**SUPPORTING INFORMATION FOR**

# Synthesis, Structure, and Properties of Magnesocene Amine Adducts. Structural Distortions Arising from N-H···$C_5H_5^-$ Hydrogen Bonding and Molecular Orbital Calculations Thereof

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1. Positional Parameters for Structures Considered by Molecular Orbital Theory

**Positional parameters for $C_{13}H_{19}MgN$ (2)**

| | | | |
|---|---|---|---|
| Mg | -0.71083200 | 0.18699100 | -0.07123000 |
| C | -3.10716800 | -0.01352900 | 0.15301900 |
| C | -2.76279700 | -0.58734700 | -1.10251200 |
| C | -1.97730700 | -1.74840500 | -0.85473600 |
| C | -1.82627800 | -1.88510300 | 0.55199400 |
| C | -2.52413500 | -0.81006300 | 1.17555400 |
| H | -3.71453700 | 0.87155300 | 0.30365500 |
| H | -3.07902400 | -0.22741500 | -2.07525200 |
| H | -1.59363100 | -2.42889100 | -1.60725400 |
| H | -1.31483900 | -2.69202100 | 1.06485700 |
| H | -2.62492000 | -0.65061000 | 2.24328600 |
| C | 1.81789800 | 2.48610200 | -0.11309300 |
| C | 0.82834100 | 2.62022200 | -1.11337400 |
| C | -0.44407800 | 2.48956400 | -0.50340200 |
| C | -0.22610800 | 2.26169900 | 0.90753600 |
| C | 1.17580900 | 2.26095700 | 1.12407000 |
| H | 2.89059900 | 2.55889800 | -0.26775900 |
| H | 1.00483800 | 2.82319800 | -2.16493500 |
| H | -1.39968600 | 2.71934200 | -0.96550000 |
| H | -0.99069800 | 2.30065600 | 1.67810400 |
| H | 1.66368500 | 2.13785000 | 2.08550100 |
| N | 1.22373400 | -0.59925400 | -0.67835100 |
| H | 1.18565800 | -0.73404300 | -1.68995400 |
| H | 1.82075800 | 0.22648700 | -0.53667100 |
| C | 1.85243900 | -1.80804500 | -0.05870700 |
| H | 1.13532700 | -2.62778400 | -0.19297100 |
| C | 2.05289400 | -1.57329200 | 1.44179200 |
| H | 1.10299200 | -1.35851900 | 1.94383800 |
| H | 2.48699300 | -2.46404000 | 1.90922200 |
| H | 2.73003800 | -0.72915100 | 1.62087300 |
| C | 3.16599000 | -2.18205300 | -0.76219300 |
| H | 3.00815600 | -2.35623700 | -1.83422200 |
| H | 3.91098600 | -1.38325700 | -0.65230800 |
| H | 3.58813300 | -3.09936800 | -0.33497400 |

**Positional Parameters for $C_{11}H_{15}MgN$ (11)**

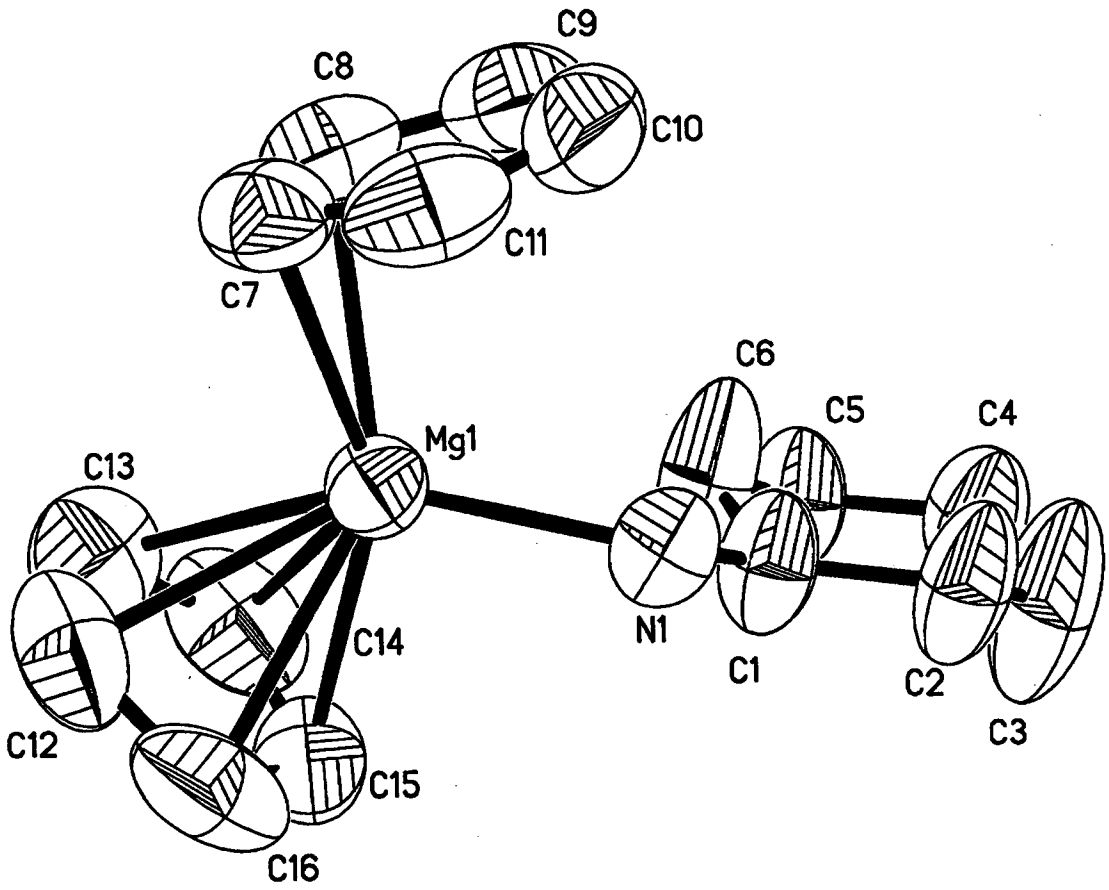
| | | | |
|---|---|---|---|
| Mg | -0.11724900 | -0.04518200 | -0.30793900 |
| C | -0.30108900 | 0.04300000 | -2.70037600 |
| C | -0.99398500 | -1.12377300 | -2.27679700 |
| C | -2.11759900 | -0.71154000 | -1.51318900 |
| C | -2.11038900 | 0.70558000 | -1.44861800 |
| C | -0.98754900 | 1.17148300 | -2.18771500 |
| H | 0.58718500 | 0.06544600 | -3.31581800 |
| H | -0.73595600 | -2.14259700 | -2.53108100 |
| H | -2.86201900 | -1.36420300 | -1.07749300 |
| H | -2.85316700 | 1.32661600 | -0.96692400 |
| H | -0.72096700 | 2.20623500 | -2.35143500 |
| C | 2.12023600 | -0.05991500 | 2.28128800 |
| C | 2.38414400 | -0.95162900 | 1.22042400 |
| C | 2.20739300 | -0.25792900 | 0.00068000 |

| | | | |
|---|---|---|---|
| C | 1.81970300 | 1.09241900 | 0.32409800 |
| C | 1.76767500 | 1.19107500 | 1.73548700 |
| H | 2.19176100 | -0.29249700 | 3.33664800 |
| H | 2.69675300 | -1.98322300 | 1.31679600 |
| H | 2.49995800 | -0.61325800 | -0.97977200 |
| H | 1.78338800 | 1.92180900 | -0.37193400 |
| H | 1.52957000 | 2.08686100 | 2.29400700 |
| N | -0.87251000 | -0.77019700 | 1.58321300 |
| H | -1.15960900 | -1.74233400 | 1.50030200 |
| H | -0.01101100 | -0.76468500 | 2.13900500 |
| C | -1.92900700 | 0.00120700 | 2.27792100 |
| H | -2.82604400 | 0.03567100 | 1.65859400 |
| H | -1.57673700 | 1.02185100 | 2.43180800 |
| H | -2.18574000 | -0.42800700 | 3.25085400 |

**Positional Parameters for $C_{11}H_{15}MgN$ (11) with Reversed $\eta^2$-Cyclopentadienyl Ligand**

| | | | |
|---|---|---|---|
| Mg | 0.04488200 | 0.12306700 | -0.04473100 |
| C | 0.29356300 | -2.23294700 | 0.00008300 |
| C | 0.99966600 | -1.79918000 | -1.15331100 |
| C | 2.14213900 | -1.07602000 | -0.71938900 |
| C | 2.13275300 | -1.05227800 | 0.69530200 |
| C | 0.98713600 | -1.75961000 | 1.14380700 |
| H | -0.60677200 | -2.82691400 | 0.00753700 |
| H | 0.73751100 | -2.02168200 | -2.17819100 |
| H | 2.89776400 | -0.64258300 | -1.36106700 |
| H | 2.88267500 | -0.59673300 | 1.32729100 |
| H | 0.71331000 | -1.94640100 | 2.17332200 |
| C | -2.46828400 | -0.03481100 | -1.06741000 |
| C | -1.93326700 | 1.23615100 | -0.74571800 |
| C | -1.83692500 | 1.31539500 | 0.68716400 |
| C | -2.32096900 | 0.08955700 | 1.21229100 |
| C | -2.70929300 | -0.73043400 | 0.13470700 |
| H | -2.66063600 | -0.40126100 | -2.06603300 |
| H | -1.75780500 | 2.04506200 | -1.44328500 |
| H | -1.59248700 | 2.19615400 | 1.26837700 |
| H | -2.38469300 | -0.16423400 | 2.26160300 |
| H | -3.09048700 | -1.73877300 | 0.21444800 |
| N | 1.13966400 | 2.06050000 | -0.35370400 |
| H | 1.24066800 | 2.15915100 | -1.36231000 |
| H | 0.44802200 | 2.75432900 | -0.08121300 |
| C | 2.43852600 | 2.37269900 | 0.29006600 |
| H | 3.18271200 | 1.65093000 | -0.03966600 |
| H | 2.33419600 | 2.27946100 | 1.37170200 |
| H | 2.78951200 | 3.38206700 | 0.05463000 |

2. Structure Report for $C_{16}H_{23}MgN$ (**5**).



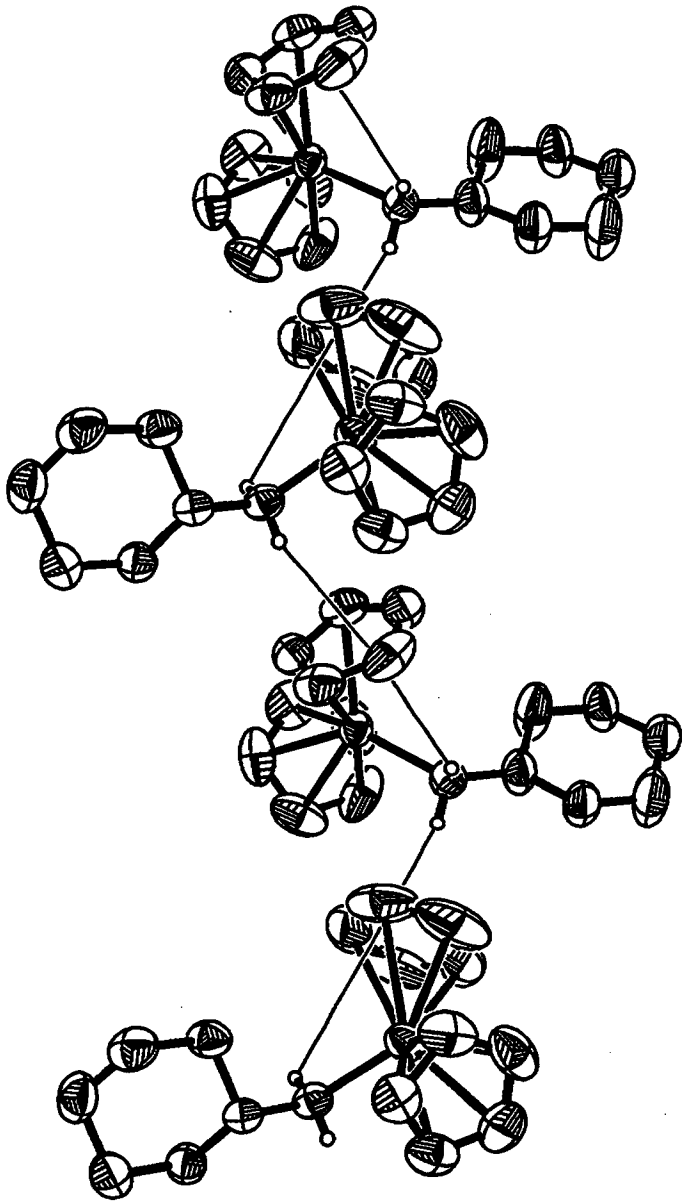


Table 1. Crystal data and structure refinement for trim.

| | |
|---|---|
| Identification code | trim |
| Empirical formula | C16 H23 Mg N |
| Formula weight | 253.66 |
| Temperature | 295(2) K |
| Wavelength | 0.71073 A |
| Crystal system | Monoclinic |
| Space group | P2(1)/c |
| Unit cell dimensions | a = 10.6243(9) A alpha = 90 deg. |
| | b = 19.9057(18) A beta = 90.972(2) deg. |
| | c = 14.3919(13) A gamma = 90 deg. |
| Volume | 3043.2(5) A^3 |
| Z | 8 |

| | |
|---|---|
| Density (calculated) | 1.107 Mg/m^3 |
| Absorption coefficient | 0.101 mm^-1 |
| F(000) | 1104 |
| Crystal size | 0.30 x 0.25 x 0.20 mm |
| Theta range for data collection | 1.75 to 28.34 deg. |
| Index ranges | -14<=h<=14, 0<=k<=25, 0<=l<=18 |
| Reflections collected | 22124 |
| Independent reflections | 7238 [R(int) = 0.063] |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9801 and 0.9704 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 7238 / 0 / 482 |
| Goodness-of-fit on F^2 | 0.821 |
| Final R indices [I>2sigma(I)] | R1 = 0.0492, wR2 = 0.1210 |
| R indices (all data) | R1 = 0.1879, wR2 = 0.1635 |
| Extinction coefficient | 0.0031(6) |
| Largest diff. peak and hole | 0.313 and -0.261 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for trim. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mg(1) | 4233(1) | 1280(1) | 3142(1) | 57(1) |
| N(1) | 5167(3) | 639(1) | 2224(2) | 63(1) |
| C(1) | 5180(3) | -88(1) | 2295(2) | 79(1) |
| C(2) | 5767(5) | -458(2) | 1525(3) | 96(2) |
| C(3) | 5794(4) | -1202(2) | 1645(4) | 152(2) |
| C(4) | 4801(4) | -1513(2) | 2081(3) | 95(1) |
| C(5) | 4235(5) | -1148(2) | 2862(3) | 91(1) |
| C(6) | 4195(4) | -406(2) | 2735(3) | 125(2) |
| C(7) | 2799(3) | 1999(2) | 2498(3) | 75(1) |
| C(8) | 2076(3) | 1431(2) | 2612(4) | 82(1) |
| C(9) | 2140(4) | 1050(2) | 1826(4) | 97(2) |
| C(10) | 2916(5) | 1383(3) | 1216(4) | 105(2) |
| C(11) | 3319(4) | 1969(2) | 1640(4) | 87(1) |
| C(12) | 4666(6) | 1976(2) | 4506(3) | 96(1) |
| C(13) | 3813(6) | 1529(3) | 4760(3) | 101(1) |
| C(14) | 4309(7) | 911(3) | 4708(3) | 106(2) |
| C(15) | 5511(7) | 961(3) | 4439(3) | 113(2) |
| C(16) | 5762(5) | 1651(4) | 4287(3) | 106(2) |
| Mg(2) | 9237(1) | 1737(1) | 403(1) | 63(1) |
| N(2) | 10189(3) | 2450(1) | 1240(2) | 57(1) |
| C(17) | 10217(2) | 3173(1) | 963(2) | 52(1) |
| C(18) | 11035(3) | 3597(2) | 1600(3) | 65(1) |
| C(19) | 11005(4) | 4336(2) | 1339(3) | 82(1) |
| C(20) | 9659(4) | 4587(2) | 1308(3) | 88(1) |
| C(21) | 8849(4) | 4178(2) | 654(3) | 85(1) |
| C(22) | 8892(3) | 3437(2) | 916(3) | 69(1) |
| C(23) | 10826(4) | 1880(3) | -785(3) | 83(1) |
| C(24) | 9792(4) | 2234(2) | -1093(2) | 80(1) |

| | | | | |
|---|---|---|---|---|
| C(25) | 8845(4) | 1780(3) | -1281(3) | 93(1) |
| C(26) | 9309(6) | 1151(3) | -1096(3) | 104(2) |
| C(27) | 10540(5) | 1216(3) | -766(3) | 91(1) |
| C(28) | 7444(9) | 1120(7) | 714(5) | 146(3) |
| C(29) | 8256(7) | 877(3) | 1355(8) | 125(3) |
| C(30) | 8299(6) | 1313(5) | 2071(5) | 117(2) |
| C(31) | 7512(8) | 1822(3) | 1857(8) | 121(2) |
| C(32) | 7027(5) | 1688(5) | 1019(9) | 138(3) |

Table 3. Bond lengths [A] and angles [deg] for trim.

| | |
|---|---|
| Mg(1)-N(1) | 2.098(3) |
| Mg(1)-C(7) | 2.276(3) |
| Mg(1)-C(14) | 2.371(4) |
| Mg(1)-C(15) | 2.376(4) |
| Mg(1)-C(16) | 2.410(4) |
| Mg(1)-C(8) | 2.422(3) |
| Mg(1)-C(13) | 2.430(4) |
| Mg(1)-C(12) | 2.441(4) |
| Mg(1)-C(11) | 2.724(4) |
| N(1)-C(1) | 1.450(4) |
| C(1)-C(6) | 1.386(4) |
| C(1)-C(2) | 1.478(4) |
| C(2)-C(3) | 1.490(5) |
| C(3)-C(4) | 1.383(5) |
| C(4)-C(5) | 1.475(5) |
| C(5)-C(6) | 1.489(5) |
| C(7)-C(11) | 1.361(5) |
| C(7)-C(8) | 1.378(5) |
| C(8)-C(9) | 1.363(6) |
| C(9)-C(10) | 1.383(6) |
| C(10)-C(11) | 1.381(6) |
| C(12)-C(13) | 1.326(6) |
| C(12)-C(16) | 1.373(6) |
| C(13)-C(14) | 1.341(7) |
| C(14)-C(15) | 1.344(7) |
| C(15)-C(16) | 1.416(7) |
| Mg(2)-N(2) | 2.110(3) |
| Mg(2)-C(28) | 2.316(5) |
| Mg(2)-C(27) | 2.430(4) |
| Mg(2)-C(29) | 2.436(5) |
| Mg(2)-C(23) | 2.439(4) |
| Mg(2)-C(24) | 2.452(4) |
| Mg(2)-C(25) | 2.455(4) |
| Mg(2)-C(26) | 2.455(4) |
| Mg(2)-C(32) | 2.525(6) |
| Mg(2)-C(30) | 2.747(6) |
| Mg(2)-C(31) | 2.809(5) |
| N(2)-C(17) | 1.493(4) |
| C(17)-C(22) | 1.503(4) |
| C(17)-C(18) | 1.510(4) |
| C(18)-C(19) | 1.519(4) |
| C(19)-C(20) | 1.515(5) |
| C(20)-C(21) | 1.504(5) |
| C(21)-C(22) | 1.524(4) |

| | |
|---|---|
| C(23)-C(27) | 1.357(5) |
| C(23)-C(24) | 1.372(5) |
| C(24)-C(25) | 1.376(5) |
| C(25)-C(26) | 1.371(6) |
| C(26)-C(27) | 1.389(6) |
| C(28)-C(32) | 1.294(9) |
| C(28)-C(29) | 1.343(9) |
| C(29)-C(30) | 1.346(9) |
| C(30)-C(31) | 1.347(9) |
| C(31)-C(32) | 1.330(9) |

| | |
|---|---|
| N(1)-Mg(1)-C(7) | 116.52(16) |
| N(1)-Mg(1)-C(14) | 113.7(2) |
| C(7)-Mg(1)-C(14) | 126.4(2) |
| N(1)-Mg(1)-C(15) | 93.59(17) |
| C(7)-Mg(1)-C(15) | 149.01(17) |
| C(14)-Mg(1)-C(15) | 32.90(16) |
| N(1)-Mg(1)-C(16) | 107.2(2) |
| C(7)-Mg(1)-C(16) | 121.6(2) |
| C(14)-Mg(1)-C(16) | 55.47(17) |
| C(15)-Mg(1)-C(16) | 34.41(17) |
| N(1)-Mg(1)-C(8) | 109.42(18) |
| C(7)-Mg(1)-C(8) | 33.94(12) |
| C(14)-Mg(1)-C(8) | 110.8(2) |
| C(15)-Mg(1)-C(8) | 143.7(2) |
| C(16)-Mg(1)-C(8) | 143.2(2) |
| N(1)-Mg(1)-C(13) | 145.50(18) |
| C(7)-Mg(1)-C(13) | 97.42(18) |
| C(14)-Mg(1)-C(13) | 32.41(16) |
| C(15)-Mg(1)-C(13) | 54.06(19) |
| C(16)-Mg(1)-C(13) | 54.18(19) |
| C(8)-Mg(1)-C(13) | 95.05(19) |
| N(1)-Mg(1)-C(12) | 140.10(19) |
| C(7)-Mg(1)-C(12) | 94.95(16) |
| C(14)-Mg(1)-C(12) | 53.69(16) |
| C(15)-Mg(1)-C(12) | 54.67(16) |
| C(16)-Mg(1)-C(12) | 32.89(15) |
| C(8)-Mg(1)-C(12) | 110.3(2) |
| C(13)-Mg(1)-C(12) | 31.58(16) |
| N(1)-Mg(1)-C(11) | 88.45(15) |
| C(7)-Mg(1)-C(11) | 29.92(12) |
| C(14)-Mg(1)-C(11) | 156.3(2) |
| C(15)-Mg(1)-C(11) | 161.6(2) |
| C(16)-Mg(1)-C(11) | 128.0(2) |
| C(8)-Mg(1)-C(11) | 50.58(14) |
| C(13)-Mg(1)-C(11) | 126.05(18) |
| C(12)-Mg(1)-C(11) | 114.33(17) |
| C(1)-N(1)-Mg(1) | 124.5(2) |
| C(6)-C(1)-N(1) | 118.9(3) |
| C(6)-C(1)-C(2) | 116.4(3) |
| N(1)-C(1)-C(2) | 116.6(3) |
| C(1)-C(2)-C(3) | 114.6(3) |
| C(4)-C(3)-C(2) | 119.0(4) |
| C(3)-C(4)-C(5) | 116.6(3) |
| C(4)-C(5)-C(6) | 114.0(3) |
| C(1)-C(6)-C(5) | 119.3(3) |

| | |
|---|---|
| C(11)-C(7)-C(8) | 107.9(4) |
| C(11)-C(7)-Mg(1) | 93.6(2) |
| C(8)-C(7)-Mg(1) | 78.8(2) |
| C(9)-C(8)-C(7) | 108.7(4) |
| C(9)-C(8)-Mg(1) | 97.6(3) |
| C(7)-C(8)-Mg(1) | 67.23(19) |
| C(8)-C(9)-C(10) | 107.5(4) |
| C(11)-C(10)-C(9) | 107.8(4) |
| C(7)-C(11)-C(10) | 108.1(4) |
| C(7)-C(11)-Mg(1) | 56.51(19) |
| C(10)-C(11)-Mg(1) | 91.7(3) |
| C(13)-C(12)-C(16) | 109.5(5) |
| C(13)-C(12)-Mg(1) | 73.8(3) |
| C(16)-C(12)-Mg(1) | 72.3(2) |
| C(12)-C(13)-C(14) | 109.2(5) |
| C(12)-C(13)-Mg(1) | 74.6(3) |
| C(14)-C(13)-Mg(1) | 71.4(3) |
| C(13)-C(14)-C(15) | 108.9(5) |
| C(13)-C(14)-Mg(1) | 76.2(3) |
| C(15)-C(14)-Mg(1) | 73.8(3) |
| C(14)-C(15)-C(16) | 107.4(4) |
| C(14)-C(15)-Mg(1) | 73.3(3) |
| C(16)-C(15)-Mg(1) | 74.1(2) |
| C(12)-C(16)-C(15) | 105.0(4) |
| C(12)-C(16)-Mg(1) | 74.8(3) |
| C(15)-C(16)-Mg(1) | 71.5(2) |
| N(2)-Mg(2)-C(28) | 129.4(2) |
| N(2)-Mg(2)-C(27) | 114.17(17) |
| C(28)-Mg(2)-C(27) | 112.8(3) |
| N(2)-Mg(2)-C(29) | 110.9(3) |
| C(28)-Mg(2)-C(29) | 32.7(2) |
| C(27)-Mg(2)-C(29) | 110.1(2) |
| N(2)-Mg(2)-C(23) | 89.46(14) |
| C(28)-Mg(2)-C(23) | 141.1(2) |
| C(27)-Mg(2)-C(23) | 32.35(13) |
| C(29)-Mg(2)-C(23) | 141.59(19) |
| N(2)-Mg(2)-C(24) | 96.28(13) |
| C(28)-Mg(2)-C(24) | 126.5(2) |
| C(27)-Mg(2)-C(24) | 54.22(16) |
| C(29)-Mg(2)-C(24) | 152.7(3) |
| C(23)-Mg(2)-C(24) | 32.59(12) |
| N(2)-Mg(2)-C(25) | 127.71(15) |
| C(28)-Mg(2)-C(25) | 94.8(2) |
| C(27)-Mg(2)-C(25) | 54.54(17) |
| C(29)-Mg(2)-C(25) | 120.9(3) |
| C(23)-Mg(2)-C(25) | 53.94(15) |
| C(24)-Mg(2)-C(25) | 32.57(13) |
| N(2)-Mg(2)-C(26) | 143.10(15) |
| C(28)-Mg(2)-C(26) | 87.5(2) |
| C(27)-Mg(2)-C(26) | 33.04(15) |
| C(29)-Mg(2)-C(26) | 100.4(3) |
| C(23)-Mg(2)-C(26) | 53.64(16) |
| C(24)-Mg(2)-C(26) | 53.71(17) |
| C(25)-Mg(2)-C(26) | 32.43(14) |
| N(2)-Mg(2)-C(32) | 105.4(4) |
| C(28)-Mg(2)-C(32) | 30.6(2) |

| | |
|---|---|
| C(27)-Mg(2)-C(32) | 140.4(4) |
| C(29)-Mg(2)-C(32) | 50.7(2) |
| C(23)-Mg(2)-C(32) | 155.4(3) |
| C(24)-Mg(2)-C(32) | 124.3(2) |
| C(25)-Mg(2)-C(32) | 101.8(3) |
| C(26)-Mg(2)-C(32) | 109.5(4) |
| N(2)-Mg(2)-C(30) | 83.44(19) |
| C(28)-Mg(2)-C(30) | 50.0(2) |
| C(27)-Mg(2)-C(30) | 133.9(3) |
| C(29)-Mg(2)-C(30) | 29.33(19) |
| C(23)-Mg(2)-C(30) | 156.0(2) |
| C(24)-Mg(2)-C(30) | 171.1(2) |
| C(25)-Mg(2)-C(30) | 144.68(17) |
| C(26)-Mg(2)-C(30) | 129.7(2) |
| C(32)-Mg(2)-C(30) | 47.8(2) |
| N(2)-Mg(2)-C(31) | 81.18(18) |
| C(28)-Mg(2)-C(31) | 48.7(2) |
| C(27)-Mg(2)-C(31) | 158.16(18) |
| C(29)-Mg(2)-C(31) | 48.20(18) |
| C(23)-Mg(2)-C(31) | 169.28(17) |
| C(24)-Mg(2)-C(31) | 143.1(3) |
| C(25)-Mg(2)-C(31) | 129.2(3) |
| C(26)-Mg(2)-C(31) | 135.5(2) |
| C(32)-Mg(2)-C(31) | 28.2(2) |
| C(30)-Mg(2)-C(31) | 28.0(2) |
| C(17)-N(2)-Mg(2) | 120.50(19) |
| N(2)-C(17)-C(22) | 109.0(2) |
| N(2)-C(17)-C(18) | 113.0(2) |
| C(22)-C(17)-C(18) | 111.2(3) |
| C(17)-C(18)-C(19) | 112.5(3) |
| C(20)-C(19)-C(18) | 110.0(3) |
| C(21)-C(20)-C(19) | 111.7(3) |
| C(20)-C(21)-C(22) | 110.8(3) |
| C(17)-C(22)-C(21) | 111.9(3) |
| C(27)-C(23)-C(24) | 109.2(4) |
| C(27)-C(23)-Mg(2) | 73.4(2) |
| C(24)-C(23)-Mg(2) | 74.2(2) |
| C(23)-C(24)-C(25) | 107.8(5) |
| C(23)-C(24)-Mg(2) | 73.2(2) |
| C(25)-C(24)-Mg(2) | 73.8(2) |
| C(26)-C(25)-C(24) | 107.6(5) |
| C(26)-C(25)-Mg(2) | 73.8(2) |
| C(24)-C(25)-Mg(2) | 73.6(2) |
| C(25)-C(26)-C(27) | 108.3(4) |
| C(25)-C(26)-Mg(2) | 73.8(2) |
| C(27)-C(26)-Mg(2) | 72.5(2) |
| C(23)-C(27)-C(26) | 107.1(5) |
| C(23)-C(27)-Mg(2) | 74.2(2) |
| C(26)-C(27)-Mg(2) | 74.5(2) |
| C(32)-C(28)-C(29) | 107.4(7) |
| C(32)-C(28)-Mg(2) | 83.6(4) |
| C(29)-C(28)-Mg(2) | 78.6(4) |
| C(28)-C(29)-C(30) | 108.0(7) |
| C(28)-C(29)-Mg(2) | 68.7(3) |
| C(30)-C(29)-Mg(2) | 88.2(3) |
| C(29)-C(30)-C(31) | 107.3(6) |

| | |
|---|---|
| C(29)-C(30)-Mg(2) | 62.4(3) |
| C(31)-C(30)-Mg(2) | 78.6(4) |
| C(32)-C(31)-C(30) | 106.6(6) |
| C(32)-C(31)-Mg(2) | 63.9(3) |
| C(30)-C(31)-Mg(2) | 73.4(3) |
| C(28)-C(32)-C(31) | 110.8(7) |
| C(28)-C(32)-Mg(2) | 65.7(3) |
| C(31)-C(32)-Mg(2) | 87.8(3) |

Symmetry transformations used to generate equivalent atoms:

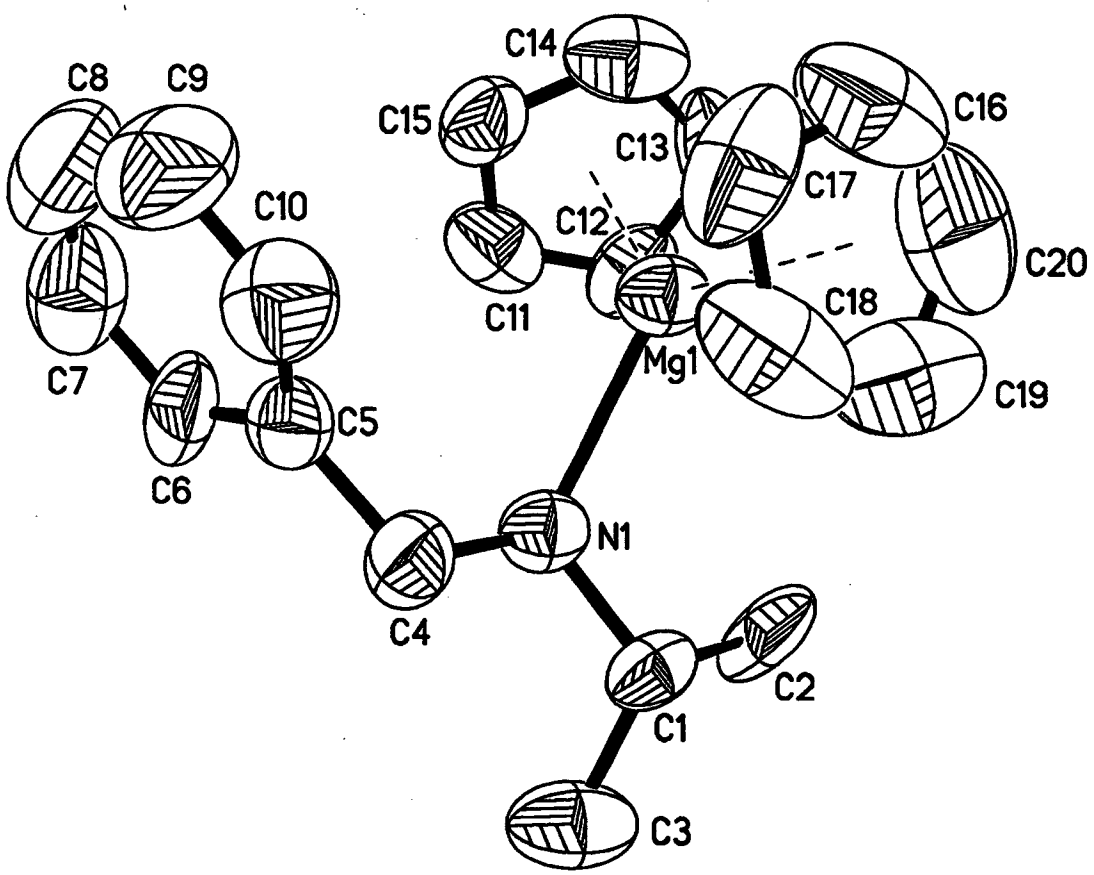
Table 4. Anisotropic displacement parameters (A^2 x 10^3) for trim.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

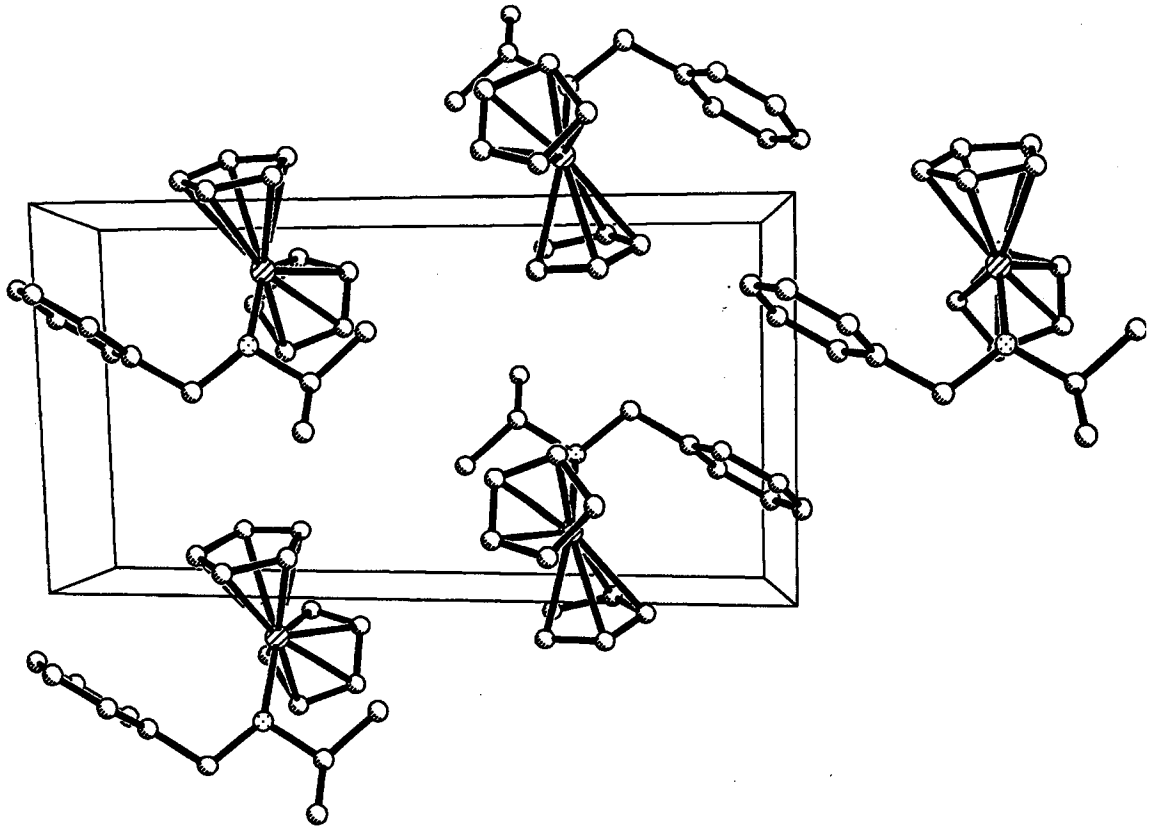
| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Mg(1) | 61(1) | 51(1) | 59(1) | 2(1) | -3(1) | 6(1) |
| N(1) | 65(2) | 52(2) | 74(2) | 6(1) | 14(2) | -3(1) |
| C(1) | 95(2) | 50(2) | 93(3) | -7(2) | 36(2) | -10(2) |
| C(2) | 100(3) | 64(2) | 126(4) | -18(2) | 65(3) | -16(2) |
| C(3) | 172(5) | 73(3) | 216(6) | -45(3) | 112(4) | -20(3) |
| C(4) | 102(3) | 65(2) | 120(3) | -12(2) | 30(2) | -5(2) |
| C(5) | 118(4) | 55(2) | 100(3) | -10(2) | 37(3) | -19(2) |
| C(6) | 163(4) | 57(2) | 158(4) | -11(2) | 105(3) | -15(2) |
| C(7) | 73(2) | 65(2) | 86(3) | 10(2) | -16(2) | 8(2) |
| C(8) | 59(2) | 93(3) | 93(3) | 24(3) | 3(2) | 12(2) |
| C(9) | 72(3) | 70(3) | 149(5) | -7(3) | -30(3) | 8(2) |
| C(10) | 104(4) | 140(5) | 71(3) | -12(3) | -8(3) | 56(4) |
| C(11) | 69(2) | 90(3) | 103(4) | 39(3) | -4(2) | 11(2) |
| C(12) | 158(5) | 62(3) | 67(3) | -4(2) | -15(3) | 3(3) |
| C(13) | 115(4) | 123(5) | 66(3) | 12(2) | 12(3) | 9(4) |
| C(14) | 164(5) | 81(4) | 73(3) | 30(2) | -25(3) | -17(4) |
| C(15) | 134(5) | 120(5) | 83(3) | -24(3) | -49(3) | 72(4) |
| C(16) | 99(4) | 157(5) | 63(3) | -1(3) | -9(2) | -48(4) |
| Mg(2) | 64(1) | 67(1) | 58(1) | 2(1) | 9(1) | -13(1) |
| N(2) | 52(2) | 64(2) | 56(2) | 9(1) | 5(1) | 5(1) |
| C(17) | 49(2) | 62(2) | 44(2) | 8(2) | 3(1) | 1(1) |
| C(18) | 62(2) | 65(2) | 67(2) | -3(2) | -4(2) | 2(2) |
| C(19) | 84(3) | 68(3) | 92(3) | -2(2) | -1(2) | -7(2) |
| C(20) | 105(3) | 57(2) | 102(3) | 7(2) | 17(3) | 11(2) |
| C(21) | 72(3) | 82(3) | 100(3) | 32(2) | 0(2) | 17(2) |
| C(22) | 53(2) | 72(2) | 80(3) | 17(2) | -3(2) | 0(2) |
| C(23) | 71(3) | 121(4) | 58(2) | -9(2) | 12(2) | -17(3) |
| C(24) | 94(3) | 89(3) | 56(2) | 3(2) | 7(2) | -5(3) |
| C(25) | 76(3) | 143(5) | 59(2) | -6(3) | 1(2) | -18(3) |
| C(26) | 131(5) | 108(4) | 73(3) | -29(3) | 28(3) | -54(4) |
| C(27) | 103(4) | 94(4) | 76(3) | -1(2) | 19(2) | 18(3) |
| C(28) | 126(6) | 236(10) | 78(4) | 6(6) | 18(4) | -104(7) |
| C(29) | 101(4) | 64(3) | 212(8) | -2(5) | 77(5) | -17(3) |
| C(30) | 84(4) | 152(7) | 114(5) | 53(5) | -21(4) | -51(4) |
| C(31) | 110(5) | 91(4) | 164(6) | -22(5) | 61(5) | -35(4) |
| C(32) | 62(3) | 149(6) | 204(10) | 99(7) | 20(4) | -10(4) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for trim.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 5840 | -142 | 2774 | 95 |
| H(3A) | 5867 | -1401 | 1034 | 183 |
| H(3B) | 6557 | -1314 | 1991 | 183 |
| H(4A) | 5091 | -1946 | 2309 | 115 |
| H(4B) | 4145 | -1598 | 1619 | 115 |
| H(6A) | 3429 | -301 | 2389 | 150 |
| H(6B) | 4118 | -205 | 3345 | 150 |
| H(1N1) | 4950(40) | 740(20) | 1720(30) | 130(20) |
| H(2N1) | 5920(40) | 792(17) | 2190(30) | 111(15) |
| H(2A) | 6370(30) | -272(16) | 1290(20) | 98(13) |
| H(2B) | 4950(50) | -380(20) | 1050(30) | 190(20) |
| H(5A) | 3420(40) | -1301(19) | 3000(30) | 136(16) |
| H(5B) | 4950(60) | -1200(30) | 3320(40) | 240(30) |
| H(7) | 2810(30) | 2387(17) | 2960(20) | 111(13) |
| H(8) | 1660(30) | 1363(15) | 3130(20) | 83(12) |
| H(9) | 1770(40) | 710(20) | 1790(30) | 118(18) |
| H(10) | 3130(30) | 1271(15) | 690(20) | 82(13) |
| H(11) | 3840(30) | 2280(17) | 1390(20) | 99(13) |
| H(12) | 4590(40) | 2400(20) | 4490(30) | 137(18) |
| H(13) | 3150(60) | 1550(30) | 4930(50) | 220(40) |
| H(14) | 3900(40) | 540(20) | 4890(30) | 146(18) |
| H(15) | 6040(40) | 697(19) | 4350(30) | 112(16) |
| H(16) | 6410(40) | 1870(20) | 4070(30) | 132(17) |
| H(1N2) | 9900(30) | 2471(14) | 1790(20) | 79(11) |
| H(2N2) | 10860(30) | 2324(14) | 1300(20) | 66(11) |
| H(17) | 10540(20) | 3192(10) | 356(17) | 46(7) |
| H(18A) | 11870(30) | 3436(14) | 1580(20) | 85(11) |
| H(18B) | 10750(20) | 3561(12) | 2250(20) | 68(9) |
| H(19A) | 11350(30) | 4380(14) | 690(20) | 92(11) |
| H(19B) | 11510(30) | 4622(14) | 1780(20) | 86(10) |
| H(20A) | 9640(20) | 5032(15) | 1163(18) | 66(9) |
| H(20B) | 9300(30) | 4598(14) | 1960(20) | 98(11) |
| H(21A) | 8000(40) | 4314(17) | 730(30) | 122(14) |
| H(21B) | 9160(20) | 4245(13) | 0(20) | 71(9) |
| H(22A) | 8530(20) | 3387(12) | 1560(20) | 68(8) |
| H(22B) | 8380(30) | 3182(13) | 480(20) | 71(10) |
| H(23) | 11470(30) | 2086(17) | -660(20) | 97(14) |
| H(24) | 9710(30) | 2657(16) | -1160(20) | 87(13) |
| H(25) | 8040(40) | 1873(18) | -1480(30) | 112(15) |
| H(26) | 8970(30) | 803(18) | -1090(20) | 95(15) |
| H(27) | 11080(30) | 904(16) | -550(20) | 80(12) |
| H(28) | 7290(50) | 910(30) | 220(40) | 180(30) |
| H(29) | 8590(30) | 554(19) | 1290(30) | 96(15) |
| H(30) | 8670(40) | 1250(20) | 2440(30) | 100(20) |
| H(31) | 7540(50) | 2130(30) | 2350(40) | 170(20) |
| H(32) | 6520(50) | 2060(30) | 770(40) | 200(20) |

3. Structure Report for $C_{20}H_{25}MgN$ (**9**).





No significant intramolecular or intermolecular hydrogen bonding interactions.

Table 1. Crystal data and structure refinement for bliM.

| | |
|---|---|
| Identification code | blim |
| Empirical formula | C20 H25 Mg N |
| Formula weight | 303.72 |
| Temperature | 295(2) K |
| Wavelength | 0.71073 A |
| Crystal system | Triclinic |
| Space group | p(-1) |
| Unit cell dimensions | a = 7.7678(13) A alpha = 79.116(3) deg. |
| | b = 7.8924(14) A beta = 89.416(3) deg. |
| | c = 15.083(3) A gamma = 80.735(3) deg. |
| Volume | 896.0(3) A^3 |
| Z | 2 |
| Density (calculated) | 1.126 Mg/m^3 |
| Absorption coefficient | 0.096 mm^-1 |
| F(000) | 328 |
| Crystal size | 0.35 x 0.35 x 0.30 mm |
| Theta range for data collection | 2.97 to 28.27 deg. |
| Index ranges | -10<=h<=10, -6<=k<=6, 0<=l<=12 |
| Reflections collected | 6358 |
| Independent reflections | 1037 [R(int) = 0.012] |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9718 and 0.9672 |

| | |
|---|---|
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 1037 / 0 / 230 |
| Goodness-of-fit on F^2 | 1.018 |
| Final R indices [I>2sigma(I)] | R1 = 0.0377, wR2 = 0.0929 |
| R indices (all data) | R1 = 0.0493, wR2 = 0.0989 |
| Extinction coefficient | 0.000(7) |
| Largest diff. peak and hole | 0.078 and -0.087 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for bliM. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mg(1) | 1490(1) | 4541(2) | 7116(1) | 54(1) |
| N(1) | 3559(2) | 2229(5) | 7224(3) | 53(2) |
| C(1) | 4512(3) | 2040(8) | 6380(3) | 53(2) |
| C(2) | 3209(4) | 2249(9) | 5602(4) | 81(3) |
| C(3) | 5763(3) | 340(8) | 6415(5) | 87(3) |
| C(4) | 4767(3) | 1972(6) | 8028(4) | 68(2) |
| C(5) | 3827(3) | 2009(10) | 8876(5) | 55(2) |
| C(6) | 3112(4) | 572(8) | 9316(4) | 72(2) |
| C(7) | 2238(5) | 572(14) | 10082(8) | 97(3) |
| C(8) | 2064(6) | 2020(19) | 10464(8) | 121(5) |
| C(9) | 2807(9) | 3480(12) | 10067(7) | 124(4) |
| C(10) | 3689(5) | 3426(13) | 9282(7) | 90(3) |
| C(11) | -422(5) | 2230(12) | 7721(8) | 73(4) |
| C(12) | -817(6) | 2762(13) | 6830(7) | 67(3) |
| C(13) | -1480(6) | 4519(17) | 6721(9) | 106(5) |
| C(14) | -1465(7) | 5020(17) | 7572(8) | 85(4) |
| C(15) | -793(5) | 3555(14) | 8179(7) | 66(3) |
| C(16) | 978(5) | 7963(12) | 6791(9) | 121(5) |
| C(17) | 2290(7) | 7274(12) | 7436(6) | 108(4) |
| C(18) | 3619(5) | 6440(9) | 6951(8) | 119(4) |
| C(19) | 2975(11) | 6565(12) | 6089(9) | 137(5) |
| C(20) | 1387(11) | 7510(18) | 6033(10) | 140(5) |

Table 3. Bond lengths [A] and angles [deg] for bliM.

| | |
|---|---|
| Mg(1)-N(1) | 2.210(4) |
| Mg(1)-C(14) | 2.382(6) |
| Mg(1)-C(18) | 2.386(5) |
| Mg(1)-C(13) | 2.392(5) |
| Mg(1)-C(19) | 2.430(9) |
| Mg(1)-C(17) | 2.471(8) |
| Mg(1)-C(15) | 2.497(7) |
| Mg(1)-C(12) | 2.535(6) |
| Mg(1)-C(11) | 2.565(7) |
| Mg(1)-C(20) | 2.582(14) |
| Mg(1)-C(16) | 2.618(10) |
| N(1)-C(1) | 1.486(6) |
| N(1)-C(4) | 1.503(6) |

| | |
|---|---|
| C(1)-C(3) | 1.517(8) |
| C(1)-C(2) | 1.525(6) |
| C(4)-C(5) | 1.470(9) |
| C(5)-C(10) | 1.362(9) |
| C(5)-C(6) | 1.395(9) |
| C(6)-C(7) | 1.334(12) |
| C(7)-C(8) | 1.362(11) |
| C(8)-C(9) | 1.402(14) |
| C(9)-C(10) | 1.366(12) |
| C(11)-C(15) | 1.351(9) |
| C(11)-C(12) | 1.354(10) |
| C(12)-C(13) | 1.379(13) |
| C(13)-C(14) | 1.414(12) |
| C(14)-C(15) | 1.365(14) |
| C(16)-C(20) | 1.282(14) |
| C(16)-C(17) | 1.388(14) |
| C(17)-C(18) | 1.407(12) |
| C(18)-C(19) | 1.378(16) |
| C(19)-C(20) | 1.330(13) |

| | |
|---|---|
| N(1)-Mg(1)-C(14) | 134.8(3) |
| N(1)-Mg(1)-C(18) | 90.93(17) |
| C(14)-Mg(1)-C(18) | 130.1(4) |
| N(1)-Mg(1)-C(13) | 123.4(4) |
| C(14)-Mg(1)-C(13) | 34.4(3) |
| C(18)-Mg(1)-C(13) | 140.8(3) |
| N(1)-Mg(1)-C(19) | 97.3(2) |
| C(14)-Mg(1)-C(19) | 127.1(4) |
| C(18)-Mg(1)-C(19) | 33.2(4) |
| C(13)-Mg(1)-C(19) | 115.5(4) |
| N(1)-Mg(1)-C(17) | 118.11(19) |
| C(14)-Mg(1)-C(17) | 97.1(3) |
| C(18)-Mg(1)-C(17) | 33.6(3) |
| C(13)-Mg(1)-C(17) | 118.5(4) |
| C(19)-Mg(1)-C(17) | 54.5(3) |
| N(1)-Mg(1)-C(15) | 104.7(2) |
| C(14)-Mg(1)-C(15) | 32.4(3) |
| C(18)-Mg(1)-C(15) | 140.7(4) |
| C(13)-Mg(1)-C(15) | 54.2(3) |
| C(19)-Mg(1)-C(15) | 157.7(3) |
| C(17)-Mg(1)-C(15) | 110.1(3) |
| N(1)-Mg(1)-C(12) | 91.3(2) |
| C(14)-Mg(1)-C(12) | 54.8(3) |
| C(18)-Mg(1)-C(12) | 164.4(4) |
| C(13)-Mg(1)-C(12) | 32.3(3) |
| C(19)-Mg(1)-C(12) | 131.2(4) |
| C(17)-Mg(1)-C(12) | 150.1(3) |
| C(15)-Mg(1)-C(12) | 52.9(3) |
| N(1)-Mg(1)-C(11) | 82.96(19) |
| C(14)-Mg(1)-C(11) | 52.4(3) |
| C(18)-Mg(1)-C(11) | 164.5(3) |
| C(13)-Mg(1)-C(11) | 51.9(3) |
| C(19)-Mg(1)-C(11) | 161.7(4) |
| C(17)-Mg(1)-C(11) | 140.8(3) |
| C(15)-Mg(1)-C(11) | 30.9(2) |
| C(12)-Mg(1)-C(11) | 30.8(2) |

| | |
|---|---|
| N(1)-Mg(1)-C(20) | 127.0(3) |
| C(14)-Mg(1)-C(20) | 96.5(4) |
| C(18)-Mg(1)-C(20) | 52.0(2) |
| C(13)-Mg(1)-C(20) | 89.7(3) |
| C(19)-Mg(1)-C(20) | 30.6(3) |
| C(17)-Mg(1)-C(20) | 51.6(4) |
| C(15)-Mg(1)-C(20) | 128.1(3) |
| C(12)-Mg(1)-C(20) | 115.6(3) |
| C(11)-Mg(1)-C(20) | 141.6(2) |
| N(1)-Mg(1)-C(16) | 142.45(14) |
| C(14)-Mg(1)-C(16) | 81.7(3) |
| C(18)-Mg(1)-C(16) | 51.78(15) |
| C(13)-Mg(1)-C(16) | 91.2(3) |
| C(19)-Mg(1)-C(16) | 50.1(3) |
| C(17)-Mg(1)-C(16) | 31.5(3) |
| C(15)-Mg(1)-C(16) | 107.9(3) |
| C(12)-Mg(1)-C(16) | 123.2(3) |
| C(11)-Mg(1)-C(16) | 134.1(2) |
| C(20)-Mg(1)-C(16) | 28.5(3) |
| C(1)-N(1)-C(4) | 112.4(2) |
| C(1)-N(1)-Mg(1) | 115.5(3) |
| C(4)-N(1)-Mg(1) | 113.9(3) |
| N(1)-C(1)-C(3) | 115.7(5) |
| N(1)-C(1)-C(2) | 109.6(2) |
| C(3)-C(1)-C(2) | 108.6(5) |
| C(5)-C(4)-N(1) | 112.6(3) |
| C(10)-C(5)-C(6) | 117.5(8) |
| C(10)-C(5)-C(4) | 120.9(8) |
| C(6)-C(5)-C(4) | 121.5(7) |
| C(7)-C(6)-C(5) | 122.9(7) |
| C(6)-C(7)-C(8) | 118.8(12) |
| C(7)-C(8)-C(9) | 120.7(12) |
| C(10)-C(9)-C(8) | 118.6(9) |
| C(5)-C(10)-C(9) | 121.4(10) |
| C(15)-C(11)-C(12) | 111.9(9) |
| C(15)-C(11)-Mg(1) | 71.7(5) |
| C(12)-C(11)-Mg(1) | 73.4(4) |
| C(11)-C(12)-C(13) | 105.5(9) |
| C(11)-C(12)-Mg(1) | 75.9(4) |
| C(13)-C(12)-Mg(1) | 68.1(4) |
| C(12)-C(13)-C(14) | 108.5(10) |
| C(12)-C(13)-Mg(1) | 79.5(3) |
| C(14)-C(13)-Mg(1) | 72.4(4) |
| C(15)-C(14)-C(13) | 106.6(9) |
| C(15)-C(14)-Mg(1) | 78.5(3) |
| C(13)-C(14)-Mg(1) | 73.2(4) |
| C(11)-C(15)-C(14) | 107.5(9) |
| C(11)-C(15)-Mg(1) | 77.3(5) |
| C(14)-C(15)-Mg(1) | 69.2(4) |
| C(20)-C(16)-C(17) | 111.0(7) |
| C(20)-C(16)-Mg(1) | 74.2(8) |
| C(17)-C(16)-Mg(1) | 68.4(5) |
| C(16)-C(17)-C(18) | 103.5(8) |
| C(16)-C(17)-Mg(1) | 80.1(4) |
| C(18)-C(17)-Mg(1) | 69.9(4) |
| C(19)-C(18)-C(17) | 107.3(5) |

| | |
|---|---|
| C(19)-C(18)-Mg(1) | 75.1(4) |
| C(17)-C(18)-Mg(1) | 76.5(3) |
| C(20)-C(19)-C(18) | 107.6(10) |
| C(20)-C(19)-Mg(1) | 81.0(6) |
| C(18)-C(19)-Mg(1) | 71.6(6) |
| C(16)-C(20)-C(19) | 110.4(12) |
| C(16)-C(20)-Mg(1) | 77.3(9) |
| C(19)-C(20)-Mg(1) | 68.4(7) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for bliM.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

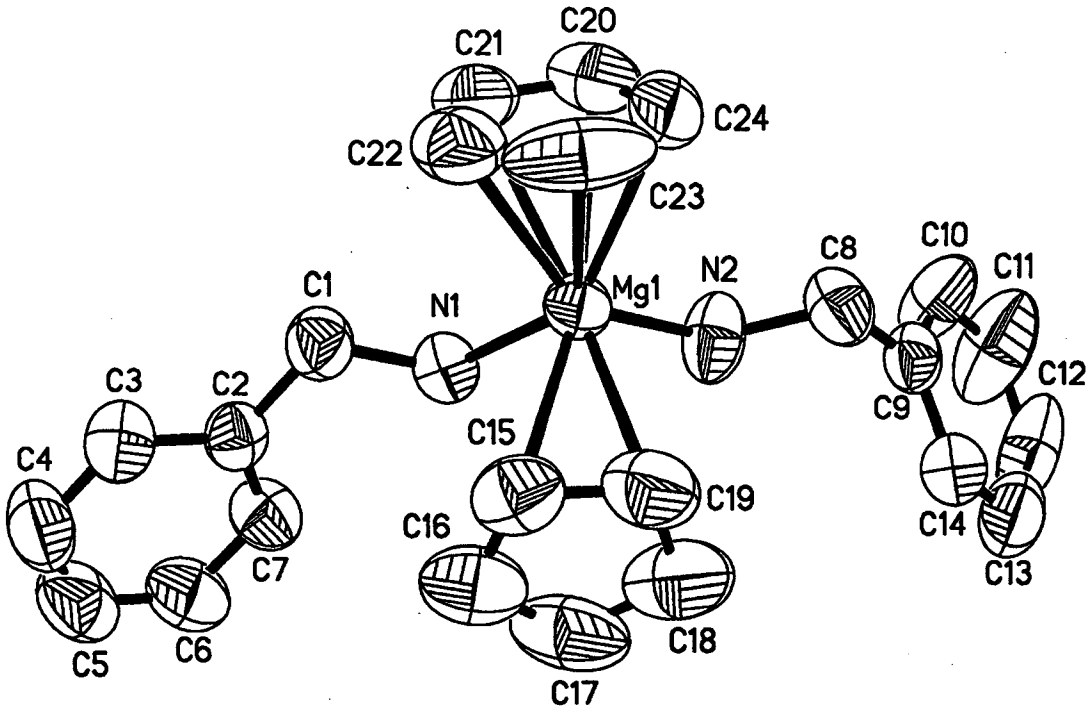
| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Mg(1) | 45(1) | 56(2) | 64(2) | -15(1) | 8(1) | -11(1) |
| N(1) | 43(1) | 58(4) | 61(5) | -12(2) | 7(1) | -13(1) |
| C(1) | 56(1) | 54(6) | 55(6) | -18(3) | 20(2) | -20(2) |
| C(2) | 84(2) | 130(8) | 37(8) | -31(4) | 21(2) | -23(2) |
| C(3) | 73(2) | 70(8) | 130(8) | -44(4) | 24(2) | -14(2) |
| C(4) | 48(1) | 99(6) | 51(7) | -5(3) | -2(2) | -7(1) |
| C(5) | 55(1) | 61(8) | 50(7) | -12(4) | -7(2) | -7(2) |
| C(6) | 72(2) | 103(8) | 36(8) | -1(4) | -9(2) | -19(2) |
| C(7) | 86(2) | 123(13) | 80(11) | 5(5) | -6(3) | -38(3) |
| C(8) | 98(3) | 190(20) | 69(12) | -20(9) | 10(3) | -22(4) |
| C(9) | 133(4) | 152(15) | 98(14) | -66(7) | -1(5) | -5(5) |
| C(10) | 96(3) | 91(12) | 86(11) | -19(6) | -4(3) | -19(3) |
| C(11) | 47(2) | 57(9) | 108(11) | 0(6) | 8(3) | -10(3) |
| C(12) | 58(2) | 93(9) | 57(10) | -18(6) | 8(3) | -32(3) |
| C(13) | 61(2) | 106(13) | 126(14) | 52(8) | -26(4) | -26(4) |
| C(14) | 63(2) | 79(12) | 122(13) | -39(8) | 18(4) | -12(4) |
| C(15) | 54(2) | 83(10) | 59(9) | -8(5) | 13(2) | -13(3) |
| C(16) | 74(2) | 81(9) | 202(15) | -19(7) | 5(4) | -1(2) |
| C(17) | 169(5) | 116(14) | 65(12) | -31(6) | 10(5) | -82(5) |
| C(18) | 63(2) | 66(8) | 223(13) | -5(5) | -1(3) | -22(2) |
| C(19) | 164(6) | 49(12) | 216(19) | -48(8) | 104(6) | -55(5) |
| C(20) | 155(6) | 97(15) | 160(20) | 25(8) | -26(6) | -43(6) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for bliM.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 2609 | 1260 | 5687 | 97 |
| H(2B) | 3818 | 2323 | 5042 | 97 |
| H(2C) | 2379 | 3298 | 5587 | 97 |
| H(3A) | 6581 | 184 | 6908 | 105 |
| H(3B) | 6380 | 380 | 5859 | 105 |
| H(3C) | 5120 | -618 | 6501 | 105 |
| H(4A) | 5533 | 857 | 8076 | 81 |

| | | | | |
|---|---|---|---|---|
| H(4B) | 5488 | 2884 | 7935 | 81 |
| H(6) | 3250 | -429 | 9065 | 86 |
| H(7) | 1755 | -400 | 10350 | 117 |
| H(8) | 1446 | 2041 | 10994 | 145 |
| H(9) | 2703 | 4463 | 10332 | 149 |
| H(10) | 4207 | 4378 | 9018 | 108 |
| H(16) | -60 | 8661 | 6894 | 145 |
| H(17) | 2292 | 7347 | 8045 | 130 |
| H(18) | 4726 | 5904 | 7172 | 143 |
| H(19) | 3548 | 6077 | 5631 | 164 |
| H(20) | 673 | 7801 | 5518 | 168 |
| H(1N1) | 2990(30) | 1310(60) | 7320(30) | 54(10) |
| H(1) | 5130(30) | 3000(70) | 6330(30) | 59(10) |
| H(11) | -10(40) | 1250(80) | 8000(30) | 48(14) |
| H(12) | -680(60) | 2340(120) | 6220(70) | 130(30) |
| H(13) | -1760(30) | 5280(70) | 6380(30) | 24(11) |
| H(14) | -1770(50) | 5820(100) | 7610(50) | 70(30) |
| H(15) | -650(50) | 3340(90) | 9000(50) | 120(20) |

4. Structure Report for $C_{24}H_{28}MgN_2$ (**10**).



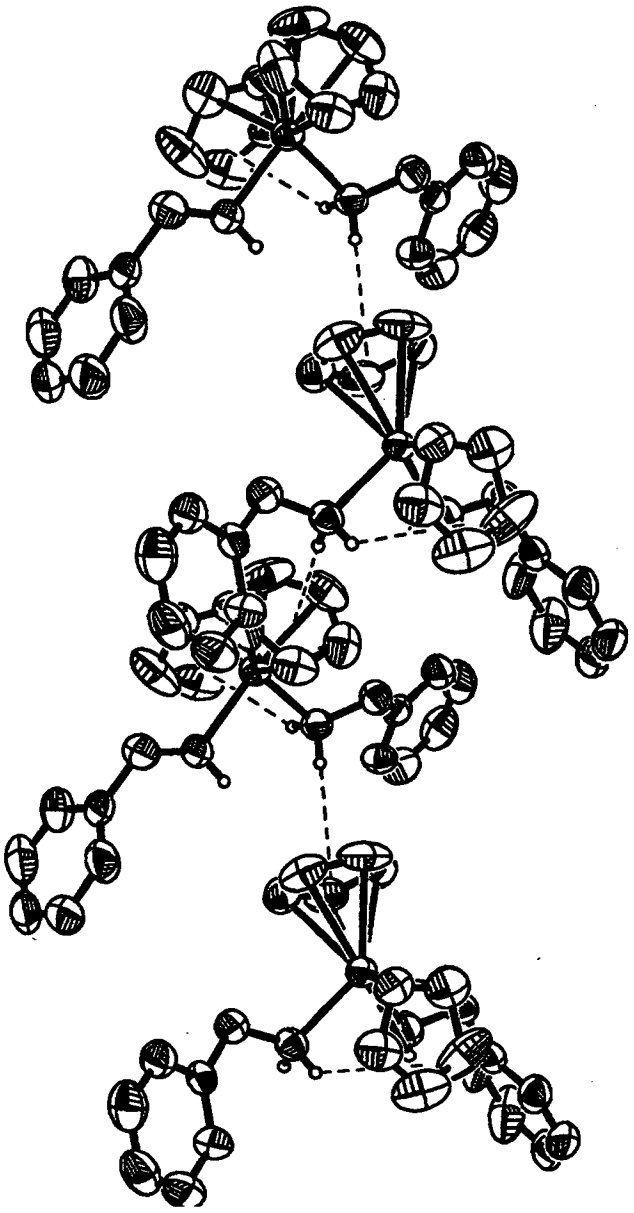


Table 1. Crystal data and structure refinement for mina.

| | |
|---|---|
| Identification code | mina |
| Empirical formula | C24 H28 Mg N2 |
| Formula weight | 368.79 |
| Temperature | 295(2) K |
| Wavelength | 0.71073 A |
| Crystal system | Monoclinic |
| Space group | C2/c |
| Unit cell dimensions | a = 25.648(9) A alpha = 90 deg. |
| | b = 11.527(4) A beta = 119.418(6) deg. |
| | c = 16.783(5) A gamma = 90 deg. |
| Volume | 4322(2) A^3 |
| Z | 8 |
| Density (calculated) | 1.134 Mg/m^3 |

| | |
|---|---|
| Absorption coefficient | 0.092 mm^-1 |
| F(000) | 1584 |
| Crystal size | 0.50 x 0.20 x 0.10 mm |
| Theta range for data collection | 1.99 to 28.26 deg. |
| Index ranges | -32<=h<=28, 0<=k<=15, 0<=l<=22 |
| Reflections collected | 30847 |
| Independent reflections | 4911 [R(int) = 0.027] |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9908 and 0.9554 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4911 / 0 / 357 |
| Goodness-of-fit on F^2 | 0.904 |
| Final R indices [I>2sigma(I)] | R1 = 0.0529, wR2 = 0.1459 |
| R indices (all data) | R1 = 0.1307, wR2 = 0.1771 |
| Extinction coefficient | 0.0006(4) |
| Largest diff. peak and hole | 0.331 and -0.183 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for mina. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mg(1) | 1933(1) | 3966(1) | 2835(1) | 55(1) |
| N(1) | 2582(1) | 5181(2) | 3779(1) | 59(1) |
| C(1) | 3165(1) | 4720(3) | 4481(2) | 68(1) |
| C(2) | 3441(1) | 5295(2) | 5398(2) | 56(1) |
| C(3) | 3858(1) | 4676(3) | 6152(2) | 77(1) |
| C(4) | 4126(2) | 5161(5) | 7016(2) | 101(1) |
| C(5) | 3986(2) | 6257(4) | 7149(2) | 97(1) |
| C(6) | 3576(2) | 6877(3) | 6415(2) | 88(1) |
| C(7) | 3307(1) | 6403(3) | 5543(2) | 70(1) |
| N(2) | 1407(1) | 5363(2) | 1965(3) | 77(1) |
| C(8) | 868(2) | 5186(3) | 1083(2) | 73(1) |
| C(9) | 500(1) | 6257(2) | 686(2) | 61(1) |
| C(10) | 551(2) | 6914(4) | 59(3) | 102(1) |
| C(11) | 221(2) | 7927(4) | -272(4) | 138(2) |
| C(12) | -156(2) | 8253(4) | 33(4) | 125(2) |
| C(13) | -226(2) | 7602(4) | 638(3) | 105(1) |
| C(14) | 99(1) | 6621(3) | 951(2) | 81(1) |
| C(15) | 1717(2) | 3368(3) | 4101(2) | 77(1) |
| C(16) | 1848(2) | 4306(3) | 4679(3) | 95(1) |
| C(17) | 1418(3) | 5105(4) | 4270(3) | 114(1) |
| C(18) | 998(2) | 4704(4) | 3434(3) | 131(2) |
| C(19) | 1184(2) | 3572(4) | 3313(2) | 95(1) |
| C(20) | 2248(2) | 3237(3) | 1753(2) | 87(1) |
| C(21) | 2703(2) | 3000(3) | 2579(3) | 86(1) |
| C(22) | 2539(2) | 2238(4) | 3003(3) | 94(1) |
| C(23) | 1954(3) | 1940(4) | 2425(5) | 125(2) |
| C(24) | 1766(2) | 2588(5) | 1626(3) | 108(2) |

Table 3. Bond lengths [A] and angles [deg] for mina.

| | |
|---|---|
| Mg(1)-N(2) | 2.146(3) |
| Mg(1)-N(1) | 2.156(2) |
| Mg(1)-C(24) | 2.444(3) |
| Mg(1)-C(23) | 2.443(4) |
| Mg(1)-C(22) | 2.457(3) |
| Mg(1)-C(19) | 2.459(4) |
| Mg(1)-C(20) | 2.471(3) |
| Mg(1)-C(21) | 2.483(3) |
| Mg(1)-C(15) | 2.540(3) |
| N(1)-C(1) | 1.474(3) |
| C(1)-C(2) | 1.496(4) |
| C(2)-C(7) | 1.375(4) |
| C(2)-C(3) | 1.388(4) |
| C(3)-C(4) | 1.381(5) |
| C(4)-C(5) | 1.362(5) |
| C(5)-C(6) | 1.365(5) |
| C(6)-C(7) | 1.387(4) |
| N(2)-C(8) | 1.461(4) |
| C(8)-C(9) | 1.497(4) |
| C(9)-C(10) | 1.356(4) |
| C(9)-C(14) | 1.371(4) |
| C(10)-C(11) | 1.388(6) |
| C(11)-C(12) | 1.350(7) |
| C(12)-C(13) | 1.344(6) |
| C(13)-C(14) | 1.348(5) |
| C(15)-C(19) | 1.378(5) |
| C(15)-C(16) | 1.379(5) |
| C(16)-C(17) | 1.338(5) |
| C(17)-C(18) | 1.363(6) |
| C(18)-C(19) | 1.437(6) |
| C(20)-C(21) | 1.329(5) |
| C(20)-C(24) | 1.370(6) |
| C(21)-C(22) | 1.323(5) |
| C(22)-C(23) | 1.371(7) |
| C(23)-C(24) | 1.397(7) |

| | |
|---|---|
| N(2)-Mg(1)-N(1) | 90.75(11) |
| N(2)-Mg(1)-C(24) | 97.33(17) |
| N(1)-Mg(1)-C(24) | 142.08(16) |
| N(2)-Mg(1)-C(23) | 128.2(2) |
| N(1)-Mg(1)-C(23) | 135.4(2) |
| C(24)-Mg(1)-C(23) | 33.21(17) |
| N(2)-Mg(1)-C(22) | 146.79(15) |
| N(1)-Mg(1)-C(22) | 103.02(15) |
| C(24)-Mg(1)-C(22) | 53.88(14) |
| C(23)-Mg(1)-C(22) | 32.49(17) |
| N(2)-Mg(1)-C(19) | 91.76(15) |
| N(1)-Mg(1)-C(19) | 108.99(12) |
| C(24)-Mg(1)-C(19) | 107.71(18) |
| C(23)-Mg(1)-C(19) | 92.54(15) |
| C(22)-Mg(1)-C(19) | 111.36(16) |
| N(2)-Mg(1)-C(20) | 94.47(15) |
| N(1)-Mg(1)-C(20) | 110.32(13) |
| C(24)-Mg(1)-C(20) | 32.36(14) |
| C(23)-Mg(1)-C(20) | 53.61(14) |

| | |
|---|---|
| C(22)-Mg(1)-C(20) | 52.47(11) |
| C(19)-Mg(1)-C(20) | 140.07(15) |
| N(2)-Mg(1)-C(21) | 120.36(16) |
| N(1)-Mg(1)-C(21) | 91.46(11) |
| C(24)-Mg(1)-C(21) | 52.68(13) |
| C(23)-Mg(1)-C(21) | 52.59(15) |
| C(22)-Mg(1)-C(21) | 31.07(12) |
| C(19)-Mg(1)-C(21) | 142.07(15) |
| C(20)-Mg(1)-C(21) | 31.12(11) |
| N(2)-Mg(1)-C(15) | 116.82(15) |
| N(1)-Mg(1)-C(15) | 88.22(11) |
| C(24)-Mg(1)-C(15) | 119.77(19) |
| C(23)-Mg(1)-C(15) | 91.15(15) |
| C(22)-Mg(1)-C(15) | 93.97(13) |
| C(19)-Mg(1)-C(15) | 31.94(11) |
| C(20)-Mg(1)-C(15) | 143.80(12) |
| C(21)-Mg(1)-C(15) | 122.82(13) |
| C(1)-N(1)-Mg(1) | 117.84(17) |
| N(1)-C(1)-C(2) | 116.4(2) |
| C(7)-C(2)-C(3) | 117.6(3) |
| C(7)-C(2)-C(1) | 124.1(2) |
| C(3)-C(2)-C(1) | 118.3(3) |
| C(4)-C(3)-C(2) | 120.8(4) |
| C(5)-C(4)-C(3) | 120.8(4) |
| C(4)-C(5)-C(6) | 119.1(3) |
| C(5)-C(6)-C(7) | 120.6(4) |
| C(2)-C(7)-C(6) | 121.0(3) |
| C(8)-N(2)-Mg(1) | 123.4(2) |
| N(2)-C(8)-C(9) | 114.4(2) |
| C(10)-C(9)-C(14) | 117.1(3) |
| C(10)-C(9)-C(8) | 121.7(3) |
| C(14)-C(9)-C(8) | 121.3(3) |
| C(9)-C(10)-C(11) | 120.5(4) |
| C(12)-C(11)-C(10) | 119.5(4) |
| C(13)-C(12)-C(11) | 121.1(4) |
| C(12)-C(13)-C(14) | 118.4(4) |
| C(13)-C(14)-C(9) | 123.3(4) |
| C(19)-C(15)-C(16) | 109.0(4) |
| C(19)-C(15)-Mg(1) | 70.80(18) |
| C(16)-C(15)-Mg(1) | 107.3(2) |
| C(17)-C(16)-C(15) | 109.0(4) |
| C(16)-C(17)-C(18) | 109.2(4) |
| C(17)-C(18)-C(19) | 107.8(4) |
| C(15)-C(19)-C(18) | 105.1(4) |
| C(15)-C(19)-Mg(1) | 77.3(2) |
| C(18)-C(19)-Mg(1) | 104.1(3) |
| C(21)-C(20)-C(24) | 108.2(4) |
| C(21)-C(20)-Mg(1) | 74.96(18) |
| C(24)-C(20)-Mg(1) | 72.7(2) |
| C(22)-C(21)-C(20) | 110.4(4) |
| C(22)-C(21)-Mg(1) | 73.36(19) |
| C(20)-C(21)-Mg(1) | 73.92(19) |
| C(21)-C(22)-C(23) | 108.2(4) |
| C(21)-C(22)-Mg(1) | 75.6(2) |
| C(23)-C(22)-Mg(1) | 73.2(2) |
| C(22)-C(23)-C(24) | 106.7(4) |

| | |
|---|---|
| C(22)-C(23)-Mg(1) | 74.3(2) |
| C(24)-C(23)-Mg(1) | 73.4(2) |
| C(20)-C(24)-C(23) | 106.5(4) |
| C(20)-C(24)-Mg(1) | 74.9(2) |
| C(23)-C(24)-Mg(1) | 73.4(2) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for mina.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Mg(1) | 57(1) | 51(1) | 55(1) | -5(1) | 27(1) | 0(1) |
| N(1) | 62(1) | 53(1) | 57(1) | 3(1) | 27(1) | -4(1) |
| C(1) | 63(2) | 65(2) | 65(2) | -7(1) | 24(2) | 2(2) |
| C(2) | 49(1) | 59(2) | 58(1) | 0(1) | 24(1) | -8(1) |
| C(3) | 69(2) | 74(2) | 76(2) | 2(2) | 27(2) | 2(2) |
| C(4) | 79(2) | 137(4) | 63(2) | 9(2) | 17(2) | 2(2) |
| C(5) | 88(2) | 124(3) | 70(2) | -27(2) | 33(2) | -31(2) |
| C(6) | 105(3) | 84(2) | 78(2) | -22(2) | 46(2) | -14(2) |
| C(7) | 83(2) | 60(2) | 64(2) | -2(1) | 34(2) | -2(2) |
| N(2) | 55(2) | 57(2) | 90(2) | 0(2) | 13(1) | -3(1) |
| C(8) | 78(2) | 66(2) | 59(2) | -6(2) | 22(2) | 0(2) |
| C(9) | 51(1) | 64(2) | 58(1) | -7(1) | 18(1) | -7(1) |
| C(10) | 68(2) | 127(3) | 124(3) | 45(3) | 56(2) | 26(2) |
| C(11) | 85(3) | 138(4) | 184(5) | 87(4) | 60(3) | 19(3) |
| C(12) | 55(2) | 82(3) | 183(5) | 1(3) | 15(3) | 7(2) |
| C(13) | 62(2) | 115(3) | 110(3) | -30(3) | 21(2) | 11(2) |
| C(14) | 65(2) | 106(3) | 67(2) | -9(2) | 27(2) | 2(2) |
| C(15) | 88(2) | 69(2) | 93(2) | 14(2) | 59(2) | 4(2) |
| C(16) | 127(3) | 84(3) | 106(3) | -1(2) | 82(3) | -16(2) |
| C(17) | 192(5) | 91(3) | 108(3) | 27(2) | 112(3) | 28(3) |
| C(18) | 164(4) | 153(4) | 111(3) | 70(3) | 96(3) | 97(4) |
| C(19) | 112(3) | 109(3) | 82(2) | -1(2) | 61(2) | 3(3) |
| C(20) | 121(3) | 76(2) | 78(2) | -2(2) | 61(2) | 10(2) |
| C(21) | 81(2) | 101(3) | 88(2) | -25(2) | 50(2) | 1(2) |
| C(22) | 125(3) | 86(3) | 81(2) | 11(2) | 59(2) | 40(3) |
| C(23) | 198(6) | 54(2) | 218(7) | -37(3) | 176(6) | -29(3) |
| C(24) | 80(3) | 124(4) | 81(3) | -55(3) | 10(2) | 26(3) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for mina.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(01) | 2359(13) | 5460(30) | 4037(19) | 94(10) |
| H(02) | 2626(13) | 5810(30) | 3530(20) | 92(11) |
| H(1A) | 3100(12) | 3890(30) | 4570(18) | 88(9) |
| H(1B) | 3465(12) | 4730(20) | 4285(17) | 84(9) |
| H(3) | 3946(12) | 3950(20) | 6032(17) | 75(9) |

| | | | | |
|---|---|---|---|---|
| H(4) | 4343(16) | 4770(30) | 7460(20) | 106(13) |
| H(5) | 4136(15) | 6600(30) | 7750(20) | 116(11) |
| H(6) | 3418(13) | 7690(30) | 6470(19) | 92(9) |
| H(7) | 3058(12) | 6880(20) | 5064(18) | 71(8) |
| H(03) | 1670(20) | 5800(50) | 1900(30) | 190(20) |
| H(04) | 1400(20) | 5690(40) | 2290(30) | 130(20) |
| H(8A) | 634(13) | 4640(30) | 1135(18) | 86(10) |
| H(8B) | 993(14) | 4840(30) | 710(20) | 115(12) |
| H(10) | 775(14) | 6680(30) | -118(19) | 84(10) |
| H(11) | 280(20) | 8230(40) | -720(30) | 153(17) |
| H(12) | -370(20) | 8840(40) | -140(30) | 158(19) |
| H(13) | -540(20) | 7960(40) | 820(30) | 182(18) |
| H(14) | 80(15) | 6200(30) | 1430(20) | 114(12) |
| H(15) | 1938(14) | 2670(30) | 4200(20) | 101(11) |
| H(16) | 2260(20) | 4520(40) | 5350(30) | 172(17) |
| H(17) | 1470(30) | 6060(50) | 4520(40) | 220(20) |
| H(18) | 735(18) | 5190(30) | 3110(30) | 133(15) |
| H(19) | 992(12) | 3010(20) | 2895(17) | 65(8) |
| H(20) | 2234(16) | 3810(30) | 1230(20) | 123(11) |
| H(21) | 3120(20) | 3330(30) | 2810(30) | 146(15) |
| H(22) | 2818(16) | 1930(30) | 3650(20) | 119(12) |
| H(23) | 1886(15) | 1580(30) | 2630(20) | 75(12) |
| H(24) | 1541(16) | 2690(30) | 1200(20) | 106(15) |