Table 1. Crystal data and structure refinement for eva12.

Identification code eva12

Empirical formula C28 H56 N3 Na O Si Zn

Formula weight 567.21

Temperature 123(2) K

Wavelength 0.71073 Å

Crystal system Orthorhombic

Space group Pna21

Unit cell dimensions a = 22.0991(9) Å = 90°.

b = 10.3628(4) Å = 90°.

c = 14.3036(7) Å  = 90°.

Volume 3275.6(2) Å3

Z 4

Density (calculated) 1.150 Mg/m3

Absorption coefficient 0.822 mm-1

F(000) 1232

Crystal size 0.2 x 0.12 x 0.10 mm3

Theta range for data collection 2.43 to 27.49°.

Index ranges -26<=h<=28, -13<=k<=10, -18<=l<=12

Reflections collected 16094

Independent reflections 6089 [R(int) = 0.0648]

Completeness to theta = 26.00° 99.9 %

Absorption correction None

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 6089 / 1 / 330

Goodness-of-fit on F2 0.870

Final R indices [I>2sigma(I)] R1 = 0.0471, wR2 = 0.0910

R indices (all data) R1 = 0.0849, wR2 = 0.0974

Absolute structure parameter 0.037(16)

Largest diff. peak and hole 1.226 and -0.458 e.Å-3

Table 2. Atomic coordinates ( x 104) and equivalent isotropic displacement parameters (Å2x 103)

for eva12. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Zn(1) 9902(1) 9052(1) 7569(1) 28(1)

Na(1) 8930(1) 6717(1) 7611(2) 35(1)

Si(1) 8508(1) 9538(1) 6679(1) 28(1)

O(1) 8402(1) 7941(3) 6459(2) 29(1)

N(1) 10013(1) 7117(3) 7607(4) 29(1)

N(2) 8424(2) 4495(4) 7400(4) 49(1)

N(3) 8163(2) 6496(4) 8953(3) 44(1)

C(1) 10274(3) 6670(6) 8516(4) 32(1)

C(2) 10966(3) 6706(6) 8512(4) 48(2)

C(3) 11219(2) 5986(5) 7676(5) 54(2)

C(4) 10973(3) 6596(6) 6780(5) 45(2)

C(5) 10294(3) 6593(5) 6755(4) 30(1)

C(6) 10047(3) 7589(7) 9252(4) 42(2)

C(7) 10040(3) 5322(6) 8816(5) 51(2)

C(8) 10086(2) 7430(6) 5928(4) 37(2)

C(9) 10078(3) 5215(6) 6513(4) 43(2)

C(10) 10499(2) 10552(4) 7490(4) 31(1)

C(11) 11169(2) 10243(4) 7534(6) 59(1)

C(12) 10384(3) 11295(6) 6602(5) 58(2)

C(13) 10363(3) 11475(6) 8320(4) 48(2)

C(14) 8995(2) 9579(4) 7668(4) 34(1)

C(15) 8837(2) 10283(4) 5627(3) 38(1)

C(16) 7738(2) 10224(5) 6817(3) 36(1)

C(17) 8051(2) 7454(4) 5735(3) 27(1)

C(18) 8307(2) 7153(5) 4895(4) 34(1)

C(19) 7961(2) 6607(5) 4205(4) 42(1)

C(20) 7355(2) 6369(5) 4359(4) 44(1)

C(21) 7096(2) 6704(5) 5194(4) 40(1)

C(22) 7435(2) 7263(4) 5882(4) 34(1)

C(23) 8282(3) 4212(5) 6434(4) 63(2)

C(24) 8796(2) 3424(4) 7766(5) 63(2)

C(25) 7877(3) 4618(5) 7940(4) 59(2)

C(26) 7960(3) 5139(5) 8932(4) 59(2)

C(27) 7647(2) 7347(6) 8760(4) 56(2)

C(28) 8384(3) 6815(7) 9873(4) 65(2)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_Table 3. Bond lengths [Å] and angles [°] for eva12.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Zn(1)-N(1) 2.021(3)

Zn(1)-C(10) 2.041(4)

Zn(1)-C(14) 2.083(4)

Zn(1)-Na(1) 3.2377(15)

Na(1)-O(1) 2.385(4)

Na(1)-N(1) 2.430(3)

Na(1)-N(3) 2.571(5)

Na(1)-N(2) 2.577(4)

Na(1)-C(14) 2.971(4)

Na(1)-Si(1) 3.346(2)

Si(1)-O(1) 1.701(3)

Si(1)-C(14) 1.778(5)

Si(1)-C(15) 1.842(5)

Si(1)-C(16) 1.855(4)

O(1)-C(17) 1.388(5)

N(1)-C(5) 1.471(7)

N(1)-C(1) 1.496(7)

N(2)-C(25) 1.439(7)

N(2)-C(23) 1.447(7)

N(2)-C(24) 1.477(6)

N(3)-C(28) 1.441(7)

N(3)-C(27) 1.468(6)

N(3)-C(26) 1.476(7)

C(1)-C(6) 1.506(8)

C(1)-C(2) 1.530(8)

C(1)-C(7) 1.550(9)

C(2)-C(3) 1.517(9)

C(2)-H(2A) 0.9900

C(2)-H(2B) 0.9900

C(3)-C(4) 1.530(9)

C(3)-H(3A) 0.9900

C(3)-H(3B) 0.9900

C(4)-C(5) 1.502(8)

C(4)-H(4A) 0.9900

C(4)-H(4B) 0.9900

C(5)-C(8) 1.537(8)

C(5)-C(9) 1.545(8)

C(6)-H(6A) 0.9800

C(6)-H(6B) 0.9800

C(6)-H(6C) 0.9800

C(7)-H(7A) 0.9800

C(7)-H(7B) 0.9800

C(7)-H(7C) 0.9800

C(8)-H(8A) 0.9800

C(8)-H(8B) 0.9800

C(8)-H(8C) 0.9800

C(9)-H(9A) 0.9800

C(9)-H(9B) 0.9800

C(9)-H(9C) 0.9800

C(10)-C(12) 1.508(8)

C(10)-C(11) 1.516(5)

C(10)-C(13) 1.554(8)

C(11)-H(11A) 0.9800

C(11)-H(11B) 0.9800

C(11)-H(11C) 0.9800

C(12)-H(12A) 0.9800

C(12)-H(12B) 0.9800

C(12)-H(12C) 0.9800

C(13)-H(13A) 0.9800

C(13)-H(13B) 0.9800

C(13)-H(13C) 0.9800

C(14)-H(14A) 0.9900

C(14)-H(14B) 0.9900

C(15)-H(15A) 0.9800

C(15)-H(15B) 0.9800

C(15)-H(15C) 0.9800

C(16)-H(16A) 0.9800

C(16)-H(16B) 0.9800

C(16)-H(16C) 0.9800

C(17)-C(18) 1.364(6)

C(17)-C(22) 1.392(6)

C(18)-C(19) 1.370(6)

C(18)-H(18) 0.9500

C(19)-C(20) 1.380(7)

C(19)-H(19) 0.9500

C(20)-C(21) 1.370(7)

C(20)-H(20) 0.9500

C(21)-C(22) 1.365(6)

C(21)-H(21) 0.9500

C(22)-H(22) 0.9500

C(23)-H(23A) 0.9800

C(23)-H(23B) 0.9800

C(23)-H(23C) 0.9800

C(24)-H(24A) 0.9800

C(24)-H(24B) 0.9800

C(24)-H(24C) 0.9800

C(25)-C(26) 1.529(8)

C(25)-H(25A) 0.9900

C(25)-H(25B) 0.9900

C(26)-H(26A) 0.9900

C(26)-H(26B) 0.9900

C(27)-H(27A) 0.9800

C(27)-H(27B) 0.9800

C(27)-H(27C) 0.9800

C(28)-H(28A) 0.9800

C(28)-H(28B) 0.9800

C(28)-H(28C) 0.9800

N(1)-Zn(1)-C(10) 132.74(14)

N(1)-Zn(1)-C(14) 112.01(14)

C(10)-Zn(1)-C(14) 115.23(16)

N(1)-Zn(1)-Na(1) 48.55(9)

C(10)-Zn(1)-Na(1) 177.51(17)

C(14)-Zn(1)-Na(1) 63.61(12)

O(1)-Na(1)-N(1) 112.94(15)

O(1)-Na(1)-N(3) 103.96(13)

N(1)-Na(1)-N(3) 131.75(19)

O(1)-Na(1)-N(2) 100.50(14)

N(1)-Na(1)-N(2) 125.43(13)

N(3)-Na(1)-N(2) 73.87(16)

O(1)-Na(1)-C(14) 60.77(12)

N(1)-Na(1)-C(14) 77.38(10)

N(3)-Na(1)-C(14) 95.75(15)

N(2)-Na(1)-C(14) 156.40(13)

O(1)-Na(1)-Zn(1) 85.10(8)

N(1)-Na(1)-Zn(1) 38.56(7)

N(3)-Na(1)-Zn(1) 121.16(13)

N(2)-Na(1)-Zn(1) 162.51(12)

C(14)-Na(1)-Zn(1) 38.90(7)

O(1)-Na(1)-Si(1) 28.77(7)

N(1)-Na(1)-Si(1) 97.14(10)

N(3)-Na(1)-Si(1) 101.05(11)

N(2)-Na(1)-Si(1) 127.83(12)

C(14)-Na(1)-Si(1) 32.01(10)

Zn(1)-Na(1)-Si(1) 61.60(4)

O(1)-Si(1)-C(14) 104.73(17)

O(1)-Si(1)-C(15) 108.13(19)

C(14)-Si(1)-C(15) 113.6(2)

O(1)-Si(1)-C(16) 105.44(18)

C(14)-Si(1)-C(16) 117.5(2)

C(15)-Si(1)-C(16) 106.8(2)

O(1)-Si(1)-Na(1) 42.44(11)

C(14)-Si(1)-Na(1) 62.31(14)

C(15)-Si(1)-Na(1) 125.58(16)

C(16)-Si(1)-Na(1) 123.25(16)

C(17)-O(1)-Si(1) 124.7(3)

C(17)-O(1)-Na(1) 126.5(3)

Si(1)-O(1)-Na(1) 108.79(15)

C(5)-N(1)-C(1) 116.2(3)

C(5)-N(1)-Zn(1) 113.3(3)

C(1)-N(1)-Zn(1) 112.2(3)

C(5)-N(1)-Na(1) 110.8(3)

C(1)-N(1)-Na(1) 109.0(3)

Zn(1)-N(1)-Na(1) 92.89(11)

C(25)-N(2)-C(23) 110.4(5)

C(25)-N(2)-C(24) 110.1(4)

C(23)-N(2)-C(24) 107.9(5)

C(25)-N(2)-Na(1) 102.8(3)

C(23)-N(2)-Na(1) 112.7(3)

C(24)-N(2)-Na(1) 112.8(3)

C(28)-N(3)-C(27) 107.3(5)

C(28)-N(3)-C(26) 109.9(5)

C(27)-N(3)-C(26) 109.4(4)

C(28)-N(3)-Na(1) 116.0(3)

C(27)-N(3)-Na(1) 108.5(3)

C(26)-N(3)-Na(1) 105.6(3)

N(1)-C(1)-C(6) 106.4(5)

N(1)-C(1)-C(2) 112.0(4)

C(6)-C(1)-C(2) 108.7(5)

N(1)-C(1)-C(7) 113.0(4)

C(6)-C(1)-C(7) 105.4(5)

C(2)-C(1)-C(7) 110.9(5)

C(3)-C(2)-C(1) 111.1(5)

C(3)-C(2)-H(2A) 109.4

C(1)-C(2)-H(2A) 109.4

C(3)-C(2)-H(2B) 109.4

C(1)-C(2)-H(2B) 109.4

H(2A)-C(2)-H(2B) 108.0

C(2)-C(3)-C(4) 109.0(4)

C(2)-C(3)-H(3A) 109.9

C(4)-C(3)-H(3A) 109.9

C(2)-C(3)-H(3B) 109.9

C(4)-C(3)-H(3B) 109.9

H(3A)-C(3)-H(3B) 108.3

C(5)-C(4)-C(3) 112.0(5)

C(5)-C(4)-H(4A) 109.2

C(3)-C(4)-H(4A) 109.2

C(5)-C(4)-H(4B) 109.2

C(3)-C(4)-H(4B) 109.2

H(4A)-C(4)-H(4B) 107.9

N(1)-C(5)-C(4) 113.7(5)

N(1)-C(5)-C(8) 107.6(4)

C(4)-C(5)-C(8) 108.4(5)

N(1)-C(5)-C(9) 113.4(4)

C(4)-C(5)-C(9) 108.4(5)

C(8)-C(5)-C(9) 104.9(5)

C(1)-C(6)-H(6A) 109.5

C(1)-C(6)-H(6B) 109.5

H(6A)-C(6)-H(6B) 109.5

C(1)-C(6)-H(6C) 109.5

H(6A)-C(6)-H(6C) 109.5

H(6B)-C(6)-H(6C) 109.5

C(1)-C(7)-H(7A) 109.5

C(1)-C(7)-H(7B) 109.5

H(7A)-C(7)-H(7B) 109.5

C(1)-C(7)-H(7C) 109.5

H(7A)-C(7)-H(7C) 109.5

H(7B)-C(7)-H(7C) 109.5

C(5)-C(8)-H(8A) 109.5

C(5)-C(8)-H(8B) 109.5

H(8A)-C(8)-H(8B) 109.5

C(5)-C(8)-H(8C) 109.5

H(8A)-C(8)-H(8C) 109.5

H(8B)-C(8)-H(8C) 109.5

C(5)-C(9)-H(9A) 109.5

C(5)-C(9)-H(9B) 109.5

H(9A)-C(9)-H(9B) 109.5

C(5)-C(9)-H(9C) 109.5

H(9A)-C(9)-H(9C) 109.5

H(9B)-C(9)-H(9C) 109.5

C(12)-C(10)-C(11) 107.9(5)

C(12)-C(10)-C(13) 107.2(4)

C(11)-C(10)-C(13) 106.7(5)

C(12)-C(10)-Zn(1) 109.1(4)

C(11)-C(10)-Zn(1) 117.9(3)

C(13)-C(10)-Zn(1) 107.5(4)

C(10)-C(11)-H(11A) 109.5

C(10)-C(11)-H(11B) 109.5

H(11A)-C(11)-H(11B) 109.5

C(10)-C(11)-H(11C) 109.5

H(11A)-C(11)-H(11C) 109.5

H(11B)-C(11)-H(11C) 109.5

C(10)-C(12)-H(12A) 109.5

C(10)-C(12)-H(12B) 109.5

H(12A)-C(12)-H(12B) 109.5

C(10)-C(12)-H(12C) 109.5

H(12A)-C(12)-H(12C) 109.5

H(12B)-C(12)-H(12C) 109.5

C(10)-C(13)-H(13A) 109.5

C(10)-C(13)-H(13B) 109.5

H(13A)-C(13)-H(13B) 109.5

C(10)-C(13)-H(13C) 109.5

H(13A)-C(13)-H(13C) 109.5

H(13B)-C(13)-H(13C) 109.5

Si(1)-C(14)-Zn(1) 121.5(3)

Si(1)-C(14)-Na(1) 85.68(17)

Zn(1)-C(14)-Na(1) 77.48(12)

Si(1)-C(14)-H(14A) 106.9

Zn(1)-C(14)-H(14A) 106.9

Na(1)-C(14)-H(14A) 54.2

Si(1)-C(14)-H(14B) 106.9

Zn(1)-C(14)-H(14B) 106.9

Na(1)-C(14)-H(14B) 160.3

H(14A)-C(14)-H(14B) 106.7

Si(1)-C(15)-H(15A) 109.5

Si(1)-C(15)-H(15B) 109.5

H(15A)-C(15)-H(15B) 109.5

Si(1)-C(15)-H(15C) 109.5

H(15A)-C(15)-H(15C) 109.5

H(15B)-C(15)-H(15C) 109.5

Si(1)-C(16)-H(16A) 109.5

Si(1)-C(16)-H(16B) 109.5

H(16A)-C(16)-H(16B) 109.5

Si(1)-C(16)-H(16C) 109.5

H(16A)-C(16)-H(16C) 109.5

H(16B)-C(16)-H(16C) 109.5

C(18)-C(17)-O(1) 120.6(4)

C(18)-C(17)-C(22) 120.4(5)

O(1)-C(17)-C(22) 119.0(4)

C(17)-C(18)-C(19) 119.9(5)

C(17)-C(18)-H(18) 120.1

C(19)-C(18)-H(18) 120.1

C(18)-C(19)-C(20) 120.0(5)

C(18)-C(19)-H(19) 120.0

C(20)-C(19)-H(19) 120.0

C(21)-C(20)-C(19) 119.9(5)

C(21)-C(20)-H(20) 120.0

C(19)-C(20)-H(20) 120.0

C(22)-C(21)-C(20) 120.5(5)

C(22)-C(21)-H(21) 119.7

C(20)-C(21)-H(21) 119.7

C(21)-C(22)-C(17) 119.2(5)

C(21)-C(22)-H(22) 120.4

C(17)-C(22)-H(22) 120.4

N(2)-C(23)-H(23A) 109.5

N(2)-C(23)-H(23B) 109.5

H(23A)-C(23)-H(23B) 109.5

N(2)-C(23)-H(23C) 109.5

H(23A)-C(23)-H(23C) 109.5

H(23B)-C(23)-H(23C) 109.5

N(2)-C(24)-H(24A) 109.5

N(2)-C(24)-H(24B) 109.5

H(24A)-C(24)-H(24B) 109.5

N(2)-C(24)-H(24C) 109.5

H(24A)-C(24)-H(24C) 109.5

H(24B)-C(24)-H(24C) 109.5

N(2)-C(25)-C(26) 115.4(5)

N(2)-C(25)-H(25A) 108.4

C(26)-C(25)-H(25A) 108.4

N(2)-C(25)-H(25B) 108.4

C(26)-C(25)-H(25B) 108.4

H(25A)-C(25)-H(25B) 107.5

N(3)-C(26)-C(25) 113.1(4)

N(3)-C(26)-H(26A) 109.0

C(25)-C(26)-H(26A) 109.0

N(3)-C(26)-H(26B) 109.0

C(25)-C(26)-H(26B) 109.0

H(26A)-C(26)-H(26B) 107.8

N(3)-C(27)-H(27A) 109.5

N(3)-C(27)-H(27B) 109.5

H(27A)-C(27)-H(27B) 109.5

N(3)-C(27)-H(27C) 109.5

H(27A)-C(27)-H(27C) 109.5

H(27B)-C(27)-H(27C) 109.5

N(3)-C(28)-H(28A) 109.5

N(3)-C(28)-H(28B) 109.5

H(28A)-C(28)-H(28B) 109.5

N(3)-C(28)-H(28C) 109.5

H(28A)-C(28)-H(28C) 109.5

H(28B)-C(28)-H(28C) 109.5

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103)for eva12. The anisotropic

displacement factor exponent takes the form: -22[ h2a\*2U11 + ... + 2 h k a\* b\* U12 ]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

U11 U22 U33 U23 U13 U12

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Zn(1) 32(1) 25(1) 29(1) -2(1) -2(1) 3(1)

Na(1) 35(1) 29(1) 40(1) 4(1) 0(1) 1(1)

Si(1) 33(1) 24(1) 29(1) 1(1) 0(1) 2(1)

O(1) 35(2) 24(2) 27(2) -3(1) 1(2) 3(1)

N(1) 43(2) 24(2) 21(2) -6(3) 4(3) 8(2)

N(2) 46(2) 26(2) 75(4) 8(3) 5(3) -2(2)

N(3) 43(3) 51(3) 38(3) 14(2) 3(2) -2(2)

C(1) 44(4) 29(3) 23(3) 3(3) -7(3) -2(3)

C(2) 50(4) 56(4) 37(4) 4(3) -4(3) 15(3)

C(3) 34(2) 59(3) 70(5) 16(4) -2(4) 14(3)

C(4) 40(3) 37(3) 59(4) -5(3) 15(3) 5(3)

C(5) 42(3) 27(3) 21(3) -3(3) 2(3) 6(3)

C(6) 55(4) 47(4) 25(4) -10(3) -1(3) -5(3)

C(7) 68(4) 37(4) 48(4) -2(3) -1(3) 0(3)

C(8) 41(3) 34(3) 36(4) -16(3) 6(3) 5(3)

C(9) 68(4) 31(3) 30(3) -17(3) 12(3) -1(3)

C(10) 38(2) 24(2) 31(3) -6(3) -3(3) 1(2)

C(11) 41(3) 41(3) 95(4) 8(5) 12(5) -6(2)

C(12) 78(5) 37(3) 57(4) 6(3) -13(4) -23(3)

C(13) 48(4) 35(3) 60(4) -6(3) -15(3) -5(3)

C(14) 38(2) 24(2) 40(3) -1(3) 1(3) 2(2)

C(15) 43(3) 36(3) 33(3) 3(2) -2(2) -1(2)

C(16) 33(3) 39(3) 35(3) 4(2) -4(2) -2(2)

C(17) 36(3) 19(2) 27(3) -8(2) -7(2) -2(2)

C(18) 40(3) 32(3) 30(3) -5(2) 7(3) -2(2)

C(19) 50(3) 40(3) 36(3) -10(3) 6(3) -1(3)

C(20) 58(4) 35(3) 38(3) -10(2) -11(3) -2(3)

C(21) 39(3) 40(3) 41(3) -8(3) 0(3) -7(3)

C(22) 41(3) 26(3) 35(3) -7(2) 0(3) -2(2)

C(23) 80(4) 34(3) 74(5) -3(3) 6(4) -5(3)

C(24) 50(3) 27(2) 111(6) 9(4) -2(4) -3(2)

C(25) 56(4) 36(3) 86(5) 19(3) 0(3) -6(3)

C(26) 59(4) 46(4) 73(5) 26(3) 11(3) -1(3)

C(27) 54(4) 54(4) 59(4) 8(3) 13(3) 11(3)

C(28) 50(4) 96(6) 48(4) 17(4) 16(3) -2(4)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_Table 5. Hydrogen coordinates ( x 104) and isotropic displacement parameters (Å2x 103)

for eva12.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

H(2A) 11104 7614 8493 57

H(2B) 11121 6311 9095 57

H(3A) 11100 5066 7707 65

H(3B) 11667 6032 7680 65

H(4A) 11121 7495 6733 54

H(4B) 11129 6113 6233 54

H(6A) 9603 7593 9249 64

H(6B) 10197 8459 9119 64

H(6C) 10192 7312 9867 64

H(7A) 10151 4683 8341 77

H(7B) 9599 5348 8882 77

H(7C) 10223 5082 9416 77

H(8A) 10226 8318 6020 56

H(8B) 9644 7419 5891 56

H(8C) 10257 7086 5347 56

H(9A) 9636 5204 6466 65

H(9B) 10208 4616 7004 65

H(9C) 10254 4949 5914 65

H(11A) 11402 11048 7530 88

H(11B) 11283 9718 6992 88

H(11C) 11256 9764 8110 88

H(12A) 10474 10745 6062 86

H(12B) 10644 12060 6586 86

H(12C) 9959 11562 6580 86

H(13A) 10609 12256 8258 72

H(13B) 10461 11042 8910 72

H(13C) 9933 11708 8314 72

H(14A) 8810 9021 8151 41

H(14B) 8985 10471 7915 41

H(15A) 8580 10096 5085 56

H(15B) 9243 9931 5519 56

H(15C) 8864 11219 5715 56

H(16A) 7561 9922 7407 53

H(16B) 7482 9945 6295 53

H(16C) 7762 11169 6823 53

H(18) 8724 7321 4789 41

H(19) 8139 6394 3620 50

H(20) 7117 5972 3886 52

H(21) 6678 6547 5296 48

H(22) 7252 7519 6453 41

H(23A) 8081 4958 6150 94

H(23B) 8012 3462 6404 94

H(23C) 8656 4023 6092 94

H(24A) 8564 2620 7741 94

H(24B) 8910 3607 8415 94

H(24C) 9162 3336 7384 94

H(25A) 7683 3759 7980 71

H(25B) 7597 5196 7601 71

H(26A) 7571 5068 9272 71

H(26B) 8261 4599 9264 71

H(27A) 7336 7222 9239 84

H(27B) 7479 7140 8144 84

H(27C) 7783 8248 8766 84

H(28A) 8723 6246 10033 97

H(28B) 8058 6702 10331 97

H(28C) 8521 7715 9881 97

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_Table 6. Torsion angles [°] for eva12.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

N(1)-Zn(1)-Na(1)-O(1) -137.3(2)

C(10)-Zn(1)-Na(1)-O(1) -15(3)

C(14)-Zn(1)-Na(1)-O(1) 47.6(2)

C(10)-Zn(1)-Na(1)-N(1) 122(3)

C(14)-Zn(1)-Na(1)-N(1) -175.1(3)

N(1)-Zn(1)-Na(1)-N(3) 119.3(3)

C(10)-Zn(1)-Na(1)-N(3) -119(3)

C(14)-Zn(1)-Na(1)-N(3) -55.7(2)

N(1)-Zn(1)-Na(1)-N(2) -27.6(5)

C(10)-Zn(1)-Na(1)-N(2) 94(3)

C(14)-Zn(1)-Na(1)-N(2) 157.3(5)

N(1)-Zn(1)-Na(1)-C(14) 175.1(3)

C(10)-Zn(1)-Na(1)-C(14) -63(3)

N(1)-Zn(1)-Na(1)-Si(1) -154.8(2)

C(10)-Zn(1)-Na(1)-Si(1) -33(3)

C(14)-Zn(1)-Na(1)-Si(1) 30.11(18)

N(1)-Na(1)-Si(1)-O(1) 126.0(2)

N(3)-Na(1)-Si(1)-O(1) -98.91(18)

N(2)-Na(1)-Si(1)-O(1) -20.8(2)

C(14)-Na(1)-Si(1)-O(1) 178.0(2)

Zn(1)-Na(1)-Si(1)-O(1) 141.51(16)

O(1)-Na(1)-Si(1)-C(14) -178.0(2)

N(1)-Na(1)-Si(1)-C(14) -52.0(2)

N(3)-Na(1)-Si(1)-C(14) 83.1(2)

N(2)-Na(1)-Si(1)-C(14) 161.2(2)

Zn(1)-Na(1)-Si(1)-C(14) -36.47(18)

O(1)-Na(1)-Si(1)-C(15) -77.6(2)

N(1)-Na(1)-Si(1)-C(15) 48.4(3)

N(3)-Na(1)-Si(1)-C(15) -176.5(2)

N(2)-Na(1)-Si(1)-C(15) -98.4(3)

C(14)-Na(1)-Si(1)-C(15) 100.4(3)

Zn(1)-Na(1)-Si(1)-C(15) 64.0(2)

O(1)-Na(1)-Si(1)-C(16) 75.8(2)

N(1)-Na(1)-Si(1)-C(16) -158.2(2)

N(3)-Na(1)-Si(1)-C(16) -23.1(2)

N(2)-Na(1)-Si(1)-C(16) 55.0(3)

C(14)-Na(1)-Si(1)-C(16) -106.2(3)

Zn(1)-Na(1)-Si(1)-C(16) -142.70(19)

C(14)-Si(1)-O(1)-C(17) -179.5(3)

C(15)-Si(1)-O(1)-C(17) -58.1(4)

C(16)-Si(1)-O(1)-C(17) 55.9(4)

Na(1)-Si(1)-O(1)-C(17) 178.6(4)

C(14)-Si(1)-O(1)-Na(1) 1.8(2)

C(15)-Si(1)-O(1)-Na(1) 123.31(19)

C(16)-Si(1)-O(1)-Na(1) -122.75(19)

N(1)-Na(1)-O(1)-C(17) 120.8(3)

N(3)-Na(1)-O(1)-C(17) -91.0(3)

N(2)-Na(1)-O(1)-C(17) -15.2(4)

C(14)-Na(1)-O(1)-C(17) -179.8(4)

Zn(1)-Na(1)-O(1)-C(17) 148.1(3)

Si(1)-Na(1)-O(1)-C(17) -178.6(4)

N(1)-Na(1)-O(1)-Si(1) -60.7(2)

N(3)-Na(1)-O(1)-Si(1) 87.59(18)

N(2)-Na(1)-O(1)-Si(1) 163.40(17)

C(14)-Na(1)-O(1)-Si(1) -1.23(14)

Zn(1)-Na(1)-O(1)-Si(1) -33.33(13)

C(10)-Zn(1)-N(1)-C(5) -63.0(5)

C(14)-Zn(1)-N(1)-C(5) 118.9(3)

Na(1)-Zn(1)-N(1)-C(5) 114.1(4)

C(10)-Zn(1)-N(1)-C(1) 71.0(5)

C(14)-Zn(1)-N(1)-C(1) -107.1(3)

Na(1)-Zn(1)-N(1)-C(1) -111.8(4)

C(10)-Zn(1)-N(1)-Na(1) -177.1(3)

C(14)-Zn(1)-N(1)-Na(1) 4.7(3)

O(1)-Na(1)-N(1)-C(5) -69.1(3)

N(3)-Na(1)-N(1)-C(5) 154.1(3)

N(2)-Na(1)-N(1)-C(5) 53.8(4)

C(14)-Na(1)-N(1)-C(5) -119.5(3)

Zn(1)-Na(1)-N(1)-C(5) -116.3(4)

Si(1)-Na(1)-N(1)-C(5) -94.1(3)

O(1)-Na(1)-N(1)-C(1) 161.8(3)

N(3)-Na(1)-N(1)-C(1) 25.0(3)

N(2)-Na(1)-N(1)-C(1) -75.2(4)

C(14)-Na(1)-N(1)-C(1) 111.5(3)

Zn(1)-Na(1)-N(1)-C(1) 114.6(4)

Si(1)-Na(1)-N(1)-C(1) 136.8(3)

O(1)-Na(1)-N(1)-Zn(1) 47.2(2)

N(3)-Na(1)-N(1)-Zn(1) -89.6(2)

N(2)-Na(1)-N(1)-Zn(1) 170.1(2)

C(14)-Na(1)-N(1)-Zn(1) -3.16(19)

Si(1)-Na(1)-N(1)-Zn(1) 22.18(19)

O(1)-Na(1)-N(2)-C(25) -82.4(3)

N(1)-Na(1)-N(2)-C(25) 149.4(3)

N(3)-Na(1)-N(2)-C(25) 19.3(3)

C(14)-Na(1)-N(2)-C(25) -47.1(7)

Zn(1)-Na(1)-N(2)-C(25) 170.2(4)

Si(1)-Na(1)-N(2)-C(25) -72.3(4)

O(1)-Na(1)-N(2)-C(23) 36.5(4)

N(1)-Na(1)-N(2)-C(23) -91.6(4)

N(3)-Na(1)-N(2)-C(23) 138.2(4)

C(14)-Na(1)-N(2)-C(23) 71.8(6)

Zn(1)-Na(1)-N(2)-C(23) -70.9(6)

Si(1)-Na(1)-N(2)-C(23) 46.6(4)

O(1)-Na(1)-N(2)-C(24) 159.0(4)

N(1)-Na(1)-N(2)-C(24) 30.8(5)

N(3)-Na(1)-N(2)-C(24) -99.3(4)

C(14)-Na(1)-N(2)-C(24) -165.7(5)

Zn(1)-Na(1)-N(2)-C(24) 51.6(8)

Si(1)-Na(1)-N(2)-C(24) 169.0(4)

O(1)-Na(1)-N(3)-C(28) -130.7(4)

N(1)-Na(1)-N(3)-C(28) 8.8(5)

N(2)-Na(1)-N(3)-C(28) 132.2(4)

C(14)-Na(1)-N(3)-C(28) -69.4(4)

Zn(1)-Na(1)-N(3)-C(28) -37.9(4)

Si(1)-Na(1)-N(3)-C(28) -101.3(4)

O(1)-Na(1)-N(3)-C(27) -9.9(4)

N(1)-Na(1)-N(3)-C(27) 129.6(3)

N(2)-Na(1)-N(3)-C(27) -107.0(4)

C(14)-Na(1)-N(3)-C(27) 51.4(4)

Zn(1)-Na(1)-N(3)-C(27) 82.9(4)

Si(1)-Na(1)-N(3)-C(27) 19.5(4)

O(1)-Na(1)-N(3)-C(26) 107.3(3)

N(1)-Na(1)-N(3)-C(26) -113.2(3)

N(2)-Na(1)-N(3)-C(26) 10.2(3)

C(14)-Na(1)-N(3)-C(26) 168.6(3)

Zn(1)-Na(1)-N(3)-C(26) -159.9(3)

Si(1)-Na(1)-N(3)-C(26) 136.7(3)

C(5)-N(1)-C(1)-C(6) 164.3(5)

Zn(1)-N(1)-C(1)-C(6) 31.7(5)

Na(1)-N(1)-C(1)-C(6) -69.7(4)

C(5)-N(1)-C(1)-C(2) 45.6(5)

Zn(1)-N(1)-C(1)-C(2) -87.0(5)

Na(1)-N(1)-C(1)-C(2) 171.6(4)

C(5)-N(1)-C(1)-C(7) -80.5(5)

Zn(1)-N(1)-C(1)-C(7) 146.8(4)

Na(1)-N(1)-C(1)-C(7) 45.4(5)

N(1)-C(1)-C(2)-C(3) -52.6(7)

C(6)-C(1)-C(2)-C(3) -170.0(5)

C(7)-C(1)-C(2)-C(3) 74.7(6)

C(1)-C(2)-C(3)-C(4) 58.6(6)

C(2)-C(3)-C(4)-C(5) -57.4(6)

C(1)-N(1)-C(5)-C(4) -44.8(5)

Zn(1)-N(1)-C(5)-C(4) 87.3(5)

Na(1)-N(1)-C(5)-C(4) -169.9(4)

C(1)-N(1)-C(5)-C(8) -164.8(5)

Zn(1)-N(1)-C(5)-C(8) -32.7(5)

Na(1)-N(1)-C(5)-C(8) 70.1(4)

C(1)-N(1)-C(5)-C(9) 79.7(5)

Zn(1)-N(1)-C(5)-C(9) -148.2(4)

Na(1)-N(1)-C(5)-C(9) -45.4(5)

C(3)-C(4)-C(5)-N(1) 50.4(6)

C(3)-C(4)-C(5)-C(8) 170.0(5)

C(3)-C(4)-C(5)-C(9) -76.7(6)

N(1)-Zn(1)-C(10)-C(12) 118.2(4)

C(14)-Zn(1)-C(10)-C(12) -63.7(5)

Na(1)-Zn(1)-C(10)-C(12) -2(3)

N(1)-Zn(1)-C(10)-C(11) -5.3(7)

C(14)-Zn(1)-C(10)-C(11) 172.8(5)

Na(1)-Zn(1)-C(10)-C(11) -125(3)

N(1)-Zn(1)-C(10)-C(13) -125.8(4)

C(14)-Zn(1)-C(10)-C(13) 52.3(4)

Na(1)-Zn(1)-C(10)-C(13) 114(3)

O(1)-Si(1)-C(14)-Zn(1) 71.1(3)

C(15)-Si(1)-C(14)-Zn(1) -46.7(3)

C(16)-Si(1)-C(14)-Zn(1) -172.4(2)

Na(1)-Si(1)-C(14)-Zn(1) 72.5(2)

O(1)-Si(1)-C(14)-Na(1) -1.41(17)

C(15)-Si(1)-C(14)-Na(1) -119.19(19)

C(16)-Si(1)-C(14)-Na(1) 115.15(19)

N(1)-Zn(1)-C(14)-Si(1) -80.9(3)

C(10)-Zn(1)-C(14)-Si(1) 100.6(3)

Na(1)-Zn(1)-C(14)-Si(1) -76.9(2)

N(1)-Zn(1)-C(14)-Na(1) -4.0(2)

C(10)-Zn(1)-C(14)-Na(1) 177.5(2)

O(1)-Na(1)-C(14)-Si(1) 1.11(13)

N(1)-Na(1)-C(14)-Si(1) 126.8(2)

N(3)-Na(1)-C(14)-Si(1) -101.68(19)

N(2)-Na(1)-C(14)-Si(1) -39.5(6)

Zn(1)-Na(1)-C(14)-Si(1) 123.6(3)

O(1)-Na(1)-C(14)-Zn(1) -122.5(2)

N(1)-Na(1)-C(14)-Zn(1) 3.14(19)

N(3)-Na(1)-C(14)-Zn(1) 134.69(18)

N(2)-Na(1)-C(14)-Zn(1) -163.1(4)

Si(1)-Na(1)-C(14)-Zn(1) -123.6(3)

Si(1)-O(1)-C(17)-C(18) 93.2(5)

Na(1)-O(1)-C(17)-C(18) -88.4(5)

Si(1)-O(1)-C(17)-C(22) -87.5(5)

Na(1)-O(1)-C(17)-C(22) 90.8(5)

O(1)-C(17)-C(18)-C(19) 176.4(4)

C(22)-C(17)-C(18)-C(19) -2.8(7)

C(17)-C(18)-C(19)-C(20) 0.3(7)

C(18)-C(19)-C(20)-C(21) 1.5(8)

C(19)-C(20)-C(21)-C(22) -0.6(8)

C(20)-C(21)-C(22)-C(17) -1.9(7)

C(18)-C(17)-C(22)-C(21) 3.6(7)

O(1)-C(17)-C(22)-C(21) -175.6(4)

C(23)-N(2)-C(25)-C(26) -170.1(4)

C(24)-N(2)-C(25)-C(26) 70.9(6)

Na(1)-N(2)-C(25)-C(26) -49.5(5)

C(28)-N(3)-C(26)-C(25) -164.8(5)

C(27)-N(3)-C(26)-C(25) 77.6(6)

Na(1)-N(3)-C(26)-C(25) -39.0(5)

N(2)-C(25)-C(26)-N(3) 66.8(6)

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Symmetry transformations used to generate equivalent atoms:

ORTEP001.Hgl

ORTEP002.Hgl

ORTEP003.Hgl