Department of Pure and Applied Chemistry

EXPERIMENTAL AND COMPUTATIONAL STUDIES ON THE ROLE OF SINGLE ELECTRON TRANSFER IN SELECTED ORGANIC REACTIONS

by

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Appendix

A.1 The X-ray diffraction data for analysis of product 6.42

Crystallographic measurements for **6.42** were made at 123 K using an Oxford Diffraction Xcalibur E diffractometer equipped with a CCD detector, performed by Dr Alan Kennedy at the University of Strathclyde. The structure was refined against F^2 to convergence using all unique reflections and the program Shelxl[1] Selected crystallographic and refinement parameters are presented in Table A1 – A6.

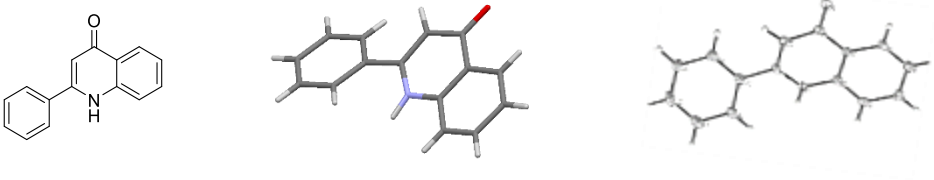


Table A1. Crystal data and structure refinement for **6.42.**

Identification code	jam_emery
Empirical formula	C15 H11 N O
Formula weight	221.25
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 11.4794(3) Å b = 7.0970(2) Å c = 13.2228(3) Å
Volume	1075.12(5) $Å^3$
Z	4
Density (calculated)	1.367 Mg/m^3
Absorption coefficient	0.086 mm^{-1}
F(000)	464
Crystal size	0.30 x 0.26 x 0.05 mm^3
Theta range for data collection	3.26 to 29.00°.
Index ranges	-15<=h<=15, -9<=k<=9, -17<=l<=18
Reflections collected	8625
Independent reflections	2817 [R(int) = 0.0194]
Completeness to theta = 27.00°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.92935
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2817 / 0 / 158
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0425, wR2 = 0.1135
R indices (all data)	R1 = 0.0548, wR2 = 0.1222
Largest diff. peak and hole	0.422 and -0.190 $e.Å^{-3}$

Table A2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6.42**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5702(1)	3258(1)	6579(1)	23(1)
N(1)	5315(1)	1769(1)	3602(1)	15(1)
C(1)	4358(1)	2187(2)	4108(1)	14(1)

C(2)	4467(1)	2628(2)	5121(1)	16(1)
C(3)	5574(1)	2753(2)	5669(1)	16(1)
C(4)	6581(1)	2220(2)	5106(1)	15(1)
C(5)	6417(1)	1712(2)	4081(1)	14(1)
C(6)	7370(1)	1105(2)	3542(1)	18(1)
C(7)	8461(1)	1048(2)	4026(1)	20(1)
C(8)	8645(1)	1593(2)	5047(1)	21(1)
C(9)	7716(1)	2155(2)	5577(1)	18(1)
C(10)	3211(1)	2113(2)	3524(1)	16(1)
C(11)	3052(1)	1039(2)	2638(1)	19(1)
C(12)	1963(1)	969(2)	2113(1)	24(1)
C(13)	1027(1)	1950(2)	2465(1)	26(1)
C(14)	1180(1)	3016(2)	3345(1)	24(1)
C(15)	2266(1)	3102(2)	3867(1)	20(1)

Table A3. Bond lengths [Å] and angles [°] for **6.42**.

O(1)-C(3)	1.2550(13)
N(1)-C(1)	1.3550(14)
N(1)-C(5)	1.3785(14)
N(1)-H(1N)	0.908(15)
C(1)-C(2)	1.3742(15)
C(1)-C(10)	1.4847(15)
C(2)-C(3)	1.4247(15)
C(2)-H(2)	0.9500
C(3)-C(4)	1.4636(16)
C(4)-C(5)	1.4048(14)
C(4)-C(9)	1.4090(15)
C(5)-C(6)	1.4100(16)
C(6)-C(7)	1.3703(16)
C(6)-H(6)	0.9500
C(7)-C(8)	1.4080(16)
C(7)-H(7)	0.9500
C(8)-C(9)	1.3716(17)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(15)	1.3919(17)
C(10)-C(11)	1.4004(16)
C(11)-C(12)	1.3921(16)
C(11)-H(11)	0.9500
C(12)-C(13)	1.3852(19)
C(12)-H(12)	0.9500
C(13)-C(14)	1.3898(19)
C(13)-H(13)	0.9500
C(14)-C(15)	1.3879(16)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(1)-N(1)-C(5)	121.89(9)
C(1)-N(1)-H(1N)	120.6(10)
C(5)-N(1)-H(1N)	117.1(10)
N(1)-C(1)-C(2)	120.30(10)
N(1)-C(1)-C(10)	117.13(9)
C(2)-C(1)-C(10)	122.57(10)
C(1)-C(2)-C(3)	122.26(10)
C(1)-C(2)-H(2)	118.9
C(3)-C(2)-H(2)	118.9
O(1)-C(3)-C(2)	123.56(11)
O(1)-C(3)-C(4)	120.79(10)
C(2)-C(3)-C(4)	115.64(10)
C(5)-C(4)-C(9)	118.81(10)
C(5)-C(4)-C(3)	119.67(10)
C(9)-C(4)-C(3)	121.50(10)
N(1)-C(5)-C(4)	119.97(10)

N(1)-C(5)-C(6)	119.71(10)
C(4)-C(5)-C(6)	120.31(10)
C(7)-C(6)-C(5)	119.29(10)
C(7)-C(6)-H(6)	120.4
C(5)-C(6)-H(6)	120.4
C(6)-C(7)-C(8)	121.12(11)
C(6)-C(7)-H(7)	119.4
C(8)-C(7)-H(7)	119.4
C(9)-C(8)-C(7)	119.68(11)
C(9)-C(8)-H(8)	120.2
C(7)-C(8)-H(8)	120.2
C(8)-C(9)-C(4)	120.76(10)
C(8)-C(9)-H(9)	119.6
C(4)-C(9)-H(9)	119.6
C(15)-C(10)-C(11)	118.95(10)
C(15)-C(10)-C(1)	119.81(10)
C(11)-C(10)-C(1)	121.23(10)
C(12)-C(11)-C(10)	120.13(11)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(13)-C(12)-C(11)	120.42(12)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(12)-C(13)-C(14)	119.65(11)
C(12)-C(13)-H(13)	120.2
C(14)-C(13)-H(13)	120.2
C(15)-C(14)-C(13)	120.19(12)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(14)-C(15)-C(10)	120.66(11)
C(14)-C(15)-H(15)	119.7
C(10)-C(15)-H(15)	119.7

Table A4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6.42**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	24(1)	33(1)	11(1)	-3(1)	1(1)	-1(1)
N(1)	16(1)	20(1)	10(1)	0(1)	1(1)	0(1)
C(1)	15(1)	14(1)	15(1)	1(1)	1(1)	-1(1)
C(2)	16(1)	20(1)	14(1)	0(1)	3(1)	0(1)
C(3)	19(1)	17(1)	12(1)	1(1)	1(1)	-1(1)
C(4)	17(1)	14(1)	13(1)	2(1)	0(1)	-1(1)
C(5)	16(1)	14(1)	13(1)	2(1)	1(1)	-2(1)
C(6)	19(1)	20(1)	14(1)	0(1)	2(1)	0(1)
C(7)	18(1)	23(1)	20(1)	1(1)	3(1)	2(1)
C(8)	16(1)	23(1)	22(1)	1(1)	-4(1)	1(1)
C(9)	20(1)	19(1)	15(1)	1(1)	-3(1)	-1(1)
C(10)	16(1)	16(1)	15(1)	3(1)	-1(1)	-2(1)
C(11)	19(1)	20(1)	18(1)	1(1)	0(1)	-1(1)
C(12)	25(1)	26(1)	21(1)	1(1)	-4(1)	-6(1)
C(13)	19(1)	28(1)	30(1)	7(1)	-6(1)	-5(1)
C(14)	16(1)	25(1)	32(1)	4(1)	2(1)	1(1)
C(15)	18(1)	20(1)	23(1)	1(1)	1(1)	-1(1)

Table A5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **6.42**.

	x	y	z	U(eq)
H(2)	3781	2856	5469	20
H(6)	7257	740	2852	21
H(7)	9104	633	3665	24
H(8)	9409	1571	5368	25

H(9)	7839	2504	6269	21
H(11)	3689	356	2394	23
H(12)	1861	244	1510	29
H(13)	284	1895	2106	31
H(14)	539	3687	3590	29
H(15)	2365	3842	4465	24
H(1N)	5265(13)	1650(20)	2916(12)	27(4)

Table A6. Torsion angles [°] for **6.42**.

C(5)-N(1)-C(1)-C(2)	2.03(17)
C(5)-N(1)-C(1)-C(10)	-177.03(10)
N(1)-C(1)-C(2)-C(3)	3.00(18)
C(10)-C(1)-C(2)-C(3)	-178.00(10)
C(1)-C(2)-C(3)-O(1)	175.76(11)
C(1)-C(2)-C(3)-C(4)	-5.21(16)
O(1)-C(3)-C(4)-C(5)	-178.19(10)
C(2)-C(3)-C(4)-C(5)	2.76(16)
O(1)-C(3)-C(4)-C(9)	3.49(18)
C(2)-C(3)-C(4)-C(9)	-175.57(10)
C(1)-N(1)-C(5)-C(4)	-4.40(16)
C(1)-N(1)-C(5)-C(6)	174.27(11)
C(9)-C(4)-C(5)-N(1)	-179.81(10)
C(3)-C(4)-C(5)-N(1)	1.82(16)
C(9)-C(4)-C(5)-C(6)	1.53(17)
C(3)-C(4)-C(5)-C(6)	-176.84(10)
N(1)-C(5)-C(6)-C(7)	-179.80(11)
C(4)-C(5)-C(6)-C(7)	-1.13(17)
C(5)-C(6)-C(7)-C(8)	-0.32(18)
C(6)-C(7)-C(8)-C(9)	1.36(19)
C(7)-C(8)-C(9)-C(4)	-0.94(18)
C(5)-C(4)-C(9)-C(8)	-0.49(17)
C(3)-C(4)-C(9)-C(8)	177.85(11)
N(1)-C(1)-C(10)-C(15)	-158.33(11)
C(2)-C(1)-C(10)-C(15)	22.63(17)
N(1)-C(1)-C(10)-C(11)	22.69(16)
C(2)-C(1)-C(10)-C(11)	-156.34(11)
C(15)-C(10)-C(11)-C(12)	0.00(17)
C(1)-C(10)-C(11)-C(12)	178.98(11)
C(10)-C(11)-C(12)-C(13)	-0.35(18)
C(11)-C(12)-C(13)-C(14)	0.24(19)
C(12)-C(13)-C(14)-C(15)	0.22(19)
C(13)-C(14)-C(15)-C(10)	-0.59(19)
C(11)-C(10)-C(15)-C(14)	0.47(17)
C(1)-C(10)-C(15)-C(14)	-178.53(11)

Symmetry transformations used to generate equivalent atoms:

A.2 The X-ray diffraction data for analysis of product 6.73

Crystallographic data for **6.73** were measured by the UK National Crystallography Service (NCS) at the University of Southampton.[2] The structure was refined against F^2 to convergence using all unique reflections and the program Shelxl[1] Selected crystallographic and refinement parameters are presented in Table A7 – A11.

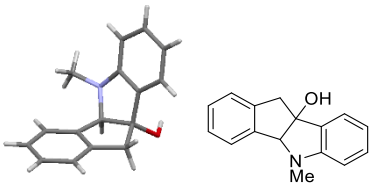


Table A7. Crystal data and structure refinement for **6.73.**

Identification code	jam_pol
Empirical formula	C16 H15 N O
Formula weight	237.29
Temperature	100(2) K
Wavelength	1.54180 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 23.5092(16) Å b = 6.3261(4) Å c = 25.0834(18) Å
Volume	3629.6(4) $Å^3$
Z	12
Density (calculated)	1.303 Mg/m^3
Absorption coefficient	0.637 mm^{-1}
F(000)	1512
Crystal size	0.52 x 0.04 x 0.01 mm^3
Theta range for data collection	3.62 to 68.35°.
Index ranges	-28<=h<=28, -7<=k<=6, -29<=l<=29
Reflections collected	34176
Independent reflections	6590 [R(int) = 0.0556]
Completeness to theta = 68.35°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.787
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6590 / 0 / 502
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.1230
R indices (all data)	R1 = 0.0501, wR2 = 0.1288
Largest diff. peak and hole	0.307 and -0.263 e.$Å^{-3}$

Table A8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6.73**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8051(1)	-10693(2)	3093(1)	22(1)
O(2)	7483(1)	-7411(2)	2435(1)	21(1)
O(3)	7307(1)	-4063(2)	3121(1)	22(1)

N(1)	8560(1)	-12884(2)	4300(1)	25(1)
N(2)	8342(1)	-8720(2)	1471(1)	25(1)
N(3)	6022(1)	-6201(2)	2758(1)	22(1)
C(1)	8473(1)	-10245(2)	3596(1)	21(1)
C(2)	8840(1)	-12204(2)	3864(1)	22(1)
C(3)	9454(1)	-11316(2)	4040(1)	21(1)
C(4)	9488(1)	-9320(2)	3819(1)	22(1)
C(5)	8910(1)	-8644(2)	3463(1)	23(1)
C(6)	9954(1)	-12279(2)	4358(1)	26(1)
C(7)	10482(1)	-11195(3)	4455(1)	29(1)
C(8)	10514(1)	-9208(3)	4231(1)	28(1)
C(9)	10019(1)	-8252(2)	3912(1)	26(1)
C(10)	8173(1)	-9607(2)	4043(1)	22(1)
C(11)	8236(1)	-11218(2)	4433(1)	24(1)
C(12)	7965(1)	-11062(3)	4869(1)	34(1)
C(13)	7628(1)	-9273(3)	4900(1)	39(1)
C(14)	7561(1)	-7677(3)	4511(1)	34(1)
C(15)	7835(1)	-7851(2)	4077(1)	27(1)
C(16)	8832(1)	-14467(2)	4695(1)	30(1)
C(17)	7719(1)	-6974(2)	1969(1)	20(1)
C(18)	7777(1)	-8996(2)	1626(1)	22(1)
C(19)	7257(1)	-8912(2)	1141(1)	22(1)
C(20)	6969(1)	-6979(2)	1125(1)	22(1)
C(21)	7271(1)	-5545(2)	1584(1)	24(1)
C(22)	7056(1)	-10442(2)	743(1)	24(1)
C(23)	6564(1)	-10025(3)	327(1)	27(1)
C(24)	6275(1)	-8096(3)	315(1)	27(1)
C(25)	6475(1)	-6562(2)	711(1)	25(1)
C(26)	8337(1)	-6152(2)	2118(1)	21(1)
C(27)	8680(1)	-7290(2)	1832(1)	23(1)
C(28)	9277(1)	-6889(3)	1917(1)	27(1)
C(29)	9515(1)	-5288(3)	2282(1)	28(1)
C(30)	9173(1)	-4115(2)	2555(1)	27(1)
C(31)	8577(1)	-4541(2)	2470(1)	24(1)
C(32)	8609(1)	-10549(3)	1284(1)	31(1)
C(33)	6714(1)	-3473(2)	3111(1)	21(1)
C(34)	6342(1)	-5287(2)	3281(1)	21(1)
C(35)	5988(1)	-4150(2)	3630(1)	22(1)
C(36)	6216(1)	-2128(2)	3772(1)	22(1)
C(37)	6731(1)	-1688(2)	3528(1)	23(1)
C(38)	5523(1)	-4878(2)	3834(1)	25(1)
C(39)	5285(1)	-3583(3)	4173(1)	28(1)
C(40)	5516(1)	-1579(3)	4315(1)	28(1)
C(41)	5983(1)	-841(2)	4117(1)	26(1)
C(42)	6376(1)	-3015(2)	2533(1)	21(1)
C(43)	5996(1)	-4705(2)	2350(1)	22(1)
C(44)	5663(1)	-4758(2)	1810(1)	25(1)
C(45)	5724(1)	-3084(3)	1469(1)	26(1)
C(46)	6092(1)	-1381(2)	1651(1)	27(1)
C(47)	6425(1)	-1348(2)	2190(1)	24(1)
C(48)	5549(1)	-7704(2)	2728(1)	26(1)

Table A9. Bond lengths [Å] and angles [°] for **6.73**.

O(1)-C(1)	1.4403(16)
O(1)-H(1H)	0.92(2)
O(2)-C(17)	1.4324(16)
O(2)-H(2H)	0.92(2)
O(3)-C(33)	1.4386(16)
O(3)-H(3H)	0.94(2)
N(1)-C(11)	1.385(2)
N(1)-C(16)	1.4497(19)
N(1)-C(2)	1.4641(18)
N(2)-C(27)	1.3924(19)

N(2)-C(32)	1.4463(19)
N(2)-C(18)	1.4762(19)
N(3)-C(43)	1.3858(19)
N(3)-C(48)	1.4512(18)
N(3)-C(34)	1.4722(18)
C(1)-C(10)	1.5115(19)
C(1)-C(5)	1.5343(19)
C(1)-C(2)	1.5711(19)
C(2)-C(3)	1.5154(19)
C(2)-H(2)	1.0000
C(3)-C(4)	1.390(2)
C(3)-C(6)	1.399(2)
C(4)-C(9)	1.389(2)
C(4)-C(5)	1.505(2)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.389(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.386(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.390(2)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(15)	1.379(2)
C(10)-C(11)	1.396(2)
C(11)-C(12)	1.391(2)
C(12)-C(13)	1.394(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.393(2)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(26)	1.5063(19)
C(17)-C(21)	1.5462(19)
C(17)-C(18)	1.5650(19)
C(18)-C(19)	1.5141(19)
C(18)-H(18)	1.0000
C(19)-C(22)	1.392(2)
C(19)-C(20)	1.394(2)
C(20)-C(25)	1.394(2)
C(20)-C(21)	1.508(2)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.393(2)
C(22)-H(22)	0.9500
C(23)-C(24)	1.394(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.390(2)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(26)-C(31)	1.380(2)
C(26)-C(27)	1.396(2)
C(27)-C(28)	1.392(2)
C(28)-C(29)	1.393(2)
C(28)-H(28)	0.9500
C(29)-C(30)	1.385(2)
C(29)-H(29)	0.9500
C(30)-C(31)	1.395(2)
C(30)-H(30)	0.9500

C(31)-H(31)	0.9500
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(42)	1.513(2)
C(33)-C(37)	1.5320(19)
C(33)-C(34)	1.5603(19)
C(34)-C(35)	1.520(2)
C(34)-H(34)	1.0000
C(35)-C(38)	1.388(2)
C(35)-C(36)	1.401(2)
C(36)-C(41)	1.391(2)
C(36)-C(37)	1.503(2)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(39)	1.388(2)
C(38)-H(38)	0.9500
C(39)-C(40)	1.393(2)
C(39)-H(39)	0.9500
C(40)-C(41)	1.387(2)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500
C(42)-C(47)	1.383(2)
C(42)-C(43)	1.401(2)
C(43)-C(44)	1.397(2)
C(44)-C(45)	1.390(2)
C(44)-H(44)	0.9500
C(45)-C(46)	1.391(2)
C(45)-H(45)	0.9500
C(46)-C(47)	1.397(2)
C(46)-H(46)	0.9500
C(47)-H(47)	0.9500
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(1)-O(1)-H(1H)	109.3(15)
C(17)-O(2)-H(2H)	111.2(13)
C(33)-O(3)-H(3H)	111.0(13)
C(11)-N(1)-C(16)	122.75(13)
C(11)-N(1)-C(2)	108.88(11)
C(16)-N(1)-C(2)	120.61(12)
C(27)-N(2)-C(32)	120.34(12)
C(27)-N(2)-C(18)	108.60(11)
C(32)-N(2)-C(18)	118.36(12)
C(43)-N(3)-C(48)	120.38(12)
C(43)-N(3)-C(34)	108.49(11)
C(48)-N(3)-C(34)	122.14(12)
O(1)-C(1)-C(10)	110.97(11)
O(1)-C(1)-C(5)	107.49(11)
C(10)-C(1)-C(5)	115.84(12)
O(1)-C(1)-C(2)	114.81(11)
C(10)-C(1)-C(2)	101.34(11)
C(5)-C(1)-C(2)	106.48(11)
N(1)-C(2)-C(3)	116.98(12)
N(1)-C(2)-C(1)	104.71(11)
C(3)-C(2)-C(1)	102.98(11)
N(1)-C(2)-H(2)	110.6
C(3)-C(2)-H(2)	110.6
C(1)-C(2)-H(2)	110.6
C(4)-C(3)-C(6)	120.22(13)
C(4)-C(3)-C(2)	111.13(12)
C(6)-C(3)-C(2)	128.58(13)

C(9)-C(4)-C(3)	120.56(13)
C(9)-C(4)-C(5)	127.84(13)
C(3)-C(4)-C(5)	111.50(12)
C(4)-C(5)-C(1)	104.07(11)
C(4)-C(5)-H(5A)	110.9
C(1)-C(5)-H(5A)	110.9
C(4)-C(5)-H(5B)	110.9
C(1)-C(5)-H(5B)	110.9
H(5A)-C(5)-H(5B)	109.0
C(7)-C(6)-C(3)	119.02(14)
C(7)-C(6)-H(6)	120.5
C(3)-C(6)-H(6)	120.5
C(8)-C(7)-C(6)	120.45(14)
C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(7)-C(8)-C(9)	120.74(14)
C(7)-C(8)-H(8)	119.6
C(9)-C(8)-H(8)	119.6
C(4)-C(9)-C(8)	119.01(14)
C(4)-C(9)-H(9)	120.5
C(8)-C(9)-H(9)	120.5
C(15)-C(10)-C(11)	120.99(14)
C(15)-C(10)-C(1)	129.37(13)
C(11)-C(10)-C(1)	109.41(12)
N(1)-C(11)-C(12)	128.37(14)
N(1)-C(11)-C(10)	111.24(12)
C(12)-C(11)-C(10)	120.31(15)
C(11)-C(12)-C(13)	118.04(15)
C(11)-C(12)-H(12)	121.0
C(13)-C(12)-H(12)	121.0
C(14)-C(13)-C(12)	121.82(15)
C(14)-C(13)-H(13)	119.1
C(12)-C(13)-H(13)	119.1
C(13)-C(14)-C(15)	119.58(16)
C(13)-C(14)-H(14)	120.2
C(15)-C(14)-H(14)	120.2
C(10)-C(15)-C(14)	119.25(15)
C(10)-C(15)-H(15)	120.4
C(14)-C(15)-H(15)	120.4
N(1)-C(16)-H(16A)	109.5
N(1)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
N(1)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(2)-C(17)-C(26)	113.39(11)
O(2)-C(17)-C(21)	106.61(11)
C(26)-C(17)-C(21)	115.66(12)
O(2)-C(17)-C(18)	112.93(11)
C(26)-C(17)-C(18)	102.56(11)
C(21)-C(17)-C(18)	105.56(11)
N(2)-C(18)-C(19)	113.08(11)
N(2)-C(18)-C(17)	104.20(11)
C(19)-C(18)-C(17)	104.84(11)
N(2)-C(18)-H(18)	111.4
C(19)-C(18)-H(18)	111.4
C(17)-C(18)-H(18)	111.4
C(22)-C(19)-C(20)	120.43(13)
C(22)-C(19)-C(18)	129.03(13)
C(20)-C(19)-C(18)	110.54(12)
C(25)-C(20)-C(19)	120.20(13)
C(25)-C(20)-C(21)	128.31(13)
C(19)-C(20)-C(21)	111.47(12)

C(20)-C(21)-C(17)	104.96(11)
C(20)-C(21)-H(21A)	110.8
C(17)-C(21)-H(21A)	110.8
C(20)-C(21)-H(21B)	110.8
C(17)-C(21)-H(21B)	110.8
H(21A)-C(21)-H(21B)	108.8
C(19)-C(22)-C(23)	119.47(14)
C(19)-C(22)-H(22)	120.3
C(23)-C(22)-H(22)	120.3
C(22)-C(23)-C(24)	119.88(14)
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-H(23)	120.1
C(25)-C(24)-C(23)	120.85(14)
C(25)-C(24)-H(24)	119.6
C(23)-C(24)-H(24)	119.6
C(24)-C(25)-C(20)	119.16(14)
C(24)-C(25)-H(25)	120.4
C(20)-C(25)-H(25)	120.4
C(31)-C(26)-C(27)	120.67(13)
C(31)-C(26)-C(17)	129.92(13)
C(27)-C(26)-C(17)	109.40(12)
C(28)-C(27)-N(2)	128.46(13)
C(28)-C(27)-C(26)	120.54(13)
N(2)-C(27)-C(26)	110.98(12)
C(27)-C(28)-C(29)	118.10(14)
C(27)-C(28)-H(28)	120.9
C(29)-C(28)-H(28)	120.9
C(30)-C(29)-C(28)	121.54(14)
C(30)-C(29)-H(29)	119.2
C(28)-C(29)-H(29)	119.2
C(29)-C(30)-C(31)	119.88(14)
C(29)-C(30)-H(30)	120.1
C(31)-C(30)-H(30)	120.1
C(26)-C(31)-C(30)	119.21(13)
C(26)-C(31)-H(31)	120.4
C(30)-C(31)-H(31)	120.4
N(2)-C(32)-H(32A)	109.5
N(2)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(2)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(3)-C(33)-C(42)	110.91(11)
O(3)-C(33)-C(37)	107.85(11)
C(42)-C(33)-C(37)	116.05(12)
O(3)-C(33)-C(34)	113.99(11)
C(42)-C(33)-C(34)	101.53(11)
C(37)-C(33)-C(34)	106.52(11)
N(3)-C(34)-C(35)	117.64(11)
N(3)-C(34)-C(33)	104.41(11)
C(35)-C(34)-C(33)	102.99(11)
N(3)-C(34)-H(34)	110.4
C(35)-C(34)-H(34)	110.4
C(33)-C(34)-H(34)	110.4
C(38)-C(35)-C(36)	119.87(13)
C(38)-C(35)-C(34)	129.57(13)
C(36)-C(35)-C(34)	110.45(12)
C(41)-C(36)-C(35)	120.59(14)
C(41)-C(36)-C(37)	128.05(13)
C(35)-C(36)-C(37)	111.29(12)
C(36)-C(37)-C(33)	104.10(11)
C(36)-C(37)-H(37A)	110.9
C(33)-C(37)-H(37A)	110.9

C(36)-C(37)-H(37B)	110.9
C(33)-C(37)-H(37B)	110.9
H(37A)-C(37)-H(37B)	109.0
C(35)-C(38)-C(39)	119.51(14)
C(35)-C(38)-H(38)	120.2
C(39)-C(38)-H(38)	120.2
C(38)-C(39)-C(40)	120.45(14)
C(38)-C(39)-H(39)	119.8
C(40)-C(39)-H(39)	119.8
C(41)-C(40)-C(39)	120.51(14)
C(41)-C(40)-H(40)	119.7
C(39)-C(40)-H(40)	119.7
C(40)-C(41)-C(36)	119.06(14)
C(40)-C(41)-H(41)	120.5
C(36)-C(41)-H(41)	120.5
C(47)-C(42)-C(43)	121.12(13)
C(47)-C(42)-C(33)	129.95(13)
C(43)-C(42)-C(33)	108.80(12)
N(3)-C(43)-C(44)	128.23(13)
N(3)-C(43)-C(42)	111.27(12)
C(44)-C(43)-C(42)	120.47(13)
C(45)-C(44)-C(43)	117.64(14)
C(45)-C(44)-H(44)	121.2
C(43)-C(44)-H(44)	121.2
C(44)-C(45)-C(46)	122.23(14)
C(44)-C(45)-H(45)	118.9
C(46)-C(45)-H(45)	118.9
C(45)-C(46)-C(47)	119.71(14)
C(45)-C(46)-H(46)	120.1
C(47)-C(46)-H(46)	120.1
C(42)-C(47)-C(46)	118.80(14)
C(42)-C(47)-H(47)	120.6
C(46)-C(47)-H(47)	120.6
N(3)-C(48)-H(48A)	109.5
N(3)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
N(3)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table A10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6.73**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	23(1)	20(1)	19(1)	-1(1)	-1(1)	-2(1)
O(2)	22(1)	21(1)	21(1)	0(1)	3(1)	2(1)
O(3)	17(1)	21(1)	27(1)	-4(1)	2(1)	0(1)
N(1)	25(1)	26(1)	23(1)	6(1)	2(1)	-2(1)
N(2)	23(1)	29(1)	23(1)	-7(1)	1(1)	5(1)
N(3)	21(1)	20(1)	24(1)	-2(1)	2(1)	-4(1)
C(1)	21(1)	20(1)	18(1)	0(1)	-1(1)	-2(1)
C(2)	23(1)	19(1)	21(1)	0(1)	2(1)	-2(1)
C(3)	24(1)	20(1)	19(1)	-2(1)	4(1)	-1(1)
C(4)	26(1)	20(1)	20(1)	-1(1)	5(1)	0(1)
C(5)	25(1)	19(1)	24(1)	1(1)	4(1)	-1(1)
C(6)	26(1)	25(1)	27(1)	4(1)	4(1)	1(1)
C(7)	23(1)	33(1)	28(1)	4(1)	1(1)	3(1)
C(8)	24(1)	32(1)	29(1)	-1(1)	4(1)	-6(1)
C(9)	27(1)	24(1)	28(1)	0(1)	6(1)	-5(1)
C(10)	20(1)	24(1)	22(1)	-3(1)	1(1)	-5(1)
C(11)	18(1)	32(1)	20(1)	0(1)	-1(1)	-7(1)
C(12)	24(1)	52(1)	23(1)	5(1)	4(1)	-4(1)

C(13)	25(1)	65(1)	26(1)	-7(1)	6(1)	-2(1)
C(14)	24(1)	42(1)	34(1)	-11(1)	5(1)	1(1)
C(15)	22(1)	28(1)	28(1)	-6(1)	1(1)	-3(1)
C(16)	31(1)	28(1)	27(1)	8(1)	-2(1)	-5(1)
C(17)	22(1)	18(1)	19(1)	0(1)	3(1)	3(1)
C(18)	25(1)	19(1)	20(1)	-1(1)	2(1)	4(1)
C(19)	22(1)	23(1)	19(1)	1(1)	3(1)	0(1)
C(20)	23(1)	22(1)	20(1)	2(1)	5(1)	1(1)
C(21)	26(1)	20(1)	23(1)	1(1)	1(1)	5(1)
C(22)	27(1)	24(1)	22(1)	-1(1)	5(1)	0(1)
C(23)	29(1)	31(1)	21(1)	-3(1)	2(1)	-5(1)
C(24)	23(1)	35(1)	22(1)	3(1)	1(1)	-2(1)
C(25)	22(1)	28(1)	23(1)	5(1)	4(1)	4(1)
C(26)	23(1)	20(1)	18(1)	3(1)	2(1)	3(1)
C(27)	25(1)	23(1)	19(1)	1(1)	2(1)	4(1)
C(28)	23(1)	34(1)	24(1)	0(1)	5(1)	6(1)
C(29)	23(1)	34(1)	27(1)	2(1)	4(1)	-1(1)
C(30)	29(1)	26(1)	25(1)	-2(1)	3(1)	-4(1)
C(31)	27(1)	21(1)	23(1)	0(1)	5(1)	1(1)
C(32)	30(1)	32(1)	31(1)	-11(1)	3(1)	8(1)
C(33)	17(1)	20(1)	26(1)	-1(1)	3(1)	0(1)
C(34)	20(1)	19(1)	24(1)	-1(1)	1(1)	-1(1)
C(35)	20(1)	23(1)	20(1)	2(1)	-1(1)	2(1)
C(36)	21(1)	22(1)	22(1)	1(1)	-1(1)	2(1)
C(37)	22(1)	20(1)	25(1)	-3(1)	2(1)	-2(1)
C(38)	22(1)	27(1)	25(1)	2(1)	1(1)	-1(1)
C(39)	22(1)	37(1)	24(1)	4(1)	4(1)	2(1)
C(40)	26(1)	35(1)	22(1)	-1(1)	3(1)	8(1)
C(41)	27(1)	25(1)	22(1)	0(1)	0(1)	3(1)
C(42)	18(1)	21(1)	24(1)	-2(1)	4(1)	2(1)
C(43)	18(1)	21(1)	26(1)	-3(1)	5(1)	2(1)
C(44)	19(1)	29(1)	26(1)	-6(1)	3(1)	1(1)
C(45)	21(1)	35(1)	23(1)	-1(1)	3(1)	7(1)
C(46)	24(1)	28(1)	30(1)	4(1)	8(1)	6(1)
C(47)	22(1)	22(1)	31(1)	1(1)	7(1)	2(1)
C(48)	23(1)	21(1)	32(1)	-2(1)	3(1)	-5(1)

Table A11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6.73**.

	x	y	z	U(eq)
H(2)	8825	-13358	3589	26
H(5A)	8918	-8705	3071	27
H(5B)	8811	-7188	3554	27
H(6)	9934	-13653	4504	31
H(7)	10823	-11819	4677	35
H(8)	10879	-8492	4295	34
H(9)	10042	-6888	3760	31
H(12)	8009	-12142	5139	40
H(13)	7439	-9144	5194	46
H(14)	7329	-6473	4541	40
H(15)	7791	-6772	3807	32
H(16A)	9157	-13828	4961	45
H(16B)	8979	-15626	4504	45
H(16C)	8543	-15018	4885	45
H(18)	7774	-10313	1846	26
H(21A)	6986	-4950	1779	28
H(21B)	7470	-4368	1441	28
H(22)	7252	-11759	756	29
H(23)	6425	-11054	52	33
H(24)	5936	-7827	33	33
H(25)	6278	-5246	698	30
H(28)	9514	-7686	1732	33

H(29)	9921	-4993	2345	34
H(30)	9345	-3021	2799	32
H(31)	8339	-3733	2652	28
H(32A)	8921	-10089	1110	47
H(32B)	8313	-11334	1018	47
H(32C)	8774	-11463	1597	47
H(34)	6602	-6372	3504	26
H(37A)	7101	-1723	3813	28
H(37B)	6693	-291	3345	28
H(38)	5369	-6253	3742	31
H(39)	4963	-4067	4309	34
H(40)	5352	-711	4550	33
H(41)	6141	524	4215	31
H(44)	5405	-5898	1682	30
H(45)	5507	-3104	1099	32
H(46)	6117	-245	1409	32
H(47)	6681	-202	2318	29
H(48A)	5189	-6943	2741	39
H(48B)	5648	-8684	3038	39
H(48C)	5490	-8499	2384	39
H(1H)	7802(10)	-11740(40)	3154(10)	57(6)
H(2H)	7697(10)	-8440(40)	2654(9)	50(6)
H(3H)	7319(9)	-5130(40)	2861(9)	51(6)

Table A12. Torsion angles [°] for **6.73**.

C(11)-N(1)-C(2)-C(3)	92.72(14)
C(16)-N(1)-C(2)-C(3)	-57.35(18)
C(11)-N(1)-C(2)-C(1)	-20.50(14)
C(16)-N(1)-C(2)-C(1)	-170.57(12)
O(1)-C(1)-C(2)-N(1)	-99.94(13)
C(10)-C(1)-C(2)-N(1)	19.72(13)
C(5)-C(1)-C(2)-N(1)	141.25(11)
O(1)-C(1)-C(2)-C(3)	137.25(11)
C(10)-C(1)-C(2)-C(3)	-103.09(12)
C(5)-C(1)-C(2)-C(3)	18.43(14)
N(1)-C(2)-C(3)-C(4)	-125.21(13)
C(1)-C(2)-C(3)-C(4)	-11.02(15)
N(1)-C(2)-C(3)-C(6)	57.9(2)
C(1)-C(2)-C(3)-C(6)	172.06(14)
C(6)-C(3)-C(4)-C(9)	-0.3(2)
C(2)-C(3)-C(4)-C(9)	-177.52(13)
C(6)-C(3)-C(4)-C(5)	176.27(13)
C(2)-C(3)-C(4)-C(5)	-0.95(16)
C(9)-C(4)-C(5)-C(1)	-170.91(14)
C(3)-C(4)-C(5)-C(1)	12.82(15)
O(1)-C(1)-C(5)-C(4)	-142.57(11)
C(10)-C(1)-C(5)-C(4)	92.72(14)
C(2)-C(1)-C(5)-C(4)	-19.06(14)
C(4)-C(3)-C(6)-C(7)	1.1(2)
C(2)-C(3)-C(6)-C(7)	177.75(14)
C(3)-C(6)-C(7)-C(8)	-1.4(2)
C(6)-C(7)-C(8)-C(9)	1.0(2)
C(3)-C(4)-C(9)-C(8)	-0.1(2)
C(5)-C(4)-C(9)-C(8)	-176.11(14)
C(7)-C(8)-C(9)-C(4)	-0.2(2)
O(1)-C(1)-C(10)-C(15)	-65.08(18)
C(5)-C(1)-C(10)-C(15)	57.82(19)
C(2)-C(1)-C(10)-C(15)	172.56(14)
O(1)-C(1)-C(10)-C(11)	109.31(13)
C(5)-C(1)-C(10)-C(11)	-127.79(13)
C(2)-C(1)-C(10)-C(11)	-13.05(14)
C(16)-N(1)-C(11)-C(12)	-21.2(2)
C(2)-N(1)-C(11)-C(12)	-170.50(14)

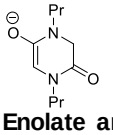
C(16)-N(1)-C(11)-C(10)	162.10(13)
C(2)-N(1)-C(11)-C(10)	12.81(16)
C(15)-C(10)-C(11)-N(1)	175.99(13)
C(1)-C(10)-C(11)-N(1)	1.05(16)
C(15)-C(10)-C(11)-C(12)	-1.0(2)
C(1)-C(10)-C(11)-C(12)	-175.95(13)
N(1)-C(11)-C(12)-C(13)	-175.76(14)
C(10)-C(11)-C(12)-C(13)	0.7(2)
C(11)-C(12)-C(13)-C(14)	-0.2(2)
C(12)-C(13)-C(14)-C(15)	0.1(2)
C(11)-C(10)-C(15)-C(14)	0.8(2)
C(1)-C(10)-C(15)-C(14)	174.67(14)
C(13)-C(14)-C(15)-C(10)	-0.4(2)
C(27)-N(2)-C(18)-C(19)	134.31(12)
C(32)-N(2)-C(18)-C(19)	-83.74(16)
C(27)-N(2)-C(18)-C(17)	21.05(14)
C(32)-N(2)-C(18)-C(17)	163.00(12)
O(2)-C(17)-C(18)-N(2)	-139.96(11)
C(26)-C(17)-C(18)-N(2)	-17.55(13)
C(21)-C(17)-C(18)-N(2)	103.95(12)
O(2)-C(17)-C(18)-C(19)	101.01(12)
C(26)-C(17)-C(18)-C(19)	-136.59(11)
C(21)-C(17)-C(18)-C(19)	-15.09(14)
N(2)-C(18)-C(19)-C(22)	75.77(18)
C(17)-C(18)-C(19)-C(22)	-171.36(14)
N(2)-C(18)-C(19)-C(20)	-104.15(14)
C(17)-C(18)-C(19)-C(20)	8.72(15)
C(22)-C(19)-C(20)-C(25)	0.2(2)
C(18)-C(19)-C(20)-C(25)	-179.89(12)
C(22)-C(19)-C(20)-C(21)	-178.41(13)
C(18)-C(19)-C(20)-C(21)	1.52(16)
C(25)-C(20)-C(21)-C(17)	170.33(14)
C(19)-C(20)-C(21)-C(17)	-11.23(16)
O(2)-C(17)-C(21)-C(20)	-104.43(12)
C(26)-C(17)-C(21)-C(20)	128.49(12)
C(18)-C(17)-C(21)-C(20)	15.90(14)
C(20)-C(19)-C(22)-C(23)	0.1(2)
C(18)-C(19)-C(22)-C(23)	-179.79(13)
C(19)-C(22)-C(23)-C(24)	-0.6(2)
C(22)-C(23)-C(24)-C(25)	0.9(2)
C(23)-C(24)-C(25)-C(20)	-0.5(2)
C(19)-C(20)-C(25)-C(24)	0.0(2)
C(21)-C(20)-C(25)-C(24)	178.35(14)
O(2)-C(17)-C(26)-C(31)	-49.63(19)
C(21)-C(17)-C(26)-C(31)	73.96(19)
C(18)-C(17)-C(26)-C(31)	-171.72(14)
O(2)-C(17)-C(26)-C(27)	130.85(12)
C(21)-C(17)-C(26)-C(27)	-105.55(14)
C(18)-C(17)-C(26)-C(27)	8.76(14)
C(32)-N(2)-C(27)-C(28)	24.1(2)
C(18)-N(2)-C(27)-C(28)	165.15(14)
C(32)-N(2)-C(27)-C(26)	-157.49(13)
C(18)-N(2)-C(27)-C(26)	-16.43(16)
C(31)-C(26)-C(27)-C(28)	3.2(2)
C(17)-C(26)-C(27)-C(28)	-177.26(13)
C(31)-C(26)-C(27)-N(2)	-175.39(13)
C(17)-C(26)-C(27)-N(2)	4.18(16)
N(2)-C(27)-C(28)-C(29)	176.44(14)
C(26)-C(27)-C(28)-C(29)	-1.8(2)
C(27)-C(28)-C(29)-C(30)	0.0(2)
C(28)-C(29)-C(30)-C(31)	0.5(2)
C(27)-C(26)-C(31)-C(30)	-2.6(2)
C(17)-C(26)-C(31)-C(30)	177.95(14)

C(29)-C(30)-C(31)-C(26)	0.7(2)
C(43)-N(3)-C(34)-C(35)	91.29(14)
C(48)-N(3)-C(34)-C(35)	-55.85(18)
C(43)-N(3)-C(34)-C(33)	-22.06(14)
C(48)-N(3)-C(34)-C(33)	-169.20(12)
O(3)-C(33)-C(34)-N(3)	-96.85(13)
C(42)-C(33)-C(34)-N(3)	22.46(13)
C(37)-C(33)-C(34)-N(3)	144.33(11)
O(3)-C(33)-C(34)-C(35)	139.73(11)
C(42)-C(33)-C(34)-C(35)	-100.96(12)
C(37)-C(33)-C(34)-C(35)	20.91(14)
N(3)-C(34)-C(35)-C(38)	56.0(2)
C(33)-C(34)-C(35)-C(38)	170.14(14)
N(3)-C(34)-C(35)-C(36)	-127.87(13)
C(33)-C(34)-C(35)-C(36)	-13.73(14)
C(38)-C(35)-C(36)-C(41)	0.3(2)
C(34)-C(35)-C(36)-C(41)	-176.29(13)
C(38)-C(35)-C(36)-C(37)	177.60(13)
C(34)-C(35)-C(36)-C(37)	1.04(16)
C(41)-C(36)-C(37)-C(33)	-170.50(14)
C(35)-C(36)-C(37)-C(33)	12.42(15)
O(3)-C(33)-C(37)-C(36)	-143.25(11)
C(42)-C(33)-C(37)-C(36)	91.66(14)
C(34)-C(33)-C(37)-C(36)	-20.49(14)
C(36)-C(35)-C(38)-C(39)	0.5(2)
C(34)-C(35)-C(38)-C(39)	176.36(13)
C(35)-C(38)-C(39)-C(40)	-1.0(2)
C(38)-C(39)-C(40)-C(41)	0.6(2)
C(39)-C(40)-C(41)-C(36)	0.2(2)
C(35)-C(36)-C(41)-C(40)	-0.7(2)
C(37)-C(36)-C(41)-C(40)	-177.50(14)
O(3)-C(33)-C(42)-C(47)	-70.31(18)
C(37)-C(33)-C(42)-C(47)	53.2(2)
C(34)-C(33)-C(42)-C(47)	168.21(14)
O(3)-C(33)-C(42)-C(43)	105.42(13)
C(37)-C(33)-C(42)-C(43)	-131.07(13)
C(34)-C(33)-C(42)-C(43)	-16.06(14)
C(48)-N(3)-C(43)-C(44)	-21.6(2)
C(34)-N(3)-C(43)-C(44)	-169.44(13)
C(48)-N(3)-C(43)-C(42)	160.24(12)
C(34)-N(3)-C(43)-C(42)	12.42(15)
C(47)-C(42)-C(43)-N(3)	179.35(12)
C(33)-C(42)-C(43)-N(3)	3.18(16)
C(47)-C(42)-C(43)-C(44)	1.1(2)
C(33)-C(42)-C(43)-C(44)	-175.13(12)
N(3)-C(43)-C(44)-C(45)	-178.15(13)
C(42)-C(43)-C(44)-C(45)	-0.2(2)
C(43)-C(44)-C(45)-C(46)	-1.1(2)
C(44)-C(45)-C(46)-C(47)	1.5(2)
C(43)-C(42)-C(47)-C(46)	-0.7(2)
C(33)-C(42)-C(47)-C(46)	174.62(13)
C(45)-C(46)-C(47)-C(42)	-0.6(2)

Symmetry transformations used to generate equivalent atoms:

A.3 XYZ files Chapter 4

Scheme 4.1B

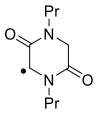


Enolate anion 4.7 in benzene

31

-651.2494131

C	1.09766	-1.31030	-1.01114
C	-0.25598	-1.54171	-0.85917
C	-0.39270	-0.68684	1.41033
C	1.06343	-1.12076	1.42370
H	-0.85494	-1.98727	-1.63940
H	1.56546	-0.62359	2.25541
H	1.07917	-2.20401	1.60368
N	-0.99541	-1.01576	0.26032
N	1.76928	-0.85118	0.18249
O	-0.93836	-0.08052	2.34605
O	1.79364	-1.46834	-2.05196
C	-2.35834	-0.56934	0.02229
H	-2.83142	-1.28472	-0.65784
H	-2.89450	-0.59066	0.97303
C	-2.40342	0.83585	-0.57339
H	-1.93962	1.52310	0.14088
H	-1.79068	0.84585	-1.47992
C	-3.83166	1.27220	-0.88615
H	-3.85914	2.28033	-1.30489
H	-4.29547	0.59608	-1.61023
H	-4.44853	1.26754	0.01701
C	2.40137	0.45497	0.06179
H	3.11381	0.57947	0.88715
H	2.97722	0.44055	-0.86702
C	1.42443	1.63540	0.04331
H	0.86835	1.66706	0.98711
H	0.68986	1.46070	-0.75085
C	2.14639	2.96162	-0.18039
H	1.45195	3.80468	-0.18617
H	2.88324	3.14111	0.60845
H	2.67871	2.95665	-1.13573



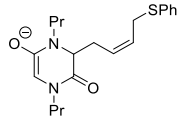
Radical 4.8 in benzene

31

-651.1544696

C	0.82862	1.18260	-0.36753
C	-0.61407	1.21798	-0.28654
C	-0.84757	-1.17041	-0.37225
C	0.64396	-1.24926	-0.12831
H	-1.11187	2.17357	-0.22355
H	0.76806	-1.48490	0.93938
H	1.01085	-2.10663	-0.69508
N	-1.39088	0.09556	-0.42397
N	1.38802	-0.06302	-0.50808
O	-1.52852	-2.17137	-0.45516
O	1.49443	2.21741	-0.36392
C	-2.85157	0.22859	-0.49793
H	-3.06657	1.17187	-1.00344
H	-3.22301	-0.58789	-1.11716
C	-3.49171	0.18724	0.88566
H	-3.23177	-0.76214	1.36156
H	-3.06628	0.98764	1.49874
C	-5.00726	0.33700	0.79433
H	-5.46295	0.30522	1.78483
H	-5.28051	1.28724	0.32856
H	-5.44285	-0.46843	0.19810
C	2.84221	-0.17387	-0.52473
H	3.09811	-1.08768	-1.06986
H	3.22702	0.67608	-1.08959
C	3.46396	-0.19278	0.87104
H	3.07282	-1.04347	1.43815
H	3.16029	0.71724	1.39592
C	4.98569	-0.27907	0.79488
H	5.43083	-0.29916	1.79079
H	5.30070	-1.18380	0.26798
H	5.39616	0.58097	0.26001

Scheme 4.5

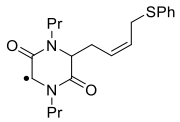


Enolate anion 4.20 in benzene

55

-1475.7389399

C	-3.54129	0.99793	-0.51346
C	-2.31126	1.52705	0.22244
C	-2.74172	0.05044	2.11482
C	-4.05758	0.16795	1.70681
H	-4.88634	-0.07324	2.35609
N	-1.76961	0.55310	1.16762
N	-4.40150	0.41461	0.33158
O	-2.31499	-0.42318	3.20244
O	-3.70364	1.07482	-1.74200
C	-0.84582	-0.45997	0.67147
H	0.03847	0.02675	0.24563
H	-0.50470	-1.01290	1.55059
C	-1.44258	-1.43817	-0.34567
H	-2.32124	-1.91251	0.10529
H	-1.79961	-0.89184	-1.22666
C	-0.42095	-2.49153	-0.76687
H	-0.83615	-3.19039	-1.49693
H	0.46031	-2.02006	-1.21311
H	-0.08094	-3.06882	0.09775
C	-5.57944	-0.24645	-0.20796
H	-6.35384	-0.23508	0.56540
H	-5.93479	0.33609	-1.06043
C	-5.28651	-1.68035	-0.64288
H	-4.86212	-2.22078	0.20875
H	-4.52007	-1.64910	-1.42330
C	-6.54081	-2.38328	-1.15328
H	-6.32392	-3.40491	-1.47237
H	-7.30600	-2.43193	-0.37305
H	-6.96861	-1.84933	-2.00664
C	-1.27081	2.06267	-0.75504
H	-0.96586	1.27682	-1.44924
H	-1.77079	2.81815	-1.36988
C	-0.09592	2.68191	-0.05690
C	1.18756	2.54864	-0.38980
C	1.73148	1.73291	-1.53470
H	1.78477	2.35236	-2.43833
H	1.06658	0.89710	-1.77265
C	3.13642	1.20201	-1.26735
H	3.52910	0.68617	-2.14455
H	3.81493	2.01618	-1.00245
S	3.10404	0.01231	0.12864
C	4.83449	-0.43433	0.14234
C	5.67166	0.05308	1.14565
C	5.35374	-1.28334	-0.83723
C	7.01762	-0.30352	1.16692
H	5.26337	0.70963	1.90496
C	6.70085	-1.62809	-0.82017
H	4.69562	-1.67572	-1.60446
C	7.53469	-1.14026	0.18321
H	7.66154	0.07589	1.95174
H	7.09683	-2.28777	-1.58354
H	8.58280	-1.41569	0.19971
H	-0.33848	3.30727	0.80025
H	1.93258	3.07871	0.20119
H	-2.67416	2.36308	0.83993

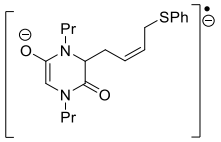


Radical 4.22 in benzene

55

-1475.6467155

C	-2.58191	-0.26983	-1.02537
C	-1.32355	0.12059	-0.27291
C	-2.38109	2.23438	0.37218
C	-3.63845	1.56545	0.10557
H	-4.56163	2.04297	0.39668
N	-1.26005	1.55122	-0.01350
N	-3.71107	0.45421	-0.69384
O	-2.34467	3.36763	0.85241
O	-2.62296	-1.21590	-1.78619
C	0.03809	2.21593	0.07387
H	0.71329	1.69367	-0.60960
H	-0.09630	3.23452	-0.29857
C	0.65388	2.27717	1.47177
H	-0.03927	2.80012	2.13524
H	0.79765	1.26713	1.86229
C	2.00399	2.98704	1.42589
H	2.43451	3.08297	2.42401
H	2.71283	2.42677	0.80858
H	1.90555	3.99114	1.00444
C	-5.01730	-0.04618	-1.13847
H	-5.69401	0.80796	-1.19559
H	-4.88973	-0.45431	-2.14125
C	-5.55341	-1.11268	-0.18837
H	-5.64765	-0.68017	0.81264
H	-4.82114	-1.92320	-0.12610
C	-6.89935	-1.65075	-0.66431
H	-7.28430	-2.40480	0.02347
H	-7.63965	-0.84967	-0.73348
H	-6.80689	-2.11038	-1.65132
C	-1.27226	-0.72745	1.03051
H	-0.49838	-0.29741	1.66230
H	-2.22734	-0.60095	1.55573
C	-1.00481	-2.17868	0.75367
C	0.05738	-2.87302	1.16331
C	1.19045	-2.38067	2.02258
H	1.39788	-3.13006	2.79262
H	0.93156	-1.45734	2.54363
C	2.49069	-2.16738	1.24036
H	3.28542	-1.85498	1.91945
H	2.79110	-3.08514	0.73040
S	2.23605	-0.84665	0.01040
C	3.88701	-0.43994	-0.49717
C	5.00992	-1.21042	-0.19269
C	4.03839	0.71804	-1.26861
C	6.26710	-0.81390	-0.64410
H	4.92023	-2.12119	0.38449
C	5.29414	1.10064	-1.71860
H	3.16910	1.31883	-1.51463
C	6.41801	0.33871	-1.40462
H	7.13163	-1.41946	-0.39748
H	5.39424	2.00127	-2.31300
H	7.39803	0.64135	-1.75218
H	-1.73524	-2.68585	0.12894
H	0.13717	-3.90953	0.84269
H	-0.47809	-0.15202	-0.90615

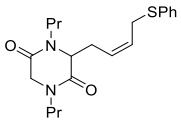


Radical dianion 4.34 in benzene

55

-1475.7309047

C	-3.14904	-1.18532	-0.49026
C	-2.16287	-0.09479	-0.90509
C	-4.00226	1.42268	-1.43768
C	-4.68508	0.25042	-1.70390
H	-5.58458	0.22879	-2.30167
N	-2.74062	1.24247	-0.75975
N	-4.36099	-0.97807	-1.02834
O	-4.35574	2.59895	-1.73100
O	-2.87514	-2.12622	0.27056
C	-2.65538	1.90565	0.53503
H	-1.60415	2.00230	0.82884
H	-3.03835	2.91757	0.38130
C	-3.45087	1.22364	1.65362
H	-4.49111	1.12634	1.32329
H	-3.07435	0.20639	1.80963
C	-3.37698	2.01265	2.95849
H	-3.94651	1.52986	3.75611
H	-2.34091	2.10697	3.29691
H	-3.77474	3.02258	2.82346
C	-5.45671	-1.85429	-0.64753
H	-6.18391	-1.85658	-1.46561
H	-5.06038	-2.86557	-0.53616
C	-6.12495	-1.41165	0.65222
H	-6.45095	-0.37347	0.53797
H	-5.37140	-1.43101	1.44511
C	-7.30516	-2.30883	1.01417
H	-7.77629	-1.99349	1.94762
H	-8.06748	-2.28628	0.22985
H	-6.98275	-3.34694	1.13535
C	-0.81662	-0.25341	-0.21017
H	-0.94855	-0.18597	0.87546
H	-0.47140	-1.27480	-0.39314
C	0.20549	0.74776	-0.69227
C	1.48456	0.77994	-0.31566
C	2.12984	-0.17571	0.65175
H	1.52154	-1.08100	0.74058
H	2.15326	0.27872	1.65208
C	3.55867	-0.55290	0.26134
H	3.92487	-1.37823	0.87437
H	3.61713	-0.84160	-0.79075
S	4.72774	0.88039	0.54101
C	6.30829	0.23370	0.18810
C	6.83500	0.22817	-1.15251
C	7.02495	-0.54974	1.16467
C	8.02077	-0.39905	-1.45214
H	6.28546	0.75086	-1.93032
C	8.20962	-1.17234	0.84916
H	6.62364	-0.62301	2.17162
C	8.77165	-1.09311	-0.45704
H	8.39298	-0.35874	-2.47292
H	8.72973	-1.73320	1.62219
H	9.69472	-1.60277	-0.70348
H	-0.15744	1.50033	-1.38872
H	2.13330	1.55204	-0.72343
H	-2.01430	-0.22962	-1.98733

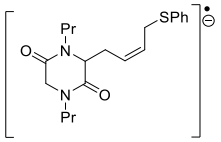


Neutral additive 4.19 in benzene

56

-1476.2833623

C	-3.62101	1.12495	-0.16366
C	-2.23326	1.27211	0.48229
C	-2.60383	-0.86476	1.56923
C	-3.96246	-0.22380	1.82247
H	-4.64537	-1.01068	2.13436
N	-1.75508	-0.06941	0.87246
N	-4.46758	0.39943	0.60306
O	-2.34434	-1.99816	1.93879
O	-3.91576	1.61526	-1.24063
C	-0.54444	-0.67560	0.31681
H	0.21374	0.09550	0.19423
H	-0.16741	-1.37902	1.06086
C	-0.81912	-1.40698	-0.99659
H	-1.57994	-2.17157	-0.81158
H	-1.24492	-0.70677	-1.72379
C	0.44773	-2.04646	-1.55855
H	0.23853	-2.58472	-2.48455
H	1.21209	-1.29241	-1.76531
H	0.87393	-2.75431	-0.84269
C	-5.77904	0.01243	0.09321
H	-6.47187	-0.03330	0.93808
H	-6.11577	0.80428	-0.57715
C	-5.73457	-1.32468	-0.64315
H	-5.33594	-2.09342	0.02759
H	-5.03359	-1.23297	-1.47811
C	-7.11561	-1.73155	-1.14775
H	-7.07736	-2.68726	-1.67245
H	-7.82123	-1.83152	-0.31888
H	-7.51319	-0.98414	-1.83891
C	-1.28203	2.05866	-0.41228
H	-0.97496	1.46081	-1.27103
H	-1.88043	2.87687	-0.82427
C	-0.11521	2.64523	0.33180
C	1.16459	2.62944	-0.03745
C	1.74583	1.97517	-1.26235
H	1.81410	2.71218	-2.07121
H	1.09932	1.17274	-1.62976
C	3.15292	1.43298	-1.02201
H	3.54121	0.95456	-1.92192
H	3.83086	2.23775	-0.72915
S	3.13070	0.18606	0.32320
C	4.83637	-0.34158	0.23097
C	5.81337	0.31179	0.98226
C	5.19150	-1.41315	-0.58890
C	7.14025	-0.10055	0.90603
H	5.52919	1.13785	1.62390
C	6.51924	-1.82298	-0.66167
H	4.42446	-1.92193	-1.16187
C	7.49416	-1.16696	0.08458
H	7.89649	0.40930	1.49118
H	6.79066	-2.65766	-1.29725
H	8.52729	-1.48904	0.02913
H	-0.37203	3.17403	1.24778
H	1.88219	3.14581	0.59714
H	-2.38015	1.85537	1.40241
H	-3.88413	0.50737	2.63634

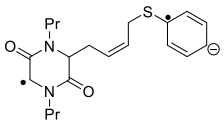


Radical anion A1 in benzene

56

-1476.3011241

C	-3.65506	1.12154	-0.15177
C	-2.25970	1.24052	0.48397
C	-2.64383	-0.91128	1.53722
C	-4.00097	-0.27164	1.80284
H	-4.68636	-1.06492	2.09273
N	-1.79540	-0.11340	0.84980
N	-4.50592	0.38832	0.60418
O	-2.39116	-2.04882	1.90390
O	-3.96122	1.64171	-1.21200
C	-0.54684	-0.69770	0.34853
H	0.20591	0.08303	0.25706
H	-0.19095	-1.39204	1.11108
C	-0.75489	-1.44023	-0.97078
H	-1.53061	-2.19790	-0.81945
H	-1.13589	-0.74336	-1.72590
C	0.53626	-2.09215	-1.45859
H	0.37619	-2.62130	-2.40003
H	1.32283	-1.34816	-1.60660
H	0.90996	-2.80970	-0.72361
C	-5.82638	0.03701	0.09571
H	-6.51125	-0.03283	0.94569
H	-6.16056	0.85726	-0.54115
C	-5.80796	-1.27123	-0.69222
H	-5.42027	-2.07216	-0.05368
H	-5.10790	-1.15850	-1.52510
C	-7.19734	-1.63354	-1.20764
H	-7.17835	-2.56843	-1.76978
H	-7.90304	-1.75291	-0.38118
H	-7.58277	-0.85227	-1.86773
C	-1.30655	2.02960	-0.40723
H	-0.98728	1.42627	-1.25774
H	-1.90843	2.83945	-0.83027
C	-0.14419	2.62530	0.33794
C	1.13479	2.60360	-0.03537
C	1.71470	1.93778	-1.25575
H	1.70307	2.65023	-2.09099
H	1.09493	1.08975	-1.56689
C	3.14610	1.46169	-1.02897
H	3.54141	0.96742	-1.91805
H	3.79947	2.30009	-0.77306
S	3.20806	0.22247	0.37552
C	4.83936	-0.38446	0.35082
C	5.90902	0.33037	1.00053
C	5.22610	-1.42175	-0.57438
C	7.22161	-0.03999	0.82851
H	5.65961	1.16052	1.65552
C	6.54450	-1.77845	-0.73347
H	4.45000	-1.94343	-1.12809
C	7.58630	-1.12550	-0.01793
H	7.99635	0.50841	1.35865
H	6.79079	-2.58595	-1.41853
H	8.62278	-1.40538	-0.15636
H	-0.40381	3.15726	1.25165
H	1.85615	3.11618	0.59806
H	-2.39387	1.81332	1.41338
H	-3.91892	0.43603	2.63718



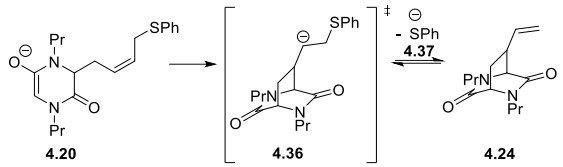
Triplet anion A2 in benzene

55

-1475.6614961

C	-3.52433	-0.72077	0.31774
C	-2.32693	0.01561	0.91807
C	-2.46861	1.67962	-0.87384
C	-3.78453	1.15303	-1.15449
H	-4.42001	1.67295	-1.85505
N	-1.68497	0.92244	-0.03747
N	-4.19676	-0.06915	-0.69333
O	-2.08515	2.71876	-1.41163
O	-3.91619	-1.78592	0.75187
C	-0.36957	1.46624	0.31040
H	0.31428	0.63789	0.50023
H	0.00119	1.98402	-0.57385
C	-0.40860	2.42763	1.49627
H	-1.08568	3.25393	1.25789
H	-0.81903	1.91812	2.37587
C	0.98964	2.95177	1.81316
H	0.97378	3.63878	2.66140
H	1.66793	2.12769	2.04825
H	1.40821	3.48124	0.95373
C	-5.45129	-0.64808	-1.18653
H	-5.58603	-0.30277	-2.21318
H	-5.33037	-1.73138	-1.19918
C	-6.63994	-0.25327	-0.31563
H	-6.71560	0.83815	-0.29071
H	-6.45084	-0.59191	0.70642
C	-7.93405	-0.86374	-0.84542
H	-8.78515	-0.57800	-0.22558
H	-8.13507	-0.53069	-1.86696
H	-7.87428	-1.95486	-0.85253
C	-1.34909	-1.00168	1.51514
H	-0.63492	-0.48037	2.15323
H	-1.94164	-1.64844	2.16779
C	-0.65360	-1.82644	0.46796
C	0.62988	-2.18525	0.47841
C	1.65894	-1.86485	1.52936
H	1.68125	-2.68692	2.25700
H	1.38342	-0.96513	2.09046
C	3.05628	-1.68329	0.94704
H	3.79574	-1.53998	1.73660
H	3.34619	-2.54892	0.34562
S	3.10944	-0.16305	-0.14612
C	4.78767	0.00879	-0.57535
C	5.35127	-0.72415	-1.68089
C	5.72441	0.61624	0.33855
C	6.70714	-0.74294	-1.90727
H	4.68009	-1.24735	-2.35618
C	7.07756	0.58695	0.09558
H	5.34085	1.12501	1.21857
C	7.61735	-0.06493	-1.04725
H	7.08780	-1.28496	-2.76935
H	7.74718	1.08123	0.79519
H	8.68464	-0.09188	-1.22616
H	-1.27592	-2.16444	-0.35817
H	0.99168	-2.79528	-0.34751
H	-2.75544	0.59833	1.75167

Scheme 4.6



Ionic cyclisation of 4.20 – starting species 4.20 in benzene

52

-1436.4472934

C	-1.61570	-1.02625	-0.06472
C	-0.45075	-0.10265	-0.39184
C	-1.99927	1.57283	-1.28609
C	-2.86753	0.51127	-1.47847
N	-0.91635	1.26932	-0.41098
N	-2.74427	-0.69537	-0.70827
O	-2.07780	2.72837	-1.79187
O	-1.50762	-1.98191	0.72210
C	-0.00333	2.31429	0.00664
H	1.02691	1.94353	-0.05934
H	-0.10260	3.15164	-0.68990
C	-0.26475	2.79462	1.43455
H	-1.28248	3.19309	1.48771
H	-0.22498	1.93101	2.10797
C	0.74773	3.85307	1.86370
H	0.58600	4.17882	2.89390
H	1.76939	3.46635	1.78830
H	0.68436	4.73414	1.21877
C	-3.95717	-1.44800	-0.42900
H	-4.58212	-1.41932	-1.32713
H	-3.67794	-2.48554	-0.23564
C	-4.72139	-0.88104	0.76508
H	-4.91968	0.17806	0.57624
H	-4.07193	-0.93958	1.64350
C	-6.02303	-1.63713	1.01351
H	-6.56450	-1.22901	1.86954
H	-6.68149	-1.57876	0.14194
H	-5.82796	-2.69460	1.21331
H	0.27785	-0.20818	0.41258
C	0.19842	-0.58449	-1.71860
H	0.58679	-1.59252	-1.55304
H	-0.59959	-0.64255	-2.46791
C	1.24796	0.36175	-2.21301
H	0.87724	1.35759	-2.44994
C	2.55179	0.13314	-2.38767
H	3.17998	0.94870	-2.73727
C	3.27116	-1.14734	-2.11773
H	3.93645	-1.40874	-2.94373
S	4.40798	-1.02042	-0.67278
C	3.21951	-0.87235	0.65240
C	2.43720	-1.96892	1.02227
C	3.10183	0.32834	1.35133
C	1.54292	-1.86369	2.08093
H	2.52906	-2.90196	0.47706
C	2.22144	0.42252	2.42740
H	3.69628	1.18317	1.04947
C	1.44244	-0.67038	2.79229
H	0.91036	-2.70412	2.33682
H	2.13275	1.35843	2.96742
H	0.73992	-0.58774	3.61318
H	2.59959	-1.98652	-1.94526
H	-3.69449	0.55436	-2.16911

Ionic cyclisation of 4.20 – transition state 4.36 in benzene

52

-1436.4179170

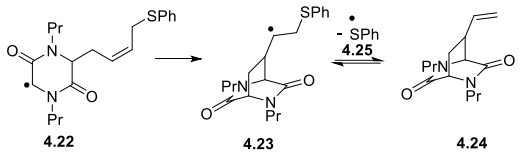
C	1.36917	1.16214	1.33077
C	2.27016	-0.05661	1.19765
C	1.81131	-0.27293	-1.13717
C	0.52222	0.11560	-0.63627
N	2.79736	-0.11880	-0.16457
N	0.47589	1.17942	0.32683
O	2.02453	-0.81405	-2.22862
O	1.45674	1.99417	2.23613
C	4.12300	-0.67722	-0.35625
H	4.27564	-1.51743	0.33639
H	4.15938	-1.08046	-1.36989
C	5.22585	0.36034	-0.15573
H	5.08760	1.15674	-0.89253
H	5.11655	0.82167	0.83146
C	6.61447	-0.25821	-0.29307
H	7.39946	0.48953	-0.16342
H	6.76907	-1.04046	0.45532
H	6.74157	-0.71248	-1.27960
C	-0.59486	2.15831	0.25325
H	-1.52652	1.61831	0.04756
H	-0.68169	2.62751	1.23522
C	-0.34923	3.21156	-0.82337
H	-0.16751	2.70655	-1.77729
H	0.56274	3.76213	-0.57334
C	-1.53482	4.16449	-0.94812
H	-1.35404	4.93168	-1.70379
H	-2.43902	3.61766	-1.22885
H	-1.73233	4.66791	0.00263
H	3.09645	0.05298	1.89926
C	1.44190	-1.32835	1.50236
H	2.09745	-2.19247	1.35216
H	1.14933	-1.30783	2.55695
C	0.21668	-1.47515	0.61459
H	-0.65158	-0.92012	0.98161
H	-0.29623	0.13415	-1.34506
C	-0.04892	-2.70692	0.01728
H	0.70322	-3.48730	-0.00523
C	-1.25767	-2.87330	-0.78178
H	-1.30519	-3.82747	-1.30504
S	-2.93637	-2.83664	0.20548
C	-3.40148	-1.12837	0.08396
C	-3.54970	-0.49131	-1.15525
C	-3.68526	-0.40155	1.24748
C	-3.97851	0.83129	-1.22546
H	-3.35622	-1.04379	-2.06747
C	-4.13541	0.91210	1.17204
H	-3.55011	-0.87907	2.21140
C	-4.28641	1.53582	-0.06456
H	-4.08817	1.30557	-2.19485
H	-4.35769	1.45385	2.08458
H	-4.63158	2.56163	-0.12124
H	-1.43645	-2.06827	-1.50456

Ionic cyclisation of 4.20 – products 4.24 and 4.37 in benzene

52

-1436.4979773

C	-1.27020	0.34615	-1.53844
C	-2.07929	-0.91338	-1.21155
C	-1.79431	-0.40127	1.09894
C	-0.37308	-0.42513	0.53416
N	-2.67403	-0.74421	0.12224
N	-0.34821	0.54223	-0.57182
O	-2.09436	-0.08943	2.23997
O	-1.44535	1.04394	-2.52612
C	-4.09901	-0.49070	0.26753
H	-4.64291	-1.24474	-0.30960
H	-4.34645	-0.62882	1.32154
C	-4.48154	0.91612	-0.18984
H	-3.91338	1.63704	0.40651
H	-4.17323	1.05214	-1.23171
C	-5.97938	1.16519	-0.04256
H	-6.24621	2.17380	-0.36233
H	-6.55446	0.45851	-0.64709
H	-6.29237	1.04776	0.99824
C	0.55659	1.68280	-0.55351
H	1.54489	1.32968	-0.24816
H	0.62873	2.04854	-1.57964
C	0.06649	2.78844	0.37804
H	-0.01213	2.39013	1.39577
H	-0.94162	3.08604	0.07078
C	1.01069	3.98710	0.35595
H	0.66745	4.77527	1.02895
H	2.01571	3.68709	0.66258
H	1.07900	4.40776	-0.65095
H	-2.86954	-1.04140	-1.94861
C	-1.10390	-2.10222	-1.15914
H	-1.67394	-3.00686	-0.93800
H	-0.61873	-2.22621	-2.12924
C	-0.05376	-1.81524	-0.04838
H	0.93183	-1.73820	-0.52543
H	0.34036	-0.11518	1.29555
C	0.02173	-2.91587	0.96868
H	0.21042	-3.90053	0.54377
C	-0.08626	-2.79445	2.28925
H	0.00967	-3.66170	2.93247
S	3.29876	-1.83730	-1.68363
C	3.50419	-0.58635	-0.47277
C	3.06394	-0.75278	0.85815
C	4.10850	0.65341	-0.77865
C	3.18966	0.25856	1.80583
H	2.61252	-1.69795	1.14248
C	4.24356	1.65825	0.17097
H	4.46619	0.81358	-1.78979
C	3.77754	1.47829	1.47472
H	2.82621	0.08797	2.81513
H	4.71083	2.59679	-0.11144
H	3.87667	2.26540	2.21338
H	-0.27535	-1.84273	2.77478



Radical cyclisation of 4.22 – starting species 4.22 in benzene

52

-1436.3403354

C	2.51442	-0.98285	-0.49034
C	1.44924	0.08518	-0.31860
C	2.93266	1.29333	1.21241
C	3.61359	0.02605	1.38662
N	1.98769	1.32363	0.22346
N	3.48950	-1.00043	0.48482
O	3.23665	2.28202	1.88020
O	2.45915	-1.81623	-1.37192
C	1.37857	2.60296	-0.13548
H	0.42450	2.39308	-0.62358
H	1.16843	3.15902	0.78214
C	2.27629	3.42756	-1.05453
H	3.23304	3.58879	-0.55122
H	2.47867	2.84998	-1.96217
C	1.62963	4.76359	-1.40772
H	2.27247	5.35313	-2.06322
H	0.67460	4.61460	-1.91876
H	1.43894	5.35235	-0.50684
C	4.49553	-2.06925	0.46340
H	4.80246	-2.24574	1.49686
H	4.01106	-2.96955	0.08586
C	5.69226	-1.69615	-0.40572
H	6.12177	-0.76113	-0.03307
H	5.33760	-1.51030	-1.42306
C	6.74216	-2.80276	-0.40193
H	7.59577	-2.53297	-1.02516
H	7.11128	-2.98966	0.60976
H	6.32629	-3.73688	-0.78726
H	1.05719	0.28890	-1.31687
C	0.32259	-0.52078	0.55813
H	0.02959	-1.47822	0.12225
H	0.74371	-0.72776	1.54787
C	-0.85474	0.40167	0.70039
H	-0.75157	1.19848	1.43254
C	-1.99141	0.32599	0.00690
H	-2.77773	1.04631	0.21679
C	-2.31309	-0.68948	-1.04262
H	-1.43290	-1.22153	-1.40325
S	-3.43828	-2.01145	-0.42478
C	-4.87096	-1.00997	-0.05024
C	-5.69299	-0.55189	-1.08102
C	-5.17541	-0.69197	1.27306
C	-6.80528	0.23025	-0.78911
H	-5.46133	-0.81514	-2.10716
C	-6.29617	0.08240	1.56177
H	-4.53143	-1.04859	2.06818
C	-7.10936	0.54634	0.53287
H	-7.44020	0.58351	-1.59305
H	-6.52975	0.32545	2.59181
H	-7.98015	1.14981	0.76042
H	-2.79828	-0.22199	-1.90082
H	4.35641	-0.07081	2.16378

Radical cyclisation of 4.22 – transition state cyclisation in benzene

52
-1436.3236327

C	1.60080	1.02777	1.17158
C	1.62562	-0.49111	1.17274
C	1.87491	-0.55144	-1.20390
C	0.91811	0.56430	-1.04486
N	2.34549	-0.97870	0.00216
N	1.16381	1.50128	-0.03242
O	2.14895	-1.04971	-2.28775
O	1.87450	1.72650	2.12976
C	3.22804	-2.13064	0.12622
H	2.74649	-2.88022	0.76653
H	3.32942	-2.56140	-0.87101
C	4.59675	-1.75573	0.68709
H	5.07309	-1.05608	-0.00534
H	4.46966	-1.22681	1.63723
C	5.47323	-2.98854	0.88604
H	6.46466	-2.71241	1.24774
H	5.02894	-3.67396	1.61254
H	5.59842	-3.53216	-0.05392
C	0.95103	2.93018	-0.25171
H	0.07789	3.03883	-0.90182
H	0.71775	3.37698	0.71608
C	2.17418	3.60044	-0.87065
H	2.42939	3.08200	-1.80023
H	3.01953	3.47559	-0.18795
C	1.91835	5.08006	-1.13886
H	2.79876	5.55943	-1.56904
H	1.08937	5.21232	-1.83919
H	1.66623	5.60640	-0.21497
H	2.13471	-0.82113	2.07632
C	0.16489	-1.01745	1.14043
H	0.21600	-2.10842	1.18987
H	-0.35823	-0.66912	2.03534
C	-0.60426	-0.60552	-0.10037
H	-1.17856	0.31662	-0.02513
H	0.49759	0.96456	-1.95844
C	-1.07186	-1.55829	-0.99189
H	-0.70020	-2.57705	-0.93639
C	-2.07023	-1.23872	-2.03872
H	-1.90987	-1.80534	-2.95668
S	-3.79182	-1.71271	-1.51548
C	-3.91176	-0.66498	-0.07571
C	-4.20469	0.69188	-0.21982
C	-3.66091	-1.18830	1.19224
C	-4.23147	1.52153	0.89693
H	-4.40501	1.09323	-1.20700
C	-3.69753	-0.35766	2.30902
H	-3.42714	-2.24136	1.29563
C	-3.97618	0.99806	2.16215
H	-4.45566	2.57515	0.77909
H	-3.50248	-0.77002	3.29223
H	-3.99796	1.64420	3.03173
H	-2.08847	-0.17397	-2.27760

Radical cyclisation of 4.22 – intermediate 4.23 in benzene

52
-1436.3557025

C	-1.92479	0.72265	-1.58262
C	-2.43863	-0.68051	-1.25656
C	-1.17314	-0.62616	0.76244
C	-0.16129	-0.29188	-0.33353
N	-2.37976	-0.87720	0.19664
N	-0.67103	0.85664	-1.08783
O	-0.91899	-0.65961	1.95456
O	-2.54346	1.56235	-2.21306
C	-3.59729	-0.96662	0.99107
H	-4.26377	-1.69503	0.51969
H	-3.31286	-1.35381	1.97104
C	-4.29025	0.38724	1.13127
H	-3.58711	1.08767	1.59305
H	-4.52310	0.77936	0.13550
C	-5.56227	0.28033	1.96661
H	-6.05203	1.25032	2.06388
H	-6.27444	-0.41119	1.50874
H	-5.33812	-0.08584	2.97161
C	0.08011	2.10036	-1.17544
H	1.10149	1.86623	-1.49278
H	-0.39300	2.69638	-1.95800
C	0.10192	2.86764	0.14329
H	0.58237	2.25342	0.91258
H	-0.92969	3.04065	0.46565
C	0.84192	4.19319	-0.01002
H	0.92334	4.71498	0.94503
H	1.85316	4.03157	-0.39306
H	0.32066	4.85009	-0.71093
H	-3.46636	-0.78352	-1.59798
C	-1.47861	-1.67700	-1.93495
H	-1.85615	-2.68930	-1.78278
H	-1.45355	-1.47823	-3.00748
C	-0.07351	-1.51205	-1.28832
H	0.65812	-1.24083	-2.06354
H	0.79447	-0.02949	0.11587
C	0.36775	-2.76527	-0.60110
H	0.15016	-3.69893	-1.10857
C	1.36876	-2.79307	0.48134
H	1.43666	-3.78193	0.93133
S	3.10212	-2.42636	-0.13910
C	3.26061	-0.70120	0.28274
C	3.11378	-0.27721	1.60628
C	3.55287	0.23132	-0.71275
C	3.23213	1.07030	1.92341
H	2.90779	-1.00191	2.38586
C	3.69557	1.57815	-0.38480
H	3.65856	-0.09919	-1.73972
C	3.52778	2.00114	0.92965
H	3.10506	1.39247	2.95015
H	3.92354	2.29735	-1.16369
H	3.62564	3.05068	1.18101
H	1.16979	-2.06622	1.27128

Radical cyclisation of 4.22 – transition state C-S cleavage in benzene

52
-1436.3453638

C	-2.00798	0.54352	-1.59482
C	-2.40760	-0.88262	-1.21133
C	-1.06731	-0.66397	0.74596
C	-0.12014	-0.31194	-0.40362
N	-2.27298	-1.03198	0.24296
N	-0.74674	0.78071	-1.15946
O	-0.77887	-0.59773	1.92788
O	-2.71307	1.32196	-2.21236
C	-3.45618	-1.10205	1.09173
H	-4.12926	-1.85936	0.67979
H	-3.12716	-1.44091	2.07529
C	-4.16179	0.24848	1.19850
H	-3.44953	0.97768	1.59794
H	-4.44144	0.59040	0.19633
C	-5.39624	0.16471	2.09098
H	-5.89476	1.13224	2.16525
H	-6.11713	-0.55483	1.69402
H	-5.12552	-0.15297	3.10095
C	-0.11167	2.08524	-1.27431
H	0.93059	1.93440	-1.57203
H	-0.62375	2.61547	-2.07935
C	-0.18218	2.88528	0.02316
H	0.32300	2.32802	0.81932
H	-1.23235	2.98476	0.31548
C	0.45691	4.25994	-0.14863
H	0.46854	4.81338	0.79179
H	1.48874	4.16791	-0.49917
H	-0.09176	4.85400	-0.88376
H	-3.43949	-1.06606	-1.50307
C	-1.41582	-1.83715	-1.89885
H	-1.70249	-2.86411	-1.66641
H	-1.46794	-1.70226	-2.98009
C	0.01252	-1.52488	-1.35369
H	0.64642	-1.19856	-2.18745
H	0.83465	0.02735	-0.00338
C	0.63383	-2.74393	-0.74490
H	0.64290	-3.61975	-1.38884
C	1.25320	-2.82941	0.47002
H	1.53486	-3.80435	0.84717
S	3.48797	-2.25650	-0.03497
C	3.37416	-0.54376	0.33663
C	3.11723	-0.11788	1.64882
C	3.52623	0.41729	-0.67351
C	3.00394	1.23461	1.93984
H	3.00211	-0.85752	2.43295
C	3.43519	1.77185	-0.37163
H	3.71842	0.09050	-1.68894
C	3.16805	2.18373	0.93202
H	2.79250	1.54989	2.95479
H	3.56659	2.50744	-1.15766
H	3.08639	3.23933	1.16361
H	1.14682	-2.04524	1.21202

Radical cyclisation of 4.22 – products 4.24 in benzene

40
-806.5874061

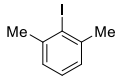
C	0.29707	0.44476	1.51284
C	-0.08337	-1.02144	1.29426
C	-0.26338	-0.55455	-1.03796
C	-1.17098	0.47968	-0.36717
N	0.25811	-1.37623	-0.09002
N	-0.36453	1.21556	0.61246
O	-0.04430	-0.61706	-2.23413
O	1.07341	0.84554	2.36156
C	1.39065	-2.24704	-0.37750
H	1.30945	-3.13646	0.25414
H	1.29899	-2.56178	-1.41837
C	2.72542	-1.54081	-0.14662
H	2.76134	-0.65608	-0.79042
H	2.77034	-1.18460	0.88811
C	3.90518	-2.46181	-0.44089
H	4.85462	-1.95041	-0.27621
H	3.88350	-3.34416	0.20411
H	3.88271	-2.80399	-1.47862
C	-0.02544	2.61609	0.39921
H	-0.94291	3.15777	0.15060
H	0.34922	3.00284	1.34842
C	1.01923	2.79272	-0.70087
H	0.64297	2.35220	-1.63024
H	1.91423	2.22887	-0.41943
C	1.36083	4.26404	-0.91482
H	2.10812	4.38507	-1.70033
H	0.47358	4.83294	-1.20497
H	1.75972	4.70779	0.00084
H	0.47822	-1.65085	1.98127
C	-1.60673	-1.15377	1.46333
H	-1.88324	-2.20164	1.33359
H	-1.89637	-0.84970	2.47022
C	-2.29958	-0.26507	0.39059
H	-2.91374	0.49797	0.87409
H	-1.56108	1.16669	-1.11554
C	-3.15423	-1.06210	-0.55307
H	-2.65182	-1.86583	-1.09095
C	-4.44910	-0.84507	-0.75247
H	-5.02406	-1.44934	-1.44391
H	-4.97510	-0.05434	-0.22616

Radical cyclisation of 4.22 – products 4.25 in benzene

12
-629.7431433

C	-2.23859	0.00003	0.00000
C	-1.53711	1.20175	-0.00001
C	-0.14683	1.21039	0.00001
C	0.55154	-0.00006	-0.00001
C	-0.14689	-1.21043	-0.00001
C	-1.53720	-1.20169	0.00002
H	-3.32135	0.00009	0.00000
H	-2.07227	2.14410	-0.00001
H	0.39209	2.15074	0.00002
H	0.39193	-2.15083	-0.00002
H	-2.07238	-2.14404	0.00002
S	2.31327	-0.00000	0.00000

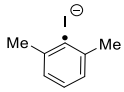
Scheme 4.7



Iodo-*m*-xylene 4.43 in benzene

18
-321.5822874

C	-3.27884	-0.00020	-0.00002
C	-2.58373	1.20071	-0.00001
C	-1.18681	1.23054	0.00000
C	-0.52099	0.00001	0.00001
C	-1.18661	-1.23058	0.00002
C	-2.58356	-1.20097	-0.00001
H	-4.36212	-0.00025	-0.00004
H	-3.12450	2.14050	-0.00000
H	-3.12415	-2.14087	-0.00001
I	1.62271	0.00005	-0.00001
C	-0.47060	-2.55398	0.00002
H	0.17028	-2.65497	-0.87955
H	0.17029	-2.65497	0.87958
H	-1.18969	-3.37302	0.00003
C	-0.47103	2.55407	0.00002
H	0.16984	2.65516	0.87958
H	0.16980	2.65522	-0.87955
H	-1.19027	3.37299	0.00007

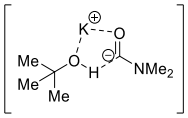


Radical anion A3 in benzene

18
-321.6512155

C	3.93898	-0.00006	-0.00108
C	3.24948	1.21084	-0.00064
C	1.84785	1.23178	0.00042
C	1.22920	0.00002	0.00093
C	1.84777	-1.23179	0.00051
C	3.24940	-1.21092	-0.00050
H	5.02324	-0.00010	-0.00188
H	3.79777	2.14841	-0.00114
H	3.79764	-2.14853	-0.00085
I	-2.31150	0.00001	-0.00024
C	1.05527	-2.51331	0.00096
H	0.40417	-2.55732	0.87635
H	0.40500	-2.55838	-0.87501
H	1.71598	-3.38220	0.00172
C	1.05542	2.51335	0.00101
H	0.40323	2.55741	-0.87356
H	0.40625	2.55846	0.87780
H	1.71618	3.38221	-0.00056

Scheme 4.9



Neutral complex 4.53 in DMF - *Method A/B*

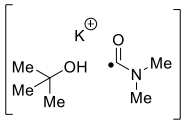
27
-1081.4834832

C	-3.63144	-0.50075	0.58763
H	-3.75586	-1.33954	1.28111
H	-3.64035	0.43296	1.14585
H	-4.47457	-0.51220	-0.11182
N	-2.36875	-0.60556	-0.12223
C	-2.19095	-1.80740	-0.90571
H	-1.22679	-1.75784	-1.41173
H	-2.21320	-2.70255	-0.27220
H	-2.98284	-1.90709	-1.65705
C	-1.38343	0.35336	-0.08887
H	0.25372	-0.01403	-0.64607
O	-1.62055	1.38981	0.59744
O	1.26562	-0.05435	-0.86717
C	1.93565	-0.83173	0.12040
C	3.35716	-1.06084	-0.38051
H	3.85352	-0.10253	-0.55335
H	3.93993	-1.62809	0.34981
H	3.34027	-1.61716	-1.32094
C	1.95881	-0.06420	1.44679
H	0.93733	0.16627	1.76423
H	2.44180	-0.64775	2.23495
H	2.51397	0.87185	1.33277
C	1.21809	-2.17123	0.30749
H	1.15011	-2.69674	-0.64882
H	1.75869	-2.80461	1.01585
H	0.20489	-2.01191	0.68649
K	0.51246	2.54331	-0.35258

Iodobenzene 4.1 in DMF - *Method A/B*

12
-242.9682233

C	2.64531	-1.20411	0.00000
C	1.25223	-1.21321	-0.00001
C	0.57437	-0.00002	0.00000
C	1.25222	1.21321	0.00000
C	2.64527	1.20413	-0.00001
C	3.34252	0.00001	0.00001
H	3.18144	-2.14575	0.00000
H	0.71162	-2.15110	-0.00000
H	0.71156	2.15107	0.00001
H	3.18142	2.14576	-0.00001
H	4.42555	0.00004	0.00002
I	-1.55628	0.00000	0.00000

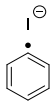


Radical cation complex 4.58 in DMF - *Method A*

27

-1081.3428081

C	-3.76359	0.09866	0.77174
H	-3.80707	-0.51501	1.67320
H	-3.55731	1.13248	1.03861
H	-4.71713	0.03596	0.24507
N	-2.69286	-0.39313	-0.10095
C	-2.80009	-1.76712	-0.57718
H	-1.95294	-1.98869	-1.22399
H	-2.80261	-2.45303	0.27245
H	-3.72805	-1.88898	-1.13847
C	-1.66189	0.35764	-0.41662
H	0.59821	-0.24458	-1.12871
O	-1.36650	1.49106	-0.13437
O	1.43198	0.01958	-0.71844
C	1.88987	-1.07217	0.10499
C	3.20594	-0.60335	0.70782
H	3.04909	0.27414	1.33993
H	3.64136	-1.39402	1.32167
H	3.91341	-0.34614	-0.08332
C	0.85736	-1.34912	1.19561
H	-0.07969	-1.70948	0.76017
H	1.22474	-2.11326	1.88444
H	0.65090	-0.43715	1.76160
C	2.09596	-2.30251	-0.77246
H	2.83446	-2.09584	-1.54995
H	2.44392	-3.14701	-0.17349
H	1.15532	-2.59088	-1.25141
K	1.07991	2.63032	-0.12116

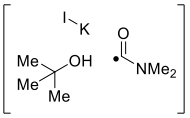


Radical anion 4.59 in DMF - *Method A*

12

-243.0754418

C	3.64561	-1.21088	-0.00014
C	2.24659	-1.22152	0.00032
C	1.61468	0.00002	0.00052
C	2.24663	1.22155	0.00032
C	3.64564	1.21087	-0.00014
C	4.33623	-0.00002	-0.00036
H	4.19115	-2.14790	-0.00032
H	1.69441	-2.15461	0.00049
H	1.69446	2.15464	0.00049
H	4.19122	2.14786	-0.00032
H	5.41963	-0.00003	-0.00072
I	-2.33213	0.00000	-0.00005



Radical complex 4.60 in DMF - *Method B*

28

-1092.9131822

C	-2.81033	2.85784	-0.33002
H	-3.27667	2.36903	-1.18899
H	-3.33023	2.57135	0.58158
H	-2.86277	3.94028	-0.45987
N	-1.40942	2.44292	-0.23547
C	-0.54704	2.75523	-1.36852
H	0.44402	2.34185	-1.18711
H	-0.96359	2.31361	-2.27737
H	-0.48474	3.83775	-1.49750
C	-0.95905	1.76641	0.79998
H	-0.04916	-1.03740	-0.39833
O	-1.49564	1.39572	1.81467
O	-0.70550	-1.47161	0.16964
C	-1.84419	-1.86038	-0.61424
C	-2.71486	-2.69398	0.31468
H	-2.99797	-2.10597	1.19125
H	-3.62378	-3.01195	-0.20000
H	-2.17161	-3.58128	0.64717
C	-2.58741	-0.60832	-1.07407
H	-1.93215	0.01973	-1.68647
H	-3.46344	-0.87525	-1.67010
H	-2.91539	-0.03005	-0.20669
C	-1.37094	-2.68153	-1.81032
H	-0.81964	-3.56125	-1.47094
H	-2.22174	-3.01029	-2.41146
H	-0.71393	-2.08202	-2.44799
K	0.31561	-0.59836	2.43781
I	2.45027	-0.00819	-0.40314

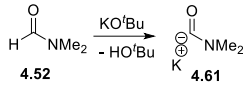
Phenyl radical 4.2 in DMF - *Method B*

11

-231.5160855

C	1.21101	0.63045	0.00000
C	1.22267	-0.76846	0.00000
C	0.00000	-1.39689	-0.00000
C	-1.22267	-0.76845	0.00000
C	-1.21101	0.63045	0.00000
C	0.00000	1.32045	0.00000
H	2.14820	1.17539	0.00000
H	2.15590	-1.31991	0.00000
H	-2.15589	-1.31992	0.00000
H	-2.14820	1.17539	0.00000
H	-0.00001	2.40379	0.00000

Scheme 4.10



4.52 4.61

Deprotonation of 4.52 – starting species 4.52 and KO^{t}Bu in benzene

27
-1081.4907677

C	-4.11082	-0.27327	0.00089
H	-4.61986	-0.66223	0.88675
H	-4.14733	0.81320	0.00654
H	-4.61856	-0.65281	-0.88982
N	-2.72300	-0.69696	0.00010
C	-2.47056	-2.12621	-0.00096
H	-1.39684	-2.30678	-0.00311
H	-2.90809	-2.58860	0.88792
H	-2.91147	-2.58779	-0.88860
C	-1.71539	0.19002	-0.00027
H	-0.70109	-0.24373	-0.00085
O	-1.86838	1.41425	0.00011
O	1.40077	0.35365	-0.00030
C	2.25686	-0.72177	0.00014
C	3.16040	-0.70149	-1.24988
H	3.74417	0.22391	-1.26095
H	3.85273	-1.54989	-1.28388
H	2.53737	-0.72231	-2.14920
C	3.15907	-0.70146	1.25113
H	2.53508	-0.72224	2.14978
H	3.85139	-1.54985	1.28590
H	3.74282	0.22395	1.26278
C	1.46758	-2.04818	-0.00028
H	0.83005	-2.09080	-0.89019
H	2.11846	-2.92896	0.00007
H	0.82906	-2.09081	0.88893
K	0.50427	2.55081	-0.00031

Deprotonation of 4.52 – transition state in benzene

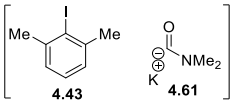
27
-1081.4684972

C	-3.84968	-0.38208	0.00007
H	-4.34860	-0.78581	0.88769
H	-3.93325	0.70237	-0.00143
H	-4.34851	-0.78828	-0.88647
N	-2.44180	-0.73563	0.00060
C	-2.14899	-2.14997	0.00062
H	-1.06895	-2.28723	0.00281
H	-2.57040	-2.63922	0.88642
H	-2.56676	-2.63869	-0.88722
C	-1.43475	0.18864	-0.00072
H	0.06117	0.01741	-0.00071
O	-1.76317	1.40744	-0.00152
O	1.17577	0.31538	-0.00077
C	2.05088	-0.78664	-0.00012
C	3.48357	-0.25280	-0.00109
H	3.65255	0.36391	0.88585
H	4.21238	-1.06855	-0.00025
H	3.65213	0.36170	-0.88965
C	1.82196	-1.63493	1.25765
H	0.79030	-1.99400	1.29198
H	2.49100	-2.49991	1.28521
H	1.99849	-1.02824	2.14976
C	1.82098	-1.63710	-1.25624
H	1.99585	-1.03168	-2.14953
H	2.49062	-2.50162	-1.28331
H	0.78951	-1.99696	-1.28864
K	0.42266	2.69005	0.00056

Deprotonation of 4.52 – products 4.61 and HO^{t}Bu in benzene

27
-1081.4692339

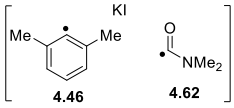
C	-3.59384	-0.49645	0.62918
H	-3.70492	-1.34500	1.31326
H	-3.56933	0.42905	1.20082
H	-4.45899	-0.48609	-0.04306
N	-2.35676	-0.60368	-0.12222
C	-2.21063	-1.78920	-0.93409
H	-1.26029	-1.73562	-1.46562
H	-2.22345	-2.69739	-0.31865
H	-3.02314	-1.86696	-1.66609
C	-1.36677	0.34722	-0.09921
H	0.26212	-0.02069	-0.68055
O	-1.57551	1.36986	0.61575
O	1.28255	-0.03054	-0.87444
C	1.93908	-0.80378	0.12342
C	3.36886	-1.02792	-0.35510
H	3.86373	-0.06804	-0.52415
H	3.94402	-1.59137	0.38432
H	3.36593	-1.58377	-1.29542
C	1.93616	-0.03313	1.44941
H	0.90854	0.19711	1.74746
H	2.40597	-0.61129	2.24941
H	2.49561	0.90254	1.34269
C	1.22266	-2.14510	0.30061
H	1.16984	-2.66776	-0.65785
H	1.75503	-2.77835	1.01533
H	0.20406	-1.98881	0.66584
K	0.47016	2.47968	-0.36989



Neutral complex 4.43 and 4.61 in benzene

30
-1169.4058004

C	2.75646	0.14492	-0.81912
N	3.67501	-0.61011	-0.11799
C	3.67219	-2.06041	-0.08181
H	2.88427	-2.41813	-0.74309
H	4.63606	-2.46253	-0.41355
H	3.48544	-2.42591	0.93640
O	1.88854	-0.51024	-1.46874
C	0.60501	1.63148	1.58430
C	0.06801	0.38858	1.23068
C	-1.15158	0.39169	0.54202
C	-1.84832	1.56650	0.22297
C	-1.27253	2.78028	0.61291
C	-0.05560	2.81600	1.28540
H	1.55984	1.65472	2.09646
H	-1.79625	3.70265	0.38678
H	0.37594	3.76640	1.57666
I	-1.97647	-1.48381	-0.06483
C	0.80675	-0.87123	1.58060
H	0.19920	-1.50808	2.22899
H	1.04689	-1.42619	0.67094
H	1.74175	-0.63123	2.08751
C	-3.16791	1.56710	-0.50142
H	-3.08200	1.09877	-1.48521
H	-3.91798	1.00229	0.05672
H	-3.52821	2.58735	-0.63129
C	4.65449	0.03452	0.72014
H	4.50423	-0.22107	1.77842
H	5.67377	-0.26466	0.44707
H	4.55424	1.11310	0.59732
K	0.79899	1.74162	-1.67571



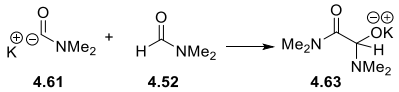
4.46 4.62

Triplet complex 4.46, 4.62 and KI in benzene

30
-1169.3863592

C	-2.85334	1.16624	0.81818
N	-3.62545	0.42494	0.05152
C	-3.30924	-0.97872	-0.23363
H	-2.33297	-1.22494	0.18179
H	-4.07576	-1.62522	0.19872
H	-3.28200	-1.12613	-1.31559
O	-1.84220	0.90991	1.41959
C	0.35285	2.82967	-0.33764
C	0.34451	1.68439	-1.14879
C	1.53421	0.98943	-1.20953
C	2.70891	1.28956	-0.55064
C	2.67520	2.44540	0.24581
C	1.50795	3.20354	0.34854
H	-0.55476	3.41732	-0.23993
H	3.56799	2.74526	0.78597
H	1.49936	4.09266	0.96842
I	0.59071	-2.32324	-0.07870
C	-0.88005	1.22149	-1.89047
H	-0.69454	1.21142	-2.96647
H	-1.12673	0.19884	-1.59038
H	-1.73037	1.87519	-1.68834
C	3.93272	0.42178	-0.67666
H	3.67724	-0.61979	-0.46703
H	4.32777	0.46508	-1.69385
H	4.71444	0.74616	0.01114
C	-4.80509	0.98762	-0.58949
H	-4.68432	0.96313	-1.67521
H	-5.68713	0.40478	-0.31643
H	-4.93412	2.01677	-0.25975
K	0.67749	0.40920	1.78245

Scheme 4.11



4.61 4.52 4.63

Formation of 4.63 – starting species 4.61 and 4.52 in benzene

24
-1096.3073305

C	-2.75173	-0.62803	1.03220
H	-3.49920	-1.42668	1.11207
H	-2.12349	-0.63527	1.92170
H	-3.29039	0.32595	0.97185
N	-1.90243	-0.81656	-0.12895
C	-2.56415	-0.74742	-1.40726
H	-1.81999	-0.90912	-2.18765
H	-3.34855	-1.50975	-1.49827
H	-3.03514	0.23359	-1.55801
C	-0.55375	-1.12149	-0.05737
O	-0.06908	-1.17764	1.10966
K	2.08198	-1.76177	-0.07872
C	1.23040	1.29293	-0.87503
N	0.41046	1.92741	-0.03094
C	0.67998	1.92798	1.39712
H	1.75336	1.85038	1.55723
H	0.31170	2.86083	1.82725
H	0.18161	1.06959	1.86083
C	-0.91943	2.33548	-0.44301
H	-1.66794	1.73212	0.07692
H	-1.07691	3.39196	-0.21370
H	-1.03606	2.18056	-1.51591
O	2.31247	0.78928	-0.57329
H	0.86212	1.28359	-1.91024

Formation of 4.63 – transition state in benzene

24
-1096.2951509

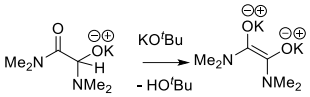
C	-2.43393	-1.72298	0.93357
H	-2.81352	-2.68937	0.58363
H	-1.76800	-1.88118	1.77936
H	-3.29004	-1.11600	1.24950
N	-1.69161	-1.04598	-0.11654
C	-2.44185	-0.72339	-1.30703
H	-1.77040	-0.27707	-2.03949
H	-2.88467	-1.62594	-1.74375
H	-3.25582	-0.01978	-1.09001
C	-0.36085	-0.72008	-0.01549
O	0.24483	-1.09389	1.01888
K	2.50249	-1.36540	-0.10958
C	0.58363	1.12623	-0.88465
N	0.00293	2.03627	-0.00813
C	0.55981	2.13137	1.32640
H	1.64328	2.04883	1.26629
H	0.29407	3.09840	1.75900
H	0.17587	1.32688	1.97013
C	-1.43065	2.21780	-0.06838
H	-1.96020	1.48205	0.55355
H	-1.68660	3.22151	0.27844
H	-1.77332	2.11175	-1.09916
O	1.81487	0.89426	-0.84286
H	0.02828	1.07383	-1.82754

Formation of 4.63 – product 4.63 in benzene

24

-1096.3224629

C	2.04604	-2.09262	-0.86077
H	1.94527	-3.06758	-0.37194
H	1.40651	-2.07216	-1.73902
H	3.08698	-1.95773	-1.16047
N	1.67521	-1.01183	0.04271
C	2.72610	-0.62381	0.97061
H	2.34486	0.01225	1.76088
H	3.14789	-1.52432	1.42644
H	3.52729	-0.09498	0.44541
C	0.39281	-0.56605	0.04542
O	-0.44383	-1.12120	-0.68180
K	-2.90038	-0.83477	0.04744
C	-0.05321	0.69758	0.87823
N	0.19247	1.90079	0.01747
C	-0.59638	1.92878	-1.19694
H	-1.63241	1.69620	-0.94846
H	-0.56222	2.93374	-1.62782
H	-0.24449	1.21524	-1.96256
C	1.58638	2.18961	-0.24899
H	2.06350	1.47358	-0.94284
H	1.67319	3.18520	-0.69338
H	2.15144	2.18938	0.68679
O	-1.32276	0.57175	1.25184
H	0.64802	0.84378	1.71863



4.63 **4.64**

Deprotonation of 4.63 – starting species 4.63 and KO^{t}Bu in benzene

39

-1929.3495378

C	-1.97233	3.41002	-0.23503
H	-2.11677	3.70446	-1.28007
H	-2.94353	3.22193	0.21505
H	-1.47328	4.22550	0.29076
N	-1.14353	2.21618	-0.13940
C	0.28964	2.47169	-0.25261
H	0.87718	1.55729	-0.29953
H	0.47545	3.05396	-1.16090
H	0.62731	3.05918	0.60643
C	-1.74540	1.00457	-0.12845
O	-2.98011	0.91999	-0.22226
K	-3.80385	-1.28213	-1.24807
C	-0.89526	-0.28691	0.06055
N	-0.71873	-0.54418	1.52740
C	-1.97374	-0.70219	2.24083
H	-2.62435	-1.36790	1.67209
H	-1.78377	-1.14892	3.22091
H	-2.49984	0.25437	2.39748
C	0.16643	0.39509	2.20256
H	-0.27084	1.40369	2.29997
H	0.37141	0.02689	3.21222
H	1.10978	0.45421	1.65272
O	-1.46038	-1.34606	-0.56021
H	0.12479	-0.07834	-0.28759
O	2.36366	-0.53192	-0.23782
C	3.57131	0.09697	-0.41287
C	4.72840	-0.92617	-0.42471
H	5.70991	-0.45808	-0.56171
H	4.73602	-1.47669	0.52141
H	4.57014	-1.64370	-1.23620
C	3.60373	0.86679	-1.75088
H	4.56064	1.37195	-1.92447
H	3.42174	0.16933	-2.57398
H	2.80806	1.61802	-1.76180
C	3.83721	1.10308	0.72843
H	3.04223	1.85555	0.74828
H	3.82817	0.57588	1.68764
H	4.79872	1.61785	0.62201
K	0.89024	-2.43547	0.10169

Deprotonation of 4.63 – transition state in benzene

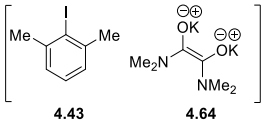
39
-1929.2931514

C	-2.62035	1.86386	-1.96883
H	-2.44118	1.42109	-2.95790
H	-3.52563	1.42100	-1.55515
H	-2.77657	2.93815	-2.09135
N	-1.50149	1.66761	-1.06043
C	-0.31595	2.38274	-1.53400
H	0.57818	2.04276	-1.02156
H	-0.17483	2.20283	-2.61078
H	-0.44031	3.45850	-1.38220
C	-1.34929	0.34357	-0.59065
O	-1.95433	-0.57209	-1.21636
K	-2.81676	-1.94498	0.82999
C	-0.44235	0.05867	0.52927
N	-0.48545	0.99705	1.66247
C	-1.79418	1.08622	2.27262
H	-2.12630	0.08336	2.55719
H	-1.74797	1.67893	3.19194
H	-2.54773	1.54915	1.60766
C	0.13635	2.29897	1.54020
H	-0.46447	3.02790	0.97228
H	0.30036	2.71340	2.54175
H	1.10751	2.19926	1.05210
O	-0.46340	-1.26368	0.92742
H	0.82393	0.22344	-0.05894
O	1.91301	0.11750	-0.65417
C	3.07697	-0.07144	0.11128
C	2.72826	-0.33903	1.58137
H	3.62514	-0.58738	2.15758
H	2.25401	0.53654	2.03198
H	2.00582	-1.15737	1.64672
C	3.84336	-1.27876	-0.44937
H	4.80312	-1.42369	0.05574
H	3.25790	-2.19507	-0.31428
H	4.03087	-1.13513	-1.51741
C	3.96168	1.17656	0.00390
H	4.21471	1.36445	-1.04329
H	3.41945	2.04644	0.38497
H	4.88916	1.06893	0.57538
K	0.47645	-1.92407	-1.34928

Deprotonation of 4.63 – products 4.64 and HO^{t}Bu in benzene

39
-1929.3380828

C	-3.46651	1.81716	-0.32656
H	-4.14086	1.18553	-0.92646
H	-3.62717	1.59715	0.73243
H	-3.73094	2.86487	-0.50117
N	-2.06409	1.60509	-0.65499
C	-1.82387	1.95392	-2.04940
H	-0.76492	1.80739	-2.28235
H	-2.42105	1.34476	-2.74455
H	-2.06743	3.00826	-2.21365
C	-1.65711	0.24604	-0.37151
O	-2.25655	-0.72283	-1.07186
K	-2.88579	-1.81804	1.09565
C	-0.70116	-0.05212	0.57946
N	0.20109	0.89332	1.22138
C	0.24013	0.72884	2.66906
H	0.27889	-0.33270	2.90461
H	1.13043	1.22072	3.07257
H	-0.64685	1.17549	3.15016
C	0.19273	2.30324	0.86234
H	-0.71316	2.82665	1.18997
H	1.06258	2.77136	1.33577
H	0.27792	2.41615	-0.21762
O	-0.41632	-1.31160	0.89056
O	2.10159	-0.01730	-0.60398
C	3.44401	-0.02548	-0.12282
C	3.58931	-1.09923	0.95657
H	4.61308	-1.13562	1.33836
H	2.91225	-0.88667	1.78893
H	3.33091	-2.07993	0.54931
C	4.32996	-0.33843	-1.32137
H	5.38209	-0.36802	-1.02849
H	4.06044	-1.30953	-1.74466
H	4.20218	0.42519	-2.09217
C	3.78070	1.35009	0.45332
H	3.62572	2.12211	-0.30435
H	3.13128	1.56746	1.30646
H	4.81926	1.39031	0.79170
K	0.13907	-1.56346	-1.61718
H	1.51508	0.25840	0.14739



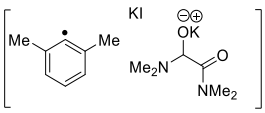
4.43 **4.64**

Neutral complex of 4.43 and 4.64 in benzene

42

-2017.2699655

N	-2.23797	-1.38573	1.66632
C	-1.00479	-1.31280	2.42541
H	-0.89830	-0.30717	2.83419
H	-1.02579	-2.02787	3.25404
H	-0.12234	-1.54367	1.79769
C	-2.42086	-0.23910	0.81517
O	-2.54421	0.90560	1.48299
K	-4.72588	1.24910	0.25142
C	-2.47685	-0.26010	-0.56532
N	-2.16996	-1.45990	-1.31367
C	-0.92217	-1.30330	-2.04654
H	-0.11692	-1.09421	-1.33607
H	-0.67580	-2.23193	-2.57231
H	-0.96687	-0.48698	-2.78759
O	-2.76741	0.83828	-1.27895
K	-0.78860	1.88607	-0.07518
C	2.13667	2.65352	-1.30282
C	2.30730	1.26443	-1.28742
C	2.38576	0.63887	-0.03518
C	2.28814	1.34190	1.17401
C	2.12011	2.72915	1.10042
C	2.05397	3.38349	-0.12347
H	2.08079	3.16051	-2.25970
H	2.05242	3.29439	2.02327
H	1.93651	4.46027	-0.15809
I	2.76201	-1.46317	0.03435
C	2.42582	0.51843	-2.58873
H	3.40874	0.04895	-2.67733
H	1.67881	-0.27486	-2.66311
H	2.29150	1.20101	-3.42729
C	2.38145	0.67485	2.51899
H	1.62909	-0.10981	2.62349
H	3.36033	0.20714	2.65044
H	2.23612	1.40557	3.31399
C	-3.24517	-1.81656	-2.22845
H	-3.42360	-1.04252	-2.98976
H	-3.00321	-2.75605	-2.73490
H	-4.16931	-1.96175	-1.66155
C	-2.49647	-2.72811	1.19005
H	-3.41741	-2.74411	0.60610
H	-1.69658	-3.13467	0.55569
H	-2.61882	-3.38197	2.06207



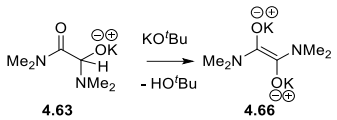
4.46 **4.65**

Triplet complex of 4.46 and 4.65 in benzene

42

-2017.2898503

N	-2.12251	0.46575	1.96555
C	-1.84445	1.55966	2.87988
H	-2.42021	2.44059	2.60182
H	-2.12543	1.24671	3.88710
H	-0.78022	1.83435	2.88117
C	-2.03703	0.79630	0.60850
O	-1.64737	1.96978	0.26834
K	-2.99167	2.52895	-1.82511
C	-2.42044	-0.13427	-0.44037
N	-3.06286	-1.33750	-0.16539
C	-3.13441	-2.28577	-1.26312
H	-2.15892	-2.37278	-1.73836
H	-3.42069	-3.25804	-0.85783
H	-3.87168	-1.98771	-2.02136
O	-2.08853	0.14148	-1.64624
K	0.44728	0.67784	-0.97598
C	3.12861	2.44639	-0.92254
C	3.60871	1.14034	-0.73395
C	3.28921	0.56023	0.47558
C	2.54419	1.11420	1.49604
C	2.07125	2.41390	1.26004
C	2.36518	3.06999	0.06449
H	3.35187	2.96694	-1.84891
H	1.47126	2.90908	2.01691
H	1.99556	4.07591	-0.09753
I	1.29865	-2.43505	-0.22792
C	4.40385	0.40337	-1.77903
H	5.42935	0.24509	-1.43838
H	3.96212	-0.57947	-1.96035
H	4.43336	0.96225	-2.71507
C	2.27730	0.37019	2.77676
H	2.01004	-0.66616	2.55880
H	3.17409	0.36126	3.40147
H	1.47145	0.84080	3.34216
C	-4.22698	-1.35773	0.70790
H	-5.14518	-1.13594	0.14459
H	-4.33058	-2.35059	1.15244
H	-4.11418	-0.62742	1.50622
C	-1.53814	-0.79731	2.41814
H	-1.98335	-1.07389	3.37697
H	-1.71833	-1.58872	1.69477
H	-0.45198	-0.69834	2.54637



4.63 **4.66**

Deprotonation of 4.63 – starting species 4.63 and KO^{t}Bu in benzene

39

-1929.3539175

C	-4.43257	1.67476	-0.00334
H	-3.94649	2.38427	0.66173
H	-4.65253	2.17350	-0.95325
H	-5.37033	1.33566	0.43951
N	-3.57352	0.51790	-0.20935
C	-4.25552	-0.70096	-0.63024
H	-3.51564	-1.43067	-0.95044
H	-4.86667	-1.08986	0.18963
H	-4.91472	-0.46188	-1.47076
C	-2.23825	0.68395	-0.18479
O	-1.74538	1.81060	0.00984
K	0.82486	2.28193	-0.35557
C	-1.24521	-0.51698	-0.34534
N	-0.99810	-1.15994	0.99462
C	-2.12272	-1.94261	1.47856
H	-2.47382	-2.59289	0.67760
H	-1.80006	-2.56257	2.31965
H	-2.96164	-1.31456	1.82434
C	-0.51094	-0.24377	2.01271
H	-1.25777	0.50855	2.31629
H	-0.22408	-0.81172	2.90231
H	0.38077	0.26760	1.63813
O	-1.50240	-1.40596	-1.29984
H	-0.29548	0.04142	-0.49769
O	2.21682	0.19924	-0.42761
C	3.49665	0.15399	0.09146
C	3.67989	1.22757	1.18614
H	4.67055	1.19330	1.65069
H	3.55472	2.22766	0.75441
H	2.92669	1.08729	1.96849
C	3.77996	-1.22308	0.72884
H	4.76396	-1.27523	1.20538
H	3.01800	-1.43975	1.48537
H	3.74673	-2.00520	-0.03859
C	4.54566	0.40184	-1.00958
H	4.43562	-0.35235	-1.79441
H	4.37923	1.38479	-1.46100
H	5.57251	0.36303	-0.63011
K	1.01187	-2.02169	-0.90442

Deprotonation of 4.63 – transition state in benzene

39

-1929.2988349

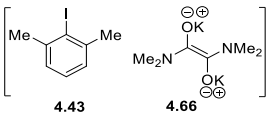
C	2.39253	-2.66222	-0.75964
H	3.43548	-2.62405	-0.41504
H	1.79445	-3.10879	0.03469
H	2.34296	-3.30283	-1.64393
N	1.87496	-1.35493	-1.10913
C	2.46226	-0.79643	-2.31948
H	2.00400	0.17642	-2.50255
H	3.55354	-0.69651	-2.21683
H	2.26120	-1.46183	-3.16467
C	1.60702	-0.47762	-0.05266
O	1.93184	-0.85431	1.12459
K	-0.19785	-1.28543	2.35034
C	0.79458	0.68969	-0.30585
N	1.06140	1.85216	0.60100
C	2.41585	2.35519	0.40787
H	2.59147	2.45234	-0.66548
H	2.53741	3.33965	0.87457
H	3.16876	1.67287	0.83329
C	0.74686	1.73089	2.01296
H	1.40343	1.03123	2.55175
H	0.84495	2.71335	2.49008
H	-0.29751	1.41680	2.13059
O	0.47147	1.10045	-1.55805
H	-0.54656	0.14906	0.16287
O	-1.64858	-0.00358	0.49220
C	-2.36760	-0.84187	-0.40249
C	-3.62733	-1.31502	0.32061
H	-4.23321	-1.96165	-0.32081
H	-3.36082	-1.87837	1.22022
H	-4.23368	-0.45685	0.62204
C	-2.74849	-0.05663	-1.66203
H	-3.28682	-0.68498	-2.37625
H	-3.40518	0.78063	-1.39820
H	-1.83470	0.31671	-2.13667
C	-1.50550	-2.04257	-0.80954
H	-0.57788	-1.70294	-1.27899
H	-1.24939	-2.65229	0.06544
H	-2.04414	-2.68980	-1.50725
K	-1.30116	2.56176	-0.60563

Deprotonation of 4.63 – products 4.66 and HO^{t}Bu in benzene

39

-1929.3098428

C	-1.79960	-2.44559	0.51207
H	-2.85923	-2.36060	0.82502
H	-1.76452	-2.47597	-0.57919
H	-1.42544	-3.40082	0.89374
N	-0.96496	-1.37998	1.00931
C	-0.95523	-1.33397	2.46082
H	-0.25076	-0.56551	2.77998
H	-1.95537	-1.11265	2.87736
H	-0.62987	-2.30085	2.86117
C	-1.20944	-0.08392	0.39345
O	-2.35075	0.06821	-0.25063
K	-4.44720	-0.65663	-1.02035
C	-0.23439	0.85188	0.54395
N	-0.40422	2.18873	-0.02750
C	-1.41176	2.97170	0.68101
H	-1.16281	2.99494	1.74399
H	-1.42636	4.00200	0.30606
H	-2.41535	2.53785	0.56334
C	-0.64816	2.19774	-1.46670
H	-1.61129	1.74131	-1.72677
H	-0.62577	3.22981	-1.83774
H	0.14005	1.62929	-1.97009
O	0.90590	0.68095	1.24641
H	1.91072	0.08914	0.46683
O	2.75353	-0.10785	-0.15837
C	2.74358	-1.46193	-0.57004
C	4.07214	-1.73607	-1.26900
H	4.12409	-2.76878	-1.62472
H	4.18852	-1.06648	-2.12581
H	4.90161	-1.56178	-0.57864
C	2.58414	-2.36554	0.65708
H	2.59497	-3.42191	0.37124
H	3.40110	-2.18576	1.36139
H	1.63241	-2.14062	1.14781
C	1.57317	-1.69485	-1.53097
H	0.63878	-1.44199	-1.02113
H	1.68224	-1.05461	-2.41175
H	1.53281	-2.73789	-1.86107
K	2.35286	2.45576	0.15176



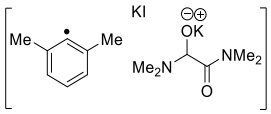
4.43 **4.66**

Neutral complex of 4.43 and 4.66 in benzene

42

-2017.2647450

C	2.18815	2.53121	-1.69313
H	2.90363	2.14290	-2.43053
H	1.18558	2.27962	-2.04551
H	2.28008	3.62105	-1.64894
N	2.39819	1.98487	-0.36220
C	3.72539	2.34096	0.13623
H	3.82647	1.96411	1.15533
H	4.52141	1.91208	-0.49386
H	3.84494	3.43006	0.14461
C	2.20849	0.52539	-0.31142
O	2.34638	-0.14445	-1.44443
C	2.06429	-0.00138	0.95311
N	2.14838	-1.47091	1.03568
C	1.47378	-1.98773	2.21845
H	0.42838	-1.67043	2.20886
H	1.50687	-3.08270	2.20553
H	1.92723	-1.62788	3.15067
C	3.55846	-1.86410	1.04158
H	4.10068	-1.42842	1.89448
H	3.65023	-2.95604	1.10171
H	4.02502	-1.51519	0.11570
O	2.01573	0.66128	2.09027
K	1.57103	-2.45155	-1.41746
K	0.21850	2.12978	1.25259
I	-1.89126	-1.73835	-0.16908
C	-2.09791	0.38920	-0.25958
C	-2.82467	1.02026	0.75804
C	-1.52213	1.07666	-1.33669
C	-2.97523	2.40909	0.67206
C	-1.70600	2.46527	-1.37029
C	-2.42502	3.12650	-0.38284
H	-3.53772	2.92178	1.44428
H	-1.27774	3.02389	-2.19512
H	-2.55953	4.20038	-0.43754
C	-3.43436	0.27856	1.91698
H	-4.16427	-0.45644	1.57004
H	-2.67243	-0.26350	2.48266
H	-3.93670	0.97426	2.58837
C	-0.72944	0.40755	-2.42335
H	0.26398	0.10637	-2.05435
H	-1.25333	-0.46943	-2.80911
H	-0.57274	1.10242	-3.24929



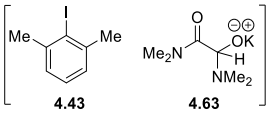
4.46 **4.67**

Triplet complex of 4.46, 4.67 and KI in benzene

42

-2017.3078987

C	-0.70339	3.46373	1.02403
H	-1.59129	3.98199	1.41065
H	-0.28343	2.86860	1.83103
H	0.02709	4.20969	0.70485
N	-1.02840	2.62055	-0.12087
C	-1.49367	3.44786	-1.24053
H	-1.72316	2.82808	-2.10254
H	-2.38759	4.02180	-0.95758
H	-0.70500	4.15487	-1.50856
C	-1.85299	1.50619	0.21793
O	-2.16227	1.29921	1.42932
C	-2.22831	0.61663	-0.85873
N	-3.22361	-0.35795	-0.54481
C	-3.38903	-1.36376	-1.58889
H	-2.42409	-1.81235	-1.82077
H	-4.06536	-2.13719	-1.21830
H	-3.80766	-0.93756	-2.50959
C	-4.51101	0.19993	-0.12221
H	-5.02649	0.69076	-0.95984
H	-5.15044	-0.60721	0.24485
H	-4.35996	0.92199	0.67805
O	-1.68335	0.62274	-1.99682
K	-2.05547	-1.24704	1.82587
K	0.82004	0.72348	-1.40163
I	0.45982	-2.42381	-0.05208
C	2.94556	-0.10066	0.80604
C	3.79481	-0.03879	-0.28218
C	2.29939	0.95128	1.41616
C	4.02280	1.24468	-0.79675
C	2.57014	2.22218	0.88082
C	3.41790	2.36139	-0.21530
H	4.68324	1.36641	-1.64976
H	2.11113	3.09778	1.32746
H	3.61473	3.34792	-0.61890
C	4.42205	-1.27600	-0.86640
H	5.16377	-1.68732	-0.17781
H	3.65985	-2.04217	-1.02510
H	4.91620	-1.05552	-1.81322
C	1.33085	0.74757	2.55227
H	0.30067	0.76875	2.17842
H	1.49986	-0.21692	3.03112
H	1.42937	1.53998	3.29742



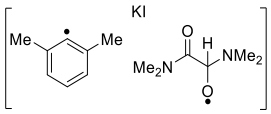
4.43 **4.63**

Neutral complex of 4.43 and 4.63 in benzene

42

-1417.9221716

N	4.01628	-0.15888	-1.25012
C	4.06206	-0.26151	-2.69921
H	3.23613	0.29919	-3.12709
H	5.00934	0.14388	-3.06691
H	3.99044	-1.30829	-3.00962
C	2.99201	0.47961	-0.63759
O	2.03547	0.91811	-1.28905
C	3.04412	0.67968	0.91758
N	2.81897	-0.68688	1.50047
C	1.47707	-1.16290	1.20761
H	1.33323	-1.26502	0.12924
H	1.32485	-2.14587	1.66184
H	0.70048	-0.48196	1.59616
O	2.20392	1.62569	1.32958
K	0.22541	2.21362	0.02885
C	-2.83738	2.09007	1.23257
C	-2.53469	0.72498	1.17599
C	-2.35843	0.15622	-0.09347
C	-2.47547	0.89380	-1.28021
C	-2.79162	2.25192	-1.16597
C	-2.97350	2.84782	0.07614
H	-2.97842	2.55182	2.20341
H	-2.89623	2.83964	-2.07119
H	-3.22219	3.90039	0.14250
I	-1.94287	-1.93389	-0.22604
C	-2.43176	-0.06457	2.45243
H	-3.18084	-0.85976	2.47618
H	-1.45217	-0.53804	2.55002
H	-2.58975	0.58609	3.31185
C	-2.27583	0.28878	-2.64304
H	-1.27605	-0.14219	-2.73732
H	-2.99381	-0.51491	-2.82155
H	-2.40312	1.04656	-3.41549
C	3.02585	-0.63613	2.94105
H	2.30977	0.03399	3.43854
H	2.92413	-1.63950	3.36320
H	4.03578	-0.27379	3.15183
C	5.17058	-0.70913	-0.55323
H	4.90466	-0.96686	0.46762
H	5.47809	-1.62194	-1.06872
H	6.01062	-0.00640	-0.56616
H	4.10469	0.89831	1.16333



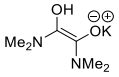
4.46 **4.70**

Triplet complex of 4.46, 4.70 and KI in benzene

42

-1417.8457768

N	3.52692	-0.75150	-0.75421
C	3.38796	-2.16867	-1.07363
H	2.34059	-2.38584	-1.27150
H	3.99521	-2.43326	-1.94386
H	3.71663	-2.75204	-0.21248
C	2.59614	0.10779	-1.19887
O	1.69713	-0.21151	-1.96930
C	2.64915	1.58059	-0.72074
N	2.78130	1.70625	0.73000
C	1.89153	0.95222	1.59918
H	1.56319	0.03190	1.11444
H	2.44491	0.69597	2.50685
H	1.01462	1.54172	1.88178
O	1.48151	2.22693	-0.88167
K	-0.68610	0.63684	-1.29747
C	-2.82401	2.49544	0.30873
C	-2.69374	1.37004	1.13692
C	-3.19932	0.19308	0.62566
C	-3.79419	0.00801	-0.60531
C	-3.90707	1.15866	-1.40078
C	-3.42637	2.38680	-0.94486
H	-2.44739	3.45472	0.65015
H	-4.36916	1.08463	-2.38049
H	-3.51861	3.26548	-1.57259
I	-0.47773	-2.11709	0.70651
C	-2.03994	1.42604	2.49178
H	-2.78555	1.30212	3.28054
H	-1.31858	0.61093	2.58976
H	-1.53538	2.38156	2.64360
C	-4.27070	-1.34646	-1.05685
H	-3.48184	-2.08680	-0.90500
H	-5.13675	-1.66113	-0.47017
H	-4.55456	-1.33107	-2.10986
C	3.27938	2.96179	1.25886
H	2.46554	3.66916	1.44192
H	3.78419	2.75816	2.20624
H	3.98715	3.40017	0.55601
C	4.69512	-0.37119	0.02862
H	4.95540	0.67354	-0.12876
H	4.53053	-0.54477	1.09620
H	5.53863	-0.98079	-0.29961
H	3.51661	2.07970	-1.18122

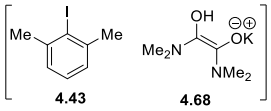


Enolate anion 4.68 in benzene

24

-1096.2939315

C	-2.59975	-0.51051	1.12671
H	-2.85809	-1.52960	0.79944
H	-1.99735	-0.57915	2.03556
H	-3.52888	0.01650	1.36255
N	-1.85670	0.22809	0.11627
C	-2.67175	0.47591	-1.07029
H	-2.09976	1.08482	-1.77279
H	-2.97497	-0.45626	-1.57246
H	-3.57729	1.02252	-0.79249
C	-0.59047	-0.32096	-0.18100
O	-0.61884	-1.63155	-0.77119
K	1.60274	-2.10101	0.51314
C	0.55317	0.41635	-0.44793
N	0.64832	1.77790	-0.04412
C	1.92807	2.39962	-0.34354
H	2.21180	2.19919	-1.37363
H	1.82794	3.47771	-0.19967
H	2.73695	2.03646	0.30974
C	0.19744	2.10780	1.30080
H	0.87984	1.69510	2.06359
H	0.18144	3.19445	1.41569
H	-0.80358	1.72144	1.46630
O	1.55644	-0.10345	-1.05376
H	-0.39253	-1.53515	-1.70527



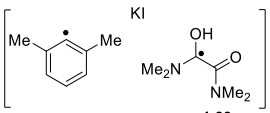
4.43 **4.68**

Neutral complex of 4.43 and 4.68 in benzene

42

-1417.8869054

N	-2.68596	-0.73886	1.70339
C	-1.74823	-1.09345	2.75597
H	-1.49487	-0.20666	3.33099
H	-2.20522	-1.83215	3.41892
H	-0.82646	-1.53653	2.34034
C	-2.44255	0.51872	1.10045
O	-2.08854	1.47716	1.89374
C	-2.57448	0.77634	-0.25201
N	-3.06497	-0.04339	-1.28499
C	-2.19338	-0.11483	-2.44880
H	-1.21511	-0.48376	-2.13495
H	-2.60837	-0.81734	-3.17778
H	-2.06773	0.85996	-2.94763
O	-2.53876	2.17310	-0.59454
K	-0.10916	2.16830	0.46421
C	2.82742	2.12845	-1.07012
C	2.31424	0.84239	-1.27145
C	2.16036	0.02519	-0.14246
C	2.52148	0.43741	1.14865
C	3.03478	1.73135	1.29178
C	3.18361	2.57305	0.19687
H	2.95415	2.77909	-1.92808
H	3.32251	2.07101	2.28030
H	3.58613	3.57032	0.32909
I	1.33294	-1.92596	-0.39725
C	1.95860	0.39644	-2.66363
H	2.51928	-0.49954	-2.93906
H	0.89729	0.15086	-2.74224
H	2.18556	1.18344	-3.38197
C	2.37077	-0.43895	2.36169
H	1.32385	-0.70632	2.52442
H	2.92850	-1.37033	2.24253
H	2.73822	0.07603	3.24862
C	-4.44087	0.26009	-1.67051
H	-4.53526	1.24248	-2.15609
H	-4.80677	-0.50359	-2.36304
H	-5.07194	0.25386	-0.77936
C	-3.05863	-1.89271	0.90591
H	-3.92733	-1.67521	0.29089
H	-2.24664	-2.22948	0.24368
H	-3.30667	-2.70618	1.59294
H	-2.91900	2.63474	0.16535



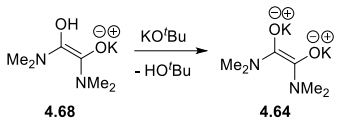
4.46 **4.69**

Triplet complex of 4.46, 4.69 and KI in benzene

42

-1417.8817045

N	-3.23299	1.67563	0.63355
C	-2.87826	2.98558	1.15613
H	-2.53445	3.62766	0.34822
H	-3.76500	3.42344	1.61704
H	-2.08334	2.91661	1.90876
C	-2.33139	1.11428	-0.25170
O	-1.26045	1.70234	-0.52328
C	-2.65729	-0.12363	-0.91276
N	-3.90677	-0.63251	-1.09731
C	-4.06023	-2.02179	-1.50025
H	-3.30469	-2.63700	-1.01705
H	-5.05095	-2.35949	-1.19124
H	-3.97047	-2.13683	-2.58617
O	-1.63511	-0.85094	-1.43669
K	0.96218	0.74797	-1.25501
C	4.14899	0.31788	-1.84538
C	3.87314	-0.61345	-0.83234
C	3.54350	-0.07553	0.39431
C	3.43813	1.26105	0.71860
C	3.72354	2.15856	-0.32255
C	4.07482	1.68792	-1.58769
H	4.41973	-0.03702	-2.83488
H	3.66330	3.22618	-0.13588
H	4.29139	2.39428	-2.38063
I	0.36803	-1.52973	1.26185
C	3.91677	-2.10105	-1.05987
H	4.75822	-2.54500	-0.52339
H	3.00262	-2.56384	-0.68054
H	4.02471	-2.33099	-2.12043
C	3.02552	1.71422	2.09345
H	2.12126	1.18580	2.40440
H	3.80822	1.48762	2.82079
H	2.83843	2.78834	2.11067
C	-5.05827	0.21816	-1.36269
H	-5.33666	0.14583	-2.42024
H	-5.90724	-0.10537	-0.75509
H	-4.82584	1.25250	-1.12381
C	-3.96939	0.85079	1.58606
H	-4.95852	1.28238	1.75714
H	-4.08609	-0.16359	1.21536
H	-3.43397	0.81036	2.54149
H	-1.05258	-1.14850	-0.70151



4.68 **4.64**

Deprotonation of 4.68 – starting species 4.68 and KO^{t}Bu in benzene

39
-1929.3320675

C	3.39832	2.27193	1.17084
H	2.66422	2.96505	1.61755
H	3.72030	1.56334	1.93689
H	4.26042	2.86992	0.86341
N	2.86998	1.53725	0.02896
C	2.48699	2.43474	-1.05610
H	2.24013	1.84114	-1.93880
H	1.62463	3.06916	-0.79544
H	3.32441	3.09040	-1.30960
C	1.89011	0.57831	0.35186
O	0.66330	1.08192	0.90597
K	-0.99084	-1.04425	1.79137
C	1.86848	-0.73930	-0.03871
N	3.02896	-1.31409	-0.64356
C	2.84395	-2.68620	-1.09165
H	1.93503	-2.77244	-1.68265
H	3.70037	-2.96313	-1.71053
H	2.77227	-3.39875	-0.25654
C	4.27916	-1.16513	0.09076
H	4.25774	-1.72043	1.04268
H	5.09634	-1.56379	-0.51535
H	4.47894	-0.11618	0.28981
O	0.81534	-1.47625	0.05743
H	0.86380	1.55108	1.72121
O	-2.58122	-0.07984	0.17566
C	-3.89716	0.14233	-0.17240
C	-4.76339	-1.08585	0.16836
H	-4.38524	-1.96174	-0.36722
H	-4.69934	-1.28816	1.24205
H	-5.81741	-0.94462	-0.09361
C	-4.45920	1.36150	0.58334
H	-4.39763	1.18271	1.66097
H	-3.85643	2.24459	0.35061
H	-5.50265	1.57274	0.32543
C	-4.01991	0.41434	-1.68704
H	-3.61698	-0.43702	-2.24630
H	-5.05481	0.57379	-2.00649
H	-3.44678	1.31076	-1.95099
K	-0.60903	0.32861	-1.31257

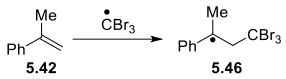
Deprotonation of 4.68 – products 4.64 and HO^{t}Bu in benzene

39
-1929.3401951

C	0.59076	2.75421	0.84862
H	-0.43440	2.60844	1.22198
H	1.28589	2.51884	1.66068
H	0.71869	3.80758	0.58286
N	0.89298	1.91831	-0.30419
C	0.00171	2.24249	-1.41261
H	0.29337	1.65886	-2.28891
H	-1.05364	2.02873	-1.18213
H	0.09266	3.30413	-1.66216
C	0.84186	0.51944	0.02879
O	-0.27868	0.05991	0.65139
K	1.19005	-0.97795	2.41665
C	1.90919	-0.30592	-0.22848
N	3.11477	0.23671	-0.82366
C	3.94338	-0.78094	-1.44648
H	3.35194	-1.36144	-2.15607
H	4.75237	-0.28700	-1.99156
H	4.38205	-1.48647	-0.72519
C	3.88636	1.04221	0.10918
H	4.20999	0.46161	0.99342
H	4.78460	1.42280	-0.38647
H	3.28693	1.89235	0.43459
O	1.89423	-1.59771	0.05773
O	-2.37569	-0.38463	-0.65849
C	-3.59035	-0.00211	-0.03443
C	-3.64182	-0.59143	1.37799
H	-3.58782	-1.68240	1.32939
H	-2.79047	-0.22702	1.95967
H	-4.56455	-0.31030	1.89251
C	-3.67485	1.52440	0.03432
H	-2.83664	1.91839	0.61595
H	-3.62250	1.94762	-0.97191
H	-4.60833	1.84757	0.50319
C	-4.72553	-0.55862	-0.88632
H	-4.64891	-1.64719	-0.94918
H	-5.69793	-0.30171	-0.45861
H	-4.66942	-0.14844	-1.89755
K	-0.25768	-1.79361	-1.32674
H	-1.57622	-0.07337	-0.08643

A.4 XYZ files Chapter 5

Scheme 5.10



5.42 5.46

CBr_3 radical addition onto 5.42 – starting species 5.42 and CBr_3 radical in benzene

23
-426.9053843

C	2.56909	-2.37892	0.15786
C	2.63360	-1.59259	-0.98579
C	2.42682	-0.21876	-0.90545
C	2.14585	0.40002	0.31844
C	2.09707	-0.40669	1.46471
C	2.29691	-1.77781	1.38491
H	2.73098	-3.44865	0.09770
H	2.84130	-2.04748	-1.94748
H	2.47790	0.37212	-1.81200
H	1.92241	0.04526	2.43386
H	2.25694	-2.37799	2.28671
C	1.93011	1.87080	0.39192
C	1.29281	2.44486	1.41628
C	2.43383	2.70291	-0.75931
H	3.48322	2.48544	-0.97494
H	1.86303	2.49460	-1.66912
H	2.33304	3.76467	-0.53583
C	-0.90555	-0.08223	-0.07253
Br	-1.69918	0.23213	1.63523
Br	-1.01515	-1.87330	-0.71355
Br	-1.15601	1.28540	-1.37967
H	1.15329	3.51943	1.44712
H	0.87648	1.87467	2.23705

CBr_3 radical addition onto 5.42 – transition state in benzene

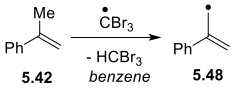
23
-426.9005195

C	4.54807	-0.84266	-0.44886
C	4.09818	0.37395	-0.95127
C	3.02847	1.02688	-0.34963
C	2.37345	0.46706	0.75474
C	2.84783	-0.75268	1.25898
C	3.92297	-1.39908	0.66491
H	5.38502	-1.34941	-0.91449
H	4.58006	0.81698	-1.81481
H	2.68786	1.96979	-0.76016
H	2.38421	-1.18730	2.13678
H	4.27881	-2.33718	1.07479
C	1.20099	1.14191	1.34914
C	0.19709	0.42882	1.90967
C	1.10061	2.63575	1.22117
H	2.01695	3.11895	1.57024
H	0.95297	2.93043	0.17778
H	0.25516	3.01606	1.79391
C	-1.17706	-0.10819	0.00346
Br	-2.71611	-0.96261	0.81490
Br	-0.10755	-1.30415	-1.06793
Br	-1.60534	1.54968	-0.89481
H	-0.63397	0.93301	2.39051
H	0.26427	-0.64417	2.04578

CBr_3 radical addition onto 5.42 – product 5.46 in benzene

23
-426.9505972

C	-4.91518	-0.82592	0.05320
C	-4.75164	0.55341	0.16680
C	-3.53267	1.14386	-0.12291
C	-2.41599	0.37399	-0.53499
C	-2.60849	-1.02660	-0.63426
C	-3.83199	-1.60736	-0.34933
H	-5.86994	-1.28623	0.27620
H	-5.58221	1.17342	0.48378
H	-3.43504	2.21666	-0.01757
H	-1.79311	-1.67360	-0.92897
H	-3.94423	-2.68159	-0.43974
C	-1.17252	1.01886	-0.84546
C	0.04217	0.24069	-1.25344
C	-1.09081	2.51686	-0.87006
H	-1.90807	2.94139	-1.46153
H	-1.16243	2.94714	0.13563
H	-0.14945	2.85403	-1.30128
C	1.06761	-0.05267	-0.14745
Br	2.54779	-1.11000	-0.94482
Br	0.27289	-1.09074	1.32683
Br	1.82875	1.61317	0.59472
H	0.59132	0.79130	-2.02359
H	-0.22010	-0.72815	-1.68142



5.42 5.48

H atom abstraction of 5.42 CBr_3 radical – starting species 5.42 and CBr_3 radical in benzene

23
-426.9051125

C	-3.90491	-0.96580	-0.22621
C	-3.75423	0.22028	-0.93490
C	-2.81466	1.16321	-0.53024
C	-2.01249	0.94800	0.59521
C	-2.18151	-0.24924	1.30281
C	-3.11299	-1.19521	0.89682
H	-4.62615	-1.70798	-0.54756
H	-4.36334	0.41279	-1.81055
H	-2.70514	2.07400	-1.10586
H	-1.55768	-0.45941	2.16292
H	-3.21328	-2.12069	1.45215
C	-0.98211	1.94772	0.98847
C	-0.47340	2.00075	2.22312
H	-0.80937	1.34756	3.01932
H	0.29386	2.72463	2.47338
C	-0.53525	2.92369	-0.07065
H	-0.28316	2.40786	-1.00190
H	-1.32946	3.64039	-0.29914
H	0.33765	3.48289	0.26573
C	0.98108	-0.25076	-0.12691
Br	0.07561	-0.85567	-1.68954
Br	1.21401	-1.53394	1.26330
Br	2.45321	0.93081	-0.41129

H atom abstraction of 5.42 CBr_3 radical – transition state in benzene

23
-426.8834349

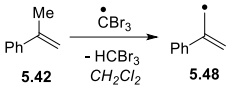
C	4.17606	-1.13666	-0.53288
C	3.82027	-1.28025	0.80551
C	2.92644	-0.39085	1.38987
C	2.38639	0.66507	0.65015
C	2.75495	0.80453	-0.69065
C	3.64219	-0.09082	-1.27887
H	4.86504	-1.83688	-0.99040
H	4.23815	-2.08797	1.39485
H	2.65968	-0.51158	2.43379
H	2.31817	1.60298	-1.27986
H	3.90778	0.02362	-2.32324
C	1.40737	1.60667	1.26104
C	1.48234	2.93075	1.04236
H	2.29363	3.36218	0.46779
H	0.73944	3.60649	1.45056
C	0.29768	1.01752	2.02100
H	0.53096	0.13828	2.62011
H	-0.34978	1.72754	2.53226
H	-0.44283	0.49086	1.12809
C	-1.17109	-0.08734	0.05548
Br	-0.29117	-1.76801	-0.34876
Br	-1.03658	1.20776	-1.37934
Br	-2.98928	-0.31824	0.70604

H atom abstraction of 5.42 – products 5.48 and $HCBr_3$ in benzene

23
-426.9178080

C	-3.43817	-1.67132	-0.27794
C	-3.64023	-0.56709	-1.10143
C	-3.10845	0.66920	-0.75541
C	-2.37730	0.82307	0.42482
C	-2.19771	-0.28572	1.25574
C	-2.71640	-1.52726	0.90250
H	-3.84107	-2.63822	-0.55513
H	-4.20963	-0.66968	-2.01787
H	-3.26482	1.52608	-1.40150
H	-1.62590	-0.18269	2.17282
H	-2.54776	-2.38216	1.54689
C	-1.75329	2.13504	0.76979
C	-1.82435	2.60181	2.07395
H	-2.37191	2.06320	2.83593
H	-1.34882	3.53447	2.35094
C	-1.08500	2.83989	-0.22445
H	-1.00182	2.45018	-1.23132
H	-0.62342	3.79539	-0.00779
C	1.01894	-0.02651	0.04643
Br	0.18676	-0.65225	-1.59916
Br	1.41858	-1.50066	1.26207
Br	2.60186	1.06525	-0.31788
H	0.31481	0.62475	0.54665

Scheme 5.15C



H atom abstraction of 5.42 – starting species 5.42 and CBr_3 radical in dichloromethane

23
-426.9068042

C	-0.59175	3.06143	0.44122
C	-1.02673	2.66498	-0.82260
C	-1.80766	1.52723	-0.96838
C	-2.18557	0.76412	0.14608
C	-1.73160	1.16674	1.40583
C	-0.94354	2.30540	1.55306
H	0.03010	3.94199	0.55238
H	-0.73792	3.23400	-1.69904
H	-2.10703	1.20768	-1.96006
H	-1.99174	0.58985	2.28556
H	-0.60309	2.59794	2.53975
C	-3.03071	-0.45118	-0.00387
C	-2.86318	-1.54062	1.02446
C	-3.91791	-0.56892	-0.99594
H	-4.08513	0.22324	-1.71640
H	-4.51586	-1.46719	-1.10062
C	0.89088	-0.29981	-0.06697
Br	1.20544	-0.97081	1.69270
Br	2.20482	0.90390	-0.74481
Br	0.18166	-1.55165	-1.32107
H	-3.41533	-2.43363	0.73161
H	-3.23589	-1.21965	2.00120
H	-1.80850	-1.80068	1.14977

H atom abstraction of 5.42 – transition state in dichloromethane

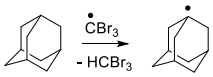
23
-426.8841066

C	-4.93425	-0.93960	0.31081
C	-4.45968	-1.10433	-0.98683
C	-3.35036	-0.38621	-1.42252
C	-2.70425	0.51624	-0.57224
C	-3.18871	0.67134	0.73140
C	-4.29340	-0.04975	1.16937
H	-5.79446	-1.50352	0.65184
H	-4.95357	-1.79168	-1.66365
H	-3.00198	-0.51388	-2.44109
H	-2.67823	1.34348	1.41216
H	-4.64978	0.07666	2.18501
C	-1.53952	1.31267	-1.05076
C	-1.39905	2.60647	-0.70624
H	-2.13987	3.11551	-0.10122
H	-0.54483	3.18284	-1.04387
C	-0.51527	0.64293	-1.86737
H	-0.82085	-0.25558	-2.39869
H	0.10015	1.30802	-2.47133
H	0.32769	0.19521	-1.04441
C	1.31070	-0.12675	-0.04838
Br	0.28971	-0.44313	1.56750
Br	2.43186	1.45424	0.06253
Br	2.26696	-1.69725	-0.67083

H atom abstraction of 5.42 CBr_3 radical – products 5.48 and $HCBr_3$ in dichloromethane

23
-426.9183180

C	4.11587	0.97577	-0.96558
C	4.15326	-0.41515	-1.02216
C	3.34429	-1.17143	-0.18125
C	2.48362	-0.55089	0.72891
C	2.46284	0.84529	0.78609
C	3.26953	1.60346	-0.05627
H	4.74458	1.56573	-1.62210
H	4.81842	-0.91153	-1.71908
H	3.39178	-2.25371	-0.22384
H	1.78713	1.34464	1.47062
H	3.22978	2.68531	-0.00560
C	1.59060	-1.36238	1.60902
C	1.28807	-0.91016	2.88641
H	1.72996	-0.00937	3.29075
H	0.61904	-1.47671	3.52222
C	1.05011	-2.55022	1.12671
H	1.23036	-2.88931	0.11532
H	0.41636	-3.15755	1.76138
C	-1.19716	-0.04895	0.03483
Br	-0.29426	-0.28200	-1.67931
Br	-1.15922	1.80871	0.63442
Br	-3.02314	-0.74819	-0.01312
H	-0.65202	-0.63812	0.76026



5.50 **5.54**

H atom abstraction of 5.50 – starting species 5.50 in dichloromethane

26
-390.6458290

C	-1.10154	0.02223	-1.38950
H	-0.87252	-0.32352	-2.40376
H	-2.13602	0.38348	-1.39153
C	-0.14894	1.16304	-0.99714
H	-0.25448	1.98966	-1.70645
C	-0.95480	-1.14017	-0.39527
H	-1.63379	-1.95113	-0.67608
C	0.49445	-1.65081	-0.41808
H	0.74433	-2.02000	-1.41905
H	0.60526	-2.48969	0.27824
C	1.29871	0.64722	-1.01915
H	1.98763	1.45755	-0.75565
H	1.55958	0.30977	-2.02852
C	1.45112	-0.51376	-0.02418
H	2.48252	-0.87897	-0.04101
C	1.10161	-0.02221	1.38921
H	1.22124	-0.83941	2.10939
H	1.78726	0.77959	1.68541
C	-0.49477	1.65065	0.41869
H	-1.52101	2.03405	0.44120
H	0.17003	2.47435	0.70211
C	-1.29900	-0.64750	1.01887
H	-2.33607	-0.29479	1.04870
H	-1.21276	-1.47342	1.73385
C	-0.34658	0.49150	1.41647
H	-0.59276	0.84140	2.42368

H atom abstraction of 5.50 – starting species CBr_3 radical in dichloromethane

4
-78.0020647

C	0.00044	-0.00044	0.33966
Br	1.85239	-0.26784	-0.01942
Br	-1.15836	-1.46920	-0.01941
Br	-0.69410	1.73712	-0.01940

H atom abstraction of 5.50 – transition state in dichloromethane

30
-468.6412626

C	-1.69951	0.40968	-1.37350
H	-1.35970	-0.26981	-2.16298
H	-1.26297	1.39556	-1.56598
C	-1.27870	-0.11942	-0.01398
H	-0.01580	-0.12510	-0.00522
C	-3.24812	0.48677	-1.37206
H	-3.58923	0.88147	-2.33389
C	-3.81937	-0.91892	-1.13979
H	-3.51459	-1.58326	-1.95483
H	-4.91350	-0.87447	-1.13991
C	-1.77575	-1.53624	0.19124
H	-1.39852	-1.96322	1.12699
H	-1.45054	-2.17692	-0.63501
C	-3.32356	-1.47091	0.21180
H	-3.72308	-2.47631	0.36899
C	-3.79325	-0.53614	1.33668
H	-4.88798	-0.50047	1.33763
H	-3.47812	-0.92654	2.31069
C	-1.68675	0.80869	1.11071
H	-1.28831	1.81234	0.92686
H	-1.29891	0.46045	2.07465
C	-3.71027	1.41610	-0.24248
H	-3.32890	2.43104	-0.39422
H	-4.80407	1.47528	-0.24405
C	-3.23091	0.87094	1.11601
H	-3.55531	1.52897	1.92712
C	1.37627	-0.02003	-0.01850
Br	1.72052	1.87164	-0.36574
Br	2.14090	-1.19722	-1.37614
Br	1.91769	-0.54391	1.78549

H atom abstraction of 5.50 – product 5.54 in dichloromethane

25
-389.9798509

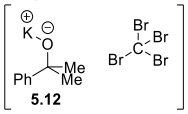
C	-0.90747	-1.12797	1.07358
H	-1.92515	-0.97635	1.44813
H	-0.54442	-2.09287	1.44230
C	0.00178	-0.00498	1.48362
C	-0.91612	-1.13082	-0.48126
H	-1.56639	-1.93233	-0.84494
C	-1.43462	0.22863	-0.97862
H	-2.45908	0.39005	-0.62550
H	-1.46100	0.23602	-2.07377
C	-0.51662	1.34640	1.08041
H	0.12724	2.14995	1.45289
H	-1.53112	1.51522	1.45616
C	-0.52385	1.36006	-0.47432
H	-0.89524	2.32476	-0.83336
C	0.90989	1.13046	-0.98045
H	0.92292	1.14984	-2.07578
H	1.56426	1.93703	-0.63197
C	1.42982	-0.22903	1.07371
H	1.80724	-1.18921	1.44059
H	2.08563	0.56422	1.44743
C	0.51992	-1.34927	-0.98734
H	0.89383	-2.31972	-0.64288
H	0.52654	-1.36656	-2.08268
C	1.43704	-0.22444	-0.48103
H	2.45613	-0.38419	-0.84639

H atom abstraction of 5.50 – product $HCBr_3$ in dichloromethane

5
-78.6661292

C	0.00056	-0.00040	0.53201
Br	1.75864	-0.62524	-0.04580
Br	-1.42110	-1.20979	-0.04575
Br	-0.33767	1.83511	-0.04573
H	0.00105	-0.00068	1.61262

Figure 5.1

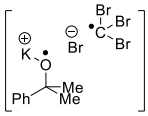


5.12

Neutral complex of 5.12 and CBr_4 in dichloromethane

27
-1116.1116760

C	3.10600	0.93009	0.61016
C	2.68297	0.81112	2.08946
H	3.50789	0.50312	2.73667
H	2.32364	1.78662	2.42866
H	1.87227	0.08711	2.19661
C	4.31261	1.88956	0.52154
H	4.62136	1.99333	-0.52192
H	4.01315	2.87211	0.89887
H	5.16877	1.53943	1.10545
O	2.07777	1.45022	-0.15433
C	3.56206	-0.44960	0.10293
C	3.03091	-0.98119	-1.07248
C	4.53174	-1.19650	0.78308
C	3.44692	-2.22296	-1.55210
H	2.28262	-0.40565	-1.60253
C	4.95150	-2.43506	0.30863
H	4.97143	-0.80792	1.69593
C	4.40798	-2.95647	-0.86405
H	3.01802	-2.61808	-2.46680
H	5.70410	-2.99399	0.85377
H	4.73220	-3.92206	-1.23477
Br	-0.06633	0.46111	-0.01173
C	-1.95735	-0.26662	0.04902
Br	-3.14756	0.82699	-1.09293
Br	-2.64399	-0.22230	1.90371
Br	-1.99814	-2.13452	-0.59663
K	1.24586	3.63343	-0.93669



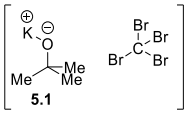
5.65

Triplet complex 5.65 in dichloromethane

27

-1116.0776501

C	2.30193	-1.04484	0.70234
C	1.46279	-1.77821	-0.35183
H	2.01937	-2.61793	-0.77089
H	0.54809	-2.15406	0.11012
H	1.19767	-1.08111	-1.14787
C	2.57293	-1.99402	1.90724
H	3.15012	-1.47761	2.67451
H	1.62566	-2.33948	2.32256
H	3.14293	-2.85097	1.54593
O	1.56608	-0.03774	1.28604
C	3.62712	-0.54028	0.13215
C	3.95004	0.81504	0.16401
C	4.53801	-1.43677	-0.43376
C	5.16100	1.26634	-0.35685
H	3.23946	1.51694	0.58047
C	5.74696	-0.98756	-0.95468
H	4.30882	-2.49665	-0.47177
C	6.06335	0.36839	-0.91725
H	5.39506	2.32445	-0.32957
H	6.44147	-1.69666	-1.38991
H	7.00381	0.72032	-1.32460
Br	0.49425	1.83738	-1.00419
C	-2.22121	-0.32519	-0.17504
Br	-2.02620	-1.20291	1.51587
Br	-2.12953	-1.44307	-1.71261
Br	-3.51162	1.07993	-0.23179
K	0.06526	1.94213	2.09261



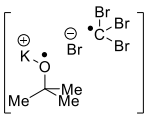
5.1

Neutral complex of 5.1 and CBr_4 in dichloromethane

20

-924.4005342

C	3.68603	-0.95755	-0.00045
C	3.38994	-1.79739	1.25294
H	4.00014	-2.70535	1.28365
H	3.59906	-1.20742	2.15015
H	2.33679	-2.08982	1.27196
C	5.17655	-0.58026	-0.00169
H	5.40793	0.01591	-0.88910
H	5.40934	0.01548	0.88565
H	5.81889	-1.46676	-0.00236
O	2.93691	0.21790	0.00033
C	3.38738	-1.79711	-1.25348
C	-1.41957	-0.05845	-0.00013
K	2.83217	2.66403	0.00262
H	3.99700	-2.70543	-1.28527
H	2.33392	-2.08900	-1.27099
H	3.59542	-1.20717	-2.15097
Br	-2.07517	-1.39505	-1.30191
Br	-2.09604	-0.54006	1.79686
Br	-2.14752	1.71745	-0.49499
Br	0.62939	-0.00450	-0.00076



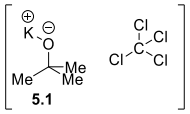
5.66

Triplet complex 5.66 in dichloromethane

20

-924.3685022

C	4.70433	-0.31992	0.25852
C	4.59623	-1.79140	0.66061
H	5.48883	-2.33459	0.34233
H	4.49407	-1.87981	1.74398
H	3.71962	-2.23312	0.18318
C	5.90609	0.34368	0.98065
H	5.96968	1.40266	0.72715
H	5.81279	0.23106	2.06114
H	6.81402	-0.15968	0.64270
O	3.62317	0.39507	0.75021
C	4.83439	-0.14945	-1.25482
C	-2.06866	-0.03608	0.11930
K	1.78092	2.04832	-0.29321
H	5.71972	-0.67292	-1.62259
H	3.94853	-0.56239	-1.74140
H	4.92257	0.90922	-1.51111
Br	-3.15680	-1.15085	-0.97859
Br	-2.04671	-0.44498	1.98252
Br	-2.06619	1.82747	-0.32393
Br	1.05408	-0.94765	-0.84691



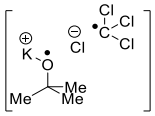
5.1

Neutral complex of 5.1 and CCl_4 in dichloromethane

20

-2711.8762101

C	3.01232	-0.79293	0.00159
C	2.70002	-1.62311	1.26359
H	3.25532	-2.56692	1.28841
H	2.96022	-1.04408	2.15525
H	1.63053	-1.84887	1.30286
C	4.52953	-0.51911	-0.02838
H	4.78268	0.05568	-0.92456
H	4.81439	0.07065	0.84837
H	5.11933	-1.44225	-0.03129
O	2.30580	0.39308	0.00785
C	2.65434	-1.63914	-1.23779
C	-2.09751	-0.19329	0.00094
K	1.55916	2.67352	-0.00023
Cl	-2.81655	1.36171	-0.48430
Cl	-0.32257	-0.05211	0.01953
Cl	-2.69153	-0.62662	1.62064
Cl	-2.58705	-1.45000	-1.15849
H	3.21033	-2.58227	-1.27123
H	1.58463	-1.86744	-1.23563
H	2.88067	-1.07098	-2.14558



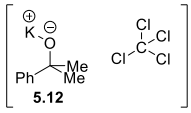
5.68

Triplet complex 5.68 in dichloromethane

20

-2711.8403776

C	3.38838	-0.55717	-0.00831
C	3.05140	-1.04432	1.42947
H	3.80780	-1.78228	1.70329
H	3.08585	-0.21288	2.13344
H	2.06613	-1.50991	1.45583
C	4.76011	0.12021	-0.02574
H	4.96964	0.51439	-1.02216
H	4.78630	0.94067	0.69309
H	5.53771	-0.60193	0.23032
O	2.38946	0.36441	-0.25403
C	3.30098	-1.72279	-0.99461
C	-2.07642	-0.83817	-0.01765
K	0.67789	2.46561	-0.15220
Cl	-2.26335	2.42518	0.16392
Cl	-0.37608	-0.75785	-0.26852
Cl	-2.60274	-1.34644	1.53255
Cl	-3.03085	-1.31090	-1.36041
H	4.05492	-2.47549	-0.75634
H	2.31309	-2.18482	-0.94896
H	3.47740	-1.36620	-2.01143



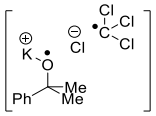
5.12

Neutral complex of 5.12 and CCl_4 in carbon tetrachloride

27

-2903.5754123

C	2.29240	1.12884	0.64758
C	1.95731	0.99349	2.15010
H	2.78116	0.58595	2.74215
H	1.71297	1.98667	2.53662
H	1.08514	0.34798	2.27901
C	3.56417	1.99612	0.50483
H	3.80938	2.10474	-0.55511
H	3.36302	2.98780	0.92066
H	4.42902	1.56777	1.02040
O	1.24533	1.71555	-0.01778
C	2.62482	-0.26963	0.08274
C	2.00048	-0.72218	-1.07906
C	3.56668	-1.11112	0.68725
C	2.29093	-1.97510	-1.61611
H	1.27553	-0.07034	-1.54943
C	3.86206	-2.36313	0.15710
H	4.08170	-0.78798	1.58596
C	3.22166	-2.80411	-0.99896
H	1.78737	-2.30502	-2.51865
H	4.59301	-2.99670	0.64743
H	3.44763	-3.78058	-1.41161
C	-2.55237	-0.56021	0.18435
K	-0.27510	3.08460	-1.15816
Cl	-3.75660	0.46765	-0.64398
Cl	-0.98260	0.27978	0.21369
Cl	-3.10512	-0.88079	1.84009
Cl	-2.39511	-2.09310	-0.69620



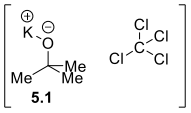
5.67

Triplet complex of 5.67 in carbon tetrachloride

27

-2903.5364951

C	-1.80480	1.60632	-0.46437
C	-2.30812	1.27837	-1.87784
H	-3.35447	0.97347	-1.85532
H	-2.21206	2.16235	-2.50998
H	-1.71792	0.46443	-2.30189
C	-2.66274	2.76194	0.14295
H	-2.28228	3.03372	1.12724
H	-2.65176	3.62725	-0.51988
H	-3.68247	2.38795	0.24419
O	-0.55857	2.18283	-0.53988
C	-1.83634	0.40052	0.47379
C	-0.72678	0.06598	1.24467
C	-2.98897	-0.38387	0.57314
C	-0.75446	-1.04480	2.08541
H	0.18814	0.64186	1.19501
C	-3.02018	-1.48943	1.41537
H	-3.87150	-0.13999	-0.00853
C	-1.89894	-1.82777	2.17097
H	0.13462	-1.28744	2.65710
H	-3.92019	-2.08997	1.47852
H	-1.92202	-2.69508	2.82015
C	0.82704	-1.51652	-0.84676
K	2.02323	2.65420	-0.00182
Cl	2.79126	0.59266	1.80325
Cl	1.19342	-0.13550	-1.82774
Cl	2.15241	-2.43336	-0.29053
Cl	-0.58621	-2.38118	-1.30128



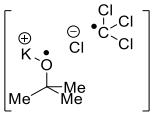
5.1

Neutral complex of 5.1 and CCl_4 in carbon tetrachloride

20

-2711.8636814

C	-3.02634	-0.76219	0.00198
C	-2.69791	-1.61317	-1.24061
H	-3.28973	-2.53383	-1.28056
H	-2.89900	-1.03050	-2.14476
H	-1.63798	-1.88314	-1.23742
C	-4.52907	-0.42322	-0.02676
H	-4.78689	0.17543	0.85221
H	-4.75553	0.16477	-0.92150
H	-5.15837	-1.31976	-0.03256
O	-2.27628	0.39675	0.01073
C	-2.74169	-1.60166	1.26262
C	2.09086	-0.20150	0.00142
K	-1.49979	2.60659	-0.00004
Cl	2.78925	1.37273	-0.46841
Cl	0.31288	-0.07798	0.02300
Cl	2.59502	-1.43469	-1.17262
Cl	2.69393	-0.63997	1.61483
H	-3.33004	-2.52506	1.28827
H	-1.68088	-1.86538	1.29983
H	-2.97875	-1.01277	2.15387



5.68

Triplet complex 5.68 in carbon tetrachloride

20

-2711.8260835

C	-2.83443	-0.68658	-0.00449
C	-2.28839	-1.77393	-0.93147
H	-2.61761	-2.75876	-0.59371
H	-2.65334	-1.61892	-1.94951
H	-1.19800	-1.74960	-0.93819
C	-4.36360	-0.70193	0.07124
H	-4.71590	0.08841	0.73563
H	-4.79215	-0.54819	-0.92155
H	-4.70979	-1.66542	0.45062
O	-2.38719	0.55854	-0.39227
C	-2.22821	-0.84550	1.42033
C	1.95988	-0.55890	-0.13473
K	-0.64093	2.50685	-0.67527
Cl	0.56444	1.52425	1.71236
Cl	1.23764	-0.16704	-1.66020
Cl	3.60471	-0.12491	0.05089
Cl	1.46236	-2.04237	0.56768
H	-2.51259	-1.83854	1.77564
H	-1.14322	-0.74953	1.39094
H	-2.62952	-0.08559	2.09070

Hypochlorite A3 in carbon tetrachloride

22

-884.8685868

C	0.74259	0.48886	0.00004
C	1.09705	1.26323	-1.26671
H	0.51317	2.18316	-1.31597
H	2.15463	1.53256	-1.27290
H	0.87253	0.65961	-2.14787
C	1.09709	1.26324	1.26677
H	0.87258	0.65968	2.14796
H	2.15467	1.53258	1.27294
H	0.51323	2.18318	1.31598
O	1.41708	-0.79480	-0.00001
C	-0.73739	0.10744	0.00005
C	-1.16834	-1.21869	0.00007
C	-1.69515	1.12574	-0.00002
C	-2.52971	-1.51702	0.00003
H	-0.44363	-2.02108	0.00013
C	-3.05197	0.82629	-0.00006
H	-1.38511	2.16521	-0.00005
C	-3.47548	-0.49996	-0.00003
H	-2.84710	-2.55341	0.00005
H	-3.77785	1.63092	-0.00010
H	-4.53321	-0.73506	-0.00007
Cl	3.11160	-0.70081	-0.00005

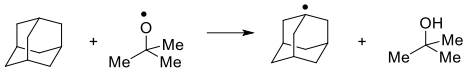
Triplet hypochlorite A4 in carbon tetrachloride

22

-884.8123022

C	-0.60377	0.39066	0.04098
C	-0.97207	1.19904	1.32397
H	-0.40954	2.13274	1.29394
H	-2.04124	1.40655	1.33050
H	-0.69118	0.63679	2.21400
C	-1.04722	1.16241	-1.21542
H	-0.88614	0.54519	-2.10033
H	-2.10066	1.42740	-1.14126
H	-0.44813	2.06851	-1.30601
O	-1.33948	-0.76835	0.17304
C	0.89157	0.06913	0.01364
C	1.34745	-1.24682	0.04286
C	1.82127	1.10918	-0.05079
C	2.71313	-1.51815	0.00638
H	0.63642	-2.06149	0.09438
C	3.18394	0.83711	-0.08598
H	1.48791	2.14124	-0.07343
C	3.63453	-0.47968	-0.05831
H	3.05455	-2.54639	0.02720
H	3.89286	1.65507	-0.13630
H	4.69648	-0.69216	-0.08772
Cl	-3.66404	-0.57082	-0.09431

Scheme 5.20



5.50 5.5 5.54 5.7

H atom abstraction of 5.50 – starting species 5.50 and 5.5 in dichloromethane

40

-623.6102168

C	-3.42491	0.00692	0.00269
C	-3.10835	-1.05501	-1.05336
H	-3.87636	-1.05672	-1.82997
H	-2.14443	-0.84409	-1.52273
H	-3.06645	-2.04388	-0.59290
C	-3.46991	1.41428	-0.59661
H	-3.69027	2.14798	0.18097
H	-2.50721	1.66073	-1.05038
H	-4.23990	1.47417	-1.36892
O	-2.51844	-0.05644	1.04839
C	-4.77073	-0.31874	0.69920
H	-4.98538	0.41590	1.47588
H	-5.55496	-0.27855	-0.05935
H	-4.74317	-1.31698	1.13671
H	-0.63107	0.40171	-0.21725
C	0.34943	0.51279	-0.69365
H	0.19451	0.99413	-1.66667
C	0.99045	-0.87038	-0.88304
C	1.24673	1.38648	0.19545
H	0.35010	-1.48940	-1.51995
C	1.15407	-1.54231	0.48919
C	2.36910	-0.70771	-1.54239
H	0.78660	2.37102	0.32568
C	1.40942	0.70830	1.56499
C	2.62450	1.54321	-0.46602
H	1.59554	-2.53797	0.36779
H	0.17141	-1.67101	0.95730
C	2.05328	-0.67553	1.38484
H	2.25904	-0.24266	-2.52856
H	2.82871	-1.69111	-1.69272
C	3.27014	0.16080	-0.65031
H	0.43006	0.60487	2.04573
H	2.03419	1.32900	2.21712
H	2.51834	2.03778	-1.43819
H	3.26734	2.17598	0.15618
H	2.17080	-1.15504	2.36155
C	3.43019	-0.51392	0.72122
H	4.25220	0.27420	-1.11985
H	4.08326	0.09101	1.36031
H	3.90421	-1.49473	0.60190

H atom abstraction of 5.50 – transition state in dichloromethane

40

-623.5964200

C	-3.10325	0.00166	-0.00523
C	-3.08191	-1.20849	-0.94124
H	-3.99558	-1.25049	-1.53944
H	-2.22917	-1.15142	-1.62284
H	-3.00090	-2.13008	-0.35932
C	-3.18438	1.31192	-0.79113
H	-3.18387	2.16077	-0.10285
H	-2.32780	1.40851	-1.46347
H	-4.09665	1.34735	-1.39238
O	-1.97527	-0.00113	0.84301
C	-4.29048	-0.10389	0.96559
H	-4.30487	0.75332	1.64128
H	-5.22257	-0.12185	0.39605
H	-4.21841	-1.02080	1.55389
H	-0.88667	0.10227	0.05676
C	0.10334	0.16192	-0.64250
H	-0.26371	0.32688	-1.66048
C	0.83563	-1.16380	-0.49024
C	0.93950	1.32588	-0.12862
H	0.20551	-1.98242	-0.85133
C	1.19580	-1.38751	0.98761
C	2.12918	-1.09191	-1.32906
H	0.38131	2.26120	-0.23530
C	1.30002	1.09096	1.34719
C	2.23322	1.38921	-0.96904
H	1.73003	-2.33769	1.09687
H	0.27973	-1.44899	1.58381
C	2.07313	-0.22931	1.48751
H	1.88213	-0.94613	-2.38623
H	2.67213	-2.03985	-1.24468
C	3.00414	0.06766	-0.82765
H	0.38643	1.05612	1.94950
H	1.90917	1.92393	1.71505
H	1.98734	1.57109	-2.02073
H	2.85013	2.22616	-0.62346
H	2.32762	-0.39289	2.53910
C	3.35902	-0.16148	0.65027
H	3.92115	0.11667	-1.42296
H	3.99642	0.65369	1.01064
H	3.92543	-1.09327	0.75763

H atom abstraction of 5.50 – products 5.54 and 5.7 in dichloromethane

40

-623.6241434

C	-3.30498	0.00556	0.00032
C	-2.89852	-1.13296	-0.93392
H	-3.68694	-1.33522	-1.66301
H	-1.98761	-0.87052	-1.48054
H	-2.70927	-2.04335	-0.36026
C	-3.53367	1.29270	-0.79004
H	-3.80484	2.10681	-0.11424
H	-2.62338	1.57499	-1.32717
H	-4.33469	1.16275	-1.52172
O	-2.26886	0.22068	0.96889
C	-4.54512	-0.36689	0.80020
H	-4.80762	0.44107	1.48672
H	-5.38978	-0.54571	0.13153
H	-4.36051	-1.27347	1.38084
C	0.45567	0.70106	-0.77390
H	0.00485	1.29775	-1.56223
C	0.97417	-0.67013	-1.09824
C	1.21619	1.39148	0.32212
H	0.37782	-1.14127	-1.88407
C	0.96340	-1.54007	0.17405
C	2.43802	-0.50940	-1.58496
H	0.78779	2.37395	0.53719
C	1.21692	0.51848	1.59328
C	2.67932	1.55543	-0.16705
H	1.37313	-2.52994	-0.05432
H	-0.06648	-1.67923	0.52026
C	1.80292	-0.86490	1.27021
H	2.46007	0.08762	-2.50233
H	2.85629	-1.49481	-1.81935
C	3.26909	0.17202	-0.48673
H	0.19947	0.41463	1.98400
H	1.81597	1.00615	2.36978
H	2.70336	2.19125	-1.05782
H	3.27154	2.04930	0.61152
H	1.79040	-1.48469	2.17168
C	3.24887	-0.69856	0.77888
H	4.29977	0.29032	-0.83460
H	3.85693	-0.23260	1.56209
H	3.68616	-1.67974	0.56355
H	-1.45529	0.42553	0.48601

5.54 **5.83** **5.69** **5.5**

Cl abstraction of 5.83 – starting species 5.54 and 5.83 in dichloromethane

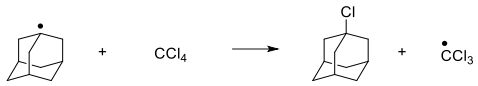
25
-389.9787578

C	1.25958	-1.21146	0.30720
H	2.15841	-1.04459	0.91215
H	1.28647	-2.24614	-0.04961
C	1.25632	-0.23910	-0.89902
H	2.14286	-0.41326	-1.51406
C	0.00009	-0.97690	1.15805
H	0.00017	-1.66874	2.00589
C	-0.00057	0.46994	1.67516
H	0.88261	0.64453	2.29962
H	-0.88417	0.64393	2.29922
C	1.25596	1.20874	-0.36549
H	1.27791	1.91142	-1.20471
H	2.15506	1.38132	0.23669
C	-0.00056	1.44414	0.48793
H	-0.00097	2.47407	0.85759
C	-1.25657	1.20799	-0.36601
H	-2.15600	1.37998	0.23582
H	-1.27862	1.91067	-1.20523
C	0.00046	-0.47349	-1.68393
H	0.00080	-1.13093	-2.54645
C	-1.25886	-1.21235	0.30669
H	-1.28476	-2.24705	-0.05013
H	-2.15805	-1.04622	0.91131
C	-1.25581	-0.23990	-0.89946
H	-2.14201	-0.41466	-1.51482

Cl abstraction of 5.83 – products 5.69 and 5.5 dichloromethane

40
-1083.2201766

C	0.94175	-0.08291	-0.69188
H	0.69362	-0.04390	-1.75329
C	1.84639	-1.28100	-0.39802
C	1.60627	1.22181	-0.24969
H	1.33285	-2.20030	-0.69102
C	2.22126	-1.32695	1.09047
C	3.12301	-1.10026	-1.24206
H	0.92436	2.05478	-0.43929
C	1.98202	1.16360	1.23822
C	2.88324	1.38683	-1.09495
H	2.88377	-2.18078	1.26578
H	1.32648	-1.47550	1.70167
C	2.92680	-0.02191	1.48884
H	2.87115	-1.08284	-2.30775
H	3.78515	-1.95571	-1.07511
C	3.82963	0.20358	-0.84352
H	1.08185	1.06805	1.85182
H	2.47286	2.10097	1.51904
H	2.62682	1.44438	-2.15822
H	3.37239	2.32789	-0.82438
H	3.18992	-0.05924	2.54977
C	4.19948	0.15078	0.64661
H	4.73479	0.32603	-1.44510
H	4.71722	1.07208	0.93487
H	4.88589	-0.68295	0.83041
Cl	-0.68541	-0.28519	0.11879
O	-3.61021	-0.08282	1.13598
C	-4.38060	0.04668	-0.00738
C	-5.81978	0.13303	0.56072
H	-5.92173	1.00112	1.21269
H	-6.50483	0.23494	-0.28326
H	-6.06721	-0.77216	1.11603
C	-4.23705	-1.18738	-0.90021
H	-3.20748	-1.27182	-1.25421
H	-4.49292	-2.08870	-0.34001
H	-4.89770	-1.10934	-1.76650
C	-4.03019	1.33601	-0.75350
H	-4.14041	2.19677	-0.09135
H	-2.99778	1.29134	-1.10652
H	-4.68870	1.46423	-1.61544



5.54 **5.69**

Cl abstraction of CCl_4 – starting species CCl_4 and 5.54 in dichloromethane

30

-2268.8442784

C	-1.70633	-0.00075	-1.27199
H	-1.40594	-0.00053	-2.31553
C	-2.24373	1.25671	-0.65558
C	-2.24679	-1.25755	-0.65693
H	-1.79936	2.14176	-1.11831
C	-1.96852	1.25352	0.86154
C	-3.77896	1.26152	-0.87995
H	-1.80459	-2.14320	-1.12059
C	-1.97155	-1.25665	0.86019
C	-3.78204	-1.25842	-0.88131
H	-2.39911	2.15341	1.31423
H	-0.88967	1.27464	1.04467
C	-2.58623	-0.00117	1.49782
H	-3.99726	1.28780	-1.95241
H	-4.21512	2.16047	-0.42961
C	-4.39177	0.00194	-0.24566
H	-0.89275	-1.28065	1.04327
H	-2.40434	-2.15598	1.31191
H	-4.00039	-1.28303	-1.95379
H	-4.22037	-2.15679	-0.43191
H	-2.38096	-0.00199	2.57264
C	-4.10454	0.00077	1.26299
H	-5.47318	0.00335	-0.41315
H	-4.55593	-0.88223	1.72865
H	-4.55381	0.88434	1.72961
Cl	1.28256	-0.00112	-0.64777
C	2.94381	0.00002	-0.00840
Cl	3.18743	1.44949	0.98816
Cl	4.10668	-0.00022	-1.34805
Cl	3.18880	-1.44820	0.98967

Cl abstraction of CCl_4 – transition state in dichloromethane

30

-2268.8362837

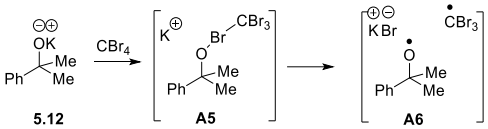
C	-1.34484	1.06143	0.36895
H	-1.12708	2.07691	0.69060
C	-1.96806	0.15035	1.38463
C	-1.89261	0.89363	-1.01778
H	-1.49563	0.27987	2.36136
C	-1.88831	-1.31663	0.92899
C	-3.46247	0.57336	1.46451
H	-1.36567	1.54247	-1.72134
C	-1.81621	-0.57624	-1.46737
C	-3.38721	1.31471	-0.93036
H	-2.40032	-1.94852	1.66187
H	-0.84412	-1.63818	0.88741
C	-2.54445	-1.46880	-0.45134
H	-3.54024	1.61056	1.80511
H	-3.96817	-0.05780	2.20282
C	-4.11315	0.41589	0.08191
H	-0.77245	-0.88812	-1.56227
H	-2.28164	-0.67155	-2.45372
H	-3.46321	2.36394	-0.62825
H	-3.83906	1.22165	-1.92348
H	-2.47712	-2.51259	-0.77127
C	-4.01830	-1.04944	-0.36764
H	-5.16329	0.71670	0.14163
H	-4.49743	-1.16969	-1.34530
H	-4.55218	-1.69095	0.34169
Cl	0.87696	0.48822	0.22435
C	2.79197	-0.00719	-0.00477
Cl	3.69291	1.45240	-0.39512
Cl	2.88347	-1.17837	-1.31744
Cl	3.34957	-0.71407	1.51027

Cl abstraction of CCl_4 – products 5.69 and CCl_3 radical in dichloromethane

30

-2268.8829758

C	-1.58604	-1.46703	0.00019
H	-2.21505	-2.35788	0.00028
C	-1.83404	-0.63474	-1.25885
C	-1.83402	-0.63445	1.25903
H	-1.61769	-1.24319	-2.14078
C	-0.96150	0.62779	-1.25309
C	-3.32163	-0.23217	-1.25070
H	-1.61771	-1.24271	2.14110
C	-0.96148	0.62805	1.25306
C	-3.32161	-0.23182	1.25079
H	-1.16916	1.21111	-2.15594
H	0.09560	0.34834	-1.27951
C	-1.26408	1.46426	-0.00013
H	-3.95438	-1.12586	-1.26913
H	-3.54069	0.34311	-2.15577
C	-3.62563	0.60597	-0.00007
H	0.09574	0.34882	1.27958
H	-1.16921	1.21159	2.15575
H	-3.95437	-1.12548	1.26961
H	-3.54060	0.34378	2.15568
H	-0.63892	2.36138	-0.00026
C	-2.74716	1.86611	-0.00020
H	-4.68150	0.89140	-0.00010
H	-2.97002	2.47461	0.88295
H	-2.97000	2.47439	-0.88351
Cl	0.11380	-2.14257	0.00013
C	2.54831	0.26743	-0.00006
Cl	3.07425	-0.46121	1.46149
Cl	2.40267	1.97875	-0.00008
Cl	3.07406	-0.46143	-1.46152



5.12 A5 A6

Formation of hypobromite – starting species CBr_4 in dichloromethane

5

-91.3749874

C	-0.00010	0.00000	-0.00027
Br	0.94937	1.60555	-0.62222
Br	0.94937	-1.60555	-0.62222
Br	-1.82999	0.00000	-0.71935
Br	-0.06873	0.00000	1.96384

Formation of hypobromite – starting species 5.12 in dichloromethane

22

-1024.7206284

C	0.38785	1.09159	-0.00012
C	0.33782	1.99933	-1.25339
H	-0.54742	2.64158	-1.28603
H	1.22826	2.63458	-1.25821
H	0.35053	1.37836	-2.15363
C	0.33866	1.99798	1.25416
H	0.35204	1.37606	2.15373
H	1.22904	2.63331	1.25903
H	-0.54663	2.64011	1.28808
O	1.52414	0.33350	-0.00093
C	-0.89167	0.22239	-0.00009
C	-0.78881	-1.16814	-0.00024
C	-2.17656	0.78133	0.00016
C	-1.92357	-1.97968	-0.00016
H	0.20598	-1.59702	-0.00047
C	-3.31357	-0.02114	0.00020
H	-2.29758	1.86005	0.00031
C	-3.19255	-1.40998	0.00003
H	-1.81514	-3.05923	-0.00028
H	-4.29674	0.43687	0.00037
H	-4.07717	-2.03669	0.00006
K	3.43980	-1.08726	0.00006

Formation of hypobromite – intermediate A5 in dichloromethane

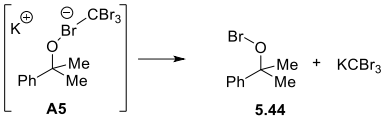
27
-1116.1116760

C	3.10600	0.93009	0.61016
C	2.68297	0.81112	2.08946
H	3.50789	0.50312	2.73667
H	2.32364	1.78662	2.42866
H	1.87227	0.08711	2.19661
C	4.31261	1.88956	0.52154
H	4.62136	1.99333	-0.52192
H	4.01315	2.87211	0.89887
H	5.16877	1.53943	1.10545
O	2.07777	1.45022	-0.15433
C	3.56206	-0.44960	0.10293
C	3.03091	-0.98119	-1.07248
C	4.53174	-1.19650	0.78308
C	3.44692	-2.22296	-1.55210
H	2.28262	-0.40565	-1.60253
C	4.95150	-2.43506	0.30863
H	4.97143	-0.80792	1.69593
C	4.40798	-2.95647	-0.86405
H	3.01802	-2.61808	-2.46680
H	5.70410	-2.99399	0.85377
H	4.73220	-3.92206	-1.23477
Br	-0.06633	0.46111	-0.01173
C	-1.95735	-0.26662	0.04902
Br	-3.14756	0.82699	-1.09293
Br	-2.64399	-0.22230	1.90371
Br	-1.99814	-2.13452	-0.59663
K	1.24586	3.63343	-0.93669

Formation of hypobromite – triplet complex A6 in dichloromethane

27
-1116.0776501

C	2.30193	-1.04484	0.70234
C	1.46279	-1.77821	-0.35183
H	2.01937	-2.61793	-0.77089
H	0.54809	-2.15406	0.11012
H	1.19767	-1.08111	-1.14787
C	2.57293	-1.99402	1.90724
H	3.15012	-1.47761	2.67451
H	1.62566	-2.33948	2.32256
H	3.14293	-2.85097	1.54593
O	1.56608	-0.03774	1.28604
C	3.62712	-0.54028	0.13215
C	3.95004	0.81504	0.16401
C	4.53801	-1.43677	-0.43376
C	5.16100	1.26634	-0.35685
H	3.23946	1.51694	0.58047
C	5.74696	-0.98756	-0.95468
H	4.30882	-2.49665	-0.47177
C	6.06335	0.36839	-0.91725
H	5.39506	2.32445	-0.32957
H	6.44147	-1.69666	-1.38991
H	7.00381	0.72032	-1.32460
Br	0.49425	1.83738	-1.00419
C	-2.22121	-0.32519	-0.17504
Br	-2.02620	-1.20291	1.51587
Br	-2.12953	-1.44307	-1.71261
Br	-3.51162	1.07993	-0.23179
K	0.06526	1.94213	2.0926



Formation of hypobromite – product 5.44 in dichloromethane

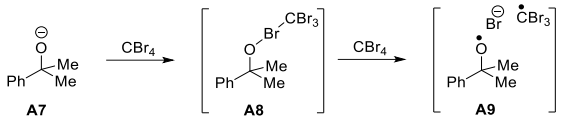
22
-438.0104873

C	0.12234	0.62608	0.01800
C	0.41146	1.50337	-1.19738
H	-0.22757	2.38689	-1.19214
H	1.44901	1.84224	-1.18420
H	0.22793	0.94294	-2.11582
C	0.40541	1.35561	1.32936
H	0.25581	0.67837	2.17229
H	1.42866	1.73501	1.34817
H	-0.27209	2.20362	1.43748
O	0.88194	-0.59598	-0.05934
C	-1.32762	0.13132	-0.00363
C	-1.65981	-1.22373	0.01178
C	-2.35888	1.07570	-0.02208
C	-2.99549	-1.62266	0.00474
H	-0.87731	-1.96997	0.02934
C	-3.68973	0.67612	-0.02808
H	-2.12911	2.13544	-0.02905
C	-4.01425	-0.67831	-0.01557
H	-3.23474	-2.67984	0.01593
H	-4.47368	1.42426	-0.04272
H	-5.05152	-0.99191	-0.02078
Br	2.75682	-0.40001	-0.01505

Formation of hypobromite – product $KCBr_3$ in dichloromethane

5
-678.0521668

K	2.61070	0.02488	-1.58802
Br	0.94280	-0.24319	1.55205
C	0.05720	0.00347	-0.33842
Br	-1.32859	-1.50525	-0.46152
Br	-1.04125	1.73434	-0.17045



Formation of hypobromite – starting species A7 in dichloromethane

21
-424.8255260

C	-1.51472	0.15336	-0.00006
C	-2.02244	-0.61058	-1.25318
H	-1.70772	-1.65902	-1.28625
H	-3.11601	-0.57608	-1.25903
H	-1.65788	-0.10892	-2.15441
C	-2.02220	-0.60961	1.25377
H	-1.65772	-0.10705	2.15454
H	-3.11578	-0.57541	1.25965
H	-1.70713	-1.65793	1.28770
O	-1.94998	1.43975	-0.00055
C	0.03385	0.04884	-0.00008
C	0.80063	1.21439	-0.00009
C	0.71237	-1.17753	0.00003
C	2.19473	1.16515	-0.00005
H	0.26608	2.15698	-0.00015
C	2.10310	-1.23544	0.00004
H	0.15035	-2.10637	0.00010
C	2.85409	-0.06026	-0.00001
H	2.76818	2.08653	-0.00005
H	2.60362	-2.19801	0.00007
H	3.93744	-0.10261	-0.00001

Formation of hypobromite – starting species CBr_4 in dichloromethane

5
-91.3749874

C	-0.00010	0.00000	-0.00027
Br	0.94937	1.60555	-0.62222
Br	0.94937	-1.60555	-0.62222
Br	-1.82999	0.00000	-0.71935
Br	-0.06873	0.00000	1.96384

Formation of hypobromite – intermediate A8 in dichloromethane

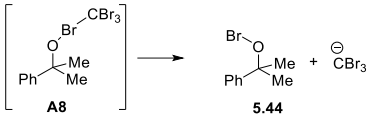
26
-516.2221446

C	-2.90165	0.50095	0.00152
C	-2.65060	1.35894	-1.25663
H	-3.29805	2.23884	-1.29643
H	-1.61134	1.69679	-1.26512
H	-2.82694	0.75482	-2.15062
C	-2.65500	1.35959	1.26001
H	-2.83640	0.75655	2.15369
H	-1.61527	1.69537	1.27253
H	-3.30108	2.24066	1.29614
O	-2.09258	-0.62436	0.00335
C	-4.37917	0.06491	-0.00030
C	-4.71885	-1.28811	0.00185
C	-5.41707	1.00510	-0.00286
C	-6.05361	-1.69291	0.00145
H	-3.91473	-2.01324	0.00395
C	-6.74970	0.60622	-0.00332
H	-5.18766	2.06590	-0.00445
C	-7.07529	-0.74928	-0.00107
H	-6.29421	-2.75076	0.00322
H	-7.53592	1.35329	-0.00532
H	-8.11304	-1.06303	-0.00130
Br	0.10247	-0.29061	0.00098
C	2.17957	-0.06575	-0.00095
Br	3.05225	-1.52618	-1.02537
Br	2.89300	-0.09576	1.85452
Br	2.68953	1.66746	-0.83103

Formation of hypobromite – triplet complex A9 in dichloromethane

26
-516.1897768

C	3.24535	0.10769	0.20526
C	2.84554	0.45227	1.64893
H	3.30010	1.39479	1.95670
H	1.76034	0.54248	1.71305
H	3.18338	-0.33438	2.32603
C	2.69730	1.19235	-0.76620
H	2.92222	0.92146	-1.79829
H	1.62020	1.29877	-0.63610
H	3.18971	2.13681	-0.52980
O	2.58516	-1.03422	-0.18782
C	4.76096	-0.02231	0.04283
C	5.32599	-1.18742	-0.47268
C	5.60434	1.03108	0.40589
C	6.70699	-1.29906	-0.62223
H	4.68080	-2.00862	-0.75832
C	6.98248	0.92183	0.25543
H	5.18844	1.94969	0.80608
C	7.53993	-0.24629	-0.25944
H	7.12986	-2.21309	-1.02339
H	7.62082	1.75018	0.54017
H	8.61386	-0.33296	-0.37612
Br	-0.48875	-0.79591	0.00481
C	-2.36187	-0.26535	0.02392
Br	-3.39291	-1.13646	-1.39236
Br	-2.36391	2.42212	-0.49406
Br	-3.18224	-0.51662	1.78196

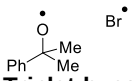


Formation of hypobromite – product 5.44 in dichloromethane

22

-438.0104873

C	0.12234	0.62608	0.01800
C	0.41146	1.50337	-1.19738
H	-0.22757	2.38689	-1.19214
H	1.44901	1.84224	-1.18420
H	0.22793	0.94294	-2.11582
C	0.40541	1.35561	1.32936
H	0.25581	0.67837	2.17229
H	1.42866	1.73501	1.34817
H	-0.27209	2.20362	1.43748
O	0.88194	-0.59598	-0.05934
C	-1.32762	0.13132	-0.00363
C	-1.65981	-1.22373	0.01178
C	-2.35888	1.07570	-0.02208
C	-2.99549	-1.62266	0.00474
H	-0.87731	-1.96997	0.02934
C	-3.68973	0.67612	-0.02808
H	-2.12911	2.13544	-0.02905
C	-4.01425	-0.67831	-0.01557
H	-3.23474	-2.67984	0.01593
H	-4.47368	1.42426	-0.04272
H	-5.05152	-0.99191	-0.02078
Br	2.75682	-0.40001	-0.01505



Triplet hypobromite A10 in dichloromethane

22

-437.9669470

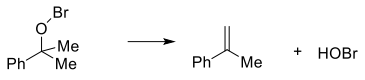
C	0.08972	0.51344	0.07762
C	-0.18634	1.32096	1.38781
H	0.43916	2.21371	1.35444
H	-1.23727	1.60537	1.42857
H	0.07934	0.72406	2.25949
C	-0.32959	1.34124	-1.14861
H	-0.25256	0.72945	-2.04868
H	-1.35454	1.69043	-1.03171
H	0.33239	2.20082	-1.25018
O	-0.72218	-0.58932	0.22276
C	1.55944	0.09115	0.01552
C	1.92913	-1.25100	0.07703
C	2.55351	1.06562	-0.10169
C	3.27308	-1.61297	0.01837
H	1.16831	-2.01552	0.17125
C	3.89438	0.70305	-0.15851
H	2.28969	2.11671	-0.14684
C	4.25881	-0.63947	-0.09936
H	3.54687	-2.66060	0.06407
H	4.65368	1.47077	-0.25023
H	5.30365	-0.92280	-0.14526
Br	-3.18412	-0.33229	-0.07418

Formation of hypobromite – product CBr_3 anion in dichloromethane

4

-78.1736580

C	0.00062	-0.00048	0.83266
Br	1.81980	-0.57410	-0.04762
Br	-1.40751	-1.28785	-0.04757
Br	-0.41240	1.86204	-0.04755



5.44 **5.42** **A11**

Elimination of HOBr from hypobromite 5.44 – starting species 5.44 in dichloromethane

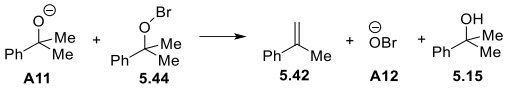
22
-438.0104870

C	0.12236	0.62625	0.01793
C	0.41124	1.50205	-1.19855
H	-0.22804	2.38542	-1.19449
H	1.44870	1.84128	-1.18581
H	0.22776	0.94034	-2.11622
C	0.40565	1.35707	1.32845
H	0.25573	0.68082	2.17211
H	1.42907	1.73610	1.34680
H	-0.27130	2.20562	1.43589
O	0.88194	-0.59589	-0.05815
C	-1.32761	0.13129	-0.00325
C	-1.65977	-1.22378	0.01187
C	-2.35887	1.07565	-0.02181
C	-2.99545	-1.62267	0.00481
H	-0.87732	-1.97011	0.02926
C	-3.68976	0.67608	-0.02791
H	-2.12912	2.13539	-0.02897
C	-4.01425	-0.67832	-0.01542
H	-3.23474	-2.67984	0.01588
H	-4.47365	1.42429	-0.04260
H	-5.05148	-0.99206	-0.02070
Br	2.75679	-0.40005	-0.01493

Elimination of HOBr from hypobromite 5.44 – products 5.42 and HOBr in dichloromethane

22
-437.9891740

C	-0.51196	1.13568	0.63212
C	0.00834	2.15293	-0.35088
H	-0.67007	3.00706	-0.42216
H	0.98412	2.52409	-0.03740
H	0.09540	1.72022	-1.35108
C	0.12015	0.91069	1.79243
H	-0.26542	0.21821	2.53204
H	0.90056	-0.52459	0.17169
H	1.02867	1.44748	2.04196
O	1.43663	-1.03654	-0.46035
C	-1.74781	0.38940	0.26412
C	-1.97264	-0.90994	0.73751
C	-2.71164	0.96751	-0.56918
C	-3.13399	-1.59804	0.40975
H	-1.22506	-1.39743	1.35352
C	-3.87817	0.28104	-0.89294
H	-2.56161	1.96613	-0.96157
C	-4.09481	-1.00300	-0.40407
H	-3.28366	-2.60462	0.78209
H	-4.61664	0.75110	-1.53171
H	-4.99969	-1.54031	-0.66179
Br	3.16159	-0.32094	-0.22702



A11 **5.44** **5.42** **A12** **5.15**

Based-induced elimination on hypobromite 5.44 – starting species A11 and 5.86 in dichloromethane

43
-862.8454498

C	2.24596	-0.23388	0.11835
C	2.02136	-0.65250	1.57044
H	1.02327	-0.33813	1.88108
H	2.08739	-1.73666	1.68206
H	2.75954	-0.17587	2.21940
C	1.32410	-0.98234	-0.83306
H	1.52324	-0.67050	-1.86132
H	1.50460	-2.05646	-0.74910
H	0.27378	-0.78641	-0.59618
O	3.63002	-0.42590	-0.27138
C	2.09164	1.28620	0.00787
C	3.18490	2.13660	0.19170
C	0.82237	1.83760	-0.19926
C	3.02011	3.51854	0.14900
H	4.16733	1.71670	0.36525
C	0.66619	3.22177	-0.23121
H	-0.05405	1.19309	-0.30609
C	1.75966	4.06726	-0.06544
H	3.87912	4.16548	0.28614
H	-0.32282	3.64132	-0.38491
H	1.62936	5.14297	-0.09662
Br	4.28311	-2.18950	-0.09343
C	-2.82506	0.58898	-0.10497
C	-2.99417	1.58173	-1.28510
H	-3.86980	2.23267	-1.19236
H	-2.09819	2.20828	-1.33617
H	-3.07284	1.02143	-2.22130
C	-2.74122	1.41823	1.20436
H	-2.63408	0.73764	2.05393
H	-1.84959	2.05128	1.15724
H	-3.61407	2.05687	1.37703
O	-1.70548	-0.16717	-0.26994
C	-4.11405	-0.26682	-0.02558
C	-4.01960	-1.65629	-0.09817
C	-5.38903	0.29441	0.12700
C	-5.15434	-2.46425	-0.02588
H	-3.02835	-2.07900	-0.21400
C	-6.52642	-0.50490	0.19967
H	-5.50019	1.37262	0.19083
C	-6.41453	-1.89267	0.12298
H	-5.05430	-3.54325	-0.08619
H	-7.50242	-0.04583	0.31780
H	-7.29914	-2.51723	0.17777

Based-induced elimination on hypobromite 5.44 – transition state in dichloromethane

43
-862.8194036

C	1.98491	-0.26045	0.38527
C	2.12789	-0.76014	1.81863
H	1.17423	-0.68475	2.34447
H	2.41852	-1.81210	1.80225
H	2.88569	-0.19938	2.37010
C	1.15082	-1.12424	-0.42885
H	1.06209	-0.83259	-1.47572
H	1.38888	-2.18418	-0.31352
H	-0.54433	-0.98671	0.17756
O	3.48098	-0.04526	-0.11272
C	1.61098	1.21530	0.28043
C	1.36351	2.00649	1.40312
C	1.49042	1.80999	-0.98329
C	0.97317	3.33953	1.27073
H	1.45725	1.58663	2.39686
C	1.10588	3.13715	-1.11898
H	1.70689	1.21974	-1.86568
C	0.83941	3.91071	0.01138
H	0.77189	3.92825	2.15885
H	1.01488	3.57273	-2.10797
H	0.53606	4.94607	-0.09225
Br	4.47812	-1.64033	-0.33642
C	-2.30935	-0.03368	-0.24155
C	-1.91905	-0.08705	-1.72596
H	-2.59182	0.52651	-2.32943
H	-0.90014	0.28448	-1.84994
H	-1.96367	-1.11702	-2.08918
C	-2.14120	1.40089	0.28227
H	-2.42064	1.44369	1.33821
H	-1.09480	1.69729	0.18342
H	-2.75909	2.11244	-0.27150
O	-1.51247	-0.90861	0.52285
C	-3.77011	-0.46590	-0.08648
C	-4.11378	-1.59539	0.65654
C	-4.79913	0.26729	-0.68910
C	-5.44634	-1.98233	0.79571
H	-3.32259	-2.16551	1.12491
C	-6.12887	-0.11569	-0.55301
H	-4.56308	1.15016	-1.27398
C	-6.45976	-1.24597	0.19266
H	-5.69100	-2.86365	1.37864
H	-6.90853	0.46777	-1.02990
H	-7.49557	-1.54629	0.30040

Based-induced elimination on hypobromite 5.44 – products 5.42, A12 and 5.15 in dichloromethane

43
-862.8492165

C	-1.36789	-0.53368	0.23772
C	-1.76460	-1.38552	-0.93606
H	-1.00050	-1.36596	-1.71889
H	-1.90823	-2.42189	-0.62847
H	-2.69995	-0.99466	-1.34257
C	-1.11832	-1.06506	1.44169
H	-0.81292	-0.45411	2.28492
H	-1.23023	-2.13003	1.61520
H	0.93107	-1.12101	0.20582
O	-4.26834	0.41175	-0.15828
C	-1.21876	0.92734	0.00717
C	-1.53698	1.84774	1.01191
C	-0.71645	1.41345	-1.20367
C	-1.33169	3.20874	0.82368
H	-1.97103	1.49049	1.93843
C	-0.50713	2.77694	-1.39377
H	-0.46680	0.72494	-2.00219
C	-0.80829	3.67968	-0.37956
H	-1.59096	3.90575	1.61243
H	-0.10659	3.13239	-2.33645
H	-0.64954	4.74151	-0.52806
Br	-5.41871	-1.10451	-0.18228
C	2.70513	-0.51270	0.73724
C	2.72827	-1.31627	2.04223
H	3.39866	-0.86522	2.77628
H	1.72216	-1.34809	2.47015
H	3.05912	-2.33797	1.84485
C	2.22979	0.92083	0.99506
H	2.16569	1.46917	0.05259
H	1.23674	0.90590	1.45343
H	2.91086	1.44685	1.66685
O	1.81725	-1.14709	-0.18111
C	4.08627	-0.50613	0.09646
C	4.30494	-1.04351	-1.17162
C	5.17097	0.04845	0.78377
C	5.57790	-1.02604	-1.74009
H	3.47350	-1.47619	-1.71202
C	6.44045	0.06623	0.21825
H	5.02790	0.47298	1.77204
C	6.64975	-0.47194	-1.04994
H	5.72809	-1.44885	-2.72720
H	7.26744	0.50174	0.76735
H	7.63892	-0.45838	-1.49233

A.5 XYZ files Chapter 6

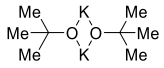
Table 6.2

6.13

KO^{t}Bu 6.13 in benzene

15
-832.9947940

C	-1.08912	0.00048	-0.00110
C	-1.63447	-1.15166	-0.86972
H	-1.26563	-2.10548	-0.48086
H	-2.72954	-1.18344	-0.88742
H	-1.27442	-1.03818	-1.89705
C	-1.63253	1.33130	-0.56007
H	-2.72777	1.36847	-0.56747
H	-1.26043	2.16096	0.04895
H	-1.27497	1.47256	-1.58523
C	-1.62988	-0.17835	1.43295
H	-1.26446	-1.12456	1.84465
H	-1.26058	0.63453	2.06545
H	-2.72448	-0.18057	1.47288
O	0.28573	-0.00248	-0.00282
K	2.60066	0.00026	-0.00019

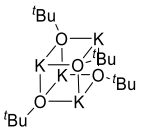


6.14

KO^{t}Bu dimer 6.14 in benzene

30
-1666.0362918

C	0.62927	-3.05346	0.00000
C	0.00110	-3.70210	1.25011
H	-1.07444	-3.50019	1.26622
H	0.15102	-4.78630	1.28575
H	0.44681	-3.26711	2.15133
C	2.13932	-3.36032	0.00000
H	2.35201	-4.43469	0.00000
H	2.60199	-2.91357	-0.88519
H	2.60199	-2.91357	0.88519
C	0.00110	-3.70210	-1.25011
H	-1.07444	-3.50019	-1.26622
H	0.44681	-3.26711	-2.15133
H	0.15102	-4.78630	-1.28575
O	0.41164	-1.69156	0.00000
K	-0.00047	-0.00032	1.78177
K	-0.00047	-0.00032	-1.78177
O	-0.41180	1.69163	0.00000
C	-0.62890	3.05358	0.00000
C	-2.13868	3.36152	0.00000
H	-2.35028	4.43612	0.00000
H	-2.60199	2.91540	-0.88519
H	-2.60199	2.91540	0.88519
C	-0.00047	3.70204	1.25012
H	-0.15001	4.78629	1.28553
H	-0.44647	3.26731	2.15130
H	1.07498	3.49967	1.26629
C	-0.00047	3.70204	-1.25012
H	1.07498	3.49967	-1.26629
H	-0.44647	3.26731	-2.15130
H	-0.15001	4.78629	-1.28553



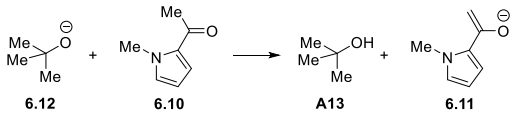
6.15

KO^{t}Bu cubic tetramer 6.15 in benzene

60
-3332.1275140

O	-2.10499	-0.66083	-0.39249
K	-0.36415	-1.97065	0.97625
K	-1.42382	1.50990	0.81846
O	0.30768	0.19875	2.19744
O	0.36173	1.97362	-0.97891
O	1.42392	-1.51907	-0.81755
K	-0.31418	-0.19583	-2.19446
K	2.09561	0.65667	0.39673
C	0.58729	3.19291	-1.58912
C	-0.66584	3.65550	-2.35946
H	-0.52607	4.62078	-2.85797
H	-0.92603	2.91075	-3.11917
H	-1.51075	3.74240	-1.66813
C	0.93374	4.26628	-0.53859
H	1.82120	3.95844	0.02434
H	1.13095	5.24780	-0.98357
H	0.10403	4.36960	0.16884
C	1.76064	3.09003	-2.58427
H	1.53324	2.33840	-3.34737
H	1.97513	4.03840	-3.08891
H	2.66462	2.77079	-2.05518
C	0.50544	0.31966	3.56013
C	0.89046	1.76674	3.92683
H	1.80459	2.05066	3.39503
H	0.09289	2.45116	3.61922
H	1.06144	1.90015	5.00032
C	-0.78024	-0.04842	4.32807
H	-1.07433	-1.07517	4.08614
H	-0.66300	0.03041	5.41434
H	-1.59453	0.61658	4.02108
C	1.63738	-0.61629	4.02981
H	1.81997	-0.55169	5.10790
H	1.38406	-1.65298	3.78443
H	2.56628	-0.36364	3.50796
C	-3.40248	-1.06486	-0.64594
C	-4.12433	-0.03956	-1.54329
H	-3.58538	0.06637	-2.49055
H	-5.15812	-0.32380	-1.76785
H	-4.13571	0.93827	-1.05047
C	-4.19298	-1.19702	0.67054
H	-5.22810	-1.51832	0.51335
H	-3.70028	-1.92539	1.32332
H	-4.20635	-0.23271	1.18939
C	-3.41281	-2.43107	-1.35954
H	-2.91662	-3.17933	-0.73228
H	-4.42408	-2.78768	-1.58311
H	-2.85785	-2.35758	-2.30075
C	2.31152	-2.44944	-1.32580
C	3.20107	-1.81264	-2.41236
H	3.74949	-0.96458	-1.98859
H	3.92713	-2.51702	-2.83226
H	2.57529	-1.43648	-3.22879
C	3.22368	-2.99074	-0.20777

H	2.61209	-3.46202	0.56853
H	3.94843	-3.72811	-0.56964
H	3.77485	-2.16358	0.25206
C	1.55103	-3.63607	-1.95107
H	0.92185	-4.11097	-1.19087
H	0.89709	-3.27413	-2.75174
H	2.21861	-4.39718	-2.36882



6.12 6.10 A13 6.11

Deprotonation of 6.10 – starting material 6.12 and 6.10 in benzene

32

-635.1652092

C	2.26087	-0.20305	-0.09778
C	1.49045	-0.95263	-1.21386
H	1.09456	-0.22521	-1.93022
H	2.11543	-1.67583	-1.75392
H	0.63600	-1.47948	-0.77629
C	2.83070	-1.26684	0.87640
H	3.49711	-1.98899	0.38747
H	3.38428	-0.75984	1.67342
H	2.00137	-1.81431	1.33638
C	3.46324	0.51648	-0.76009
H	3.08546	1.26489	-1.46471
H	4.03890	1.03868	0.01061
H	4.13246	-0.16690	-1.29891
O	1.45271	0.68171	0.55030
C	-2.01947	-1.89086	-0.01091
C	-2.39255	-1.51467	-1.28784
C	-2.09139	-0.13860	-1.40922
C	-1.55978	0.27557	-0.19785
N	-1.53764	-0.80293	0.64715
H	-2.03851	-2.85561	0.47218
H	-2.81997	-2.16088	-2.03840
H	-2.25400	0.48791	-2.27243
C	-0.87679	-0.82678	1.94924
H	0.08223	-0.30549	1.83109
H	-1.49534	-0.33539	2.69970
H	-0.71644	-1.87061	2.22150
C	-1.16360	1.62683	0.24816
C	-0.57011	2.53515	-0.79062
H	-1.01439	2.38508	-1.77577
H	-0.66687	3.57381	-0.47595
H	0.48553	2.23869	-0.81628
O	-1.32942	1.98160	1.40053

Deprotonation of 6.10 – transition state in benzene

32

-635.1602401

C	2.47261	-0.24863	0.20353
C	1.51746	-1.15248	1.01371
H	0.50094	-1.05604	0.61913
H	1.80623	-2.20981	0.97330
H	1.51561	-0.82825	2.05913
C	3.90371	-0.44860	0.73747
H	4.23244	-1.49300	0.67595
H	4.59501	0.17325	0.16116
H	3.94770	-0.12683	1.78216
C	2.43346	-0.71067	-1.26947
H	1.41325	-0.62789	-1.65511
H	3.08327	-0.06716	-1.87084
H	2.76282	-1.74985	-1.38438
O	2.11779	1.07999	0.32305
C	-2.41527	-1.71398	0.16850
C	-2.07567	-1.85634	-1.16197
C	-1.50558	-0.62824	-1.56878
C	-1.52727	0.22792	-0.47994
N	-2.09750	-0.45221	0.57186
H	-2.84541	-2.41736	0.86484
H	-2.22011	-2.74250	-1.75961
H	-1.12575	-0.38112	-2.54764
C	-2.20620	0.01441	1.94808
H	-1.24537	0.40556	2.28170
H	-2.95025	0.80375	2.03149
H	-2.48768	-0.83807	2.56573
C	-1.05043	1.63244	-0.34939
C	0.09142	2.00267	-1.17024
H	0.13670	1.49482	-2.13339
H	0.20411	3.08289	-1.25751
H	1.05171	1.54311	-0.49945
O	-1.55806	2.35613	0.50962

Deprotonation of 6.10 – products 6.11 and A13 in benzene

32

-635.1839562

C	2.76882	0.26793	-0.26672
C	1.74929	0.84069	-1.25295
H	1.63397	1.91559	-1.08940
H	2.07193	0.67295	-2.28500
H	0.77858	0.35850	-1.11106
C	2.87794	-1.24638	-0.45170
H	3.24775	-1.48383	-1.45390
H	3.57200	-1.66238	0.28411
H	1.89458	-1.71167	-0.32750
C	4.12617	0.93749	-0.44830
H	4.03819	2.01368	-0.27813
H	4.84351	0.53102	0.26919
H	4.50711	0.77202	-1.45927
O	2.36964	0.56655	1.06946
C	-3.27970	1.18470	-0.44019
C	-2.53279	2.07668	0.29856
C	-1.43938	1.34839	0.83640
C	-1.55233	0.03656	0.41009
N	-2.67749	-0.04312	-0.37458
H	-4.19207	1.31710	-1.00104
H	-2.74802	3.12652	0.42698
H	-0.63071	1.72824	1.44229
C	-3.19942	-1.24226	-1.01166
H	-2.59119	-1.52012	-1.87082
H	-3.18435	-2.07295	-0.30791
H	-4.22566	-1.03952	-1.32035
C	-0.65330	-1.14964	0.62927
C	-0.02491	-1.22135	1.85659
H	-0.29080	-0.54596	2.65965
H	0.64175	-2.05052	2.06757
O	-0.52351	-1.95284	-0.35073
H	1.56450	0.04670	1.27057

6.13 **6.10** **A14** **A15**

Deprotonation of 6.10 – starting material 6.13 and 6.10 in benzene

33

-1235.0881477

C	1.70680	1.49924	0.14743
C	0.38383	2.17108	0.56806
H	0.02710	1.73410	1.50567
H	0.49473	3.25226	0.70863
H	-0.38434	1.99633	-0.19274
C	2.17962	2.15367	-1.16773
H	2.32409	3.23579	-1.07444
H	3.12686	1.70286	-1.48117
H	1.43771	1.96979	-1.95168
C	2.76017	1.78693	1.23728
H	2.43696	1.33618	2.18115
H	3.71442	1.33258	0.95197
H	2.92013	2.85848	1.40041
O	1.54314	0.14254	-0.01965
K	2.06436	-2.09892	-0.57413
C	-2.90109	0.91119	-1.09108
C	-3.45162	1.15730	0.15521
C	-2.75752	0.34544	1.07039
C	-1.81823	-0.38495	0.35214
N	-1.93384	-0.03106	-0.97383
H	-3.11619	1.35449	-2.05124
H	-4.25585	1.84336	0.36662
H	-2.93206	0.27794	2.13252
C	-1.00157	-0.39498	-2.03648
H	0.01324	-0.20013	-1.67199
H	-1.11918	-1.44443	-2.30240
H	-1.22050	0.23140	-2.90058
C	-0.87252	-1.39084	0.82179
C	-0.42364	-1.29454	2.25233
H	-1.19587	-0.90676	2.91531
H	-0.07555	-2.26679	2.59946
H	0.41372	-0.58746	2.23661
O	-0.43322	-2.26507	0.08181

Deprotonation of 6.10 – transition state in benzene

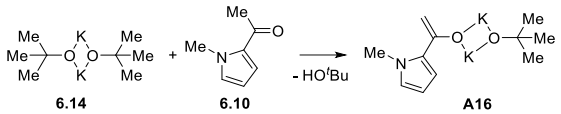
33
-1235.0770131

C	-1.99134	-1.38225	-0.28355
C	-1.09306	-1.08956	-1.49874
H	-0.11341	-0.73718	-1.15989
H	-0.94189	-1.97581	-2.12307
H	-1.54980	-0.30935	-2.11793
C	-3.35486	-1.88462	-0.77259
H	-3.26091	-2.79336	-1.37564
H	-3.99729	-2.09882	0.08543
H	-3.83967	-1.11391	-1.37921
C	-1.32920	-2.47347	0.57290
H	-0.33350	-2.15258	0.89228
H	-1.93484	-2.66082	1.46391
H	-1.22517	-3.41048	0.01756
O	-2.17750	-0.21458	0.46452
K	-2.11366	2.21735	-0.07417
C	3.49284	-0.71612	-0.70339
C	3.40437	-1.50621	0.42681
C	2.35983	-0.97663	1.20795
C	1.83917	0.12224	0.53661
N	2.55528	0.26495	-0.63711
H	4.15570	-0.77845	-1.55261
H	4.02529	-2.35791	0.65403
H	2.01884	-1.34475	2.16233
C	2.35589	1.25643	-1.68722
H	1.34862	1.17829	-2.09490
H	2.49466	2.26103	-1.29479
H	3.08541	1.05659	-2.47109
C	0.72026	1.00022	0.91423
C	-0.15866	0.57469	1.98223
H	0.23268	-0.17576	2.66290
H	-0.59938	1.42075	2.51212
H	-1.13833	0.06666	1.27717
O	0.47428	2.01373	0.22787

Deprotonation of 6.10 – products A14 and A15 in benzene

33
-1235.0961986

C	2.02878	-1.27864	0.11805
C	2.03720	-2.43410	-0.87931
H	2.72209	-2.21932	-1.70274
H	2.35143	-3.36110	-0.39356
H	1.03244	-2.58227	-1.28570
C	1.05120	-1.55773	1.25669
H	1.36607	-2.43500	1.82759
H	1.00196	-0.69841	1.93084
H	0.04980	-1.74588	0.85839
C	3.42825	-1.00098	0.64727
H	4.10059	-0.74718	-0.17550
H	3.40901	-0.16944	1.35713
H	3.82292	-1.87985	1.16097
O	1.62867	-0.07627	-0.56311
K	1.52089	2.47504	0.10953
C	-2.51177	-1.82351	0.21830
C	-2.06173	-2.02667	-1.06719
C	-1.50595	-0.79710	-1.50253
C	-1.63138	0.11754	-0.46527
N	-2.24386	-0.53124	0.57863
H	-3.00464	-2.49086	0.90802
H	-2.12904	-2.94853	-1.62349
H	-1.06896	-0.58652	-2.46788
C	-2.58448	0.02627	1.88163
H	-1.69145	0.14577	2.49339
H	-3.04822	1.00257	1.76088
H	-3.28268	-0.65853	2.36254
C	-1.16632	1.53914	-0.36857
C	-1.03027	2.23925	-1.54059
H	-1.35844	1.83098	-2.48615
H	-0.73750	3.28434	-1.51033
O	-0.84900	1.96787	0.80432
H	0.71611	-0.20147	-0.86644



6.14 6.10 A16

Deprotonation of 6.10 – starting material 6.14 and 6.10 in benzene

48

-2068.1329744

C	2.90465	-1.49115	-0.47325
C	3.58477	-0.56412	-1.50475
H	3.85438	0.38753	-1.03693
H	4.49209	-1.00435	-1.93181
H	2.89223	-0.35121	-2.32691
C	2.57886	-2.82583	-1.17683
H	3.46784	-3.31540	-1.58885
H	2.10421	-3.50832	-0.46528
H	1.87481	-2.65168	-1.99792
C	3.91348	-1.78077	0.65648
H	4.16969	-0.85151	1.17406
H	3.45922	-2.45987	1.38516
H	4.83828	-2.23821	0.28868
O	1.75639	-0.91394	0.02939
K	-0.12865	-0.21119	-1.50221
K	0.06461	-1.32688	1.83756
O	-1.79625	-1.03939	0.20644
C	-3.09780	-1.35517	-0.12591
C	-3.63605	-0.39349	-1.20840
H	-4.68006	-0.59570	-1.46999
H	-3.56320	0.63818	-0.85097
H	-3.04016	-0.48369	-2.12413
C	-3.18291	-2.79242	-0.67629
H	-4.20244	-3.07710	-0.95820
H	-2.54027	-2.88524	-1.55787
H	-2.82131	-3.49510	0.08018
C	-4.01926	-1.25416	1.10657
H	-3.65359	-1.92752	1.88782
H	-4.00396	-0.23390	1.50196
H	-5.05704	-1.51961	0.87812
C	-1.23782	2.82836	-1.20993
C	-0.05189	3.03839	-1.89900
C	0.99202	2.73491	-1.00647
C	0.41445	2.33256	0.19423
N	-0.95656	2.39868	0.04434
H	-2.26181	2.97053	-1.52016
H	0.03439	3.38847	-2.91517
H	2.05203	2.77520	-1.20524
C	-1.97274	2.09420	1.05333
H	-2.04176	1.01043	1.17202
H	-1.70913	2.57236	1.99381
H	-2.92077	2.49083	0.69057
C	1.07963	1.83252	1.40053
C	2.57703	1.94196	1.44647
H	2.93568	2.89170	1.04964
H	2.91220	1.80628	2.47336
H	2.95499	1.11886	0.83274
O	0.45078	1.31657	2.31398

Deprotonation of 6.10 – transition state in benzene

48

-2068.1198875

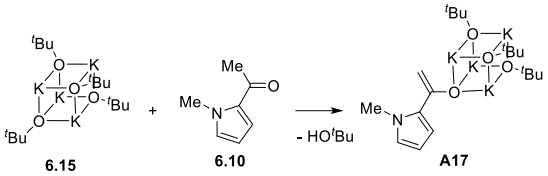
C	3.08154	-1.20390	-0.49229
C	3.93586	-0.32078	-1.41333
H	4.23901	0.58622	-0.88313
H	4.83527	-0.84055	-1.75655
H	3.35124	-0.02501	-2.28999
C	2.64919	-2.46459	-1.24840
H	3.51000	-3.06226	-1.56341
H	2.01127	-3.08426	-0.61117
H	2.07816	-2.19414	-2.14199
C	3.90992	-1.60785	0.73679
H	4.20096	-0.71679	1.29943
H	3.31355	-2.24943	1.39338
H	4.81530	-2.15432	0.45699
O	1.93602	-0.50135	-0.08584
K	-0.12723	0.05342	-1.58736
K	0.23374	-1.32136	1.79352
O	-1.52166	-1.24267	0.03252
C	-2.78425	-1.74425	-0.21457
C	-3.57086	-0.80149	-1.14985
H	-4.58841	-1.15479	-1.34755
H	-3.63074	0.19518	-0.70225
H	-3.05365	-0.71522	-2.11243
C	-2.69486	-3.12714	-0.88895
H	-3.67970	-3.55708	-1.10113
H	-2.14331	-3.04155	-1.83057
H	-2.14757	-3.81609	-0.23855
C	-3.57652	-1.89840	1.09929
H	-3.02416	-2.55537	1.77919
H	-3.69113	-0.92431	1.58434
H	-4.57328	-2.32434	0.94355
C	-1.69339	2.87268	-0.97629
C	-0.57991	3.29532	-1.68159
C	0.53966	3.02178	-0.86883
C	0.08067	2.43455	0.30561
N	-1.29510	2.35741	0.21740
H	-2.74211	2.91642	-1.22738
H	-0.58731	3.76328	-2.65319
H	1.57346	3.21893	-1.10551
C	-2.22865	1.81130	1.20396
H	-2.12104	0.72571	1.23669
H	-2.03107	2.24301	2.18121
H	-3.23419	2.07429	0.87538
C	0.85869	1.84579	1.42578
C	2.28367	1.74635	1.25189
H	2.75296	2.50316	0.62922
H	2.81195	1.55474	2.18357
H	2.23288	0.61109	0.55407
O	0.24803	1.30105	2.36253

Deprotonation of 6.10 – products A16 in benzene

48

-2068.1406255

C	2.96848	-1.63844	-0.60284
C	3.41500	-0.40449	-1.38934
H	3.28974	0.49473	-0.77758
H	4.46663	-0.48134	-1.67716
H	2.81987	-0.29981	-2.30173
C	3.06186	-2.89173	-1.46188
H	4.08904	-3.05496	-1.79599
H	2.73648	-3.76528	-0.89224
H	2.42145	-2.79440	-2.34215
C	3.80537	-1.77853	0.66788
H	3.69937	-0.88042	1.28381
H	3.47075	-2.64311	1.24704
H	4.86254	-1.91077	0.42502
O	1.59170	-1.48921	-0.24418
K	-0.24917	0.11960	-1.45561
K	-0.48458	-1.74920	1.73516
O	-1.99046	-1.03436	-0.10022
C	-3.36169	-1.02440	-0.26545
C	-3.81109	0.27012	-0.97380
H	-4.89490	0.31643	-1.12306
H	-3.50671	1.13845	-0.38126
H	-3.33178	0.34012	-1.95681
C	-3.81642	-2.22620	-1.11455
H	-4.90123	-2.24906	-1.26330
H	-3.33201	-2.18556	-2.09488
H	-3.51206	-3.15610	-0.62511
C	-4.07199	-1.09841	1.10175
H	-3.78038	-2.02002	1.61707
H	-3.77191	-0.24687	1.72123
H	-5.16325	-1.09026	1.01188
C	-0.97212	3.11002	-0.72854
C	0.11930	3.38694	-1.52409
C	1.26017	2.85917	-0.85955
C	0.82651	2.27437	0.31770
N	-0.53843	2.42987	0.37929
H	-2.01520	3.36038	-0.84492
H	0.09723	3.92292	-2.46012
H	2.28583	2.88568	-1.19463
C	-1.39973	1.97135	1.46392
H	-1.71572	0.94183	1.27687
H	-0.85187	2.03138	2.40319
H	-2.27092	2.62544	1.51027
C	1.55949	1.45076	1.32469
C	2.68799	1.94399	1.88135
H	3.02220	2.94686	1.65278
H	3.26283	1.34283	2.57605
O	1.03449	0.26437	1.53968
H	1.52165	-0.76922	0.45358



Deprotonation of 6.10 – starting material 6.15 and 6.10 in benzene

78

-3734.2095005

O	2.61460	0.91392	1.23517
K	2.10730	-1.61195	1.36667
K	2.50010	0.72673	-1.31971
O	1.96418	-1.74226	-1.22831
O	-0.05908	1.64718	-1.26981
O	-0.40106	-1.03041	1.38636
K	0.11493	1.45109	1.38474
K	-0.48883	-1.01945	-1.17964
C	-0.03818	2.95928	-1.72690
C	-0.16552	3.95970	-0.55727
H	-0.18599	4.99848	-0.90101
H	-1.09159	3.77341	-0.00187
H	0.68670	3.85623	0.12488
C	1.27874	3.29230	-2.46494
H	1.44810	2.56898	-3.26976
H	1.25374	4.29066	-2.91099
H	2.12880	3.27613	-1.77402
C	-1.18825	3.24091	-2.71398
H	-2.15475	3.13411	-2.21587
H	-1.13193	4.25357	-3.12482
H	-1.14877	2.52735	-3.54240
C	2.49969	-2.81162	-1.92363
C	2.17854	-2.69429	-3.42573
H	1.09363	-2.68450	-3.57217
H	2.58273	-1.75429	-3.81529
H	2.59633	-3.51951	-4.01177
C	4.03146	-2.84844	-1.75500
H	4.28489	-2.93429	-0.69302
H	4.49726	-3.68412	-2.28760
H	4.46508	-1.91603	-2.13157
C	1.91698	-4.14047	-1.40407
H	2.31398	-5.01161	-1.93557
H	2.14668	-4.25770	-0.33963
H	0.82811	-4.13422	-1.51558
C	3.64068	1.56947	1.88841
C	4.53657	2.31440	0.87863
H	3.93286	3.03373	0.31388
H	5.35504	2.85922	1.35980
H	4.97702	1.59853	0.17540
C	4.51555	0.56495	2.66350
H	5.34863	1.04473	3.18715
H	3.90435	0.03954	3.40514
H	4.92869	-0.17289	1.96713
C	3.07713	2.59874	2.88714
H	2.43667	2.09029	3.61560
H	3.86267	3.13081	3.43340
H	2.47419	3.34024	2.35155
C	-1.27821	-1.71020	2.21496
C	-2.32079	-0.73650	2.79603
H	-2.84736	-0.24328	1.97260
H	-3.06463	-1.23435	3.42669
H	-1.81793	0.02678	3.40151
C	-2.01478	-2.81362	1.43433
H	-1.28320	-3.50964	1.00916
H	-2.70576	-3.38349	2.06499

H	-2.59067	-2.37410	0.61466
C	-0.52053	-2.36818	3.38606
H	0.18219	-3.11818	3.00522
H	0.04404	-1.60730	3.93578
H	-1.19268	-2.87221	4.08796
H	-2.16888	0.90809	-2.07593
C	-3.09252	0.45638	-2.46401
C	-3.58533	-0.62150	-1.53166
H	-2.87497	-0.00303	-3.42819
H	-3.82449	1.25459	-2.59298
C	-4.36933	-0.28135	-0.34096
O	-3.33354	-1.79391	-1.77210
C	-5.22010	-1.14426	0.33626
N	-4.45129	0.95703	0.27284
C	-5.83281	-0.41750	1.37046
H	-5.37044	-2.17919	0.07146
C	-5.32312	0.86692	1.31021
C	-3.64362	2.14210	0.01003
H	-6.55375	-0.77728	2.08691
H	-5.50038	1.72015	1.94690
H	-2.60902	1.86278	-0.20068
H	-4.03953	2.71127	-0.83282
H	-3.66715	2.77087	0.89912

Deprotonation of 6.10 – transition state in benzene

78

-3734.2025619

O	2.35788	1.01753	0.94230
K	2.09832	-1.47188	1.57433
K	1.01951	0.43237	-1.27823
O	1.69367	-2.09112	-0.84001
O	-0.69970	2.45115	-0.55680
O	-0.48423	-1.02866	1.68230
K	0.05741	1.54275	1.77037
K	-0.75030	-2.58680	-0.40136
C	-0.55358	3.83085	-0.77338
C	0.29664	4.43545	0.35135
H	0.50430	5.49497	0.17534
H	-0.22743	4.35706	1.31136
H	1.24958	3.90258	0.42219
C	0.14795	4.08307	-2.11733
H	-0.44341	3.66372	-2.93537
H	0.29034	5.15095	-2.30760
H	1.13007	3.60060	-2.11919
C	-1.92925	4.51726	-0.78217
H	-2.43607	4.34317	0.17205
H	-1.84018	5.59723	-0.93372
H	-2.55334	4.10742	-1.58120
C	2.47239	-2.75130	-1.77220
C	3.04511	-1.75484	-2.79957
H	2.22579	-1.27019	-3.34251
H	3.62546	-0.98665	-2.27622
H	3.69728	-2.23433	-3.53636
C	3.64804	-3.46609	-1.07931
H	3.25979	-4.17720	-0.34259
H	4.28641	-4.01146	-1.78214
H	4.26664	-2.73045	-0.55467
C	1.63527	-3.80174	-2.52873
H	2.21266	-4.33454	-3.29108
H	1.24570	-4.54226	-1.82093
H	0.78921	-3.31000	-3.02092
C	3.63413	1.52994	0.80196
C	3.82561	2.13989	-0.60119
H	3.06375	2.90683	-0.77286
H	4.81149	2.59772	-0.73041
H	3.71893	1.36266	-1.36676
C	4.69088	0.42046	0.98500
H	5.71620	0.78254	0.85920
H	4.61157	-0.00719	1.99111
H	4.51984	-0.37360	0.24893
C	3.89708	2.62693	1.85053
H	3.77345	2.20820	2.85409
H	4.90386	3.05045	1.77242
H	3.17159	3.43641	1.72646
C	-1.33065	-1.38834	2.71945
C	-2.39807	-0.30292	2.98014
H	-2.91159	-0.07678	2.04099
H	-3.14353	-0.62786	3.71308
H	-1.94846	0.61876	3.36917
C	-2.08762	-2.69660	2.39974
H	-1.37145	-3.50372	2.19564
H	-2.72182	-3.01954	3.23072
H	-2.73646	-2.55192	1.52581
C	-0.52553	-1.60728	4.01582
H	0.18248	-2.43165	3.87871
H	0.04464	-0.70293	4.25454
H	-1.16210	-1.84821	4.87337
H	-1.48816	1.91930	-1.52778
C	-2.16661	1.33691	-2.46592
C	-2.19889	-0.04366	-2.04770
H	-1.56256	1.46130	-3.36449
H	-3.13894	1.81838	-2.54353
C	-3.31061	-0.55314	-1.20627
O	-1.28413	-0.84514	-2.31677
C	-3.79490	-1.85337	-1.20897
N	-4.10119	0.18480	-0.35250
C	-4.90315	-1.90134	-0.33520
H	-3.41405	-2.64753	-1.83382
C	-5.05210	-0.63194	0.18327
C	-3.92646	1.57935	0.04092
H	-5.52173	-2.75428	-0.10550
H	-5.74981	-0.24814	0.91175
H	-2.86507	1.82219	0.10488
H	-4.40020	2.25065	-0.67779
H	-4.39206	1.71623	1.01665

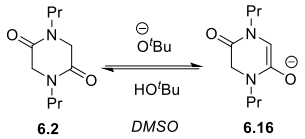
Deprotonation of 6.10 – product A17 in benzene

78

-3734.2326320

O	-1.40749	1.83943	-1.15262
K	-3.00773	-0.08977	-0.92028
K	-0.87444	1.73772	1.37290
O	-2.52177	-0.24340	1.61263
O	1.69041	2.26763	0.20098
O	-1.05937	-1.77424	-1.36937
K	0.56951	0.23389	-1.60963
K	-0.78038	-2.06976	1.17395
C	3.06843	2.63473	0.26993
C	3.15248	4.07144	-0.22723
H	4.18456	4.42938	-0.20648
H	2.77864	4.13772	-1.25185
H	2.54230	4.72160	0.40425
C	3.54470	2.52955	1.71873
H	3.38757	1.51328	2.09471
H	4.60688	2.77385	1.80305
H	2.97745	3.21798	2.35028
C	3.88124	1.70084	-0.63010
H	3.53308	1.78283	-1.66402
H	4.94421	1.95508	-0.60549
H	3.76772	0.66017	-0.30655
C	-3.48057	-0.32256	2.60528
C	-3.33697	0.84980	3.59578
H	-2.33894	0.82872	4.04680
H	-3.46200	1.80026	3.06548
H	-4.07632	0.81300	4.40214
C	-4.89567	-0.27301	1.99630
H	-5.02485	-1.10722	1.29827
H	-5.68413	-0.33746	2.75310
H	-5.02646	0.66498	1.44623
C	-3.33758	-1.64020	3.39288
H	-4.08101	-1.74047	4.19008
H	-3.45557	-2.49008	2.71157
H	-2.34230	-1.69195	3.84779
C	-1.34149	3.07329	-1.77531
C	-1.13102	4.19809	-0.74106
H	-0.18593	4.03032	-0.21364
H	-1.09341	5.18951	-1.20412
H	-1.95641	4.19439	-0.01975
C	-2.64352	3.35047	-2.54924
H	-2.63301	4.31805	-3.06226
H	-2.79797	2.56535	-3.29657
H	-3.49108	3.33616	-1.85651
C	-0.16053	3.12401	-2.76774
H	-0.27916	2.34042	-3.52534
H	-0.09190	4.08517	-3.28742
H	0.77643	2.96497	-2.22246
C	-1.22982	-2.77888	-2.30634
C	-0.22403	-2.62155	-3.46530
H	0.80086	-2.67002	-3.08310
H	-0.33840	-3.39809	-4.22847
H	-0.36952	-1.64875	-3.94794
C	-1.02053	-4.16423	-1.66260
H	-1.74882	-4.30795	-0.85674
H	-1.14304	-4.98320	-2.37873
H	-0.01358	-4.23031	-1.23741
C	-2.65195	-2.73466	-2.90117
H	-3.39241	-2.85689	-2.10272
H	-2.81800	-1.76884	-3.39144
H	-2.82183	-3.52150	-3.64285
C	2.11764	-1.08691	2.92614
C	1.94710	-0.89940	1.59487
H	1.51589	-0.52577	3.63201
H	2.84176	-1.79284	3.30955
C	2.75976	-1.65748	0.60265
O	1.03173	-0.11885	1.06041
C	2.29951	-2.24351	-0.56485
N	4.10956	-1.90840	0.69057
C	3.40392	-2.87373	-1.19395
H	1.26665	-2.24147	-0.89277
C	4.50288	-2.64010	-0.39926
C	5.03169	-1.42320	1.70594
H	3.39953	-3.43271	-2.11699
H	5.53763	-2.91863	-0.52354
H	4.70811	-0.44479	2.05651
H	5.07918	-2.10441	2.55751
H	6.02207	-1.33846	1.25979
H	1.59417	1.35659	0.57783

Table 6.3



6.2 *DMSO* 6.16

Deprotonation of 6.2 – starting species 6.2 and *tert*-butoxide in DMSO

46
-884.9356036

C	-1.36374	-0.79822	-0.05487
C	-0.09272	-0.05446	0.28824
C	-1.11425	2.07147	-0.36904
C	-2.44057	1.39005	-0.08628
H	0.75743	-0.62637	-0.11841
H	-2.70782	1.59702	0.95824
H	-3.18663	1.86852	-0.72031
N	-0.02520	1.29665	-0.25986
N	-2.43981	-0.03982	-0.36031
O	-1.08861	3.26245	-0.67126
O	-1.38720	-2.02482	-0.04216
C	1.30419	1.88034	-0.44844
H	1.96759	1.06261	-0.74770
H	1.23498	2.60439	-1.26300
C	1.82201	2.56699	0.81368
H	1.07879	3.29453	1.15303
H	1.93685	1.82225	1.60746
C	3.15517	3.26223	0.55111
H	3.54831	3.72302	1.45897
H	3.90058	2.55208	0.18378
H	3.04047	4.04551	-0.20296
C	-3.73030	-0.68246	-0.59575
H	-4.30059	-0.04580	-1.27767
H	-3.53927	-1.63155	-1.09763
C	-4.51247	-0.91900	0.69444
H	-4.68095	0.03770	1.19845
H	-3.90142	-1.53409	1.36132
C	-5.84790	-1.60262	0.41523
H	-6.40277	-1.77410	1.33888
H	-6.46988	-0.98996	-0.24250
H	-5.69571	-2.56978	-0.07064
H	-0.01199	-0.03565	1.38443
O	2.39950	-1.31171	-1.09539
C	3.27185	-1.78200	-0.14304
C	4.63482	-2.15855	-0.76476
H	5.06976	-1.27906	-1.25024
H	5.34989	-2.53395	-0.02339
H	4.48951	-2.93105	-1.52685
C	2.70922	-3.03820	0.56209
H	1.75369	-2.79344	1.03705
H	2.53016	-3.82578	-0.17693
H	3.38613	-3.43163	1.32941
C	3.53125	-0.71644	0.94931
H	3.93310	0.19257	0.49048
H	2.58925	-0.45771	1.44271
H	4.23692	-1.06021	1.71435

Deprotonation of 6.2 – transition state in DMSO

46
-884.9266175

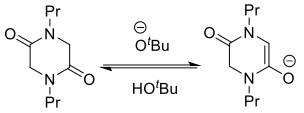
C	1.23006	-0.66572	-0.29670
C	-0.06711	0.01566	-0.38903
C	0.91891	2.07679	0.58258
C	2.27370	1.41055	0.46208
H	-0.94805	-0.74574	0.26462
H	2.77028	1.83917	-0.41974
H	2.85148	1.71419	1.33721
N	-0.13690	1.35665	0.19703
N	2.23191	-0.04056	0.40169
O	0.85738	3.23008	1.02475
O	1.39190	-1.80257	-0.75824
C	-1.47495	1.92986	0.31939
H	-2.13978	1.11927	0.62533
H	-1.45153	2.68310	1.10831
C	-1.96077	2.56031	-0.98390
H	-1.28238	3.37410	-1.25815
H	-1.91255	1.81876	-1.78762
C	-3.38882	3.08008	-0.84426
H	-3.73634	3.54224	-1.76993
H	-4.07300	2.26404	-0.59666
H	-3.45615	3.82709	-0.04872
C	3.50841	-0.72514	0.57338
H	3.97855	-0.32422	1.47739
H	3.29668	-1.78111	0.74482
C	4.45489	-0.57713	-0.61750
H	4.68217	0.48083	-0.78016
H	3.94440	-0.94176	-1.51305
C	5.74963	-1.35282	-0.39015
H	6.43184	-1.24523	-1.23508
H	6.26539	-0.99608	0.50549
H	5.54530	-2.41829	-0.25570
H	-0.39322	0.03501	-1.43401
O	-1.80671	-1.39696	0.99301
C	-2.85744	-1.94263	0.25097
C	-3.79594	-2.70398	1.19560
H	-4.18882	-2.02238	1.95553
H	-4.63994	-3.15026	0.65929
H	-3.24555	-3.50199	1.70224
C	-2.32417	-2.91742	-0.81328
H	-1.65424	-2.39042	-1.49858
H	-1.75431	-3.71618	-0.32921
H	-3.13394	-3.37030	-1.39430
C	-3.66310	-0.83640	-0.45592
H	-4.07598	-0.14524	0.28534
H	-3.01488	-0.26745	-1.13043
H	-4.49083	-1.25020	-1.04081

Deprotonation of 6.2 – products 6.16 and *tert*-butanol in DMSO

46

-884.9401085

C	1.14689	-0.41369	-0.63019
C	0.02355	0.38278	-0.79957
C	0.76359	2.09557	0.75506
C	2.12425	1.46907	0.51647
H	-1.00391	-0.95525	0.45807
H	2.55324	1.92962	-0.39122
H	2.76245	1.72874	1.36193
N	-0.22071	1.51767	0.05307
N	2.02432	0.02301	0.40394
O	0.61653	3.04921	1.53398
O	1.41488	-1.47135	-1.27037
C	-1.60273	1.95637	0.21921
H	-2.19976	1.08593	0.50837
H	-1.62283	2.67453	1.03920
C	-2.18547	2.59151	-1.04083
H	-1.58617	3.46745	-1.30788
H	-2.11666	1.89020	-1.87756
C	-3.64338	2.98825	-0.82374
H	-4.06918	3.44069	-1.72084
H	-4.24755	2.11317	-0.56835
H	-3.73514	3.70835	-0.00639
C	3.28586	-0.68931	0.55563
H	3.66495	-0.48733	1.56442
H	3.07240	-1.75700	0.49036
C	4.35838	-0.32384	-0.47323
H	4.64226	0.72689	-0.35614
H	3.93005	-0.43589	-1.47329
C	5.59373	-1.20720	-0.32029
H	6.37197	-0.93698	-1.03659
H	6.01698	-1.11448	0.68403
H	5.34065	-2.25896	-0.47916
H	-0.63047	0.26594	-1.64971
O	-1.55898	-1.46684	1.08139
C	-2.51896	-2.19660	0.31008
C	-3.27532	-3.07360	1.29873
H	-3.77278	-2.45513	2.04981
H	-4.03160	-3.66829	0.78132
H	-2.58456	-3.75127	1.80582
C	-1.79079	-3.04940	-0.72779
H	-1.16386	-2.41538	-1.36186
H	-1.14303	-3.77457	-0.22839
H	-2.50266	-3.59085	-1.35599
C	-3.47881	-1.22386	-0.37907
H	-3.97383	-0.59276	0.36384
H	-2.93594	-0.57939	-1.07697
H	-4.24443	-1.76722	-0.93866



6.2 *benzene* **6.16**

Deprotonation of 6.2 – starting species 6.2 and *tert*-butoxide in benzene

46

-884.8938973

C	-1.39618	-0.79264	-0.11444
C	-0.13049	-0.03769	0.21737
C	-1.20083	2.10288	-0.30656
C	-2.50669	1.38004	-0.01783
H	0.74825	-0.56438	-0.19831
H	-2.74108	1.52394	1.04624
H	-3.28000	1.88558	-0.59651
N	-0.10268	1.33560	-0.28116
N	-2.49228	-0.02874	-0.37690
O	-1.21463	3.30820	-0.54112
O	-1.42552	-2.01376	-0.12304
C	1.21796	1.92645	-0.51275
H	1.84290	1.15049	-0.96639
H	1.08461	2.77144	-1.19000
C	1.86860	2.38342	0.79069
H	1.21575	3.10350	1.29540
H	1.97959	1.51231	1.44470
C	3.24063	2.99575	0.52403
H	3.73371	3.29395	1.45188
H	3.88349	2.27399	0.01364
H	3.15541	3.88096	-0.11289
C	-3.77427	-0.68456	-0.59507
H	-4.37597	-0.04033	-1.24393
H	-3.57872	-1.61646	-1.12704
C	-4.52281	-0.97723	0.70435
H	-4.69956	-0.04045	1.24278
H	-3.88277	-1.60034	1.33533
C	-5.84992	-1.68081	0.43457
H	-6.38586	-1.88805	1.36246
H	-6.49687	-1.06612	-0.19749
H	-5.68593	-2.63182	-0.07849
H	-0.02987	-0.05267	1.31270
O	2.61202	-0.79913	-0.85451
C	3.37217	-1.65499	-0.11138
C	4.77097	-1.85500	-0.74207
H	5.27232	-0.88494	-0.82074
H	5.40936	-2.53489	-0.16357
H	4.65333	-2.25778	-1.75283
C	2.69914	-3.04446	0.00384
H	1.70911	-2.92993	0.45651
H	2.56263	-3.46137	-0.99867
H	3.28128	-3.75494	0.60446
C	3.57453	-1.11114	1.32604
H	4.05753	-0.12954	1.27470
H	2.59594	-0.98162	1.80090
H	4.18427	-1.77092	1.95623

Deprotonation of 6.2 – transition state in benzene

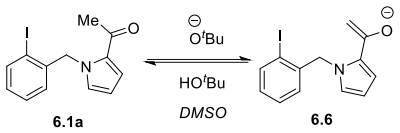
46
-884.8883013

C	1.22521	-0.65288	-0.28132
C	-0.08105	0.01670	-0.36513
C	0.89037	2.10184	0.57550
C	2.25095	1.43772	0.48029
H	-0.93544	-0.70658	0.29578
H	2.76196	1.87196	-0.39152
H	2.80656	1.75090	1.36702
N	-0.15883	1.36540	0.20052
N	2.22196	-0.01214	0.42225
O	0.82418	3.26265	0.98886
O	1.40595	-1.77596	-0.75255
C	-1.50267	1.92196	0.32519
H	-2.15563	1.10086	0.63238
H	-1.48448	2.67684	1.11318
C	-1.99198	2.54802	-0.97933
H	-1.32529	3.37366	-1.24719
H	-1.92777	1.80747	-1.78309
C	-3.42989	3.04209	-0.84751
H	-3.78358	3.49787	-1.77474
H	-4.09848	2.21278	-0.60163
H	-3.51391	3.78766	-0.05191
C	3.49929	-0.69049	0.58130
H	3.99101	-0.26993	1.46571
H	3.28983	-1.74276	0.77918
C	4.41967	-0.57634	-0.63452
H	4.63464	0.47731	-0.83981
H	3.88837	-0.97848	-1.50090
C	5.72485	-1.33555	-0.41087
H	6.38520	-1.26231	-1.27722
H	6.26317	-0.94157	0.45604
H	5.52776	-2.39512	-0.22739
H	-0.41152	0.02039	-1.40933
O	-1.86816	-1.31424	1.04334
C	-2.80641	-1.96183	0.25373
C	-3.76147	-2.76322	1.15209
H	-4.25230	-2.08765	1.85865
H	-4.53052	-3.28837	0.57368
H	-3.18982	-3.49827	1.72532
C	-2.12251	-2.93133	-0.73038
H	-1.41784	-2.38824	-1.36632
H	-1.55024	-3.67512	-0.16882
H	-2.84772	-3.45082	-1.36720
C	-3.63813	-0.94180	-0.55412
H	-4.14304	-0.25787	0.13553
H	-2.98134	-0.34971	-1.20018
H	-4.39451	-1.42668	-1.18135

Deprotonation of 6.2 – products 6.16 and *tert*-butanol in benzene

46
-884.9027601

C	1.13092	-0.42327	-0.57318
C	-0.01873	0.34347	-0.73148
C	0.76417	2.15701	0.69671
C	2.12179	1.51482	0.47058
H	-1.06328	-0.92885	0.58418
H	2.53997	1.93654	-0.46145
H	2.76556	1.81760	1.29789
N	-0.23746	1.52525	0.06489
N	2.02453	0.06660	0.42709
O	0.63498	3.16361	1.40370
O	1.41159	-1.48347	-1.19009
C	-1.61148	1.97116	0.24906
H	-2.21135	1.10156	0.53725
H	-1.61910	2.68790	1.07168
C	-2.19735	2.61597	-1.00546
H	-1.59376	3.49044	-1.26770
H	-2.12864	1.91674	-1.84432
C	-3.65342	3.01803	-0.78650
H	-4.08041	3.47946	-1.67922
H	-4.26116	2.14403	-0.53546
H	-3.74079	3.73208	0.03703
C	3.28122	-0.64507	0.58501
H	3.69494	-0.38537	1.56768
H	3.05353	-1.71215	0.58958
C	4.32336	-0.36289	-0.50106
H	4.62083	0.69078	-0.46765
H	3.85512	-0.54364	-1.47216
C	5.55340	-1.25003	-0.32907
H	6.30928	-1.04780	-1.09123
H	6.01562	-1.09424	0.65068
H	5.27729	-2.30565	-0.40140
H	-0.63130	0.23869	-1.61453
O	-1.69559	-1.42037	1.15078
C	-2.48851	-2.23700	0.29412
C	-3.34335	-3.10220	1.21267
H	-3.96805	-2.47144	1.85030
H	-3.99062	-3.76182	0.62850
H	-2.70257	-3.71375	1.85203
C	-1.57795	-3.10283	-0.57624
H	-0.89223	-2.47698	-1.15578
H	-0.97083	-3.75437	0.05771
H	-2.16609	-3.72500	-1.25758
C	-3.38549	-1.35412	-0.58003
H	-4.00992	-0.71596	0.05150
H	-2.77539	-0.71418	-1.22283
H	-4.03540	-1.96402	-1.21430



6.1a 6.6

Deprotonation of 6.1a – starting species 6.1a and *tert*-butoxide in DMSO

42
-876.9881769

C	3.51999	1.86939	0.74825
C	2.28579	1.87535	0.10880
C	1.61787	0.68651	-0.20105
C	2.25041	-0.50898	0.14465
C	3.48496	-0.53420	0.78385
C	4.12095	0.66408	1.09066
H	4.00980	2.80795	0.97760
H	1.82594	2.82225	-0.15280
H	3.94827	-1.47810	1.04199
H	5.08048	0.64728	1.59307
C	0.27021	0.70267	-0.89719
H	0.38892	0.31795	-1.91410
H	-0.47729	0.06019	-0.41962
N	-0.27630	2.04806	-1.02282
C	-0.12070	2.78828	-2.15166
C	-0.85751	2.84309	-0.04548
C	-0.61279	4.06230	-1.93643
H	0.32904	2.34807	-3.02880
C	-1.07502	4.09408	-0.60863
H	-1.53512	4.92050	-0.09011
H	-0.63938	4.86051	-2.66096
C	-1.20193	2.48612	1.34540
C	-0.97248	1.10061	1.87641
H	0.08644	0.83353	1.82704
H	-1.30447	1.07164	2.91350
O	-1.70633	3.34934	2.05120
I	1.34734	-2.38779	-0.31158
H	-1.54320	0.38371	1.26423
O	-2.52358	-0.55540	-0.34453
C	-3.39011	-1.54086	0.06698
C	-4.86302	-1.11899	-0.13705
H	-5.06636	-0.20359	0.42777
H	-5.04187	-0.91213	-1.19698
H	-5.57180	-1.88928	0.18824
C	-3.19405	-1.85761	1.56806
H	-3.85972	-2.65376	1.92043
H	-2.15779	-2.16696	1.74411
H	-3.38538	-0.95952	2.16423
C	-3.16634	-2.85061	-0.72203
H	-3.30423	-2.66091	-1.79131
H	-2.14127	-3.20239	-0.56831
H	-3.85413	-3.64912	-0.42051

Deprotonation of 6.1a – transition state in DMSO

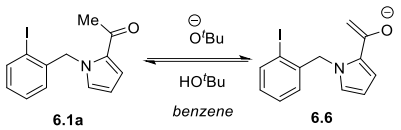
42
-876.9818173

C	0.34025	-2.76997	2.42937
C	0.89692	-2.10487	1.34366
C	0.09849	-1.47341	0.38609
C	-1.28486	-1.55056	0.55469
C	-1.85981	-2.21014	1.63589
C	-1.04076	-2.81938	2.58046
H	0.98673	-3.24798	3.15534
H	1.97545	-2.06658	1.23046
H	-2.93655	-2.25428	1.73918
H	-1.48767	-3.33298	3.42307
C	0.71744	-0.72736	-0.78031
H	0.25990	-1.07244	-1.71030
N	2.15121	-0.94864	-0.90542
C	2.64809	-2.02992	-1.57524
C	3.20867	-0.18589	-0.43812
C	4.02497	-1.98523	-1.54662
H	1.97408	-2.73893	-2.03224
C	4.37627	-0.81598	-0.83569
H	5.36675	-0.45428	-0.60871
H	4.69081	-2.70722	-1.99276
C	3.16155	1.04445	0.40365
C	1.97069	1.36582	1.16993
H	1.43272	0.49770	1.54940
H	2.19943	2.07877	1.96293
O	4.16774	1.76387	0.38606
I	-2.61648	-0.70614	-0.88686
H	1.15486	1.95563	0.38802
O	0.22746	2.53640	-0.46108
C	-0.64879	3.36417	0.23885
C	0.07228	4.64889	0.68691
H	0.92735	4.38976	1.31862
H	0.44607	5.18675	-0.18958
H	-0.58570	5.31812	1.25123
C	-1.20152	2.64989	1.48907
H	-1.92067	3.27555	2.02789
H	-1.70247	1.72207	1.19456
H	-0.38750	2.39620	2.17379
C	-1.82885	3.74489	-0.66618
H	-1.45868	4.24667	-1.56491
H	-2.36376	2.84114	-0.97298
H	-2.53430	4.41293	-0.16043
H	0.51035	0.34467	-0.69942

Deprotonation of 6.1a – products 6.6 and *tert*-butanol in DMSO

42
-877.0023769

C	2.69497	2.61842	1.45047
C	1.59535	2.33744	0.64847
C	1.41930	1.07633	0.07229
C	2.39166	0.11060	0.33257
C	3.49981	0.37377	1.13030
C	3.64944	1.63700	1.69304
H	2.80501	3.60450	1.88555
H	0.84981	3.10397	0.46534
H	4.24035	-0.39542	1.30995
H	4.51112	1.84716	2.31512
C	0.21502	0.78234	-0.80575
H	0.55934	0.45459	-1.78995
H	-0.37621	-0.03330	-0.38554
N	-0.63594	1.93814	-1.00747
C	-0.39087	2.82675	-2.02396
C	-1.68676	2.40442	-0.23216
C	-1.28454	3.86642	-1.92658
H	0.39765	2.63214	-2.73522
C	-2.10494	3.59358	-0.80267
H	-2.92691	4.18288	-0.42954
H	-1.34532	4.71180	-2.59444
C	-2.31103	1.77948	0.98861
C	-1.61702	0.86227	1.75074
H	-0.56973	0.64252	1.60834
H	-2.09552	0.47112	2.64256
O	-3.50431	2.17508	1.22630
I	2.22546	-1.84586	-0.50579
H	-2.71992	-0.43731	0.36791
O	-3.21196	-1.01027	-0.25067
C	-3.05535	-2.36573	0.17901
C	-3.64270	-2.52860	1.58092
H	-3.10929	-1.88889	2.28944
H	-4.69790	-2.24458	1.58163
H	-3.55911	-3.56420	1.92003
C	-1.57124	-2.72763	0.17605
H	-1.41789	-3.76683	0.47909
H	-1.15260	-2.59031	-0.82435
H	-1.02244	-2.08268	0.86975
C	-3.81920	-3.21680	-0.82625
H	-4.87298	-2.92810	-0.84094
H	-3.40554	-3.07936	-1.82814
H	-3.75087	-4.27472	-0.56298



Deprotonation of 6.1a – starting species 6.1a and *tert*-butoxide in benzene

42
-876.9509341

C	-1.10231	-3.82205	0.25083
C	-0.21375	-2.82173	-0.12513
C	-0.61524	-1.48569	-0.22747
C	-1.95551	-1.20299	0.04581
C	-2.85869	-2.19145	0.41947
C	-2.42781	-3.50900	0.52824
H	-0.75518	-4.84565	0.32661
H	0.81922	-3.07502	-0.33994
H	-3.89053	-1.93537	0.62482
H	-3.12840	-4.28026	0.82533
C	0.35273	-0.39263	-0.62649
H	0.00096	0.06424	-1.55600
H	0.42373	0.44398	0.09649
N	1.69184	-0.89818	-0.89973
C	2.09640	-1.21187	-2.15915
C	2.70092	-1.23565	-0.01233
C	3.37032	-1.74510	-2.11316
H	1.44354	-1.01967	-2.99701
C	3.74782	-1.75987	-0.75754
H	4.67743	-2.10006	-0.32963
H	3.95210	-2.06650	-2.96257
C	2.71881	-1.12470	1.46642
C	1.54130	-0.59176	2.22758
H	0.63217	-1.14890	1.98868
H	1.75754	-0.68551	3.29094
O	3.73328	-1.47895	2.04677
I	-2.69706	0.78751	-0.13478
H	1.38278	0.46280	1.95147
O	1.07975	2.07440	0.91107
C	1.20306	3.19338	0.13683
C	2.62908	3.78259	0.23958
H	2.84379	4.02112	1.28573
H	3.35235	3.03068	-0.09146
H	2.76209	4.68954	-0.36355
C	0.20025	4.28569	0.57656
H	0.26969	5.20041	-0.02545
H	-0.81698	3.88878	0.49796
H	0.38451	4.53956	1.62497
C	0.93022	2.87568	-1.35499
H	1.62096	2.09302	-1.68938
H	-0.09290	2.50061	-1.46484
H	1.05236	3.75091	-2.00471

Deprotonation of 6.1a – transition state in benzene

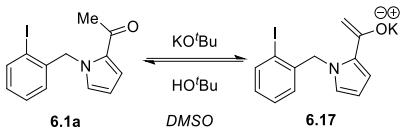
42
-876.9444239

C	0.37815	-2.71351	2.43847
C	0.92199	-2.04338	1.35019
C	0.11263	-1.42732	0.39103
C	-1.26830	-1.53039	0.56158
C	-1.83088	-2.19587	1.64548
C	-1.00151	-2.78669	2.59196
H	1.03468	-3.17467	3.16663
H	1.99938	-1.98414	1.23427
H	-2.90695	-2.25509	1.74856
H	-1.43836	-3.30248	3.43878
C	0.71976	-0.67128	-0.77407
H	0.25063	-1.00774	-1.70177
N	2.14971	-0.90348	-0.91506
C	2.62663	-1.99403	-1.58675
C	3.22024	-0.16172	-0.44676
C	4.00348	-1.97282	-1.55974
H	1.93843	-2.69069	-2.04140
C	4.37519	-0.81062	-0.84582
H	5.36872	-0.45554	-0.62293
H	4.65619	-2.70314	-2.01187
C	3.20220	1.07744	0.39526
C	2.01609	1.41632	1.16510
H	1.49449	0.55196	1.57785
H	2.25704	2.14717	1.93777
O	4.22458	1.76406	0.37494
I	-2.61304	-0.71389	-0.88148
H	1.15950	1.96098	0.38952
O	0.16129	2.43707	-0.43774
C	-0.70095	3.28670	0.23773
C	0.03174	4.57926	0.64833
H	0.88339	4.33101	1.28834
H	0.41598	5.07784	-0.24604
H	-0.62095	5.27519	1.18757
C	-1.25724	2.60891	1.50806
H	-1.96461	3.25304	2.04266
H	-1.76861	1.68132	1.23176
H	-0.43840	2.35651	2.18820
C	-1.87873	3.65279	-0.67871
H	-1.49635	4.11994	-1.59066
H	-2.41672	2.74317	-0.96041
H	-2.58010	4.34298	-0.19540
H	0.50556	0.40098	-0.68318

Deprotonation of 6.1a – products 6.6 and *tert*-butanol in benzene

42
-876.9612529

C	-2.03379	-2.92336	1.78231
C	-1.04666	-2.58914	0.86355
C	-1.10570	-1.39774	0.13564
C	-2.19105	-0.55575	0.37328
C	-3.18914	-0.87298	1.28728
C	-3.10823	-2.06698	1.99517
H	-1.95862	-3.85176	2.33574
H	-0.20019	-3.24948	0.70726
H	-4.01766	-0.19495	1.44804
H	-3.88202	-2.31763	2.71110
C	-0.02566	-1.03867	-0.86766
H	-0.48026	-0.94134	-1.85823
H	0.40791	-0.06894	-0.62127
N	1.02404	-2.02983	-0.96392
C	0.91957	-3.10630	-1.81107
C	2.21235	-2.11285	-0.25679
C	2.03976	-3.88889	-1.66305
H	0.05850	-3.20748	-2.45431
C	2.85619	-3.25547	-0.69134
H	3.82397	-3.56540	-0.33113
H	2.24996	-4.79821	-2.20503
C	2.75937	-1.16867	0.79123
C	1.88534	-0.41997	1.56469
H	0.81808	-0.59305	1.57344
H	2.30729	0.16562	2.37514
O	4.02199	-1.16099	0.88040
I	-2.37679	1.29402	-0.67959
H	1.92454	1.12316	0.18165
O	1.80123	1.86799	-0.44849
C	2.08156	3.07913	0.24302
C	3.52418	3.05371	0.75056
H	3.66834	2.20857	1.42930
H	4.21246	2.93453	-0.08935
H	3.77054	3.97743	1.28195
C	1.10683	3.24715	1.41182
H	1.28293	4.19197	1.93431
H	0.07815	3.23372	1.04297
H	1.22657	2.42660	2.12371
C	1.88533	4.19736	-0.77356
H	2.56896	4.06158	-1.61481
H	0.86026	4.17844	-1.15252
H	2.07474	5.17295	-0.31827



6.1a *DMSO* **6.17**

Deprotonation of 6.1a – starting species 6.1a and KO^{t}Bu in DMSO

43
-1476.8805597

C	2.99260	3.09117	0.30629
C	1.77409	2.60178	-0.14970
C	1.56689	1.23348	-0.34423
C	2.63292	0.37619	-0.06828
C	3.85940	0.84823	0.38589
C	4.03708	2.21470	0.57661
H	3.12341	4.15670	0.45115
H	0.96311	3.29269	-0.35462
H	4.66819	0.15894	0.59302
H	4.98965	2.58491	0.93600
C	0.23890	0.70540	-0.84491
H	0.33094	0.43854	-1.90144
H	-0.09460	-0.19914	-0.33171
N	-0.83132	1.69123	-0.75556
C	-1.26080	2.40364	-1.83278
C	-1.48578	2.15428	0.37703
C	-2.21575	3.31691	-1.42423
H	-0.85219	2.20398	-2.81191
C	-2.35107	3.16182	-0.03176
H	-3.00830	3.70254	0.63079
H	-2.74314	4.00733	-2.06272
C	-1.35501	1.68906	1.77753
C	-0.48007	0.52331	2.13665
H	0.56807	0.73940	1.91492
H	-0.58994	0.32750	3.20222
O	-2.01063	2.26729	2.63021
I	2.42185	-1.73049	-0.33134
H	-0.79997	-0.34535	1.54695
K	-3.58614	0.31131	-1.01592
O	-1.92862	-1.30645	-0.07269
C	-2.23009	-2.59811	0.31063
C	-3.75891	-2.81164	0.35887
H	-4.20851	-2.08983	1.04930
H	-4.18860	-2.65414	-0.63695
H	-4.03514	-3.81902	0.68810
C	-1.66135	-2.90621	1.71170
H	-1.88061	-3.92989	2.03437
H	-0.57472	-2.76981	1.70470
H	-2.08506	-2.21380	2.44617
C	-1.63862	-3.62260	-0.67942
H	-2.03503	-3.43610	-1.68247
H	-0.55057	-3.51118	-0.71615
H	-1.87172	-4.65690	-0.40237

Deprotonation of 6.1a – transition state in DMSO

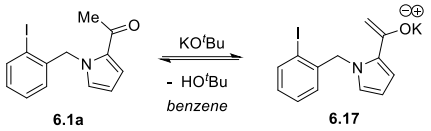
43
-1476.8690869

C	-2.56786	-3.30761	0.64319
C	-1.43416	-2.70114	0.11504
C	-1.41646	-1.33832	-0.19343
C	-2.58472	-0.61141	0.03769
C	-3.72697	-1.20108	0.56700
C	-3.71504	-2.55778	0.87375
H	-2.55210	-4.36566	0.87481
H	-0.54191	-3.29266	-0.05930
H	-4.61791	-0.61087	0.73992
H	-4.60256	-3.01904	1.28954
C	-0.17753	-0.68224	-0.77153
H	-0.36203	-0.41327	-1.81512
N	0.98402	-1.55991	-0.75946
C	1.36485	-2.25926	-1.87126
C	1.76433	-1.96354	0.31720
C	2.40782	-3.09838	-1.53987
H	0.85784	-2.10104	-2.81099
C	2.65457	-2.91203	-0.16164
H	3.40776	-3.39048	0.44376
H	2.92442	-3.76064	-2.21627
C	1.76942	-1.44287	1.72276
C	0.94129	-0.31644	2.08699
H	-0.08975	-0.34776	1.74287
H	1.01257	-0.09266	3.15020
O	2.62799	-1.92995	2.46977
I	-2.67849	1.46645	-0.43685
H	1.53772	0.60828	1.34878
K	3.56041	0.02389	-1.22165
O	2.20259	1.34032	0.47780
C	1.91231	2.71184	0.45752
C	3.19678	3.51193	0.71354
H	3.60581	3.25321	1.69419
H	3.94485	3.26542	-0.04629
H	3.01723	4.59124	0.68464
C	0.87718	3.05980	1.53812
H	0.63803	4.12722	1.52874
H	-0.04566	2.49633	1.37117
H	1.26244	2.79856	2.52804
C	1.34811	3.09551	-0.91869
H	2.08344	2.87689	-1.69973
H	0.44386	2.51545	-1.12516
H	1.09774	4.15975	-0.97469
H	0.07425	0.24035	-0.24774

Deprotonation of 6.1a – products 6.17 and *tert*-butanol in DMSO

43
-1476.8930435

C	-2.96084	-3.04404	1.01082
C	-1.82388	-2.55495	0.37817
C	-1.74772	-1.22894	-0.05459
C	-2.85587	-0.41336	0.17515
C	-4.00170	-0.88480	0.80515
C	-4.05229	-2.21006	1.22475
H	-2.99171	-4.07676	1.33658
H	-0.97265	-3.20798	0.21855
H	-4.84623	-0.22730	0.96808
H	-4.94346	-2.58151	1.71597
C	-0.50634	-0.70158	-0.75056
H	-0.76781	-0.38266	-1.76306
H	-0.12085	0.17582	-0.22809
N	0.54980	-1.68797	-0.86278
C	0.63560	-2.53610	-1.93682
C	1.55299	-1.99056	0.04217
C	1.69962	-3.38535	-1.74582
H	-0.06681	-2.44928	-2.75184
C	2.28327	-3.03367	-0.50270
H	3.14005	-3.48588	-0.02761
H	2.02176	-4.15842	-2.42582
C	1.87572	-1.31029	1.34398
C	0.91766	-0.62637	2.05174
H	-0.13251	-0.65781	1.80157
H	1.20400	-0.16017	2.98821
O	3.11608	-1.40284	1.67868
I	-2.83969	1.63040	-0.44238
H	1.92967	0.79065	0.64135
K	4.43165	-0.56019	-0.39826
O	2.45681	1.24655	-0.04132
C	2.38755	2.65734	0.21428
C	3.00747	2.94510	1.58049
H	2.45581	2.41873	2.36509
H	4.04652	2.60723	1.59987
H	2.98312	4.01488	1.80119
C	0.92466	3.09248	0.17971
H	0.83246	4.16707	0.35525
H	0.48343	2.85569	-0.79181
H	0.35366	2.56846	0.95306
C	3.18335	3.32648	-0.89657
H	4.21826	2.97560	-0.88525
H	2.74469	3.09392	-1.86960
H	3.18348	4.41039	-0.76395



6.1a **6.17**

Deprotonation of 6.1a – starting species 6.1a and KO^{t}Bu in benzene

43
-1476.8655305

C	-2.77192	-3.27213	0.02960
C	-1.57793	-2.66482	-0.33941
C	-1.46042	-1.27384	-0.41514
C	-2.59263	-0.51631	-0.10978
C	-3.79514	-1.10849	0.25949
C	-3.88315	-2.49414	0.33132
H	-2.83066	-4.35244	0.08318
H	-0.71493	-3.28075	-0.56966
H	-4.65540	-0.49441	0.49425
H	-4.81782	-2.95659	0.62465
C	-0.15708	-0.62125	-0.82804
H	-0.22578	-0.29066	-1.86841
H	0.10301	0.26892	-0.25227
N	0.97121	-1.54298	-0.75424
C	1.47945	-2.16983	-1.85020
C	1.58582	-2.05126	0.37742
C	2.44465	-3.07682	-1.44929
H	1.10537	-1.92832	-2.83352
C	2.50361	-3.00549	-0.04286
H	3.13761	-3.56704	0.62545
H	3.01910	-3.71740	-2.09967
C	1.39350	-1.65692	1.79984
C	0.48931	-0.52046	2.17933
H	-0.54673	-0.73506	1.90480
H	0.55523	-0.37834	3.25663
O	2.03495	-2.26410	2.63704
I	-2.52796	1.61153	-0.19130
H	0.82217	0.37827	1.64458
K	3.75418	-0.19431	-0.67866
O	1.99216	1.31562	-0.01090
C	2.01282	2.68596	0.14769
C	3.46592	3.20069	0.24050
H	3.97266	2.71532	1.08160
H	4.00533	2.95382	-0.68186
H	3.52579	4.28500	0.38276
C	1.27197	3.09813	1.43493
H	1.26724	4.18259	1.58832
H	0.23542	2.75010	1.38445
H	1.74741	2.62696	2.30110
C	1.33279	3.37988	-1.04911
H	1.86337	3.12233	-1.97161
H	0.30410	3.01914	-1.13754
H	1.31547	4.47099	-0.95096

Deprotonation of 6.1a – transition state in benzene

43
-1476.8560457

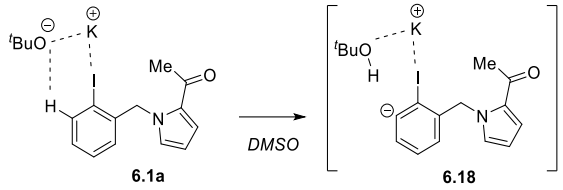
C	2.09652	2.65334	2.21905
C	1.16452	2.35845	1.23231
C	1.34008	1.27858	0.36248
C	2.49812	0.51426	0.51355
C	3.44225	0.79754	1.49453
C	3.23667	1.87033	2.35398
H	1.93020	3.49537	2.87981
H	0.27731	2.97418	1.12699
H	4.33358	0.18972	1.58326
H	3.97176	2.09084	3.11864
C	0.30186	0.95900	-0.69711
H	0.80100	0.75475	-1.64634
N	-0.63445	2.04739	-0.92813
C	-0.33958	3.07903	-1.77214
C	-1.91987	2.21980	-0.44443
C	-1.42009	3.93100	-1.83697
H	0.61582	3.11157	-2.27373
C	-2.42153	3.38031	-1.00763
H	-3.40606	3.77201	-0.80678
H	-1.47597	4.83515	-2.42203
C	-2.64113	1.38280	0.54537
C	-1.93812	0.49991	1.44806
H	-0.90806	0.76060	1.67508
H	-2.52193	0.30907	2.34891
O	-3.88529	1.43002	0.50991
I	2.92323	-1.11913	-0.79373
H	-1.98229	-0.63519	0.80826
K	-4.64268	-1.03584	0.08312
O	-2.26875	-1.75391	0.12468
C	-1.35067	-2.80312	0.24772
C	-2.09168	-4.07991	0.66902
H	-2.57736	-3.92449	1.63686
H	-2.86105	-4.31958	-0.07132
H	-1.41614	-4.93683	0.75369
C	-0.29140	-2.47064	1.31223
H	0.43486	-3.28152	1.41907
H	0.25680	-1.56135	1.04750
H	-0.77267	-2.30287	2.28041
C	-0.66438	-3.04461	-1.10348
H	-1.41321	-3.31860	-1.85217
H	-0.16685	-2.13049	-1.43682
H	0.08323	-3.84246	-1.04654
H	-0.25885	0.05800	-0.43341

Deprotonation of 6.1a – products 6.17 and *tert*-butanol in benzene

43
-1476.8753977

C	-2.87504	-3.03826	1.12095
C	-1.75486	-2.54210	0.46570
C	-1.71551	-1.22900	-0.00862
C	-2.84131	-0.43438	0.20409
C	-3.97104	-0.91357	0.85594
C	-3.98510	-2.22553	1.31682
H	-2.87655	-4.05988	1.48087
H	-0.88679	-3.17673	0.32361
H	-4.82994	-0.27151	1.00408
H	-4.86300	-2.60327	1.82688
C	-0.48928	-0.69187	-0.72335
H	-0.77124	-0.35504	-1.72456
H	-0.09034	0.17344	-0.19050
N	0.56189	-1.67755	-0.87244
C	0.61490	-2.52508	-1.94976
C	1.58319	-1.98757	0.00772
C	1.67817	-3.38030	-1.78634
H	-0.11034	-2.43596	-2.74419
C	2.29396	-3.03436	-0.55673
H	3.14464	-3.50407	-0.08737
H	1.97291	-4.15970	-2.47136
C	1.94701	-1.31355	1.30454
C	1.02088	-0.61204	2.03611
H	-0.03846	-0.64375	1.82811
H	1.34100	-0.18301	2.97914
O	3.19423	-1.42168	1.59894
I	-2.88343	1.58853	-0.47933
H	2.11297	0.83061	0.77011
K	4.40094	-0.57347	-0.42901
O	2.65529	1.32088	0.11914
C	2.36211	2.71845	0.24929
C	2.82161	3.19758	1.62502
H	2.29364	2.64980	2.41046
H	3.89377	3.02629	1.74589
H	2.62024	4.26392	1.75272
C	0.85960	2.92887	0.08068
H	0.60326	3.98883	0.15283
H	0.53015	2.55493	-0.89224
H	0.31134	2.39128	0.86076
C	3.13773	3.41573	-0.85911
H	4.20869	3.22755	-0.74786
H	2.81445	3.04690	-1.83535
H	2.97178	4.49441	-0.82191

Scheme 6.2



6.1a 6.18

Benzyne formation – starting species 6.1a and KO^{t}Bu in DMSO

43
-1476.8731516

C	-0.67449	2.75628	-0.42616
C	-1.68164	1.81817	-0.62197
C	-1.39262	0.45361	-0.70260
C	-0.05554	0.07237	-0.58163
C	0.96975	0.98965	-0.38285
C	0.64685	2.34278	-0.30475
H	-0.92600	3.80848	-0.36862
H	-2.71107	2.14809	-0.71349
H	2.00837	0.65795	-0.28937
H	1.43645	3.07000	-0.15135
C	-2.49906	-0.55905	-0.93123
H	-2.47909	-0.89888	-1.96957
H	-2.34912	-1.44269	-0.31481
N	-3.82555	-0.01266	-0.68849
C	-4.62598	0.41655	-1.70131
C	-4.38399	0.38682	0.51857
C	-5.72180	1.07063	-1.17247
H	-4.34972	0.22617	-2.72739
C	-5.56523	1.05376	0.22518
H	-6.23590	1.45524	0.96863
H	-6.53550	1.49708	-1.73682
C	-3.88226	0.14553	1.88227
C	-2.72383	-0.78564	2.14624
H	-1.80096	-0.39684	1.70817
H	-2.59613	-0.87129	3.22352
O	-4.44374	0.69664	2.81558
I	0.49833	-1.99167	-0.70851
H	-2.91543	-1.77471	1.72470
O	3.97600	-0.00846	0.09901
C	4.78869	1.06840	-0.18692
C	4.61798	2.16699	0.88532
H	5.22619	3.05600	0.68518
H	3.56646	2.46944	0.93286
H	4.90153	1.77030	1.86619
C	4.44064	1.67882	-1.56113
H	3.40146	2.02203	-1.56734
H	5.08365	2.52809	-1.81720
H	4.55037	0.91541	-2.33766
C	6.27323	0.65075	-0.21287
H	6.94185	1.49140	-0.42952
H	6.55258	0.22707	0.75697
H	6.42503	-0.11759	-0.97736
K	2.93316	-0.84513	2.17672

Benzyne formation – transition state in DMSO

43
-1476.8560648

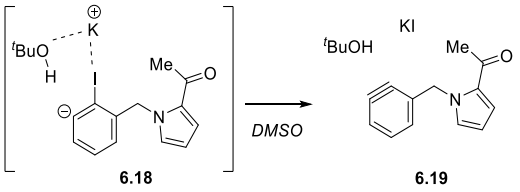
C	-0.52224	2.72389	-0.54108
C	-1.53972	1.79061	-0.72195
C	-1.25405	0.42414	-0.72744
C	0.08793	0.07162	-0.54975
C	1.14740	0.93524	-0.36031
C	0.78910	2.29653	-0.36000
H	-0.76292	3.78184	-0.53931
H	-2.56392	2.12282	-0.85666
H	2.51379	0.52719	-0.19922
H	1.56277	3.04834	-0.21566
C	-2.35862	-0.59586	-0.92768
H	-2.31732	-0.99635	-1.94345
H	-2.22836	-1.44249	-0.25805
N	-3.69120	-0.03583	-0.74796
C	-4.46948	0.33113	-1.80031
C	-4.28216	0.42043	0.42199
C	-5.58392	1.00248	-1.33364
H	-4.16682	0.08811	-2.80766
C	-5.46182	1.06037	0.06609
H	-6.15325	1.49401	0.77160
H	-6.38694	1.38972	-1.93995
C	-3.80946	0.25797	1.80710
C	-2.64847	-0.64533	2.14670
H	-1.72169	-0.27882	1.69754
H	-2.53798	-0.66362	3.22909
O	-4.39732	0.85143	2.69792
I	0.57181	-2.07649	-0.56551
H	-2.82785	-1.65986	1.78409
O	3.60719	0.11525	0.03548
C	4.61365	1.06354	-0.23121
C	4.58927	2.16580	0.83757
H	5.35015	2.92960	0.65160
H	3.60936	2.65208	0.85409
H	4.77406	1.73249	1.82533
C	4.40404	1.68981	-1.61688
H	3.44552	2.21420	-1.65906
H	5.19889	2.40309	-1.85310
H	4.40028	0.90774	-2.38134
C	5.96659	0.35026	-0.19466
H	6.78972	1.04655	-0.38075
H	6.11734	-0.11223	0.78469
H	5.99549	-0.43468	-0.95512
K	2.40816	-0.53864	2.22339

Benzyne formation – product 6.18 in DMSO

43

-1476.8579160

C	-0.50431	2.73422	-0.08616
C	-1.52135	1.84009	-0.41436
C	-1.24270	0.47995	-0.55945
C	0.09188	0.11051	-0.36154
C	1.15585	0.91444	-0.03740
C	0.79612	2.27379	0.09865
H	-0.73729	3.78859	0.02362
H	-2.53614	2.19747	-0.55568
H	2.84821	0.41511	-0.14661
H	1.56262	3.00514	0.35296
C	-2.33688	-0.50437	-0.92366
H	-2.20800	-0.83940	-1.95567
H	-2.27851	-1.39632	-0.30394
N	-3.67492	0.06446	-0.83006
C	-4.33462	0.53573	-1.92056
C	-4.39160	0.41133	0.30688
C	-5.49456	1.16994	-1.51645
H	-3.92396	0.38612	-2.90779
C	-5.52697	1.09203	-0.11321
H	-6.28985	1.46580	0.55147
H	-6.22642	1.62117	-2.16711
C	-4.06782	0.12770	1.71493
C	-2.90834	-0.75888	2.09970
H	-1.96154	-0.35267	1.73580
H	-2.87951	-0.82785	3.18527
O	-4.77681	0.61019	2.58451
I	0.54823	-2.06175	-0.61945
H	-3.03573	-1.75924	1.67916
O	3.80621	0.04365	-0.11275
C	4.73168	1.11415	-0.28104
C	4.69866	2.01978	0.95350
H	5.38799	2.86088	0.84307
H	3.69049	2.41705	1.10262
H	4.98771	1.45519	1.84455
C	4.36954	1.91915	-1.53118
H	3.37695	2.36456	-1.42114
H	5.09349	2.72069	-1.69890
H	4.36164	1.26697	-2.40819
C	6.11080	0.48418	-0.43720
H	6.87741	1.25411	-0.55519
H	6.35293	-0.11597	0.44356
H	6.12977	-0.16466	-1.31618
K	2.53097	-0.73445	2.13646



6.18 6.19

CI bond cleavage 6.18 – transition state in DMSO

43

-1476.8462671

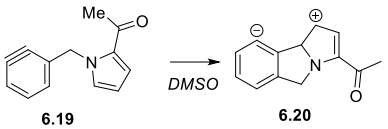
C	0.68040	-2.98420	-0.71942
C	1.65163	-1.98216	-0.85283
C	1.32378	-0.61631	-0.82083
C	-0.03715	-0.48877	-0.64475
C	-1.00144	-1.30853	-0.51639
C	-0.67053	-2.67785	-0.54749
H	0.99433	-4.02208	-0.75115
H	2.69412	-2.25932	-0.98211
H	-2.90698	-0.48009	-0.42882
H	-1.40677	-3.46828	-0.44441
C	2.33776	0.48939	-0.97154
H	2.30495	0.88310	-1.98951
H	2.08855	1.31720	-0.31312
N	3.69712	0.02810	-0.73161
C	4.55034	-0.26881	-1.74853
C	4.25690	-0.41066	0.46044
C	5.68139	-0.87312	-1.23443
H	4.28330	-0.02947	-2.76681
C	5.49222	-0.96526	0.15640
H	6.17570	-1.36363	0.88991
H	6.53935	-1.19356	-1.80357
C	3.70880	-0.29035	1.82195
C	2.50766	0.57634	2.11400
H	1.60802	0.17592	1.63908
H	2.35939	0.59973	3.19178
O	4.26904	-0.88144	2.73146
I	-0.66366	2.37522	-0.51458
H	2.66250	1.59263	1.74526
O	-3.72955	-0.12639	-0.04063
C	-4.73027	-1.15655	-0.12646
C	-4.41771	-2.24989	0.89422
H	-5.14509	-3.06220	0.82533
H	-3.42108	-2.66363	0.71566
H	-4.45208	-1.84529	1.90913
C	-4.73453	-1.72829	-1.54180
H	-3.76897	-2.19222	-1.76736
H	-5.51178	-2.48805	-1.64933
H	-4.91771	-0.93434	-2.26933
C	-6.05433	-0.47897	0.19460
H	-6.86821	-1.20690	0.17673
H	-6.01391	-0.02620	1.18811
H	-6.26593	0.30236	-0.53848
K	-2.06962	0.46462	2.04148

CI bond cleavage 6.18 – product 6.19, KI and *tert*-butanol in DMSO

43

-1476.8508356

C	1.95681	1.64693	2.74714
C	2.34921	0.67198	1.81448
C	1.49113	-0.35613	1.37667
C	0.26539	-0.20509	1.99851
C	-0.11765	0.63909	2.82883
C	0.67559	1.67264	3.31746
H	2.67497	2.40664	3.03695
H	3.35941	0.70659	1.41525
H	-1.64835	0.82110	0.52838
H	0.37825	2.42450	4.03705
C	1.90704	-1.45420	0.43048
H	2.18902	-2.33964	1.00431
H	1.06901	-1.74501	-0.19890
N	3.06686	-1.07626	-0.36658
C	4.33036	-1.45848	-0.03111
C	3.14780	-0.06716	-1.31459
C	5.23943	-0.73623	-0.77870
H	4.48443	-2.21166	0.72689
C	4.49165	0.14580	-1.58244
H	4.86262	0.84557	-2.31524
H	6.31144	-0.84808	-0.74908
C	2.03504	0.60894	-2.00082
C	0.65102	0.00968	-1.99786
H	0.18049	0.10610	-1.01451
H	0.04385	0.54951	-2.72372
O	2.26053	1.63812	-2.61732
I	-1.86645	-2.31136	0.38187
H	0.68193	-1.05162	-2.25433
O	-2.07256	1.32339	-0.18223
C	-1.75013	2.72198	-0.05807
C	-0.23848	2.90823	-0.16790
H	0.02674	3.95742	-0.01574
H	0.28109	2.31282	0.58941
H	0.11449	2.60354	-1.15559
C	-2.27466	3.24316	1.27706
H	-1.78323	2.73118	2.10843
H	-2.08049	4.31395	1.37213
H	-3.35148	3.07460	1.34934
C	-2.46157	3.40051	-1.22038
H	-2.26638	4.47458	-1.20795
H	-2.10383	2.99615	-2.17100
H	-3.54078	3.24316	-1.15067
K	-3.37479	-0.17776	-1.91160



6.19 **6.20**

Cyclisation of 6.19 – starting species 6.19 in DMSO

26

-631.7536745

C	-3.01287	-1.27646	-0.51769
C	-1.85308	-1.13014	0.26223
C	-1.37796	0.11691	0.70491
C	-2.21787	1.13823	0.26880
C	-3.23298	0.97641	-0.42418
C	-3.79910	-0.18186	-0.91685
H	-3.31741	-2.27149	-0.82319
H	-1.30519	-2.02401	0.54265
H	-4.69391	-0.28250	-1.51428
C	-0.12786	0.29048	1.52861
H	-0.30079	1.00745	2.33102
H	0.16472	-0.65277	1.98126
N	0.96869	0.81642	0.71169
C	1.06354	2.15168	0.45138
C	1.71814	0.13084	-0.23404
C	1.90419	2.34983	-0.62395
H	0.50515	2.85940	1.04563
C	2.31083	1.07228	-1.06023
H	3.00823	0.83645	-1.84914
H	2.20151	3.30468	-1.02709
C	2.01950	-1.30928	-0.26887
C	1.91824	-2.14882	0.98423
H	0.91164	-2.56216	1.08422
H	2.61058	-2.98354	0.88577
O	2.42566	-1.80643	-1.30577
H	2.15301	-1.57574	1.88144

Cyclisation of 6.19 – transition state in DMSO

26

-631.7310143

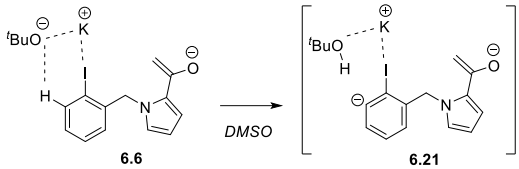
C	-3.51929	-1.07893	-0.61996
C	-2.35453	-1.61168	-0.04649
C	-1.34671	-0.75188	0.37484
C	-1.62566	0.59220	0.16395
C	-2.66950	1.16721	-0.33876
C	-3.69214	0.30019	-0.77411
H	-4.29982	-1.75685	-0.95086
H	-2.23820	-2.68446	0.06542
H	-4.61227	0.66726	-1.21986
C	-0.01640	-1.06931	1.01909
H	-0.12167	-1.30425	2.08064
H	0.49908	-1.88785	0.52409
N	0.72969	0.18819	0.86528
C	-0.03795	1.35344	1.01324
C	1.71981	0.43397	-0.02912
C	0.62150	2.36790	0.28215
H	-0.56613	1.50387	1.94721
C	1.69337	1.79030	-0.38068
H	2.40791	2.26471	-1.03444
H	0.32257	3.40500	0.26071
C	2.73885	-0.54281	-0.49987
C	3.02939	-1.78066	0.31007
H	2.52398	-2.63653	-0.14582
H	4.10166	-1.96839	0.26587
O	3.36522	-0.28125	-1.50540
H	2.70892	-1.68938	1.34713

Cyclisation of 6.19 – product 6.20 in DMSO

26

-631.7485995

C	-3.66122	-0.98075	-0.55156
C	-2.47591	-1.63265	-0.20195
C	-1.41511	-0.83381	0.19083
C	-1.56600	0.56068	0.22648
C	-2.71139	1.28523	-0.09927
C	-3.75646	0.41513	-0.50187
H	-4.51535	-1.57149	-0.87014
H	-2.38882	-2.71264	-0.24388
H	-4.71613	0.84028	-0.79659
C	-0.02704	-1.27683	0.61276
H	0.00453	-1.70057	1.61956
H	0.44684	-1.96145	-0.08741
N	0.67351	0.02484	0.60782
C	-0.25746	1.14055	0.77759
C	1.77477	0.43365	0.05036
C	0.48856	2.27750	0.19235
H	-0.36794	1.32911	1.85877
C	1.71593	1.85951	-0.18393
H	2.52673	2.42944	-0.60952
H	0.10216	3.28605	0.16309
C	2.94532	-0.44429	-0.35214
C	3.13576	-1.77356	0.31330
H	2.64342	-2.54486	-0.28609
H	4.20092	-1.99700	0.34013
O	3.68678	0.00498	-1.18741
H	2.71636	-1.79277	1.31883



6.6 6.21

Benzyne formation – starting species 6.6 and KO^{t}Bu in DMSO

42
-1476.3702982

C	0.68359	-2.62655	-0.97128
C	1.70437	-1.68371	-0.97059
C	1.43337	-0.31930	-0.83165
C	0.09609	0.05300	-0.69931
C	-0.94507	-0.86901	-0.68538
C	-0.63831	-2.22067	-0.82392
H	0.92304	-3.67753	-1.08137
H	2.73666	-2.00311	-1.07055
H	-1.98133	-0.54777	-0.55257
H	-1.43982	-2.95108	-0.81554
C	2.56298	0.69262	-0.84567
H	2.63537	1.15305	-1.83497
H	2.35528	1.48250	-0.12998
N	3.85231	0.09288	-0.54985
C	4.76621	-0.22625	-1.52606
C	4.21082	-0.52117	0.63439
C	5.73829	-1.02215	-0.96843
H	4.63828	0.14041	-2.53301
C	5.38079	-1.21451	0.39431
H	5.92300	-1.77898	1.13743
H	6.60662	-1.41004	-1.47845
C	3.44274	-0.44173	1.92999
C	2.97081	0.78527	2.32836
H	2.43121	0.87857	3.26489
O	3.33158	-1.54788	2.57103
I	-0.43935	2.12085	-0.51434
H	3.18785	1.68696	1.77094
O	-3.93315	0.01263	0.18001
C	-4.74781	-1.03392	-0.19771
C	-4.46074	-2.27700	0.67273
H	-5.06771	-3.14442	0.39067
H	-3.40387	-2.54915	0.58248
H	-4.66161	-2.04383	1.72388
C	-4.51571	-1.41899	-1.67481
H	-3.47603	-1.72574	-1.82531
H	-5.16525	-2.23940	-1.99909
H	-4.70885	-0.55132	-2.31362
C	-6.23648	-0.66607	-0.03225
H	-6.90501	-1.48625	-0.31683
H	-6.43608	-0.40387	1.01148
H	-6.47186	0.20365	-0.65359
K	-2.59283	0.53974	2.18040

Benzyne formation – transition state in DMSO

42
-1476.3517258

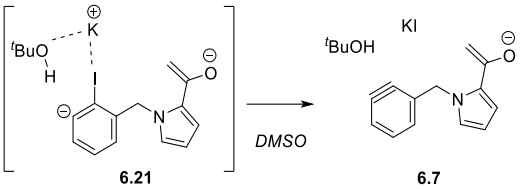
C	0.55168	-2.65323	-0.71792
C	1.56919	-1.70605	-0.79970
C	1.27995	-0.34296	-0.71019
C	-0.06974	-0.01448	-0.54975
C	-1.13193	-0.88881	-0.45076
C	-0.76687	-2.24569	-0.53944
H	0.79725	-3.70800	-0.78777
H	2.60068	-2.01958	-0.92370
H	-2.51040	-0.49049	-0.25878
H	-1.53983	-3.00906	-0.46790
C	2.38330	0.69356	-0.80107
H	2.33513	1.20361	-1.76734
H	2.24009	1.44440	-0.02964
N	3.71402	0.12199	-0.68029
C	4.48643	-0.18510	-1.77433
C	4.25535	-0.46911	0.44405
C	5.54995	-0.95026	-1.35742
H	4.20376	0.16524	-2.75520
C	5.39710	-1.13583	0.04389
H	6.05176	-1.68099	0.70671
H	6.34520	-1.32147	-1.98547
C	3.68276	-0.40183	1.83750
C	3.24454	0.81446	2.30163
H	2.84262	0.89768	3.30576
O	3.69667	-1.50793	2.48898
I	-0.56783	2.13476	-0.44844
H	3.35130	1.71857	1.71697
O	-3.59238	-0.10225	0.02022
C	-4.59252	-1.05037	-0.27263
C	-4.52512	-2.20784	0.73420
H	-5.28184	-2.97063	0.52834
H	-3.53937	-2.68066	0.69586
H	-4.68707	-1.83040	1.74848
C	-4.40884	-1.59786	-1.69465
H	-3.44363	-2.10303	-1.78792
H	-5.19851	-2.31070	-1.94904
H	-4.43647	-0.77622	-2.41587
C	-5.95300	-0.35953	-0.16448
H	-6.77136	-1.05695	-0.36680
H	-6.08521	0.04905	0.84110
H	-6.01178	0.46377	-0.88135
K	-2.30070	0.37402	2.21663

Benzyne formation – product 6.21

42

-1476.3532145

C	-0.51262	2.70532	-0.21595
C	-1.53955	1.78997	-0.44011
C	-1.26108	0.42484	-0.53063
C	0.08612	0.07854	-0.38538
C	1.16093	0.89925	-0.15651
C	0.79967	2.26287	-0.07426
H	-0.74703	3.76339	-0.15080
H	-2.56534	2.12942	-0.54199
H	2.83792	0.40189	-0.19328
H	1.57276	3.01039	0.10169
C	-2.36511	-0.58666	-0.77601
H	-2.22059	-1.06521	-1.74821
H	-2.31566	-1.36437	-0.01818
N	-3.69362	0.00253	-0.77410
C	-4.27323	0.49701	-1.91780
C	-4.39175	0.45907	0.32673
C	-5.36838	1.24850	-1.56402
H	-3.84527	0.27525	-2.88363
C	-5.43688	1.23008	-0.14382
H	-6.17849	1.70383	0.48114
H	-6.04437	1.74043	-2.24658
C	-4.06604	0.15794	1.76787
C	-3.75863	-1.13701	2.10673
H	-3.54320	-1.38866	3.13982
O	-4.15302	1.15691	2.56943
I	0.54516	-2.10920	-0.57079
H	-3.79208	-1.93775	1.37954
O	3.80017	0.03678	-0.09466
C	4.72921	1.10397	-0.25684
C	4.63103	2.05819	0.93732
H	5.31689	2.90189	0.82473
H	3.61341	2.44949	1.02510
H	4.88522	1.53337	1.86273
C	4.43037	1.85757	-1.55497
H	3.43146	2.30056	-1.51490
H	5.15903	2.65608	-1.71682
H	4.47077	1.17091	-2.40433
C	6.11770	0.47753	-0.31575
H	6.88609	1.24717	-0.42450
H	6.31567	-0.08459	0.60041
H	6.18584	-0.20644	-1.16511
K	2.44586	-0.64099	2.13820



CI bond cleavage 6.18 – transition state in DMSO

42

-1476.3437007

C	0.68858	-2.87018	-0.73413
C	1.66660	-1.87105	-0.81957
C	1.34422	-0.50676	-0.73441
C	-0.01851	-0.37650	-0.57039
C	-1.00517	-1.19029	-0.47857
C	-0.65957	-2.55723	-0.55930
H	0.99428	-3.90887	-0.80368
H	2.71125	-2.14191	-0.94469
H	-2.87983	-0.46875	-0.39995
H	-1.39961	-3.34921	-0.49049
C	2.36860	0.59646	-0.82866
H	2.29673	1.08048	-1.80582
H	2.15047	1.34758	-0.07630
N	3.72610	0.10223	-0.67983
C	4.53300	-0.16739	-1.75967
C	4.27403	-0.46333	0.45544
C	5.62355	-0.88022	-1.32208
H	4.25249	0.16997	-2.74564
C	5.45343	-1.07393	0.07628
H	6.12230	-1.58611	0.75105
H	6.44840	-1.21128	-1.93427
C	3.67382	-0.42072	1.83806
C	3.15088	0.76905	2.28244
H	2.72904	0.83562	3.27953
O	3.74648	-1.51800	2.50019
I	-0.64425	2.39373	-0.43926
H	3.20926	1.67300	1.69076
O	-3.74228	-0.13029	-0.07759
C	-4.70014	-1.19353	-0.20824
C	-4.42053	-2.25839	0.85206
H	-5.12057	-3.09208	0.75851
H	-3.40424	-2.64720	0.74071
H	-4.52649	-1.83383	1.85387
C	-4.59327	-1.79257	-1.60896
H	-3.60047	-2.22756	-1.76105
H	-5.33818	-2.57902	-1.75000
H	-4.75350	-1.01893	-2.36346
C	-6.06641	-0.55964	0.01030
H	-6.85162	-1.31611	-0.05493
H	-6.11329	-0.09356	0.99739
H	-6.25273	0.20506	-0.74699
K	-2.13279	0.45596	2.05898

CI bond cleavage 6.18 – product 6.7, KI and *tert*-butanol in DMSO

42

-1476.3410468

C	-1.31533	3.15966	-1.08685
C	-2.08264	1.98407	-1.09054
C	-1.51779	0.69785	-0.97151
C	-0.15252	0.84781	-0.85559
C	0.58659	1.85261	-0.85553
C	0.08280	3.14927	-0.95546
H	-1.82643	4.11227	-1.18034
H	-3.16459	2.05631	-1.16956
H	2.65914	0.29967	-0.39226
H	0.66777	4.06065	-0.94821
C	-2.32659	-0.57271	-0.96589
H	-2.40483	-0.96310	-1.98351
H	-1.81176	-1.31835	-0.36838
N	-3.68451	-0.34628	-0.49075
C	-4.75456	-0.25123	-1.34911
C	-4.05062	0.13501	0.75170
C	-5.82678	0.25807	-0.65697
H	-4.65279	-0.55142	-2.38074
C	-5.37612	0.51296	0.66750
H	-5.95389	0.90552	1.49037
H	-6.81653	0.41988	-1.05566
C	-3.16469	0.21046	1.96847
C	-2.33032	-0.84763	2.23344
H	-1.70034	-0.82803	3.11682
O	-3.31269	1.26334	2.68784
I	1.07399	-2.34724	-0.74223
H	-2.32218	-1.73727	1.61820
O	3.40997	0.28277	0.21855
C	4.23240	1.44818	0.02346
C	3.64926	2.61707	0.81392
H	4.25161	3.51669	0.66733
H	2.62702	2.82301	0.48999
H	3.63195	2.37865	1.88039
C	4.29692	1.77372	-1.46572
H	3.30117	2.02075	-1.84709
H	4.95227	2.62939	-1.64128
H	4.68286	0.91748	-2.02388
C	5.60722	1.07167	0.56025
H	6.28803	1.92282	0.49182
H	5.53120	0.77200	1.60825
H	6.02381	0.24059	-0.01255
K	2.14658	-0.92103	2.24050

6.7 **6.22**

Cyclisation of 6.7 – starting species 6.7 in DMSO

25

-631.2564870

C	3.32120	-0.97214	-0.60505
C	2.18469	-1.44545	0.07174
C	1.20448	-0.57879	0.59012
C	1.58129	0.71539	0.31525
C	2.55163	1.22889	-0.28925
C	3.54856	0.39469	-0.81340
H	4.03949	-1.69206	-0.98328
H	2.04995	-2.51493	0.20367
H	4.42771	0.73969	-1.34526
C	-0.03663	-1.04047	1.29924
H	0.04744	-2.10396	1.52074
H	-0.14510	-0.50902	2.24273
N	-1.23637	-0.87408	0.47916
C	-1.95587	-1.94860	0.01793
C	-1.70911	0.28119	-0.11494
C	-2.91062	-1.49417	-0.86102
H	-1.71456	-2.94720	0.34797
C	-2.74564	-0.08723	-0.95155
H	-3.32446	0.60434	-1.54403
H	-3.63756	-2.10432	-1.37444
C	-1.20868	1.68149	0.11585
C	-0.79957	2.03543	1.38811
H	-0.44727	3.04416	1.57094
O	-1.23241	2.45014	-0.90092
H	-0.93594	1.37936	2.23601

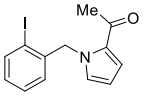
Cyclisation of 6.7 – products 6.22 in DMSO

25

-631.3484140

C	3.23835	-1.07105	-0.69639
C	2.09876	-1.58257	-0.08121
C	1.16739	-0.69727	0.45654
C	1.39006	0.68878	0.37501
C	2.52023	1.26777	-0.24261
C	3.42291	0.31240	-0.76558
H	3.97358	-1.75100	-1.11856
H	1.93088	-2.65360	-0.01922
H	4.33254	0.65638	-1.26032
C	-0.07880	-1.22839	1.12099
H	-0.05025	-2.31626	1.17857
H	-0.17689	-0.84396	2.14044
N	-1.29650	-0.88355	0.37603
C	-2.22725	-1.79045	-0.00959
C	-1.67566	0.36705	-0.07775
C	-3.22802	-1.14234	-0.71593
H	-2.10783	-2.83368	0.23969
C	-2.87714	0.21831	-0.75988
H	-3.42016	1.02586	-1.22583
H	-4.09962	-1.60987	-1.14567
C	-0.94095	1.61902	0.14497
C	0.32176	1.59748	0.97667
H	0.69892	2.61716	1.02257
O	-1.35597	2.65785	-0.34837
H	0.05216	1.27856	1.99160

Table 6.4 and 6.5

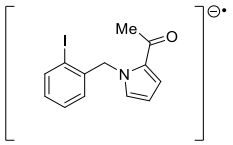


Neutral 6.1a in DMSO

28

-643.8557281

C	0.18047	3.09141	0.31026
C	0.72224	1.91757	-0.19970
C	-0.05597	0.76760	-0.35478
C	-1.39882	0.84048	0.01795
C	-1.95619	2.00733	0.52890
C	-1.15932	3.13741	0.67688
H	0.80720	3.96787	0.42030
H	1.76920	1.88943	-0.48304
H	-3.00081	2.03568	0.81181
H	-1.59042	4.04645	1.07837
C	0.54449	-0.50397	-0.92371
H	0.20556	-1.37489	-0.36709
H	0.20320	-0.64297	-1.95219
N	1.99817	-0.47976	-0.95516
C	2.88474	-0.52587	0.11295
C	2.69008	-0.16022	-2.08201
C	4.14855	-0.24928	-0.38953
C	4.02902	-0.02123	-1.77226
H	2.17213	-0.05099	-3.02279
H	5.04855	-0.24225	0.20522
H	4.81811	0.20689	-2.47062
C	2.60125	-0.83247	1.52534
C	1.24508	-1.32147	1.97376
H	0.96176	-2.22832	1.43507
H	1.29789	-1.53773	3.03880
O	3.50071	-0.70624	2.34069
I	-2.67955	-0.85625	-0.17130
H	0.47694	-0.56326	1.80143

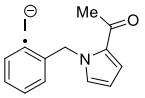


Product A18 in DMSO

28

-643.9298114

C	0.35162	3.00643	0.41367
C	0.82908	1.82249	-0.13577
C	-0.00778	0.71702	-0.32040
C	-1.33922	0.85266	0.06812
C	-1.83643	2.02848	0.62075
C	-0.98173	3.11123	0.79566
H	1.02324	3.84641	0.54479
H	1.87063	1.73919	-0.42789
H	-2.87646	2.10015	0.91227
H	-1.36305	4.02904	1.22705
C	0.53234	-0.56336	-0.93703
H	0.14328	-1.42124	-0.39304
H	0.15238	-0.65202	-1.95944
N	1.97555	-0.61415	-1.00096
C	2.85130	-0.57844	0.10601
C	2.64599	-0.13962	-2.12744
C	4.08697	-0.10265	-0.39035
C	3.94013	0.15508	-1.77581
H	2.13137	-0.07204	-3.07366
H	4.98362	-0.00315	0.20012
H	4.70606	0.50323	-2.45405
C	2.55608	-0.95218	1.44758
C	1.26588	-1.66110	1.82320
H	0.38139	-1.01000	1.80816
H	1.05017	-2.51875	1.17578
O	3.43339	-0.75799	2.37637
I	-2.72160	-0.76076	-0.18746
H	1.38065	-2.03399	2.84198

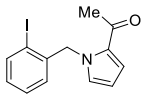


Radical anion A19 in DMSO

28

-643.9665259

C	1.61061	3.28725	0.44105
C	1.75340	2.03697	-0.15938
C	0.62506	1.28615	-0.50875
C	-0.60015	1.85200	-0.22662
C	-0.79512	3.07634	0.36547
C	0.34718	3.81050	0.70463
H	2.49453	3.85420	0.70800
H	2.74541	1.63763	-0.35100
H	-1.78794	3.46249	0.56816
H	0.24504	4.78188	1.17520
C	0.71973	-0.07087	-1.17583
H	-0.08498	-0.71316	-0.82199
H	0.58542	0.03802	-2.25394
N	2.02036	-0.70250	-0.98138
C	2.59246	-1.15269	0.20008
C	2.97907	-0.68168	-1.94603
C	3.92543	-1.43478	-0.06557
C	4.17052	-1.14312	-1.41973
H	2.73951	-0.32978	-2.93794
H	4.61727	-1.83654	0.65829
H	5.09643	-1.26054	-1.95958
C	1.93832	-1.36633	1.50217
C	0.43726	-1.34483	1.63081
H	0.03630	-0.34848	1.42834
H	-0.02447	-2.03378	0.92000
O	2.63630	-1.60308	2.47626
I	-3.21306	-0.69439	-0.16554
H	0.17380	-1.63667	2.64578

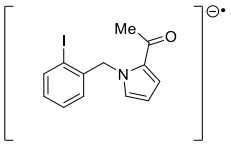


Neutral 6.1a in benzene

28

-643.8502505

C	0.18553	3.08508	0.30906
C	0.72554	1.90756	-0.19354
C	-0.05735	0.76107	-0.34803
C	-1.40133	0.84038	0.01797
C	-1.95672	2.01128	0.52064
C	-1.15580	3.13829	0.66758
H	0.81598	3.95857	0.42101
H	1.77445	1.87195	-0.46882
H	-3.00268	2.04373	0.79786
H	-1.58485	4.05078	1.06349
C	0.54055	-0.51605	-0.90721
H	0.20671	-1.37893	-0.33488
H	0.18626	-0.66938	-1.92965
N	1.99215	-0.49121	-0.95504
C	2.88893	-0.52629	0.10465
C	2.67241	-0.16776	-2.09006
C	4.14440	-0.24168	-0.40849
C	4.01111	-0.01726	-1.79172
H	2.14529	-0.06563	-3.02648
H	5.04645	-0.22608	0.18266
H	4.79300	0.21415	-2.49688
C	2.62205	-0.82680	1.52550
C	1.26975	-1.31788	1.99055
H	0.98426	-2.23013	1.46178
H	1.33850	-1.52641	3.05622
O	3.52730	-0.69384	2.32685
I	-2.68486	-0.85414	-0.16717
H	0.49659	-0.56373	1.82254

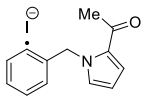


Radical anion A18 in benzene

28

-643.8897792

C	0.38728	2.98132	0.27210
C	0.84948	1.75579	-0.19225
C	-0.00954	0.65831	-0.31550
C	-1.34192	0.85102	0.03804
C	-1.82666	2.06910	0.50071
C	-0.94924	3.14059	0.62256
H	1.07741	3.81134	0.36522
H	1.89347	1.63156	-0.45993
H	-2.87079	2.17962	0.76357
H	-1.31524	4.09221	0.99012
C	0.51077	-0.67957	-0.82227
H	0.14731	-1.47099	-0.16846
H	0.07595	-0.87241	-1.80845
N	1.94480	-0.74285	-0.95719
C	2.87539	-0.56856	0.09778
C	2.54218	-0.33592	-2.15586
C	4.06149	-0.08629	-0.50208
C	3.83727	0.04137	-1.89170
H	1.98523	-0.37843	-3.07915
H	4.97332	0.10509	0.03998
H	4.55555	0.35761	-2.63507
C	2.66489	-0.82043	1.48203
C	1.41465	-1.53022	1.98023
H	0.51532	-0.89871	1.96559
H	1.18968	-2.43921	1.40976
O	3.56047	-0.50583	2.34030
I	-2.75512	-0.75310	-0.13405
H	1.60070	-1.81605	3.01655

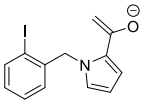


Radical anion A19 in benzene

28

-643.9288407

C	1.26617	3.30715	0.52518
C	1.52459	2.08200	-0.08792
C	0.46754	1.25222	-0.47816
C	-0.81080	1.70704	-0.22854
C	-1.11079	2.90370	0.37787
C	-0.04264	3.72196	0.75930
H	2.09477	3.93655	0.82826
H	2.55015	1.76249	-0.25237
H	-2.13815	3.19708	0.56385
H	-0.23351	4.67305	1.24450
C	0.68077	-0.08546	-1.15550
H	-0.05604	-0.80113	-0.79415
H	0.51371	0.01391	-2.23011
N	2.03961	-0.59232	-0.98916
C	2.66147	-1.02701	0.17030
C	2.98190	-0.45412	-1.96024
C	4.01074	-1.17910	-0.11282
C	4.21582	-0.82113	-1.45825
H	2.69862	-0.09610	-2.93816
H	4.73801	-1.53727	0.59864
H	5.14281	-0.83548	-2.00888
C	2.04779	-1.33503	1.47953
C	0.55202	-1.40383	1.64309
H	0.08087	-0.43394	1.46402
H	0.11003	-2.10911	0.93530
O	2.78585	-1.56912	2.42114
I	-3.07672	-0.78031	-0.17658
H	0.33345	-1.72506	2.65966

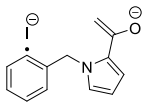


Enolate anion 6.6 in DMSO

27

-643.3534550

C	-0.19425	3.13096	0.61929
C	0.48823	2.02604	0.12417
C	-0.17065	0.82197	-0.13440
C	-1.54035	0.77040	0.12501
C	-2.24063	1.86417	0.62054
C	-1.56008	3.05215	0.86780
H	0.34214	4.05208	0.81267
H	1.55519	2.08559	-0.06185
H	-3.30395	1.79408	0.81225
H	-2.10092	3.90756	1.25428
C	0.57985	-0.38393	-0.66900
H	0.45527	-1.22759	0.01110
H	0.15768	-0.67123	-1.63589
N	1.99662	-0.15003	-0.85390
C	3.03294	-0.41830	0.02340
C	2.50025	0.40213	-2.00579
C	4.20111	-0.03457	-0.61027
C	3.86647	0.49223	-1.88521
H	1.83713	0.67086	-2.81415
H	5.18521	-0.13959	-0.18118
H	4.54178	0.88030	-2.63237
C	2.94054	-1.03489	1.39655
C	1.83748	-0.79698	2.18125
H	1.03721	-0.13556	1.88257
H	1.79595	-1.22761	3.17605
O	3.96816	-1.72501	1.73723
I	-2.63528	-1.02805	-0.23517

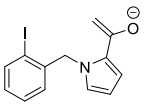


Radical dianion A20 in DMSO

27

-643.4599916

C	1.08996	3.43497	0.40198
C	1.44914	2.15214	-0.01206
C	0.47511	1.16324	-0.18882
C	-0.82665	1.53919	0.06836
C	-1.23423	2.78496	0.47838
C	-0.24179	3.75810	0.64773
H	1.85916	4.18665	0.53549
H	2.49200	1.90906	-0.19347
H	-2.27831	3.01125	0.66585
H	-0.51257	4.75720	0.96992
C	0.80446	-0.25182	-0.62616
H	0.45846	-0.96029	0.12658
H	0.27681	-0.47112	-1.55755
N	2.22107	-0.46648	-0.85392
C	3.17217	-0.95319	0.02476
C	2.81692	-0.16150	-2.05184
C	4.37810	-0.96160	-0.65432
C	4.15772	-0.45302	-1.96104
H	2.22595	0.22647	-2.86773
H	5.30861	-1.30924	-0.23302
H	4.88649	-0.32488	-2.74688
C	2.96378	-1.41266	1.44531
C	2.01637	-0.80003	2.22917
H	1.43201	0.04278	1.89019
H	1.89377	-1.12593	3.25654
O	3.75758	-2.34956	1.82339
I	-3.58070	-0.88515	-0.13706

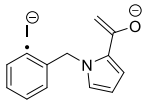


Enolate anion 6.6 in benzene

27

-643.3105041

C	-0.18927	3.12100	0.58735
C	0.49230	1.99629	0.14022
C	-0.17445	0.79333	-0.10569
C	-1.54954	0.76710	0.12079
C	-2.25060	1.88075	0.56826
C	-1.56227	3.06648	0.80074
H	0.35526	4.03859	0.77510
H	1.56565	2.03159	-0.01283
H	-3.31885	1.82497	0.73552
H	-2.10197	3.93845	1.15088
C	0.58125	-0.43302	-0.58425
H	0.50250	-1.22551	0.16299
H	0.12667	-0.79352	-1.51161
N	1.98102	-0.18229	-0.83945
C	3.05754	-0.40393	0.00198
C	2.42373	0.34838	-2.02815
C	4.18879	-0.01507	-0.68964
C	3.79149	0.46851	-1.96399
H	1.72174	0.57987	-2.81500
H	5.18798	-0.09880	-0.29290
H	4.42795	0.84543	-2.75009
C	3.03648	-0.99100	1.39692
C	1.96210	-0.72292	2.21838
H	1.16782	-0.04471	1.94020
H	1.96845	-1.11297	3.22993
O	4.07214	-1.66778	1.69508
I	-2.65835	-1.03058	-0.20895

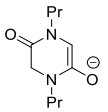


Radical dianion A20 in benzene

27

-643.3576895

C	-0.05400	-0.27796	1.58633
C	1.17450	-0.18181	0.93511
C	1.23681	-0.15230	-0.46374
C	0.02585	-0.22406	-1.11735
C	-1.21307	-0.31423	-0.53243
C	-1.24527	-0.34148	0.86592
H	-0.08071	-0.29470	2.66974
H	2.09884	-0.11374	1.50196
H	-2.13847	-0.35037	-1.09815
H	-2.20625	-0.40137	1.36627
C	2.54622	-0.05390	-1.21916
H	2.93107	-1.05034	-1.44017
H	2.37170	0.46377	-2.16619
N	3.57327	0.65683	-0.47574
C	4.78016	0.17099	-0.00853
C	3.50839	2.01194	-0.26265
C	5.47988	1.25044	0.49589
C	4.67503	2.41127	0.34585
H	2.63594	2.56902	-0.56975
H	6.46446	1.17594	0.93009
H	4.91534	3.42032	0.64560
C	5.25247	-1.26546	-0.02163
C	4.32882	-2.25325	0.24150
H	3.30255	-2.02865	0.50305
H	4.65231	-3.28794	0.27083
O	6.50058	-1.41824	-0.23247
I	-5.37621	0.03708	-0.04705

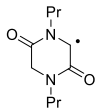


Enolate anion 6.16 in DMSO

31

-651.2914030

C	-0.56308	1.32020	-0.08500
C	0.94857	1.38523	-0.15358
C	0.68653	-0.85826	-1.02052
C	-0.53159	-1.07745	-0.40237
H	-0.95487	1.54542	-1.09451
H	-0.90990	2.09445	0.60019
H	1.20260	-1.64595	-1.54611
O	-1.22857	-2.13762	-0.46120
O	1.59237	2.38782	0.20409
N	1.49463	0.27481	-0.65443
N	-0.99909	0.01554	0.38634
C	-2.38427	-0.03585	0.83385
H	-2.56466	-1.03220	1.23938
H	-2.49823	0.68362	1.65295
C	-3.41885	0.26076	-0.25427
H	-3.23822	-0.41746	-1.09321
H	-3.28584	1.28187	-0.62565
C	-4.84129	0.08958	0.27265
H	-5.58392	0.30339	-0.49849
H	-5.00491	-0.93344	0.62248
H	-5.02903	0.76281	1.11391
C	2.94718	0.18121	-0.77356
H	3.16093	-0.58781	-1.51969
H	3.31963	1.13584	-1.14936
C	3.62809	-0.15765	0.55220
H	4.70842	-0.18723	0.37822
H	3.43912	0.65910	1.25412
C	3.15542	-1.48089	1.14836
H	3.67449	-1.69466	2.08508
H	2.08166	-1.45355	1.34828
H	3.34336	-2.30950	0.45945

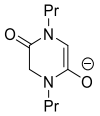


Radical A21 in DMSO

31

-651.1622504

C	-0.57919	1.33192	0.04489
C	0.92606	1.35880	-0.10831
C	0.76440	-0.92631	-0.81097
C	-0.58241	-1.08563	-0.31195
H	-0.99785	1.77704	-0.86947
H	-0.82906	1.98945	0.87778
H	1.25190	-1.76322	-1.28656
O	-1.16876	-2.17091	-0.39191
O	1.57458	2.36039	0.12621
N	1.50312	0.20889	-0.59576
N	-1.12745	0.01041	0.29637
C	-2.50434	-0.05456	0.77456
H	-2.65660	-1.04504	1.20502
H	-2.60914	0.68186	1.57636
C	-3.53705	0.20341	-0.32197
H	-3.39189	-0.53448	-1.11595
H	-3.36823	1.19176	-0.76067
C	-4.95687	0.11801	0.23111
H	-5.69665	0.28986	-0.55218
H	-5.14633	-0.86785	0.66361
H	-5.11557	0.86422	1.01395
C	2.95473	0.19775	-0.83939
H	3.14456	-0.58718	-1.57309
H	3.22041	1.15778	-1.27998
C	3.74916	-0.05130	0.44050
H	4.80882	-0.01602	0.17286
H	3.56746	0.77240	1.13528
C	3.42021	-1.38725	1.10105
H	4.05101	-1.54966	1.97649
H	2.37909	-1.42298	1.43192
H	3.58352	-2.21796	0.40879

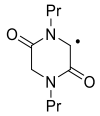


Enolate anion 6.16 in benzene

31

-651.2494131

C	1.09766	-1.31030	-1.01114
C	-0.25598	-1.54171	-0.85917
C	-0.39270	-0.68684	1.41033
C	1.06343	-1.12076	1.42370
H	-0.85494	-1.98727	-1.63940
H	1.56546	-0.62359	2.25541
H	1.07917	-2.20401	1.60368
N	-0.99541	-1.01576	0.26032
N	1.76928	-0.85118	0.18249
O	-0.93836	-0.08052	2.34605
O	1.79364	-1.46834	-2.05196
C	-2.35834	-0.56934	0.02229
H	-2.83142	-1.28472	-0.65784
H	-2.89450	-0.59066	0.97303
C	-2.40342	0.83585	-0.57339
H	-1.93962	1.52310	0.14088
H	-1.79068	0.84585	-1.47992
C	-3.83166	1.27220	-0.88615
H	-3.85914	2.28033	-1.30489
H	-4.29547	0.59608	-1.61023
H	-4.44853	1.26754	0.01701
C	2.40137	0.45497	0.06179
H	3.11381	0.57947	0.88715
H	2.97722	0.44055	-0.86702
C	1.42443	1.63540	0.04331
H	0.86835	1.66706	0.98711
H	0.68986	1.46070	-0.75085
C	2.14639	2.96162	-0.18039
H	1.45195	3.80468	-0.18617
H	2.88324	3.14111	0.60845
H	2.67871	2.95665	-1.13573

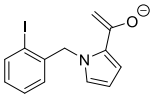


Radical A21 in benzene

31

-651.1544696

C	0.82862	1.18260	-0.36753
C	-0.61407	1.21798	-0.28654
C	-0.84757	-1.17041	-0.37225
C	0.64396	-1.24926	-0.12831
H	-1.11187	2.17357	-0.22355
H	0.76806	-1.48490	0.93938
H	1.01085	-2.10663	-0.69508
N	-1.39088	0.09556	-0.42397
N	1.38802	-0.06302	-0.50808
O	-1.52852	-2.17137	-0.45516
O	1.49443	2.21741	-0.36392
C	-2.85157	0.22859	-0.49793
H	-3.06657	1.17187	-1.00344
H	-3.22301	-0.58789	-1.11716
C	-3.49171	0.18724	0.88566
H	-3.23177	-0.76214	1.36156
H	-3.06628	0.98764	1.49874
C	-5.00726	0.33700	0.79433
H	-5.46295	0.30522	1.78483
H	-5.28051	1.28724	0.32856
H	-5.44285	-0.46843	0.19810
C	2.84221	-0.17387	-0.52473
H	3.09811	-1.08768	-1.06986
H	3.22702	0.67608	-1.08959
C	3.46396	-0.19278	0.87104
H	3.07282	-1.04347	1.43815
H	3.16029	0.71724	1.39592
C	4.98569	-0.27907	0.79488
H	5.43083	-0.29916	1.79079
H	5.30070	-1.18380	0.26798
H	5.39616	0.58097	0.26001

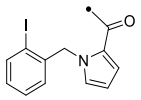


Enolate anion 6.6 in DMSO

27

-643.3534550

C	-0.19425	3.13096	0.61929
C	0.48823	2.02604	0.12417
C	-0.17065	0.82197	-0.13440
C	-1.54035	0.77040	0.12501
C	-2.24063	1.86417	0.62054
C	-1.56008	3.05215	0.86780
H	0.34214	4.05208	0.81267
H	1.55519	2.08559	-0.06185
H	-3.30395	1.79408	0.81225
H	-2.10092	3.90756	1.25428
C	0.57985	-0.38393	-0.66900
H	0.45527	-1.22759	0.01110
H	0.15768	-0.67123	-1.63589
N	1.99662	-0.15003	-0.85390
C	3.03294	-0.41830	0.02340
C	2.50025	0.40213	-2.00579
C	4.20111	-0.03457	-0.61027
C	3.86647	0.49223	-1.88521
H	1.83713	0.67086	-2.81415
H	5.18521	-0.13959	-0.18118
H	4.54178	0.88030	-2.63237
C	2.94054	-1.03489	1.39655
C	1.83748	-0.79698	2.18125
H	1.03721	-0.13556	1.88257
H	1.79595	-1.22761	3.17605
O	3.96816	-1.72501	1.73723
I	-2.63528	-1.02805	-0.23517

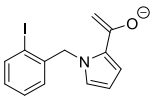


Radical A22 in DMSO

27

-643.1944220

C	-0.10861	3.13401	0.50121
C	0.54436	2.00662	0.01592
C	-0.14303	0.81040	-0.19996
C	-1.50863	0.78545	0.08904
C	-2.17613	1.90321	0.57491
C	-1.46909	3.08363	0.78068
H	0.44724	4.04970	0.66111
H	1.60722	2.05029	-0.19666
H	-3.23601	1.85761	0.79129
H	-1.98626	3.95649	1.16013
C	0.56974	-0.42150	-0.72668
H	0.39279	-1.27847	-0.07344
H	0.16320	-0.69001	-1.70463
N	2.00124	-0.23735	-0.88326
C	3.00542	-0.45767	0.04395
C	2.56253	0.21339	-2.04034
C	4.20920	-0.14145	-0.56504
C	3.93018	0.29294	-1.87671
H	1.94042	0.43291	-2.89489
H	5.17277	-0.21842	-0.08626
H	4.63648	0.61868	-2.62346
C	2.86543	-0.94594	1.43005
C	1.65439	-0.76044	2.18891
H	0.82670	-0.14877	1.86062
H	1.62121	-1.20054	3.17677
O	3.84119	-1.47815	1.97467
I	-2.64035	-0.99922	-0.20719

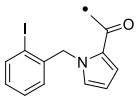


Enolate anion 6.6 in benzene

27

-643.3105041

C	-0.18927	3.12100	0.58735
C	0.49230	1.99629	0.14022
C	-0.17445	0.79333	-0.10569
C	-1.54954	0.76710	0.12079
C	-2.25060	1.88075	0.56826
C	-1.56227	3.06648	0.80074
H	0.35526	4.03859	0.77510
H	1.56565	2.03159	-0.01283
H	-3.31885	1.82497	0.73552
H	-2.10197	3.93845	1.15088
C	0.58125	-0.43302	-0.58425
H	0.50250	-1.22551	0.16299
H	0.12667	-0.79352	-1.51161
N	1.98102	-0.18229	-0.83945
C	3.05754	-0.40393	0.00198
C	2.42373	0.34838	-2.02815
C	4.18879	-0.01507	-0.68964
C	3.79149	0.46851	-1.96399
H	1.72174	0.57987	-2.81500
H	5.18798	-0.09880	-0.29290
H	4.42795	0.84543	-2.75009
C	3.03648	-0.99100	1.39692
C	1.96210	-0.72292	2.21838
H	1.16782	-0.04471	1.94020
H	1.96845	-1.11297	3.22993
O	4.07214	-1.66778	1.69508
I	-2.65835	-1.03058	-0.20895



Radical A22 in benzene

27

-643.1887007

C	-0.09337	3.12752	0.49972
C	0.55397	1.99733	0.01438
C	-0.14001	0.80482	-0.20077
C	-1.50532	0.78642	0.08861
C	-2.16682	1.90760	0.57447
C	-1.45380	3.08400	0.77967
H	0.46716	4.04032	0.65978
H	1.61718	2.03354	-0.19857
H	-3.22682	1.86604	0.79088
H	-1.96607	3.95962	1.15949
C	0.56888	-0.43025	-0.72579
H	0.39088	-1.28381	-0.06806
H	0.15659	-0.70224	-1.70070
N	1.99832	-0.24989	-0.88728
C	3.00322	-0.45798	0.04199
C	2.55850	0.20163	-2.04631
C	4.20409	-0.13679	-0.56590
C	3.92404	0.29032	-1.88051
H	1.93564	0.41484	-2.90183
H	5.16599	-0.21339	-0.08417
H	4.63009	0.61443	-2.62800
C	2.86689	-0.94690	1.43095
C	1.65192	-0.77387	2.18989
H	0.82103	-0.16275	1.86775
H	1.62766	-1.21747	3.17643
O	3.84490	-1.46475	1.97641
I	-2.64528	-0.99255	-0.20520

Dimsyl anion 6.30 in DMSO

9

-552.6394561

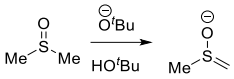
S	0.11620	0.14532	-0.41122
C	1.37804	-0.82514	0.19707
H	2.33634	-0.46410	-0.17547
H	1.34642	-0.92997	1.28568
C	-1.31527	-0.82293	0.13069
H	-1.21349	-0.99446	1.20441
H	-2.21398	-0.24264	-0.07344
H	-1.34041	-1.76910	-0.40571
O	-0.14384	1.49544	0.34718

Radical A23 in DMSO

9

-552.4905292

S	-0.10845	-0.14067	-0.41933
C	-0.99298	1.21313	0.23115
H	-0.66455	2.20876	-0.03750
H	-2.01291	1.01551	0.53267
C	1.53727	0.29296	0.20630
H	1.49395	0.31959	1.29417
H	2.21611	-0.48349	-0.14191
H	1.82330	1.26022	-0.20606
O	-0.54830	-1.38830	0.33040



A24 **6.30**

Deprotonation of DMSO – starting species

A24 O^{t}Bu anion in DMSO

24

-786.2924330

S	2.11673	-0.24854	0.29541
C	1.21519	0.92680	-0.72521
H	1.78910	1.09443	-1.63841
H	0.23537	0.46227	-0.92065
H	1.09708	1.85487	-0.16276
C	3.66873	0.66282	0.44022
H	3.48451	1.59433	0.97520
H	4.36050	0.03821	1.00290
H	4.05194	0.85321	-0.56272
O	2.43287	-1.43920	-0.61342
O	-1.49000	-0.64460	-0.94482
C	-2.30721	-0.05520	-0.00962
C	-3.64771	-0.81159	0.12509
H	-3.45579	-1.84790	0.42162
H	-4.31758	-0.35903	0.86557
H	-4.16129	-0.82486	-0.84163
C	-1.63754	-0.03496	1.38527
H	-1.38794	-1.05786	1.68561
H	-0.70761	0.54074	1.34353
H	-2.27978	0.40627	2.15627
C	-2.62818	1.40844	-0.39488
H	-3.13136	1.42962	-1.36700
H	-3.27130	1.90870	0.33850
H	-1.69621	1.97611	-0.48203

Deprotonation of DMSO – transition state in DMSO

24
-786.2817945

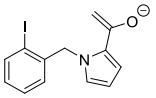
S	-2.04254	-0.16097	0.34014
C	-1.03261	0.98008	-0.55075
H	-0.88196	1.84463	0.10420
H	0.17515	0.39568	-0.80671
H	-1.56301	1.28701	-1.45866
C	-3.70226	0.53615	0.14628
H	-3.90417	0.62829	-0.92197
H	-4.41692	-0.14087	0.61383
H	-3.73213	1.51189	0.63122
O	-2.11006	-1.46513	-0.48444
O	1.29395	-0.12372	-1.08311
C	2.18351	-0.01352	-0.01063
C	3.44030	-0.83723	-0.31379
H	3.90625	-0.47652	-1.23525
H	4.17407	-0.77122	0.49613
H	3.17037	-1.88774	-0.45449
C	2.58756	1.45602	0.20474
H	3.06055	1.84674	-0.70094
H	1.69909	2.05848	0.41463
H	3.28803	1.56982	1.03842
C	1.54173	-0.54461	1.28483
H	1.21758	-1.57954	1.13924
H	2.24291	-0.51425	2.12490
H	0.66443	0.05253	1.54952

Deprotonation of DMSO – products 6.30 and HO^{t}Bu in DMSO

24
-786.2877112

S	-2.12740	-0.09450	0.35196
C	-1.17970	1.09429	-0.45970
H	-0.93049	1.87745	0.25928
H	0.53377	0.39096	-0.88787
H	-1.69619	1.49591	-1.33681
C	-3.85937	0.36593	0.03526
H	-3.98863	0.43012	-1.04715
H	-4.51722	-0.39818	0.44976
H	-4.05434	1.33135	0.50184
O	-2.04218	-1.44902	-0.41141
O	1.44345	0.05613	-1.15261
C	2.27161	-0.01203	0.00206
C	3.61656	-0.56176	-0.45987
H	4.05067	0.09614	-1.21705
H	4.31365	-0.63567	0.37850
H	3.48815	-1.55572	-0.89568
C	2.45175	1.38669	0.59949
H	2.88112	2.06034	-0.14657
H	1.48554	1.78861	0.91417
H	3.11559	1.35969	1.46795
C	1.64639	-0.94717	1.04104
H	1.49508	-1.93974	0.60860
H	2.29194	-1.04235	1.91858
H	0.67619	-0.55958	1.36354

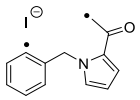
Scheme 6.6



Enolate anion 6.6 in DMSO

27
-643.3534550

C	-0.19425	3.13096	0.61929
C	0.48823	2.02604	0.12417
C	-0.17065	0.82197	-0.13440
C	-1.54035	0.77040	0.12501
C	-2.24063	1.86417	0.62054
C	-1.56008	3.05215	0.86780
H	0.34214	4.05208	0.81267
H	1.55519	2.08559	-0.06185
H	-3.30395	1.79408	0.81225
H	-2.10092	3.90756	1.25428
C	0.57985	-0.38393	-0.66900
H	0.45527	-1.22759	0.01110
H	0.15768	-0.67123	-1.63589
N	1.99662	-0.15003	-0.85390
C	3.03294	-0.41830	0.02340
C	2.50025	0.40213	-2.00579
C	4.20111	-0.03457	-0.61027
C	3.86647	0.49223	-1.88521
H	1.83713	0.67086	-2.81415
H	5.18521	-0.13959	-0.18118
H	4.54178	0.88030	-2.63237
C	2.94054	-1.03489	1.39655
C	1.83748	-0.79698	2.18125
H	1.03721	-0.13556	1.88257
H	1.79595	-1.22761	3.17605
O	3.96816	-1.72501	1.73723
I	-2.63528	-1.02805	-0.23517

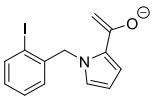


Triplet anion 6.31 in DMSO

27

-643.3070148

C	2.42454	3.05870	0.83435
C	2.28273	1.82170	0.20566
C	1.09848	1.50018	-0.46580
C	0.11395	2.46484	-0.45441
C	0.19652	3.69455	0.14834
C	1.39428	3.99435	0.80913
H	3.34805	3.29000	1.35130
H	3.08975	1.09637	0.24306
H	-0.62220	4.40440	0.12339
H	1.51234	4.95172	1.30327
C	0.86947	0.17649	-1.16622
H	-0.13084	-0.19307	-0.93372
H	0.91288	0.32288	-2.24735
N	1.85465	-0.83846	-0.82632
C	1.81153	-1.76805	0.19707
C	2.99442	-1.03203	-1.54831
C	2.95086	-2.55063	0.09671
C	3.70442	-2.07991	-0.99891
H	3.20115	-0.41299	-2.40814
H	3.19419	-3.36141	0.76529
H	4.64872	-2.45882	-1.35611
C	0.77051	-1.92585	1.23569
C	-0.03840	-0.82219	1.67093
H	0.11150	0.19425	1.34130
H	-0.77012	-1.01916	2.44174
O	0.65136	-3.02987	1.78868
I	-3.02129	-0.29998	-0.23650

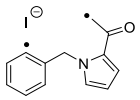


Enolate anion 6.6 in benzene

27

-643.3105041

C	-0.18927	3.12100	0.58735
C	0.49230	1.99629	0.14022
C	-0.17445	0.79333	-0.10569
C	-1.54954	0.76710	0.12079
C	-2.25060	1.88075	0.56826
C	-1.56227	3.06648	0.80074
H	0.35526	4.03859	0.77510
H	1.56565	2.03159	-0.01283
H	-3.31885	1.82497	0.73552
H	-2.10197	3.93845	1.15088
C	0.58125	-0.43302	-0.58425
H	0.50250	-1.22551	0.16299
H	0.12667	-0.79352	-1.51161
N	1.98102	-0.18229	-0.83945
C	3.05754	-0.40393	0.00198
C	2.42373	0.34838	-2.02815
C	4.18879	-0.01507	-0.68964
C	3.79149	0.46851	-1.96399
H	1.72174	0.57987	-2.81500
H	5.18798	-0.09880	-0.29290
H	4.42795	0.84543	-2.75009
C	3.03648	-0.99100	1.39692
C	1.96210	-0.72292	2.21838
H	1.16782	-0.04471	1.94020
H	1.96845	-1.11297	3.22993
O	4.07214	-1.66778	1.69508
I	-2.65835	-1.03058	-0.20895



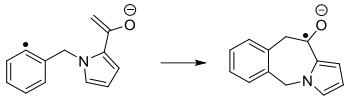
Triplet anion 6.31 in benzene

27

-643.2687235

C	1.16950	3.39675	0.96605
C	1.49399	2.21879	0.29350
C	0.51780	1.52400	-0.42800
C	-0.75127	2.06461	-0.42530
C	-1.12255	3.21392	0.22743
C	-0.12885	3.89809	0.93617
H	1.93723	3.91958	1.52432
H	2.50661	1.82870	0.33847
H	-2.14585	3.57132	0.20720
H	-0.37480	4.80916	1.47031
C	0.79712	0.23558	-1.17405
H	0.00713	-0.48841	-0.96209
H	0.77184	0.42170	-2.24994
N	2.09867	-0.33602	-0.86314
C	2.42866	-1.21794	0.14759
C	3.22520	-0.03229	-1.56775
C	3.78735	-1.46826	0.05576
C	4.29489	-0.71168	-1.02191
H	3.16950	0.63931	-2.41090
H	4.32589	-2.13246	0.71290
H	5.31414	-0.67026	-1.37181
C	1.52467	-1.82127	1.15748
C	0.31158	-1.17485	1.57164
H	0.03914	-0.16864	1.29267
H	-0.31597	-1.70551	2.27409
O	1.87706	-2.87869	1.69687
I	-2.83454	-0.85652	-0.24132

Scheme 6.7



6.33 6.34

$S_{RN}1$ cyclisation of 6.33 – starting species 6.33 in DMSO

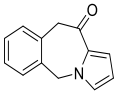
26
-631.9004297

C	-2.73321	-0.24997	1.46881
C	-1.51740	-0.34745	0.79266
C	-1.43908	-0.06963	-0.57663
C	-2.62254	0.29578	-1.18084
C	-3.84593	0.40838	-0.57080
C	-3.89495	0.12471	0.79976
H	-2.77073	-0.46932	2.52926
H	-0.61652	-0.63782	1.32527
H	-4.73703	0.70032	-1.11485
H	-4.83619	0.19696	1.33251
C	-0.14614	-0.14734	-1.36586
H	-0.29852	-0.78439	-2.24021
H	0.13102	0.84661	-1.71700
N	0.95989	-0.68853	-0.59962
C	1.13717	-2.03963	-0.43162
C	1.97371	-0.00531	0.04656
C	2.26998	-2.24094	0.32095
H	0.44438	-2.73840	-0.87608
C	2.80228	-0.95738	0.61235
H	3.69321	-0.72842	1.17614
H	2.66920	-3.19919	0.61627
C	2.16332	1.48827	0.12080
C	1.06007	2.29996	0.22510
H	0.05565	1.90693	0.29775
H	1.19697	3.37341	0.30032
O	3.38819	1.87454	0.12507

$S_{RN}1$ cyclisation of 6.33 – products 6.34 in DMSO

26
-631.9716451

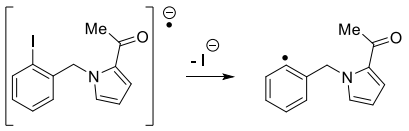
C	3.20248	-1.13436	-0.66836
C	2.07161	-1.58973	0.00598
C	1.14374	-0.69065	0.52606
C	1.33639	0.69138	0.36891
C	2.46994	1.13552	-0.31364
C	3.39892	0.23380	-0.82882
H	3.92186	-1.84193	-1.06397
H	1.90747	-2.65555	0.13099
H	2.62842	2.20195	-0.43921
H	4.27569	0.60051	-1.35047
C	-0.11209	-1.17057	1.20902
H	-0.07093	-2.24938	1.36177
H	-0.22159	-0.70211	2.19351
N	-1.28916	-0.89095	0.40117
C	-2.17400	-1.86261	-0.02910
C	-1.69304	0.36422	-0.06993
C	-3.15891	-1.25065	-0.77192
H	-2.02068	-2.89684	0.23709
C	-2.87789	0.13744	-0.80685
H	-3.44009	0.90587	-1.31317
H	-3.99182	-1.75637	-1.23877
C	-1.02377	1.60374	0.15698
C	0.31089	1.65890	0.90611
H	0.17592	1.49319	1.98467
H	0.68336	2.67795	0.79193
O	-1.52363	2.71259	-0.27614



Neutral 6.3 in DMSO

26
-631.8980850

C	3.22968	-1.12300	-0.66874
C	2.07908	-1.60447	-0.04937
C	1.13629	-0.72203	0.46962
C	1.34190	0.65928	0.37190
C	2.49217	1.13391	-0.25355
C	3.43476	0.24820	-0.77096
H	3.95928	-1.81671	-1.06914
H	1.91189	-2.67322	0.03168
H	2.65423	2.20354	-0.33074
H	4.32737	0.63173	-1.25073
C	-0.11543	-1.22897	1.13930
H	-0.09034	-2.31386	1.22672
H	-0.21084	-0.81551	2.14727
N	-1.31780	-0.89133	0.37382
C	-2.23824	-1.80310	-0.02365
C	-1.70667	0.36076	-0.07345
C	-3.23937	-1.15891	-0.73265
H	-2.11417	-2.84619	0.22367
C	-2.90235	0.20413	-0.76421
H	-3.44805	1.00927	-1.23105
H	-4.10292	-1.63170	-1.17226
C	-0.98781	1.61730	0.14334
C	0.31507	1.61627	0.92979
H	0.07974	1.35476	1.96833
H	0.69244	2.63778	0.92086
O	-1.43356	2.66291	-0.29821



6.33 **6.34**

C-I elongation of 6.33 – transition state in DMSO

28

-643.9223676

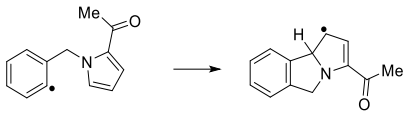
C	0.48610	3.05031	0.42108
C	0.93172	1.85744	-0.13740
C	0.06284	0.77512	-0.32724
C	-1.24423	0.97526	0.07610
C	-1.73502	2.14067	0.63405
C	-0.84252	3.19639	0.80844
H	1.18216	3.86946	0.55573
H	1.97009	1.74459	-0.43259
H	-2.77201	2.23162	0.92729
H	-1.19278	4.12390	1.24546
C	0.54580	-0.51976	-0.96062
H	0.10440	-1.36254	-0.43401
H	0.17271	-0.56746	-1.98791
N	1.98448	-0.63619	-1.00994
C	2.84452	-0.63766	0.11086
C	2.68730	-0.16627	-2.11975
C	4.09930	-0.18610	-0.35838
C	3.98248	0.09000	-1.74290
H	2.19062	-0.07141	-3.07317
H	4.98908	-0.12089	0.24740
H	4.76884	0.42441	-2.40439
C	2.51764	-1.03020	1.43920
C	1.21051	-1.72888	1.77244
H	0.34005	-1.05893	1.78323
H	0.98295	-2.54820	1.08137
O	3.37686	-0.86603	2.38843
I	-2.79681	-0.75524	-0.18895
H	1.30956	-2.15286	2.77284

C-I elongation of 6.33 – products 6.34 and iodide anion in DMSO

28

-643.9665259

C	1.61061	3.28725	0.44105
C	1.75340	2.03697	-0.15938
C	0.62506	1.28615	-0.50875
C	-0.60015	1.85200	-0.22662
C	-0.79512	3.07634	0.36547
C	0.34718	3.81050	0.70463
H	2.49453	3.85420	0.70800
H	2.74541	1.63763	-0.35100
H	-1.78794	3.46249	0.56816
H	0.24504	4.78188	1.17520
C	0.71973	-0.07087	-1.17583
H	-0.08498	-0.71316	-0.82199
H	0.58542	0.03802	-2.25394
N	2.02036	-0.70250	-0.98138
C	2.59246	-1.15269	0.20008
C	2.97907	-0.68168	-1.94603
C	3.92543	-1.43478	-0.06557
C	4.17052	-1.14312	-1.41973
H	2.73951	-0.32978	-2.93794
H	4.61727	-1.83654	0.65829
H	5.09643	-1.26054	-1.95958
C	1.93832	-1.36633	1.50217
C	0.43726	-1.34483	1.63081
H	0.03630	-0.34848	1.42834
H	-0.02447	-2.03378	0.92000
O	2.63630	-1.60308	2.47626
I	-3.21306	-0.69439	-0.16554
H	0.17380	-1.63667	2.64578



6.34 6.35

Cyclisation 6.34 – starting species 6.34 in DMSO

27
-632.4034071

C	-2.25369	-0.20247	1.70411
C	-1.21388	-0.46653	0.84509
C	-1.28560	-0.47851	-0.52875
C	-2.54046	-0.19943	-1.08451
C	-3.63157	0.06905	-0.26337
C	-3.49602	0.07024	1.12447
H	-2.12458	-0.20319	2.78022
H	-4.59502	0.28355	-0.70984
H	-4.34989	0.28617	1.75621
C	-0.09207	-0.77758	-1.41044
H	-0.21815	-1.75321	-1.88277
H	-0.01683	-0.04561	-2.21401
N	1.15349	-0.83631	-0.65611
C	1.72816	-2.02126	-0.31429
C	1.77755	0.17835	0.05605
C	2.74824	-1.79332	0.58858
H	1.35848	-2.94360	-0.73610
C	2.77384	-0.40669	0.82457
H	3.45220	0.14315	1.45794
H	3.39692	-2.54374	1.01124
C	1.51280	1.62506	-0.00086
C	0.65557	2.21983	-1.09078
H	-0.38742	1.91795	-0.96808
H	0.72046	3.30404	-1.02382
O	2.03157	2.35060	0.83278
H	-2.65589	-0.18906	-2.16420
H	0.99543	1.89255	-2.07519

Cyclisation 6.34 – transition state in DMSO

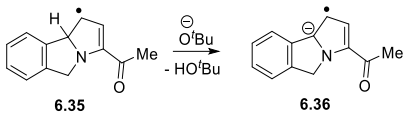
27
-632.3878362

C	-2.74967	1.07494	-0.54232
C	-1.61746	0.70058	0.14464
C	-1.32200	-0.59506	0.51610
C	-2.22651	-1.59766	0.16726
C	-3.38554	-1.26376	-0.53338
C	-3.64861	0.05837	-0.88790
H	-2.94691	2.10619	-0.81436
H	-4.08620	-2.04272	-0.80944
H	-4.55098	0.30325	-1.43708
C	-0.02968	-0.80909	1.28069
H	-0.21149	-0.81917	2.35831
H	0.45062	-1.74459	1.01004
N	0.83291	0.33286	0.96354
C	0.24381	1.57775	1.07941
C	1.71916	0.38362	-0.10557
C	0.87980	2.45738	0.19511
H	-0.35865	1.81025	1.94561
C	1.77636	1.69653	-0.56232
H	2.45290	2.04539	-1.32730
H	0.70268	3.51942	0.13248
C	2.60285	-0.69863	-0.55389
C	2.85016	-1.89756	0.33200
H	2.19547	-2.71845	0.02596
H	3.87906	-2.22193	0.18007
O	3.17941	-0.59733	-1.62623
H	-2.02802	-2.63088	0.43528
H	2.67989	-1.68267	1.38644

Cyclisation 6.34 – product 6.35 in DMSO

27
-632.4493559

C	-2.71868	1.11644	0.02551
C	-1.51273	0.49955	0.32838
C	-1.34430	-0.87105	0.16069
C	-2.38510	-1.65833	-0.31409
C	-3.59750	-1.04483	-0.62559
C	-3.76285	0.33051	-0.45860
H	-2.84779	2.18492	0.15862
H	-4.41920	-1.64168	-1.00328
H	-4.71102	0.79182	-0.70792
C	0.05215	-1.28849	0.56082
H	0.05061	-1.88389	1.47785
H	0.55191	-1.85898	-0.22248
N	0.73547	0.00368	0.77148
C	-0.24261	1.11058	0.87721
C	1.79415	0.42252	-0.00631
C	0.40706	2.22384	0.10652
H	-0.38711	1.40091	1.92724
C	1.58623	1.79857	-0.38405
H	2.30336	2.36919	-0.95532
H	-0.01639	3.21531	0.03136
C	2.96123	-0.35378	-0.32023
C	3.16882	-1.69687	0.34439
H	2.84032	-2.50092	-0.32009
H	4.23634	-1.82837	0.52208
O	3.80584	0.08803	-1.11463
H	-2.25837	-2.72711	-0.44603
H	2.62704	-1.78297	1.28659



6.35 6.36

Deprotonation of 6.35 – starting species 6.35 and O^{t}Bu anion in DMSO

41

-865.5794437

C	-0.56013	2.48129	0.96682
C	0.18440	1.51200	0.30678
C	1.21127	1.87118	-0.56259
C	1.51636	3.20692	-0.78786
C	0.77719	4.18370	-0.12118
C	-0.25134	3.82359	0.74961
H	-1.36383	2.20286	1.63963
H	1.00524	5.23125	-0.27907
H	-0.81494	4.59465	1.26185
C	1.85861	0.64032	-1.15687
H	1.65229	0.55135	-2.22750
H	2.93990	0.63218	-1.01235
N	1.22872	-0.45901	-0.40216
C	0.03174	0.01147	0.33506
C	1.93099	-1.33750	0.39134
C	0.13455	-0.70904	1.64244
H	-0.90467	-0.26952	-0.21372
C	1.22592	-1.49932	1.64089
H	1.54767	-2.17729	2.41771
H	-0.61375	-0.63777	2.42011
C	3.11927	-2.04367	0.01421
C	3.62013	-1.95970	-1.41180
H	4.40837	-1.20591	-1.49428
H	4.05396	-2.92376	-1.67866
O	3.72688	-2.74239	0.84627
H	2.31670	3.48853	-1.46328
H	2.82766	-1.70885	-2.11750
O	-2.46892	-0.56656	-1.27368
C	-3.43304	-1.02483	-0.40421
C	-4.79051	-1.20816	-1.11624
H	-4.68301	-1.93016	-1.93183
H	-5.57561	-1.56549	-0.43983
H	-5.11165	-0.25377	-1.54573
C	-3.64443	-0.03325	0.76429
H	-2.70570	0.09760	1.31175
H	-3.94428	0.94276	0.36910
H	-4.40925	-0.37153	1.47257
C	-3.02469	-2.38715	0.20158
H	-2.90086	-3.12173	-0.60055
H	-2.06452	-2.28416	0.71793
H	-3.76218	-2.77375	0.91440

Deprotonation of 6.35 – transition state in DMSO

41

-865.5785755

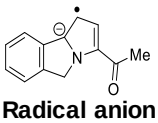
C	-0.91934	2.39230	0.99531
C	-0.03961	1.51988	0.36417
C	0.92844	2.00905	-0.51540
C	1.03104	3.36687	-0.78154
C	0.15310	4.24443	-0.14451
C	-0.81167	3.75896	0.73828
H	-1.67458	2.01964	1.67829
H	0.22313	5.30897	-0.33422
H	-1.48552	4.45164	1.22934
C	1.76063	0.87430	-1.07094
H	1.61285	0.75466	-2.14907
H	2.82821	1.01297	-0.88593
N	1.25808	-0.28973	-0.32682
C	0.02793	0.02477	0.41572
C	2.02922	-1.16648	0.40310
C	0.19606	-0.71963	1.68447
H	-0.91268	-0.41637	-0.19747
C	1.34022	-1.44091	1.64015
H	1.70448	-2.14083	2.37817
H	-0.54769	-0.74157	2.46987
C	3.25571	-1.76047	-0.01880
C	3.74462	-1.54311	-1.43630
H	2.93363	-1.31012	-2.12700
H	4.47196	-0.72667	-1.47032
O	3.92458	-2.47393	0.76081
H	1.78304	3.74341	-1.46681
O	-1.99867	-0.93909	-1.12285
C	-3.11725	-1.35790	-0.41784
C	-4.30825	-1.55068	-1.37299
H	-4.05355	-2.29124	-2.13688
H	-5.20807	-1.88951	-0.84786
H	-4.53620	-0.60574	-1.87518
C	-3.51679	-0.31462	0.64634
H	-2.70951	-0.19027	1.37465
H	-3.69172	0.65278	0.16569
H	-4.42264	-0.60335	1.18986
C	-2.83888	-2.69610	0.29579
H	-2.57958	-3.46007	-0.44381
H	-1.98978	-2.57944	0.97679
H	-3.70125	-3.04919	0.87182
H	4.25041	-2.45147	-1.76584

Deprotonation of 6.35 – products 6.36 and HO^{t}Bu in DMSO

41

-865.6231594

C	2.82167	-0.62636	1.29333
C	1.58573	-0.95655	0.72539
C	1.53381	-1.47941	-0.58724
C	2.68826	-1.68087	-1.32011
C	3.92335	-1.35190	-0.74853
C	3.97814	-0.82831	0.54667
H	2.87773	-0.21718	2.29606
H	4.83734	-1.50245	-1.31011
H	4.94043	-0.57563	0.97828
C	0.09404	-1.72900	-0.98764
H	-0.22197	-1.09386	-1.82533
H	-0.07130	-2.77399	-1.26671
N	-0.62123	-1.36368	0.23115
C	0.23900	-0.84271	1.20313
C	-1.94653	-1.02438	0.53062
C	-0.53663	-0.21253	2.17067
H	-0.82768	1.04344	-0.04327
C	-1.87708	-0.32101	1.77039
H	-2.74093	0.04755	2.30118
H	-0.16267	0.28197	3.05563
C	-3.11728	-1.30433	-0.21901
C	-3.08842	-2.16675	-1.46386
H	-3.84388	-2.95313	-1.36146
H	-3.36334	-1.57593	-2.34501
O	-4.25628	-0.84909	0.15056
H	2.64058	-2.08048	-2.32801
H	-2.13006	-2.64452	-1.65631
O	-0.66352	1.58100	-0.83054
C	-0.05613	2.81164	-0.41513
C	0.05607	3.65805	-1.67556
H	-0.93344	3.82353	-2.10815
H	0.50410	4.62726	-1.44664
H	0.68063	3.15185	-2.41548
C	1.32555	2.53025	0.17314
H	1.23758	1.92330	1.07821
H	1.93704	1.97869	-0.54627
H	1.83385	3.46447	0.42582
C	-0.95067	3.49060	0.62035
H	-1.93969	3.68218	0.19693
H	-1.06590	2.84485	1.49639
H	-0.51860	4.43997	0.94624

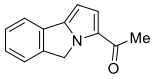


Radical anion 6.36 in DMSO

26

-631.9734622

C	-2.81274	1.23120	-0.00306
C	-1.57030	0.58300	-0.00898
C	-1.52182	-0.83264	-0.00126
C	-2.67864	-1.58706	0.01092
C	-3.91864	-0.93519	0.01658
C	-3.97235	0.46187	0.00967
H	-2.87069	2.31386	-0.00842
H	-4.83466	-1.51320	0.02634
H	-4.93694	0.95763	0.01429
C	-0.07948	-1.29990	-0.01034
H	0.16786	-1.89476	0.87690
H	0.14706	-1.90473	-0.89616
N	0.63819	-0.03275	-0.02423
C	-0.22174	1.06473	-0.01946
C	1.96950	0.38842	-0.00513
C	0.55773	2.21821	-0.00383
C	1.89838	1.81445	0.00483
H	2.76555	2.45638	0.01579
H	0.18547	3.23226	0.00206
C	3.15281	-0.39387	0.00367
C	3.13156	-1.90793	-0.01216
H	3.75343	-2.26585	-0.83992
H	3.58188	-2.29346	0.91006
O	4.30702	0.16634	0.03493
H	-2.63111	-2.67130	0.01680
H	2.14308	-2.35012	-0.11626

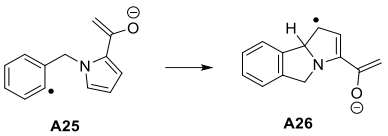


Neutral 6.4 in DMSO

26

-631.8971159

C	2.77758	1.23734	0.00042
C	1.55750	0.57055	0.00004
C	1.50265	-0.83030	-0.00034
C	2.66276	-1.58587	-0.00039
C	3.88905	-0.91886	-0.00008
C	3.94406	0.47569	0.00033
H	2.81968	2.32001	0.00075
H	4.80888	-1.49117	-0.00014
H	4.90687	0.97253	0.00064
C	0.06398	-1.29471	-0.00031
H	-0.17817	-1.88003	-0.88923
H	-0.17774	-1.88068	0.88831
N	-0.65337	-0.01546	0.00028
C	0.18581	1.05952	0.00028
C	-1.96169	0.42255	-0.00032
C	-0.56971	2.22445	-0.00015
C	-1.91551	1.81635	-0.00054
H	-2.78963	2.44927	-0.00085
H	-0.18919	3.23321	-0.00021
C	-3.16157	-0.41459	0.00011
C	-3.00852	-1.91493	0.00044
H	-3.99602	-2.37149	0.00011
H	-2.45653	-2.24442	-0.88283
O	-4.26746	0.10390	0.00014
H	2.62413	-2.66916	-0.00070
H	-2.45724	-2.24411	0.88425



A25 A26

Cyclisation A25 – starting species A25 in DMSO

26

-631.9002517

C	2.79905	-0.94212	-1.21862
C	1.64483	-0.88465	-0.47479
C	1.41100	-0.04832	0.59319
C	2.45850	0.81601	0.93481
C	3.65316	0.80191	0.21883
C	3.82960	-0.07003	-0.85450
H	2.91357	-1.62825	-2.05002
H	4.45043	1.48113	0.49604
H	4.76029	-0.07251	-1.41012
C	0.11410	-0.05963	1.37513
H	0.24800	-0.64684	2.28790
H	-0.15433	0.95661	1.66141
N	-0.98909	-0.64177	0.63177
C	-1.19529	-1.99708	0.56976
C	-1.97525	0.00916	-0.08416
C	-2.32234	-2.23322	-0.18305
H	-0.52997	-2.67246	1.08612
C	-2.81909	-0.96576	-0.58567
H	-3.69436	-0.76165	-1.18275
H	-2.74027	-3.20307	-0.40580
C	-2.11464	1.49400	-0.29380
C	-0.98146	2.25365	-0.45588
H	0.00783	1.81835	-0.47803
H	-1.07650	3.31931	-0.63549
O	-3.32524	1.91869	-0.35002
H	2.32792	1.50875	1.76100

Cyclisation A25 – transition state in DMSO

26

-631.8883080

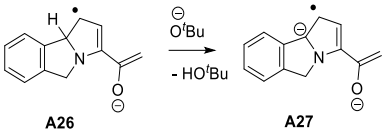
C	2.72254	1.06651	0.58404
C	1.57975	0.73495	-0.11500
C	1.30112	-0.54739	-0.55007
C	2.21671	-1.56087	-0.26378
C	3.37980	-1.26029	0.44583
C	3.63411	0.04254	0.87047
H	2.91989	2.08188	0.91313
H	4.08861	-2.04836	0.67206
H	4.53886	0.26518	1.42602
C	0.00239	-0.75238	-1.30916
H	0.17841	-0.73528	-2.38878
H	-0.47891	-1.69366	-1.05367
N	-0.87826	0.35711	-0.94990
C	-0.32417	1.63025	-1.01003
C	-1.78869	0.32265	0.09352
C	-1.00684	2.44000	-0.10199
H	0.26876	1.92094	-1.86452
C	-1.89236	1.60598	0.60962
H	-2.57539	1.89488	1.39336
H	-0.86892	3.50415	0.01521
C	-2.59390	-0.87409	0.51180
C	-2.95890	-1.76918	-0.46443
H	-2.69341	-1.61564	-1.50220
H	-3.56939	-2.62835	-0.20889
O	-2.91425	-0.91728	1.75385
H	2.02390	-2.57947	-0.58804

Cyclisation A25 – product A26 in DMSO

26

-631.9403183

C	-2.66979	1.11985	0.01693
C	-1.47624	0.49287	0.35042
C	-1.31460	-0.87755	0.17675
C	-2.34952	-1.65169	-0.33409
C	-3.54937	-1.02799	-0.67491
C	-3.70842	0.34758	-0.50136
H	-2.79295	2.18945	0.15131
H	-4.36455	-1.61541	-1.08122
H	-4.64567	0.81878	-0.77377
C	0.06615	-1.30018	0.62038
H	0.02062	-1.89715	1.53734
H	0.59490	-1.88525	-0.13274
N	0.77067	-0.02375	0.85557
C	-0.20955	1.09431	0.92641
C	1.80879	0.36653	-0.00791
C	0.44430	2.19180	0.13282
H	-0.38964	1.39414	1.96897
C	1.60536	1.70362	-0.40407
H	2.31101	2.24443	-1.01798
H	0.03938	3.18952	0.04578
C	3.00379	-0.44954	-0.32210
C	3.24492	-1.56927	0.44734
H	2.59917	-1.84348	1.27097
H	4.12585	-2.17248	0.25592
O	3.74507	-0.02217	-1.28775
H	-2.22831	-2.72094	-0.47122



A26 **A27**

Deprotonation A26 – starting species A26 and O^{t}Bu anion in DMSO

40

-865.0661243

C	-1.66618	-2.45343	0.95276
C	-1.37281	-1.26848	0.29004
C	-2.20263	-0.79195	-0.72048
C	-3.34559	-1.49336	-1.08628
C	-3.64871	-2.68051	-0.41925
C	-2.81530	-3.15716	0.59339
H	-1.01645	-2.82362	1.73899
H	-4.53960	-3.23641	-0.68798
H	-3.06393	-4.08032	1.10406
C	-1.64984	0.49779	-1.28284
H	-1.29223	0.35746	-2.30880
H	-2.38167	1.30711	-1.29470
N	-0.53592	0.83173	-0.37506
C	-0.19229	-0.34176	0.47853
C	-0.60908	1.96615	0.44564
C	0.00221	0.26353	1.84086
H	0.72721	-0.83339	0.11083
C	-0.25552	1.60702	1.76314
H	-0.17656	2.32633	2.56592
H	0.33526	-0.29582	2.70349
C	-0.87825	3.34052	-0.03528
C	-0.80508	3.57285	-1.39426
H	-0.97755	4.57078	-1.78228
O	-1.14063	4.22454	0.86857
H	-3.99527	-1.12617	-1.87374
H	-0.53906	2.78684	-2.08859
O	2.51284	-1.67724	-0.88328
C	3.48134	-0.87811	-0.32388
C	4.86594	-1.14433	-0.95837
H	4.81856	-0.94779	-2.03442
H	5.65687	-0.51946	-0.52706
H	5.13909	-2.19513	-0.81621
C	3.60260	-1.13642	1.19624
H	2.63998	-0.93235	1.67578
H	3.85657	-2.18753	1.36933
H	4.36695	-0.51250	1.67443
C	3.15827	0.62389	-0.51718
H	3.07038	0.84380	-1.58697
H	2.20091	0.86297	-0.04295
H	3.92976	1.27719	-0.09269

Deprotonation A26 – transition state in DMSO

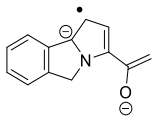
40
-865.0544641

C	-0.97476	2.33664	0.99465
C	-0.07487	1.48834	0.34934
C	0.87305	2.02601	-0.53162
C	0.92694	3.38856	-0.78428
C	0.02167	4.23632	-0.14028
C	-0.91820	3.70842	0.74562
H	-1.71000	1.93691	1.68510
H	0.05228	5.30380	-0.32502
H	-1.61272	4.37321	1.24777
C	1.74105	0.92231	-1.09381
H	1.61957	0.83517	-2.18037
H	2.80541	1.08121	-0.89775
N	1.26453	-0.28283	-0.39848
C	0.04009	0.00878	0.38816
C	2.11033	-1.10121	0.36419
C	0.25251	-0.72705	1.65108
H	-0.99487	-0.47468	-0.28785
C	1.46248	-1.38496	1.58359
H	1.87126	-2.06113	2.32219
H	-0.47106	-0.78670	2.45316
C	3.37196	-1.69723	-0.11471
C	3.69316	-1.58809	-1.45781
H	3.03268	-1.10398	-2.16482
O	4.09676	-2.30451	0.77035
H	1.66540	3.79587	-1.46810
O	-1.93436	-0.93631	-1.09227
C	-3.03030	-1.43068	-0.38231
C	-4.20294	-1.64936	-1.34783
H	-3.91179	-2.35495	-2.13121
H	-5.08498	-2.04577	-0.83380
H	-4.47483	-0.70224	-1.82274
C	-3.46735	-0.43528	0.70835
H	-2.66005	-0.29225	1.43227
H	-3.69525	0.53459	0.25592
H	-4.35388	-0.78644	1.24618
C	-2.67637	-2.77033	0.28700
H	-2.38360	-3.49813	-0.47578
H	-1.83166	-2.62777	0.96764
H	-3.51791	-3.18201	0.85425
H	4.61430	-2.02550	-1.82836

Deprotonation A26 – product A27 and HO^{t}Bu in DMSO

40
-865.0879020

C	2.91802	-0.09566	1.26263
C	1.72101	-0.65361	0.70176
C	1.80837	-1.32326	-0.56759
C	2.99342	-1.45832	-1.23810
C	4.19169	-0.91232	-0.66919
C	4.10790	-0.23978	0.56808
H	2.89452	0.43226	2.21060
H	5.14019	-1.00970	-1.18224
H	5.01414	0.18253	0.99544
C	0.42051	-1.79466	-0.97476
H	0.05728	-1.29849	-1.88294
H	0.38076	-2.87484	-1.14416
N	-0.38458	-1.40381	0.18173
C	0.37015	-0.69783	1.12212
C	-1.74582	-1.32603	0.48821
C	-0.52353	-0.21128	2.08946
H	-0.96266	0.90487	-0.17437
C	-1.82447	-0.60931	1.67456
H	-2.75450	-0.40589	2.18414
H	-0.26710	0.37893	2.95666
C	-2.88297	-1.91247	-0.27096
C	-2.64472	-2.67903	-1.39580
H	-3.48883	-3.09794	-1.93325
H	-1.65354	-2.89909	-1.76021
O	-4.05696	-1.65028	0.19479
H	3.02883	-1.96820	-2.19730
O	-0.98855	1.52027	-0.92156
C	-0.63886	2.82377	-0.43899
C	-0.75905	3.75264	-1.63927
H	-1.78146	3.74394	-2.02440
H	-0.50116	4.77584	-1.35731
H	-0.08324	3.42972	-2.43481
C	0.79350	2.80445	0.09163
H	0.88213	2.08727	0.91199
H	1.48355	2.49993	-0.70000
H	1.08597	3.79491	0.45015
C	-1.61361	3.23264	0.66422
H	-2.63752	3.23022	0.28211
H	-1.54905	2.52711	1.49760
H	-1.38149	4.23379	1.03613

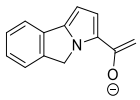


Radical dianion A27 in DMSO

25

-631.4374431

C	-2.79124	1.26514	-0.03428
C	-1.52033	0.59767	-0.01463
C	-1.50643	-0.84003	0.03415
C	-2.65735	-1.57863	0.06318
C	-3.92635	-0.90930	0.05628
C	-3.94576	0.50111	0.00413
H	-2.85017	2.34808	-0.07328
H	-4.84929	-1.47497	0.07621
H	-4.90616	1.01074	-0.00693
C	-0.06235	-1.31783	0.05460
H	0.20737	-1.80693	0.99987
H	0.15109	-2.02042	-0.75538
N	0.67435	-0.06519	-0.10493
C	-0.17549	1.04143	-0.07918
C	2.00643	0.34087	0.00070
C	0.63440	2.18704	-0.04995
C	1.97854	1.72837	0.01005
H	2.86933	2.33883	0.03823
H	0.29246	3.21106	-0.03223
C	3.21748	-0.52175	0.01397
C	3.10427	-1.88389	-0.19345
H	2.16240	-2.37461	-0.38345
H	4.00222	-2.49267	-0.18194
O	4.33494	0.09001	0.21968
H	-2.61412	-2.66400	0.10238

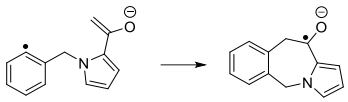


Anion A28 in DMSO

25

-631.3942397

C	2.74636	1.25209	0.01558
C	1.53102	0.57328	0.01894
C	1.49907	-0.83073	-0.01366
C	2.67026	-1.56790	-0.04680
C	3.89022	-0.88731	-0.05001
C	3.92389	0.50736	-0.01907
H	2.77656	2.33524	0.03913
H	4.81741	-1.44709	-0.07678
H	4.87920	1.01919	-0.02248
C	0.06721	-1.31760	0.00484
H	-0.19168	-1.90664	-0.87862
H	-0.14328	-1.91596	0.89487
N	-0.67293	-0.05751	0.03138
C	0.15578	1.04304	0.04473
C	-1.98882	0.33877	0.01475
C	-0.62745	2.17983	0.04665
C	-1.97294	1.72961	0.02603
H	-2.86385	2.33760	0.01929
H	-0.27532	3.19978	0.05542
C	-3.20803	-0.53368	-0.02024
C	-3.07542	-1.89403	0.13286
H	-2.12949	-2.38357	0.30019
H	-3.96596	-2.51251	0.11165
O	-4.31315	0.09649	-0.18993
H	2.64520	-2.65177	-0.07051



6.33 6.34

$S_{RN}1$ cyclisation of 6.33 – starting species 6.33 in benzene

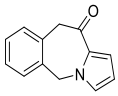
26
-631.8573282

C	2.73158	0.13430	1.48264
C	1.51391	0.22203	0.81044
C	1.44844	0.03122	-0.57467
C	2.64705	-0.24167	-1.19640
C	3.87385	-0.34112	-0.58997
C	3.90960	-0.14513	0.79548
H	2.75716	0.28290	2.55568
H	0.59713	0.43491	1.35254
H	4.77653	-0.56119	-1.14864
H	4.85231	-0.21272	1.32688
C	0.14597	0.09761	-1.34899
H	0.29848	0.69261	-2.25338
H	-0.15469	-0.90869	-1.64472
N	-0.93582	0.68359	-0.58618
C	-1.05561	2.04109	-0.40674
C	-1.98223	0.03644	0.04562
C	-2.18600	2.27948	0.33887
H	-0.32832	2.71378	-0.83597
C	-2.77379	1.01631	0.61300
H	-3.68112	0.80927	1.15791
H	-2.54812	3.25084	0.64002
C	-2.24024	-1.45337	0.10031
C	-1.16059	-2.30278	0.21461
H	-0.14894	-1.94008	0.33726
H	-1.33609	-3.36978	0.29306
O	-3.47065	-1.77794	0.07717

$S_{RN}1$ cyclisation of 6.33 – products 6.34 in benzene

26
-631.9298533

C	3.17523	-1.14539	-0.68892
C	2.04985	-1.59794	-0.00470
C	1.13565	-0.69948	0.53888
C	1.33234	0.68461	0.39034
C	2.45978	1.12538	-0.30600
C	3.37675	0.22414	-0.83958
H	3.88429	-1.85406	-1.10153
H	1.87573	-2.66405	0.10669
H	2.61632	2.19211	-0.43076
H	4.24772	0.59087	-1.37156
C	-0.12269	-1.17707	1.21786
H	-0.08572	-2.25818	1.36138
H	-0.22953	-0.71662	2.20770
N	-1.29339	-0.88635	0.41181
C	-2.18576	-1.85133	-0.02542
C	-1.67855	0.37235	-0.07086
C	-3.15314	-1.22641	-0.78276
H	-2.04792	-2.88648	0.24501
C	-2.85485	0.15462	-0.82131
H	-3.39497	0.93413	-1.33395
H	-3.98684	-1.72317	-1.25813
C	-1.00606	1.61084	0.15835
C	0.31526	1.65038	0.93878
H	0.16249	1.46830	2.01243
H	0.68821	2.67067	0.84013
O	-1.46737	2.71285	-0.29852

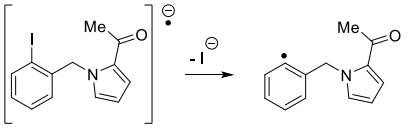


Neutral 6.3 in benzene

26

-631.8918340

C	3.23064	-1.12431	-0.66784
C	2.07944	-1.60437	-0.04983
C	1.13720	-0.72204	0.46933
C	1.34376	0.65916	0.37379
C	2.49472	1.13187	-0.25118
C	3.43646	0.24634	-0.76882
H	3.95927	-1.81827	-1.06944
H	1.91070	-2.67324	0.02802
H	2.65582	2.20143	-0.33029
H	4.32873	0.62958	-1.24932
C	-0.11679	-1.22885	1.13511
H	-0.09030	-2.31437	1.22071
H	-0.21068	-0.81847	2.14516
N	-1.31867	-0.89163	0.37258
C	-2.24278	-1.80317	-0.02372
C	-1.70806	0.36025	-0.07390
C	-3.24285	-1.15749	-0.72921
H	-2.11959	-2.84656	0.22241
C	-2.90341	0.20585	-0.76111
H	-3.44475	1.01490	-1.22572
H	-4.10790	-1.62805	-1.16783
C	-0.98776	1.61979	0.14001
C	0.31687	1.61667	0.92852
H	0.08042	1.35749	1.96755
H	0.69213	2.63896	0.91719
O	-1.43097	2.66248	-0.29917



6.33 6.34

C-I elongation of 6.33 – transition state in benzene

28

-643.8878222

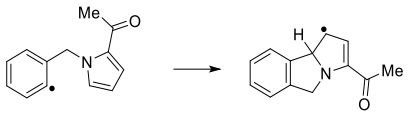
C	0.45728	2.99938	0.30352
C	0.90343	1.77418	-0.17821
C	0.07523	0.69032	-0.31691
C	-1.29197	0.91209	0.04184
C	-1.77325	2.12042	0.52019
C	-0.87703	3.17629	0.65589
H	1.19856	3.81734	0.40937
H	1.94275	1.63856	-0.44631
H	-2.81633	2.23819	0.78252
H	-1.22733	4.12906	1.03573
C	0.51819	-0.65123	-0.84581
H	0.12785	-1.44320	-0.20897
H	0.08527	-0.81232	-1.83820
N	1.95058	-0.74485	-0.97010
C	2.87093	-0.59906	0.09810
C	2.56768	-0.32506	-2.15406
C	4.06814	-0.11644	-0.47768
C	3.86290	0.03537	-1.86775
H	2.02123	-0.34487	-3.08433
H	4.97636	0.05317	0.07748
H	4.59382	0.35627	-2.59660
C	2.63912	-0.87845	1.47426
C	1.38307	-1.60322	1.93405
H	0.48767	-0.96600	1.94220
H	1.15688	-2.48337	1.32090
O	3.51747	-0.57895	2.35256
I	-2.79249	-0.74732	-0.14162
H	1.56055	-1.93659	2.95759

C-I elongation of 6.33 – products 6.34 and iodide anion in benzene

28

-643.9288407

C	1.26617	3.30715	0.52518
C	1.52459	2.08200	-0.08792
C	0.46754	1.25222	-0.47816
C	-0.81080	1.70704	-0.22854
C	-1.11079	2.90370	0.37787
C	-0.04264	3.72196	0.75930
H	2.09477	3.93655	0.82826
H	2.55015	1.76249	-0.25237
H	-2.13815	3.19708	0.56385
H	-0.23351	4.67305	1.24450
C	0.68077	-0.08546	-1.15550
H	-0.05604	-0.80113	-0.79415
H	0.51371	0.01391	-2.23011
N	2.03961	-0.59232	-0.98916
C	2.66147	-1.02701	0.17030
C	2.98190	-0.45412	-1.96024
C	4.01074	-1.17910	-0.11282
C	4.21582	-0.82113	-1.45825
H	2.69862	-0.09610	-2.93816
H	4.73801	-1.53727	0.59864
H	5.14281	-0.83548	-2.00888
C	2.04779	-1.33503	1.47953
C	0.55202	-1.40383	1.64309
H	0.08087	-0.43394	1.46402
H	0.11003	-2.10911	0.93530
O	2.78585	-1.56912	2.42114
I	-3.07672	-0.78031	-0.17658
H	0.33345	-1.72506	2.65966



6.34 **6.35**

Cyclisation 6.34 – starting species 6.34 in benzene

27

-632.3967710

C	-2.25152	-0.19440	1.70366
C	-1.21279	-0.46335	0.84550
C	-1.28790	-0.48055	-0.52763
C	-2.54304	-0.20373	-1.08291
C	-3.63284	0.06860	-0.26188
C	-3.49424	0.07599	1.12534
H	-2.11853	-0.18867	2.77913
H	-4.59701	0.28184	-0.70738
H	-4.34691	0.29609	1.75723
C	-0.09308	-0.77975	-1.40788
H	-0.22027	-1.75524	-1.88131
H	-0.01968	-0.04592	-2.21073
N	1.15246	-0.83891	-0.65787
C	1.72528	-2.02565	-0.31099
C	1.77839	0.17584	0.05326
C	2.74338	-1.79637	0.59086
H	1.35351	-2.94864	-0.72930
C	2.77163	-0.40825	0.82241
H	3.44581	0.14609	1.45600
H	3.38946	-2.54629	1.01790
C	1.51834	1.62660	-0.00269
C	0.64750	2.22247	-1.08483
H	-0.39396	1.91917	-0.95340
H	0.71376	3.30622	-1.01198
O	2.04891	2.34991	0.81898
H	-2.66073	-0.19720	-2.16269
H	0.98135	1.90101	-2.07358

Cyclisation 6.34 – transition state in benzene

27

-632.3816047

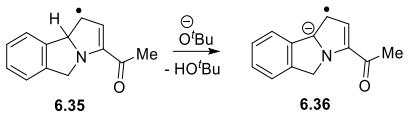
C	-2.75247	1.07209	-0.54556
C	-1.62043	0.70381	0.14435
C	-1.32387	-0.59048	0.51787
C	-2.22573	-1.59567	0.17117
C	-3.38469	-1.26664	-0.53064
C	-3.64909	0.05371	-0.88880
H	-2.94935	2.10168	-0.82354
H	-4.08309	-2.04766	-0.80626
H	-4.55070	0.29508	-1.44073
C	-0.03047	-0.80146	1.28157
H	-0.21248	-0.81269	2.35982
H	0.45063	-1.73693	1.01080
N	0.83435	0.33746	0.96646
C	0.24645	1.58477	1.07730
C	1.72017	0.38448	-0.10395
C	0.88292	2.45844	0.18988
H	-0.35579	1.82128	1.94242
C	1.77881	1.69295	-0.56548
H	2.45314	2.03208	-1.33641
H	0.70660	3.52016	0.12177
C	2.60300	-0.70166	-0.55504
C	2.84567	-1.90392	0.33228
H	2.18534	-2.72113	0.02875
H	3.87180	-2.23349	0.17382
O	3.18060	-0.60101	-1.62166
H	-2.02516	-2.62843	0.44028
H	2.68213	-1.68651	1.38763

Cyclisation 6.34 – product 6.35 in benzene

27

-632.4429452

C	-2.72298	1.11329	0.03468
C	-1.51483	0.49814	0.33099
C	-1.34520	-0.87083	0.15554
C	-2.38629	-1.65687	-0.31986
C	-3.60054	-1.04472	-0.62430
C	-3.76743	0.32891	-0.44974
H	-2.85362	2.18112	0.17199
H	-4.42220	-1.64094	-1.00286
H	-4.71694	0.78997	-0.69416
C	0.05380	-1.28653	0.54820
H	0.05541	-1.89660	1.45621
H	0.55472	-1.84421	-0.24425
N	0.73556	0.00242	0.77614
C	-0.24368	1.10951	0.87699
C	1.79361	0.42296	-0.00804
C	0.40456	2.22056	0.09991
H	-0.38844	1.40323	1.92644
C	1.58355	1.79278	-0.39181
H	2.30145	2.35589	-0.96953
H	-0.01944	3.21127	0.01883
C	2.96830	-0.35047	-0.31893
C	3.17877	-1.69093	0.35436
H	2.84637	-2.49839	-0.30395
H	4.24772	-1.82030	0.52310
O	3.80647	0.09015	-1.11064
H	-2.25862	-2.72476	-0.45884
H	2.64309	-1.76929	1.30107



6.35 6.36

Deprotonation of 6.35 – starting species 6.35 and O^{t}Bu anion in benzene

41

-865.5414505

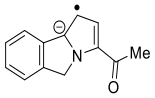
C	-1.44550	2.14282	1.20218
C	-0.46990	1.40486	0.54401
C	-0.05056	1.76949	-0.73533
C	-0.58781	2.87960	-1.37119
C	-1.55437	3.63362	-0.70512
C	-1.97912	3.26528	0.57140
H	-1.79146	1.84179	2.18479
H	-1.98229	4.50669	-1.18410
H	-2.73815	3.85348	1.07459
C	0.97265	0.78170	-1.25232
H	0.58828	0.22957	-2.11715
H	1.91159	1.26342	-1.53727
N	1.18418	-0.10652	-0.10207
C	0.19817	0.13377	0.96416
C	2.41720	-0.36217	0.46075
C	1.00953	0.04775	2.20293
H	-0.63274	-0.70828	1.00024
C	2.28358	-0.28485	1.89227
H	3.09466	-0.50253	2.57146
H	0.58449	0.12832	3.19393
C	3.59978	-0.72149	-0.25442
C	3.50356	-1.00206	-1.74351
H	2.49861	-1.30275	-2.04379
H	3.78981	-0.11813	-2.32134
O	4.69868	-0.83155	0.32233
H	-0.26541	3.15921	-2.36884
O	-1.80194	-1.73305	1.05373
C	-2.44472	-2.05176	-0.11914
C	-2.50310	-3.58342	-0.29855
H	-3.01634	-4.02722	0.55951
H	-3.02601	-3.88167	-1.21532
H	-1.48485	-3.98242	-0.32812
C	-1.71273	-1.45246	-1.34242
H	-1.71620	-0.35899	-1.27261
H	-0.67186	-1.79358	-1.34786
H	-2.18439	-1.73951	-2.28923
C	-3.88773	-1.50449	-0.11299
H	-4.43372	-1.93383	0.73232
H	-3.85722	-0.41807	0.01799
H	-4.43337	-1.73226	-1.03670
H	4.20995	-1.79790	-1.98271

Deprotonation of 6.35 – products 6.36 and HO^{t}Bu in benzene

41

-865.5881066

C	3.07456	-0.36323	1.22371
C	1.85844	-0.68374	0.59286
C	1.84017	-0.87216	-0.81774
C	2.98008	-0.71865	-1.57566
C	4.18879	-0.38626	-0.94197
C	4.21823	-0.22044	0.44757
H	3.11643	-0.21896	2.29762
H	5.09294	-0.25910	-1.52455
H	5.15610	0.03204	0.93151
C	0.44895	-1.29671	-1.24516
H	0.08808	-0.76056	-2.12604
H	0.40518	-2.37710	-1.45591
N	-0.33467	-0.98648	-0.04337
C	0.53109	-0.85633	1.06974
C	-1.57286	-1.50257	0.40823
C	-0.20612	-1.15018	2.22274
H	-0.71292	0.84944	-0.68056
C	-1.48175	-1.54714	1.82277
H	-2.30731	-1.82404	2.46116
H	0.16502	-1.09603	3.23589
C	-2.70802	-1.75413	-0.40275
C	-2.63486	-1.39762	-1.88173
H	-2.00273	-2.09357	-2.44238
H	-3.64407	-1.44668	-2.29056
O	-3.77635	-2.22873	0.06309
H	2.94962	-0.86359	-2.65130
H	-2.23607	-0.38908	-2.03103
O	-0.87087	1.72001	-1.08495
C	-0.89221	2.67683	-0.02434
C	-1.38153	3.97789	-0.64681
H	-2.37949	3.83916	-1.06910
H	-1.42391	4.77121	0.10356
H	-0.70582	4.28859	-1.44749
C	0.52001	2.84334	0.53855
H	0.87325	1.89420	0.95166
H	1.20477	3.15091	-0.25586
H	0.53828	3.59697	1.33119
C	-1.84882	2.19590	1.06581
H	-2.85024	2.05609	0.65053
H	-1.50777	1.23755	1.47095
H	-1.90372	2.91893	1.88444

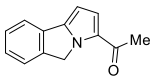


Radical anion 6.36 in benzene

26

-631.9360589

C	-2.81716	1.23354	-0.00400
C	-1.56492	0.58968	-0.01302
C	-1.52384	-0.83500	-0.00138
C	-2.67900	-1.58470	0.01539
C	-3.92532	-0.93635	0.02282
C	-3.97310	0.46364	0.01357
H	-2.87836	2.31612	-0.01101
H	-4.84121	-1.51430	0.03593
H	-4.93751	0.96133	0.02032
C	-0.08030	-1.30179	-0.01060
H	0.17357	-1.89055	0.88109
H	0.14713	-1.91489	-0.89238
N	0.63616	-0.03755	-0.03630
C	-0.22577	1.06055	-0.02863
C	1.96818	0.38507	-0.00609
C	0.56699	2.21633	-0.00723
C	1.89738	1.80923	0.00670
H	2.77318	2.43951	0.02263
H	0.19959	3.23197	-0.00018
C	3.16051	-0.38584	0.00781
C	3.13624	-1.90398	-0.02166
H	3.76880	-2.24570	-0.84704
H	3.58245	-2.28871	0.90182
O	4.30021	0.16506	0.05184
H	-2.63010	-2.66970	0.02409
H	2.14828	-2.34511	-0.13811

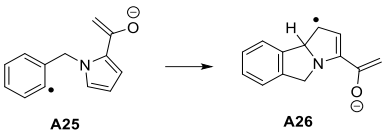


Neutral 6.4 in benzene

26

-631.8907121

C	2.77921	1.23558	0.00029
C	1.55803	0.57164	0.00007
C	1.50400	-0.82922	-0.00020
C	2.66317	-1.58516	-0.00033
C	3.89027	-0.92015	-0.00014
C	3.94510	0.47362	0.00018
H	2.82243	2.31812	0.00051
H	4.80969	-1.49297	-0.00026
H	4.90800	0.97024	0.00040
C	0.06407	-1.29229	0.00005
H	-0.17777	-1.87927	-0.88840
H	-0.17702	-1.87899	0.88894
N	-0.65279	-0.01517	0.00024
C	0.18717	1.06168	0.00026
C	-1.96101	0.42310	-0.00024
C	-0.56941	2.22384	-0.00014
C	-1.91580	1.81474	-0.00048
H	-2.79342	2.44246	-0.00085
H	-0.19102	3.23321	-0.00026
C	-3.16535	-0.41269	0.00009
C	-3.01199	-1.91596	0.00008
H	-4.00145	-2.36822	-0.00002
H	-2.46162	-2.24595	-0.88417
O	-4.26696	0.10372	0.00021
H	2.62436	-2.66863	-0.00064
H	-2.46169	-2.24597	0.88436



A25 A26

Cyclisation A25 – starting species A25 in benzene

26

-631.8555478

C	3.01738	-1.11400	-0.91319
C	1.82597	-1.04667	-0.23348
C	1.41994	-0.01870	0.58835
C	2.32281	1.04128	0.72970
C	3.55026	1.02566	0.07101
C	3.90264	-0.04365	-0.74917
H	3.26628	-1.95393	-1.55184
H	4.23032	1.86133	0.18692
H	4.85500	-0.04520	-1.26738
C	0.09421	-0.02971	1.31940
H	0.20854	-0.58354	2.25671
H	-0.20300	0.99247	1.55125
N	-0.97306	-0.65175	0.56011
C	-1.14079	-2.01394	0.49373
C	-2.00423	-0.02259	-0.11016
C	-2.28719	-2.27222	-0.22227
H	-0.43923	-2.67447	0.98042
C	-2.83561	-1.01590	-0.59110
H	-3.73692	-0.82389	-1.15153
H	-2.68288	-3.25175	-0.44442
C	-2.18813	1.46733	-0.28650
C	-1.06305	2.22908	-0.52280
H	-0.08925	1.77869	-0.66496
H	-1.17122	3.29281	-0.70364
O	-3.39436	1.87020	-0.23716
H	2.04335	1.89223	1.34394

Cyclisation A27 – transition state in benzene

26

-631.8456646

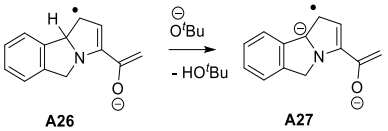
C	2.76532	1.07428	0.58402
C	1.60796	0.75090	-0.09553
C	1.32297	-0.53103	-0.52810
C	2.24428	-1.54477	-0.26118
C	3.42106	-1.24936	0.42617
C	3.68331	0.05166	0.85026
H	2.96615	2.08787	0.91724
H	4.13140	-2.03997	0.63962
H	4.59704	0.27168	1.39273
C	0.01265	-0.75382	-1.26267
H	0.17690	-0.77011	-2.34524
H	-0.46431	-1.68820	-0.97196
N	-0.87425	0.35290	-0.92476
C	-0.34858	1.63546	-0.99750
C	-1.81789	0.31439	0.08642
C	-1.06551	2.44093	-0.11320
H	0.26159	1.92510	-1.83945
C	-1.95610	1.60211	0.58347
H	-2.65997	1.87446	1.35398
H	-0.94857	3.50891	-0.00648
C	-2.61506	-0.89302	0.50763
C	-2.93240	-1.80414	-0.47773
H	-2.65999	-1.63756	-1.51216
H	-3.55102	-2.66049	-0.23469
O	-2.96269	-0.91751	1.73076
H	2.03989	-2.56350	-0.57872

Cyclisation A25 – product A26 in benzene

26

-631.8968615

C	-2.67329	1.11582	0.01557
C	-1.47728	0.49519	0.34985
C	-1.31232	-0.87553	0.17852
C	-2.34628	-1.65183	-0.32996
C	-3.54903	-1.03383	-0.67061
C	-3.71156	0.34102	-0.49950
H	-2.79662	2.18639	0.14370
H	-4.36197	-1.62451	-1.07736
H	-4.64973	0.80987	-0.77392
C	0.07203	-1.29124	0.61779
H	0.02941	-1.89564	1.53103
H	0.60784	-1.86838	-0.13709
N	0.76859	-0.01557	0.85912
C	-0.20996	1.10137	0.92144
C	1.81538	0.37177	0.00084
C	0.44701	2.19580	0.12408
H	-0.39496	1.40439	1.96373
C	1.61371	1.70079	-0.40373
H	2.32825	2.22451	-1.02201
H	0.04373	3.19367	0.03092
C	3.00786	-0.45417	-0.32755
C	3.23978	-1.56800	0.45897
H	2.60931	-1.80509	1.30617
H	4.11839	-2.17609	0.27588
O	3.72622	-0.03784	-1.30002
H	-2.21986	-2.72046	-0.46897



A26 **A27**

Deprotonation A26 – starting species A26 and O^{t}Bu anion in DMSO benzene

40

-864.9549963

C	0.85455	1.06787	-0.06983
C	-0.47646	0.81097	0.24507
C	-1.44999	1.80054	0.14536
C	-1.11651	3.07752	-0.29001
C	0.21150	3.34534	-0.62276
C	1.18393	2.35052	-0.50972
H	1.64902	0.32560	0.02139
H	0.49035	4.33499	-0.96895
H	2.21730	2.56471	-0.75955
C	-2.79363	1.26870	0.58462
H	-3.12815	1.75720	1.50748
H	-3.57628	1.40855	-0.16348
N	-2.55906	-0.17142	0.80055
C	-1.10184	-0.47177	0.75327
C	-3.22539	-1.10379	-0.01773
C	-1.01915	-1.68885	-0.12898
H	-0.71359	-0.68567	1.76122
C	-2.28526	-2.00733	-0.54735
H	-2.57679	-2.83681	-1.17571
H	-0.09333	-2.20394	-0.34030
C	-4.69759	-1.17848	-0.20120
C	-5.48330	-0.44367	0.67071
H	-5.04795	0.13087	1.47794
H	-6.56341	-0.49387	0.58772
O	-5.11535	-1.94031	-1.14293
H	-1.87306	3.85173	-0.37252
O	3.66166	-0.21646	0.13167
C	4.91207	-0.73971	0.05415
C	5.43281	-1.16975	1.45087
H	5.43538	-0.29758	2.11256
H	4.74787	-1.91178	1.87298
H	6.44430	-1.59635	1.42409
C	5.92020	0.29002	-0.52166
H	5.92636	1.17797	0.11854
H	6.94416	-0.09985	-0.59510
H	5.58743	0.59461	-1.51896
C	4.94628	-1.98885	-0.86457
H	4.25878	-2.74238	-0.46781
H	4.59541	-1.70502	-1.86170
H	5.94577	-2.43452	-0.95488

Deprotonation A26 – transition state in benzene

40

-864.9392848

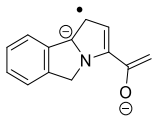
C	-1.99798	-2.10920	1.01013
C	-1.49756	-0.97287	0.37432
C	-2.24758	-0.36596	-0.64397
C	-3.47698	-0.87451	-1.02944
C	-3.97801	-2.01336	-0.39010
C	-3.23742	-2.62025	0.62453
H	-1.42512	-2.59194	1.79555
H	-4.93974	-2.42181	-0.68052
H	-3.63075	-3.50279	1.11901
C	-1.50126	0.83499	-1.18125
H	-1.21188	0.67910	-2.22895
H	-2.08396	1.75936	-1.13776
N	-0.32615	0.93066	-0.31076
C	-0.20345	-0.27201	0.54793
C	-0.03518	2.07037	0.45070
C	0.21698	0.27911	1.85690
H	0.71139	-1.10566	0.09016
C	0.32483	1.65177	1.74301
H	0.67022	2.34410	2.49862
H	0.48060	-0.32604	2.71396
C	0.02682	3.45987	-0.06817
C	-0.00388	3.64390	-1.44353
H	-0.00124	2.80613	-2.12907
H	0.06647	4.64863	-1.84685
O	0.11626	4.39581	0.80779
H	-4.05087	-0.39171	-1.81543
O	1.58865	-1.98765	-0.37859
C	2.88387	-1.49131	-0.33698
C	2.93206	-0.01598	-0.77986
H	2.50884	0.07950	-1.78431
H	2.33177	0.60661	-0.11024
H	3.95864	0.36845	-0.79215
C	3.76980	-2.32147	-1.28193
H	3.38254	-2.24572	-2.30213
H	4.81266	-1.98178	-1.27480
H	3.73952	-3.37366	-0.98203
C	3.45460	-1.59357	1.09185
H	2.83010	-1.00349	1.76862
H	3.43072	-2.63800	1.41939
H	4.48583	-1.22626	1.15578

Deprotonation A26 – product A27 and HO^{t}Bu in benzene

40

-864.9792918

C	1.85336	-1.64040	1.41101
C	0.61634	-1.34843	0.73276
C	0.51133	-1.65961	-0.66167
C	1.54468	-2.21504	-1.36879
C	2.78265	-2.51012	-0.68871
C	2.88752	-2.20717	0.68321
H	1.97785	-1.41382	2.46467
H	3.62181	-2.93307	-1.22654
H	3.82539	-2.41733	1.19270
C	-0.87248	-1.25756	-1.15132
H	-0.83630	-0.51542	-1.95608
H	-1.44855	-2.11732	-1.51007
N	-1.47349	-0.69148	0.05250
C	-0.60826	-0.74429	1.13942
C	-2.64179	-0.01127	0.38461
C	-1.24423	-0.10852	2.20801
H	2.34709	0.16200	-0.47327
C	-2.50515	0.34244	1.71614
H	-3.27096	0.87552	2.25909
H	-0.84054	0.02579	3.20069
C	-3.82106	0.27846	-0.49153
C	-3.84374	-0.20410	-1.78968
H	-3.05378	-0.80607	-2.21048
H	-4.70770	0.01444	-2.40856
O	-4.74914	0.97433	0.04908
H	1.43910	-2.42182	-2.43013
O	2.76675	0.98802	-0.75860
C	2.00604	2.09308	-0.26900
C	0.58667	2.05101	-0.83415
H	0.61954	1.99629	-1.92566
H	0.04784	1.18179	-0.44997
H	0.02510	2.94349	-0.54386
C	2.74485	3.33156	-0.76400
H	2.78707	3.33003	-1.85617
H	2.23551	4.23999	-0.43330
H	3.76717	3.33858	-0.37704
C	1.96609	2.06123	1.25842
H	1.45438	1.15634	1.59596
H	2.98313	2.06694	1.66023
H	1.42360	2.92764	1.64789

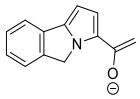


Radical dianion A27 in benzene

25

-631.3230920

C	-2.79616	1.26861	0.00015
C	-1.52389	0.59435	0.00004
C	-1.51194	-0.83559	-0.00005
C	-2.66046	-1.58186	-0.00015
C	-3.93709	-0.90684	-0.00020
C	-3.95083	0.50225	0.00006
H	-2.85190	2.35223	0.00036
H	-4.86243	-1.47021	-0.00020
H	-4.91169	1.01378	0.00010
C	-0.06641	-1.31351	-0.00001
H	0.17602	-1.91101	0.88519
H	0.17614	-1.91105	-0.88515
N	0.67585	-0.05781	-0.00000
C	-0.17135	1.04350	0.00005
C	2.00992	0.34145	-0.00004
C	0.63535	2.18530	0.00006
C	1.98545	1.72613	0.00002
H	2.88326	2.32595	-0.00012
H	0.29084	3.20876	0.00017
C	3.23170	-0.52363	-0.00003
C	3.09615	-1.90294	0.00040
H	2.14214	-2.40623	0.00069
H	3.99521	-2.51046	0.00041
O	4.35035	0.09968	-0.00038
H	-2.61396	-2.66783	-0.00023



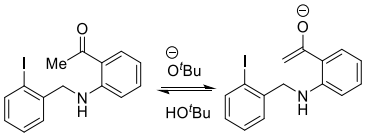
Anion A28 in benzene

25

-631.3512135

C	2.74842	1.25041	0.01241
C	1.52881	0.57753	0.01708
C	1.49794	-0.82908	-0.01138
C	2.66811	-1.56564	-0.04115
C	3.89161	-0.88963	-0.04531
C	3.92515	0.50439	-0.01881
H	2.78056	2.33361	0.03254
H	4.81784	-1.45138	-0.06942
H	4.88094	1.01613	-0.02303
C	0.06475	-1.31299	0.00664
H	-0.19781	-1.90316	-0.87556
H	-0.15083	-1.91007	0.89694
N	-0.67205	-0.05547	0.03047
C	0.15787	1.04719	0.04134
C	-1.98701	0.33549	0.01570
C	-0.63175	2.18072	0.04132
C	-1.97404	1.72659	0.02375
H	-2.87361	2.32114	0.01379
H	-0.28332	3.20213	0.04710
C	-3.21504	-0.53492	-0.01937
C	-3.06975	-1.90053	0.11270
H	-2.12065	-2.38667	0.27177
H	-3.95880	-2.52041	0.09539
O	-4.30755	0.09998	-0.16883
H	2.64008	-2.64990	-0.06167

Scheme 6.8



6.37a 6.43

Deprotonation of 6.37a – starting species 6.37a and O^{t}Bu anion in DMSO

46

-954.4014472

C	4.52224	2.80138	1.45063
C	3.54106	1.94592	1.93789
C	3.12581	0.82513	1.21543
C	3.72679	0.59444	-0.02491
C	4.71225	1.43700	-0.52690
C	5.10861	2.54501	0.21702
H	4.82530	3.66349	2.03217
H	3.07972	2.14180	2.89980
H	5.17035	1.23624	-1.48715
H	5.87569	3.20216	-0.17456
C	2.04303	-0.06100	1.77519
H	2.34030	-1.11206	1.67816
H	1.92182	0.14892	2.84282
C	-0.26778	-0.66219	1.13127
C	-1.38472	-0.53180	0.25119
C	-0.30163	-1.68664	2.10506
C	-2.47146	-1.40631	0.40396
C	-1.39202	-2.52905	2.21664
H	0.52803	-1.80122	2.78997
C	-2.49479	-2.39633	1.36943
H	-3.32701	-1.29052	-0.24944
H	-1.38506	-3.29779	2.98163
H	-3.35084	-3.05190	1.46508
N	0.80331	0.17262	1.05786
O	-0.51852	1.31102	-0.95857
C	-1.42410	0.49117	-0.81992
C	-2.61273	0.53448	-1.74166
H	-3.52046	0.81033	-1.17297
H	-2.41872	1.27845	-2.51306
H	-2.78448	-0.43751	-2.20963
I	3.16978	-1.09114	-1.21131
O	-5.12217	1.47224	0.00289
C	-6.32253	0.84854	-0.23280
C	-7.28882	1.01814	0.96111
H	-7.47031	2.08352	1.13574
H	-8.25440	0.52425	0.80132
H	-6.83088	0.59936	1.86295
C	-6.12618	-0.66805	-0.46713
H	-5.44553	-0.82196	-1.31137
H	-5.67544	-1.12112	0.42214
H	-7.06608	-1.18964	-0.68150
C	-7.01831	1.42963	-1.48619
H	-7.98089	0.94989	-1.69814
H	-7.19008	2.50141	-1.34403
H	-6.36909	1.30192	-2.35858
H	0.78390	0.86132	0.31692

Deprotonation of 6.37a – transition state in DMSO

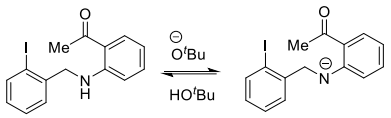
46
-954.3958219

C	-5.09263	-0.62233	2.41772
C	-4.17077	0.40122	2.22939
C	-3.36273	0.45692	1.09170
C	-3.50811	-0.56204	0.14544
C	-4.42479	-1.59277	0.31573
C	-5.21902	-1.62054	1.45927
H	-5.70751	-0.63895	3.30933
H	-4.06717	1.18072	2.97643
H	-4.52509	-2.36713	-0.43418
H	-5.93451	-2.42317	1.59143
C	-2.36919	1.58056	0.93436
H	-2.48876	2.03539	-0.05676
H	-2.58742	2.35562	1.67605
C	0.05529	1.66613	0.46641
C	1.24463	0.94336	0.16912
C	-0.01008	3.02875	0.10839
C	2.31860	1.62756	-0.41203
C	1.07040	3.66832	-0.47684
H	-0.90735	3.59378	0.32848
C	2.25351	2.97609	-0.73177
H	3.23420	1.07968	-0.60045
H	0.99088	4.72149	-0.72292
H	3.10606	3.47810	-1.17194
N	-1.01511	1.07354	1.08579
O	0.59977	-1.06567	1.25336
C	1.36567	-0.52799	0.43501
C	2.43213	-1.26618	-0.22496
H	3.50604	-1.01221	0.42306
H	2.25801	-2.34016	-0.16251
H	2.63175	-0.94566	-1.24724
I	-2.33910	-0.56655	-1.64222
O	4.65203	-0.74385	1.15411
C	5.81478	-0.93029	0.41175
C	7.03927	-0.70301	1.31056
H	7.01637	-1.40412	2.14984
H	7.98004	-0.84180	0.76716
H	7.01785	0.31373	1.71376
C	5.87686	0.06240	-0.76509
H	5.03586	-0.10812	-1.44437
H	5.81149	1.08746	-0.38706
H	6.80443	-0.03798	-1.33823
C	5.87550	-2.36271	-0.15327
H	6.78736	-2.53724	-0.73389
H	5.84445	-3.08484	0.66832
H	5.01291	-2.54541	-0.80104
H	-0.89188	0.08871	1.28871

Deprotonation of 6.37a – products 6.43 and HO^{t}Bu in DMSO

46
-954.4188824

C	-4.82281	-1.38921	2.33045
C	-3.96066	-0.29889	2.37377
C	-3.23401	0.10405	1.25096
C	-3.40109	-0.63475	0.07666
C	-4.25903	-1.72647	0.01279
C	-4.97091	-2.10433	1.14834
H	-5.37437	-1.67796	3.21697
H	-3.84111	0.25973	3.29584
H	-4.37548	-2.27929	-0.91082
H	-5.63841	-2.95629	1.10008
C	-2.29149	1.27864	1.34605
H	-2.48350	1.96639	0.51242
H	-2.50285	1.82754	2.27055
C	0.09705	1.58555	0.77268
C	1.25944	0.97785	0.22306
C	-0.00726	2.98806	0.76567
C	2.28217	1.80750	-0.23581
C	1.02152	3.78186	0.27224
H	-0.89295	3.45723	1.17797
C	2.18301	3.19772	-0.22118
H	3.18391	1.34457	-0.62139
H	0.91539	4.86101	0.29085
H	2.99937	3.80938	-0.58587
N	-0.91737	0.81727	1.29914
O	0.82910	-1.22901	1.04832
C	1.37329	-0.53045	0.11405
C	2.05475	-1.05080	-0.96287
H	3.72277	-0.93581	0.40147
H	2.12584	-2.12777	-1.07311
H	2.42125	-0.42634	-1.76638
I	-2.35730	-0.09787	-1.70722
O	4.48840	-0.90300	1.00754
C	5.67783	-1.10314	0.23926
C	6.83169	-1.03491	1.23072
H	6.71696	-1.80792	1.99438
H	7.78603	-1.18619	0.72142
H	6.84968	-0.05929	1.72248
C	5.80541	0.00105	-0.81080
H	4.96557	-0.04284	-1.51038
H	5.80698	0.98134	-0.32722
H	6.73227	-0.10930	-1.37944
C	5.62684	-2.47412	-0.43554
H	6.54054	-2.66191	-1.00512
H	5.51638	-3.25873	0.31695
H	4.77528	-2.52566	-1.11969
H	-0.72582	-0.18079	1.27692



6.37a **6.44**

Deprotonation of 6.37a – starting species 6.37a and O^{t}Bu anion in DMSO

46

-954.405613787

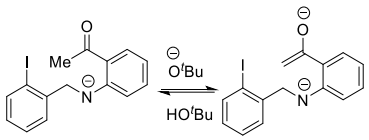
C	-2.50846	3.42287	-0.56243
C	-1.59702	2.53472	-1.12373
C	-1.66590	1.16035	-0.88208
C	-2.69999	0.70658	-0.05893
C	-3.62233	1.57743	0.51013
C	-3.51998	2.94330	0.26025
H	-2.42706	4.48319	-0.76860
H	-0.81114	2.90826	-1.77066
H	-4.41731	1.19966	1.14056
H	-4.23742	3.62260	0.70498
C	-0.62841	0.23909	-1.47724
H	-1.13152	-0.62133	-1.92871
H	-0.09305	0.76388	-2.28164
C	1.21270	-1.17775	-0.69643
C	2.17368	-1.49731	0.30100
C	1.30065	-1.83478	-1.93664
C	3.19628	-2.39504	0.00334
C	2.31138	-2.75698	-2.18978
H	0.59081	-1.60698	-2.72133
C	3.27736	-3.03641	-1.23083
H	3.93747	-2.61993	0.76227
H	2.34959	-3.24454	-3.15782
H	4.07387	-3.74170	-1.43183
N	0.25992	-0.22369	-0.43090
O	0.97279	-0.90175	2.26088
C	2.05476	-1.00189	1.71237
C	3.32736	-0.82740	2.50612
H	4.12647	-0.41121	1.89736
H	3.11960	-0.17346	3.35087
H	3.64417	-1.80135	2.89390
I	-2.96149	-1.37666	0.33025
O	2.09261	1.56443	0.95833
C	2.90794	2.23538	0.07490
C	4.34585	1.67421	0.11236
H	4.32311	0.61068	-0.14738
H	5.01554	2.19037	-0.58518
H	4.75584	1.77285	1.12247
C	2.97206	3.73991	0.41724
H	1.96383	4.16579	0.37776
H	3.35536	3.86704	1.43484
H	3.61453	4.30471	-0.26831
C	2.40097	2.10255	-1.37898
H	3.03398	2.64238	-2.09228
H	2.37184	1.04656	-1.66692
H	1.38515	2.50314	-1.44936
H	0.63904	0.51390	0.18020

Deprotonation of 6.37a – products 6.44 and HO^{t}Bu in DMSO

46

-954.4191446

C	2.66186	3.27068	0.49524
C	1.66997	2.45757	1.03144
C	1.65086	1.07552	0.82190
C	2.68476	0.54277	0.05015
C	3.68942	1.33394	-0.49710
C	3.67365	2.70793	-0.27473
H	2.64432	4.33863	0.67751
H	0.87573	2.89603	1.62576
H	4.47987	0.88726	-1.08725
H	4.45461	3.32739	-0.69940
C	0.53703	0.23859	1.40630
H	0.99488	-0.62696	1.91073
H	0.04690	0.82988	2.19810
C	-1.31764	-1.04252	0.71243
C	-2.29364	-1.54235	-0.24805
C	-1.48457	-1.53689	2.06230
C	-3.33619	-2.37825	0.18673
C	-2.51249	-2.37632	2.42601
H	-0.79040	-1.21930	2.82870
C	-3.46952	-2.81013	1.49433
H	-4.06192	-2.72535	-0.53949
H	-2.58400	-2.70070	3.46030
H	-4.27984	-3.46624	1.78489
N	-0.38639	-0.16457	0.36463
O	-1.22142	-0.81695	-2.25199
C	-2.22471	-1.23322	-1.68632
C	-3.46983	-1.46315	-2.53818
H	-4.37014	-1.06706	-2.06602
H	-3.31421	-0.97527	-3.49900
H	-3.62469	-2.53077	-2.71493
I	2.81377	-1.56335	-0.30150
O	-1.29585	2.20501	-0.78097
C	-2.49617	2.62012	-0.14014
C	-3.67774	1.79490	-0.65514
H	-3.55529	0.74622	-0.37123
H	-4.62104	2.15816	-0.23730
H	-3.73161	1.85757	-1.74556
C	-2.68224	4.08983	-0.50166
H	-1.82947	4.67431	-0.14678
H	-2.75314	4.20354	-1.58659
H	-3.59321	4.48998	-0.05023
C	-2.37388	2.45849	1.37721
H	-3.28295	2.80504	1.87637
H	-2.21345	1.40759	1.63515
H	-1.52932	3.04258	1.75214
H	-1.02193	1.30768	-0.45128



6.44 **6.45**

Deprotonation of 6.44 – starting species 6.37a and O^{t}Bu anion in DMSO

45

-953.8859693

C	4.11576	3.27706	1.03038
C	3.11773	2.43281	1.50374
C	2.95414	1.13248	1.01580
C	3.84355	0.71702	0.02392
C	4.85141	1.54119	-0.46579
C	4.98561	2.83036	0.04171
H	4.21447	4.27831	1.43274
H	2.43761	2.78083	2.27456
H	5.52749	1.18560	-1.23316
H	5.76992	3.47518	-0.33629
C	1.82875	0.27229	1.53963
H	2.22051	-0.74467	1.70053
H	1.55038	0.65316	2.53579
C	-0.29735	-0.49134	0.88249
C	-1.47883	-0.57924	0.01908
C	-0.34090	-1.34889	2.05783
C	-2.51715	-1.47029	0.35895
C	-1.38702	-2.19275	2.33237
H	0.48457	-1.31965	2.75627
C	-2.50405	-2.27699	1.47888
H	-3.38359	-1.52542	-0.28803
H	-1.34935	-2.80358	3.23030
H	-3.32921	-2.94329	1.69633
N	0.71922	0.30394	0.60867
O	-0.83158	1.04712	-1.60411
C	-1.64781	0.22196	-1.19742
C	-2.92280	0.04388	-2.02111
H	-3.80972	0.30614	-1.43603
H	-2.85404	0.70476	-2.88393
H	-3.03982	-0.98462	-2.37046
I	3.71707	-1.25439	-0.80014
O	-5.48699	1.27436	0.44631
C	-6.61095	0.74010	-0.13240
C	-7.87402	1.03605	0.71090
H	-7.99421	2.11855	0.82259
H	-8.78901	0.63097	0.26306
H	-7.75854	0.60235	1.70955
C	-6.49599	-0.79625	-0.27592
H	-5.64242	-1.04268	-0.91546
H	-6.32324	-1.24317	0.70883
H	-7.39401	-1.25083	-0.71042
C	-6.84591	1.32308	-1.54616
H	-7.73533	0.90777	-2.03417
H	-6.96364	2.40970	-1.47976
H	-5.97485	1.11285	-2.17501

Deprotonation of 6.44 – transition state in DMSO

45

-953.8762757

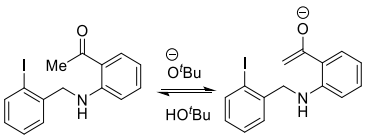
C	-1.93307	3.62466	-0.85019
C	-1.24174	2.50552	-1.30053
C	-1.63397	1.20582	-0.96316
C	-2.75613	1.08205	-0.14378
C	-3.46680	2.18480	0.31890
C	-3.04992	3.46417	-0.03762
H	-1.60102	4.61680	-1.13230
H	-0.36720	2.62742	-1.93203
H	-4.33515	2.05320	0.95222
H	-3.60124	4.32550	0.32049
C	-0.81163	0.03173	-1.43692
H	-1.50141	-0.75504	-1.79353
H	-0.24706	0.35654	-2.33021
C	0.82258	-1.46132	-0.66089
C	1.76804	-1.96280	0.31714
C	0.84661	-2.14980	-1.92466
C	2.64325	-2.98971	0.00720
C	1.72100	-3.19801	-2.18668
H	0.16745	-1.84207	-2.71006
C	2.63759	-3.64001	-1.23549
H	3.35129	-3.30866	0.76857
H	1.68525	-3.67533	-3.16258
H	3.32165	-4.45344	-1.44331
N	0.04797	-0.41649	-0.36972
O	0.85315	-1.43946	2.45464
C	1.83696	-1.37912	1.70473
C	3.07707	-0.71813	2.07533
H	3.02058	0.48835	1.57914
H	3.19950	-0.61566	3.15592
H	3.96006	-1.13572	1.59125
I	-3.46627	-0.84633	0.45506
O	3.01671	1.76772	1.12220
C	3.99301	1.95673	0.14519
C	3.87738	3.37623	-0.42946
H	4.01076	4.11464	0.36667
H	4.62719	3.56344	-1.20583
H	2.88388	3.51750	-0.86557
C	3.82059	0.94706	-1.00737
H	3.87045	-0.07637	-0.62403
H	2.83761	1.08012	-1.47124
H	4.58909	1.07462	-1.77730
C	5.40031	1.78256	0.74859
H	6.18880	1.93553	0.00422
H	5.54429	2.50288	1.55958
H	5.50620	0.77614	1.16315

Deprotonation of 6.44 – products 6.45 and HO^{t}Bu in DMSO

45

-953.8958041

C	-1.63245	3.64037	-0.44529
C	-0.95311	2.52965	-0.93191
C	-1.44371	1.22899	-0.77160
C	-2.65498	1.09692	-0.09317
C	-3.35778	2.19148	0.40113
C	-2.84040	3.47118	0.22356
H	-1.22162	4.63306	-0.58810
H	-0.00899	2.65773	-1.45243
H	-4.29904	2.05221	0.91800
H	-3.38499	4.32621	0.60610
C	-0.62922	0.06243	-1.27419
H	-1.31899	-0.67183	-1.72935
H	-0.00020	0.42832	-2.10865
C	0.92690	-1.52172	-0.52620
C	1.83585	-2.09439	0.44908
C	0.97260	-2.12721	-1.82847
C	2.67344	-3.13868	0.10139
C	1.82374	-3.18806	-2.13267
H	0.32926	-1.75041	-2.61405
C	2.68908	-3.71561	-1.18209
H	3.34794	-3.52286	0.86295
H	1.80521	-3.60213	-3.13768
H	3.35345	-4.53905	-1.41592
N	0.15218	-0.48307	-0.19396
O	0.89071	-1.77523	2.63067
C	1.89677	-1.56668	1.86823
C	3.06349	-0.92011	2.23873
H	2.93693	1.06649	1.43705
H	3.20553	-0.58831	3.26427
H	3.91413	-0.89599	1.56800
I	-3.52743	-0.83272	0.22228
O	2.94076	1.99510	1.12835
C	3.76656	2.08958	-0.03594
C	3.59019	3.51030	-0.55689
H	3.89751	4.23295	0.20319
H	4.19465	3.66944	-1.45291
H	2.54187	3.69211	-0.80599
C	3.31295	1.07219	-1.08362
H	3.37434	0.05437	-0.68559
H	2.26943	1.25028	-1.35814
H	3.93504	1.14048	-1.98022
C	5.22602	1.84299	0.35076
H	5.88088	1.94027	-0.51907
H	5.54185	2.56507	1.10787
H	5.34671	0.83660	0.76025



6.37a **6.43**

Deprotonation of 6.37a – starting species 6.37a and O^{t}Bu anion in benzene

46

-954.3624541

C	-5.11516	-0.37059	2.42726
C	-4.09437	0.56235	2.28366
C	-3.28074	0.58724	1.14946
C	-3.52497	-0.36618	0.15617
C	-4.54078	-1.30611	0.28338
C	-5.33654	-1.30735	1.42561
H	-5.72945	-0.36794	3.31966
H	-3.91314	1.29178	3.06581
H	-4.71206	-2.03386	-0.49976
H	-6.12511	-2.04369	1.52555
C	-2.17071	1.60458	1.04067
H	-2.24828	2.11596	0.07363
H	-2.30299	2.36172	1.82162
C	0.22091	1.39375	0.45271
C	1.28491	0.51612	0.09517
C	0.31247	2.74559	0.07426
C	2.40499	1.02791	-0.57559
C	1.42765	3.22054	-0.59915
H	-0.48153	3.43035	0.34562
C	2.48488	2.37153	-0.91670
H	3.25946	0.37967	-0.79473
H	1.47397	4.27206	-0.86337
H	3.36720	2.74752	-1.42010
N	-0.88066	0.94940	1.14289
O	0.39611	-1.40090	1.17250
C	1.21212	-0.94182	0.37713
C	2.12616	-1.86253	-0.38047
H	3.18304	-1.54757	-0.35190
H	1.99964	-2.87252	0.00740
H	1.83771	-1.84105	-1.43731
I	-2.35872	-0.40239	-1.62841
O	4.99999	-0.66947	-0.78205
C	5.75437	-0.66325	0.35493
C	7.11358	0.03939	0.12398
H	6.93336	1.06844	-0.20266
H	7.74521	0.06028	1.02132
H	7.65386	-0.47904	-0.67438
C	6.04415	-2.10668	0.83763
H	5.09599	-2.61966	1.02907
H	6.56814	-2.64938	0.04463
H	6.65150	-2.14218	1.75096
C	5.02948	0.08002	1.50685
H	5.60723	0.08898	2.43947
H	4.83218	1.11427	1.20642
H	4.06376	-0.40014	1.70115
H	-0.86615	-0.03720	1.37203

Deprotonation of 6.37a – transition state in benzene

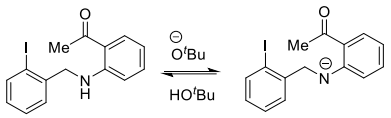
46
-954.3559457

C	-5.37903	-0.33224	1.92442
C	-4.50559	0.71612	1.65847
C	-3.49329	0.60119	0.70410
C	-3.38125	-0.61447	0.02271
C	-4.24689	-1.67228	0.27444
C	-5.24813	-1.52874	1.23088
H	-6.15272	-0.21506	2.67372
H	-4.59757	1.64997	2.20262
H	-4.14143	-2.60383	-0.26698
H	-5.91867	-2.35638	1.42943
C	-2.54873	1.75442	0.46815
H	-2.49008	1.95886	-0.60822
H	-2.95857	2.65072	0.94769
C	-0.08396	1.87160	0.34948
C	1.11339	1.11033	0.37950
C	-0.08779	3.09333	-0.34626
C	2.26636	1.63476	-0.20932
C	1.06816	3.57741	-0.94280
H	-0.99768	3.68115	-0.38318
C	2.26000	2.86237	-0.86144
H	3.18866	1.06774	-0.12430
H	1.03746	4.53136	-1.45847
H	3.17063	3.25207	-1.30022
N	-1.22954	1.42991	0.97623
O	0.36491	-0.55693	1.89208
C	1.15434	-0.26695	0.98317
C	2.16464	-1.18598	0.47669
H	3.31670	-0.81217	0.86869
H	1.97844	-2.20079	0.82748
H	2.26091	-1.14071	-0.61049
I	-1.87617	-0.89605	-1.45968
O	4.59653	-0.37603	1.21117
C	5.58033	-0.88382	0.38292
C	6.96425	-0.56608	0.97451
H	7.04997	-1.02006	1.96586
H	7.78088	-0.93762	0.34419
H	7.07121	0.51664	1.08693
C	5.49495	-0.25243	-1.02383
H	4.51845	-0.46688	-1.46954
H	5.59930	0.83426	-0.94119
H	6.27264	-0.62825	-1.69840
C	5.45022	-2.41558	0.23883
H	6.24006	-2.83989	-0.39143
H	5.50410	-2.87820	1.22873
H	4.48171	-2.66957	-0.20172
H	-1.11437	0.55389	1.47418

Deprotonation of 6.37a – products 6.43 and HO^{t}Bu in benzene

46
-954.3766453

C	-5.01236	-1.27271	2.15978
C	-4.18708	-0.15400	2.19364
C	-3.35978	0.17880	1.11969
C	-3.38523	-0.65988	0.00144
C	-4.20413	-1.78143	-0.05068
C	-5.01872	-2.08883	1.03559
H	-5.64010	-1.50893	3.01071
H	-4.17131	0.48082	3.07325
H	-4.20587	-2.41417	-0.92939
H	-5.65185	-2.96745	0.99685
C	-2.45649	1.38659	1.20821
H	-2.59512	2.00175	0.30982
H	-2.76861	1.99653	2.06626
C	-0.04195	1.67383	0.73455
C	1.16132	1.00425	0.37782
C	-0.15544	3.05330	0.49017
C	2.21045	1.76650	-0.12893
C	0.90227	3.77415	-0.05346
H	-1.06978	3.56912	0.76030
C	2.10087	3.13884	-0.35361
H	3.14439	1.26383	-0.35457
H	0.78887	4.84009	-0.22082
H	2.94054	3.69718	-0.75042
N	-1.07815	0.97175	1.30499
O	0.63602	-1.05023	1.48370
C	1.27880	-0.50436	0.52187
C	2.06328	-1.17549	-0.39529
H	3.85222	-0.85777	0.73023
H	2.10544	-2.25807	-0.34658
H	2.45419	-0.68257	-1.27574
I	-2.17679	-0.23229	-1.70024
O	4.72679	-0.73644	1.15618
C	5.74652	-1.04378	0.21461
C	7.06132	-0.94089	0.97958
H	7.06511	-1.64925	1.81123
H	7.90904	-1.16030	0.32535
H	7.17983	0.06698	1.38440
C	5.72197	-0.03177	-0.93358
H	4.77521	-0.09855	-1.47572
H	5.82406	0.98158	-0.53688
H	6.53701	-0.21778	-1.63885
C	5.55356	-2.46240	-0.32530
H	6.35590	-2.72789	-1.01964
H	5.55141	-3.17737	0.50098
H	4.59760	-2.53882	-0.84925
H	-0.83879	-0.00093	1.51053



6.37a **6.44**

Deprotonation of 6.37a – starting species 6.37a and O^{t}Bu anion in benzene

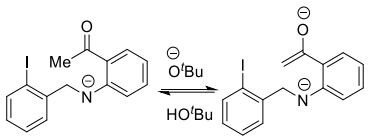
46
-954.3636946

C	-1.88415	3.56066	0.70822
C	-1.02074	2.71512	0.02208
C	-1.39266	1.40052	-0.28477
C	-2.64155	0.96532	0.15352
C	-3.52140	1.79867	0.83542
C	-3.13834	3.10842	1.10571
H	-1.57250	4.57203	0.94259
H	-0.00651	3.01307	-0.24768
H	-4.48681	1.43191	1.16002
H	-3.81855	3.76220	1.63964
C	-0.40264	0.52459	-1.02077
H	-0.94260	-0.20303	-1.62004
H	0.20106	1.15764	-1.67772
C	1.02396	-1.35419	-0.23921
C	2.05756	-1.82805	0.63011
C	0.61893	-2.22123	-1.28502
C	2.64992	-3.07231	0.38435
C	1.20921	-3.45629	-1.47477
H	-0.16285	-1.91645	-1.96572
C	2.24299	-3.89991	-0.64889
H	3.44249	-3.41091	1.04090
H	0.86399	-4.08019	-2.29249
H	2.71213	-4.86264	-0.80652
N	0.47000	-0.12651	-0.05626
O	1.76944	-0.25529	2.38777
C	2.47834	-1.07964	1.84757
C	3.83600	-1.39836	2.45321
H	4.60762	-1.49374	1.68810
H	4.09004	-0.59312	3.13986
H	3.78826	-2.33579	3.01408
I	-3.26442	-1.06141	-0.15029
O	1.93448	2.27260	-0.12724
C	3.13544	2.18121	-0.77334
C	4.13118	1.28701	0.00397
H	3.74983	0.26101	0.02540
H	5.13125	1.26890	-0.44699
H	4.21081	1.64589	1.03479
C	3.77848	3.57709	-0.94099
H	3.09271	4.22263	-1.49874
H	3.93339	4.02130	0.04717
H	4.73992	3.54570	-1.46868
C	2.96212	1.55850	-2.18123
H	3.91017	1.45351	-2.72339
H	2.50880	0.56561	-2.07966
H	2.28819	2.18396	-2.77626
H	1.07615	0.58962	0.37553

Deprotonation of 6.37a – products 6.44 and HO^{t}Bu in benzene

46
-954.3791836

C	2.50784	3.18917	0.85635
C	1.57952	2.27682	1.34616
C	1.61672	0.92287	1.00204
C	2.64207	0.51828	0.14607
C	3.58525	1.41058	-0.35216
C	3.51312	2.75468	0.00129
H	2.44231	4.23362	1.13868
H	0.79176	2.61406	2.01251
H	4.36892	1.06284	-1.01333
H	4.24391	3.45176	-0.39212
C	0.54765	-0.01138	1.51626
H	1.03283	-0.92096	1.90953
H	0.06786	0.47129	2.38767
C	-1.38905	-1.12014	0.77482
C	-2.39942	-1.44694	-0.21255
C	-1.61872	-1.66518	2.08513
C	-3.55684	-2.12643	0.15945
C	-2.76652	-2.37012	2.39955
H	-0.87954	-1.50917	2.86062
C	-3.76918	-2.59861	1.45324
H	-4.30202	-2.33953	-0.60130
H	-2.88804	-2.74774	3.41118
H	-4.66879	-3.14511	1.70663
N	-0.38551	-0.30642	0.45772
O	-1.13009	-1.37644	-2.22285
C	-2.19239	-1.18563	-1.66333
C	-3.36509	-0.68710	-2.49403
H	-4.32115	-0.70872	-1.97446
H	-3.12588	0.35260	-2.73192
H	-3.42284	-1.25314	-3.42545
I	2.84183	-1.52681	-0.42316
O	-1.58034	1.61592	-1.06092
C	-2.31062	2.53786	-0.27103
C	-3.66615	2.72646	-0.95298
H	-4.21820	1.78318	-0.94388
H	-4.26188	3.49059	-0.44540
H	-3.51773	3.02976	-1.99303
C	-1.55497	3.87012	-0.23540
H	-0.56870	3.72521	0.21255
H	-1.41427	4.24220	-1.25353
H	-2.09901	4.62373	0.34242
C	-2.52273	2.01600	1.15200
H	-3.13828	2.71698	1.72317
H	-3.01946	1.04215	1.13115
H	-1.56654	1.89289	1.66692
H	-1.05336	0.97385	-0.49999



6.44 **6.45**

Deprotonation of 6.44 – starting species 6.37a and O^{t}Bu anion in benzene

45

-953.7725938

C	-5.10006	-2.03338	-1.42362
C	-4.01896	-2.20136	-0.56712
C	-3.35481	-1.11680	0.01487
C	-3.82831	0.15283	-0.31237
C	-4.91012	0.34992	-1.16485
C	-5.54932	-0.75189	-1.72402
H	-5.58463	-2.89864	-1.86129
H	-3.65398	-3.19814	-0.34215
H	-5.24877	1.35226	-1.39558
H	-6.38836	-0.60187	-2.39361
C	-2.14837	-1.36450	0.88954
H	-2.19727	-0.67738	1.75512
H	-2.25086	-2.38158	1.31312
C	0.18691	-1.30928	0.75898
C	1.46714	-1.11501	0.08852
C	0.28719	-1.57773	2.17572
C	2.66098	-1.10278	0.81331
C	1.49664	-1.59049	2.84639
H	-0.61448	-1.78062	2.73995
C	2.70260	-1.34078	2.18694
H	3.60531	-0.93922	0.29414
H	1.49933	-1.80053	3.91396
H	3.64884	-1.34888	2.71429
N	-0.95889	-1.20229	0.09835
O	0.82868	-1.50844	-2.17878
C	1.57034	-0.95168	-1.38411
C	2.66990	-0.04233	-1.90621
H	3.67505	-0.37964	-1.61693
H	2.59261	0.00805	-2.99293
H	2.54487	0.95868	-1.48126
I	-2.90087	1.90034	0.49750
O	5.73447	-0.64638	-0.70927
C	6.22914	0.59445	-0.46331
C	7.69676	0.53071	0.03791
H	8.31006	0.03057	-0.71905
H	8.12784	1.51946	0.24589
H	7.73263	-0.06926	0.95297
C	5.39737	1.33206	0.61862
H	4.35972	1.41662	0.28112
H	5.39752	0.73831	1.53865
H	5.77874	2.33673	0.84551
C	6.21380	1.47532	-1.74207
H	6.61530	2.48427	-1.57748
H	6.80636	0.98298	-2.52024
H	5.18473	1.56108	-2.10464

Deprotonation of 6.44 – transition state in benzene

45

-953.7658645

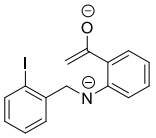
C	1.09079	-2.93380	1.21116
C	0.58676	-1.66583	0.95068
C	1.40870	-0.62680	0.49783
C	2.75540	-0.93525	0.32096
C	3.28859	-2.19391	0.57587
C	2.44389	-3.20348	1.02709
H	0.42182	-3.71405	1.55734
H	-0.46217	-1.42328	1.07828
H	4.34316	-2.38503	0.42282
H	2.84776	-4.18962	1.22721
C	0.81436	0.74153	0.21969
H	1.42070	1.47761	0.78724
H	1.03149	0.97233	-0.84485
C	-1.20644	1.91251	0.25286
C	-2.64239	2.02058	0.45968
C	-0.58383	3.08893	-0.30440
C	-3.31761	3.17465	0.09795
C	-1.30128	4.23147	-0.62900
H	0.48673	3.08894	-0.47233
C	-2.67974	4.30263	-0.44037
H	-4.39098	3.20825	0.26369
H	-0.76822	5.08521	-1.04201
H	-3.24218	5.19282	-0.69658
N	-0.57417	0.78224	0.53420
O	-3.07131	0.49258	2.23446
C	-3.44396	0.93420	1.14322
C	-4.65119	0.45282	0.47676
H	-4.43002	-0.60060	-0.27499
H	-5.38357	0.08009	1.19758
H	-5.08779	1.16382	-0.22491
I	4.12299	0.56341	-0.39008
O	-4.46470	-1.69330	-1.06689
C	-3.30805	-2.44883	-0.95859
C	-3.01243	-2.78978	0.51718
H	-3.84829	-3.36364	0.93188
H	-2.09402	-3.38068	0.62308
H	-2.90812	-1.86988	1.10024
C	-2.10168	-1.68782	-1.54155
H	-2.31549	-1.42483	-2.58292
H	-1.92020	-0.76923	-0.97429
H	-1.18202	-2.28629	-1.51116
C	-3.48883	-3.76351	-1.73796
H	-2.59651	-4.39956	-1.68639
H	-4.34078	-4.31717	-1.33073
H	-3.69856	-3.53761	-2.78816

Deprotonation of 6.44 – products 6.45 and HO^{t}Bu in benzene

45

-953.7711490

C	-1.58567	3.61594	-0.40165
C	-0.91583	2.50388	-0.89588
C	-1.42496	1.20754	-0.76394
C	-2.64286	1.08209	-0.09876
C	-3.33875	2.17835	0.40148
C	-2.80523	3.45399	0.24793
H	-1.15305	4.60369	-0.51479
H	0.04385	2.62223	-1.38857
H	-4.28360	2.03902	0.91195
H	-3.34053	4.31030	0.64204
C	-0.61406	0.03829	-1.26873
H	-1.30872	-0.69705	-1.71969
H	0.00845	0.40363	-2.11348
C	0.93734	-1.52937	-0.50522
C	1.85857	-2.07374	0.47656
C	0.98318	-2.15520	-1.79905
C	2.69576	-3.11948	0.14282
C	1.83675	-3.21900	-2.08757
H	0.33389	-1.79510	-2.58838
C	2.70642	-3.72504	-1.13073
H	3.37774	-3.48068	0.90919
H	1.81627	-3.65148	-3.08602
H	3.37359	-4.55103	-1.35129
N	0.16659	-0.48740	-0.18836
O	0.96449	-1.71307	2.66912
C	1.93902	-1.50913	1.88822
C	3.11523	-0.83128	2.20421
H	2.86431	1.13136	1.45257
H	3.28137	-0.48715	3.22223
H	3.95641	-0.84781	1.52070
I	-3.51805	-0.84444	0.20738
O	2.95132	2.06527	1.15202
C	3.67424	2.09626	-0.06994
C	3.48810	3.50597	-0.62490
H	3.85496	4.24391	0.09400
H	4.03147	3.62907	-1.56596
H	2.42665	3.69557	-0.80224
C	3.12567	1.06050	-1.05225
H	3.24627	0.04794	-0.65773
H	2.05384	1.21135	-1.20130
H	3.64318	1.13136	-2.01438
C	5.16007	1.83413	0.20170
H	5.74395	1.88407	-0.72271
H	5.54729	2.57610	0.90571
H	5.28836	0.84200	0.64072

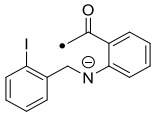


Dianion 6.45 in DMSO

30

-720.2417849

C	-2.13089	3.48667	-0.12209
C	-0.97347	2.73231	0.04084
C	-0.99777	1.33398	0.07945
C	-2.25369	0.73645	-0.05454
C	-3.42555	1.46515	-0.22085
C	-3.36283	2.85581	-0.25400
H	-2.07005	4.56888	-0.14653
H	-0.00328	3.20129	0.14433
H	-4.37746	0.95970	-0.32513
H	-4.27271	3.42997	-0.38273
I	-2.44726	-1.40102	-0.02193
C	0.27881	0.53079	0.25413
H	0.11289	-0.16544	1.09151
H	0.36219	-0.13072	-0.62542
N	1.43073	1.36730	0.42583
C	2.64890	0.85584	0.21220
C	3.74308	1.79505	0.21477
C	3.03607	-0.51994	-0.05388
C	5.03922	1.46447	-0.12249
H	3.49560	2.82383	0.46250
C	4.35689	-0.80503	-0.41034
C	5.37358	0.14917	-0.47220
H	5.80204	2.23874	-0.11717
H	4.59688	-1.84559	-0.61364
H	6.38640	-0.12705	-0.74045
C	2.14051	-1.72034	0.19779
C	1.91602	-2.60199	-0.83717
H	1.34690	-3.51182	-0.66687
H	2.29324	-2.40793	-1.83337
O	1.71046	-1.86263	1.40308

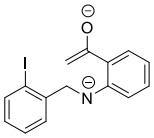


Radical anion A29 in DMSO

30

-720.1128365

C	-2.15076	3.48302	-0.05636
C	-0.98080	2.73576	0.02377
C	-1.00108	1.33810	0.03484
C	-2.25489	0.72718	-0.04190
C	-3.43696	1.45410	-0.12376
C	-3.38318	2.84458	-0.12967
H	-2.09768	4.56537	-0.06114
H	-0.01740	3.22522	0.08266
H	-4.39053	0.94485	-0.18241
H	-4.30176	3.41570	-0.19153
I	-2.42678	-1.40719	-0.03936
C	0.27620	0.52989	0.12722
H	0.22201	-0.15568	0.98640
H	0.34337	-0.14560	-0.74046
N	1.43766	1.35966	0.23231
C	2.67008	0.83590	0.12843
C	3.71419	1.81694	0.09168
C	3.05169	-0.54910	-0.00725
C	5.03058	1.48485	-0.12970
H	3.41283	2.85084	0.21586
C	4.39091	-0.84291	-0.25004
C	5.37603	0.14142	-0.32070
H	5.79022	2.25679	-0.16538
H	4.67088	-1.88520	-0.35732
H	6.40717	-0.13723	-0.50405
C	2.11159	-1.71290	0.23056
C	1.91664	-2.57833	-0.81433
H	1.25185	-3.42858	-0.70184
H	2.41462	-2.42862	-1.76366
O	1.60858	-1.78321	1.40823

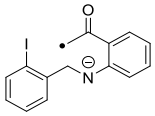


Dianion 6.45 in benzene

30

-720.1214667

C	-2.13006	3.48326	-0.08063
C	-0.97212	2.72390	0.04319
C	-1.00023	1.32366	0.06367
C	-2.26109	0.73416	-0.04657
C	-3.43479	1.46873	-0.17377
C	-3.36913	2.85950	-0.19023
H	-2.06542	4.56626	-0.09175
H	0.01026	3.17310	0.12987
H	-4.38871	0.96334	-0.26029
H	-4.28020	3.43938	-0.28789
I	-2.44519	-1.40246	-0.03073
C	0.28209	0.52787	0.20261
H	0.15756	-0.15014	1.06378
H	0.32968	-0.15607	-0.66379
N	1.42583	1.38279	0.30647
C	2.64735	0.86391	0.15422
C	3.73661	1.80906	0.13105
C	3.04676	-0.52384	-0.02686
C	5.04706	1.46495	-0.13021
H	3.46986	2.84834	0.30339
C	4.37986	-0.82164	-0.30280
C	5.40102	0.13229	-0.37588
H	5.80649	2.24427	-0.14565
H	4.62515	-1.87234	-0.43678
H	6.42636	-0.15667	-0.57852
C	2.12954	-1.71806	0.21024
C	1.92439	-2.59215	-0.84132
H	1.32158	-3.48404	-0.69331
H	2.32572	-2.38895	-1.82669
O	1.66406	-1.84866	1.39381

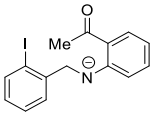


Radical anion A29 in benzene

30

-720.0741434

C	-2.14754	3.48074	-0.06301
C	-0.97917	2.73399	0.03141
C	-0.99835	1.33603	0.04211
C	-2.25085	0.72442	-0.04808
C	-3.43154	1.45203	-0.14507
C	-3.37923	2.84217	-0.15177
H	-2.09459	4.56345	-0.06660
H	-0.01300	3.21684	0.10326
H	-4.38288	0.93982	-0.21424
H	-4.29741	3.41316	-0.22533
I	-2.41074	-1.40783	-0.03724
C	0.27860	0.53260	0.15251
H	0.22917	-0.13937	1.02595
H	0.34475	-0.17006	-0.69600
N	1.43500	1.36645	0.23497
C	2.66359	0.83819	0.13695
C	3.71468	1.81308	0.09678
C	3.03761	-0.54889	-0.00061
C	5.02646	1.47353	-0.13159
H	3.41696	2.84739	0.22672
C	4.37481	-0.84916	-0.25811
C	5.36404	0.12707	-0.33086
H	5.79124	2.24119	-0.16718
H	4.64253	-1.89444	-0.36874
H	6.39327	-0.15638	-0.52000
C	2.08785	-1.70411	0.23953
C	1.91254	-2.57634	-0.81073
H	1.22067	-3.40579	-0.71399
H	2.45058	-2.44700	-1.74098
O	1.54777	-1.75137	1.39115

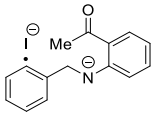


Anion 6.44 in DMSO

31

-720.7637628

C	-2.20085	3.46156	-0.07705
C	-1.04200	2.72823	0.15431
C	-1.04319	1.33020	0.16128
C	-2.26927	0.70695	-0.08198
C	-3.44070	1.41662	-0.31935
C	-3.40477	2.80811	-0.31529
H	-2.16245	4.54474	-0.07323
H	-0.09563	3.22109	0.33673
H	-4.37106	0.89531	-0.50637
H	-4.31436	3.36731	-0.49935
I	-2.41008	-1.43248	-0.10797
C	0.22554	0.53757	0.41749
H	0.03072	-0.15127	1.25273
H	0.38086	-0.13623	-0.44661
N	1.36147	1.37618	0.64572
C	2.56248	0.92364	0.35296
C	3.64247	1.89392	0.33478
C	2.94688	-0.42694	-0.04956
C	4.83261	1.64901	-0.28618
H	3.43313	2.86716	0.76734
C	4.16815	-0.60837	-0.75104
C	5.09689	0.39343	-0.89877
H	5.58578	2.43047	-0.32256
H	4.40734	-1.59716	-1.12881
H	6.03183	0.21465	-1.41465
C	2.27380	-1.61825	0.44272
C	2.47154	-2.93961	-0.28996
H	1.63342	-3.59039	-0.04261
H	2.53681	-2.81815	-1.37121
O	1.60020	-1.63374	1.47875
H	3.38859	-3.42573	0.05498

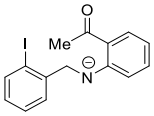


Radical dianion A30 in DMSO

31

-720.8694189

C	-0.12726	4.73811	-0.29030
C	0.59354	3.56886	-0.03737
C	-0.06068	2.35267	0.19168
C	-1.43972	2.41520	0.14479
C	-2.20452	3.52685	-0.10270
C	-1.51850	4.72849	-0.32542
H	0.40607	5.66608	-0.46306
H	1.67650	3.57633	-0.01065
H	-3.28796	3.48719	-0.12616
H	-2.07094	5.63989	-0.52472
I	-3.16960	-1.52326	-0.16550
C	0.66061	1.04467	0.46486
H	0.20811	0.58976	1.35745
H	0.40462	0.34224	-0.35134
N	2.07679	1.22118	0.58362
C	2.88005	0.21915	0.29758
C	4.29244	0.52887	0.15888
C	2.52811	-1.17000	0.01044
C	5.16694	-0.31217	-0.46550
H	4.61529	1.50592	0.50409
C	3.45646	-1.97711	-0.69851
C	4.74396	-1.57602	-0.96158
H	6.20124	-0.00669	-0.59257
H	3.15763	-2.97981	-0.98607
H	5.43604	-2.22797	-1.47949
C	1.39745	-1.84287	0.63018
C	0.87579	-3.13832	0.02083
H	-0.17265	-3.23881	0.30071
H	0.96538	-3.16478	-1.06511
O	0.87752	-1.45648	1.68292
H	1.42365	-3.99111	0.43250

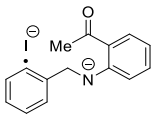


Anion 6.44 in benzene

31

-720.7285731

C	-2.18980	3.45870	-0.05112
C	-1.03485	2.71818	0.17078
C	-1.04312	1.31980	0.16445
C	-2.27245	0.70673	-0.08112
C	-3.44121	1.42377	-0.30962
C	-3.39835	2.81440	-0.29330
H	-2.14542	4.54188	-0.03705
H	-0.08056	3.19532	0.35661
H	-4.37315	0.90612	-0.49875
H	-4.30555	3.38028	-0.47054
I	-2.42166	-1.43147	-0.11951
C	0.22662	0.52742	0.41330
H	0.04317	-0.15339	1.25819
H	0.37258	-0.15199	-0.44832
N	1.35739	1.37496	0.62057
C	2.55791	0.92505	0.33874
C	3.62996	1.90546	0.30819
C	2.95605	-0.42924	-0.04229
C	4.82307	1.66330	-0.30466
H	3.40487	2.88034	0.72814
C	4.18203	-0.60738	-0.73388
C	5.10250	0.39995	-0.89545
H	5.56891	2.45178	-0.35078
H	4.43348	-1.59961	-1.09484
H	6.04137	0.22084	-1.40455
C	2.28816	-1.61958	0.46027
C	2.51571	-2.95171	-0.25343
H	1.68206	-3.60654	-0.00168
H	2.58820	-2.84432	-1.33619
O	1.59583	-1.63596	1.47951
H	3.43603	-3.41900	0.10860

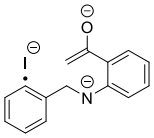


Radical dianion A30 in benzene

31

-720.7602330

C	-0.01608	4.58619	0.09895
C	0.77667	3.45780	0.30054
C	0.22023	2.17253	0.27831
C	-1.13855	2.12368	0.03455
C	-1.97289	3.19610	-0.18130
C	-1.38205	4.46482	-0.13940
H	0.43818	5.57096	0.12420
H	1.84390	3.54053	0.46829
H	-3.03180	3.06234	-0.37175
H	-1.98982	5.34934	-0.30106
I	-4.08618	-1.28295	-0.25067
C	1.04633	0.92658	0.54448
H	0.81618	0.58873	1.56452
H	0.67294	0.11511	-0.10418
N	2.44737	1.17976	0.35099
C	3.28475	0.19962	0.06265
C	4.60367	0.59925	-0.40900
C	3.05956	-1.25257	0.06143
C	5.42367	-0.24806	-1.09274
H	4.86884	1.64267	-0.27111
C	3.90981	-2.07001	-0.72305
C	5.05781	-1.60390	-1.31921
H	6.36941	0.12243	-1.47929
H	3.67669	-3.12735	-0.80592
H	5.69738	-2.26436	-1.89189
C	2.17480	-1.92161	1.00288
C	1.73663	-3.35500	0.70955
H	0.86960	-3.57069	1.33208
H	1.48100	-3.50458	-0.34033
O	1.81047	-1.42289	2.07009
H	2.53366	-4.05661	0.97234



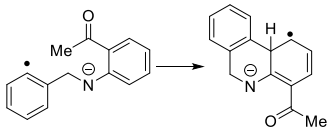
Radical trianion A31 in DMSO

30

-720.3443286

C	-0.57977	4.53469	-0.00855
C	0.31687	3.46577	0.07255
C	-0.13711	2.14321	0.15123
C	-1.51198	2.00012	0.14122
C	-2.44244	3.00519	0.05829
C	-1.95449	4.31761	-0.01640
H	-0.19722	5.54765	-0.06890
H	1.38770	3.62885	0.07119
H	-3.50786	2.80136	0.04814
H	-2.64486	5.15122	-0.08282
I	-3.41021	-1.54257	-0.24121
C	0.78877	0.94584	0.25871
H	0.56355	0.44944	1.21651
H	0.46588	0.21852	-0.50715
N	2.16839	1.31608	0.10750
C	3.08345	0.35217	-0.04701
C	4.39701	0.77627	-0.46230
C	2.93760	-1.08529	0.11904
C	5.41167	-0.09413	-0.80333
H	4.55343	1.84831	-0.54447
C	3.98533	-1.92995	-0.25723
C	5.21760	-1.48072	-0.73527
H	6.36654	0.30701	-1.13324
H	3.82722	-2.99753	-0.12737
H	6.00296	-2.17726	-1.00337
C	1.78899	-1.73937	0.86806
C	1.06583	-2.72735	0.23909
H	0.29276	-3.26830	0.77778
H	1.24134	-2.97837	-0.79969
O	1.62589	-1.36143	2.08955

Scheme 6.9



6.46 6.48

Cyclisation of 6.46 – starting species 6.46 in DMSO

30
-709.3095148

C	4.58104	-0.24887	0.06626
C	3.57387	-0.58111	-0.83645
C	2.21899	-0.46079	-0.49229
C	1.97671	-0.00355	0.78379
C	2.92485	0.34277	1.71871
C	4.26559	0.21217	1.34390
C	1.12087	-0.82697	-1.48381
C	-0.36685	1.42481	-0.78481
C	-0.87213	0.07126	-0.58955
C	-2.21732	0.00434	-0.00811
C	-2.91854	1.20227	0.25562
C	-2.40637	2.45979	0.01924
C	-1.09916	2.54725	-0.50411
H	1.42590	-1.77035	-1.94943
H	5.61919	-0.35412	-0.22673
H	3.83453	-0.94338	-1.82747
H	2.65394	0.70083	2.70582
H	5.05238	0.46664	2.04502
H	-3.91559	1.13775	0.67350
H	-2.98186	3.34884	0.24365
H	-0.65535	3.52326	-0.68079
C	-2.88338	-1.25560	0.32630
C	-4.30753	-1.20848	0.88485
H	-4.34957	-0.67120	1.83468
H	-4.99809	-0.71910	0.19502
H	-4.63309	-2.23448	1.04560
O	-2.37893	-2.37015	0.19849
N	-0.19231	-1.01092	-0.91213
H	1.14369	-0.07879	-2.29519
H	0.63770	1.55601	-1.16388

Cyclisation of 6.46 – transition state in DMSO

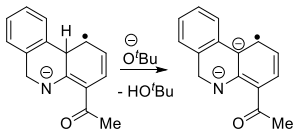
30
-709.3041328

C	4.19763	-0.64349	0.80006
C	3.28584	-1.32197	-0.01074
C	2.08972	-0.71053	-0.40197
C	1.85085	0.57069	0.05780
C	2.73377	1.27836	0.84772
C	3.92834	0.65315	1.23043
C	1.07338	-1.42647	-1.28808
C	-0.15018	1.04407	-1.18393
C	-0.80525	-0.16226	-0.66975
C	-2.07616	0.07380	0.02016
C	-2.48675	1.39350	0.27573
C	-1.80537	2.51034	-0.18632
C	-0.66445	2.31340	-0.97363
H	1.36561	-2.47703	-1.36303
H	5.11942	-1.13110	1.09659
H	3.50648	-2.33328	-0.34241
H	2.51917	2.29144	1.17643
H	4.63912	1.17743	1.86072
H	-3.40477	1.55566	0.82781
H	-2.18289	3.50581	0.01157
H	-0.16276	3.16419	-1.42482
C	-2.95718	-1.01591	0.44702
C	-4.08621	-0.70102	1.42614
H	-3.74539	-0.10841	2.27601
H	-4.88427	-0.14404	0.92813
H	-4.49551	-1.64545	1.78081
O	-2.86259	-2.17473	0.05055
N	-0.27409	-1.35800	-0.76213
H	1.15689	-1.01177	-2.30684
H	0.62029	0.92654	-1.93432

Cyclisation of 6.46 – product 6.48 in DMSO

30
-709.3701967

C	-4.04103	-0.48513	-0.88523
C	-3.20372	-1.37654	-0.21558
C	-2.01500	-0.92168	0.34469
C	-1.64738	0.42052	0.22750
C	-2.47464	1.30641	-0.45674
C	-3.67380	0.85225	-1.00717
C	-1.01094	-1.79428	1.04544
C	-0.32055	0.77450	0.87742
C	0.70707	-0.30969	0.46468
C	2.02482	0.11977	-0.00425
C	2.30288	1.51852	-0.06575
C	1.36657	2.50738	0.28221
C	0.10672	2.19800	0.71406
H	-1.25009	-2.85015	0.90623
H	-4.97119	-0.83548	-1.31794
H	-3.47397	-2.42462	-0.13281
H	-2.18644	2.34541	-0.56756
H	-4.31801	1.54417	-1.53775
H	3.27374	1.84982	-0.40641
H	1.66225	3.54939	0.20267
H	-0.59269	2.97435	1.00371
C	3.04320	-0.81538	-0.41563
C	4.39085	-0.24886	-0.86807
H	4.28464	0.39822	-1.74255
H	4.86650	0.34129	-0.08070
H	5.03830	-1.08591	-1.12429
O	2.92731	-2.05396	-0.44084
N	0.35208	-1.54778	0.57353
H	-1.06452	-1.59373	2.12848
H	-0.48168	0.57862	1.95550



6.48 **6.49**

Deprotonation 6.48 – starting species 6.48 and O^{t}Bu anion in DMSO

44

-942.4969340

C	4.69901	0.32158	-0.38556
C	3.67732	0.35918	-1.33412
C	2.35082	0.25457	-0.92980
C	2.02994	0.09139	0.42039
C	3.05361	0.03561	1.36370
C	4.38427	0.15843	0.96050
C	1.17144	0.24851	-1.86030
C	0.54593	-0.01987	0.71906
C	-0.08318	-0.98282	-0.31339
C	-1.03731	-1.99217	0.15806
C	-1.30147	-2.07116	1.56049
C	-0.68016	-1.24265	2.51166
C	0.22052	-0.27837	2.15461
H	1.49604	0.16106	-2.89935
H	5.73365	0.40984	-0.69686
H	3.91222	0.46924	-2.38848
H	2.82137	-0.11033	2.41226
H	5.17601	0.11745	1.70025
H	-2.00004	-2.81104	1.92638
H	-0.93436	-1.37734	3.55927
H	0.65675	0.37856	2.89972
C	-1.71032	-2.90058	-0.73337
C	-2.70071	-3.89547	-0.12096
H	-2.21240	-4.56772	0.58961
H	-3.50828	-3.38814	0.41333
H	-3.12782	-4.48670	-0.92957
O	-1.56445	-2.95953	-1.97113
N	0.23757	-0.83775	-1.55699
H	0.64372	1.20995	-1.75478
H	0.12352	0.97684	0.44612
O	-0.65130	3.01185	0.28832
C	-1.96551	2.80430	-0.05644
C	-2.74466	4.13726	-0.13675
H	-2.28113	4.78974	-0.88409
H	-3.79796	3.99592	-0.40670
H	-2.70216	4.64670	0.83135
C	-2.67956	1.90035	0.97654
H	-2.15790	0.93975	1.04496
H	-2.64616	2.37421	1.96390
H	-3.72908	1.71246	0.72000
C	-2.08186	2.10647	-1.43154
H	-1.58265	2.71270	-2.19520
H	-1.58542	1.13207	-1.38907
H	-3.12360	1.95308	-1.73837

Deprotonation 6.48 – transition state in DMSO

44

-942.4919052

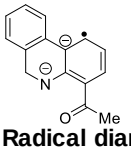
C	4.64152	-0.75862	-0.39032
C	3.63516	-0.60535	-1.34555
C	2.31639	-0.41182	-0.95126
C	1.96251	-0.40438	0.40566
C	2.97568	-0.58029	1.35611
C	4.30354	-0.74321	0.96001
C	1.17312	-0.20353	-1.90120
C	0.51175	-0.19761	0.71550
C	-0.36560	-0.92246	-0.29114
C	-1.62453	-1.52882	0.18652
C	-1.88430	-1.52253	1.59535
C	-1.01495	-0.94285	2.53233
C	0.14949	-0.33222	2.14371
H	1.46905	-0.45790	-2.92273
H	5.67252	-0.89271	-0.69711
H	3.87943	-0.62467	-2.40404
H	2.73458	-0.60015	2.41236
H	5.07436	-0.87070	1.71273
H	-2.79218	-1.97597	1.96923
H	-1.28570	-0.97162	3.58456
H	0.78166	0.15150	2.88148
C	-2.61164	-2.08008	-0.69549
C	-3.88888	-2.64827	-0.06437
H	-3.67604	-3.46828	0.62728
H	-4.43968	-1.88756	0.49619
H	-4.52316	-3.02163	-0.86719
O	-2.55295	-2.13896	-1.94734
N	-0.01742	-0.97140	-1.54021
H	0.91183	0.86601	-1.88275
H	0.34817	1.02165	0.44051
O	0.28188	2.45418	0.21862
C	-1.00262	2.88846	-0.08606
C	-1.05724	4.42466	-0.04095
H	-0.34840	4.84193	-0.76294
H	-2.05660	4.80915	-0.27380
H	-0.77468	4.77454	0.95657
C	-2.02578	2.33050	0.92326
H	-1.99784	1.23641	0.91893
H	-1.77342	2.67232	1.93255
H	-3.04541	2.65892	0.69237
C	-1.41708	2.42293	-1.49565
H	-0.71784	2.82253	-2.23739
H	-1.38216	1.33040	-1.54637
H	-2.42715	2.75673	-1.75801

Deprotonation 6.48 – products 6.49 and HO^{t}Bu in DMSO

44

-942.5251437

C	4.76189	-0.43530	-0.35936
C	3.73286	-0.43840	-1.30991
C	2.40407	-0.38475	-0.91929
C	2.03944	-0.38239	0.44847
C	3.08992	-0.38838	1.39751
C	4.42146	-0.40058	0.99373
C	1.24697	-0.24310	-1.86327
C	0.63131	-0.46252	0.78013
C	-0.24673	-1.03204	-0.24466
C	-1.54282	-1.59081	0.21639
C	-1.89770	-1.39166	1.59892
C	-1.06448	-0.76210	2.51696
C	0.19474	-0.31727	2.13227
H	1.56026	-0.45880	-2.89028
H	5.80061	-0.45149	-0.66870
H	3.97209	-0.45111	-2.37050
H	2.86243	-0.40707	2.45730
H	5.20434	-0.40009	1.74592
H	-2.85767	-1.74486	1.95177
H	-1.40414	-0.62200	3.53940
H	0.84960	0.15292	2.85890
C	-2.46449	-2.28297	-0.62847
C	-3.81792	-2.68201	-0.02528
H	-3.70818	-3.41439	0.78194
H	-4.36144	-1.82825	0.39112
H	-4.41830	-3.13006	-0.81681
O	-2.29195	-2.63301	-1.83369
N	0.10102	-1.07316	-1.51971
H	0.93940	0.82202	-1.84088
H	0.16303	1.67579	0.37362
O	0.03903	2.63386	0.24718
C	-1.30670	2.85768	-0.19104
C	-1.46584	4.36916	-0.28665
H	-0.74435	4.78180	-0.99626
H	-2.47220	4.62569	-0.62539
H	-1.29885	4.83077	0.68971
C	-2.27835	2.26912	0.82951
H	-2.11632	1.19072	0.92658
H	-2.12360	2.73201	1.80828
H	-3.31305	2.44366	0.52143
C	-1.52101	2.20390	-1.55621
H	-0.81909	2.61619	-2.28619
H	-1.35890	1.12348	-1.48801
H	-2.53916	2.38496	-1.91161



Radical dianion 6.49 in DMSO

29

-708.8734067

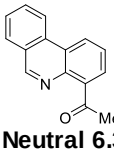
C	-4.25019	-0.50109	-0.57560
C	-3.28984	-1.37406	-0.04735
C	-2.03226	-0.91300	0.30985
C	-1.65769	0.43701	0.10194
C	-2.63749	1.30690	-0.43517
C	-3.90896	0.84192	-0.75336
C	-0.98802	-1.72824	1.01218
C	-0.28641	0.80680	0.36872
C	0.69342	-0.27642	0.30560
C	2.09655	0.10945	0.01646
C	2.43155	1.50319	0.17155
C	1.47564	2.49599	0.37116
C	0.12235	2.16991	0.41137
H	-1.24941	-2.79133	0.99673
H	-5.24052	-0.85829	-0.83280
H	-3.53739	-2.41967	0.11863
H	-2.39061	2.34569	-0.62618
H	-4.63995	1.53288	-1.16227
H	3.46815	1.80687	0.09985
H	1.79236	3.52991	0.47533
H	-0.62479	2.95048	0.51771
C	3.11218	-0.80830	-0.38136
C	4.53502	-0.26116	-0.54886
H	4.59473	0.50848	-1.32579
H	4.92091	0.18794	0.37245
H	5.18400	-1.08997	-0.83124
O	2.97164	-2.04346	-0.64101
N	0.34951	-1.54255	0.46931
H	-0.99236	-1.41083	2.07774

Anion 6.50 in DMSO

29

-708.8121885

C	-4.27740	-0.48206	-0.48141
C	-3.31826	-1.35696	0.02321
C	-2.03386	-0.90577	0.31439
C	-1.67921	0.42860	0.07110
C	-2.64292	1.29580	-0.46384
C	-3.93422	0.84900	-0.71907
C	-0.97064	-1.76748	0.93928
C	-0.27772	0.80783	0.30006
C	0.70708	-0.28460	0.25128
C	2.08607	0.14186	-0.00175
C	2.41437	1.50193	0.14408
C	1.47759	2.48844	0.39558
C	0.12092	2.12167	0.41638
H	-1.22844	-2.82367	0.82168
H	-5.28018	-0.83416	-0.69400
H	-3.57213	-2.39644	0.20886
H	-2.37869	2.32029	-0.70195
H	-4.66917	1.53461	-1.12577
H	3.45019	1.80277	0.04156
H	1.77601	3.52202	0.51334
H	-0.63507	2.89690	0.50715
C	3.14571	-0.79127	-0.38291
C	4.58982	-0.29318	-0.40224
H	4.73897	0.45334	-1.18596
H	4.87817	0.15992	0.54785
H	5.23437	-1.14623	-0.60642
O	2.94975	-1.95810	-0.71670
N	0.37398	-1.54002	0.42222
H	-0.97391	-1.56715	2.02691

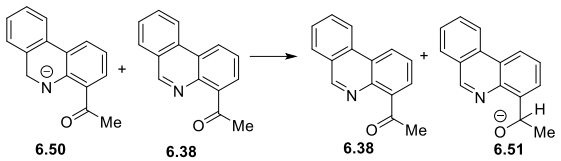


Neutral 6.38 in DMSO

28

-708.1155762

C	3.25938	-0.63601	-0.06414
O	4.24665	-0.34068	-0.70712
C	2.09626	0.31820	-0.03538
C	0.74366	-0.10641	-0.03377
C	2.39464	1.66699	0.00542
C	-0.28957	0.85812	0.03705
C	1.37277	2.62190	0.08735
H	3.43308	1.97619	-0.01018
C	-1.66469	0.39133	0.01802
C	0.05468	2.22283	0.10721
C	-0.73377	-1.86157	-0.17069
H	1.62086	3.67501	0.13614
C	-1.87838	-0.99705	-0.08649
C	-2.79075	1.23667	0.09302
H	-0.72183	2.97435	0.17003
H	-0.90814	-2.93257	-0.26350
C	-3.18383	-1.52491	-0.11479
C	-4.06322	0.70617	0.06606
H	-2.66944	2.30884	0.17371
C	-4.26810	-0.68165	-0.03855
H	-3.31751	-2.59820	-0.19716
H	-4.91838	1.36904	0.12506
H	-5.27526	-1.07911	-0.05924
C	3.22756	-1.89618	0.76159
H	2.56791	-1.80042	1.62290
H	2.84347	-2.70938	0.14365
H	4.24583	-2.12973	1.07199
N	0.49520	-1.46273	-0.14969



6.50 6.38 6.38 6.51

Hydride transfer – starting species 6.50 and 6.39 in DMSO

57

-1416.9443788

C	4.09971	0.25057	-2.25134
C	3.53712	1.22362	-1.43258
C	2.16249	1.26594	-1.20146
C	1.31106	0.34678	-1.83123
C	1.89111	-0.62327	-2.66530
C	3.26374	-0.68169	-2.86323
C	1.57702	2.27570	-0.24522
C	-0.14378	0.49252	-1.63953
C	-0.61656	1.68015	-0.91795
C	-2.06549	1.82659	-0.82784
C	-2.91246	0.92820	-1.49894
C	-2.43408	-0.16577	-2.18628
C	-1.04273	-0.36735	-2.23166
H	2.17075	3.19652	-0.29248
H	5.17049	0.22398	-2.41738
H	4.17392	1.97029	-0.96591
H	1.26734	-1.34511	-3.17795
H	3.68035	-1.44839	-3.50701
H	-3.98148	1.08693	-1.40527
H	-3.10907	-0.88226	-2.63750
H	-0.67466	-1.24261	-2.75783
C	-2.73418	2.80244	0.03771
C	-2.00088	3.46876	1.18292
H	-2.74020	3.72141	1.94559
H	-1.20646	2.83894	1.57834
H	-1.52536	4.38670	0.83015
O	-3.93949	3.05488	-0.08810
N	0.17659	2.59847	-0.41586
H	1.72458	1.89194	0.78304
C	2.58689	0.21800	2.62530
O	2.07597	0.42942	3.70393
C	1.99088	-0.75100	1.64583
C	0.58422	-0.87884	1.46711
C	2.85033	-1.58543	0.95543
C	0.08560	-1.92897	0.65910
C	2.35309	-2.60442	0.13283
H	3.92224	-1.46716	1.06391
C	-1.35264	-2.07338	0.52686
C	0.99481	-2.78174	0.00340
C	-1.51646	-0.03836	1.86080
H	3.03969	-3.25162	-0.39883
C	-2.16080	-1.10215	1.14316
C	-1.98399	-3.12321	-0.17224
H	0.62755	-3.57590	-0.63455
H	-2.14949	0.73368	2.29763
C	-3.56401	-1.17299	1.05598
C	-3.35944	-3.19145	-0.23519
H	-1.39742	-3.89332	-0.65668
C	-4.16067	-2.21162	0.37887
H	-4.16054	-0.39909	1.52982
H	-3.83029	-4.01085	-0.76626
H	-5.24012	-2.27570	0.31198
C	3.90612	0.86331	2.25857
H	4.72183	0.19117	2.54145
H	3.98283	1.05425	1.18839
H	4.01569	1.78684	2.82498
N	-0.24085	0.06858	2.04336

Hydride transfer – transition state in DMSO

57

-1416.9054801

C	-4.00974	-0.45497	2.21452
C	-3.61584	0.63311	1.45657
C	-2.25917	0.87423	1.20634
C	-1.27416	0.04718	1.77078
C	-1.69193	-1.05978	2.53163
C	-3.03627	-1.31525	2.73600
C	-1.82956	1.98574	0.34058
C	0.12643	0.43817	1.59910
C	0.39237	1.67847	0.93673
C	1.75077	2.11455	0.88006
C	2.76291	1.36967	1.47640
C	2.49238	0.15111	2.09249
C	1.18179	-0.30267	2.13741
H	-2.60113	2.73371	0.14106
H	-5.06039	-0.63931	2.40514
H	-4.35640	1.31534	1.05209
H	-0.96239	-1.72495	2.97634
H	-3.33418	-2.17675	3.32288
H	3.78081	1.73788	1.41030
H	3.29345	-0.44568	2.51088
H	0.97981	-1.25502	2.61417
C	2.18168	3.32583	0.12274
C	1.51980	3.67309	-1.18863
H	2.28329	4.07907	-1.85435
H	1.01915	2.81088	-1.62694
H	0.76147	4.43816	-1.01279
O	3.13066	3.98765	0.51431
N	-0.57262	2.47636	0.40942
H	-2.00543	1.38984	-0.94535
C	-2.33224	0.77681	-2.09406
O	-1.79839	1.36041	-3.10458
C	-1.79248	-0.57556	-1.62923
C	-0.39190	-0.80255	-1.46889
C	-2.66522	-1.58833	-1.27110
C	0.07053	-2.03139	-0.93009
C	-2.20674	-2.81595	-0.77022
H	-3.73265	-1.44264	-1.37569
C	1.49552	-2.19896	-0.70567
C	-0.86096	-3.03392	-0.59534
C	1.74347	0.05020	-1.60526
H	-2.92076	-3.58859	-0.50866
C	2.34255	-1.13338	-1.05890
C	2.07959	-3.34874	-0.13037
H	-0.52353	-3.97945	-0.19081
H	2.40477	0.87605	-1.87129
C	3.73227	-1.21361	-0.84906
C	3.44175	-3.41445	0.07355
H	1.46595	-4.19090	0.16234
C	4.28080	-2.34361	-0.28833
H	4.35484	-0.36852	-1.12491
H	3.87219	-4.30405	0.51865
H	5.34855	-2.41174	-0.11855
C	-3.85627	0.93515	-1.99638
H	-4.32972	0.36694	-2.80455
H	-4.28203	0.60963	-1.04822
H	-4.08729	1.99100	-2.14691
N	0.47840	0.21985	-1.79842

Hydride transfer – product 6.38 and 6.51 in DMSO

57

-1416.9488832

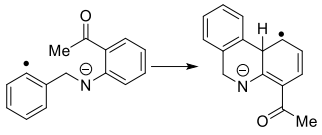
C	2.25520	-2.85565	-2.41522
C	2.22552	-1.47987	-2.43298
C	1.05134	-0.79594	-2.06654
C	-0.10567	-1.50413	-1.68867
C	-0.04911	-2.91244	-1.66131
C	1.11054	-3.56944	-2.01812
C	1.00074	0.63925	-2.07397
C	-1.28305	-0.72865	-1.34617
C	-1.19263	0.68340	-1.39061
C	-2.33816	1.46459	-1.08320
C	-3.52766	0.83883	-0.75743
C	-3.61119	-0.55768	-0.69737
C	-2.50543	-1.32637	-0.98110
H	1.90182	1.18020	-2.35861
H	3.15590	-3.38991	-2.69239
H	3.10162	-0.90620	-2.71744
H	-0.91260	-3.49280	-1.36196
H	1.13866	-4.65267	-1.99251
H	-4.39473	1.44833	-0.53170
H	-4.54258	-1.03162	-0.41212
H	-2.58265	-2.40435	-0.91943
C	-2.34907	2.96986	-1.07957
C	-1.15676	3.74524	-0.58762
H	-1.50799	4.69904	-0.19335
H	-0.58905	3.18726	0.15748
H	-0.48562	3.92552	-1.42969
O	-3.36334	3.54824	-1.42175
N	-0.03949	1.34448	-1.77110
H	2.50360	2.79620	1.98635
C	3.11098	2.34371	1.17588
O	4.45201	2.47566	1.38855
C	2.64390	0.87381	1.11157
C	1.30664	0.47302	1.39242
C	3.56484	-0.10710	0.80193
C	0.95259	-0.90080	1.39635
C	3.21126	-1.46534	0.76133
H	4.58451	0.20919	0.61442
C	-0.40402	-1.26650	1.75958
C	1.92874	-1.86137	1.06324
C	-0.82334	1.12577	1.99951
H	3.95462	-2.20982	0.49639
C	-1.29866	-0.22813	2.08331
C	-0.87984	-2.59435	1.81211
H	1.67410	-2.91309	1.03634
H	-1.53107	1.92734	2.21675
C	-2.62038	-0.51172	2.47696
C	-2.17807	-2.85769	2.19707
H	-0.22887	-3.42034	1.55549
C	-3.05724	-1.81518	2.54135
H	-3.28526	0.31149	2.71827
H	-2.52548	-3.88391	2.23558
H	-4.07340	-2.04087	2.84183
C	2.65660	3.03878	-0.12833
H	3.24457	2.63467	-0.96036
H	1.59532	2.89105	-0.34250
H	2.86655	4.11045	-0.05494
N	0.38193	1.46785	1.68357

Anion 6.51 in DMSO

29

-708.8113747

H	2.84092	-1.57502	-0.97048
C	3.20989	-0.80983	-0.25665
O	4.39887	-0.26364	-0.63469
C	2.06554	0.21834	-0.15296
C	0.69323	-0.15777	-0.12722
C	2.37601	1.56079	-0.06838
C	-0.32181	0.82525	-0.00289
C	1.37779	2.53996	0.06337
H	3.42461	1.83068	-0.11543
C	-1.70773	0.39013	0.01215
C	0.04839	2.18200	0.09796
C	-0.84045	-1.88065	-0.22892
H	1.65321	3.58664	0.13466
C	-1.96217	-0.99054	-0.10160
C	-2.81256	1.26077	0.13112
H	-0.70802	2.94979	0.19891
H	-1.04510	-2.94675	-0.32568
C	-3.28169	-1.48422	-0.09817
C	-4.09892	0.76469	0.13416
H	-2.66174	2.32849	0.22040
C	-4.34291	-0.61650	0.01892
H	-3.44426	-2.55308	-0.18959
H	-4.93421	1.44910	0.22578
H	-5.35996	-0.98899	0.02230
C	3.30292	-1.52324	1.11544
H	3.62206	-0.79827	1.87223
H	2.35366	-1.96776	1.42648
H	4.06065	-2.31021	1.05697
N	0.39629	-1.51008	-0.24243



6.46 **6.48**

Cyclisation of 6.46 – starting species 6.46 in benzene

30

-709.2689329

C	4.58455	-0.41627	0.14332
C	3.56161	-0.80707	-0.71828
C	2.22382	-0.47117	-0.46553
C	2.01126	0.25740	0.68414
C	2.97600	0.67465	1.57053
C	4.30037	0.32359	1.28946
C	1.11199	-0.90267	-1.41676
C	-0.39707	1.38724	-0.87493
C	-0.87900	0.04138	-0.58251
C	-2.22095	-0.00483	0.00959
C	-2.92019	1.19687	0.23461
C	-2.42144	2.44844	-0.06902
C	-1.13195	2.51736	-0.63361
H	1.41531	-1.87429	-1.82198
H	5.60840	-0.69720	-0.07698
H	3.79663	-1.39249	-1.60361
H	2.72610	1.25144	2.45441
H	5.09723	0.62295	1.96143
H	-3.91043	1.14571	0.67111
H	-2.99826	3.34343	0.12757
H	-0.70257	3.48588	-0.87702
C	-2.88404	-1.26087	0.37652
C	-4.29203	-1.19064	0.98660
H	-4.30397	-0.61369	1.91393
H	-5.00744	-0.73463	0.29827
H	-4.60277	-2.21232	1.19796
O	-2.40566	-2.37855	0.23483
N	-0.19018	-1.05099	-0.82292
H	1.12686	-0.20591	-2.27501
H	0.59392	1.50600	-1.29302

Cyclisation of 6.46 – transition state in benzene

30

-709.2652784

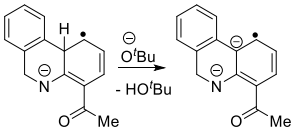
C	4.20852	-0.67887	0.78337
C	3.27799	-1.33006	-0.02784
C	2.09422	-0.69166	-0.41190
C	1.88435	0.59254	0.05417
C	2.78669	1.27162	0.84717
C	3.96899	0.62008	1.22272
C	1.06265	-1.39224	-1.29540
C	-0.17527	1.07814	-1.17429
C	-0.81141	-0.13959	-0.66575
C	-2.08668	0.07612	0.02413
C	-2.51205	1.38190	0.29336
C	-1.84170	2.51531	-0.15523
C	-0.69986	2.33903	-0.94294
H	1.35119	-2.44318	-1.38533
H	5.11921	-1.19047	1.07499
H	3.47163	-2.34582	-0.36364
H	2.59213	2.28563	1.18593
H	4.69210	1.12390	1.85648
H	-3.43344	1.52618	0.84597
H	-2.22944	3.50434	0.05571
H	-0.20496	3.20121	-1.38084
C	-2.95550	-1.03668	0.43076
C	-4.06144	-0.75443	1.45233
H	-3.70018	-0.17767	2.30504
H	-4.87970	-0.19652	0.98889
H	-4.44718	-1.71405	1.79271
O	-2.87367	-2.17453	-0.00710
N	-0.27459	-1.32839	-0.75702
H	1.13913	-0.96345	-2.31009
H	0.60399	0.97767	-1.91777

Cyclisation of 6.46 – product 6.48 in benzene

30

-709.3311818

C	-4.04792	-0.48957	-0.87668
C	-3.19979	-1.38281	-0.22408
C	-2.01073	-0.92929	0.33589
C	-1.65113	0.41672	0.23258
C	-2.48824	1.30384	-0.43724
C	-3.68888	0.85095	-0.98447
C	-0.99613	-1.80686	1.01487
C	-0.32289	0.77351	0.87574
C	0.70914	-0.30652	0.45345
C	2.02426	0.12978	-0.00725
C	2.29648	1.52499	-0.07389
C	1.35860	2.51071	0.27767
C	0.09998	2.19913	0.71482
H	-1.22917	-2.86192	0.85538
H	-4.97790	-0.84106	-1.30966
H	-3.45921	-2.43504	-0.15708
H	-2.19908	2.34309	-0.54273
H	-4.33921	1.54564	-1.50454
H	3.26694	1.85920	-0.41356
H	1.65150	3.55400	0.19953
H	-0.59714	2.97446	1.01400
C	3.04967	-0.81401	-0.40137
C	4.38633	-0.24137	-0.89102
H	4.25489	0.40623	-1.76171
H	4.87935	0.34753	-0.11274
H	5.02421	-1.08152	-1.16130
O	2.95153	-2.04557	-0.38037
N	0.36110	-1.54596	0.54670
H	-1.04978	-1.62772	2.10264
H	-0.47780	0.56827	1.95363



6.48 **6.49**

Deprotonation 6.48 – starting species 6.48 and O^{t}Bu anion in benzene

44

-942.3803722

C	-1.63032	3.69975	0.22487
C	-1.16058	3.01134	-0.89485
C	-0.53728	1.77850	-0.74466
C	-0.36563	1.22824	0.53007
C	-0.81278	1.92482	1.64726
C	-1.45191	3.15671	1.49414
C	0.02095	0.94355	-1.86244
C	0.29995	-0.13326	0.53638
C	1.53640	-0.04344	-0.39139
C	2.82389	-0.55963	0.09624
C	2.86751	-1.13819	1.39757
C	1.74835	-1.21432	2.24926
C	0.52183	-0.72948	1.88823
H	0.04156	1.50708	-2.79840
H	-2.12500	4.65814	0.10637
H	-1.28292	3.43389	-1.88811
H	-0.66849	1.50411	2.63661
H	-1.80771	3.69213	2.36832
H	3.80239	-1.53488	1.77070
H	1.87344	-1.68000	3.22395
H	-0.33414	-0.83005	2.54826
C	4.03035	-0.49074	-0.68711
C	5.30529	-1.09253	-0.07248
H	5.58709	-0.58418	0.85428
H	5.18221	-2.15429	0.15908
H	6.10615	-0.97476	-0.80171
O	4.15650	0.01257	-1.81584
N	1.37732	0.47702	-1.55791
H	-0.65690	0.08069	-1.98073
H	-0.42640	-0.76195	-0.02805
O	-2.19314	-1.44093	-1.21230
C	-3.24612	-1.72356	-0.40280
C	-3.08700	-3.11459	0.26757
H	-3.00405	-3.87942	-0.51163
H	-2.15989	-3.12331	0.84982
H	-3.92355	-3.37435	0.93044
C	-3.38764	-0.67575	0.73238
H	-2.47569	-0.67196	1.33734
H	-3.49325	0.32155	0.29231
H	-4.24622	-0.86876	1.39005
C	-4.58175	-1.73782	-1.19350
H	-4.51207	-2.48171	-1.99388
H	-5.45409	-1.97149	-0.56811
H	-4.73167	-0.75635	-1.65486

Deprotonation 6.48 – transition state in benzene

44

-942.3748136

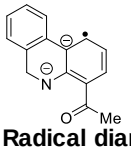
C	-2.30341	3.61536	0.28038
C	-1.58450	3.13522	-0.81723
C	-0.82797	1.97538	-0.71222
C	-0.73958	1.28428	0.50777
C	-1.44220	1.78590	1.60902
C	-2.22744	2.93286	1.49149
C	-0.04487	1.36062	-1.83673
C	0.09909	0.05309	0.50249
C	1.36294	0.28730	-0.31885
C	2.63707	-0.27307	0.17728
C	2.61106	-1.02571	1.39175
C	1.45429	-1.18907	2.17130
C	0.25563	-0.63312	1.80231
H	0.03488	2.05766	-2.67658
H	-2.90800	4.51185	0.19197
H	-1.62158	3.66269	-1.76689
H	-1.36913	1.28352	2.56713
H	-2.77218	3.30045	2.35577
H	3.52411	-1.47767	1.75615
H	1.52066	-1.76821	3.08948
H	-0.62666	-0.79097	2.41567
C	3.88674	-0.09352	-0.50704
C	5.12760	-0.76579	0.10989
H	5.33854	-0.38736	1.11504
H	5.00953	-1.85098	0.18768
H	5.97506	-0.54416	-0.53842
O	4.09340	0.55653	-1.55190
N	1.29693	0.94966	-1.42763
H	-0.59923	0.47086	-2.17437
H	-0.58822	-0.72805	-0.23267
O	-1.36866	-1.54707	-1.10831
C	-2.40775	-2.22437	-0.50704
C	-1.88003	-3.40598	0.33502
H	-1.33967	-4.10047	-0.31574
H	-1.17735	-3.02668	1.08262
H	-2.68439	-3.95192	0.84424
C	-3.22153	-1.29028	0.41549
H	-2.58476	-0.91332	1.22019
H	-3.57268	-0.42736	-0.15939
H	-4.08620	-1.79712	0.86152
C	-3.35605	-2.78072	-1.58746
H	-2.79253	-3.43514	-2.25920
H	-4.19102	-3.34861	-1.15745
H	-3.76011	-1.95260	-2.17741

Deprotonation 6.48 – products 6.49 and HO^{t}Bu in benzene

44

-942.4058202

C	3.06303	-3.28308	0.12012
C	2.14454	-2.96762	-0.89875
C	1.16474	-2.01177	-0.70661
C	1.00840	-1.35495	0.54373
C	1.94229	-1.68279	1.56444
C	2.94872	-2.61720	1.34207
C	0.25918	-1.49734	-1.78788
C	-0.09941	-0.45674	0.70468
C	-1.23984	-0.65016	-0.21621
C	-2.54817	-0.12280	0.23283
C	-2.55221	0.77440	1.35688
C	-1.42734	1.02382	2.13246
C	-0.22197	0.37751	1.85291
H	0.26618	-2.17472	-2.64942
H	3.84598	-4.01536	-0.04361
H	2.22131	-3.45391	-1.86911
H	1.85407	-1.22250	2.54252
H	3.64653	-2.84313	2.14434
H	-3.47625	1.26455	1.63669
H	-1.49508	1.71222	2.97112
H	0.64023	0.53829	2.49385
C	-3.78629	-0.43675	-0.41311
C	-5.04588	0.29536	0.08745
H	-5.27541	0.04661	1.12930
H	-4.94348	1.38393	0.02922
H	-5.87883	-0.01917	-0.54159
O	-3.97866	-1.26372	-1.33471
N	-1.11318	-1.26744	-1.36564
H	0.68782	-0.53360	-2.13403
H	0.30296	1.41135	-0.53450
O	0.58900	2.15492	-1.09528
C	1.73916	2.75579	-0.51201
C	1.32589	3.57937	0.71027
H	0.61875	4.35769	0.41123
H	0.83607	2.93040	1.44075
H	2.19571	4.05182	1.17747
C	2.75249	1.68175	-0.11444
H	2.33645	1.02903	0.65695
H	2.99898	1.05999	-0.97992
H	3.67087	2.13939	0.26593
C	2.31922	3.66317	-1.59220
H	1.56943	4.39299	-1.90837
H	3.19633	4.19800	-1.21782
H	2.61144	3.06879	-2.46134



Radical dianion 6.49 in benzene

29

-708.7533311

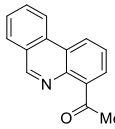
C	-4.27121	-0.50667	-0.55120
C	-3.28326	-1.38655	-0.06941
C	-2.02582	-0.92901	0.27578
C	-1.65900	0.43470	0.10360
C	-2.66776	1.31311	-0.38461
C	-3.93947	0.84473	-0.69081
C	-0.97241	-1.76012	0.94704
C	-0.29770	0.80613	0.35497
C	0.69892	-0.27876	0.28799
C	2.09658	0.12158	0.00568
C	2.42286	1.51739	0.13445
C	1.46387	2.50229	0.34206
C	0.11049	2.16711	0.40238
H	-1.21997	-2.82588	0.87870
H	-5.26398	-0.86517	-0.79965
H	-3.51463	-2.44071	0.07006
H	-2.43286	2.35857	-0.55248
H	-4.68389	1.54357	-1.06466
H	3.45603	1.82980	0.04696
H	1.77354	3.54026	0.43556
H	-0.63771	2.94575	0.51983
C	3.12520	-0.80376	-0.35655
C	4.55154	-0.24224	-0.51535
H	4.61285	0.50736	-1.31186
H	4.91518	0.23176	0.40289
H	5.20442	-1.07852	-0.76665
O	3.00884	-2.03318	-0.58460
N	0.37095	-1.54101	0.43933
H	-0.99329	-1.49379	2.02679

Anion 6.50 in benzene

29

-708.7732472

C	-4.27535	-0.49062	-0.47992
C	-3.30930	-1.36115	0.01972
C	-2.02763	-0.90668	0.31340
C	-1.67818	0.43101	0.07256
C	-2.64829	1.29291	-0.45973
C	-3.93828	0.84229	-0.71327
C	-0.96266	-1.76717	0.93874
C	-0.28045	0.81345	0.29878
C	0.70482	-0.28096	0.25684
C	2.08414	0.14626	-0.00217
C	2.41126	1.50188	0.13800
C	1.47401	2.49405	0.38683
C	0.11911	2.12804	0.40951
H	-1.21429	-2.82427	0.81091
H	-5.27651	-0.84781	-0.69316
H	-3.55544	-2.40375	0.19972
H	-2.38580	2.31746	-0.69974
H	-4.67638	1.52616	-1.11831
H	3.44734	1.80228	0.03189
H	1.77464	3.52759	0.50094
H	-0.63772	2.90302	0.50106
C	3.13947	-0.79572	-0.38585
C	4.59010	-0.30030	-0.38915
H	4.74988	0.44431	-1.17300
H	4.86991	0.15124	0.56459
H	5.22859	-1.15961	-0.58713
O	2.94472	-1.95290	-0.73157
N	0.38253	-1.53195	0.43725
H	-0.97623	-1.57345	2.02822

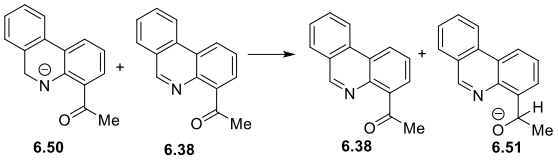


Neutral 6.38 in benzene

28

-708.1103926

C	3.26851	-0.63245	-0.06342
O	4.26867	-0.30225	-0.66285
C	2.09594	0.31516	-0.03000
C	0.74288	-0.10817	-0.02801
C	2.39238	1.66419	0.00818
C	-0.29078	0.85706	0.03846
C	1.37129	2.61944	0.08655
H	3.43164	1.96982	-0.01395
C	-1.66599	0.39150	0.01836
C	0.05330	2.22131	0.10556
C	-0.73684	-1.86158	-0.15963
H	1.61994	3.67269	0.13152
C	-1.88158	-0.99640	-0.08218
C	-2.79216	1.23734	0.08808
H	-0.72357	2.97274	0.16441
H	-0.91091	-2.93331	-0.24816
C	-3.18752	-1.52199	-0.11173
C	-4.06498	0.70922	0.05965
H	-2.66928	2.30956	0.16537
C	-4.27133	-0.67834	-0.04101
H	-3.32200	-2.59552	-0.19090
H	-4.91943	1.37348	0.11425
H	-5.27881	-1.07499	-0.06302
C	3.22484	-1.92829	0.70632
H	2.57701	-1.85983	1.57963
H	2.81625	-2.70632	0.06008
H	4.24369	-2.18906	0.99131
N	0.49121	-1.46417	-0.13700



Hydride transfer – starting species 6.50 and 6.39 in benzene

57

-1416.9065168

C	4.40909	1.35674	-1.49923
C	3.76213	1.63235	-0.29955
C	2.37217	1.58684	-0.19783
C	1.59103	1.30597	-1.32826
C	2.25616	1.06341	-2.54218
C	3.64138	1.06735	-2.62545
C	1.69213	1.79715	1.13196
C	0.12511	1.33007	-1.19322
C	-0.43269	1.82950	0.07492
C	-1.89272	1.93133	0.11956
C	-2.65428	1.60694	-1.01388
C	-2.09638	1.13974	-2.18461
C	-0.69952	1.00260	-2.24588
H	2.26061	2.53910	1.70688
H	5.49122	1.38184	-1.56127
H	4.34466	1.89209	0.58071
H	1.68723	0.87099	-3.44321
H	4.12247	0.86213	-3.57579
H	-3.73053	1.70069	-0.92266
H	-2.71390	0.86867	-3.03199
H	-0.26375	0.61981	-3.16376
C	-2.67361	2.25174	1.32372
C	-2.00174	2.60845	2.62977
H	-2.77841	2.74187	3.38356
H	-1.28848	1.83440	2.91779
H	-1.40097	3.51235	2.51659
O	-3.91016	2.21940	1.30981
N	0.30220	2.18321	1.10125
H	1.77792	0.85796	1.71311
C	2.46361	-1.62500	2.29208
O	1.96397	-2.13205	3.27209
C	1.80851	-1.69478	0.94282
C	0.39784	-1.58741	0.78970
C	2.60353	-1.93672	-0.16090
C	-0.17932	-1.86986	-0.46985
C	2.03048	-2.16240	-1.42025
H	3.68182	-1.96817	-0.05463
C	-1.62351	-1.81191	-0.59023
C	0.66252	-2.15295	-1.56331
C	-1.61498	-0.99147	1.70911
H	2.66758	-2.33897	-2.27832
C	-2.34503	-1.34671	0.52312
C	-2.34121	-2.19504	-1.74159
H	0.23053	-2.33202	-2.54021
H	-2.17690	-0.57759	2.54628
C	-3.74604	-1.22380	0.46944
C	-3.71565	-2.10202	-1.77063
H	-1.81845	-2.57771	-2.60909
C	-4.42658	-1.60031	-0.66594
H	-4.27143	-0.82169	1.32916
H	-4.25385	-2.40647	-2.66112
H	-5.50523	-1.50812	-0.71332
C	3.83424	-0.98112	2.37535
H	4.59076	-1.75209	2.19659
H	3.96789	-0.19018	1.63853
H	3.97587	-0.60009	3.38583

N	-0.34038	-1.13747	1.86626

Hydride transfer – transition state in benzene

57

-1416.8637978

C	-4.00972	-0.55095	2.16211
C	-3.61331	0.57575	1.46569
C	-2.25549	0.84034	1.24728
C	-1.27193	-0.00671	1.78582
C	-1.69295	-1.15270	2.48455
C	-3.03713	-1.42823	2.65615
C	-1.82435	1.99409	0.44644
C	0.12744	0.39208	1.63832
C	0.39447	1.64736	1.00727
C	1.75516	2.07173	0.92723
C	2.76701	1.30977	1.49760
C	2.49453	0.08643	2.10578
C	1.18371	-0.36342	2.15496
H	-2.59352	2.74532	0.25574
H	-5.06191	-0.75357	2.32486
H	-4.35172	1.26979	1.07766
H	-0.96304	-1.83582	2.90061
H	-3.33666	-2.32116	3.19341
H	3.78578	1.67278	1.41794
H	3.29695	-0.52161	2.50541
H	0.98211	-1.32552	2.61214
C	2.18873	3.27762	0.15453
C	1.43908	3.68772	-1.08979
H	2.15008	4.16048	-1.76909
H	0.92459	2.84616	-1.55668
H	0.66718	4.40803	-0.81364
O	3.20121	3.87550	0.48009
N	-0.57107	2.46519	0.51546
H	-2.02269	1.43659	-0.92627
C	-2.32497	0.86023	-2.06329
O	-1.78487	1.44784	-3.06296
C	-1.79526	-0.51263	-1.62661
C	-0.39546	-0.74522	-1.47348
C	-2.66505	-1.53646	-1.29566
C	0.07027	-1.98964	-0.97449
C	-2.20498	-2.77816	-0.83186
H	-3.73267	-1.38633	-1.39264
C	1.49558	-2.15847	-0.75696
C	-0.85899	-3.00293	-0.66793
C	1.73508	0.11678	-1.59382
H	-2.91899	-3.55759	-0.58931
C	2.33965	-1.08314	-1.08643
C	2.08410	-3.31771	-0.20558
H	-0.52007	-3.96038	-0.29319
H	2.39187	0.95459	-1.83374
C	3.72852	-1.16518	-0.87617
C	3.44570	-3.38516	-0.00091
H	1.47031	-4.16561	0.07046
C	4.28142	-2.30456	-0.33920
H	4.34686	-0.30985	-1.12964
H	3.87761	-4.28255	0.42761
H	5.34925	-2.37085	-0.16780
C	-3.85870	0.99990	-1.99361
H	-4.30690	0.43947	-2.82149
H	-4.30419	0.66028	-1.05800
H	-4.08931	2.05635	-2.13979
N	0.47041	0.28953	-1.76965

Hydride transfer – product 6.38 and 6.51 in benzene

57

-1416.9002204

C	2.37325	-2.72111	-2.41218
C	2.29733	-1.34716	-2.39372
C	1.09152	-0.71261	-2.04508
C	-0.04887	-1.46795	-1.71345
C	0.05442	-2.87371	-1.72319
C	1.24311	-3.48283	-2.06848
C	0.99190	0.72101	-2.02487
C	-1.25756	-0.74082	-1.37356
C	-1.21487	0.67449	-1.38825
C	-2.38772	1.41105	-1.07366
C	-3.55770	0.73770	-0.77468
C	-3.59558	-0.66141	-0.74720
C	-2.46196	-1.38659	-1.03459
H	1.88019	1.29983	-2.27039
H	3.30065	-3.21632	-2.67342
H	3.16255	-0.73636	-2.62954
H	-0.79698	-3.48785	-1.45824
H	1.30693	-4.56515	-2.07127
H	-4.44505	1.31688	-0.54799
H	-4.51311	-1.17276	-0.48165
H	-2.50142	-2.46749	-0.99321
C	-2.45426	2.91828	-1.02492
C	-1.27372	3.72682	-0.55950
H	-1.64272	4.67979	-0.18036
H	-0.68507	3.19667	0.19072
H	-0.60764	3.90109	-1.40648
O	-3.50491	3.46027	-1.30669
N	-0.08003	1.38108	-1.73560
H	2.53972	2.80053	2.04525
C	3.10717	2.37019	1.18901
O	4.44547	2.47544	1.31653
C	2.62440	0.89823	1.11758
C	1.29241	0.47579	1.38605
C	3.56842	-0.07040	0.83645
C	0.96007	-0.90550	1.39200
C	3.23738	-1.43294	0.79640
H	4.58249	0.28454	0.68429
C	-0.39279	-1.29219	1.74260
C	1.95563	-1.85085	1.07560
C	-0.85248	1.09269	1.98056
H	3.99870	-2.16799	0.55445
C	-1.30729	-0.26972	2.06165
C	-0.84994	-2.62775	1.78973
H	1.71944	-2.90710	1.05091
H	-1.57508	1.88312	2.19250
C	-2.62624	-0.57768	2.44442
C	-2.14560	-2.91486	2.16494
H	-0.18083	-3.44095	1.53845
C	-3.04417	-1.88767	2.50467
H	-3.30575	0.23503	2.68162
H	-2.47502	-3.94752	2.20169
H	-4.05870	-2.12935	2.79917
C	2.58200	3.10469	-0.07216
H	3.13864	2.72985	-0.93881
H	1.51047	2.97278	-0.24436
H	2.80808	4.16982	0.03203
N	0.34653	1.45320	1.66887

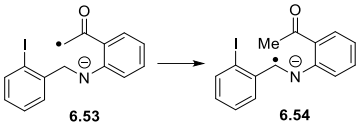
Anion 6.51 in benzene

29

-708.7642915

H	2.90016	-1.53626	-1.02537
C	3.23607	-0.79724	-0.26243
O	4.41349	-0.21043	-0.55373
C	2.06507	0.20995	-0.15585
C	0.69283	-0.16123	-0.13494
C	2.37702	1.55290	-0.07347
C	-0.32240	0.82427	-0.00740
C	1.38132	2.53239	0.05705
H	3.43188	1.80073	-0.12635
C	-1.70733	0.39097	0.01112
C	0.04963	2.17948	0.09379
C	-0.84584	-1.87945	-0.24616
H	1.65888	3.57933	0.12565
C	-1.96678	-0.98841	-0.10789
C	-2.81220	1.26157	0.14080
H	-0.70519	2.94924	0.19472
H	-1.05200	-2.94524	-0.35080
C	-3.28781	-1.47663	-0.09810
C	-4.09989	0.77074	0.15001
H	-2.65571	2.32818	0.23466
C	-4.34806	-0.60926	0.03011
H	-3.45220	-2.54526	-0.19320
H	-4.93244	1.45772	0.25069
H	-5.36578	-0.98066	0.03893
C	3.28402	-1.57414	1.08267
H	3.53567	-0.87047	1.88336
H	2.34439	-2.07965	1.32450
H	4.08645	-2.31435	1.01774
N	0.38915	-1.51077	-0.26008

Scheme 6.11



6.53 6.54

H atom abstraction of 6.53 – starting species 6.53 in DMSO

30

-720.1128365

C	-2.15076	3.48302	-0.05636
C	-0.98080	2.73576	0.02377
C	-1.00108	1.33810	0.03484
C	-2.25489	0.72718	-0.04190
C	-3.43696	1.45410	-0.12376
C	-3.38318	2.84458	-0.12967
H	-2.09768	4.56537	-0.06114
H	-0.01740	3.22522	0.08266
H	-4.39053	0.94485	-0.18241
H	-4.30176	3.41570	-0.19153
I	-2.42678	-1.40719	-0.03936
C	0.27620	0.52989	0.12722
H	0.22201	-0.15568	0.98640
H	0.34337	-0.14560	-0.74046
N	1.43766	1.35966	0.23231
C	2.67008	0.83590	0.12843
C	3.71419	1.81694	0.09168
C	3.05169	-0.54910	-0.00725
C	5.03058	1.48485	-0.12970
H	3.41283	2.85084	0.21586
C	4.39091	-0.84291	-0.25004
C	5.37603	0.14142	-0.32070
H	5.79022	2.25679	-0.16538
H	4.67088	-1.88520	-0.35732
H	6.40717	-0.13723	-0.50405
C	2.11159	-1.71290	0.23056
C	1.91664	-2.57833	-0.81433
H	1.25185	-3.42858	-0.70184
H	2.41462	-2.42862	-1.76366
O	1.60858	-1.78321	1.40823

H atom abstraction of 6.53 – transition state in DMSO

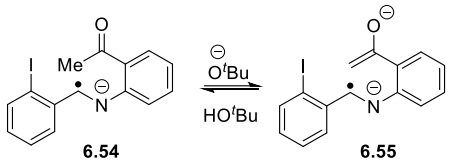
30
-720.0955497

C	2.33489	3.38090	0.34782
C	1.11275	2.72770	0.26375
C	1.02803	1.34363	0.05858
C	2.23805	0.65036	-0.04463
C	3.47225	1.28582	0.03397
C	3.52114	2.66208	0.23193
H	2.36188	4.45323	0.50264
H	0.18268	3.27583	0.34837
H	4.38884	0.71602	-0.05373
H	4.48083	3.16072	0.29588
I	2.26154	-1.47207	-0.33030
C	-0.30219	0.66172	0.00329
H	-0.32318	-0.15041	-0.74278
H	-0.41585	-0.07214	0.98565
N	-1.40325	1.49114	-0.00257
C	-2.63689	0.90641	-0.10047
C	-3.68948	1.75940	-0.52765
C	-2.97921	-0.45438	0.18412
C	-4.97858	1.30520	-0.72755
H	-3.43403	2.79458	-0.72630
C	-4.28800	-0.88675	-0.03609
C	-5.28970	-0.03729	-0.49256
H	-5.74422	1.99195	-1.07099
H	-4.51794	-1.92559	0.17979
H	-6.29502	-0.40958	-0.64860
C	-2.04686	-1.47746	0.80687
C	-1.33265	-1.08840	1.95321
H	-0.66803	-1.80560	2.42207
H	-1.67766	-0.24483	2.54078
O	-1.91980	-2.57952	0.22045

H atom abstraction of 6.53 – product 6.54 in DMSO

30
-720.1524777

C	2.44456	3.28542	0.45865
C	1.19789	2.73232	0.24976
C	1.01754	1.34617	-0.05010
C	2.21776	0.58239	-0.08479
C	3.46864	1.13109	0.12671
C	3.60067	2.49745	0.39652
H	2.52610	4.34495	0.67676
H	0.30667	3.34584	0.30108
H	4.35021	0.50224	0.08904
H	4.58173	2.92530	0.55978
I	2.14751	-1.53236	-0.44900
C	-0.28051	0.81407	-0.26682
H	-0.36059	-0.25068	-0.48948
H	-0.12544	-0.63452	2.09108
N	-1.38505	1.56286	-0.23343
C	-2.59991	0.95088	-0.22801
C	-3.69767	1.66898	-0.78175
C	-2.87353	-0.37384	0.24520
C	-4.92955	1.08640	-0.97476
H	-3.51326	2.69039	-1.09653
C	-4.13068	-0.95491	-0.00243
C	-5.15536	-0.25367	-0.60782
H	-5.72990	1.66516	-1.42358
H	-4.29505	-1.96824	0.34834
H	-6.12280	-0.71452	-0.76454
C	-1.97384	-1.15062	1.13288
C	-1.19233	-0.43302	2.21580
H	-1.50881	-0.85956	3.17081
H	-1.35417	0.64313	2.21496
O	-1.94495	-2.37363	1.09739



6.54 **6.55**

Deprotonation of 6.54 – starting species 6.54 and O^{t}Bu anion in DMSO

44
-953.2772133

C	-3.48496	3.03921	-1.47257
C	-2.37228	2.62827	-0.76778
C	-2.26266	1.31680	-0.20688
C	-3.37862	0.46897	-0.45603
C	-4.49483	0.87551	-1.16183
C	-4.56653	2.17383	-1.67933
H	-3.51838	4.04751	-1.87166
H	-1.53896	3.30198	-0.60983
H	-5.31625	0.18679	-1.31863
H	-5.44227	2.48896	-2.23238
I	-3.37969	-1.55779	0.25486
C	-1.10704	0.93570	0.52443
H	-1.08117	-0.07484	0.93309
H	0.06821	-1.23361	-1.66188
N	-0.09237	1.77203	0.75566
C	1.05797	1.28493	1.30227
C	1.85883	2.18888	2.05344
C	1.51832	-0.06930	1.23282
C	2.95212	1.76956	2.78100
H	1.54781	3.22800	2.07346
C	2.60661	-0.47632	2.01944
C	3.32501	0.41524	2.79715
H	3.52005	2.49356	3.35586
H	2.91115	-1.51615	1.96059
H	4.17872	0.08236	3.37477
C	1.02958	-1.07492	0.24788
C	0.85292	-0.64343	-1.18511
H	1.82715	-0.84708	-1.66020
H	0.64060	0.41914	-1.28044
O	0.93984	-2.25810	0.54652
O	3.97145	-0.94344	-2.07496
C	5.09637	-0.37871	-1.52559
C	6.19112	-0.15419	-2.59419
H	5.80708	0.50917	-3.37582
H	7.10387	0.29099	-2.18125
H	6.45317	-1.11079	-3.05799
C	5.69402	-1.28349	-0.42310
H	5.95374	-2.25815	-0.84940
H	6.59292	-0.85612	0.03682
H	4.94628	-1.44115	0.36070
C	4.77849	0.99309	-0.88307
H	4.37541	1.66847	-1.64550
H	4.02226	0.86842	-0.09998
H	5.66212	1.46586	-0.43738

Deprotonation of 6.54 – transition state in DMSO

44
-953.2692603

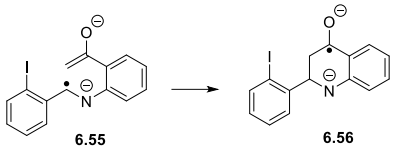
C	-2.84406	2.63231	2.32412
C	-1.84831	1.69189	2.16351
C	-1.92147	0.65453	1.17725
C	-3.09393	0.69312	0.36715
C	-4.09266	1.63484	0.52171
C	-3.98521	2.62236	1.51005
H	-2.73598	3.39335	3.09021
H	-0.96639	1.70922	2.79185
H	-4.96228	1.61430	-0.12473
H	-4.76964	3.35875	1.62987
I	-3.37052	-0.75143	-1.19714
C	-0.87475	-0.29501	1.05180
H	-0.96361	-1.04223	0.26338
H	0.56342	0.87815	-1.95839
N	0.18012	-0.31031	1.86688
C	1.24140	-1.12641	1.56615
C	2.01465	-1.60675	2.65456
C	1.63837	-1.54621	0.26062
C	3.05630	-2.49924	2.48461
H	1.73834	-1.26729	3.64726
C	2.67424	-2.47555	0.11949
C	3.38754	-2.96436	1.20629
H	3.61012	-2.84620	3.35087
H	2.94244	-2.78348	-0.88652
H	4.19651	-3.67064	1.06378
C	1.12977	-0.94695	-1.02836
C	1.20671	0.49341	-1.16450
H	2.43987	0.71300	-1.52176
H	1.08170	1.03134	-0.22658
O	0.84632	-1.70574	-1.96705
O	3.71339	0.97042	-1.91751
C	4.39157	1.71795	-0.95551
C	5.83995	1.94755	-1.41123
H	5.84924	2.48263	-2.36551
H	6.41040	2.53136	-0.68080
H	6.34084	0.98530	-1.55327
C	4.41063	0.97830	0.39602
H	4.90044	0.00649	0.27665
H	4.94456	1.54615	1.16551
H	3.38871	0.79339	0.74096
C	3.71465	3.08826	-0.75916
H	3.69600	3.62958	-1.70986
H	2.68285	2.95062	-0.42399
H	4.23934	3.70254	-0.01991

Deprotonation of 6.54 – product 6.55 and HO^{t}Bu in DMSO

44

-953.2870449

C	-3.03547	3.44386	0.67746
C	-1.97240	2.60221	0.92547
C	-2.00857	1.19986	0.61657
C	-3.22283	0.76809	0.00369
C	-4.28942	1.60702	-0.24785
C	-4.21747	2.96603	0.09194
H	-2.95214	4.49388	0.93971
H	-1.06377	2.98025	1.37824
H	-5.18630	1.21602	-0.71313
H	-5.05605	3.62154	-0.10508
I	-3.45596	-1.28108	-0.60472
C	-0.90348	0.36380	0.91804
H	-0.98456	-0.69128	0.66096
H	0.67944	-0.42880	-2.46042
N	0.19246	0.81978	1.51501
C	1.26241	-0.03750	1.68696
C	2.04463	0.17271	2.84931
C	1.65730	-1.09512	0.81568
C	3.10717	-0.64468	3.19161
H	1.75960	0.99843	3.49344
C	2.71597	-1.92290	1.20346
C	3.44482	-1.72438	2.37117
H	3.66611	-0.44896	4.10096
H	2.98428	-2.73266	0.53198
H	4.26864	-2.38105	2.62631
C	1.11363	-1.35428	-0.58293
C	1.05884	-0.28649	-1.45282
H	3.16453	-0.37334	-1.66286
H	1.17593	0.72544	-1.08503
O	0.85297	-2.57411	-0.87582
O	4.13423	-0.37030	-1.80909
C	4.64775	0.90588	-1.42020
C	6.16489	0.78690	-1.49347
H	6.47325	0.50327	-2.50283
H	6.63771	1.73861	-1.24001
H	6.51810	0.02483	-0.79441
C	4.20341	1.23978	0.00436
H	4.47027	0.42978	0.68835
H	4.67506	2.16600	0.34464
H	3.11872	1.36447	0.05019
C	4.14761	1.97460	-2.39429
H	4.47065	1.73963	-3.41157
H	3.05498	2.01456	-2.37643
H	4.53383	2.96101	-2.12395



6.55 6.56

S$_{RN}$1 cyclisation 6.55 – starting species 6.55 in DMSO

29

-719.6364475

C	2.41851	3.31312	0.49110
C	1.18132	2.73280	0.31111
C	1.01506	1.33434	0.02563
C	2.24113	0.60558	-0.03850
C	3.48233	1.18070	0.14420
C	3.59528	2.55316	0.41063
H	2.47870	4.37624	0.70177
H	0.27944	3.32885	0.37797
H	4.37585	0.57016	0.08425
H	4.57002	3.00221	0.55291
I	2.22457	-1.50799	-0.43230
C	-0.27922	0.78251	-0.16129
H	-0.35243	-0.28822	-0.34838
N	-1.37866	1.53048	-0.13435
C	-2.61322	0.91403	-0.21199
C	-3.63984	1.65192	-0.85422
C	-2.95884	-0.37221	0.29795
C	-4.91335	1.14622	-1.05089
H	-3.38352	2.64169	-1.21810
C	-4.24517	-0.86647	0.06173
C	-5.22777	-0.13897	-0.60228
H	-5.65909	1.74816	-1.55970
H	-4.47718	-1.85620	0.44460
H	-6.21730	-0.55543	-0.75168
C	-2.07514	-1.26093	1.16431
C	-1.66291	-0.75766	2.37158
H	-1.04350	-1.35804	3.03128
H	-1.86720	0.27127	2.64208
O	-1.85805	-2.44742	0.71759

$S_{RN}1$ cyclisation 6.55 – transition state in DMSO

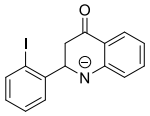
29
-719.6065580

C	2.13213	3.33574	0.49459
C	0.94696	2.67314	0.23573
C	0.89485	1.27778	-0.05881
C	2.15685	0.62736	-0.03989
C	3.34920	1.27914	0.21509
C	3.35502	2.65351	0.48723
H	2.11100	4.40055	0.70398
H	0.00261	3.20357	0.23761
H	4.28182	0.72742	0.20483
H	4.28815	3.16316	0.69152
I	2.28613	-1.48355	-0.42771
C	-0.37356	0.62165	-0.23308
H	-0.31917	-0.37026	-0.69080
N	-1.48497	1.39677	-0.53297
C	-2.68739	0.80472	-0.36783
C	-3.83903	1.39578	-0.97504
C	-2.92973	-0.41083	0.38415
C	-5.08779	0.80585	-0.94033
H	-3.69254	2.32927	-1.51158
C	-4.19869	-0.99960	0.36198
C	-5.28544	-0.42452	-0.28712
H	-5.92116	1.29589	-1.43572
H	-4.32135	-1.93120	0.90827
H	-6.25957	-0.89905	-0.27383
C	-1.85278	-1.02034	1.20949
C	-0.84015	-0.12878	1.64275
H	0.01661	-0.56174	2.15525
H	-1.10344	0.88490	1.92743
O	-1.78700	-2.29194	1.33863

$S_{RN}1$ cyclisation 6.55 – product 6.56 in DMSO

29
-719.6427170

C	1.99970	3.32703	0.59693
C	0.84976	2.57504	0.39414
C	0.89358	1.20646	0.09781
C	2.16443	0.63669	0.00725
C	3.33322	1.36881	0.19996
C	3.24991	2.72406	0.50021
H	1.92148	4.38364	0.82647
H	-0.13274	3.02809	0.44841
H	4.30044	0.88997	0.11321
H	4.15796	3.29592	0.65049
I	2.43357	-1.44364	-0.46376
C	-0.40898	0.43502	-0.03970
H	-0.22620	-0.37294	-0.77201
N	-1.47728	1.28848	-0.50511
C	-2.70574	0.74632	-0.43084
C	-3.79422	1.36120	-1.10177
C	-3.01006	-0.47613	0.32937
C	-5.09384	0.81793	-1.11209
H	-3.58432	2.27464	-1.65286
C	-4.33399	-1.01725	0.26055
C	-5.35778	-0.38381	-0.44475
H	-5.88406	1.32705	-1.65639
H	-4.53259	-1.92839	0.81559
H	-6.35424	-0.81551	-0.46682
C	-2.03526	-1.01886	1.19862
C	-0.72411	-0.26584	1.29314
H	0.07473	-0.96220	1.57228
H	-0.77637	0.49885	2.08570
O	-2.22028	-2.04319	1.95724

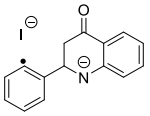


Anion 6.57 in DMSO

29

-719.5859468

C	2.01189	3.33512	0.56672
C	0.85506	2.58962	0.37861
C	0.89470	1.22002	0.09290
C	2.15923	0.63518	-0.00006
C	3.33172	1.36397	0.17864
C	3.25638	2.72246	0.46617
H	1.94215	4.39372	0.78799
H	-0.12105	3.05479	0.43957
H	4.29617	0.87993	0.09128
H	4.16853	3.29042	0.60492
I	2.40019	-1.44823	-0.44527
C	-0.40626	0.45148	-0.03700
H	-0.25381	-0.34681	-0.78492
N	-1.48630	1.30283	-0.49702
C	-2.68299	0.75904	-0.39067
C	-3.81592	1.42251	-1.00356
C	-2.98773	-0.49000	0.28008
C	-5.05855	0.85865	-1.02614
H	-3.63255	2.38044	-1.47941
C	-4.29029	-1.03935	0.22670
C	-5.31971	-0.40515	-0.42064
H	-5.86952	1.38579	-1.52009
H	-4.45706	-1.98122	0.74029
H	-6.31323	-0.83411	-0.45528
C	-1.99126	-1.07086	1.15069
C	-0.72521	-0.24675	1.29071
H	0.09066	-0.88660	1.63200
H	-0.90624	0.51734	2.06010
O	-2.14206	-2.10661	1.80536



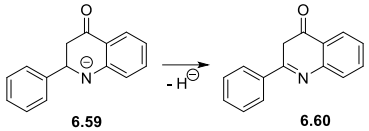
Radical dianion 6.58 in DMSO

29

-719.6931479

C	0.53756	4.49515	0.22893
C	-0.33505	3.41199	0.10845
C	0.15365	2.10818	-0.03499
C	1.52922	1.99037	-0.04976
C	2.43620	3.01471	0.05966
C	1.91685	4.30794	0.20519
H	0.13379	5.49525	0.33863
H	-1.40863	3.55810	0.11390
H	3.50616	2.83952	0.03402
H	2.58882	5.15414	0.29464
I	3.11042	-1.73631	-0.29779
C	-0.75268	0.89666	-0.11977
H	-0.32176	0.22660	-0.88977
N	-2.10020	1.25415	-0.51360
C	-2.97896	0.28071	-0.37064
C	-4.31072	0.44502	-0.91796
C	-2.73326	-0.99135	0.28248
C	-5.23050	-0.56332	-0.89908
H	-4.54292	1.39929	-1.37957
C	-3.71563	-2.00854	0.27467
C	-4.94294	-1.82934	-0.31137
H	-6.20709	-0.39704	-1.34443
H	-3.47309	-2.94131	0.77442
H	-5.68763	-2.61537	-0.31032
C	-1.54401	-1.13888	1.09244
C	-0.69620	0.11307	1.19567
H	0.32799	-0.16096	1.45676
H	-1.10800	0.73133	2.00660
O	-1.24493	-2.15477	1.72750

Scheme 6.12



6.59 6.60

Hydride elimination – starting species 6.59 in DMSO

29

-708.8185638

C	4.33215	0.59416	0.64822
C	2.96723	0.77402	0.84986
C	2.03292	-0.06256	0.23323
C	2.49720	-1.08991	-0.58829
C	3.86349	-1.27256	-0.79468
C	4.78598	-0.43179	-0.17847
H	5.04198	1.25096	1.13835
H	2.61949	1.57372	1.49776
H	4.20775	-2.07661	-1.43574
H	5.84850	-0.57664	-0.33621
C	0.55090	0.19523	0.41572
C	-1.53530	-0.79846	0.13176
C	-2.17683	0.49738	0.01256
C	-2.43743	-1.93308	0.15084
C	-3.58717	0.60838	0.02064
C	-3.79342	-1.77981	0.15206
H	-1.99105	-2.92119	0.19861
C	-4.40243	-0.49152	0.10411
H	-4.01112	1.60426	-0.06573
H	-4.42535	-2.66226	0.19037
H	-5.48081	-0.39403	0.10860
N	-0.23858	-1.00815	0.24035
O	-1.79151	2.79616	-0.45597
C	-1.36108	1.64988	-0.29353
C	0.10892	1.34040	-0.50367
H	1.77470	-1.74966	-1.05350
H	0.69918	2.24416	-0.33899
H	0.23987	1.03357	-1.55156
H	0.40831	0.56277	1.45105

Hydride elimination – transition state in DMSO

29

-708.7451341

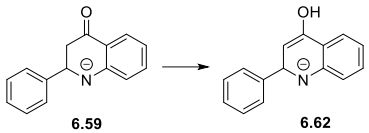
C	3.93692	-1.44068	0.53080
C	2.56527	-1.23457	0.50288
C	2.03273	-0.03996	0.00437
C	2.90731	0.93933	-0.47275
C	4.28478	0.72895	-0.45271
C	4.80403	-0.45761	0.05160
H	4.33514	-2.36645	0.93008
H	1.88458	-1.98884	0.87826
H	4.94985	1.49530	-0.83330
H	5.87545	-0.61837	0.07303
C	0.55519	0.14745	-0.03861
C	-1.55266	-0.76893	-0.17483
C	-2.20432	0.45497	0.09072
C	-2.34393	-1.92184	-0.33320
C	-3.59955	0.50766	0.19625
C	-3.72173	-1.85401	-0.23827
H	-1.84285	-2.86477	-0.51962
C	-4.36069	-0.63492	0.03148
H	-4.06540	1.46686	0.39268
H	-4.31203	-2.75424	-0.36663
H	-5.44057	-0.59049	0.10343
N	-0.17480	-0.91877	-0.18756
O	-1.87225	2.78068	0.43657
C	-1.40132	1.69128	0.15815
C	0.01939	1.53063	-0.30984
H	0.63591	2.31231	0.12463
H	-0.00053	1.67379	-1.40521
H	2.52452	1.86810	-0.87846
H	0.12903	0.66632	2.04534

Hydride elimination – product 6.60 and hydride anion in DMSO

29

-708.7506846

C	3.95531	-1.48963	0.36020
C	2.58193	-1.29730	0.31379
C	2.05053	-0.05496	-0.05336
C	2.92554	0.98875	-0.36989
C	4.30265	0.79137	-0.33187
C	4.82081	-0.44596	0.03445
H	4.35393	-2.45322	0.65481
H	1.90318	-2.10111	0.56906
H	4.96816	1.60694	-0.58789
H	5.89316	-0.59761	0.06968
C	0.57643	0.13321	-0.09738
C	-1.56587	-0.76926	-0.10948
C	-2.23052	0.46350	0.00646
C	-2.32656	-1.94004	-0.18989
C	-3.62463	0.51462	0.04531
C	-3.71241	-1.87967	-0.16193
H	-1.80858	-2.88816	-0.27061
C	-4.36855	-0.65158	-0.04403
H	-4.10572	1.48107	0.14164
H	-4.28920	-2.79481	-0.22755
H	-5.45051	-0.61270	-0.02152
N	-0.16850	-0.90888	-0.11302
O	-1.91833	2.79115	0.30296
C	-1.42915	1.69903	0.09506
C	0.05178	1.54517	-0.14428
H	0.58801	2.18818	0.55594
H	0.24339	1.95066	-1.14810
H	2.54460	1.96019	-0.66053
H	-0.35810	0.65009	3.17342



6.59 **6.62**

Enol formation from 6.59 – starting species 6.59 in DMSO

29
-708.8185638

C	4.33215	0.59416	0.64822
C	2.96723	0.77402	0.84986
C	2.03292	-0.06256	0.23323
C	2.49720	-1.08991	-0.58829
C	3.86349	-1.27256	-0.79468
C	4.78598	-0.43179	-0.17847
H	5.04198	1.25096	1.13835
H	2.61949	1.57372	1.49776
H	4.20775	-2.07661	-1.43574
H	5.84850	-0.57664	-0.33621
C	0.55090	0.19523	0.41572
C	-1.53530	-0.79846	0.13176
C	-2.17683	0.49738	0.01256
C	-2.43743	-1.93308	0.15084
C	-3.58717	0.60838	0.02064
C	-3.79342	-1.77981	0.15206
H	-1.99105	-2.92119	0.19861
C	-4.40243	-0.49152	0.10411
H	-4.01112	1.60426	-0.06573
H	-4.42535	-2.66226	0.19037
H	-5.48081	-0.39403	0.10860
N	-0.23858	-1.00815	0.24035
O	-1.79151	2.79616	-0.45597
C	-1.36108	1.64988	-0.29353
C	0.10892	1.34040	-0.50367
H	1.77470	-1.74966	-1.05350
H	0.69918	2.24416	-0.33899
H	0.23987	1.03357	-1.55156
H	0.40831	0.56277	1.45105

Enol formation from 6.59 – transition state in DMSO

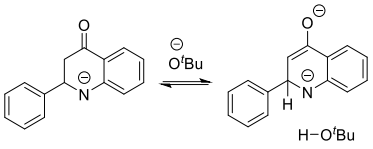
29
-708.7131734

C	4.33989	0.56196	0.66081
C	2.97782	0.74989	0.86950
C	2.03342	-0.07040	0.24504
C	2.48666	-1.08849	-0.59327
C	3.85160	-1.27929	-0.80770
C	4.78308	-0.45601	-0.18279
H	5.05693	1.20641	1.15697
H	2.63489	1.54517	1.52494
H	4.18685	-2.07662	-1.46192
H	5.84385	-0.60708	-0.34652
C	0.55962	0.20581	0.44412
C	-1.54052	-0.80475	0.11195
C	-2.19775	0.50464	0.02308
C	-2.44670	-1.94304	0.08236
C	-3.61739	0.62313	0.09232
C	-3.79561	-1.78070	0.12289
H	-2.00524	-2.93400	0.07083
C	-4.41206	-0.48241	0.15168
H	-4.04845	1.61951	0.07375
H	-4.43292	-2.65962	0.13649
H	-5.49049	-0.39805	0.19951
N	-0.25445	-1.00053	0.22108
O	-1.60482	2.80844	-0.55478
C	-1.33981	1.54916	-0.30643
C	0.09850	1.37935	-0.41038
H	1.75886	-1.73581	-1.06759
H	0.42230	0.48822	1.50395
H	-0.36335	2.81260	-0.44964
H	0.37210	1.26233	-1.46911

Enol formation from 6.59 – product 6.62 in DMSO

29
-708.7875514

C	-4.39623	0.43940	-0.55700
C	-3.07001	0.60165	-0.94755
C	-2.04281	-0.10296	-0.31531
C	-2.37312	-0.98091	0.71561
C	-3.69937	-1.15052	1.10875
C	-4.71604	-0.43999	0.47554
H	-5.18081	0.99229	-1.06166
H	-2.82545	1.28222	-1.75857
H	-3.94025	-1.84075	1.90995
H	-5.74786	-0.57350	0.77942
C	-0.59454	0.13700	-0.72576
C	1.52989	-0.81783	-0.25750
C	2.13926	0.47284	-0.02183
C	2.44210	-1.92936	-0.22260
C	3.51679	0.60981	0.15853
C	3.79983	-1.76138	-0.05580
H	2.02456	-2.92246	-0.35787
C	4.37075	-0.48673	0.12438
H	3.91594	1.60288	0.34011
H	4.44231	-2.63747	-0.06419
H	5.43950	-0.36628	0.24985
N	0.23460	-1.02604	-0.45390
O	1.75998	2.72211	0.67951
C	1.20874	1.57069	0.17379
C	-0.10061	1.41793	-0.07335
H	-1.57502	-1.53561	1.19489
H	-0.63335	0.30671	-1.82314
H	1.07660	3.39889	0.72775
H	-0.80593	2.22068	0.12527



6.59 **6.63**

Deprotonation of 6.59 – starting species 6.59 and O^{t}Bu anion in DMSO

43
-941.9423188

C	-2.40412	2.63236	1.03236
C	-1.31683	1.78209	1.23161
C	-0.36976	1.58227	0.22737
C	-0.53631	2.25193	-0.98845
C	-1.61898	3.09972	-1.19359
C	-2.55801	3.29494	-0.18044
H	-3.12988	2.77524	1.82539
H	-1.20161	1.26889	2.18160
H	-1.73125	3.61269	-2.14239
H	-3.40074	3.95808	-0.33851
C	0.80288	0.64556	0.42689
C	3.10439	0.51998	0.07980
C	3.05096	-0.93002	0.06089
C	4.43697	1.08732	0.01084
C	4.23887	-1.69614	0.07878
C	5.55780	0.30803	0.02430
H	4.51486	2.16947	-0.02036
C	5.48196	-1.11388	0.07697
H	4.13468	-2.77696	0.06802
H	6.53329	0.78461	-0.00707
H	6.38471	-1.71194	0.08779
N	2.06532	1.32626	0.17353
O	1.61549	-2.79896	-0.24053
C	1.77519	-1.57572	-0.16546
C	0.62393	-0.62414	-0.41188
H	0.20158	2.11230	-1.77169
H	-0.33624	-1.11077	-0.21407
H	0.65204	-0.35545	-1.47916
H	0.78605	0.32298	1.48599
O	-2.49498	-1.87033	-0.18338
C	-3.83718	-1.62297	-0.03429
C	-4.68765	-2.83190	-0.48903
H	-5.76473	-2.65871	-0.38015
H	-4.47723	-3.05186	-1.54069
H	-4.41760	-3.71269	0.10269
C	-4.27016	-0.39743	-0.87279
H	-3.69374	0.47968	-0.55926
H	-4.05657	-0.58728	-1.92996
H	-5.33757	-0.16709	-0.77172
C	-4.18984	-1.32971	1.44254
H	-5.25830	-1.13777	1.59610
H	-3.89885	-2.18367	2.06318
H	-3.62880	-0.45299	1.78226

Deprotonation of 6.59 – transition state in DMSO

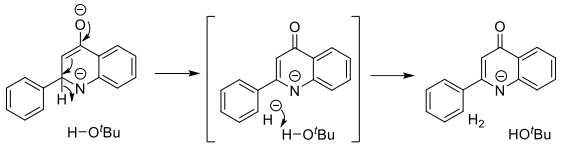
43
-941.9287739

C	4.22704	-2.19490	0.08914
C	2.84892	-2.12873	-0.09427
C	2.21044	-0.91742	-0.37897
C	2.99735	0.23197	-0.48392
C	4.37725	0.17423	-0.29276
C	4.99925	-1.03837	-0.00589
H	4.70035	-3.14782	0.29996
H	2.25219	-3.03409	-0.01784
H	4.97002	1.07930	-0.37280
H	6.07293	-1.08342	0.13615
C	0.68465	-0.87695	-0.51095
C	-0.08329	1.34072	-0.78402
C	-0.15658	1.56123	0.64569
C	-0.40773	2.49458	-1.59481
C	-0.46033	2.82702	1.16332
C	-0.69801	3.71912	-1.04729
H	-0.39643	2.36263	-2.67270
C	-0.71882	3.91974	0.35369
H	-0.50082	2.92309	2.24465
H	-0.91787	4.55309	-1.70861
H	-0.94666	4.89212	0.77276
N	0.24755	0.20860	-1.37835
O	-0.09932	0.52778	2.78694
C	-0.02970	0.40182	1.54174
C	0.03786	-0.88321	0.88006
H	2.51757	1.17466	-0.72160
H	-1.23447	-1.29345	0.80920
H	0.45747	-1.65460	1.53358
H	0.41126	-1.82266	-1.00177
O	-2.41164	-1.87291	0.89797
C	-3.28299	-1.54413	-0.14217
C	-4.63240	-2.23534	0.09515
H	-5.35301	-2.00444	-0.69673
H	-4.49407	-3.31987	0.13178
H	-5.05187	-1.90997	1.05167
C	-2.70897	-2.01146	-1.49120
H	-1.74937	-1.51648	-1.66690
H	-2.54826	-3.09404	-1.46872
H	-3.38131	-1.77907	-2.32433
C	-3.50321	-0.02196	-0.19985
H	-4.18979	0.26066	-1.00516
H	-3.92168	0.32592	0.75014
H	-2.54587	0.48156	-0.35982

Deprotonation of 6.59 – product 6.63 and HO^{t}Bu in DMSO

43
-941.9454129

C	4.52548	-1.98616	0.02516
C	3.14025	-1.99015	-0.13094
C	2.42748	-0.80183	-0.30538
C	3.14315	0.39854	-0.33591
C	4.52635	0.41078	-0.17729
C	5.22527	-0.78233	0.00574
H	5.05821	-2.92203	0.15582
H	2.59921	-2.93288	-0.11580
H	5.06479	1.35238	-0.20102
H	6.30268	-0.77316	0.12473
C	0.89457	-0.81708	-0.39937
C	-0.09825	1.31767	-0.75664
C	-0.35556	1.51750	0.65384
C	-0.46519	2.42169	-1.60458
C	-0.87328	2.72163	1.11838
C	-0.97409	3.60579	-1.10510
H	-0.31725	2.30019	-2.67419
C	-1.17992	3.79003	0.27158
H	-1.05348	2.79719	2.18677
H	-1.21770	4.40746	-1.79785
H	-1.57431	4.72173	0.66003
N	0.40735	0.21583	-1.30083
O	-0.54867	0.48259	2.81209
C	-0.18029	0.36276	1.58092
C	0.31222	-0.78731	1.00181
H	2.59891	1.32446	-0.48990
H	-1.68775	-1.44136	0.91602
H	0.48565	-1.65866	1.63319
H	0.65818	-1.79672	-0.85019
O	-2.55281	-1.90229	0.96478
C	-3.27225	-1.64127	-0.24267
C	-4.58143	-2.41170	-0.12866
H	-5.19757	-2.25185	-1.01667
H	-4.38422	-3.48205	-0.02990
H	-5.14199	-2.07850	0.74839
C	-2.45628	-2.13194	-1.43861
H	-1.51634	-1.57458	-1.49711
H	-2.23660	-3.19751	-1.33025
H	-3.00748	-1.98343	-2.37133
C	-3.53662	-0.14023	-0.36371
H	-4.09822	0.08425	-1.27483
H	-4.11529	0.20834	0.49636
H	-2.58857	0.40520	-0.39288



6.63 **6.64** **6.65**

Hydride elimination from 6.63 – starting species 6.63 + HO^{t}Bu in DMSO

43
-941.9444083

C	4.29886	-2.23872	-0.02344
C	2.92812	-2.08145	-0.22709
C	2.34902	-0.81331	-0.29392
C	3.18199	0.30177	-0.16548
C	4.55021	0.15350	0.03819
C	5.11612	-1.12015	0.11175
H	4.72882	-3.23358	0.02367
H	2.29436	-2.95821	-0.33460
H	5.18143	1.03057	0.13502
H	6.18260	-1.23725	0.26695
C	0.83054	-0.64719	-0.44611
C	-0.02038	1.56129	-0.77540
C	-0.40837	1.71066	0.61103
C	-0.27011	2.71254	-1.60380
C	-0.93402	2.91038	1.07735
C	-0.79039	3.89145	-1.10219
H	-0.01594	2.63324	-2.65712
C	-1.12661	4.02337	0.25364
H	-1.20507	2.95010	2.12845
H	-0.93967	4.72942	-1.77856
H	-1.53133	4.94966	0.64425
N	0.51131	0.47280	-1.31819
O	-0.71836	0.62809	2.73311
C	-0.29670	0.53005	1.51576
C	0.20232	-0.61467	0.93527
H	2.73759	1.28995	-0.23250
H	-1.95627	-1.00363	1.03865
H	0.31990	-1.50535	1.55263
H	0.50719	-1.57252	-0.95750
O	-2.88739	-1.30076	1.05465
C	-3.19198	-1.83041	-0.23802
C	-2.33237	-3.06863	-0.49469
H	-2.55124	-3.50015	-1.47504
H	-1.27301	-2.79878	-0.46258
H	-2.52289	-3.82512	0.27091
C	-2.92037	-0.76437	-1.29903
H	-3.53259	0.12042	-1.10152
H	-1.86541	-0.46911	-1.27857
H	-3.16329	-1.13923	-2.29728
C	-4.66876	-2.20112	-0.20370
H	-4.98286	-2.61605	-1.16425
H	-4.85387	-2.94576	0.57459
H	-5.27431	-1.31677	0.00920

Hydride elimination from 6.63 – transition state (1) in DMSO

43
-941.9073462

C	-4.72378	1.36066	0.53814
C	-3.37042	1.08710	0.68388
C	-2.75351	0.07267	-0.05776
C	-3.53542	-0.65705	-0.95302
C	-4.89420	-0.37763	-1.11236
C	-5.49596	0.62871	-0.36709
H	-5.17926	2.15387	1.12087
H	-2.76880	1.68389	1.36108
H	-5.48180	-0.95477	-1.81817
H	-6.55095	0.84646	-0.48773
C	-1.29669	-0.27249	0.14052
C	0.46197	-1.58546	-0.56298
C	1.10739	-1.50747	0.70727
C	1.16772	-2.25179	-1.60688
C	2.40003	-2.02371	0.87189
C	2.43947	-2.74917	-1.41896
H	0.67877	-2.33554	-2.57265
C	3.08074	-2.62956	-0.17131
H	2.85363	-1.93737	1.85394
H	2.95227	-3.23423	-2.24391
H	4.08361	-3.01634	-0.03087
N	-0.76255	-1.07513	-0.82394
O	0.85875	-0.97345	3.02718
C	0.36977	-0.93048	1.84711
C	-0.86610	-0.38004	1.51126
H	-3.06271	-1.44554	-1.52455
H	0.78128	1.66852	0.24454
H	-1.44831	0.09944	2.29144
H	-0.79056	1.29033	-0.32671
O	1.62856	1.95390	0.65470
C	2.57366	2.26927	-0.36758
C	2.16619	3.57013	-1.06243
H	2.88831	3.84345	-1.83681
H	1.18492	3.45381	-1.53093
H	2.10851	4.38406	-0.33526
C	2.66336	1.13023	-1.38410
H	2.86685	0.18205	-0.87950
H	1.72124	1.02390	-1.92837
H	3.45752	1.33003	-2.10952
C	3.90968	2.44393	0.34567
H	4.69306	2.72302	-0.36303
H	3.83153	3.22602	1.10515
H	4.19691	1.51014	0.83593

Hydride elimination from 6.63 – intermediate 6.64 and hydride anion and HO^{t}Bu in DMSO

43

-941.9511334

C	-4.29359	-0.35691	0.75613
C	-2.91868	-0.37921	0.97175
C	-2.07856	-1.15317	0.16410
C	-2.65534	-1.91016	-0.86135
C	-4.02908	-1.89483	-1.07378
C	-4.85523	-1.11458	-0.26747
H	-4.92501	0.26078	1.38472
H	-2.49811	0.23503	1.75888
H	-4.45719	-2.49131	-1.87147
H	-5.92552	-1.09630	-0.43680
C	-0.59357	-1.15539	0.34933
C	1.47608	-1.44893	-0.59541
C	2.14209	-1.12122	0.61272
C	2.27087	-1.75721	-1.73318
C	3.55054	-1.10706	0.65382
C	3.64351	-1.73653	-1.66884
H	1.75773	-2.00465	-2.65620
C	4.29888	-1.40725	-0.46232
H	4.02722	-0.84870	1.59267
H	4.22815	-1.97446	-2.55091
H	5.38172	-1.39197	-0.42078
N	0.12012	-1.46806	-0.73212
O	1.89982	-0.48168	2.89759
C	1.35463	-0.78514	1.80107
C	-0.04687	-0.83660	1.59629
H	-2.00828	-2.50544	-1.49334
H	-0.68879	-0.61964	2.44130
H	-2.33873	1.64316	-2.25097
H	-1.23986	2.80547	-1.71740
O	-0.65182	3.56344	-1.48464
C	0.17630	3.20407	-0.37781
C	1.02173	4.43327	-0.06678
H	1.69325	4.23442	0.77188
H	1.62351	4.70619	-0.93727
H	0.38056	5.27928	0.19293
C	1.07028	2.02249	-0.75513
H	0.46363	1.14487	-0.99531
H	1.68297	2.27698	-1.62482
H	1.73102	1.75333	0.07391
C	-0.69593	2.83628	0.82352
H	-1.31305	1.96609	0.58459
H	-0.07831	2.58524	1.69057
H	-1.35001	3.67236	1.08510

Hydride elimination from 6.63 – transition state (2) in DMSO

43

-941.9382458

C	-4.51461	0.60183	0.83251
C	-3.21494	0.13101	0.99742
C	-2.55143	-0.51470	-0.05044
C	-3.21848	-0.67422	-1.26896
C	-4.51995	-0.21313	-1.43211
C	-5.17344	0.42822	-0.38129
H	-5.01001	1.11103	1.65137
H	-2.70329	0.28916	1.94007
H	-5.02584	-0.35325	-2.38064
H	-6.18570	0.79358	-0.50924
C	-1.14524	-0.99470	0.10570
C	0.91857	-1.28950	-0.84559
C	1.47860	-1.75395	0.37216
C	1.77100	-1.19137	-1.97926
C	2.84627	-2.09058	0.42856
C	3.10119	-1.52569	-1.89902
H	1.33954	-0.83251	-2.90772
C	3.65346	-1.97938	-0.68119
H	3.24203	-2.43978	1.37589
H	3.73351	-1.43834	-2.77592
H	4.70467	-2.23775	-0.62647
N	-0.38565	-0.91522	-0.98511
O	1.07539	-2.30618	2.65705
C	0.62745	-1.87627	1.55977
C	-0.71460	-1.47046	1.34859
H	-2.70176	-1.16458	-2.08510
H	-1.40851	-1.53732	2.17837
H	-1.20793	2.73899	-1.25177
H	-0.26556	2.75093	-1.15190
O	1.05604	2.75462	-1.12849
C	1.64544	2.77221	0.13789
C	2.97013	1.99487	0.10059
H	3.48607	2.02727	1.06665
H	2.77948	0.94763	-0.15593
H	3.63120	2.42383	-0.65891
C	0.73209	2.11397	1.18884
H	-0.21522	2.65453	1.27130
H	0.51223	1.08168	0.89919
H	1.20833	2.10185	2.17501
C	1.93158	4.22182	0.56846
H	0.99686	4.78955	0.60159
H	2.40449	4.27397	1.55499
H	2.59496	4.69882	-0.15946

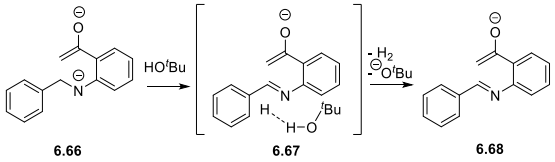
Hydride elimination from 6.63 – product complex 6.65 and H_2 and O^tBu anion in DMSO

43

-941.9468177

C	4.82143	-1.97082	0.19592
C	3.55797	-1.46360	0.48603
C	3.16329	-0.21133	0.00461
C	4.06314	0.51731	-0.77992
C	5.32871	0.01621	-1.06283
C	5.71334	-1.23139	-0.57585
H	5.10724	-2.94769	0.56876
H	2.86667	-2.05527	1.07530
H	6.01693	0.59982	-1.66374
H	6.69830	-1.62511	-0.79834
C	1.80966	0.34910	0.30253
C	0.04219	1.62887	-0.39654
C	-0.68231	1.38774	0.79858
C	-0.56747	2.43643	-1.39486
C	-1.96381	1.95011	0.96566
C	-1.82016	2.97111	-1.21014
H	-0.01337	2.61576	-2.30996
C	-2.53283	2.72988	-0.01582
H	-2.49044	1.74047	1.89012
H	-2.26563	3.58185	-1.98787
H	-3.52264	3.15087	0.11879
N	1.28584	1.12494	-0.64364
O	-0.68072	0.33864	2.94057
C	-0.08795	0.55681	1.84990
C	1.19383	0.04618	1.52185
H	3.75570	1.48373	-1.16000
H	1.70635	-0.56214	2.25778
H	0.21948	-1.62265	-1.36272
H	-0.51945	-1.52865	-1.29777
O	-2.98781	-1.08576	-1.57410
C	-3.67476	-1.68873	-0.54860
C	-4.76257	-0.75519	0.03361
H	-5.33549	-1.22658	0.84106
H	-4.29339	0.15310	0.42645
H	-5.45936	-0.46535	-0.76000
C	-2.73055	-2.08109	0.61352
H	-1.95765	-2.76212	0.24323
H	-2.23606	-1.18859	1.01304
H	-3.26259	-2.57686	1.43455
C	-4.37634	-2.98069	-1.03109
H	-3.62933	-3.67201	-1.43473
H	-4.92228	-3.49183	-0.22932
H	-5.08452	-2.73987	-1.83043

Scheme 6.13A



Hydride elimination from 6.66 – starting species 6.66 and HO^tBu in DMSO

45

-943.1293587

C	-5.23735	-0.27394	-0.59614
C	-3.96667	-0.47743	-1.13464
C	-2.85164	0.17476	-0.60948
C	-3.03607	1.03916	0.47325
C	-4.30002	1.24833	1.01547
C	-5.40740	0.59037	0.48082
H	-6.09253	-0.78941	-1.01892
H	-3.83857	-1.15349	-1.97462
H	-4.42485	1.92637	1.85246
H	-6.39354	0.75200	0.90100
C	-1.46609	-0.06119	-1.16278
H	-1.56862	-0.48060	-2.18116
C	0.55913	-1.13162	-0.65825
C	1.44179	-1.92094	0.18160
C	1.16364	-0.61023	-1.85408
C	2.75875	-2.12377	-0.17749
C	2.50109	-0.84983	-2.18412
H	0.56126	-0.03935	-2.55133
C	3.32412	-1.59898	-1.35760
H	3.38248	-2.71272	0.49117
H	2.89449	-0.43235	-3.10792
H	4.36333	-1.77896	-1.60608
N	-0.70524	-0.91594	-0.28080
O	0.24402	-3.64201	1.33505
C	0.93253	-2.56167	1.45785
C	1.28368	-1.95994	2.64456
H	1.88426	-1.05791	2.65444
H	0.95847	-2.37902	3.59316
H	-2.17290	1.54908	0.89029
O	2.09105	2.38109	-1.07642
C	2.10343	2.49480	0.35317
C	0.70113	2.21858	0.89353
H	0.38264	1.20444	0.62785
H	0.68035	2.31388	1.98299
H	-0.01074	2.93251	0.46902
C	2.53080	3.92489	0.65178
H	2.57061	4.09315	1.73025
H	3.52076	4.11875	0.23176
H	1.82084	4.63181	0.21547
C	3.10195	1.49242	0.92888
H	4.10307	1.69105	0.53671
H	3.13435	1.56177	2.01971
H	2.81195	0.47286	0.65411
H	1.84930	1.46629	-1.29206
H	-0.98122	0.92627	-1.29984

Hydride elimination from 6.66 – transition state (1) in DMSO

45

-943.0712535

C	-2.96816	-2.69682	-1.45585
C	-1.78774	-1.99552	-1.68319
C	-0.97821	-1.60934	-0.61276
C	-1.36355	-1.93096	0.69300
C	-2.53893	-2.63228	0.91887
C	-3.34469	-3.01525	-0.15468
H	-3.59260	-2.99035	-2.29138
H	-1.49326	-1.73731	-2.69552
H	-2.83628	-2.87698	1.93203
H	-4.26556	-3.55746	0.02615
C	0.25058	-0.84433	-0.88645
H	0.42934	-0.58526	-1.93748
H	-1.60185	1.64143	-2.19435
C	2.14615	0.33568	-0.32007
C	3.43253	0.04241	0.16686
C	1.92286	1.49924	-1.06347
C	4.46960	0.92222	-0.14080
C	2.97328	2.36577	-1.35331
H	0.91156	1.73217	-1.38291
C	4.25294	2.07562	-0.89448
H	5.46610	0.69192	0.22074
H	2.78506	3.26676	-1.92592
H	5.07795	2.74332	-1.11458
N	1.05953	-0.49581	0.02920
O	3.48487	-2.32897	0.31745
C	3.70203	-1.23181	0.94435
C	4.16426	-1.07967	2.22742
H	4.31413	-0.09577	2.65340
H	4.38874	-1.95000	2.83592
H	-0.73541	-1.61692	1.51830
H	-2.10082	2.09023	-1.53161
O	-2.80929	2.80234	-0.65617
C	-3.09870	2.10073	0.51502
C	-3.89236	0.81836	0.20020
H	-3.29862	0.15219	-0.43247
H	-4.16069	0.27088	1.11000
H	-4.81234	1.07661	-0.33378
C	-3.94222	2.98667	1.44291
H	-4.19636	2.47193	2.37575
H	-3.38984	3.89834	1.68896
H	-4.87075	3.27328	0.94034
C	-1.80244	1.71116	1.24967
H	-1.23382	2.61307	1.49782
H	-2.00712	1.16289	2.17604
H	-1.18239	1.07749	0.61042

Hydride elimination from 6.66 – intermediate complex 6.67 in DMSO

45

-943.0842956

C	-2.94408	-2.67901	-1.46906
C	-1.76638	-1.97331	-1.69657
C	-0.95756	-1.58562	-0.62589
C	-1.34051	-1.91086	0.67980
C	-2.51243	-2.61825	0.90544
C	-3.31803	-3.00159	-0.16798
H	-3.56833	-2.97307	-2.30453
H	-1.47384	-1.71194	-2.70854
H	-2.80759	-2.86635	1.91840
H	-4.23663	-3.54770	0.01259
C	0.27176	-0.82056	-0.89928
H	0.45165	-0.56197	-1.95060
H	-1.85358	1.61560	-2.64167
C	2.17225	0.35198	-0.32387
C	3.45212	0.05099	0.17583
C	1.96483	1.51615	-1.07055
C	4.49807	0.92317	-0.12285
C	3.02352	2.37543	-1.35128
H	0.95953	1.75867	-1.40088
C	4.29657	2.07711	-0.87978
H	5.48938	0.68633	0.24852
H	2.84658	3.27700	-1.92641
H	5.12799	2.73916	-1.09262
N	1.07909	-0.47330	0.01842
O	3.48587	-2.32020	0.32869
C	3.70520	-1.22439	0.95698
C	4.15710	-1.07436	2.24392
H	4.30994	-0.09123	2.67059
H	4.36978	-1.94578	2.85506
H	-0.71191	-1.59756	1.50510
H	-2.62543	2.31243	-1.34486
O	-3.10956	2.81318	-0.64358
C	-3.15993	2.03563	0.55201
C	-3.88567	0.71488	0.28819
H	-3.33081	0.10678	-0.43211
H	-3.98401	0.13567	1.21045
H	-4.88419	0.91069	-0.11175
C	-3.93413	2.87117	1.56458
H	-4.00608	2.34789	2.52105
H	-3.43112	3.82750	1.72721
H	-4.94460	3.06722	1.19735
C	-1.74045	1.76790	1.05643
H	-1.22264	2.71278	1.24270
H	-1.75789	1.18852	1.98418
H	-1.17374	1.19989	0.31446

Hydride elimination from 6.66 – transition state (2) in DMSO

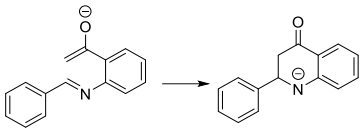
45
-943.0712537

C	-2.96849	-2.69734	-1.45564
C	-1.78799	-1.99622	-1.68312
C	-0.97847	-1.60983	-0.61277
C	-1.36388	-1.93109	0.69307
C	-2.53933	-2.63225	0.91907
C	-3.34510	-3.01540	-0.15440
H	-3.59293	-2.99102	-2.29112
H	-1.49345	-1.73830	-2.69551
H	-2.83672	-2.87668	1.93228
H	-4.26602	-3.55748	0.02654
C	0.25032	-0.84486	-0.88659
H	0.42923	-0.58628	-1.93770
H	-1.60184	1.64056	-2.19466
C	2.14583	0.33542	-0.32023
C	3.43215	0.04226	0.16694
C	1.92268	1.49874	-1.06403
C	4.46932	0.92186	-0.14096
C	2.97319	2.36511	-1.35406
H	0.91143	1.73161	-1.38368
C	4.25280	2.07502	-0.89505
H	5.46577	0.69161	0.22072
H	2.78507	3.26592	-1.92699
H	5.07787	2.74260	-1.11531
N	1.05919	-0.49596	0.02913
O	3.48456	-2.32906	0.31811
C	3.70149	-1.23175	0.94483
C	4.16338	-1.07930	2.22797
H	4.31307	-0.09530	2.65378
H	4.38772	-1.94950	2.83673
H	-0.73576	-1.61689	1.51831
H	-2.10032	2.08961	-1.53188
O	-2.80733	2.80300	-0.65600
C	-3.09768	2.10155	0.51501
C	-3.89171	0.81950	0.19980
H	-3.29791	0.15295	-0.43241
H	-4.16086	0.27225	1.10950
H	-4.81123	1.07815	-0.33480
C	-3.94136	2.98783	1.44243
H	-4.19587	2.47336	2.37533
H	-3.38894	3.89948	1.68843
H	-4.86970	3.27443	0.93950
C	-1.80193	1.71156	1.25033
H	-1.23321	2.61332	1.49880
H	-2.00717	1.16331	2.17659
H	-1.18171	1.07779	0.61133

Hydride elimination from 6.66 – product complex 6.68 and H_2 and HO^tBu anion in DMSO

45
-943.0786893

C	3.07899	-3.99769	-0.72763
C	2.23204	-2.91419	-0.94389
C	2.38035	-1.74282	-0.19844
C	3.39198	-1.66337	0.76521
C	4.23763	-2.74229	0.97739
C	4.08160	-3.91276	0.23308
H	2.95635	-4.90485	-1.30716
H	1.44885	-2.97688	-1.69299
H	5.02102	-2.67529	1.72323
H	4.74312	-4.75410	0.40318
C	1.46123	-0.61553	-0.43995
H	0.72928	-0.75630	-1.24565
H	-0.78823	-2.44165	0.20896
C	0.54388	1.46020	-0.00928
C	0.94756	2.80630	-0.06828
C	-0.81251	1.12976	-0.08742
C	-0.03413	3.78262	-0.23488
C	-1.77626	2.12112	-0.24717
H	-1.11183	0.09244	0.01680
C	-1.38667	3.45336	-0.32552
H	0.27551	4.82078	-0.29311
H	-2.82328	1.84436	-0.29693
H	-2.12862	4.23391	-0.44917
N	1.51100	0.46024	0.23347
O	3.13925	2.73131	-0.98313
C	2.41697	3.17994	-0.02335
C	2.81702	3.96732	1.02675
H	2.11126	4.29059	1.78132
H	3.85283	4.27876	1.11568
H	3.50179	-0.74927	1.33634
H	-1.52296	-2.34885	0.29592
O	-4.27389	-2.61632	0.32458
C	-4.68032	-1.31566	0.17176
C	-4.15006	-0.42483	1.31945
H	-3.05622	-0.46794	1.33857
H	-4.45448	0.62413	1.22217
H	-4.52143	-0.80380	2.27730
C	-6.22326	-1.20331	0.16751
H	-6.57518	-0.17075	0.05870
H	-6.63154	-1.79594	-0.65763
H	-6.61993	-1.60728	1.10464
C	-4.16338	-0.72052	-1.15897
H	-4.52160	-1.33103	-1.99436
H	-4.49219	0.31288	-1.32166
H	-3.06844	-0.74151	-1.16837



6.68 6.59

Cyclisation of 6.68 – starting species 6.68 in DMSO

29
-708.7846080

C	-4.29013	0.72485	-0.70348
C	-2.90515	0.75633	-0.83984
C	-2.10969	-0.20185	-0.20762
C	-2.71712	-1.19791	0.56519
C	-4.09779	-1.23069	0.69857
C	-4.88726	-0.26882	0.06558
H	-4.89972	1.47314	-1.19577
H	-2.43333	1.53001	-1.43723
H	-4.56509	-2.00466	1.29611
H	-5.96526	-0.29690	0.17344
C	-0.64640	-0.12564	-0.36956
C	1.53684	-0.78276	0.03370
C	2.19669	0.45935	0.09403
C	2.28047	-1.95682	-0.14422
C	3.58474	0.47636	-0.07020
C	3.65669	-1.91421	-0.31597
H	1.74980	-2.90239	-0.15509
C	4.31651	-0.68734	-0.27885
H	4.09522	1.43346	-0.02355
H	4.21126	-2.83298	-0.46700
H	5.39277	-0.64016	-0.39823
N	0.14161	-0.94650	0.20111
O	1.25250	2.46369	-0.76015
C	1.48779	1.78957	0.30769
C	1.19765	2.13616	1.59841
H	-2.09345	-1.93772	1.05269
H	0.69616	3.07367	1.81614
H	1.45222	1.47908	2.42076
H	-0.27489	0.68191	-1.00942

Cyclisation of 6.68 – transition state in DMSO

29
-708.7668121

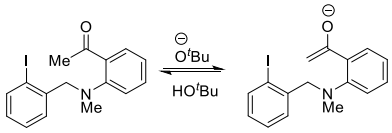
C	-4.21948	0.65038	-0.69114
C	-2.84346	0.72995	-0.87634
C	-1.98817	-0.18163	-0.25266
C	-2.53313	-1.18088	0.55727
C	-3.90873	-1.26168	0.74348
C	-4.75617	-0.34620	0.12151
H	-4.87350	1.36326	-1.17987
H	-2.42246	1.50829	-1.50555
H	-4.32315	-2.03947	1.37476
H	-5.82813	-0.41007	0.26787
C	-0.52180	-0.07294	-0.45335
C	1.61437	-0.81541	-0.14551
C	2.11657	0.48036	0.16129
C	2.54511	-1.84516	-0.36863
C	3.48945	0.68571	0.24388
C	3.91301	-1.61795	-0.27779
H	2.16635	-2.83168	-0.61352
C	4.39924	-0.34992	0.03406
H	3.84517	1.68423	0.47837
H	4.60345	-2.43584	-0.45391
H	5.46490	-0.16826	0.10489
N	0.25844	-1.09151	-0.14800
O	1.44500	2.71887	-0.22969
C	1.17841	1.65403	0.37644
C	-0.00608	1.41171	1.09527
H	-1.86287	-1.88745	1.03224
H	-0.71960	2.22409	1.18851
H	-0.05692	0.60962	1.81922
H	-0.23710	0.63069	-1.24633

Cyclisation of 6.68 – product 6.59 in DMSO

29
-708.8185638

C	4.33215	0.59416	0.64822
C	2.96723	0.77402	0.84986
C	2.03292	-0.06256	0.23323
C	2.49720	-1.08991	-0.58829
C	3.86349	-1.27256	-0.79468
C	4.78598	-0.43179	-0.17847
H	5.04198	1.25096	1.13835
H	2.61949	1.57372	1.49776
H	4.20775	-2.07661	-1.43574
H	5.84850	-0.57664	-0.33621
C	0.55090	0.19523	0.41572
C	-1.53530	-0.79846	0.13176
C	-2.17683	0.49738	0.01256
C	-2.43743	-1.93308	0.15084
C	-3.58717	0.60838	0.02064
C	-3.79342	-1.77981	0.15206
H	-1.99105	-2.92119	0.19861
C	-4.40243	-0.49152	0.10411
H	-4.01112	1.60426	-0.06573
H	-4.42535	-2.66226	0.19037
H	-5.48081	-0.39403	0.10860
N	-0.23858	-1.00815	0.24035
O	-1.79151	2.79616	-0.45597
C	-1.36108	1.64988	-0.29353
C	0.10892	1.34040	-0.50367
H	1.77470	-1.74966	-1.05350
H	0.69918	2.24416	-0.33899
H	0.23987	1.03357	-1.55156
H	0.40831	0.56277	1.45105

Scheme 6.14B-C



6.69 **6.70**

Deprotonation of 6.69 – starting species 6.69 and O^{t}Bu anion in DMSO

49
-993.6862317

C	2.33914	2.46998	1.85356
C	1.75622	1.83461	0.76374
C	2.41549	0.80401	0.08575
C	3.68118	0.44171	0.54461
C	4.27956	1.06421	1.63495
C	3.60078	2.08374	2.29375
H	1.80655	3.26609	2.36027
H	0.76943	2.12979	0.41966
H	5.26366	0.75989	1.96750
H	4.06233	2.56945	3.14507
C	1.76844	0.14749	-1.12315
H	2.25046	0.53688	-2.02291
H	1.97198	-0.92830	-1.11678
C	-0.51814	-0.13389	-0.30583
C	-1.86457	0.30242	-0.18135
C	-0.09063	-1.17236	0.54900
C	-2.76077	-0.40320	0.63216
C	-0.98333	-1.81973	1.38952
H	0.94206	-1.49462	0.54710
C	-2.33026	-1.46685	1.41539
H	-3.80202	-0.07838	0.69354
H	-0.61785	-2.62100	2.02237
H	-3.02546	-1.98788	2.06241
N	0.34910	0.40655	-1.23496
O	-1.60913	2.61075	-0.58995
C	-2.32974	1.63169	-0.69042
C	-3.71104	1.72466	-1.27256
H	-4.47482	1.35272	-0.57114
H	-3.91743	2.75680	-1.55426
H	-3.76312	1.08159	-2.15723
I	4.80154	-1.09634	-0.43297
O	-5.91168	0.51514	0.76085
C	-6.56818	-0.57783	0.24576
C	-8.09575	-0.35044	0.20463
H	-8.31780	0.53306	-0.40271
H	-8.63964	-1.20478	-0.21523
H	-8.46839	-0.16862	1.21782
C	-6.30100	-1.84097	1.09636
H	-5.22722	-2.05227	1.10621
H	-6.62401	-1.66386	2.12730
H	-6.82277	-2.72714	0.71670
C	-6.09948	-0.88432	-1.19708
H	-6.60267	-1.75935	-1.62411
H	-6.29779	-0.02206	-1.84203
H	-5.01999	-1.06760	-1.20239
C	-0.10719	1.05054	-2.45534
H	-1.13234	0.74784	-2.67594
H	-0.07583	2.14188	-2.39148
H	0.51962	0.72013	-3.28549

Deprotonation of 6.69 – transition state in DMSO

49
-993.6790290

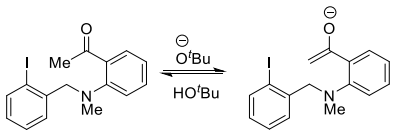
C	-1.91139	2.79450	-1.14290
C	-1.46672	1.79217	-0.28820
C	-2.30829	0.74415	0.09873
C	-3.60986	0.74908	-0.40142
C	-4.07205	1.74226	-1.25763
C	-3.21285	2.76987	-1.63266
H	-1.23911	3.59520	-1.42759
H	-0.45040	1.81041	0.09589
H	-5.08920	1.71773	-1.62711
H	-3.56691	3.54445	-2.30234
C	-1.80988	-0.32774	1.05669
H	-2.28362	-0.16673	2.02815
H	-2.15523	-1.31069	0.72064
C	0.46551	-0.68227	0.21932
C	1.83985	-0.33557	0.20550
C	-0.02635	-1.43609	-0.86647
C	2.68019	-0.86470	-0.77652
C	0.82309	-1.91598	-1.85427
H	-1.08048	-1.66873	-0.93743
C	2.19062	-1.66200	-1.80509
H	3.72822	-0.57883	-0.75377
H	0.40480	-2.50324	-2.66431
H	2.85573	-2.04444	-2.56997
N	-0.37889	-0.31640	1.25535
O	1.83633	1.83584	1.11535
C	2.42427	0.74999	1.07955
C	3.70560	0.49194	1.70893
H	4.61122	0.66966	0.80870
H	3.91808	1.19979	2.51063
H	3.83257	-0.54586	2.01772
I	-4.99780	-0.78062	0.15849
O	5.55377	0.92030	-0.14672
C	6.59466	0.00496	-0.28875
C	7.93952	0.68125	0.02786
H	7.93408	1.04985	1.05788
H	8.78473	-0.00510	-0.09058
H	8.08940	1.53441	-0.64034
C	6.63692	-0.51903	-1.73483
H	5.69433	-1.01903	-1.97820
H	6.76743	0.31831	-2.42661
H	7.45483	-1.23005	-1.89201
C	6.42009	-1.19675	0.66036
H	7.23712	-1.91576	0.54600
H	6.39956	-0.85815	1.70070
H	5.47634	-1.71161	0.45543
C	0.09941	-0.00191	2.59069
H	1.09046	-0.43188	2.74106
H	0.15992	1.07488	2.77524
H	-0.57322	-0.45479	3.32231

Deprotonation of 6.69 – products 6.70 and HO^{t}Bu anion in DMSO

49

-993.7021697

C	-1.38499	2.87009	-0.26495
C	-1.14969	1.63088	0.31897
C	-2.15447	0.65805	0.37884
C	-3.39483	0.98249	-0.16699
C	-3.64715	2.21673	-0.75833
C	-2.63164	3.16530	-0.80786
H	-0.59037	3.60647	-0.29927
H	-0.17189	1.39514	0.73643
H	-4.62233	2.43693	-1.17433
H	-2.82051	4.12729	-1.26950
C	-1.87105	-0.67656	1.05336
H	-2.31562	-0.65687	2.05238
H	-2.38870	-1.47832	0.51795
C	0.33199	-1.13604	0.07769
C	1.73413	-0.91384	0.08669
C	-0.26557	-1.54343	-1.13258
C	2.46950	-1.21946	-1.06035
C	0.49253	-1.81141	-2.26535
H	-1.33877	-1.67317	-1.19081
C	1.87573	-1.67810	-2.23319
H	3.53913	-1.04144	-1.03638
H	-0.00843	-2.13275	-3.17197
H	2.47674	-1.89119	-3.10927
N	-0.46319	-0.96164	1.20478
O	1.95511	0.96015	1.51799
C	2.44855	-0.17778	1.21040
C	3.58174	-0.75236	1.74175
H	4.68669	0.48310	0.41186
H	4.11537	-0.25252	2.54439
H	3.89921	-1.74435	1.44489
I	-5.02220	-0.40798	-0.09598
O	5.22379	1.07525	-0.15207
C	6.52089	0.49361	-0.30644
C	7.17671	0.32686	1.06473
H	6.58155	-0.34555	1.68852
H	8.18163	-0.09152	0.96594
H	7.24860	1.29473	1.56694
C	7.31767	1.46551	-1.16651
H	6.82934	1.60095	-2.13449
H	7.38776	2.43725	-0.67195
H	8.32821	1.08679	-1.33586
C	6.39781	-0.86225	-1.00298
H	7.38270	-1.30975	-1.15906
H	5.80109	-1.54749	-0.39378
H	5.91057	-0.74346	-1.97437
C	0.04328	-1.06591	2.56145
H	0.99553	-1.59267	2.56120
H	0.19806	-0.08656	3.02502
H	-0.66482	-1.64424	3.16121



6.69 **6.70**

Deprotonation of 6.69 – starting species 6.69 and O^{t}Bu anion in benzene

49

-993.6470894

C	2.18800	2.36083	1.94923
C	1.65847	1.75276	0.81794
C	2.37702	0.77880	0.11645
C	3.64347	0.44982	0.59492
C	4.18968	1.04551	1.72601
C	3.45187	2.00614	2.40834
H	1.60754	3.10948	2.47492
H	0.66921	2.02475	0.46012
H	5.17622	0.76374	2.07090
H	3.86901	2.47010	3.29418
C	1.78564	0.14380	-1.13272
H	2.28527	0.57802	-2.00273
H	2.02765	-0.92517	-1.15214
C	-0.51497	-0.20981	-0.37613
C	-1.85589	0.23421	-0.24802
C	-0.09769	-1.27669	0.44150
C	-2.76263	-0.48030	0.54383
C	-0.99956	-1.93744	1.26494
H	0.93235	-1.60819	0.42927
C	-2.33981	-1.56896	1.29853
H	-3.80539	-0.14561	0.61359
H	-0.64395	-2.75985	1.87656
H	-3.04460	-2.09511	1.93109
N	0.36780	0.36592	-1.28042
O	-1.55933	2.54035	-0.64558
C	-2.30639	1.58020	-0.73550
C	-3.69871	1.70454	-1.27887
H	-4.45898	1.37912	-0.54258
H	-3.87400	2.73477	-1.58715
H	-3.80655	1.03155	-2.13626
I	4.85163	-1.00145	-0.41567
O	-5.73468	0.47561	0.74287
C	-6.54559	-0.52027	0.28036
C	-8.03912	-0.14840	0.43825
H	-8.24215	0.77216	-0.11780
H	-8.71716	-0.93290	0.07887
H	-8.25037	0.04203	1.49513
C	-6.30509	-1.84157	1.05299
H	-5.26539	-2.15575	0.91684
H	-6.47106	-1.66548	2.12026
H	-6.96011	-2.65802	0.72371
C	-6.28363	-0.80426	-1.22117
H	-6.91911	-1.60321	-1.62287
H	-6.46198	0.10925	-1.79814
H	-5.23477	-1.08988	-1.35782
C	-0.07531	0.99447	-2.51151
H	-1.09970	0.69195	-2.73434
H	-0.04638	2.08682	-2.45912
H	0.55673	0.65290	-3.33549

Deprotonation of 6.69 – transition state in benzene

49
-993.6422758

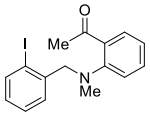
C	-1.87745	2.72660	-1.21736
C	-1.43370	1.73532	-0.34971
C	-2.28543	0.70512	0.06303
C	-3.59238	0.72330	-0.42039
C	-4.05411	1.70475	-1.28876
C	-3.18374	2.71132	-1.69337
H	-1.19514	3.51094	-1.52270
H	-0.41213	1.75690	0.02263
H	-5.07667	1.68646	-1.64333
H	-3.53380	3.47800	-2.37453
C	-1.79127	-0.36733	1.02418
H	-2.27780	-0.21136	1.99081
H	-2.13772	-1.34681	0.67902
C	0.49759	-0.70784	0.20492
C	1.84125	-0.26812	0.16017
C	0.04402	-1.53499	-0.84012
C	2.70173	-0.75447	-0.82640
C	0.90800	-1.97787	-1.83291
H	-0.98998	-1.85203	-0.87688
C	2.25001	-1.61350	-1.82231
H	3.72589	-0.38559	-0.83347
H	0.52141	-2.62111	-2.61602
H	2.92628	-1.96130	-2.59415
N	-0.36627	-0.36046	1.24104
O	1.71462	1.91789	1.01831
C	2.36417	0.87171	1.00948
C	3.65093	0.68480	1.65908
H	4.56238	0.77581	0.77411
H	3.83989	1.45091	2.41142
H	3.77913	-0.32786	2.04553
I	-5.00187	-0.76816	0.19916
O	5.53294	0.88164	-0.21132
C	6.56579	-0.03805	-0.23345
C	7.89754	0.65002	0.12291
H	7.82399	1.08406	1.12432
H	8.74755	-0.04204	0.10033
H	8.08513	1.46166	-0.58580
C	6.69001	-0.64723	-1.64374
H	5.75810	-1.15772	-1.90623
H	6.85417	0.15340	-2.37033
H	7.51423	-1.36615	-1.71830
C	6.32962	-1.18737	0.77000
H	7.13917	-1.92430	0.73501
H	6.26444	-0.79039	1.78751
H	5.38614	-1.69523	0.54509
C	0.09656	0.04478	2.55570
H	1.10921	-0.32431	2.72090
H	0.10414	1.13116	2.68954
H	-0.55052	-0.40925	3.31128

Deprotonation of 6.69 – products 6.70 and HO^{t}Bu anion in benzene

49
-993.6649597

C	-1.72628	2.64279	-1.24787
C	-1.33905	1.59043	-0.42457
C	-2.26940	0.64153	0.00996
C	-3.58993	0.80253	-0.40575
C	-3.99607	1.84603	-1.22794
C	-3.04925	2.77222	-1.65476
H	-0.98301	3.36320	-1.56935
H	-0.30039	1.51366	-0.10249
H	-5.03179	1.93757	-1.52974
H	-3.35387	3.58960	-2.29801
C	-1.84070	-0.51074	0.91102
H	-2.36085	-0.41144	1.86885
H	-2.21250	-1.44281	0.48095
C	0.46330	-1.00555	0.18623
C	1.78422	-0.50948	0.05475
C	0.03967	-1.99920	-0.71786
C	2.61516	-1.05973	-0.92416
C	0.88278	-2.51169	-1.69395
H	-0.96096	-2.40409	-0.64547
C	2.19045	-2.05376	-1.79892
H	3.61515	-0.65081	-1.02237
H	0.51017	-3.27759	-2.36559
H	2.85959	-2.44185	-2.55799
N	-0.42644	-0.58560	1.18678
O	1.66255	1.78222	0.62714
C	2.31533	0.70793	0.80440
C	3.46377	0.53806	1.55139
H	4.93060	0.88836	0.06923
H	3.86120	1.36975	2.12434
H	3.86626	-0.45384	1.71999
I	-5.10557	-0.57011	0.24615
O	5.69049	0.99802	-0.54066
C	6.76176	0.17395	-0.09677
C	7.10240	0.49249	1.36086
H	6.25095	0.26700	2.00755
H	7.96104	-0.09612	1.69627
H	7.34159	1.55379	1.46352
C	7.94228	0.50839	-1.00157
H	7.68390	0.30469	-2.04348
H	8.19438	1.56737	-0.90889
H	8.81793	-0.08800	-0.73281
C	6.38429	-1.30248	-0.24350
H	7.21636	-1.94897	0.04992
H	5.52135	-1.54098	0.38349
H	6.12230	-1.51787	-1.28281
C	0.00590	0.10212	2.39289
H	1.02395	-0.19229	2.63987
H	-0.01090	1.19266	2.29345
H	-0.65019	-0.20280	3.21334

Table 6.9

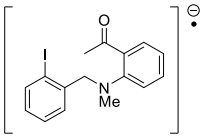


Neutral 6.69 in DMSO

35

-760.5580475

C	1.17159	2.91478	-1.35050
C	0.39692	1.79919	-1.05438
C	0.96541	0.63198	-0.53866
C	2.34386	0.63423	-0.32314
C	3.13636	1.73911	-0.61173
C	2.54405	2.88513	-1.13258
H	0.70187	3.80519	-1.75025
H	-0.67450	1.83050	-1.21893
H	4.20336	1.70937	-0.43265
H	3.15798	3.74771	-1.36207
I	3.31460	-1.08076	0.50404
C	0.10841	-0.58845	-0.22601
H	0.50454	-1.44412	-0.78291
H	0.20766	-0.84492	0.83225
N	-1.29351	-0.46107	-0.55722
C	-2.17786	0.11159	0.34451
C	-1.70761	0.90016	1.41330
C	-3.57716	-0.05282	0.21581
C	-2.58790	1.53872	2.27296
H	-0.64412	1.04926	1.54950
C	-4.44414	0.64770	1.06088
C	-3.96658	1.44078	2.09212
H	-2.18769	2.14153	3.08020
H	-5.51064	0.51279	0.91895
H	-4.65090	1.95635	2.75365
C	-4.22614	-1.05657	-0.68456
C	-3.69737	-2.47242	-0.67154
H	-3.77441	-2.90892	-1.66778
H	-2.67948	-2.54373	-0.29411
O	-5.23879	-0.78360	-1.29844
C	-1.60837	-0.61690	-1.97276
H	-1.71214	-1.66758	-2.25759
H	-2.52963	-0.08735	-2.21793
H	-0.80659	-0.17886	-2.57418
H	-4.35511	-3.03815	-0.00457

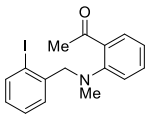


Radical anion 6.80 in DMSO

35

-760.6360878

C	-1.28159	2.92099	1.34846
C	-0.47075	1.84238	1.01702
C	-1.00016	0.65891	0.49258
C	-2.38104	0.61684	0.30140
C	-3.21250	1.68403	0.62430
C	-2.65691	2.84220	1.15687
H	-0.83876	3.82322	1.75305
H	0.60273	1.91189	1.14984
H	-4.28031	1.61524	0.46125
H	-3.29946	3.67589	1.41326
I	-3.30856	-1.11024	-0.55715
C	-0.09955	-0.52611	0.14646
H	-0.53105	-1.41513	0.62346
H	-0.14663	-0.70099	-0.93346
N	1.28045	-0.44230	0.54767
C	2.23469	0.18996	-0.28266
C	1.82818	1.13168	-1.22130
C	3.64485	-0.14034	-0.16981
C	2.74029	1.86313	-2.00335
H	0.77153	1.35258	-1.32292
C	4.54328	0.74744	-0.85358
C	4.10843	1.69586	-1.75970
H	2.37932	2.58421	-2.72683
H	5.60317	0.58080	-0.70649
H	4.83536	2.29727	-2.29701
C	4.22621	-1.27000	0.49627
C	3.43661	-2.52164	0.83636
H	3.43290	-2.70287	1.91769
H	2.40862	-2.50622	0.47984
O	5.48414	-1.33347	0.71672
C	1.49760	-0.53977	1.98416
H	1.22014	-1.53661	2.34180
H	2.54962	-0.37562	2.20910
H	0.90599	0.19667	2.54148
H	3.95840	-3.36711	0.37692

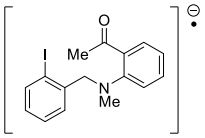


Neutral 6.69 in benzene

35

-760.5528685

C	1.17064	2.91392	-1.34787
C	0.39581	1.80080	-1.04477
C	0.96569	0.63368	-0.53082
C	2.34506	0.63355	-0.32293
C	3.13734	1.73630	-0.61900
C	2.54411	2.88176	-1.13880
H	0.69997	3.80483	-1.74537
H	-0.67708	1.83368	-1.19925
H	4.20513	1.70376	-0.44559
H	3.15806	3.74280	-1.37400
I	3.31647	-1.07943	0.50486
C	0.10797	-0.58486	-0.21153
H	0.50997	-1.44434	-0.75892
H	0.20403	-0.83227	0.84937
N	-1.29224	-0.46377	-0.54826
C	-2.18307	0.11612	0.34770
C	-1.72013	0.91778	1.40785
C	-3.57909	-0.05876	0.21437
C	-2.60789	1.55806	2.25910
H	-0.65789	1.07681	1.54337
C	-4.45357	0.64475	1.04718
C	-3.98403	1.44955	2.07324
H	-2.21503	2.17159	3.06177
H	-5.51823	0.50633	0.89566
H	-4.67402	1.96898	2.72573
C	-4.21838	-1.07102	-0.68716
C	-3.68598	-2.48741	-0.65231
H	-3.77642	-2.94187	-1.63928
H	-2.66346	-2.54903	-0.28505
O	-5.21979	-0.80533	-1.31608
C	-1.60157	-0.61381	-1.96492
H	-1.70887	-1.66372	-2.25367
H	-2.52182	-0.08306	-2.21159
H	-0.79677	-0.17651	-2.56355
H	-4.33416	-3.04155	0.03328

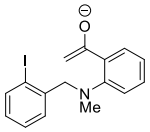


Radical anion 6.80 in benzene

35

-760.5987172

C	-1.27974	2.92331	1.33531
C	-0.46954	1.84840	0.99360
C	-1.00141	0.66291	0.47487
C	-2.38346	0.61916	0.30102
C	-3.21568	1.68247	0.63392
C	-2.65734	2.84122	1.16087
H	-0.83349	3.82712	1.73281
H	0.60618	1.91911	1.10698
H	-4.28473	1.60863	0.48135
H	-3.29889	3.67354	1.42498
I	-3.31652	-1.10828	-0.55460
C	-0.09505	-0.51724	0.12097
H	-0.53540	-1.41169	0.58148
H	-0.13149	-0.67393	-0.96243
N	1.27689	-0.43700	0.53460
C	2.24630	0.19544	-0.28947
C	1.85441	1.15446	-1.21444
C	3.64908	-0.15210	-0.16559
C	2.77914	1.88368	-1.98363
H	0.80025	1.38804	-1.31995
C	4.56255	0.73286	-0.83299
C	4.14505	1.69403	-1.72959
H	2.43246	2.61605	-2.70267
H	5.61783	0.55002	-0.67239
H	4.88392	2.29181	-2.25510
C	4.21975	-1.29083	0.49928
C	3.41095	-2.53918	0.82168
H	3.39799	-2.72612	1.90222
H	2.38714	-2.51298	0.45224
O	5.46387	-1.36608	0.73638
C	1.48624	-0.53031	1.97019
H	1.18120	-1.51848	2.33234
H	2.54354	-0.39708	2.19225
H	0.91705	0.22543	2.52787
H	3.93566	-3.38245	0.36247

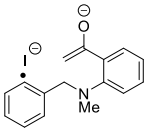


Enolate anion 6.70 in DMSO

34

-760.0540185

C	1.10317	2.95839	-1.21223
C	0.34944	1.81571	-0.97215
C	0.93793	0.63535	-0.51100
C	2.31536	0.65403	-0.29513
C	3.08908	1.78556	-0.52685
C	2.47607	2.94464	-0.99176
H	0.61775	3.85860	-1.56958
H	-0.72282	1.82904	-1.13443
H	4.15660	1.76629	-0.34843
H	3.07381	3.82903	-1.17678
I	3.32002	-1.08871	0.43335
C	0.09410	-0.61069	-0.25803
H	0.50511	-1.42861	-0.86055
H	0.20993	-0.91637	0.78614
N	-1.30606	-0.48919	-0.57416
C	-2.20050	0.03460	0.35991
C	-1.71345	0.76590	1.46304
C	-3.59808	-0.15726	0.24979
C	-2.57206	1.31749	2.40536
H	-0.64908	0.93206	1.57414
C	-4.43539	0.44762	1.18760
C	-3.94905	1.17864	2.26694
H	-2.15581	1.87252	3.23881
H	-5.50547	0.29998	1.07479
H	-4.62828	1.61458	2.98990
C	-4.27713	-1.02947	-0.79815
C	-4.09119	-2.38033	-0.67816
H	-4.55271	-3.06408	-1.38395
H	-3.44126	-2.78461	0.08817
O	-4.99815	-0.41656	-1.66733
C	-1.62969	-0.60499	-1.98951
H	-1.73882	-1.64958	-2.29449
H	-2.56231	-0.08776	-2.21003
H	-0.83169	-0.14374	-2.58152

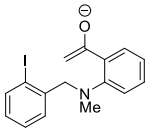


Radical dianion A32 in DMSO

34

-760.1608524

C	-0.08793	3.88895	-0.46274
C	-0.51017	2.56010	-0.50459
C	0.41306	1.51192	-0.41907
C	1.73347	1.88821	-0.29312
C	2.20806	3.17555	-0.24215
C	1.26180	4.20397	-0.33187
H	-0.82136	4.68372	-0.53236
H	-1.56625	2.32683	-0.60049
H	3.26496	3.39481	-0.13841
H	1.58291	5.23899	-0.29935
I	4.06952	-1.34618	0.20229
C	0.00211	0.04343	-0.46170
H	0.57196	-0.44550	-1.25831
H	0.30973	-0.44240	0.46822
N	-1.40012	-0.20127	-0.70118
C	-2.31284	-0.19776	0.35285
C	-1.95134	0.36198	1.59611
C	-3.60717	-0.75748	0.22363
C	-2.84376	0.40830	2.65914
H	-0.96769	0.79613	1.72584
C	-4.49556	-0.64979	1.29393
C	-4.13807	-0.08057	2.51199
H	-2.52575	0.84918	3.59757
H	-5.48959	-1.06749	1.16352
H	-4.84656	-0.03427	3.33042
C	-4.10417	-1.54433	-0.98245
C	-3.47595	-2.73512	-1.23176
H	-3.78464	-3.35557	-2.06743
H	-2.62370	-3.04630	-0.64004
O	-5.10289	-1.04414	-1.61810
C	-1.82033	-0.04486	-2.08653
H	-1.67056	-0.96348	-2.66083
H	-2.87676	0.21640	-2.13601
H	-1.24481	0.76353	-2.55067

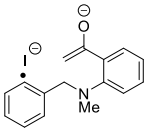


Enolate anion 6.70 in benzene

34

-760.0128981

C	1.09738	2.96578	-1.17597
C	0.34622	1.82122	-0.94106
C	0.93858	0.63743	-0.49306
C	2.31605	0.65793	-0.28593
C	3.08877	1.79103	-0.51229
C	2.47170	2.95270	-0.96380
H	0.60754	3.86807	-1.52217
H	-0.72761	1.82968	-1.09364
H	4.15725	1.76895	-0.33986
H	3.06700	3.83978	-1.14501
I	3.32796	-1.09211	0.41862
C	0.08851	-0.60794	-0.24737
H	0.50220	-1.42409	-0.85135
H	0.20165	-0.91531	0.79705
N	-1.30407	-0.47543	-0.57001
C	-2.20638	0.03111	0.36981
C	-1.72297	0.74641	1.48373
C	-3.60158	-0.16744	0.25163
C	-2.58537	1.26945	2.44004
H	-0.65982	0.92174	1.59618
C	-4.44071	0.40528	1.20492
C	-3.95935	1.11579	2.30127
H	-2.17301	1.81163	3.28422
H	-5.50859	0.25093	1.08361
H	-4.64240	1.52780	3.03511
C	-4.27742	-0.98861	-0.84479
C	-4.21461	-2.35012	-0.69650
H	-4.68783	-3.00029	-1.42517
H	-3.69416	-2.79474	0.14299
O	-4.85424	-0.31951	-1.76686
C	-1.62784	-0.61240	-1.98389
H	-1.74306	-1.66224	-2.26946
H	-2.55995	-0.09832	-2.21427
H	-0.82479	-0.16359	-2.58072



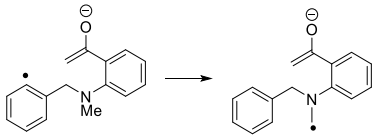
Radical dianion A32 in benzene

34

-760.0619544

C	-0.86869	0.38184	1.54492
C	0.32970	0.07187	0.90057
C	0.32681	-0.45906	-0.39382
C	-0.91809	-0.64967	-0.95517
C	-2.12851	-0.36316	-0.37665
C	-2.09366	0.17177	0.91697
H	-0.84187	0.79127	2.54825
H	1.28364	0.23667	1.39379
H	-3.08269	-0.53119	-0.86614
H	-3.03037	0.41252	1.40874
I	-6.24127	0.04238	-0.05047
C	1.60859	-0.79982	-1.14733
H	1.48547	-1.79534	-1.59014
H	1.72572	-0.10370	-1.98266
N	2.81324	-0.80106	-0.35876
C	3.62290	0.33097	-0.27381
C	3.06359	1.60435	-0.50383
C	5.00123	0.24471	0.03115
C	3.82937	2.75937	-0.40825
H	2.00624	1.69193	-0.72653
C	5.72994	1.42472	0.16718
C	5.17210	2.68091	-0.05339
H	3.36234	3.72167	-0.58969
H	6.78144	1.33329	0.42209
H	5.77515	3.57721	0.03707
C	5.78312	-1.05826	0.18873
C	6.00580	-1.76452	-0.96666
H	6.56924	-2.69176	-0.93897
H	5.60057	-1.42374	-1.91181
O	6.18349	-1.33379	1.36947
C	3.00733	-1.97024	0.48072
H	3.36365	-2.82830	-0.09903
H	3.74304	-1.76336	1.25663
H	2.05582	-2.23022	0.96071

Scheme 6.16B



6.77 6.81

H atom abstraction 6.77 – starting species 6.77 in DMSO

33
-748.6003293

C	-4.13227	1.19690	0.77983
C	-2.81680	1.04009	0.42253
C	-2.30591	0.05521	-0.39807
C	-3.24156	-0.85698	-0.89875
C	-4.59558	-0.74533	-0.58005
C	-5.04608	0.27272	0.25457
H	-4.46101	1.99584	1.43497
H	-2.90046	-1.66371	-1.54054
H	-5.30040	-1.46484	-0.98008
H	-6.09802	0.35261	0.50405
C	-0.83806	-0.02742	-0.74943
H	-0.62654	-0.98364	-1.24943
H	-0.60023	0.77586	-1.45228
C	1.32874	0.61456	0.13190
C	2.47003	-0.19974	0.00320
C	1.45782	2.00155	-0.00869
C	3.70788	0.42270	-0.20283
C	2.68842	2.59745	-0.25348
H	0.56369	2.60767	0.10042
C	3.82849	1.80176	-0.33338
H	4.58690	-0.20638	-0.29423
H	2.75861	3.67419	-0.35866
H	4.80035	2.24986	-0.50701
N	0.01516	0.13415	0.42444
O	1.57793	-2.18830	-0.92643
C	2.39134	-1.71554	-0.05384
C	3.20463	-2.42287	0.79398
H	3.85361	-1.91802	1.49826
H	3.20768	-3.50773	0.77014
C	-0.11131	-0.97044	1.36681
H	-1.11379	-0.94135	1.80280
H	0.04630	-1.94801	0.89635
H	0.61502	-0.84267	2.16983

H atom abstraction 6.77 – transition state in DMSO

33
-748.5874472

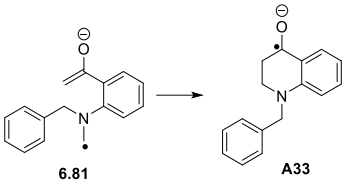
C	-3.25610	-0.84811	1.51199
C	-2.21373	-0.97949	0.60979
C	-2.19194	-0.31976	-0.60589
C	-3.26499	0.51434	-0.93225
C	-4.32784	0.66148	-0.04262
C	-4.32752	-0.01503	1.17570
H	-3.25278	-1.37273	2.46174
H	-3.26788	1.05187	-1.87643
H	-5.15692	1.31086	-0.29912
H	-5.15583	0.10694	1.86517
C	-1.01399	-0.53337	-1.55586
H	-1.20361	-1.43267	-2.15184
H	-0.91559	0.29945	-2.25220
C	0.95814	0.37039	-0.37787
C	2.28286	0.23029	0.10730
C	0.37999	1.64907	-0.40701
C	2.95133	1.37523	0.54211
C	1.08180	2.77363	0.01582
H	-0.64078	1.77543	-0.74219
C	2.37539	2.64289	0.50125
H	3.96807	1.25903	0.90062
H	0.60308	3.74534	-0.02763
H	2.93344	3.50994	0.83460
N	0.23587	-0.74936	-0.84427
O	3.14215	-1.67934	-1.04177
C	3.05891	-1.08134	0.08715
C	3.61041	-1.48385	1.27833
H	3.47980	-0.90364	2.18263
H	4.19300	-2.39810	1.32713
C	0.15854	-1.90893	-0.02109
H	-0.89872	-1.72802	0.63108
H	-0.02789	-2.81389	-0.60325
H	0.98674	-2.01423	0.67248

H atom abstraction 6.77 – product 6.81 in DMSO

33

-748.6348906

C	-3.49171	0.45919	1.48549
C	-2.29102	0.09820	0.87707
C	-2.28151	-0.39511	-0.42580
C	-3.49183	-0.52527	-1.11003
C	-4.69100	-0.16438	-0.50551
C	-4.69399	0.33020	0.79711
H	-3.48574	0.84038	2.50016
H	-3.49314	-0.91365	-2.12410
H	-5.62299	-0.27091	-1.04855
H	-5.62700	0.61010	1.27189
C	-0.99511	-0.78043	-1.13790
H	-1.12323	-1.77450	-1.57849
H	-0.81371	-0.09186	-1.96633
C	1.03773	0.30034	-0.22218
C	2.41602	0.18094	0.05991
C	0.49483	1.58048	-0.43951
C	3.17656	1.34753	0.15239
C	1.28454	2.71963	-0.36934
H	-0.56380	1.68749	-0.64389
C	2.63714	2.61220	-0.06034
H	4.23524	1.24421	0.37035
H	0.83419	3.69055	-0.54201
H	3.26245	3.49485	0.00274
N	0.19146	-0.82156	-0.29952
O	3.40832	-1.47166	1.46136
C	3.16629	-1.13190	0.24684
C	3.54799	-1.78173	-0.89536
H	4.10323	-2.71272	-0.83896
H	3.28553	-1.39098	-1.87062
C	0.31586	-1.90774	0.54028
H	1.14378	-1.93634	1.22978
H	-0.23041	-2.79957	0.26701
H	-1.35599	0.19430	1.41801



6.81 A33

$S_{RN}1$ cyclisation 6.81 – transition state in DMSO

33

-748.6199687

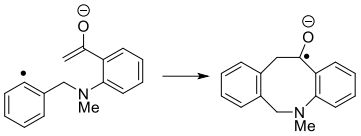
C	-3.33798	0.39382	1.61348
C	-2.18570	0.01891	0.92489
C	-2.25883	-0.38226	-0.40736
C	-3.50257	-0.40145	-1.04156
C	-4.65402	-0.02692	-0.35694
C	-4.57447	0.37203	0.97624
H	-3.26786	0.70398	2.64989
H	-3.56853	-0.71530	-2.07926
H	-5.61290	-0.04815	-0.86202
H	-5.47017	0.66219	1.51287
C	-1.01786	-0.79239	-1.18521
H	-1.17489	-1.79515	-1.59522
H	-0.88716	-0.12584	-2.04234
C	1.03475	0.29856	-0.34941
C	2.40232	0.19374	0.04282
C	0.51017	1.58034	-0.62584
C	3.13384	1.37365	0.21714
C	1.28466	2.72160	-0.49440
H	-0.53123	1.68467	-0.90706
C	2.60738	2.62952	-0.05067
H	4.16317	1.27109	0.54439
H	0.84527	3.68851	-0.71369
H	3.21179	3.52027	0.07332
N	0.20251	-0.81573	-0.40505
O	3.97694	-1.19247	1.18630
C	3.10590	-1.11528	0.24676
C	2.66725	-2.18565	-0.52998
H	3.13298	-3.15617	-0.38427
H	2.15501	-2.01756	-1.46801
C	0.50361	-1.97702	0.31246
H	0.82893	-1.84893	1.34016
H	-0.14655	-2.81721	0.09996
H	-1.22155	0.03628	1.42168

$S_{RN}1$ cyclisation 6.81 – product A33 in DMSO

33

-748.6938199

C	-3.01829	0.45070	1.68042
C	-1.94970	0.10432	0.85439
C	-2.17258	-0.30007	-0.46083
C	-3.48676	-0.35082	-0.93332
C	-4.55461	-0.00247	-0.11357
C	-4.32299	0.40041	1.20018
H	-2.82757	0.76242	2.70110
H	-3.67289	-0.66946	-1.95491
H	-5.56733	-0.04844	-0.49751
H	-5.15292	0.67049	1.84257
C	-1.04195	-0.69370	-1.40350
H	-1.29591	-1.65951	-1.85091
H	-1.00295	0.01928	-2.23268
C	1.01813	0.33186	-0.51542
C	2.30809	0.15256	0.11682
C	0.57045	1.61073	-0.81546
C	3.06263	1.33316	0.40243
C	1.35117	2.75435	-0.53402
H	-0.40939	1.75099	-1.25608
C	2.59514	2.59816	0.08155
H	4.03239	1.20587	0.86954
H	0.97155	3.73784	-0.78379
H	3.20072	3.46979	0.31058
N	0.27861	-0.81654	-0.82995
O	3.99634	-1.33312	0.89284
C	2.83888	-1.13834	0.39170
C	1.99042	-2.33985	0.02773
H	2.17325	-3.13280	0.75953
H	2.29659	-2.72850	-0.95297
C	0.51007	-1.99524	-0.00033
H	0.15350	-1.83468	1.02821
H	-0.07252	-2.81795	-0.42175
H	-0.93615	0.16073	1.23351



6.77 6.78

$S_{RN}1$ cyclisation 6.77 – starting species 6.77 in DMSO

33

-748.6017885

C	-3.58497	1.23402	0.50896
C	-2.32613	0.81357	0.15848
C	-2.01264	-0.38378	-0.45232
C	-3.09389	-1.22640	-0.73056
C	-4.39768	-0.85289	-0.39986
C	-4.64829	0.36862	0.21766
H	-3.75999	2.19156	0.98689
H	-2.90822	-2.18403	-1.20848
H	-5.21983	-1.52255	-0.62291
H	-5.66226	0.65413	0.47462
C	-0.58992	-0.74580	-0.80212
H	-0.58702	-1.66619	-1.40845
H	-0.16748	0.06057	-1.39881
C	1.62403	-0.64130	0.16007
C	2.02873	0.69534	-0.04826
C	2.58420	-1.65779	0.13688
C	3.37077	0.95130	-0.32223
C	3.92673	-1.37370	-0.11083
H	2.28628	-2.68568	0.30375
C	4.32396	-0.06701	-0.35745
H	3.67555	1.98071	-0.48278
H	4.65096	-2.18041	-0.12210
H	5.36329	0.16400	-0.56120
N	0.24853	-0.92203	0.38862
O	0.87422	2.18813	1.38239
C	1.09035	1.87863	0.15598
C	0.62482	2.52339	-0.95945
H	0.88157	2.17483	-1.95246
H	-0.03153	3.38282	-0.86446
C	-0.05506	-2.17199	1.06539
H	-1.10609	-2.16120	1.36204
H	0.10489	-3.05696	0.42935
H	0.55634	-2.26760	1.96350

$S_{RN}1$ cyclisation 6.77 – transition state in DMSO

33

-748.5990491

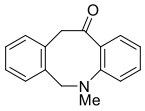
C	-3.40678	1.36530	0.04122
C	-2.17026	0.85432	-0.29235
C	-1.93485	-0.49576	-0.50101
C	-3.02070	-1.36792	-0.37328
C	-4.28611	-0.88516	-0.03424
C	-4.48239	0.47681	0.17531
H	-3.55806	2.42994	0.19469
H	-2.87461	-2.43148	-0.54419
H	-5.11705	-1.57422	0.06324
H	-5.46658	0.85087	0.43725
C	-0.54886	-0.98756	-0.84279
H	-0.60841	-1.97245	-1.33163
H	-0.09797	-0.29111	-1.54688
C	1.65227	-0.63568	0.11220
C	1.89079	0.74724	-0.01647
C	2.72347	-1.52902	0.01236
C	3.18495	1.18215	-0.29586
C	4.01498	-1.07103	-0.24246
H	2.54973	-2.59269	0.12433
C	4.24819	0.28761	-0.41499
H	3.36442	2.24880	-0.39086
H	4.83044	-1.78152	-0.31788
H	5.24737	0.65212	-0.62366
N	0.32101	-1.07787	0.34102
O	0.77148	2.11378	1.54631
C	0.82800	1.78647	0.31183
C	0.04972	2.29664	-0.70312
H	0.19271	1.98481	-1.72999
H	-0.63832	3.10991	-0.50229
C	0.16346	-2.35025	1.02493
H	-0.88180	-2.45737	1.32425
H	0.42167	-3.21579	0.39512
H	0.78210	-2.36996	1.92321

$S_{RN}1$ cyclisation 6.77 – product 6.78 in DMSO

33

-748.6670331

C	2.95787	1.40855	-0.15517
C	1.85409	0.75931	0.39822
C	1.88541	-0.63931	0.52352
C	3.00966	-1.35001	0.11163
C	4.10612	-0.69149	-0.44471
C	4.07410	0.69152	-0.58514
H	2.94683	2.49079	-0.24150
H	3.02545	-2.43011	0.22391
H	4.97574	-1.25488	-0.76305
H	4.92049	1.21516	-1.01513
C	0.63948	-1.34340	0.99464
H	0.87288	-2.37664	1.27923
H	0.21994	-0.86235	1.87900
C	-1.59823	-0.66753	0.07743
C	-1.66647	0.77410	-0.01274
C	-2.77357	-1.41284	0.10614
C	-2.97452	1.32148	-0.19740
C	-4.04357	-0.83264	-0.00230
H	-2.69584	-2.49347	0.16572
C	-4.12393	0.55357	-0.17872
H	-3.04176	2.39391	-0.33613
H	-4.93309	-1.45093	0.01638
H	-5.09030	1.03319	-0.30057
N	-0.35740	-1.34437	-0.08113
O	-0.69001	2.85996	-0.55717
C	-0.56404	1.70821	-0.01184
C	0.66430	1.54150	0.89808
H	0.34790	1.12905	1.86157
H	0.99291	2.56542	1.08946
C	-0.36045	-2.59636	-0.81633
H	0.65895	-2.80423	-1.15510
H	-0.69286	-3.45837	-0.21674
H	-1.00274	-2.51363	-1.69370

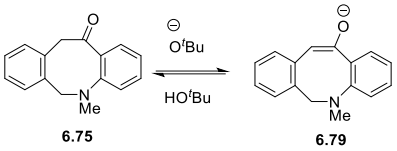


Neutral 6.75

33

-748.5884117

C	3.04806	-1.38735	0.00123
C	1.86468	-0.78877	-0.42655
C	1.79792	0.60921	-0.52760
C	2.92181	1.37327	-0.22202
C	4.10299	0.76875	0.20234
C	4.16347	-0.61483	0.31871
H	3.10054	-2.46822	0.07693
H	2.86968	2.45336	-0.31644
H	4.96882	1.37552	0.44008
H	5.07709	-1.09627	0.64707
C	0.49598	1.26968	-0.90450
H	0.68146	2.29386	-1.24513
H	0.02377	0.74616	-1.73878
C	-1.67024	0.63501	0.05914
C	-1.68171	-0.77066	0.01954
C	-2.89174	1.31199	-0.00656
C	-2.88263	-1.46177	-0.12241
C	-4.08673	0.61359	-0.15087
H	-2.90771	2.39323	0.05231
C	-4.08822	-0.77466	-0.22437
H	-2.87068	-2.54618	-0.13112
H	-5.01973	1.16211	-0.20838
H	-5.01746	-1.31925	-0.33656
N	-0.43937	1.30592	0.23614
O	-0.34289	-2.23742	1.27771
C	-0.43466	-1.58168	0.26482
C	0.66873	-1.64565	-0.78669
H	0.26623	-1.36307	-1.76101
H	0.98028	-2.69052	-0.83399
C	-0.47932	2.60771	0.88600
H	0.53490	2.87156	1.19266
H	-0.85457	3.40450	0.22835
H	-1.10434	2.55818	1.77807



6.75 6.79

Deprotonation 6.75 – starting species 6.75 and O^{t}Bu anion in DMSO

47

-981.7268409

C	0.50269	2.97545	0.01083
C	-0.31472	1.84961	-0.08191
C	-1.69754	2.01813	-0.24993
C	-2.23048	3.30404	-0.30489
C	-1.40891	4.42502	-0.20412
C	-0.03775	4.25891	-0.04787
H	1.57189	2.82496	0.12691
H	-3.30155	3.42953	-0.43058
H	-1.83929	5.41860	-0.24931
H	0.61177	5.12365	0.02602
C	-2.60338	0.81627	-0.42041
H	-3.64603	1.15277	-0.44225
H	-2.41353	0.35002	-1.39121
C	-2.05159	-1.48016	0.27782
C	-0.98240	-1.64840	-0.63183
C	-2.66485	-2.63106	0.79983
C	-0.62395	-2.92374	-1.06928
C	-2.26125	-3.89410	0.38506
H	-3.47963	-2.53915	1.50612
C	-1.25378	-4.05380	-0.56537
H	0.19290	-3.01311	-1.77752
H	-2.75687	-4.76545	0.79804
H	-0.95502	-5.04190	-0.89169
N	-2.46401	-0.20097	0.62196
O	0.30952	-0.40284	-2.17462
C	-0.11924	-0.49968	-1.04015
C	0.30989	0.47706	0.04041
H	0.06639	0.05847	1.02029
H	1.40565	0.57707	-0.04499
C	-3.35617	-0.01627	1.75246
H	-3.34507	1.03934	2.02891
H	-4.39081	-0.30367	1.52068
H	-3.00819	-0.59442	2.60876
O	3.45405	0.84966	-0.17901
C	3.97309	-0.30491	0.35639
C	3.35462	-1.56313	-0.30140
H	2.27411	-1.58480	-0.12589
H	3.52120	-1.53178	-1.38317
H	3.78080	-2.49463	0.08868
C	3.68900	-0.38644	1.87435
H	4.07691	-1.30425	2.33139
H	4.14663	0.47158	2.37728
H	2.60835	-0.34304	2.04380
C	5.50380	-0.37993	0.15835
H	5.73731	-0.35479	-0.91100
H	5.97560	0.48843	0.62923
H	5.94346	-1.28828	0.58677

Deprotonation 6.75 – transition state in DMSO

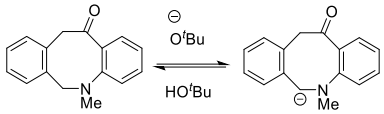
47
-981.7162527

C	0.55625	2.99815	0.07557
C	-0.22127	1.84940	-0.08300
C	-1.61227	1.99847	-0.26448
C	-2.17661	3.27239	-0.28192
C	-1.38708	4.41036	-0.12198
C	-0.01622	4.27003	0.05857
H	1.62632	2.87433	0.20761
H	-3.24905	3.37726	-0.41917
H	-1.84202	5.39409	-0.13610
H	0.60898	5.14730	0.18346
C	-2.50376	0.78639	-0.47623
H	-3.54496	1.12352	-0.53240
H	-2.28304	0.32978	-1.44423
C	-1.93628	-1.51245	0.24550
C	-0.81731	-1.65911	-0.61058
C	-2.53028	-2.67808	0.75892
C	-0.38823	-2.92633	-0.99310
C	-2.05395	-3.93496	0.40063
H	-3.38473	-2.60759	1.41964
C	-0.99253	-4.07426	-0.48934
H	0.45953	-2.99956	-1.66716
H	-2.53617	-4.81551	0.81036
H	-0.63711	-5.05616	-0.77625
N	-2.41637	-0.24549	0.55958
O	0.19192	-0.27350	-2.24632
C	-0.05100	-0.44065	-1.05015
C	0.38817	0.47428	0.00670
H	0.13751	0.05201	0.98374
H	1.72317	0.58721	-0.07039
C	-3.38394	-0.09651	1.62977
H	-3.43611	0.95910	1.90154
H	-4.39059	-0.42965	1.33951
H	-3.06720	-0.65619	2.51074
O	3.00095	0.79349	-0.13007
C	3.70060	-0.30631	0.37529
C	3.24098	-1.60787	-0.30812
H	2.18537	-1.79683	-0.09298
H	3.35882	-1.52023	-1.39255
H	3.81909	-2.47168	0.03574
C	3.46744	-0.43760	1.89115
H	4.00522	-1.29107	2.31685
H	3.80430	0.47234	2.39638
H	2.39986	-0.56579	2.09155
C	5.19996	-0.11408	0.11708
H	5.38531	-0.03277	-0.95789
H	5.54455	0.80732	0.59542
H	5.78874	-0.95006	0.50907

Deprotonation 6.75 – products 6.79 and HO^{t}Bu in DMSO

47
-981.7275513

C	-1.38218	2.56355	-0.08239
C	-0.28886	1.72115	0.13253
C	0.99252	2.30863	0.28378
C	1.12718	3.69446	0.24659
C	0.02014	4.52053	0.04509
C	-1.23592	3.95062	-0.12698
H	-2.36325	2.11521	-0.20669
H	2.11225	4.13790	0.36383
H	0.14398	5.59703	0.01398
H	-2.10199	4.58235	-0.29214
C	2.22626	1.43984	0.50390
H	3.10374	2.09481	0.54669
H	2.15968	0.95308	1.47882
C	2.39528	-0.94356	-0.23511
C	1.34893	-1.45886	0.57818
C	3.31770	-1.85920	-0.77161
C	1.28833	-2.81713	0.85995
C	3.21436	-3.22241	-0.50384
H	4.13338	-1.51024	-1.39192
C	2.20783	-3.71558	0.31818
H	0.48362	-3.17478	1.49564
H	3.94347	-3.89957	-0.93541
H	2.13545	-4.77560	0.52962
N	2.48340	0.42145	-0.52272
O	0.28386	-0.25293	2.33664
C	0.33395	-0.46749	1.09296
C	-0.35100	0.23642	0.09701
H	-0.18507	-0.15246	-0.90712
H	-2.22025	-0.28485	0.57623
C	3.37945	0.85939	-1.57481
H	3.13064	1.89056	-1.83173
H	4.43873	0.82520	-1.27932
H	3.24686	0.24937	-2.46995
O	-3.16299	-0.50124	0.78211
C	-3.70537	-1.19642	-0.34009
C	-2.90551	-2.47704	-0.58967
H	-1.86492	-2.23167	-0.81960
H	-2.92359	-3.11027	0.30116
H	-3.32507	-3.04069	-1.42726
C	-3.65923	-0.29616	-1.57673
H	-4.09237	-0.80249	-2.44353
H	-4.22161	0.62294	-1.39238
H	-2.62440	-0.02928	-1.80888
C	-5.14733	-1.53021	0.02116
H	-5.17611	-2.15850	0.91487
H	-5.70691	-0.61339	0.22255
H	-5.63627	-2.06441	-0.79701



6.75 **6.80**

Deprotonation 6.75 – starting species 6.75 and O^{t}Bu anion in DMSO

47
-981.7280946

C	3.91574	-0.11221	-1.10856
C	2.64768	-0.35110	-0.58037
C	2.21140	0.40250	0.52009
C	3.06057	1.36311	1.06702
C	4.32720	1.59433	0.53530
C	4.75579	0.85338	-0.55925
H	4.24953	-0.69226	-1.96264
H	2.72217	1.93935	1.92265
H	4.97230	2.34588	0.97518
H	5.73788	1.02119	-0.98585
C	0.81294	0.23377	1.07273
H	0.73780	0.78812	2.01568
H	0.08730	0.71449	0.39989
C	-0.65711	-1.68425	0.64802
C	-0.76790	-1.47684	-0.74579
C	-1.67631	-2.40325	1.29609
C	-1.93426	-1.84876	-1.41874
C	-2.80578	-2.80506	0.59711
H	-1.60916	-2.60125	2.35792
C	-2.96053	-2.50690	-0.75768
H	-1.99670	-1.65126	-2.48312
H	-3.58883	-3.33843	1.12456
H	-3.85365	-2.80847	-1.29034
N	0.42595	-1.15597	1.32974
O	0.20292	-0.36026	-2.59061
C	0.37498	-0.99158	-1.56544
C	1.78457	-1.43916	-1.18409
H	1.72786	-2.28704	-0.49935
H	2.24297	-1.77343	-2.11723
C	0.70871	-1.61608	2.67767
H	1.72162	-1.30764	2.94122
H	0.01425	-1.19389	3.41693
H	0.66117	-2.70452	2.72514
O	-1.01047	2.52026	-0.36242
C	-2.34304	2.47556	-0.03251
C	-2.82133	3.82551	0.55104
H	-2.24498	4.06193	1.45138
H	-2.64909	4.62108	-0.18120
H	-3.88571	3.82198	0.81411
C	-2.62503	1.37817	1.02136
H	-3.67472	1.35769	1.33806
H	-2.37174	0.39679	0.60770
H	-1.99953	1.54605	1.90487
C	-3.21732	2.16120	-1.26846
H	-3.06702	2.93108	-2.03235
H	-2.91408	1.19658	-1.68945
H	-4.28668	2.11376	-1.03085

Deprotonation 6.75 – transition state in DMSO

47
-981.7140300

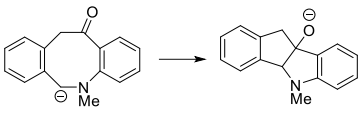
C	3.92765	-0.82851	-0.65598
C	2.60433	-0.75629	-0.22571
C	2.14085	0.38675	0.45902
C	3.06056	1.42725	0.67559
C	4.37663	1.35310	0.23250
C	4.82346	0.21636	-0.43529
H	4.25958	-1.71793	-1.18341
H	2.72532	2.31290	1.20819
H	5.05557	2.17843	0.41840
H	5.84732	0.14247	-0.78218
C	0.71936	0.57039	0.83659
H	0.66094	1.39300	1.56071
H	-0.04542	1.17705	-0.15021
C	-1.00087	-1.21141	0.82489
C	-0.89723	-1.53363	-0.54903
C	-2.19207	-1.56435	1.49164
C	-1.98614	-2.07742	-1.23309
C	-3.25000	-2.13616	0.79923
H	-2.30536	-1.34803	2.54635
C	-3.16791	-2.38157	-0.57283
H	-1.86865	-2.29873	-2.28848
H	-4.16056	-2.37738	1.33692
H	-4.00144	-2.82203	-1.10566
N	0.04910	-0.58153	1.45869
O	0.46693	-1.22818	-2.45865
C	0.40071	-1.46688	-1.26531
C	1.65958	-1.90022	-0.51620
H	1.37835	-2.41004	0.40646
H	2.15707	-2.61655	-1.17487
C	0.08600	-0.59915	2.91084
H	1.10489	-0.37453	3.22935
H	-0.58393	0.15304	3.35345
H	-0.18667	-1.58316	3.29853
O	-0.67320	1.91135	-0.93586
C	-1.90645	2.37772	-0.46549
C	-2.13548	3.79880	-0.99872
H	-1.34101	4.46240	-0.64515
H	-2.11434	3.79168	-2.09232
H	-3.09860	4.20506	-0.67271
C	-1.94565	2.41502	1.07310
H	-2.90143	2.81077	1.43010
H	-1.81442	1.40843	1.48218
H	-1.14287	3.05008	1.45944
C	-3.04383	1.46915	-0.95778
H	-3.02984	1.42000	-2.05108
H	-2.90395	0.45769	-0.56759
H	-4.02508	1.83699	-0.63891

Deprotonation 6.75 – products 6.80 and HO^{t}Bu in DMSO

47

-981.7207122

C	4.06524	-0.63097	-0.62269
C	2.73889	-0.63938	-0.21008
C	2.17221	0.48393	0.45406
C	3.02573	1.60291	0.63063
C	4.34378	1.60425	0.19531
C	4.89013	0.47994	-0.42560
H	4.45759	-1.50627	-1.13386
H	2.62723	2.48175	1.13039
H	4.95684	2.48573	0.35655
H	5.91976	0.47144	-0.76226
C	0.77921	0.54337	0.81448
H	0.54551	1.44459	1.39149
H	-0.45776	1.43762	-0.47184
C	-0.86287	-1.30285	0.81642
C	-0.73698	-1.57530	-0.56675
C	-2.02179	-1.76524	1.47199
C	-1.77622	-2.18488	-1.26862
C	-3.03440	-2.39500	0.75831
H	-2.15349	-1.58875	2.53181
C	-2.93350	-2.59634	-0.61882
H	-1.64129	-2.36687	-2.32968
H	-3.92587	-2.71601	1.28645
H	-3.73199	-3.08263	-1.16554
N	0.14024	-0.60409	1.45135
O	0.61285	-1.03820	-2.43804
C	0.55748	-1.36136	-1.26172
C	1.83444	-1.80080	-0.53797
H	1.56113	-2.35952	0.35932
H	2.34439	-2.47928	-1.22801
C	0.14090	-0.58437	2.90619
H	1.13387	-0.28506	3.24124
H	-0.58754	0.13394	3.31145
H	-0.07951	-1.57294	3.31694
O	-0.98972	2.08899	-0.99877
C	-2.27219	2.29091	-0.40489
C	-2.74861	3.66158	-0.87546
H	-2.06285	4.43874	-0.52932
H	-2.78517	3.69138	-1.96738
H	-3.74740	3.87773	-0.48855
C	-2.17041	2.26034	1.12107
H	-3.14409	2.47471	1.56958
H	-1.84271	1.27375	1.46217
H	-1.45263	3.00642	1.47261
C	-3.23706	1.20350	-0.87922
H	-3.28924	1.19989	-1.97137
H	-2.89326	0.22216	-0.54418
H	-4.24215	1.37434	-0.48274



6.80 **A34**

Nucleophilic attack of 6.80 – starting species 6.80 in DMSO

32

-748.0665397

C	3.10061	-0.99463	0.91698
C	1.86670	-0.46060	0.57690
C	1.75868	0.60213	-0.37665
C	2.98496	1.02461	-0.97116
C	4.20567	0.46628	-0.62747
C	4.29199	-0.54226	0.33760
H	3.13149	-1.81316	1.63221
H	2.95038	1.82143	-1.70942
H	5.10885	0.83132	-1.10800
H	5.24447	-0.97927	0.61081
C	0.50763	1.12326	-0.79475
H	0.56111	1.92227	-1.53973
C	-1.74320	0.62787	0.07323
C	-1.65844	-0.76410	-0.16426
C	-3.02497	1.19146	0.22353
C	-2.81161	-1.52158	-0.36011
C	-4.16369	0.41236	0.05111
H	-3.13533	2.24877	0.42579
C	-4.07246	-0.94346	-0.26210
H	-2.70309	-2.58453	-0.54838
H	-5.13806	0.87962	0.14647
H	-4.96614	-1.53877	-0.40205
N	-0.57550	1.35872	0.14155
O	-0.09447	-2.44763	-0.73952
C	-0.35084	-1.46302	-0.06378
C	0.58725	-1.07451	1.08648
H	0.05710	-0.40768	1.76907
H	0.81046	-2.00692	1.61337
C	-0.66447	2.72391	0.64001
H	0.33957	3.05461	0.90311
H	-1.06721	3.41595	-0.11440
H	-1.29218	2.77990	1.53319

Nucleophilic attack of 6.80 – transition state in DMSO

32

-748.0659566

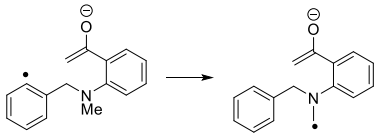
C	3.10118	-0.99582	1.00100
C	1.86825	-0.52209	0.57842
C	1.77100	0.52389	-0.38099
C	2.98890	1.00403	-0.92032
C	4.21901	0.50521	-0.50551
C	4.29386	-0.48571	0.47392
H	3.13565	-1.80805	1.72243
H	2.95307	1.79213	-1.66755
H	5.13056	0.90377	-0.94034
H	5.25128	-0.87388	0.80049
C	0.47942	0.93435	-0.85708
H	0.52132	1.64244	-1.69369
C	-1.74516	0.64300	0.09035
C	-1.68915	-0.74194	-0.18697
C	-3.00149	1.22296	0.33472
C	-2.85493	-1.48617	-0.31429
C	-4.15948	0.45420	0.22402
H	-3.08607	2.27701	0.56518
C	-4.10303	-0.89441	-0.11734
H	-2.77237	-2.54535	-0.53579
H	-5.12089	0.92854	0.39008
H	-5.01099	-1.47793	-0.20838
N	-0.55141	1.33180	0.08602
O	-0.12445	-2.36596	-0.95089
C	-0.35557	-1.40594	-0.21868
C	0.56773	-1.15122	0.99141
H	0.03408	-0.52553	1.71064
H	0.74450	-2.12877	1.45075
C	-0.58050	2.74221	0.44110
H	0.44542	3.07931	0.58475
H	-1.04033	3.35628	-0.34787
H	-1.13007	2.90580	1.37180

Nucleophilic attack of 6.80 – product A34 in DMSO

32

-748.1071091

C	-3.11162	-1.14171	-1.05056
C	-1.87630	-0.82133	-0.50129
C	-1.75125	0.29425	0.33635
C	-2.85359	1.08051	0.64450
C	-4.09472	0.75847	0.08926
C	-4.21993	-0.34315	-0.75395
H	-3.22136	-2.00817	-1.69483
H	-2.75840	1.92801	1.31619
H	-4.96515	1.36110	0.32268
H	-5.18868	-0.59057	-1.17356
C	-0.32928	0.41932	0.80449
H	-0.23703	0.73939	1.85335
C	1.74961	0.69497	-0.17514
C	1.70254	-0.66105	0.18629
C	2.94351	1.28894	-0.57869
C	2.84572	-1.43210	0.13850
C	4.09243	0.48984	-0.63475
H	2.99571	2.34041	-0.83627
C	4.05399	-0.85520	-0.28233
H	2.80613	-2.47451	0.44020
H	5.03035	0.93714	-0.94554
H	4.95887	-1.45073	-0.32040
N	0.48708	1.28222	-0.06818
O	0.15025	-1.85221	1.66525
C	0.27910	-1.03062	0.60717
C	-0.54859	-1.51862	-0.64992
H	-0.07840	-1.21271	-1.59237
H	-0.62440	-2.60797	-0.64088
C	0.38767	2.71231	0.13429
H	-0.66474	3.00049	0.12680
H	0.83317	3.02517	1.09091
H	0.88663	3.24611	-0.67620



6.77 6.81

H atom abstraction 6.77 – starting species 6.77 in benzene

33

-748.5611009

C	-4.12495	1.20792	0.75190
C	-2.80403	1.03867	0.42030
C	-2.28731	0.04678	-0.38833
C	-3.22410	-0.85696	-0.90232
C	-4.58263	-0.73085	-0.61096
C	-5.03926	0.29364	0.21215
H	-4.45552	2.01119	1.40103
H	-2.87579	-1.67111	-1.53056
H	-5.28635	-1.44613	-1.02110
H	-6.09512	0.38416	0.44193
C	-0.81548	-0.05505	-0.71638
H	-0.58759	-1.03371	-1.16085
H	-0.57215	0.71176	-1.45798
C	1.34103	0.62811	0.14480
C	2.45512	-0.21642	-0.01866
C	1.50005	2.01162	0.01626
C	3.69995	0.37631	-0.26140
C	2.73820	2.57884	-0.25949
H	0.62321	2.63531	0.16005
C	3.85169	1.75314	-0.38497
H	4.55590	-0.27820	-0.38582
H	2.83440	3.65480	-0.35590
H	4.82924	2.17695	-0.58804
N	0.01840	0.17777	0.45936
O	1.46120	-2.18746	-0.87557
C	2.33092	-1.73301	-0.05824
C	3.16613	-2.44363	0.76816
H	3.85816	-1.94058	1.43171
H	3.13481	-3.52768	0.76897
C	-0.10078	-0.89213	1.44561
H	-1.09967	-0.84379	1.88971
H	0.05604	-1.88561	1.01054
H	0.63475	-0.73396	2.23486

H atom abstraction 6.77 – transition state in benzene

33

-748.5452234

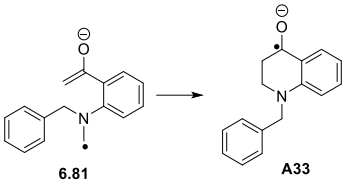
C	3.34033	-0.81390	-1.44741
C	2.25745	-0.96373	-0.59699
C	2.18732	-0.32401	0.62741
C	3.24702	0.49966	1.01633
C	4.34897	0.66105	0.17892
C	4.39903	0.00796	-1.05076
H	3.37554	-1.31747	-2.40817
H	3.20741	1.02079	1.96943
H	5.16714	1.30404	0.48320
H	5.25636	0.14161	-1.70214
C	0.96831	-0.54255	1.52511
H	1.13657	-1.44457	2.12519
H	0.84295	0.29072	2.21776
C	-0.97401	0.37516	0.31064
C	-2.30743	0.22803	-0.12619
C	-0.39229	1.65209	0.31823
C	-2.99124	1.36134	-0.56053
C	-1.10993	2.76979	-0.09377
H	0.63816	1.77779	0.62575
C	-2.41722	2.62931	-0.54314
H	-4.01338	1.23157	-0.90152
H	-0.63469	3.74425	-0.07455
H	-2.98433	3.49326	-0.87067
N	-0.25170	-0.75150	0.77111
O	-3.12909	-1.64034	-1.33230
C	-3.06070	-1.09964	-0.17627
C	-3.59844	-1.53956	1.00365
H	-4.16392	-2.46495	1.03251
H	-3.45926	-0.97973	1.92017
C	-0.15428	-1.88966	-0.07865
H	-0.96707	-1.97348	-0.79635
H	0.01505	-2.80799	0.48923
H	0.92063	-1.70065	-0.68866

H atom abstraction 6.77 – product 6.81 in benzene

33

-748.5921792

C	-3.51057	0.40350	1.49075
C	-2.30458	0.04181	0.89484
C	-2.27767	-0.40319	-0.42478
C	-3.47621	-0.48546	-1.13595
C	-4.68115	-0.12426	-0.54354
C	-4.70126	0.32324	0.77536
H	-3.51770	0.74749	2.51877
H	-3.46258	-0.83712	-2.16365
H	-5.60372	-0.19246	-1.10897
H	-5.63833	0.60429	1.24182
C	-0.98027	-0.78307	-1.12126
H	-1.10120	-1.77856	-1.56348
H	-0.79705	-0.09135	-1.94741
C	1.03852	0.30931	-0.20191
C	2.42051	0.18675	0.05332
C	0.48659	1.58838	-0.39726
C	3.17942	1.35300	0.14274
C	1.27618	2.72875	-0.33347
H	-0.57709	1.69346	-0.57800
C	2.63375	2.61870	-0.05063
H	4.24021	1.24407	0.34537
H	0.82167	3.70107	-0.48918
H	3.25920	3.50205	0.00871
N	0.19455	-0.81636	-0.27571
O	3.39920	-1.47790	1.43568
C	3.16812	-1.13353	0.22893
C	3.53589	-1.77005	-0.92789
H	4.08580	-2.70423	-0.88455
H	3.27596	-1.35766	-1.89500
C	0.33146	-1.90985	0.55607
H	1.17212	-1.93704	1.23240
H	-0.16809	-2.81657	0.24179
H	-1.37707	0.09597	1.45396



6.81 A33

$S_{RN}1$ cyclisation 6.81 – transition state in benzene

33

-748.5797844

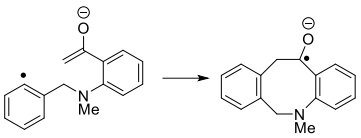
C	-3.39545	0.45421	1.57517
C	-2.22702	0.07908	0.91627
C	-2.27507	-0.37390	-0.40016
C	-3.51025	-0.44636	-1.04619
C	-4.67854	-0.07150	-0.39108
C	-4.62376	0.38085	0.92545
H	-3.34436	0.80497	2.59971
H	-3.55544	-0.80275	-2.07146
H	-5.63090	-0.13406	-0.90564
H	-5.53203	0.67186	1.44038
C	-1.01120	-0.77312	-1.14660
H	-1.15545	-1.77514	-1.56677
H	-0.86600	-0.09875	-1.99601
C	1.04583	0.30716	-0.31931
C	2.41796	0.17737	0.03889
C	0.53640	1.59591	-0.58751
C	3.17516	1.34103	0.18904
C	1.33664	2.72313	-0.48527
H	-0.51254	1.71732	-0.83442
C	2.66708	2.60631	-0.07563
H	4.20651	1.21107	0.49964
H	0.91003	3.69764	-0.69797
H	3.29259	3.48539	0.02769
N	0.18777	-0.79084	-0.34267
O	4.00555	-1.21398	1.14112
C	3.11486	-1.14421	0.23677
C	2.65159	-2.20857	-0.53731
H	3.12074	-3.17928	-0.40988
H	2.10666	-2.02981	-1.45480
C	0.47884	-1.95476	0.38070
H	0.83835	-1.82465	1.39548
H	-0.18868	-2.78531	0.18648
H	-1.26676	0.13362	1.41777

$S_{RN}1$ cyclisation 6.81 – product A33 in benzene

33

-748.6544530

C	-3.00664	0.50616	1.66388
C	-1.94208	0.16355	0.83277
C	-2.17485	-0.28274	-0.46735
C	-3.49420	-0.37992	-0.91604
C	-4.55887	-0.03465	-0.09066
C	-4.31724	0.41064	1.20670
H	-2.80769	0.85286	2.67163
H	-3.68671	-0.73314	-1.92534
H	-5.57592	-0.11665	-0.45755
H	-5.14361	0.67934	1.85458
C	-1.04349	-0.67156	-1.41236
H	-1.30734	-1.62982	-1.87262
H	-0.99768	0.05356	-2.23121
C	1.02815	0.33451	-0.52645
C	2.30933	0.13671	0.11264
C	0.59372	1.61658	-0.82483
C	3.07793	1.30733	0.40205
C	1.38654	2.75191	-0.53926
H	-0.38572	1.76927	-1.26329
C	2.62778	2.57553	0.08009
H	4.04261	1.15935	0.87310
H	1.01988	3.74055	-0.78804
H	3.24467	3.43899	0.31154
N	0.27215	-0.81076	-0.84164
O	3.96309	-1.37010	0.91681
C	2.82485	-1.15929	0.40186
C	1.95737	-2.35003	0.03460
H	2.13138	-3.14163	0.77002
H	2.26162	-2.74116	-0.94558
C	0.48261	-1.98253	0.00121
H	0.12830	-1.80637	1.02889
H	-0.11546	-2.79991	-0.41251
H	-0.92351	0.25757	1.19028



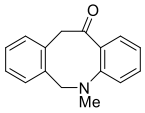
6.77 6.78

$S_{RN}1$ cyclisation 6.77 – product 6.78 in benzene

33

-748.6424854

C	3.12564	-1.10191	0.68063
C	1.86789	-0.54916	0.43315
C	1.79132	0.58175	-0.39931
C	2.95654	1.13288	-0.92694
C	4.20609	0.57349	-0.66600
C	4.28760	-0.55542	0.13873
H	3.19055	-1.98323	1.31098
H	2.88266	2.01231	-1.56041
H	5.10122	1.01435	-1.08993
H	5.24915	-1.01148	0.34727
C	0.44751	1.15388	-0.78801
H	0.59449	2.12370	-1.28312
H	-0.00731	0.48744	-1.52517
C	-1.71329	0.62449	0.18602
C	-1.65549	-0.79872	-0.05164
C	-2.93199	1.28447	0.20093
C	-2.87241	-1.41417	-0.48072
C	-4.13708	0.61028	-0.08064
H	-2.95815	2.35221	0.39024
C	-4.07644	-0.73496	-0.46765
H	-2.82976	-2.46390	-0.74626
H	-5.07960	1.14379	-0.05244
H	-4.98676	-1.25797	-0.74559
N	-0.48195	1.31294	0.33209
O	-0.39383	-2.78151	-0.35361
C	-0.48562	-1.60943	0.12248
C	0.63670	-1.16064	1.06936
H	0.24609	-0.46195	1.81167
H	0.94665	-2.07161	1.58858
C	-0.50282	2.65432	0.86484
H	0.52314	2.95987	1.08718
H	-0.93483	3.39294	0.16750
H	-1.07826	2.67812	1.79235

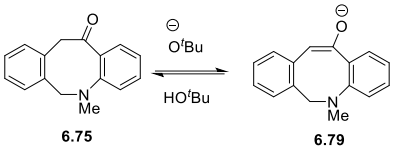


Neutral 6.75

33

-748.5933166

C	3.07550	-1.11816	0.84233
C	1.84290	-0.61645	0.42964
C	1.81484	0.49160	-0.42962
C	3.01047	1.07408	-0.84090
C	4.23754	0.56945	-0.41871
C	4.26820	-0.53258	0.42564
H	3.10127	-1.98087	1.49946
H	2.97946	1.93380	-1.50290
H	5.15895	1.03471	-0.74811
H	5.21497	-0.93895	0.76153
C	0.49697	1.02689	-0.94376
H	0.67883	1.94395	-1.51668
H	0.05936	0.30999	-1.64361
C	-1.70057	0.65194	0.08880
C	-1.72729	-0.74107	-0.13886
C	-2.91957	1.32042	0.27856
C	-2.94576	-1.40542	-0.28117
C	-4.12079	0.63008	0.18251
H	-2.93091	2.38613	0.46627
C	-4.14709	-0.73024	-0.11888
H	-2.92738	-2.47151	-0.47764
H	-5.05060	1.16925	0.32386
H	-5.08919	-1.25601	-0.20802
N	-0.47826	1.31310	0.10789
O	-0.35624	-2.54848	-0.80925
C	-0.48541	-1.57112	-0.10513
C	0.56839	-1.24541	0.95474
H	0.13054	-0.59497	1.71492
H	0.81484	-2.20396	1.41616
C	-0.40609	2.66544	0.62788
H	0.64247	2.90783	0.80951
H	-0.81896	3.40660	-0.07083
H	-0.93927	2.73349	1.57651



6.75 **6.79**

Deprotonation 6.75 – starting species 6.75 and O^{t}Bu anion in benzene

47

-981.6838637

C	1.39365	2.42079	0.00428
C	0.22650	1.66292	-0.10495
C	-1.00293	2.30890	-0.29851
C	-1.04827	3.69979	-0.36423
C	0.11598	4.45556	-0.24797
C	1.33532	3.81179	-0.06653
H	2.33335	1.88633	0.14327
H	-2.00436	4.19403	-0.51160
H	0.06798	5.53754	-0.30044
H	2.24787	4.39143	0.01897
C	-2.26945	1.50069	-0.47784
H	-3.12664	2.18218	-0.54693
H	-2.23045	0.96000	-1.42718
C	-2.59567	-0.81699	0.29852
C	-1.64102	-1.39068	-0.57093
C	-3.59185	-1.64837	0.83492
C	-1.75641	-2.72439	-0.95317
C	-3.66110	-2.98914	0.47517
H	-4.33133	-1.23982	1.51197
C	-2.75963	-3.53484	-0.43504
H	-1.01314	-3.12480	-1.63412
H	-4.44350	-3.60848	0.89974
H	-2.82609	-4.57742	-0.71999
N	-2.52671	0.53766	0.59323
O	-0.00018	-0.74706	-2.14357
C	-0.41703	-0.63721	-1.00934
C	0.32728	0.15969	0.04260
H	-0.04141	-0.12266	1.03249
H	1.39843	-0.10321	-0.01313
C	-3.28306	1.07157	1.70596
H	-2.88186	2.05690	1.95106
H	-4.35414	1.17928	1.47782
H	-3.16977	0.43259	2.58269
O	3.36979	0.06570	0.36274
C	3.98735	-1.15099	0.37774
C	2.96890	-2.29915	0.15497
H	2.20885	-2.26701	0.94344
H	2.46614	-2.15565	-0.80759
H	3.43635	-3.29150	0.16165
C	4.69241	-1.40454	1.73272
H	5.19066	-2.38113	1.78283
H	5.43820	-0.62132	1.90096
H	3.95264	-1.34552	2.53728
C	5.05639	-1.24985	-0.73741
H	4.57651	-1.09237	-1.70824
H	5.79803	-0.45786	-0.59354
H	5.57396	-2.21760	-0.75317

Deprotonation 6.75 – transition state in benzene

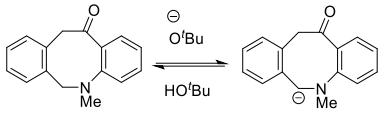
47
-981.6767959

C	0.86660	2.86018	0.26028
C	-0.03663	1.82231	0.02159
C	-1.36828	2.14932	-0.30589
C	-1.75747	3.48496	-0.38233
C	-0.84636	4.51154	-0.13941
C	0.46825	4.19389	0.18247
H	1.89193	2.59321	0.49728
H	-2.78690	3.72585	-0.63439
H	-1.16370	5.54655	-0.20163
H	1.18818	4.98365	0.36863
C	-2.37784	1.05729	-0.61417
H	-3.35503	1.52234	-0.79497
H	-2.10395	0.55514	-1.54491
C	-2.20090	-1.28234	0.19912
C	-1.01892	-1.59759	-0.51297
C	-2.99536	-2.34237	0.66512
C	-0.70637	-2.92053	-0.79804
C	-2.64018	-3.66286	0.40589
H	-3.90670	-2.13675	1.21242
C	-1.50427	-3.96527	-0.33759
H	0.20157	-3.12130	-1.35787
H	-3.27377	-4.46068	0.77793
H	-1.23865	-4.99476	-0.54537
N	-2.54461	0.04617	0.43200
O	0.29084	-0.39352	-2.07287
C	-0.06645	-0.49363	-0.90341
C	0.37929	0.38526	0.18133
H	-0.01287	0.01987	1.13503
H	1.70162	0.35647	0.26586
C	-3.56010	0.36110	1.41183
H	-3.48010	1.42118	1.66086
H	-4.58123	0.16708	1.04807
H	-3.39839	-0.21211	2.32630
O	2.98431	0.50227	0.44515
C	3.74017	-0.65749	0.33337
C	2.86960	-1.86749	-0.06263
H	2.07527	-2.02296	0.67510
H	2.40057	-1.68891	-1.03469
H	3.46786	-2.78273	-0.12478
C	4.42409	-0.96267	1.67821
H	5.05729	-1.85615	1.63025
H	5.04188	-0.10930	1.97236
H	3.66281	-1.11323	2.44910
C	4.82459	-0.46752	-0.74173
H	4.34828	-0.25593	-1.70300
H	5.45339	0.38724	-0.47631
H	5.46100	-1.35352	-0.84966

Deprotonation 6.75 – products 6.79 and HO^{t}Bu in benzene

47
-981.6884259

C	-1.02221	2.78710	-0.05615
C	-0.06252	1.79660	0.17277
C	1.29299	2.19589	0.28381
C	1.62986	3.54387	0.19267
C	0.65493	4.51860	-0.02396
C	-0.67410	4.13373	-0.15515
H	-2.06117	2.48330	-0.13982
H	2.67249	3.83895	0.27928
H	0.93537	5.56360	-0.09549
H	-1.44247	4.88071	-0.32516
C	2.39132	1.16322	0.50266
H	3.35555	1.68623	0.52360
H	2.27053	0.70039	1.48344
C	2.19782	-1.22696	-0.23059
C	1.10627	-1.58146	0.60670
C	2.95848	-2.26441	-0.79448
C	0.84700	-2.91552	0.88241
C	2.65514	-3.59923	-0.53271
H	3.80356	-2.03317	-1.43091
C	1.60540	-3.93847	0.31145
H	0.01387	-3.14848	1.53851
H	3.26137	-4.37574	-0.98702
H	1.37683	-4.97732	0.51904
N	2.48124	0.11103	-0.51676
O	0.32874	-0.21794	2.38809
C	0.27231	-0.44594	1.15774
C	-0.35785	0.34195	0.17908
H	-0.29594	-0.07957	-0.82474
H	-2.29723	0.06506	0.64365
C	3.35843	0.42609	-1.62130
H	3.22890	1.48044	-1.87424
H	4.42287	0.25593	-1.39256
H	3.09410	-0.16458	-2.50083
O	-3.27304	-0.05610	0.75636
C	-3.75386	-0.81227	-0.34481
C	-3.01181	-2.14949	-0.42905
H	-1.94608	-1.98223	-0.60454
H	-3.12191	-2.69146	0.51377
H	-3.40922	-2.76781	-1.23945
C	-3.56787	-0.01917	-1.64200
H	-3.95247	-0.57487	-2.50253
H	-4.09942	0.93377	-1.57319
H	-2.50741	0.18940	-1.80403
C	-5.23698	-1.04743	-0.07909
H	-5.36488	-1.60316	0.85291
H	-5.75431	-0.08957	0.01639
H	-5.69380	-1.61489	-0.89440



6.75 **6.80**

Deprotonation 6.75 – starting species 6.75 and O^{t}Bu anion in benzene

47
-981.6817071

C	4.13108	-0.45909	-0.59342
C	2.78165	-0.48545	-0.24370
C	2.19546	0.65835	0.31801
C	2.98288	1.79142	0.51834
C	4.32993	1.81075	0.16853
C	4.90827	0.67797	-0.39059
H	4.57752	-1.34336	-1.03668
H	2.52377	2.67626	0.94772
H	4.91957	2.70573	0.33081
H	5.95503	0.67661	-0.67259
C	0.72223	0.71125	0.64422
H	0.52478	1.61595	1.22926
H	0.09601	0.86161	-0.25513
C	-0.74433	-1.25524	0.86587
C	-0.60412	-1.71247	-0.46327
C	-1.88174	-1.65803	1.58756
C	-1.62906	-2.44241	-1.06575
C	-2.86709	-2.42581	0.98310
H	-2.01834	-1.32543	2.60852
C	-2.76214	-2.80761	-0.35347
H	-1.49576	-2.74801	-2.09740
H	-3.74384	-2.70388	1.55789
H	-3.54666	-3.38547	-0.82584
N	0.22988	-0.43747	1.41622
O	0.69600	-1.49564	-2.42928
C	0.67332	-1.58055	-1.22054
C	1.98541	-1.75502	-0.45072
H	1.77924	-2.22010	0.51544
H	2.57871	-2.44560	-1.05404
C	0.25303	-0.23969	2.85196
H	1.22011	0.18852	3.12246
H	-0.53564	0.44732	3.19226
H	0.14454	-1.19365	3.37129
O	-1.27455	2.02148	-1.14155
C	-2.49144	2.18578	-0.55595
C	-3.14081	3.52876	-0.97556
H	-2.48054	4.35303	-0.68736
H	-3.24804	3.54714	-2.06456
H	-4.12704	3.69214	-0.52146
C	-2.38080	2.18530	0.99349
H	-3.34675	2.33247	1.49360
H	-1.96373	1.22706	1.32188
H	-1.69810	2.98278	1.30665
C	-3.46538	1.04595	-0.94636
H	-3.56964	1.02307	-2.03580
H	-3.04230	0.08850	-0.62608
H	-4.46175	1.15797	-0.49831

Deprotonation 6.75 – transition state in benzene

47
-981.6749539

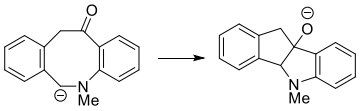
C	3.93132	-0.81603	-0.66124
C	2.60841	-0.74051	-0.23165
C	2.15177	0.40405	0.45211
C	3.07230	1.44148	0.66803
C	4.38816	1.36283	0.22752
C	4.83070	0.22441	-0.43892
H	4.25834	-1.70407	-1.19397
H	2.73404	2.33141	1.19073
H	5.06855	2.18799	0.40939
H	5.85362	0.14796	-0.78866
C	0.73043	0.59008	0.83397
H	0.67109	1.41582	1.55429
H	-0.01916	1.13528	-0.12739
C	-0.98897	-1.19074	0.83474
C	-0.89614	-1.51909	-0.53800
C	-2.17428	-1.53716	1.51327
C	-1.99160	-2.06312	-1.20690
C	-3.23922	-2.11396	0.83498
H	-2.27860	-1.30872	2.56641
C	-3.16833	-2.36487	-0.53485
H	-1.88230	-2.27959	-2.26390
H	-4.14604	-2.34961	1.38188
H	-4.00834	-2.80176	-1.06066
N	0.07030	-0.56574	1.46166
O	0.44666	-1.29970	-2.47471
C	0.39753	-1.47600	-1.27513
C	1.66531	-1.88569	-0.52071
H	1.38787	-2.39214	0.40564
H	2.16775	-2.60114	-1.17627
C	0.11797	-0.57990	2.91053
H	1.13905	-0.35024	3.21965
H	-0.55123	0.17135	3.35824
H	-0.14835	-1.56494	3.30224
O	-0.71895	1.84383	-0.95067
C	-1.92486	2.34286	-0.48105
C	-2.13500	3.76202	-1.03735
H	-1.31536	4.40851	-0.71077
H	-2.12556	3.72746	-2.13034
H	-3.08401	4.19986	-0.70652
C	-1.95498	2.41609	1.06055
H	-2.90264	2.83057	1.42099
H	-1.83122	1.41563	1.48814
H	-1.13844	3.04840	1.42290
C	-3.09382	1.45365	-0.94281
H	-3.07274	1.36706	-2.03319
H	-2.98386	0.45114	-0.52158
H	-4.06649	1.85864	-0.63844

Deprotonation 6.75 – products 6.80 and HO^{t}Bu in benzene

47

-981.6845553

C	4.09018	-0.59050	-0.58003
C	2.75878	-0.60518	-0.18698
C	2.16764	0.53124	0.43141
C	3.00212	1.66835	0.57834
C	4.32515	1.67365	0.16329
C	4.89740	0.53647	-0.40860
H	4.50005	-1.47520	-1.06046
H	2.58014	2.55955	1.03455
H	4.92152	2.57110	0.29809
H	5.93092	0.53233	-0.73368
C	0.77345	0.57972	0.77855
H	0.51331	1.49493	1.32055
H	-0.49476	1.50131	-0.54906
C	-0.83623	-1.29383	0.82717
C	-0.69774	-1.60953	-0.54570
C	-1.99208	-1.75029	1.49158
C	-1.72575	-2.25193	-1.23076
C	-2.99517	-2.41300	0.79349
H	-2.13051	-1.53853	2.54425
C	-2.88440	-2.65422	-0.57510
H	-1.58081	-2.45803	-2.28595
H	-3.88707	-2.72509	1.32681
H	-3.67662	-3.16108	-1.11257
N	0.15260	-0.56131	1.44447
O	0.65295	-1.16566	-2.43852
C	0.60106	-1.41196	-1.24870
C	1.87991	-1.79210	-0.49184
H	1.60581	-2.32822	0.41967
H	2.41475	-2.47930	-1.15365
C	0.16249	-0.51427	2.89617
H	1.15438	-0.19464	3.21611
H	-0.57204	0.20327	3.29467
H	-0.04273	-1.49832	3.32795
O	-1.04709	2.17305	-1.01775
C	-2.33560	2.26551	-0.42802
C	-2.90362	3.60863	-0.87869
H	-2.26603	4.42219	-0.52444
H	-2.93829	3.64850	-1.97017
H	-3.91464	3.75530	-0.48917
C	-2.24025	2.21839	1.09912
H	-3.22586	2.37027	1.54886
H	-1.85793	1.24712	1.42566
H	-1.56409	2.99780	1.46072
C	-3.22406	1.12338	-0.92544
H	-3.26000	1.13058	-2.01777
H	-2.82136	0.16176	-0.60062
H	-4.24276	1.22128	-0.53712



6.80 **A34**

Nucleophilic attack of 6.80 – starting species 6.80 in benzene

32

-748.0309499

C	3.10684	-0.96942	0.92380
C	1.87035	-0.44529	0.58343
C	1.75326	0.60474	-0.38501
C	2.97397	1.00630	-1.00766
C	4.19599	0.45658	-0.66160
C	4.29387	-0.52621	0.32916
H	3.14281	-1.78061	1.64743
H	2.93008	1.78215	-1.76728
H	5.09414	0.80718	-1.16272
H	5.24882	-0.95858	0.60135
C	0.50456	1.12710	-0.78450
H	0.51981	1.87900	-1.57717
C	-1.74189	0.62946	0.07490
C	-1.65468	-0.76256	-0.15976
C	-3.02356	1.19419	0.21422
C	-2.80525	-1.51594	-0.36750
C	-4.16265	0.41730	0.02821
H	-3.13214	2.25210	0.41529
C	-4.06843	-0.93641	-0.28555
H	-2.69067	-2.57767	-0.55887
H	-5.13769	0.88620	0.11218
H	-4.96056	-1.53090	-0.44036
N	-0.57296	1.35702	0.15522
O	-0.11182	-2.47544	-0.69248
C	-0.34765	-1.47236	-0.04480
C	0.59636	-1.06634	1.09782
H	0.06131	-0.40090	1.77924
H	0.83001	-1.99526	1.62639
C	-0.65829	2.71355	0.67031
H	0.34813	3.03504	0.93604
H	-1.05796	3.41824	-0.07568
H	-1.28753	2.76014	1.56459

Nucleophilic attack of 6.80 – transition state in benzene

32

-748.0303177

C	3.10343	-0.97492	1.01492
C	1.86914	-0.51582	0.58441
C	1.76747	0.51554	-0.39083
C	2.98252	0.98655	-0.94384
C	4.21396	0.50143	-0.51980
C	4.29399	-0.46755	0.48069
H	3.14119	-1.77983	1.74457
H	2.94078	1.75652	-1.70933
H	5.12380	0.89324	-0.96498
H	5.25334	-0.84705	0.81240
C	0.47357	0.91207	-0.85982
H	0.48474	1.57412	-1.73321
C	-1.74446	0.64648	0.09179
C	-1.69120	-0.73848	-0.18318
C	-2.99725	1.23215	0.33459
C	-2.85728	-1.47659	-0.31206
C	-4.15914	0.46735	0.22194
H	-3.07605	2.28737	0.56277
C	-4.10567	-0.87966	-0.11901
H	-2.77266	-2.53440	-0.53910
H	-5.11965	0.94548	0.38477
H	-5.01560	-1.45979	-0.21553
N	-0.54505	1.32461	0.08794
O	-0.14122	-2.37845	-0.93540
C	-0.35533	-1.40947	-0.21781
C	0.57151	-1.15169	0.99413
H	0.03395	-0.52975	1.71474
H	0.75275	-2.13047	1.44919
C	-0.55806	2.73135	0.44630
H	0.47301	3.05559	0.58391
H	-1.01641	3.35390	-0.33860
H	-1.10137	2.89796	1.38152

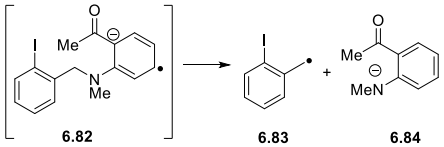
Nucleophilic attack of 6.80 – product A34 in benzene

32

-748.0629296

C	-3.11022	-1.12742	-1.05971
C	-1.87379	-0.81536	-0.50848
C	-1.74976	0.29071	0.34256
C	-2.85381	1.06977	0.66061
C	-4.09539	0.75642	0.10194
C	-4.21956	-0.33404	-0.75497
H	-3.21896	-1.98844	-1.71161
H	-2.75810	1.90542	1.34730
H	-4.96661	1.35489	0.34478
H	-5.18853	-0.57793	-1.17713
C	-0.33003	0.41292	0.81295
H	-0.23459	0.72302	1.86391
C	1.74671	0.69518	-0.17801
C	1.70354	-0.66111	0.17971
C	2.93830	1.29453	-0.57913
C	2.84990	-1.42478	0.14250
C	4.09141	0.50011	-0.63226
H	2.98736	2.34716	-0.83391
C	4.05717	-0.84327	-0.27607
H	2.80545	-2.46247	0.45876
H	5.02885	0.95146	-0.93997
H	4.96616	-1.43371	-0.30654
N	0.48294	1.27827	-0.06194
O	0.16022	-1.87163	1.64216
C	0.28194	-1.04500	0.60903
C	-0.54986	-1.51438	-0.66283
H	-0.07859	-1.20337	-1.60356
H	-0.62841	-2.60323	-0.64909
C	0.37955	2.70527	0.13166
H	-0.67463	2.98898	0.12762
H	0.82975	3.02895	1.08407
H	0.87196	3.23707	-0.68536

Scheme 6.16C



6.82 6.83 6.84

CN cleavage of 6.81 – transition state in DMSO

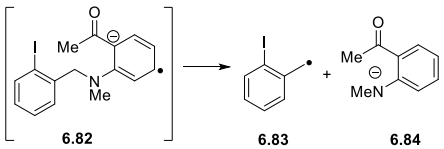
35
-760.5905567

C	-2.69899	3.29057	0.44189
C	-1.56304	2.77252	-0.14371
C	-1.38412	1.37302	-0.38558
C	-2.47975	0.56034	0.02461
C	-3.62596	1.07187	0.60414
C	-3.74944	2.44805	0.83291
H	-2.77710	4.36097	0.60035
H	-4.43691	0.40774	0.87866
H	-4.64537	2.84312	1.29442
C	-0.12108	0.91790	-0.86280
H	-0.01755	-0.12208	-1.15233
H	0.43624	1.62018	-1.47291
C	2.42582	0.83986	0.12344
C	3.32954	-0.28398	0.19932
C	2.95471	2.03232	-0.47079
C	4.70526	-0.07073	-0.05602
C	4.28131	2.17427	-0.78782
H	2.26753	2.86322	-0.59834
C	5.19398	1.12355	-0.53834
H	5.39346	-0.89962	0.07036
H	4.63693	3.11155	-1.20342
H	6.24851	1.24307	-0.75333
N	1.15747	0.92742	0.58405
O	1.79165	-2.05985	-0.08607
C	2.88953	-1.67592	0.31864
C	3.85494	-2.71299	0.87274
H	4.50702	-2.31284	1.64876
H	3.26949	-3.54094	1.27113
C	0.66616	-0.02985	1.55091
H	0.33835	-0.97757	1.11412
H	1.44697	-0.26173	2.28781
H	-0.18385	0.42059	2.07303
H	-0.75451	3.43594	-0.43557
H	4.48273	-3.10521	0.06718
I	-2.46643	-1.54876	-0.36662

CN cleavage of 6.81 – products 6.83 and 6.84 in DMSO

35
-760.6046657

C	2.03457	3.37251	-0.60934
C	1.57725	2.80456	0.56216
C	1.78436	1.43099	0.86935
C	2.50108	0.67947	-0.09891
C	2.96030	1.24348	-1.27572
C	2.72767	2.59429	-1.53888
H	1.85079	4.42166	-0.80771
H	3.49707	0.64012	-1.99676
H	3.08909	3.02746	-2.46347
C	1.25232	0.90486	2.06237
H	1.36673	-0.13314	2.33622
H	0.70446	1.55399	2.73185
C	-2.94097	0.81897	0.07546
C	-3.43638	-0.52136	-0.24841
C	-3.93621	1.70590	0.66076
C	-4.83975	-0.72302	-0.34456
C	-5.27123	1.43362	0.61647
H	-3.57480	2.64770	1.06213
C	-5.75699	0.22047	0.04926
H	-5.20316	-1.68902	-0.68050
H	-5.97708	2.15728	1.01388
H	-6.82004	0.02336	-0.00887
N	-1.75834	1.33035	-0.17006
O	-1.51175	-1.74982	0.37856
C	-2.58998	-1.69807	-0.22658
C	-3.07670	-2.97630	-0.90157
H	-3.64371	-2.78535	-1.81279
H	-2.20475	-3.58660	-1.13488
C	-0.82249	0.60286	-0.99029
H	-0.24652	-0.14823	-0.43648
H	-1.32659	0.05519	-1.80599
H	-0.11000	1.31076	-1.42664
H	1.02835	3.40442	1.27971
H	-3.71190	-3.54588	-0.21717
I	2.88082	-1.39674	0.19925



6.82 **6.83** **6.84**

CN cleavage of 6.81 – transition state in benzene

35

-760.5585428

C	-2.70397	3.28389	0.45696
C	-1.56839	2.76966	-0.12993
C	-1.39203	1.37263	-0.38743
C	-2.48769	0.55802	0.01905
C	-3.63344	1.06584	0.60031
C	-3.75802	2.44055	0.83709
H	-2.77811	4.35273	0.62861
H	-4.44243	0.39783	0.87083
H	-4.65433	2.83328	1.30014
C	-0.13560	0.92049	-0.87763
H	-0.02719	-0.11876	-1.16754
H	0.42339	1.62569	-1.48216
C	2.42310	0.83942	0.11761
C	3.33298	-0.27965	0.20612
C	2.95034	2.02886	-0.48757
C	4.70720	-0.06250	-0.04623
C	4.27700	2.17378	-0.79739
H	2.25830	2.85425	-0.62234
C	5.19436	1.12996	-0.53467
H	5.39816	-0.88808	0.08844
H	4.63041	3.10974	-1.21862
H	6.24955	1.25250	-0.74551
N	1.15907	0.92685	0.57433
O	1.79293	-2.05891	-0.06010
C	2.89142	-1.67135	0.32687
C	3.86787	-2.71067	0.86854
H	4.51137	-2.31591	1.65517
H	3.28454	-3.54840	1.24894
C	0.66144	-0.02003	1.54608
H	0.33576	-0.97277	1.11770
H	1.43921	-0.24409	2.28922
H	-0.19067	0.43936	2.05709
H	-0.75279	3.43106	-0.40511
H	4.50299	-3.08315	0.05947
I	-2.46046	-1.55048	-0.36831

CN cleavage of 6.81 – products 6.83 and 6.84 in benzene

35

-760.5719419

C	-1.59237	3.07639	0.62609
C	-0.82792	1.96219	0.34530
C	-1.42238	0.70236	0.03872
C	-2.84218	0.66987	0.03822
C	-3.60974	1.78629	0.31922
C	-2.98759	2.99908	0.61696
H	-1.10269	4.01573	0.85572
H	-4.69036	1.72067	0.30942
H	-3.59296	3.86976	0.83897
C	-0.58211	-0.39552	-0.22917
H	-0.98177	-1.37424	-0.45222
H	0.49416	-0.27807	-0.18773
C	3.35232	0.79831	-0.06078
C	4.06928	-0.46380	0.13347
C	3.83033	1.60115	-1.17620
C	5.34473	-0.61961	-0.47169
C	5.02889	1.36703	-1.77977
H	3.22386	2.45870	-1.44974
C	5.84850	0.26916	-1.38950
H	5.91933	-1.51305	-0.24812
H	5.36946	2.03408	-2.56662
H	6.81437	0.10685	-1.85196
N	2.40305	1.31967	0.67705
O	2.20835	-1.78994	0.75530
C	3.43191	-1.64362	0.68453
C	4.30311	-2.82194	1.11985
H	5.21723	-2.50714	1.62491
H	3.70800	-3.44555	1.78595
C	2.07189	0.72445	1.94667
H	1.32630	-0.07919	1.87231
H	2.94837	0.27494	2.44224
H	1.66511	1.50403	2.59998
H	0.26002	2.00828	0.35231
H	4.58314	-3.42406	0.25073
I	-3.88962	-1.13888	-0.40621

References

1. G. Sheldrick, *Acta Cryst. A*, 2008, **64**, 112-122.
2. S. J. Coles, P. A. Gale, *Chem. Sci.*, 2012, **3**, 683-689.