Chapter 1 and 2 Computational Details

Computational Details

Density functional theory[1,2] (DFT) was employed to calculate the electronic structures and energies for all species involved in oxabispidine syntheses. All structures thus far have been optimised with the hybrid meta-GGA exchange correlation functional M06-2X.[3] The M06-2X density functional was used in conjunction with the 6-311++G(*d*,*p*)[4] basis set for all main group atoms. All calculations on bispidine species were run in conjunction with the polarisable continuum model (PCM) for DCM solvation (ε = 8.93), employing the Gaussian keyword scrf=(solvent=dichloromethane).[5] Alternatively, the PCM for THF solvation (ε = 7.4257) was employed for calculations involving magnesium amides. The participating transition states (TS) are located at the same level of theory, using the Berny algorithm[6] through the Gaussian keyword opt=(ts,calcfc,noeigentest). Harmonic vibrational frequencies are calculated at the same level of theory to characterise respective minima (reactants, intermediates, and products with no imaginary frequency) and first order saddle points (TSs with one imaginary frequency). All calculations using the M06-2X functional have been performed using Gaussian 09 quantum chemistry program package.[7] All coordinates provided are listed in Cartesian (xyz) format, with charge and multiplicity of each system given at the top of the coordinate list (e.g. 0 1 = neutral singlet; 1 1 = 1+ charged singlet).

Chapter 1: Oxabispidine formation mechanism

Optimised Coordinates for Iminium Cyclisation

Protonated Iminium (conformer 1)

```
1 1
 C                  2.86125000   -1.14375100    0.16727600
 C                  1.11590400   -0.13825600    1.48102500
 C                  0.63875900   -1.36759700    1.69172800
 C                  1.84904700   -2.24226300   -0.14982200
 H                  0.79758500    0.70751200    2.07009600
 H                  3.49487600   -0.94345500   -0.69419200
 H                  3.48312700   -1.45139600    1.01135400
 H                 -0.07227300   -1.59096200    2.47359500
 H                  2.36934800   -3.18553100   -0.30681000
 N                  2.11903100    0.05619500    0.51191600
 O                  0.98346000   -2.46967600    0.96286700
 C                  2.42274500    1.26601000   -0.05321600
 O                  3.34153200    1.45202300   -0.81838700
 O                  1.55301800    2.20774300    0.33362300
 C                  1.02412700   -1.90260700   -1.42320100
 H                  1.44974000   -1.04226900   -1.94216900
 C                  1.81393400    3.52779600   -0.16563100
 H                  1.03873100    4.15669400    0.26224200
 H                  2.79892800    3.86242400    0.15641400
 H                  1.75838900    3.53575200   -1.25335900
 H                  1.01003200   -2.74744400   -2.10859800
 C                 -0.80876100   -0.39374400   -0.88061000
 H                 -0.09133900    0.41245800   -1.01997100
 N                 -0.37032300   -1.58499400   -1.10227500
 H                 -0.98885100   -2.37728100   -0.95204800
 C                 -2.14607600   -0.04042500   -0.47102800
 C                 -2.38547200    1.31793800   -0.22110100
 C                 -3.17322400   -0.98215800   -0.30053200
 C                 -3.64063200    1.73344100    0.19906700
 H                 -1.58329800    2.03656500   -0.35145900
 C                 -4.42245200   -0.55926500    0.11488400
 H                 -3.01276500   -2.03661500   -0.49420600
 C                 -4.65475300    0.79569600    0.36522600
 H                 -3.82792400    2.78121600    0.39549400
 H                 -5.21953700   -1.27984800    0.24518800
 H                 -5.63617900    1.11817400    0.69173400
```

Transition State (conformer 1)

```
1 1
 C                 -2.33941500   -1.67348600   -0.35150600
 C                 -0.97632200    0.25416200   -0.87010600
 C                  0.13716200   -0.57674400   -1.04622300
 C                 -1.00101900   -2.33618000   -0.05152500
 H                 -0.87365800    1.32667000   -0.98072400
 H                 -3.06413500   -1.87719300    0.43462400
 H                 -2.73710100   -2.02472700   -1.30377000
 H                  0.89972000   -0.25603900   -1.74302500
 H                 -1.10186800   -3.41251400   -0.16993300
 N                 -2.13841700   -0.21804800   -0.42621500
 O                 -0.03842900   -1.93782800   -1.03393600
 C                 -3.23207900    0.62591400   -0.07070400
 O                 -4.28659700    0.17209400    0.26310400
 O                 -2.90348200    1.89479500   -0.16770400
 C                 -0.46230800   -1.98411400    1.36671200
 H                 -1.09640700   -1.23265500    1.84799200
 C                 -3.94951600    2.83417700    0.16073900
 H                 -3.50122000    3.81403600    0.03495800
 H                 -4.78728100    2.69750000   -0.52031600
 H                 -4.26786700    2.67906800    1.18983900
 H                 -0.45233300   -2.87169800    1.99501300
 C                  0.99116400   -0.21931000    0.66697100
 H                  0.35971900    0.52977300    1.13791700
 N                  0.88218600   -1.44618900    1.27435800
 H                  1.58386400   -2.12652500    1.00595300
 C                  2.34907900    0.27306800    0.32210800
 C                  2.66880200    1.60877000    0.56434900
 C                  3.30183000   -0.57659900   -0.24734300
 C                  3.93928300    2.08727800    0.26045300
 H                  1.92781800    2.27110500    0.99875300
 C                  4.56854200   -0.09669800   -0.54811300
 H                  3.05473000   -1.60822400   -0.47918300
 C                  4.88973200    1.23572000   -0.29224400
 H                  4.18493700    3.12351700    0.45834200
 H                  5.30422200   -0.75906500   -0.98750100
 H                  5.87893700    1.60840400   -0.52905100
```

Cyclised Iminium (conformer 1)

```
1 1
 C                 -2.22765300   -1.69908700   -0.24925300
 C                 -1.13337300    0.44703800   -0.53134000
 C                  0.17025200   -0.21701100   -0.73395100
 C                 -0.80711300   -2.18159100   -0.01286500
 H                 -1.19334700    1.53072900   -0.52728200
 H                 -2.89772300   -1.98766400    0.55983900
 H                 -2.62819900   -2.06338100   -1.19515400
 H                  0.65918400    0.25837300   -1.58584800
 H                 -0.76268600   -3.25331800   -0.19369600
 N                 -2.21734800   -0.21719500   -0.30599100
 O                  0.03301300   -1.58293300   -1.00177500
 C                 -3.51201800    0.44594800   -0.10587500
 O                 -4.48997700   -0.20635100    0.06338700
 O                 -3.37514500    1.73971000   -0.15219800
 C                 -0.27521000   -1.83002000    1.40895900
 H                 -0.94117500   -1.11923400    1.91072700
 C                 -4.59299700    2.50762700    0.02002500
 H                 -4.28030300    3.54453900   -0.03131700
 H                 -5.28409300    2.26351100   -0.78390000
 H                 -5.02931400    2.27439400    0.98899900
 H                 -0.24723900   -2.73029700    2.02027400
 C                  1.07418500   -0.01023900    0.57976200
 H                  0.64194900    0.78677900    1.19148500
 N                  1.05136200   -1.24079200    1.34878500
 H                  1.71768200   -1.90322300    0.96207500
 C                  2.49050800    0.36259400    0.21403700
 C                  3.13967200    1.39035400    0.89326200
 C                  3.17612400   -0.35388500   -0.76919700
 C                  4.46265600    1.70353100    0.59232400
 H                  2.61144100    1.94396200    1.66219300
 C                  4.49676400   -0.04132200   -1.06964900
 H                  2.67700300   -1.15791400   -1.30373000
 C                  5.14181500    0.98878900   -0.38863200
 H                  4.96084400    2.50526100    1.12433400
 H                  5.02215600   -0.59921600   -1.83544700
 H                  6.17092300    1.23283900   -0.62406100
```

Protonated Iminium (conformer 2)

```
1 1
 C                  2.86125000   -1.14375100    0.16727600
 C                  1.11590400   -0.13825600    1.48102500
 C                  0.63875900   -1.36759700    1.69172800
 C                  1.84904700   -2.24226300   -0.14982200
 H                  0.79758500    0.70751200    2.07009600
 H                  3.49487600   -0.94345500   -0.69419200
 H                  3.48312700   -1.45139600    1.01135400
 H                 -0.07227300   -1.59096200    2.47359500
 H                  2.36934800   -3.18553100   -0.30681000
 N                  2.11903100    0.05619500    0.51191600
 O                  0.98346000   -2.46967600    0.96286700
 C                  2.42274500    1.26601000   -0.05321600
 O                  3.34153200    1.45202300   -0.81838700
 O                  1.55301800    2.20774300    0.33362300
 C                  1.02412700   -1.90260700   -1.42320100
 H                  1.44974000   -1.04226900   -1.94216900
 C                  1.81393400    3.52779600   -0.16563100
 H                  1.03873100    4.15669400    0.26224200
 H                  2.79892800    3.86242400    0.15641400
 H                  1.75838900    3.53575200   -1.25335900
 H                  1.01003200   -2.74744400   -2.10859800
 C                 -0.80876100   -0.39374400   -0.88061000
 H                 -0.09133900    0.41245800   -1.01997100
 N                 -0.37032300   -1.58499400   -1.10227500
 H                 -0.98885100   -2.37728100   -0.95204800
 C                 -2.14607600   -0.04042500   -0.47102800
 C                 -2.38547200    1.31793800   -0.22110100
 C                 -3.17322400   -0.98215800   -0.30053200
 C                 -3.64063200    1.73344100    0.19906700
 H                 -1.58329800    2.03656500   -0.35145900
 C                 -4.42245200   -0.55926500    0.11488400
 H                 -3.01276500   -2.03661500   -0.49420600
 C                 -4.65475300    0.79569600    0.36522600
 H                 -3.82792400    2.78121600    0.39549400
 H                 -5.21953700   -1.27984800    0.24518800
 H                 -5.63617900    1.11817400    0.69173400
```

Transition State (conformer 2)

```
1 1
 C                 -2.33941500   -1.67348600   -0.35150600
 C                 -0.97632200    0.25416200   -0.87010600
 C                  0.13716200   -0.57674400   -1.04622300
 C                 -1.00101900   -2.33618000   -0.05152500
 H                 -0.87365800    1.32667000   -0.98072400
 H                 -3.06413500   -1.87719300    0.43462400
 H                 -2.73710100   -2.02472700   -1.30377000
 H                  0.89972000   -0.25603900   -1.74302500
 H                 -1.10186800   -3.41251400   -0.16993300
 N                 -2.13841700   -0.21804800   -0.42621500
 O                 -0.03842900   -1.93782800   -1.03393600
 C                 -3.23207900    0.62591400   -0.07070400
 O                 -4.28659700    0.17209400    0.26310400
 O                 -2.90348200    1.89479500   -0.16770400
 C                 -0.46230800   -1.98411400    1.36671200
 H                 -1.09640700   -1.23265500    1.84799200
 C                 -3.94951600    2.83417700    0.16073900
 H                 -3.50122000    3.81403600    0.03495800
 H                 -4.78728100    2.69750000   -0.52031600
 H                 -4.26786700    2.67906800    1.18983900
 H                 -0.45233300   -2.87169800    1.99501300
 C                  0.99116400   -0.21931000    0.66697100
 H                  0.35971900    0.52977300    1.13791700
 N                  0.88218600   -1.44618900    1.27435800
 H                  1.58386400   -2.12652500    1.00595300
 C                  2.34907900    0.27306800    0.32210800
 C                  2.66880200    1.60877000    0.56434900
 C                  3.30183000   -0.57659900   -0.24734300
 C                  3.93928300    2.08727800    0.26045300
 H                  1.92781800    2.27110500    0.99875300
 C                  4.56854200   -0.09669800   -0.54811300
 H                  3.05473000   -1.60822400   -0.47918300
 C                  4.88973200    1.23572000   -0.29224400
 H                  4.18493700    3.12351700    0.45834200
 H                  5.30422200   -0.75906500   -0.98750100
 H                  5.87893700    1.60840400   -0.52905100
```

Cyclised Iminium (conformer 2)

```
1 1
 C                -2.52426800   -1.11140900    0.10317400
 C                -0.62996700    0.06214600   -0.89192600
 C                 0.02248700   -1.23428500   -1.16436100
 C                -1.67848000   -2.37618700   -0.04245200
 H                -0.13819900    1.00028800   -1.12822100
 H                -2.86627800   -0.97017700    1.12759000
 H                -3.39491500   -1.14007900   -0.55181300
 H                 0.55116800   -1.18031200   -2.11583600
 H                -2.36224700   -3.21212100   -0.18701200
 N                -1.75898200    0.10670900   -0.27302400
 O                -0.91067900   -2.28145400   -1.24424400
 C                -2.41540000    1.38268600    0.05561900
 O                -3.45219600    1.37982200    0.63459200
 O                -1.70488500    2.38522400   -0.37145600
 C                -0.74571600   -2.67688500    1.13205300
 H                -1.30602300   -2.70446900    2.06711100
 C                -2.24802200    3.70176500   -0.09713900
 H                -1.52640200    4.39543900   -0.51373900
 H                -3.21544900    3.79690500   -0.58559500
 H                -2.34436600    3.83075900    0.97890800
 H                -0.31681800   -3.66858800    0.96472100
 C                 1.04835200   -1.50456800    0.01275200
 H                 1.50445500   -2.45750600   -0.27999100
 N                 0.34770200   -1.71856600    1.25577200
 H                 0.03226000   -0.85235000    1.68076900
 C                 2.11329700   -0.42896500    0.08781500
 C                 2.33807800    0.30667900    1.25045300
 C                 2.89323200   -0.16381500   -1.04255200
 C                 3.31055100    1.30446800    1.27604100
 H                 1.78370200    0.09282800    2.15557000
 C                 3.86228500    0.83094800   -1.01581700
 H                 2.75946800   -0.74738900   -1.94779800
 C                 4.06955200    1.57369000    0.14420800
 H                 3.47771400    1.86310700    2.18917000
 H                 4.46085700    1.02165000   -1.89846200
 H                 4.82623300    2.34865500    0.16705800
```

Optimised Coordinates for Oxabispidine Products

Conformer 1

0 1

C	-2.20898400	1.73280600	0.12840200
C	0.28631600	0.56434300	0.80448900
C	-0.87757100	2.46688000	0.10010400
H	-2.85304400	2.08254000	-0.67709600
H	-2.71338400	1.90119300	1.08509000
H	0.92748900	0.22787400	1.61910500
H	-1.03785200	3.50330600	0.39656800
N	-1.96480900	0.30134600	-0.06577800
O	-0.01802200	1.91646500	1.09871400
C	-2.96759200	-0.44648100	-0.62371700
O	-3.95209800	0.01884400	-1.15598100
O	-2.72150000	-1.76236600	-0.54536600
C	-0.17969300	2.39051700	-1.28718300
H	-0.79332900	1.80275700	-1.97737200
C	-3.70346000	-2.60653900	-1.15543900
H	-3.35013500	-3.62197500	-0.99912800
H	-4.67335600	-2.46231100	-0.68083000
H	-3.78054000	-2.38940600	-2.22033800
H	-0.06971800	3.38966800	-1.70872600
C	1.04030200	0.45656300	-0.56330800
H	0.45270300	-0.17826800	-1.23638200
N	1.13713400	1.76312900	-1.21850800
H	1.76117500	2.35504200	-0.67606600
C	2.41452300	-0.15393300	-0.41508100
C	2.79696600	-1.24214000	-1.19691700
C	3.33502800	0.38648800	0.48736000
C	4.07496100	-1.78468000	-1.08219800
H	2.09025700	-1.66592300	-1.90298200
C	4.61341600	-0.14809500	0.59992300
H	3.05164200	1.23102600	1.10979900
C	4.98593900	-1.23778100	-0.18474600
H	4.35730600	-2.63344900	-1.69420600
H	5.31842000	0.28150600	1.30216000
H	5.98061100	-1.65803400	-0.09354800
C	-0.97885800	-0.30115200	0.80298500
H	-0.72305000	-1.29152200	0.41503700
C	-0.94257900	-1.44106900	2.87502700
H	0.11232100	-1.23035700	3.07868900
H	-1.48188600	-1.47560400	3.81971500
H	-1.02409800	-2.41265200	2.37476200
O	-1.54464000	-0.42557900	2.09232700

Conformer 2

```
0 1
 C                  2.53086100   -1.11687200   -0.20353600
 C                 -0.07763200   -1.31151000    0.91888500
 C                  1.70555300   -2.39553500   -0.14123600
 H                  3.09649900   -1.07250300   -1.13324500
 H                  3.23599600   -1.10034900    0.63410700
 H                 -0.65848300   -1.34564400    1.84223100
 H                  2.38913800   -3.23361200    0.00575000
 N                  1.65534400    0.05954700   -0.13966100
 O                  0.87863300   -2.35533400    1.02438500
 C                  2.18846600    1.24933000   -0.56473400
 O                  3.23292700    1.35069300   -1.17133600
 O                  1.40146300    2.29144200   -0.26260400
 C                  0.83737700   -2.66504600   -1.37385400
 H                  1.45252700   -2.65057800   -2.27587500
 C                  1.88003300    3.56844700   -0.69755500
 H                  1.14142800    4.28728100   -0.35384600
 H                  2.85206700    3.77812400   -0.25246800
 H                  1.96084300    3.59374000   -1.78379500
 H                  0.41342200   -3.66903800   -1.27206400
 C                 -1.01209700   -1.58701400   -0.28338500
 H                 -1.45783900   -2.56857500   -0.07925400
 N                 -0.27206800   -1.72075000   -1.53697100
 H                  0.11480900   -0.81815300   -1.79581100
 C                 -2.12941200   -0.56803600   -0.35451300
 C                 -2.26882000    0.32409500   -1.41682100
 C                 -3.04223100   -0.50007600    0.70299300
 C                 -3.29167700    1.27138300   -1.41588400
 H                 -1.59425700    0.27725300   -2.26303500
 C                 -4.06220600    0.44318800    0.70565600
 H                 -2.96278100   -1.20365900    1.52608900
 C                 -4.18795800    1.33726400   -0.35554700
 H                 -3.38758700    1.95544900   -2.25107200
 H                 -4.76327100    0.47614200    1.53142300
 H                 -4.98410200    2.07228000   -0.35812500
 C                  0.60957800    0.05892700    0.86108600
 H                 -0.12835300    0.81943900    0.59254400
 C                  0.28696700    1.05088800    2.97904200
 H                 -0.57786800    0.42494900    3.22624100
 H                  0.83122800    1.27478700    3.89465300
 H                 -0.06579800    1.98430900    2.52611600
 O                  1.18805700    0.38697200    2.11108900
```

Chapter 2: Magnesium amide base structures

Optimised Coordinates for Magnesium Amides

Structure A

```
0 1
 C                  0.55623000   -3.06125200   -1.00609600
 C                  2.41698800   -1.04566400   -0.42699800
 C                  1.33132800   -2.96908800    0.31339600
 H                 -0.39406300   -3.57931800   -0.82474500
 H                  1.15562000   -3.71500800   -1.66709500
 H                  3.41924000   -0.65593700   -0.62068500
 H                  1.53913200   -3.96856100    0.70523300
 N                  0.32421500   -1.75646700   -1.60454600
 O                  2.60574500   -2.37072100    0.06645300
 C                  0.63644900   -2.17468800    1.41982200
 H                 -0.35542000   -2.59347500    1.62126300
 H                  1.23111600   -2.27755900    2.33888000
 C                  1.80689900   -0.18875400    0.70982200
 H                  2.48946800   -0.30908000    1.56764800
 C                  1.81527500    1.27921100    0.32481100
 C                  0.68383900    2.01872500   -0.02095300
 C                  3.06102000    1.91264500    0.26553300
 C                  0.79591800    3.34538100   -0.43386000
 H                 -0.31173200    1.59452700    0.05353400
 C                  3.17730300    3.23447800   -0.14550500
 H                  3.95229500    1.36157700    0.54962100
 C                  2.04129200    3.95696000   -0.50256300
 H                 -0.09897700    3.89851500   -0.69450800
 H                  4.15432700    3.70176100   -0.18354800
 H                  2.12700600    4.98835100   -0.82285900
 N                  0.48219300   -0.72066600    1.12296400
 C                  0.01993400   -0.06507300    2.35874400
 H                  0.75935800   -0.18921500    3.16064800
 H                 -0.14716200    0.99733400    2.19349000
 H                 -0.92141900   -0.52039500    2.67152600
 C                  1.61425500   -1.09663200   -1.73749300
 H                  2.26490800   -1.62977300   -2.45582900
 H                  1.49107600   -0.07730300   -2.12189400
 Mg                -1.01117300   -0.69981100   -0.54846000
 C                 -2.68169400    0.55727000   -0.14976100
 H                 -2.53066400    1.00527100    0.84584600
 H                 -2.61937100    1.40520300   -0.85065900
 C                 -4.10328900   -0.01727500   -0.21478300
 H                 -4.28127500   -0.48049800   -1.19441200
 H                 -4.21920300   -0.82760000    0.51763400
 C                 -5.21529000    1.00759500    0.03224400
 H                 -5.12072000    1.81179400   -0.70648000
 H                 -5.05794600    1.47053100    1.01336900
 C                 -6.61603500    0.40184500   -0.03716500
 H                 -7.39324800    1.15145300    0.12931800
 H                 -6.79287900   -0.05234800   -1.01647200
 H                 -6.73873500   -0.38094200    0.71698100
```

Structure B

```
0 1
 C                -2.75274600   -2.01246000    0.17715800
 C                -2.49197700    0.79813500    0.37469300
 C                -3.29769900   -1.02345600   -0.85358800
 H                -2.45852800   -2.94661000   -0.31095100
 H                -3.55089700   -2.23942000    0.89975800
 H                -2.86037100    1.69595200    0.87404400
 H                -4.23114600   -1.43131500   -1.25015100
 O                -3.65638300    0.18501200   -0.17912800
 C                -2.33934400   -0.68154400   -2.00075200
 H                -2.07490700   -1.60511800   -2.53037900
 H                -2.92033200   -0.06180000   -2.70845300
 C                -1.52948900    1.17155300   -0.78323900
 H                -2.13000800    1.86018400   -1.41189100
 C                -0.31424800    1.95704400   -0.29791600
 C                 0.92229400    1.79160500   -0.92880300
 C                -0.39212600    2.87411600    0.75790200
 C                 2.04703300    2.50066600   -0.51091800
 H                 0.98783200    1.11303900   -1.77113000
 C                 0.72781500    3.58523600    1.17574100
 H                -1.33306100    3.04921000    1.26642400
 C                 1.95617200    3.39833200    0.54601900
 H                 2.99387700    2.35243700   -1.01820900
 H                 0.64000100    4.28801500    1.99642300
 H                 2.82904000    3.95084600    0.87359700
 N                -1.13631400    0.00352300   -1.55728300
 C                -1.91679100   -0.13390000    1.44544900
 H                -2.67033300   -0.24681400    2.23890300
 H                -1.01603600    0.29658800    1.89511700
 Mg                0.11145100   -1.15941800   -0.46714900
 C                 1.97988500   -1.69380800    0.40240300
 H                 2.02475800   -1.14435200    1.35700900
 H                 1.98280800   -2.75672200    0.68707700
 C                 3.25352300   -1.38585500   -0.39543800
 H                 3.25933200   -1.95589400   -1.33444200
 H                 3.26428100   -0.32842900   -0.69405600
 C                 4.56136500   -1.68111600    0.34651500
 H                 4.56801800   -2.73628600    0.64413700
 H                 4.57725400   -1.09899100    1.27512600
 C                 5.80600900   -1.36874400   -0.48254300
 H                 6.72640300   -1.58542200    0.06489300
 H                 5.81696900   -1.95993400   -1.40286100
 H                 5.82656100   -0.31286300   -0.76813100
 N                -1.58185900   -1.47359700    0.90667100
 C                -1.21429600   -2.37294400    2.00609700
 H                -0.96723500   -3.35727000    1.60365500
 H                -0.33723700   -1.97616000    2.52063400
 H                -2.03845900   -2.47658900    2.72426800
```

Structure D

```
0 1
 C                  1.51782100    2.75991400    0.47603800
 C                  0.50933000    0.61840700   -1.08591600
 C                  0.22720400    2.02411000    0.78564400
 H                  1.95822200    3.10417400    1.41703600
 H                  1.30249400    3.64642500   -0.14860600
 H                  0.03238400    0.38847200   -2.04052800
 H                 -0.49748000    2.72399300    1.20731200
 O                 -0.38218600    1.56710700   -0.44944500
 C                  0.43041800    0.77127700    1.70222100
 H                  1.50804900    0.65591700    1.87301600
 H                 -0.03486500    0.96082100    2.67421100
 C                  0.50178500   -0.68539200   -0.16658100
 H                 -0.11910900   -1.40840900   -0.71379300
 C                  1.85983100   -1.37770000   -0.06145500
 C                  2.41350800   -1.71987400    1.17098600
 C                  2.53148000   -1.77676500   -1.22159200
 C                  3.63279500   -2.39039100    1.24383000
 H                  1.86806900   -1.47085800    2.07256700
 C                  3.74703300   -2.44945400   -1.15572400
 H                  2.09040500   -1.57308700   -2.19378500
 C                  4.31001200   -2.74929100    0.08259500
 H                  4.05094800   -2.63990800    2.21279100
 H                  4.24957200   -2.74827800   -2.06879700
 H                  5.25759200   -3.27224400    0.14034500
 N                 -0.17661900   -0.41041800    1.09453500
 C                  1.82124400    1.33147100   -1.39037500
 H                  1.59547900    2.14816300   -2.10275700
 H                  2.51462100    0.64776300   -1.88042400
 Mg                -1.99195600    0.27131200    0.44493000
 C                 -4.04470900    0.63116700    0.02772500
 H                 -4.44510100    1.34255400    0.76369100
 H                 -4.11298400    1.14900800   -0.93956400
 C                 -4.95294500   -0.60720800   -0.00821900
 H                 -4.57819500   -1.33325400   -0.74230200
 H                 -4.92238400   -1.12840200    0.95794900
 C                 -6.41912600   -0.31454100   -0.34297500
 H                 -6.46558600    0.19224800   -1.31381200
 H                 -6.81588600    0.39375900    0.39334600
 C                 -7.28572700   -1.57259300   -0.37357800
 H                 -8.32689200   -1.34549500   -0.61455800
 H                 -6.91512200   -2.27978000   -1.12134400
 H                 -7.26863400   -2.07870600    0.59585600
 N                  2.44330800    1.85681500   -0.18765000
 C                  3.70659700    2.50560000   -0.48799700
 H                  4.15243400    2.88419700    0.43389200
 H                  4.39290900    1.78188200   -0.93257300
 H                  3.58388400    3.34925500   -1.18874200
```

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Chapter 2 Appendix: X-ray Crystallography Data for 55a and 55b

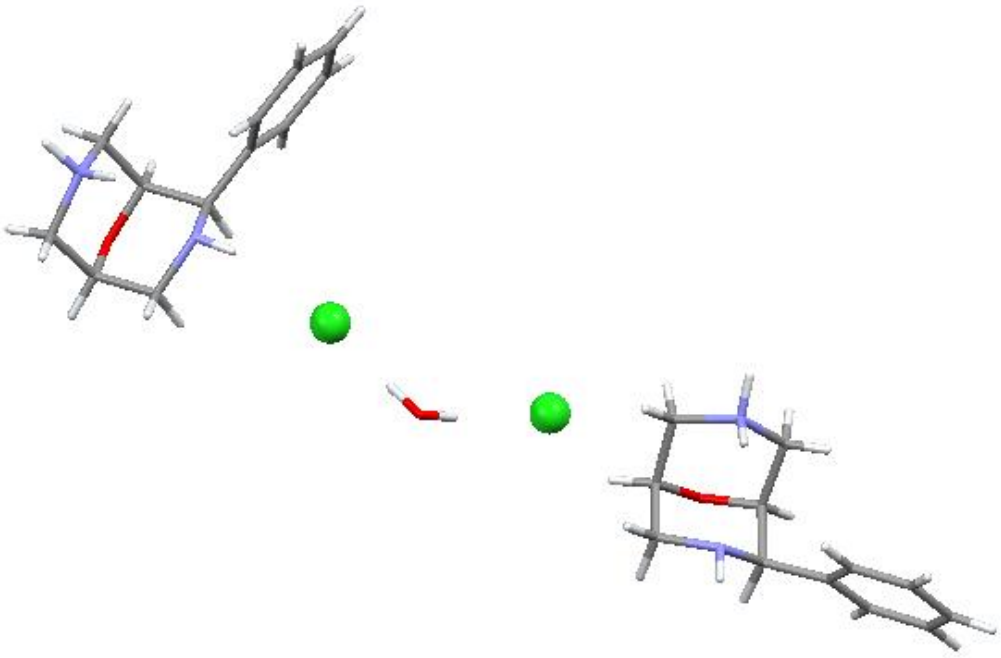

Figure 2.11: X-ray crystal structure of precipitate. Depicts a mixture of mono-HCl salts **55a** and **55b** in addition to a single water molecule.

Table 1. Crystal data and structure refinement for kerrmay2012lp.

Identification code	kerrmay2012lp	
Empirical formula	C12 H18 Cl N2 O1.50	
Formula weight	249.73	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.3808(2) Å	α= 90°.
	b = 13.9143(2) Å	β= 90°.
	c = 17.1550(3) Å	γ = 90°.
Volume	2477.90(7) $Å^3$	
Z	8	
Density (calculated)	1.339 Mg/m^3	
Absorption coefficient	0.295 mm^{-1}	
F(000)	1064	
Crystal size	0.30 x 0.12 x 0.10 mm^3	
Theta range for data collection	3.08 to 29.83°.	
Index ranges	-14<=h<=14, -18<=k<=19, -22<=l<=23	
Reflections collected	12376	

Independent reflections	6266 [R(int) = 0.0244]
Completeness to theta = 27.00°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.98175
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6266 / 0 / 331
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0364, wR2 = 0.0711
R indices (all data)	R1 = 0.0432, wR2 = 0.0743
Absolute structure parameter	0.01(4)
Largest diff. peak and hole	0.278 and -0.220 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for kerrmay2012lp. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	2966(1)	4013(1)	8498(1)	20(1)
Cl(2)	2292(1)	7584(1)	8282(1)	25(1)
O(1)	5755(1)	625(1)	8395(1)	16(1)
N(1)	3405(2)	-408(1)	8273(1)	20(1)
N(2)	3356(1)	1607(1)	8291(1)	14(1)
C(1)	4277(2)	1607(1)	7642(1)	15(1)
C(2)	5045(2)	666(1)	7672(1)	15(1)
C(3)	4270(2)	-255(1)	7590(1)	19(1)
C(4)	4108(2)	-318(1)	9027(1)	20(1)
C(5)	4875(2)	616(1)	9046(1)	16(1)
C(6)	4050(2)	1524(1)	9037(1)	16(1)
C(7)	3604(2)	1751(1)	6865(1)	15(1)
C(8)	4304(2)	2115(1)	6236(1)	22(1)
C(9)	3706(2)	2269(1)	5521(1)	24(1)
C(10)	2418(2)	2064(1)	5423(1)	23(1)
C(11)	1715(2)	1690(1)	6038(1)	22(1)
C(12)	2313(2)	1543(1)	6755(1)	18(1)
O(2)	799(1)	10086(1)	8620(1)	23(1)
N(4)	-1397(2)	10577(1)	9522(1)	19(1)
N(3)	-1727(2)	9922(1)	7988(1)	18(1)
C(13)	-505(2)	11312(1)	9231(1)	17(1)

C(14)	74(2)	10945(1)	8468(1)	18(1)
C(15)	-881(2)	10759(1)	7811(1)	19(1)
C(16)	-987(2)	9066(1)	8264(1)	22(1)
C(17)	-54(2)	9344(1)	8911(1)	23(1)
C(18)	-688(2)	9677(1)	9660(1)	25(1)
C(19)	-1119(2)	12293(1)	9135(1)	16(1)
C(20)	-2446(2)	12420(1)	9143(1)	18(1)
C(21)	-2969(2)	13337(1)	9076(1)	21(1)
C(22)	-2171(2)	14130(1)	9008(1)	24(1)
C(23)	-852(2)	14007(1)	8980(1)	25(1)
C(24)	-325(2)	13093(1)	9043(1)	22(1)
O(1W)	1428(2)	5763(1)	9304(1)	34(1)

Table 3. Bond lengths [Å] and angles [°] for kerrmay2012lp.

O(1)-C(5)	1.443(2)
O(1)-C(2)	1.4449(19)
N(1)-C(4)	1.491(2)
N(1)-C(3)	1.491(2)
N(1)-H(2N)	0.85(2)
N(1)-H(1N)	1.05(2)
N(2)-C(1)	1.468(2)
N(2)-C(6)	1.473(2)
N(2)-H(3N)	0.874(18)
C(1)-C(7)	1.518(2)
C(1)-C(2)	1.534(2)
C(1)-H(1)	1.0000
C(2)-C(3)	1.519(2)
C(2)-H(2)	1.0000
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.524(2)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.526(2)
C(5)-H(5)	1.0000
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(12)	1.384(2)
C(7)-C(8)	1.397(2)
C(8)-C(9)	1.391(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.377(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.385(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.393(2)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
O(2)-C(14)	1.436(2)
O(2)-C(17)	1.448(2)

N(4)-C(13)	1.467(2)
N(4)-C(18)	1.472(2)
N(4)-H(6N)	0.86(2)
N(3)-C(15)	1.490(2)
N(3)-C(16)	1.495(2)
N(3)-H(4N)	0.91(2)
N(3)-H(5N)	0.95(2)
C(13)-C(19)	1.516(2)
C(13)-C(14)	1.529(2)
C(13)-H(13)	1.0000
C(14)-C(15)	1.523(2)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.523(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.515(3)
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.389(2)
C(19)-C(24)	1.394(2)
C(20)-C(21)	1.391(2)
C(20)-H(20)	0.9500
C(21)-C(22)	1.384(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.381(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.389(3)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
O(1W)-H(1W)	1.05(3)
O(1W)-H(2W)	0.86(3)

C(5)-O(1)-C(2)	110.00(12)
C(4)-N(1)-C(3)	112.06(14)
C(4)-N(1)-H(2N)	109.4(13)

C(3)-N(1)-H(2N)	107.9(13)
C(4)-N(1)-H(1N)	108.6(13)
C(3)-N(1)-H(1N)	109.2(13)
H(2N)-N(1)-H(1N)	109.6(18)
C(1)-N(2)-C(6)	109.90(13)
C(1)-N(2)-H(3N)	106.5(12)
C(6)-N(2)-H(3N)	106.0(13)
N(2)-C(1)-C(7)	111.50(14)
N(2)-C(1)-C(2)	108.29(13)
C(7)-C(1)-C(2)	112.42(13)
N(2)-C(1)-H(1)	108.2
C(7)-C(1)-H(1)	108.2
C(2)-C(1)-H(1)	108.2
O(1)-C(2)-C(3)	108.49(13)
O(1)-C(2)-C(1)	109.12(13)
C(3)-C(2)-C(1)	116.15(14)
O(1)-C(2)-H(2)	107.6
C(3)-C(2)-H(2)	107.6
C(1)-C(2)-H(2)	107.6
N(1)-C(3)-C(2)	111.50(14)
N(1)-C(3)-H(3A)	109.3
C(2)-C(3)-H(3A)	109.3
N(1)-C(3)-H(3B)	109.3
C(2)-C(3)-H(3B)	109.3
H(3A)-C(3)-H(3B)	108.0
N(1)-C(4)-C(5)	110.25(14)
N(1)-C(4)-H(4A)	109.6
C(5)-C(4)-H(4A)	109.6
N(1)-C(4)-H(4B)	109.6
C(5)-C(4)-H(4B)	109.6
H(4A)-C(4)-H(4B)	108.1
O(1)-C(5)-C(4)	108.74(14)
O(1)-C(5)-C(6)	109.86(13)
C(4)-C(5)-C(6)	114.36(15)
O(1)-C(5)-H(5)	107.9
C(4)-C(5)-H(5)	107.9
C(6)-C(5)-H(5)	107.9
N(2)-C(6)-C(5)	110.44(13)

N(2)-C(6)-H(6A)	109.6
C(5)-C(6)-H(6A)	109.6
N(2)-C(6)-H(6B)	109.6
C(5)-C(6)-H(6B)	109.6
H(6A)-C(6)-H(6B)	108.1
C(12)-C(7)-C(8)	118.34(16)
C(12)-C(7)-C(1)	122.50(16)
C(8)-C(7)-C(1)	119.15(16)
C(9)-C(8)-C(7)	120.32(18)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(10)-C(9)-C(8)	120.59(18)
C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7
C(9)-C(10)-C(11)	119.79(18)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-H(10)	120.1
C(10)-C(11)-C(12)	119.55(18)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(7)-C(12)-C(11)	121.41(17)
C(7)-C(12)-H(12)	119.3
C(11)-C(12)-H(12)	119.3
C(14)-O(2)-C(17)	109.63(13)
C(13)-N(4)-C(18)	109.34(15)
C(13)-N(4)-H(6N)	110.1(14)
C(18)-N(4)-H(6N)	109.3(14)
C(15)-N(3)-C(16)	112.59(14)
C(15)-N(3)-H(4N)	109.0(12)
C(16)-N(3)-H(4N)	108.8(13)
C(15)-N(3)-H(5N)	111.2(13)
C(16)-N(3)-H(5N)	105.4(13)
H(4N)-N(3)-H(5N)	109.7(18)
N(4)-C(13)-C(19)	113.51(14)
N(4)-C(13)-C(14)	107.91(14)
C(19)-C(13)-C(14)	111.88(14)
N(4)-C(13)-H(13)	107.8
C(19)-C(13)-H(13)	107.8

C(14)-C(13)-H(13)	107.8
O(2)-C(14)-C(15)	109.56(14)
O(2)-C(14)-C(13)	109.11(14)
C(15)-C(14)-C(13)	115.75(14)
O(2)-C(14)-H(14)	107.4
C(15)-C(14)-H(14)	107.4
C(13)-C(14)-H(14)	107.4
N(3)-C(15)-C(14)	111.43(14)
N(3)-C(15)-H(15A)	109.3
C(14)-C(15)-H(15A)	109.3
N(3)-C(15)-H(15B)	109.3
C(14)-C(15)-H(15B)	109.3
H(15A)-C(15)-H(15B)	108.0
N(3)-C(16)-C(17)	110.84(14)
N(3)-C(16)-H(16A)	109.5
C(17)-C(16)-H(16A)	109.5
N(3)-C(16)-H(16B)	109.5
C(17)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	108.1
O(2)-C(17)-C(18)	109.84(15)
O(2)-C(17)-C(16)	108.56(14)
C(18)-C(17)-C(16)	114.79(16)
O(2)-C(17)-H(17)	107.8
C(18)-C(17)-H(17)	107.8
C(16)-C(17)-H(17)	107.8
N(4)-C(18)-C(17)	109.97(15)
N(4)-C(18)-H(18A)	109.7
C(17)-C(18)-H(18A)	109.7
N(4)-C(18)-H(18B)	109.7
C(17)-C(18)-H(18B)	109.7
H(18A)-C(18)-H(18B)	108.2
C(20)-C(19)-C(24)	119.06(17)
C(20)-C(19)-C(13)	122.05(15)
C(24)-C(19)-C(13)	118.89(16)
C(19)-C(20)-C(21)	120.20(16)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(22)-C(21)-C(20)	120.26(19)

C(22)-C(21)-H(21)	119.9
C(20)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	119.88(18)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	120.07(18)
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
C(23)-C(24)-C(19)	120.48(18)
C(23)-C(24)-H(24)	119.8
C(19)-C(24)-H(24)	119.8
H(1W)-O(1W)-H(2W)	100(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for kerrmay2012lp. 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}
Cl(1)	24(1)	17(1)	19(1)	2(1)	1(1)	0(1)
Cl(2)	29(1)	16(1)	30(1)	-4(1)	-2(1)	-5(1)
O(1)	12(1)	21(1)	15(1)	-2(1)	-1(1)	0(1)
N(1)	14(1)	14(1)	31(1)	-2(1)	1(1)	0(1)
N(2)	16(1)	13(1)	14(1)	0(1)	2(1)	4(1)
C(1)	15(1)	14(1)	15(1)	-1(1)	1(1)	-2(1)
C(2)	14(1)	19(1)	13(1)	-2(1)	1(1)	0(1)
C(3)	18(1)	17(1)	21(1)	-5(1)	-1(1)	4(1)
C(4)	22(1)	16(1)	23(1)	3(1)	3(1)	0(1)
C(5)	17(1)	19(1)	14(1)	0(1)	0(1)	-1(1)
C(6)	19(1)	15(1)	15(1)	-2(1)	3(1)	-1(1)
C(7)	19(1)	12(1)	14(1)	0(1)	0(1)	0(1)
C(8)	20(1)	24(1)	21(1)	1(1)	2(1)	-3(1)
C(9)	33(1)	23(1)	18(1)	3(1)	4(1)	-1(1)
C(10)	32(1)	16(1)	19(1)	-1(1)	-6(1)	3(1)
C(11)	23(1)	18(1)	26(1)	-1(1)	-6(1)	-2(1)
C(12)	21(1)	16(1)	18(1)	1(1)	2(1)	-1(1)
O(2)	14(1)	26(1)	29(1)	-1(1)	1(1)	5(1)
N(4)	22(1)	19(1)	15(1)	1(1)	6(1)	3(1)
N(3)	17(1)	21(1)	17(1)	-4(1)	0(1)	1(1)
C(13)	15(1)	22(1)	15(1)	-2(1)	-2(1)	0(1)
C(14)	14(1)	20(1)	21(1)	-1(1)	2(1)	1(1)
C(15)	23(1)	20(1)	14(1)	0(1)	2(1)	1(1)
C(16)	25(1)	16(1)	25(1)	-1(1)	3(1)	2(1)
C(17)	25(1)	21(1)	22(1)	4(1)	-1(1)	9(1)
C(18)	29(1)	24(1)	21(1)	4(1)	0(1)	4(1)
C(19)	19(1)	19(1)	11(1)	-4(1)	1(1)	-3(1)
C(20)	20(1)	16(1)	16(1)	-1(1)	-1(1)	-4(1)
C(21)	21(1)	22(1)	20(1)	-1(1)	-3(1)	1(1)
C(22)	38(1)	18(1)	18(1)	2(1)	-8(1)	-3(1)
C(23)	37(1)	22(1)	16(1)	4(1)	-2(1)	-16(1)
C(24)	20(1)	30(1)	14(1)	-1(1)	1(1)	-8(1)
O(1W)	33(1)	25(1)	44(1)	0(1)	7(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for kerrmay2012lp.

	x	y	z	U(eq)
H(1)	4890	2152	7721	18
H(2)	5686	681	7237	18
H(3A)	3745	-223	7108	22
H(3B)	4865	-807	7541	22
H(4A)	4699	-870	9092	24
H(4B)	3484	-326	9464	24
H(5)	5397	621	9536	20
H(6A)	3423	1502	9471	19
H(6B)	4606	2094	9111	19
H(8)	5193	2259	6296	26
H(9)	4190	2518	5096	29
H(10)	2013	2179	4935	27
H(11)	830	1536	5972	27
H(12)	1824	1293	7177	22
H(13)	211	11375	9618	21
H(14)	695	11443	8279	22
H(15A)	-1419	11338	7731	23
H(15B)	-403	10635	7321	23
H(16A)	-500	8786	7822	26
H(16B)	-1593	8573	8459	26
H(17)	482	8767	9036	27
H(18A)	-1288	9176	9849	30
H(18B)	-23	9781	10064	30
H(20)	-2998	11879	9194	21
H(21)	-3877	13420	9077	25
H(22)	-2530	14757	8981	29
H(23)	-304	14549	8918	30
H(24)	583	13013	9023	26
H(3N)	2995(18)	2175(13)	8294(11)	21(5)
H(2N)	2809(19)	14(13)	8253(11)	19(5)
H(1N)	3000(20)	-1100(18)	8240(14)	56(7)
H(4N)	-2300(20)	10094(14)	8361(12)	27(5)

H(6N)	-1740(20)	10764(14)	9949(12)	27(6)
H(5N)	-2170(20)	9714(14)	7538(13)	36(6)
H(1W)	1990(30)	5220(20)	9058(18)	96(11)
H(2W)	1720(30)	6260(20)	9059(17)	68(10)

Table 6. Torsion angles [°] for kerrmay2012lp.

C(6)-N(2)-C(1)-C(7)	-176.64(13)
C(6)-N(2)-C(1)-C(2)	59.17(16)
C(5)-O(1)-C(2)-C(3)	-64.78(16)
C(5)-O(1)-C(2)-C(1)	62.65(15)
N(2)-C(1)-C(2)-O(1)	-61.92(17)
C(7)-C(1)-C(2)-O(1)	174.44(13)
N(2)-C(1)-C(2)-C(3)	61.04(18)
C(7)-C(1)-C(2)-C(3)	-62.60(19)
C(4)-N(1)-C(3)-C(2)	-50.52(18)
O(1)-C(2)-C(3)-N(1)	56.28(18)
C(1)-C(2)-C(3)-N(1)	-67.01(18)
C(3)-N(1)-C(4)-C(5)	50.85(19)
C(2)-O(1)-C(5)-C(4)	66.01(16)
C(2)-O(1)-C(5)-C(6)	-59.83(16)
N(1)-C(4)-C(5)-O(1)	-57.89(18)
N(1)-C(4)-C(5)-C(6)	65.30(18)
C(1)-N(2)-C(6)-C(5)	-57.26(17)
O(1)-C(5)-C(6)-N(2)	56.88(18)
C(4)-C(5)-C(6)-N(2)	-65.71(18)
N(2)-C(1)-C(7)-C(12)	-22.7(2)
C(2)-C(1)-C(7)-C(12)	99.17(19)
N(2)-C(1)-C(7)-C(8)	156.76(15)
C(2)-C(1)-C(7)-C(8)	-81.41(19)
C(12)-C(7)-C(8)-C(9)	0.5(3)
C(1)-C(7)-C(8)-C(9)	-178.95(16)
C(7)-C(8)-C(9)-C(10)	0.0(3)
C(8)-C(9)-C(10)-C(11)	-0.8(3)
C(9)-C(10)-C(11)-C(12)	1.2(3)
C(8)-C(7)-C(12)-C(11)	-0.1(2)
C(1)-C(7)-C(12)-C(11)	179.34(15)
C(10)-C(11)-C(12)-C(7)	-0.8(3)
C(18)-N(4)-C(13)-C(19)	-175.15(14)
C(18)-N(4)-C(13)-C(14)	60.27(18)
C(17)-O(2)-C(14)-C(15)	-64.92(17)
C(17)-O(2)-C(14)-C(13)	62.75(17)
N(4)-C(13)-C(14)-O(2)	-62.75(18)

C(19)-C(13)-C(14)-O(2)	171.69(14)
N(4)-C(13)-C(14)-C(15)	61.34(19)
C(19)-C(13)-C(14)-C(15)	-64.22(19)
C(16)-N(3)-C(15)-C(14)	-48.04(19)
O(2)-C(14)-C(15)-N(3)	55.15(18)
C(13)-C(14)-C(15)-N(3)	-68.70(19)
C(15)-N(3)-C(16)-C(17)	49.4(2)
C(14)-O(2)-C(17)-C(18)	-60.15(18)
C(14)-O(2)-C(17)-C(16)	66.11(17)
N(3)-C(16)-C(17)-O(2)	-57.50(19)
N(3)-C(16)-C(17)-C(18)	65.8(2)
C(13)-N(4)-C(18)-C(17)	-58.5(2)
O(2)-C(17)-C(18)-N(4)	57.8(2)
C(16)-C(17)-C(18)-N(4)	-64.9(2)
N(4)-C(13)-C(19)-C(20)	-14.4(2)
C(14)-C(13)-C(19)-C(20)	108.02(18)
N(4)-C(13)-C(19)-C(24)	165.00(15)
C(14)-C(13)-C(19)-C(24)	-72.6(2)
C(24)-C(19)-C(20)-C(21)	-1.3(2)
C(13)-C(19)-C(20)-C(21)	178.07(15)
C(19)-C(20)-C(21)-C(22)	-0.6(2)
C(20)-C(21)-C(22)-C(23)	2.2(3)
C(21)-C(22)-C(23)-C(24)	-1.9(3)
C(22)-C(23)-C(24)-C(19)	0.0(3)
C(20)-C(19)-C(24)-C(23)	1.7(2)
C(13)-C(19)-C(24)-C(23)	-177.75(15)

Symmetry transformations used to generate equivalent atoms: