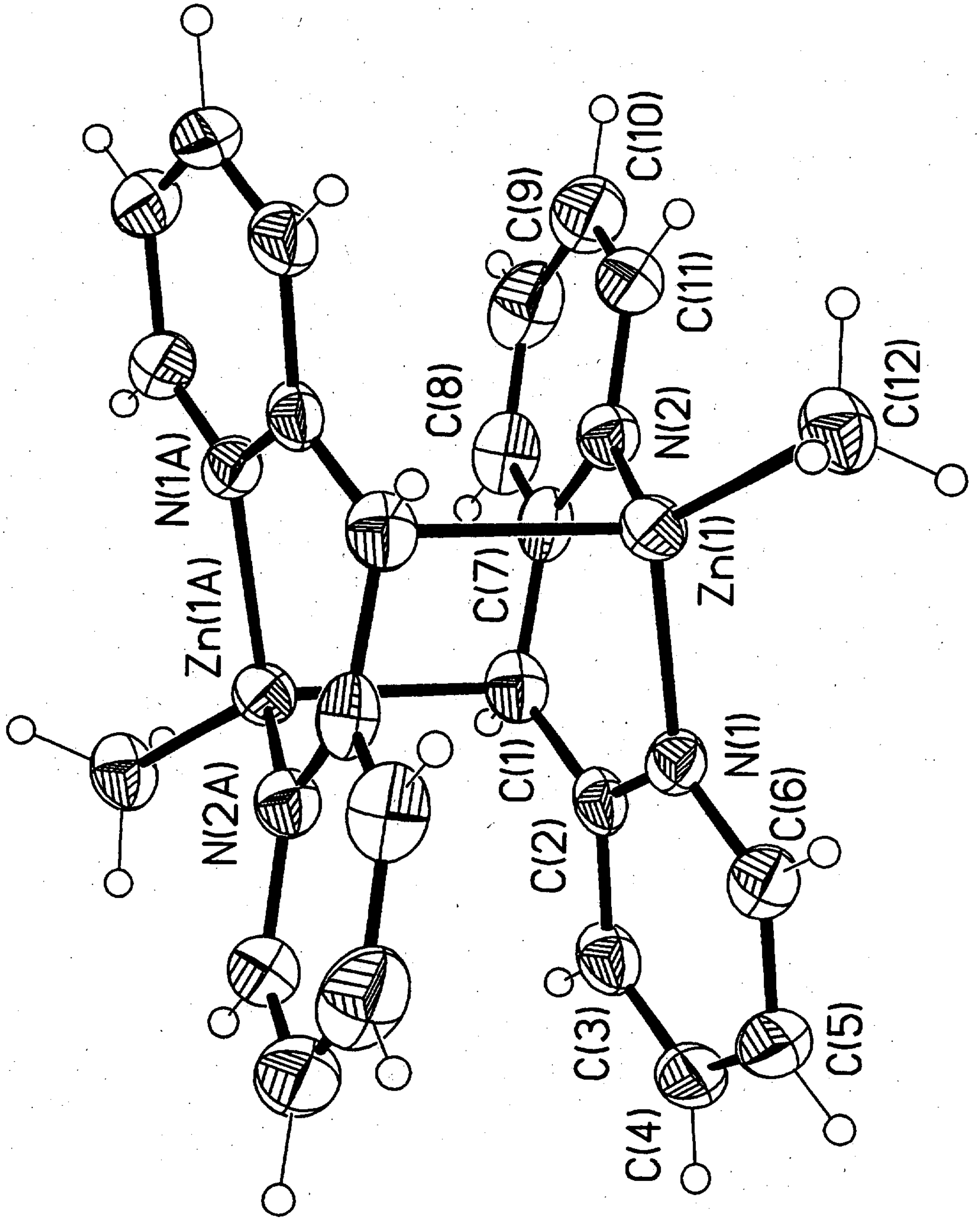
C(10)
C(9)
C(11)
C(12)
C(8)
N(2)
N(1A)
C(7)
Zn(1)
Zn(1A)
C(1)
N(1)
N(2A)
C(2)
C(6)
C(3)
C(5)
C(4)

Table 1. Crystal data and structure refinement for helgneu.

| | |
|---|---|
| Identification code | helgneu |
| Empirical formula | C15.50 H16 N2 Zn |
| Formula weight | 295.67 |
| Temperature | 153(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Monoclinic, P2(1)/n |
| Unit cell dimensions | a = 9.270(2) A alpha = 90 deg.<br>b = 13.491(3) A beta = 98.10(3) deg.<br>c = 11.000(2) A gamma = 90 deg. |
| Volume | 1362.0(5) A^3 |
| Z, Calculated density | 4, 1.442 Mg/m^3 |
| Absorption coefficient | 1.788 mm^-1 |
| F(000) | 612 |
| Crystal size | 0.3 x 0.3 x 0.3 mm |
| Theta range for data collection | 4.04 to 25.05 deg. |
| Index ranges | -11<=h<=11, 0<=k<=16, -11<=l<=13 |
| Reflections collected / unique | 2428 / 2393 [R(int) = 0.0177] |
| Completeness to 2theta = 25.05 | 95.1% |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 2393 / 67 / 205 |
| Goodness-of-fit on F^2 | 1.038 |
| Final R indices [I>2sigma(I)] | R1 = 0.0353, wR2 = 0.0927 |
| R indices (all data) | R1 = 0.0426, wR2 = 0.0980 |
| Largest diff. peak and hole | 0.533 and -0.712 e.A^-3 |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Zn(1) | 1883(1) | 9285(1) | 5087(1) | 30(1) |
| N(1) | 453(2) | 8679(2) | 6133(2) | 29(1) |
| N(2) | 496(3) | 9083(2) | 3499(2) | 31(1) |
| C(1) | -1626(3) | 9068(2) | 4593(3) | 32(1) |
| C(2) | -1008(3) | 8699(2) | 5774(3) | 30(1) |
| C(3) | -1935(3) | 8358(2) | 6611(3) | 37(1) |
| C(4) | -1356(4) | 8012(2) | 7736(3) | 42(1) |
| C(5) | 135(4) | 7990(2) | 8079(3) | 41(1) |
| C(6) | 988(3) | 8331(2) | 7249(3) | 36(1) |
| C(7) | -973(3) | 9050(2) | 3480(3) | 33(1) |
| C(8) | -1874(4) | 9036(2) | 2332(3) | 43(1) |
| C(9) | -1277(5) | 9063(3) | 1262(3) | 53(1) |
| C(10) | 213(4) | 9089(2) | 1303(3) | 49(1) |
| C(11) | 1051(4) | 9095(2) | 2431(3) | 39(1) |
| C(12) | 3932(3) | 8841(2) | 5292(3) | 39(1) |
| C(13) | -5055(12) | 8398(7) | -932(9) | 55(2) |
| C(14) | -5045(7) | 9373(5) | -306(6) | 39(1) |
| C(15) | -4470(2) | 10200(9) | -756(16) | 63(3) |
| C(16) | -4419(11) | 11084(7) | -188(16) | 93(3) |
| C(17) | -4953(13) | 11139(8) | 926(14) | 88(4) |
| C(18) | -5543(9) | 10321(7) | 1412(9) | 69(2) |
| C(19) | -5570(2) | 9459(8) | 782(11) | 42(2) |

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

| | |
|---|---|
| Zn(1)-C(12) | 1.974(3) |
| Zn(1)-N(2) | 2.035(2) |
| Zn(1)-N(1) | 2.045(2) |
| Zn(1)-C(1)#1 | 2.268(3) |
| N(1)-C(6) | 1.342(4) |
| N(1)-C(2) | 1.356(3) |
| N(2)-C(11) | 1.348(4) |
| N(2)-C(7) | 1.359(4) |
| C(1)-C(2) | 1.433(4) |
| C(1)-C(7) | 1.440(4) |
| C(1)-Zn(1)#1 | 2.268(3) |
| C(1)-H(1) | 0.88(4) |
| C(2)-C(3) | 1.422(4) |
| C(3)-C(4) | 1.361(4) |
| C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.381(5) |
| C(4)-H(4) | 0.9500 |
| C(5)-C(6) | 1.369(4) |
| C(5)-H(5) | 0.9500 |
| C(6)-H(6) | 0.9500 |
| C(7)-C(8) | 1.413(4) |
| C(8)-C(9) | 1.370(5) |
| C(8)-H(8) | 0.9500 |
| C(9)-C(10) | 1.376(5) |
| C(9)-H(9) | 0.9500 |
| C(10)-C(11) | 1.368(5) |
| C(10)-H(10) | 0.9500 |
| C(11)-H(11) | 0.9500 |
| C(12)-H(12A) | 0.9800 |
| C(12)-H(12B) | 0.9800 |
| C(12)-H(12C) | 0.9800 |
| C(13)-C(14) | 1.484(11) |
| C(13)-H(13A) | 0.9800 |
| C(13)-H(13B) | 0.9800 |
| C(13)-H(13C) | 0.9800 |
| C(14)-C(15) | 1.359(10) |
| C(14)-C(19) | 1.359(10) |
| C(15)-C(16) | 1.345(12) |
| C(15)-H(15) | 0.9500 |
| C(16)-C(17) | 1.386(14) |
| C(16)-H(16) | 0.9500 |
| C(17)-C(18) | 1.374(13) |
| C(17)-H(17) | 0.9500 |
| C(18)-C(19) | 1.353(11) |
| C(18)-H(18) | 0.9500 |
| C(19)-H(19) | 0.9500 |
| | |
| C(12)-Zn(1)-N(2) | 122.61(12) |
| C(12)-Zn(1)-N(1) | 120.28(11) |
| N(2)-Zn(1)-N(1) | 92.77(9) |
| C(12)-Zn(1)-C(1)#1 | 113.58(12) |
| N(2)-Zn(1)-C(1)#1 | 101.35(10) |
| N(1)-Zn(1)-C(1)#1 | 102.31(10) |
| C(6)-N(1)-C(2) | 119.9(2) |
| C(6)-N(1)-Zn(1) | 118.00(19) |
| C(2)-N(1)-Zn(1) | 121.85(18) |
| C(11)-N(2)-C(7) | 119.4(3) |
| C(11)-N(2)-Zn(1) | 118.3(2) |
| C(7)-N(2)-Zn(1) | 121.89(19) |
| C(2)-C(1)-C(7) | 127.0(3) |

| | |
|---|---|
| C(2)-C(1)-Zn(1)#1 | 103.68(19) |
| C(7)-C(1)-Zn(1)#1 | 102.40(18) |
| C(2)-C(1)-H(1) | 114(2) |
| C(7)-C(1)-H(1) | 110(2) |
| Zn(1)#1-C(1)-H(1) | 93(2) |
| N(1)-C(2)-C(3) | 118.4(3) |
| N(1)-C(2)-C(1) | 121.8(2) |
| C(3)-C(2)-C(1) | 119.9(3) |
| C(4)-C(3)-C(2) | 120.2(3) |
| C(4)-C(3)-H(3) | 119.9 |
| C(2)-C(3)-H(3) | 119.9 |
| C(3)-C(4)-C(5) | 120.5(3) |
| C(3)-C(4)-H(4) | 119.8 |
| C(5)-C(4)-H(4) | 119.8 |
| C(6)-C(5)-C(4) | 117.4(3) |
| C(6)-C(5)-H(5) | 121.3 |
| C(4)-C(5)-H(5) | 121.3 |
| N(1)-C(6)-C(5) | 123.6(3) |
| N(1)-C(6)-H(6) | 118.2 |
| C(5)-C(6)-H(6) | 118.2 |
| N(2)-C(7)-C(8) | 118.7(3) |
| N(2)-C(7)-C(1) | 121.7(3) |
| C(8)-C(7)-C(1) | 119.6(3) |
| C(9)-C(8)-C(7) | 120.5(3) |
| C(9)-C(8)-H(8) | 119.7 |
| C(7)-C(8)-H(8) | 119.7 |
| C(8)-C(9)-C(10) | 119.8(3) |
| C(8)-C(9)-H(9) | 120.1 |
| C(10)-C(9)-H(9) | 120.1 |
| C(11)-C(10)-C(9) | 118.0(3) |
| C(11)-C(10)-H(10) | 121.0 |
| C(9)-C(10)-H(10) | 121.0 |
| N(2)-C(11)-C(10) | 123.6(3) |
| N(2)-C(11)-H(11) | 118.2 |
| C(10)-C(11)-H(11) | 118.2 |
| Zn(1)-C(12)-H(12A) | 109.5 |
| Zn(1)-C(12)-H(12B) | 109.5 |
| H(12A)-C(12)-H(12B) | 109.5 |
| Zn(1)-C(12)-H(12C) | 109.5 |
| H(12A)-C(12)-H(12C) | 109.5 |
| H(12B)-C(12)-H(12C) | 109.5 |
| C(15)-C(14)-C(19) | 117.3(8) |
| C(15)-C(14)-C(13) | 122.4(9) |
| C(19)-C(14)-C(13) | 120.3(8) |
| C(16)-C(15)-C(14) | 123.3(12) |
| C(16)-C(15)-H(15) | 118.4 |
| C(14)-C(15)-H(15) | 118.4 |
| C(15)-C(16)-C(17) | 117.7(12) |
| C(15)-C(16)-H(16) | 121.1 |
| C(17)-C(16)-H(16) | 121.1 |
| C(18)-C(17)-C(16) | 120.8(12) |
| C(18)-C(17)-H(17) | 119.6 |
| C(16)-C(17)-H(17) | 119.6 |
| C(19)-C(18)-C(17) | 118.1(11) |
| C(19)-C(18)-H(18) | 121.0 |
| C(17)-C(18)-H(18) | 121.0 |
| C(18)-C(19)-C(14) | 122.8(10) |
| C(18)-C(19)-H(19) | 118.6 |
| C(14)-C(19)-H(19) | 118.6 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+2,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for helgneu.
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 |
|---|---|---|---|---|---|---|
| Zn(1) | 24(1) | 33(1) | 33(1) | 2(1) | 6(1) | 2(1) |
| N(1) | 29(1) | 25(1) | 35(1) | 3(1) | 7(1) | 0(1) |
| N(2) | 34(1) | 28(1) | 32(1) | -1(1) | 5(1) | 1(1) |
| C(1) | 22(1) | 31(1) | 44(2) | -1(1) | 4(1) | -2(1) |
| C(2) | 28(1) | 20(1) | 42(2) | -3(1) | 10(1) | 1(1) |
| C(3) | 32(2) | 30(1) | 54(2) | -1(1) | 18(1) | 0(1) |
| C(4) | 53(2) | 30(2) | 49(2) | 4(1) | 27(2) | -2(1) |
| C(5) | 54(2) | 34(2) | 37(2) | 4(1) | 14(1) | 1(1) |
| C(6) | 37(2) | 33(2) | 37(2) | 3(1) | 6(1) | 1(1) |
| C(7) | 33(2) | 22(1) | 40(2) | -1(1) | -2(1) | 1(1) |
| C(8) | 41(2) | 37(2) | 47(2) | -3(1) | -7(1) | -1(1) |
| C(9) | 73(3) | 43(2) | 36(2) | -1(1) | -12(2) | -1(2) |
| C(10) | 71(3) | 42(2) | 34(2) | -3(1) | 8(2) | 3(2) |
| C(11) | 48(2) | 35(2) | 35(2) | 0(1) | 12(1) | 4(1) |
| C(12) | 26(2) | 41(2) | 52(2) | -2(1) | 6(1) | 3(1) |
| C(13) | 50(5) | 54(6) | 60(5) | -3(4) | 7(4) | 9(5) |
| C(14) | 28(3) | 39(4) | 50(4) | 7(3) | 6(3) | 3(3) |
| C(15) | 40(5) | 56(7) | 94(7) | 37(6) | 17(5) | -2(8) |
| C(16) | 48(5) | 44(5) | 182(11) | 40(7) | -3(7) | -11(5) |
| C(17) | 49(6) | 36(6) | 168(10) | -24(7) | -24(6) | 10(5) |
| C(18) | 47(4) | 76(6) | 83(6) | -25(5) | 2(4) | 12(4) |
| C(19) | 37(5) | 36(6) | 55(5) | 20(5) | 11(4) | 1(6) |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | -2570(4) | 8970(3) | 4420(3) | 47(9) |
| H(3) | -2963 | 8372 | 6383 | 45 |
| H(4) | -1982 | 7783 | 8290 | 51 |
| H(5) | 553 | 7747 | 8861 | 49 |
| H(6) | 2016 | 8321 | 7476 | 43 |
| H(8) | -2903 | 9007 | 2302 | 51 |
| H(9) | -1890 | 9063 | 493 | 63 |
| H(10) | 647 | 9103 | 571 | 59 |
| H(11) | 2081 | 9109 | 2463 | 46 |
| H(12A) | 3985 | 8141 | 5534 | 59 |
| H(12B) | 4508 | 9240 | 5929 | 59 |
| H(12C) | 4321 | 8921 | 4514 | 59 |
| H(13A) | -4187 | 8021 | -595 | 82 |
| H(13B) | -5056 | 8501 | -1814 | 82 |
| H(13C) | -5930 | 8029 | -800 | 82 |
| H(15) | -4083 | 10150 | -1509 | 75 |
| H(16) | -4032 | 11652 | -538 | 112 |
| H(17) | -4911 | 11751 | 1358 | 106 |
| H(18) | -5921 | 10359 | 2170 | 83 |
| H(19) | -5972 | 8889 | 1114 | 51 |