Table 5. Bond angles [deg] for **4a**.

C(11)-Co(1)-C(7) 103.9(6) C(11)-Co(1)-C(5) 121.2(4)

C(7)-Co(1)-C(5) 63.3(4) C(11)-Co(1)-C(6) 96.0(3)

C(7)-Co(1)-C(6) 38.2(6) C(5)-Co(1)-C(6) 37.0(5)

C(11)-Co(1)-C(3) 139.3(6) C(7)-Co(1)-C(3) 38.5(6)

C(5)-Co(1)-C(3) 64.0(3) C(6)-Co(1)-C(3) 64.0(5)

C(11)-Co(1)-C(4) 158.9(3) C(7)-Co(1)-C(4) 63.5(5)

C(5)-Co(1)-C(4) 38.9(3) C(6)-Co(1)-C(4) 63.5(3)

C(3)-Co(1)-C(4) 37.6(4) C(11)-Co(1)-S(2) 72.38(15)

C(7)-Co(1)-S(2) 105.2(5) C(5)-Co(1)-S(2) 163.1(2)

C(6)-Co(1)-S(2) 139.1(6) C(3)-Co(1)-S(2) 99.2(2)

C(4)-Co(1)-S(2) 125.9(3) C(11)-Co(1)-S(1) 92.80(14)

C(7)-Co(1)-S(1) 157.9(3) C(5)-Co(1)-S(1) 95.7(3)

C(6)-Co(1)-S(1) 126.7(6) C(3)-Co(1)-S(1) 127.8(6)

C(4)-Co(1)-S(1) 96.1(3) S(2)-Co(1)-S(1) 93.51(5)

C(1)-S(1)-Co(1) 103.77(16)C(10)-S(2)-C(2) 106.7(2)

C(10)-S(2)-Co(1) 79.29(16)C(2)-S(2)-Co(1) 105.73(15)

C(9)-O(2)-C(8) 116.8(5) C(12)-O(4)-C(13) 115.9(5)

C(2)-C(1)-B(5) 108.4(4) C(2)-C(1)-B(4) 109.0(4)

B(5)-C(1)-B(4) 62.8(4) C(2)-C(1)-B(3) 60.8(3)

B(5)-C(1)-B(3) 112.8(4) B(4)-C(1)-B(3) 61.4(3)

C(2)-C(1)-B(6) 60.4(3) B(5)-C(1)-B(6) 61.2(3)

B(4)-C(1)-B(6) 112.8(4) B(3)-C(1)-B(6) 112.7(4)

C(2)-C(1)-S(1) 118.4(3) B(5)-C(1)-S(1) 122.2(3)

B(4)-C(1)-S(1) 123.5(4) B(3)-C(1)-S(1) 118.5(4)

B(6)-C(1)-S(1) 116.3(3) C(1)-C(2)-B(11) 112.9(4)

C(1)-C(2)-B(7) 112.4(4) B(11)-C(2)-B(7) 62.5(3)

C(1)-C(2)-B(6) 62.1(3) B(11)-C(2)-B(6) 63.2(3)

B(7)-C(2)-B(6) 115.0(4) C(1)-C(2)-B(3) 61.9(3)

B(11)-C(2)-B(3) 114.6(4) B(7)-C(2)-B(3) 62.5(3)

B(6)-C(2)-B(3) 115.1(4) C(1)-C(2)-S(2) 115.0(3)

B(11)-C(2)-S(2) 125.3(3) B(7)-C(2)-S(2) 117.9(3)

B(6)-C(2)-S(2) 121.5(3) B(3)-C(2)-S(2) 110.1(3)

C(4)-C(3)-C(7) 106.8(10) C(4)-C(3)-Co(1) 71.7(4)

C(7)-C(3)-Co(1) 68.3(6) C(3)-C(4)-C(5) 106.2(9)

C(3)-C(4)-Co(1) 70.6(5) C(5)-C(4)-Co(1) 67.7(4)

C(6)-C(5)-C(4) 109.5(10) C(6)-C(5)-Co(1) 72.0(5)

C(4)-C(5)-Co(1) 73.4(4) C(5)-C(6)-C(7) 108.4(12)

C(5)-C(6)-Co(1) 71.0(5) C(7)-C(6)-Co(1) 70.3(6)

C(6)-C(7)-C(3) 108.9(10) C(6)-C(7)-Co(1) 71.5(6)

C(3)-C(7)-Co(1) 73.2(6) O(1)-C(9)-O(2) 125.8(5)

O(1)-C(9)-C(10) 122.8(5) O(2)-C(9)-C(10) 111.4(4)

C(11)-C(10)-C(9) 134.2(5) C(11)-C(10)-S(2) 104.0(4)

C(9)-C(10)-S(2) 121.4(4) C(10)-C(11)-C(12) 125.5(5)

C(10)-C(11)-Co(1) 104.4(4) C(12)-C(11)-Co(1) 129.7(4)

O(3)-C(12)-O(4) 125.1(5) O(3)-C(12)-C(11) 123.2(5)

O(4)-C(12)-C(11) 111.7(4) C(2)-B(3)-C(1) 57.3(3)

C(2)-B(3)-B(8) 104.2(4) C(1)-B(3)-B(8) 105.5(5)

C(2)-B(3)-B(4) 104.0(4) C(1)-B(3)-B(4) 58.6(3)

B(8)-B(3)-B(4) 60.3(4) C(2)-B(3)-B(7) 58.2(3)

C(1)-B(3)-B(7) 105.2(4) B(8)-B(3)-B(7) 60.0(4)

B(4)-B(3)-B(7) 108.0(5) C(1)-B(4)-B(9) 104.8(5)

C(1)-B(4)-B(3) 59.9(3) B(9)-B(4)-B(3) 107.8(5)

C(1)-B(4)-B(8) 106.1(4) B(9)-B(4)-B(8) 60.3(4)

B(3)-B(4)-B(8) 59.8(4) C(1)-B(4)-B(5) 58.1(3)

B(9)-B(4)-B(5) 59.5(4) B(3)-B(4)-B(5) 107.8(4)

B(8)-B(4)-B(5) 107.9(5) C(1)-B(5)-B(6) 60.5(3)

C(1)-B(5)-B(9) 105.8(5) B(6)-B(5)-B(9) 108.3(5)

C(1)-B(5)-B(10) 106.7(4) B(6)-B(5)-B(10) 59.8(4)

B(9)-B(5)-B(10) 60.3(4) C(1)-B(5)-B(4) 59.1(3)

B(6)-B(5)-B(4) 109.3(4) B(9)-B(5)-B(4) 59.8(4)

B(10)-B(5)-B(4) 108.5(5) C(2)-B(6)-C(1) 57.5(3)

C(2)-B(6)-B(10) 104.3(4) C(1)-B(6)-B(10) 105.4(4)

C(2)-B(6)-B(5) 103.8(4) C(1)-B(6)-B(5) 58.3(3)

B(10)-B(6)-B(5) 60.4(4) C(2)-B(6)-B(11) 58.1(3)

C(1)-B(6)-B(11) 105.1(4) B(10)-B(6)-B(11) 60.0(4)

B(5)-B(6)-B(11) 107.8(4) C(2)-B(7)-B(11) 58.7(3)

C(2)-B(7)-B(12) 103.9(4) B(11)-B(7)-B(12) 59.5(4)

C(2)-B(7)-B(8) 104.7(4) B(11)-B(7)-B(8) 108.3(5)

B(12)-B(7)-B(8) 60.3(4) C(2)-B(7)-B(3) 59.3(3)

B(11)-B(7)-B(3) 108.8(4) B(12)-B(7)-B(3) 107.7(5)

B(8)-B(7)-B(3) 59.6(4) B(3)-B(8)-B(7) 60.3(4)

B(3)-B(8)-B(4) 59.9(4) B(7)-B(8)-B(4) 107.9(4)

B(3)-B(8)-B(9) 107.3(5) B(7)-B(8)-B(9) 107.1(5)

B(4)-B(8)-B(9) 59.6(4) B(3)-B(8)-B(12) 108.0(5)

B(7)-B(8)-B(12) 59.9(4) B(4)-B(8)-B(12) 107.3(5)

B(9)-B(8)-B(12) 59.4(4) B(5)-B(9)-B(12) 108.2(5)

B(5)-B(9)-B(4) 60.7(4) B(12)-B(9)-B(4) 108.6(5)

B(5)-B(9)-B(10) 59.9(4) B(12)-B(9)-B(10) 60.2(4)

B(4)-B(9)-B(10) 108.9(5) B(5)-B(9)-B(8) 108.6(5)

B(12)-B(9)-B(8) 60.3(4) B(4)-B(9)-B(8) 60.1(4)

B(10)-B(9)-B(8) 108.8(5) B(6)-B(10)-B(5) 59.8(4)

B(6)-B(10)-B(9) 107.9(5) B(5)-B(10)-B(9) 59.8(4)

B(6)-B(10)-B(11) 61.1(3) B(5)-B(10)-B(11) 108.1(4)

B(9)-B(10)-B(11) 107.3(5) B(6)-B(10)-B(12) 108.5(5)

B(5)-B(10)-B(12) 107.6(5) B(9)-B(10)-B(12) 59.7(4)

B(11)-B(10)-B(12) 59.5(4) C(2)-B(11)-B(12) 104.5(4)

C(2)-B(11)-B(7) 58.8(3) B(12)-B(11)-B(7) 60.4(4)

C(2)-B(11)-B(10) 103.8(4) B(12)-B(11)-B(10) 60.3(4)

B(7)-B(11)-B(10) 108.4(5) C(2)-B(11)-B(6) 58.6(3)

B(12)-B(11)-B(6) 107.4(4) B(7)-B(11)-B(6) 108.2(4)

B(10)-B(11)-B(6) 58.9(3) B(11)-B(12)-B(9) 108.3(4)

B(11)-B(12)-B(10) 60.3(4) B(9)-B(12)-B(10) 60.1(4)

B(11)-B(12)-B(7) 60.1(4) B(9)-B(12)-B(7) 107.9(5)

B(10)-B(12)-B(7) 108.2(5) B(11)-B(12)-B(8) 108.5(5)

B(9)-B(12)-B(8) 60.3(4) B(10)-B(12)-B(8) 108.7(5)

B(7)-B(12)-B(8) 59.9(4)

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Symmetry transformations used to generate equivalent atoms:

Table 6. Least-squares planes (x,y,z in crystal coordinates and deviations from them * indicates atom used to define plane)

* 0.0000 (0) S1

* 0.0000 (0) Co1

* 0.0000 (0) S2

Angle to previous plane (with approximate esd) = 16.63 ( 19 )

* 0.0237 (14) S1

* -0.0464 (26) C1

* 0.0455 (26) C2

* -0.0228 (13) S2

* -0.1307 (11) Co1

* 0.1509 (18) S1

* -0.1076 (27) C1

* -0.0192 (26) C2

* 0.1067 (16) S2

Angle to previous plane (with approximate esd) = 81.02 ( 12 )

* 0.0057 (14) Co1

* -0.0098 (23) C11

* 0.0102 (25) C10

* -0.0062 (15) S2

* -0.1307 (0.0011) Co1

* 0.1509 (0.0018) S1

* -0.1076 (0.0027) C1

* -0.0192 (0.0026) C2

* 0.1067 (0.0016) S2

Angle to previous plane (with approximate esd) = 54.76 ( 0.32 )

* -0.0004 (0.0059) C3

* -0.0104 (0.0048) C4

* 0.0180 (0.0047) C5

* -0.0186 (0.0059) C6

* 0.0114 (0.0065) C7

Experimental (KOR099, complex **5**)

A crystal size was 0.3 x 0.2 x 0.2 mm , mounted at the tip of a glass fiber. The accurate cell parameters were obtained by least-squares refinement from 25 reflections in the ranges 11.25 deg < theta < 14.22 deg measured with graphite monochromated Mo-Kα radiation on Enraf-Nonious CAD-4 diffractometer.

X-ray intinsity data were collected by omega-2theta scan method with theta=25.97 for the ranges $0 \le h \le 9$ , $-11 \le k \le 11$ , $-18 \le l \le 17$. Three standard reflections were checked every 100 reflections ; they showed no significant change. The intensity data were corrected for Lorentz and polarization factors.

The structure was solved by the application of Direct methods (SHELXS-86) and refined by full-matrix least-squares on $Fo^2$ (SHELXL-93). After four cycles of full matrix least-squares adjuntment,a difference Fourier map indicated the locations of the hydrogen atoms refined isotropically.

The final R value was 0.037 with 4107 (I>2sigmaI) observed reflections and 244 parameters.

Table 1. Crystal data and structure refinement for complex **5**.

| | |
|---|---|
| Identification code | KOR099 |
| Empirical formula | C11 B10 H25 SI S2 CO |
| Formula weight | 416.54 |
| Temperature | 293(2) K |
| Wavelength | 0.71070 Å |
| Crystal system, space group | TRICLINIC , P-1 |
| Unit cell dimensions | a = 7.8599(4) Å alpha = 102.517(5) deg. |
| | b = 9.7306(8) Å beta = 104.820(4) deg. |
| | c = 14.7510(7) Å gamma = 96.329(5) deg. |
| Volume | 1048.19(11) $Å^3$ |
| Z, Calculated density | 2, 1.317 $Mg/m^3$ |
| Absorption coefficient | 1.067 $mm^{-1}$ |
| F(000) | 426 |
| Crystal size | 0.3 x 0.2 x 0.2 mm |
| Theta range for data collection | 1.48 to 25.97 deg. |
| Index ranges | $0 \le h \le 9, -11 \le k \le 11, -18 \le l \le 17$ |
| Reflections collected / unique | 4460 / 4107 [R(int) = 0.0202] |
| Completeness to 2theta = 25.97 | 100.0% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4107 / 0 / 244 |
| Goodness-of-fit on F^2 | 0.837 |
| Final R indices [I>2sigma(I)] | R1 = 0.0374, wR2 = 0.1028 |
| R indices (all data) | R1 = 0.0803, wR2 = 0.1270 |
| Largest diff. peak and hole | 0.362 and -0.269 $e.Å^{-3}$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for complex **5**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Co(1) | 8070(1) | 6466(1) | 3864(1) | 36(1) |
| S(2) | 6878(1) | 6240(1) | 2339(1) | 32(1) |
| S(1) | 10911(1) | 7049(1) | 3817(1) | 44(1) |
| Si(1) | 5810(1) | 3094(1) | 2332(1) | 41(1) |
| C(1) | 10604(4) | 7595(4) | 2721(2) | 33(1) |
| C(2) | 8595(4) | 7121(3) | 1940(2) | 28(1) |
| C(3) | 6895(7) | 7944(6) | 4651(3) | 67(1) |
| C(4) | 8596(7) | 7889(6) | 5210(3) | 71(1) |
| C(5) | 8663(6) | 6493(6) | 5303(3) | 63(1) |
| C(6) | 6997(6) | 5673(5) | 4814(3) | 58(1) |
| C(7) | 5887(6) | 6547(6) | 4390(3) | 62(1) |
| C(8) | 7575(4) | 4763(4) | 2741(2) | 35(1) |
| C(9) | 3564(5) | 3520(5) | 2323(4) | 69(1) |
| C(10) | 6474(6) | 1899(5) | 3142(4) | 65(1) |
| C(11) | 5822(6) | 2227(5) | 1084(3) | 66(1) |
| B(3) | 9288(5) | 8893(4) | 2579(3) | 37(1) |
| B(4) | 11582(6) | 9215(5) | 2644(3) | 43(1) |
| B(5) | 12140(6) | 7597(5) | 2085(3) | 45(1) |
| B(6) | 10205(6) | 6247(4) | 1636(3) | 38(1) |
| B(7) | 8020(6) | 8396(4) | 1340(3) | 42(1) |
| B(8) | 9959(6) | 9735(5) | 1754(3) | 47(1) |
| B(9) | 11737(6) | 8939(5) | 1446(3) | 49(1) |
| B(10) | 10897(7) | 7117(5) | 836(3) | 51(1) |

| | | | | |
|---|---|---|---|---|
| B(11) | 8583(6) | 6777(5) | 760(3) | 44(1) |
| B(12) | 9523(7) | 8428(5) | 627(3) | 54(1) |

Table 3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **5**. 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 |
|---|---|---|---|---|---|---|
| Co(1) | 30(1) | 46(1) | 31(1) | 11(1) | 10(1) | 3(1) |
| S(2) | 26(1) | 35(1) | 35(1) | 11(1) | 7(1) | 4(1) |
| S(1) | 27(1) | 67(1) | 38(1) | 21(1) | 5(1) | 3(1) |
| Si(1) | 35(1) | 36(1) | 49(1) | 14(1) | 7(1) | -1(1) |
| C(1) | 26(2) | 36(2) | 36(2) | 8(1) | 8(1) | 3(1) |
| C(2) | 29(2) | 24(2) | 29(2) | 6(1) | 6(1) | 2(1) |
| C(3) | 93(4) | 75(3) | 56(3) | 21(2) | 46(3) | 39(3) |
| C(4) | 70(3) | 82(4) | 47(2) | -12(2) | 25(2) | -5(3) |
| C(5) | 58(3) | 95(4) | 38(2) | 19(2) | 16(2) | 14(3) |
| C(6) | 65(3) | 73(3) | 52(2) | 23(2) | 37(2) | 8(2) |
| C(7) | 44(2) | 102(4) | 49(2) | 22(2) | 25(2) | 16(2) |
| C(8) | 35(2) | 35(2) | 41(2) | 16(2) | 14(2) | 8(2) |
| C(9) | 35(2) | 64(3) | 99(4) | 15(3) | 15(2) | -1(2) |
| C(10) | 67(3) | 46(3) | 78(3) | 30(2) | 7(2) | -2(2) |
| C(11) | 67(3) | 58(3) | 58(3) | 4(2) | 7(2) | -2(2) |
| B(3) | 37(2) | 27(2) | 42(2) | 0(2) | 10(2) | 0(2) |
| B(4) | 40(2) | 37(2) | 48(2) | 7(2) | 14(2) | -7(2) |
| B(5) | 36(2) | 45(3) | 58(3) | 12(2) | 22(2) | 5(2) |
| B(6) | 44(2) | 32(2) | 41(2) | 6(2) | 22(2) | 8(2) |
| B(7) | 46(2) | 34(2) | 45(2) | 18(2) | 5(2) | 4(2) |
| B(8) | 54(3) | 28(2) | 60(3) | 14(2) | 16(2) | 3(2) |
| B(9) | 54(3) | 43(3) | 54(3) | 17(2) | 24(2) | -8(2) |
| B(10) | 64(3) | 43(3) | 49(3) | 6(2) | 31(2) | -2(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| B(11) | 59(3) | 38(2) | 30(2) | 7(2) | 11(2) | -5(2) |
| B(12) | 77(3) | 46(3) | 46(3) | 23(2) | 22(2) | 2(2) |

Table 4. Bond lengths [Å] for complex **5**.

| | | | |
|---|---|---|---|
| Co(1)-C(8) | 1.994(4) | Co(1)-C(5) | 2.047(4) |
| Co(1)-C(6) | 2.049(4) | Co(1)-C(7) | 2.058(4) |
| Co(1)-C(4) | 2.072(4) | Co(1)-C(3) | 2.095(4) |
| Co(1)-S(2) | 2.1567(9) | Co(1)-S(1) | 2.2643(10) |
| S(2)-C(8) | 1.760(3) | S(2)-C(2) | 1.808(3) |
| S(1)-C(1) | 1.776(3) | Si(1)-C(9) | 1.855(4) |
| Si(1)-C(11) | 1.855(5) | Si(1)-C(10) | 1.862(4) |
| Si(1)-C(8) | 1.891(4) | C(1)-C(2) | 1.647(4) |
| C(1)-B(5) | 1.708(5) | C(1)-B(4) | 1.716(5) |
| C(1)-B(3) | 1.732(5) | C(1)-B(6) | 1.767(5) |
| C(2)-B(11) | 1.698(5) | C(2)-B(6) | 1.700(5) |
| C(2)-B(7) | 1.710(5) | C(2)-B(3) | 1.727(5) |
| C(3)-C(4) | 1.393(7) | C(3)-C(7) | 1.415(7) |
| C(4)-C(5) | 1.400(7) | C(5)-C(6) | 1.381(6) |
| C(6)-C(7) | 1.411(6) | B(3)-B(8) | 1.759(6) |
| B(3)-B(4) | 1.769(6) | B(3)-B(7) | 1.774(6) |
| B(4)-B(9) | 1.767(6) | B(4)-B(5) | 1.768(6) |
| B(4)-B(8) | 1.783(6) | B(5)-B(6) | 1.773(6) |
| B(5)-B(9) | 1.780(6) | B(5)-B(10) | 1.781(7) |
| B(6)-B(10) | 1.751(6) | B(6)-B(11) | 1.776(6) |
| B(7)-B(8) | 1.770(6) | B(7)-B(12) | 1.772(7) |
| B(7)-B(11) | 1.781(6) | B(8)-B(9) | 1.781(7) |
| B(8)-B(12) | 1.788(7) | B(9)-B(10) | 1.771(7) |
| B(9)-B(12) | 1.791(7) | B(10)-B(11) | 1.782(6) |
| B(10)-B(12) | 1.787(7) | B(11)-B(12) | 1.765(6) |

Table 5. Bond angles [deg] for complex **5**.

C(8)-Co(1)-C(5) 127.30(19) C(8)-Co(1)-C(6) 102.62(17)
C(5)-Co(1)-C(6) 39.42(18) C(8)-Co(1)-C(7) 109.94(18)
C(5)-Co(1)-C(7) 66.97(18) C(6)-Co(1)-C(7) 40.18(18)
C(8)-Co(1)-C(4) 166.97(19) C(5)-Co(1)-C(4) 39.7(2)
C(6)-Co(1)-C(4) 66.1(2) C(7)-Co(1)-C(4) 66.2(2)
C(8)-Co(1)-C(3) 144.37(19) C(5)-Co(1)-C(3) 66.7(2)
C(6)-Co(1)-C(3) 66.80(19) C(7)-Co(1)-C(3) 39.8(2)
C(4)-Co(1)-C(3) 39.06(19) C(8)-Co(1)-S(2) 49.97(10)
C(5)-Co(1)-S(2) 167.72(13) C(6)-Co(1)-S(2) 128.52(14)
C(7)-Co(1)-S(2) 101.88(13) C(4)-Co(1)-S(2) 142.00(17)
C(3)-Co(1)-S(2) 108.50(14) C(8)-Co(1)-S(1) 91.86(10)
C(5)-Co(1)-S(1) 97.33(13) C(6)-Co(1)-S(1) 133.17(14)
C(7)-Co(1)-S(1) 157.91(15) C(4)-Co(1)-S(1) 91.76(14)
C(3)-Co(1)-S(1) 120.70(17) S(2)-Co(1)-S(1) 94.78(3)
C(8)-S(2)-C(2) 110.14(15) C(8)-S(2)-Co(1) 60.22(12)
C(2)-S(2)-Co(1) 105.11(10) C(1)-S(1)-Co(1) 102.73(11)
C(9)-Si(1)-C(11) 110.0(2) C(9)-Si(1)-C(10) 111.0(2)
C(11)-Si(1)-C(10) 109.8(2) C(9)-Si(1)-C(8) 111.82(19)
C(11)-Si(1)-C(8) 105.37(19) C(10)-Si(1)-C(8) 108.76(18)
C(2)-C(1)-B(5) 108.2(3) C(2)-C(1)-B(4) 109.3(3)
B(5)-C(1)-B(4) 62.2(2) C(2)-C(1)-B(3) 61.4(2)
B(5)-C(1)-B(3) 112.8(3) B(4)-C(1)-B(3) 61.8(2)
C(2)-C(1)-B(6) 59.6(2) B(5)-C(1)-B(6) 61.3(2)
B(4)-C(1)-B(6) 112.1(3) B(3)-C(1)-B(6) 112.4(3)
C(2)-C(1)-S(1) 116.9(2) B(5)-C(1)-S(1) 124.2(2)

B(4)-C(1)-S(1) 124.1(2) B(3)-C(1)-S(1) 116.6(2)

B(6)-C(1)-S(1) 117.4(2) C(1)-C(2)-B(11) 114.3(3)

C(1)-C(2)-B(6) 63.7(2) B(11)-C(2)-B(6) 63.0(2)

C(1)-C(2)-B(7) 112.6(3) B(11)-C(2)-B(7) 63.0(2)

B(6)-C(2)-B(7) 115.5(3) C(1)-C(2)-B(3) 61.7(2)

B(11)-C(2)-B(3) 114.9(3) B(6)-C(2)-B(3) 116.0(3)

B(7)-C(2)-B(3) 62.2(2) C(1)-C(2)-S(2) 116.2(2)

B(11)-C(2)-S(2) 122.6(2) B(6)-C(2)-S(2) 120.7(2)

B(7)-C(2)-S(2) 116.8(2) B(3)-C(2)-S(2) 111.7(2)

C(4)-C(3)-C(7) 106.9(4) C(4)-C(3)-Co(1) 69.6(3)

C(7)-C(3)-Co(1) 68.7(2) C(3)-C(4)-C(5) 109.2(5)

C(3)-C(4)-Co(1) 71.4(3) C(5)-C(4)-Co(1) 69.2(3)

C(6)-C(5)-C(4) 107.8(4) C(6)-C(5)-Co(1) 70.4(2)

C(4)-C(5)-Co(1) 71.1(3) C(5)-C(6)-C(7) 108.4(5)

C(5)-C(6)-Co(1) 70.2(2) C(7)-C(6)-Co(1) 70.3(2)

C(6)-C(7)-C(3) 107.7(4) C(6)-C(7)-Co(1) 69.6(2)

C(3)-C(7)-Co(1) 71.5(2) S(2)-C(8)-Si(1) 115.08(18)

S(2)-C(8)-Co(1) 69.81(12) Si(1)-C(8)-Co(1) 130.70(18)

C(2)-B(3)-C(1) 56.87(19) C(2)-B(3)-B(8) 104.0(3)

C(1)-B(3)-B(8) 106.0(3) C(2)-B(3)-B(4) 103.3(3)

C(1)-B(3)-B(4) 58.7(2) B(8)-B(3)-B(4) 60.7(2)

C(2)-B(3)-B(7) 58.5(2) C(1)-B(3)-B(7) 105.7(3)

B(8)-B(3)-B(7) 60.1(2) B(4)-B(3)-B(7) 108.4(3)

C(1)-B(4)-B(9) 105.7(3) C(1)-B(4)-B(5) 58.7(2)

B(9)-B(4)-B(5) 60.5(3) C(1)-B(4)-B(3) 59.6(2)

B(9)-B(4)-B(3) 107.8(3) B(5)-B(4)-B(3) 108.1(3)

C(1)-B(4)-B(8) 105.7(3) B(9)-B(4)-B(8) 60.2(3)

B(5)-B(4)-B(8) 108.5(3) B(3)-B(4)-B(8) 59.4(2)

C(1)-B(5)-B(4) 59.1(2) C(1)-B(5)-B(6) 61.0(2)

B(4)-B(5)-B(6) 109.4(3) C(1)-B(5)-B(9) 105.5(3)

B(4)-B(5)-B(9) 59.7(3) B(6)-B(5)-B(9) 107.3(3)

C(1)-B(5)-B(10) 106.3(3) B(4)-B(5)-B(10) 107.9(3)

B(6)-B(5)-B(10) 59.0(2) B(9)-B(5)-B(10) 59.6(3)

C(2)-B(6)-B(10) 104.4(3) C(2)-B(6)-C(1) 56.68(18)

B(10)-B(6)-C(1) 105.0(3) C(2)-B(6)-B(5) 103.0(3)

B(10)-B(6)-B(5) 60.7(3) C(1)-B(6)-B(5) 57.7(2)

C(2)-B(6)-B(11) 58.4(2) B(10)-B(6)-B(11) 60.7(3)

C(1)-B(6)-B(11) 105.0(3) B(5)-B(6)-B(11) 108.6(3)

C(2)-B(7)-B(8) 104.2(3) C(2)-B(7)-B(12) 103.6(3)

B(8)-B(7)-B(12) 60.6(3) C(2)-B(7)-B(3) 59.4(2)

B(8)-B(7)-B(3) 59.5(2) B(12)-B(7)-B(3) 108.2(3)

C(2)-B(7)-B(11) 58.2(2) B(8)-B(7)-B(11) 108.2(3)

B(12)-B(7)-B(11) 59.6(3) B(3)-B(7)-B(11) 108.6(3)

B(3)-B(8)-B(7) 60.4(2) B(3)-B(8)-B(9) 107.6(3)

B(7)-B(8)-B(9) 107.8(3) B(3)-B(8)-B(4) 59.9(2)

B(7)-B(8)-B(4) 108.0(3) B(9)-B(8)-B(4) 59.5(2)

B(3)-B(8)-B(12) 108.2(3) B(7)-B(8)-B(12) 59.8(3)

B(9)-B(8)-B(12) 60.3(3) B(4)-B(8)-B(12) 107.9(3)

B(4)-B(9)-B(10) 108.4(3) B(4)-B(9)-B(5) 59.8(2)

B(10)-B(9)-B(5) 60.2(3) B(4)-B(9)-B(8) 60.3(3)

B(10)-B(9)-B(8) 108.4(3) B(5)-B(9)-B(8) 108.0(3)

B(4)-B(9)-B(12) 108.4(3) B(10)-B(9)-B(12) 60.2(3)

B(5)-B(9)-B(12) 108.2(3) B(8)-B(9)-B(12) 60.0(3)

| | | | |
|---|---|---|---|
| B(6)-B(10)-B(9) | 108.7(3) | B(6)-B(10)-B(5) | 60.2(2) |
| B(9)-B(10)-B(5) | 60.2(3) | B(6)-B(10)-B(11) | 60.3(2) |
| B(9)-B(10)-B(11) | 107.8(3) | B(5)-B(10)-B(11) | 108.0(3) |
| B(6)-B(10)-B(12) | 108.3(3) | B(9)-B(10)-B(12) | 60.5(3) |
| B(5)-B(10)-B(12) | 108.3(3) | B(11)-B(10)-B(12) | 59.3(3) |
| C(2)-B(11)-B(12) | 104.4(3) | C(2)-B(11)-B(6) | 58.5(2) |
| B(12)-B(11)-B(6) | 108.2(3) | C(2)-B(11)-B(7) | 58.8(2) |
| B(12)-B(11)-B(7) | 60.0(3) | B(6)-B(11)-B(7) | 108.4(3) |
| C(2)-B(11)-B(10) | 103.1(3) | B(12)-B(11)-B(10) | 60.5(3) |
| B(6)-B(11)-B(10) | 59.0(2) | B(7)-B(11)-B(10) | 107.8(3) |
| B(11)-B(12)-B(7) | 60.5(2) | B(11)-B(12)-B(10) | 60.2(3) |
| B(7)-B(12)-B(10) | 108.0(3) | B(11)-B(12)-B(8) | 108.2(3) |
| B(7)-B(12)-B(8) | 59.6(3) | B(10)-B(12)-B(8) | 107.4(3) |
| B(11)-B(12)-B(9) | 107.6(3) | B(7)-B(12)-B(9) | 107.2(3) |
| B(10)-B(12)-B(9) | 59.3(3) | B(8)-B(12)-B(9) | 59.7(3) |

Symmetry transformations used to generate equivalent atoms:

Table 6. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

* 0.0000 (0) Co1

* 0.0000 (0) S1

* 0.0000 (0) S2

Angle to previous plane (with approximate esd) = 19.26 ( 10 )

* -0.0160 (10) S1

* 0.0315 (19) C1

* -0.0312 (18) C2

* 0.0157 ( 9) S2

* 0.1519 ( 8) Co1

* -0.1596 (13) S1

* 0.1015 (19) C1

* 0.0394 (18) C2

* -0.1332 (12) S2

Angle to previous plane (with approximate esd) = 83.00 ( 12 )

* 0.0000 (0) Co1

* 0.0000 (0) S2

* 0.0000 (0) C8

* 0.1519 (08) Co1

* -0.1595 (13) S1

* 0.1015 (19) C1

* 0.0394 (18) C2

* -0.1332 (12) S2

Angle to previous plane (with approximate esd) = 60.50 ( 14 )

* 0.0038 (26) C3

* 0.0016 (26) C4

* -0.0065 (26) C5

* 0.0088 (25) C6

* -0.0077 (25) C7