OM990269V

SUPPORTING INFORMATION

Addition Reactions of the Novel Mononuclear Dithio-*o*-carboranylcobalt(III) Complex (η^5-C_5H_5)Co(η^2-$S_2C_2B_{10}H_{10}$)

Dae-Hyun Kim, Jaejung Ko*, Kwonil Park†, Sungil Cho†, and Sang Ook Kang*

Department of Chemistry, Korea University, 208 Seochang, Chochiwon, Chung-nam 339-700, Korea. †Department of Chemical Engineering, Junnong-dong 90, Seoul City University, Seoul 130-743, Korea.

Experimental (KOR026, Complex **2**)

A crystal size was 0.2 x 0.2 x 0.3 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 11.62 deg < theta < 13.76 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 = 24.97 for the ranges $-12 \leq h \leq 12$, $-13 \leq k \leq 13$, $0 \leq l \leq 14$. 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 0.175 with 5070 (I > 2sigmaI) observed reflections and 323 parameters.

Table 1. Crystal data and structure refinement for complex **2**.

Identification code	KOR026
Empirical formula	C7 B10 H15 S2 Co1
Formula weight	330.37
Temperature	293(2) K
Wavelength	0.71070 A
Crystal system, space group	TRICLINIC , P-1
Unit cell dimensions	a = 11.2866(12) A alpha = 114.12(3) deg. b = 12.677(6) A beta = 104.985(10) deg. c = 13.2760(19) A gamma = 107.18(3) deg.
Volume	1491.5(8) $Å^3$
Z, Calculated density	2, 1.471 Mg/m^3
Absorption coefficient	7.855 mm^{-1}
F(000)	1312
Crystal size	0.2 x 0.2 x 0.3 mm
Theta range for data collection	1.87 to 24.97 deg.
Index ranges	$-12 \le h \le 12, -13 \le k \le 13, 0 \le l \le 14$
Reflections collected / unique	5315 / 5070 [R(int) = 0.0350]
Completeness to 2theta = 24.97	96.9%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5070 / 0 / 323
Goodness-of-fit on F^2	1.723
Final R indices [I>2sigma(I)]	R1 = 0.1751, wR2 = 0.5016
R indices (all data)	R1 = 0.3344, wR2 = 0.5447
Largest diff. peak and hole	3.966 and -4.761 $e.Å^{-3}$

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

	x	y	z	U(eq)
Co(1)	6058(4)	9947(4)	2426(3)	29(1)
S(1)	5177(8)	9976(8)	3660(6)	36(2)
S(2)	4453(7)	9976(7)	1164(6)	27(2)
C(1)	3540(3)	9960(3)	3120(2)	21(6)
C(2)	3130(3)	9850(2)	1600(2)	19(6)
C(3)	8130(5)	10960(4)	3320(4)	80(13)
C(4)	7640(3)	10490(3)	1950(3)	32(7)
C(5)	6990(8)	9400(8)	1160(8)	210(3)
C(6)	6900(4)	8710(4)	1980(4)	64(10)
C(7)	7970(4)	10300(4)	3550(3)	51(9)
B(3)	2250(3)	8590(3)	1660(3)	24(7)
B(4)	2110(3)	9180(3)	3050(2)	21(6)
B(5)	3010(3)	10890(3)	3910(3)	22(7)
B(6)	3570(3)	11330(3)	3050(2)	21(7)
B(7)	1530(3)	9230(3)	860(3)	31(8)
B(8)	640(4)	8670(3)	1670(2)	49(12)
B(9)	1180(4)	9930(3)	2960(3)	41(10)
B(10)	2140(3)	11440(3)	3070(3)	30(8)
B(11)	2360(4)	10960(4)	1720(3)	66(15)
B(12)	740(4)	10010(3)	1800(3)	35(9)
Co(1')	4007(4)	5183(4)	2659(4)	38(1)
S(1')	5548(8)	5089(9)	3863(8)	44(2)
S(2')	4896(9)	5113(10)	1401(9)	53(3)

C(1')	6730(2)	4890(3)	3160(2)	27(7)
C(2')	6380(3)	5030(3)	2090(2)	22(6)
C(3')	1930(3)	4080(3)	2010(3)	45(8)
C(4')	2770(4)	5270(4)	3540(4)	64(11)
C(5')	3180(3)	6120(3)	3660(3)	41(8)
C(6')	2930(3)	6160(3)	2440(3)	43(8)
C(7')	2370(3)	5240(3)	1680(3)	27(6)
B(3')	6180(4)	3690(4)	1890(4)	41(10)
B(4')	7630(4)	4240(3)	3310(3)	35(9)
B(5')	8560(4)	5960(3)	4110(3)	45(11)
B(6')	7610(5)	6520(4)	3290(3)	55(14)
B(7')	7130(5)	4350(3)	1110(3)	54(12)
B(8')	7790(7)	3730(5)	1880(4)	100(2)
B(9')	9300(5)	5060(4)	3450(3)	55(12)
B(10')	9190(4)	6440(4)	3280(5)	80(2)
B(11')	7910(5)	6050(3)	1930(8)	160(4)
B(12')	8808(13)	4886(12)	1789(12)	73(18)
Q(1)	7530(13)	9988(12)	2416(12)	34(4)
Q(2)	2622(13)	5365(12)	2650(12)	42(4)

Table 3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **2**. 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)	36(3)	45(3)	16(2)	18(2)	13(2)	26(2)
S(1)	46(5)	71(6)	19(4)	37(4)	22(4)	34(4)
S(2)	32(4)	40(4)	18(3)	19(3)	15(3)	18(3)
C(1)	42(18)	25(14)	7(13)	9(11)	24(13)	17(13)
C(2)	30(17)	0(11)	7(12)	-9(9)	1(11)	5(11)
B(4)	30(15)	30(16)	0(11)	1(11)	15(11)	12(13)
B(5)	23(16)	6(13)	37(17)	9(13)	10(14)	12(12)
B(6)	28(16)	32(15)	14(14)	11(12)	8(12)	28(13)
B(7)	36(19)	60(2)	25(17)	34(17)	21(15)	37(17)
B(8)	40(2)	40(2)	0(13)	-7(14)	-7(14)	-25(18)
B(9)	40(2)	60(2)	7(14)	23(15)	14(13)	-1(18)
B(10)	26(17)	50(2)	50(2)	42(19)	26(16)	33(16)
B(11)	50(2)	80(3)	30(2)	-5(19)	-20(18)	60(2)
B(12)	40(2)	60(2)	12(16)	10(15)	14(15)	40(18)
Co(1')	25(2)	50(3)	50(3)	29(2)	21(2)	21(2)
S(1')	38(5)	73(6)	44(5)	37(5)	27(4)	34(5)
S(2')	40(5)	85(7)	56(6)	41(5)	27(5)	43(5)
C(1')	7(13)	56(19)	23(15)	23(15)	8(11)	16(13)
C(2')	28(14)	37(15)	8(12)	13(11)	14(11)	16(12)
B(4')	80(3)	21(16)	44(19)	32(16)	50(2)	28(18)
B(5')	40(2)	0(13)	40(2)	-5(13)	1(18)	-11(14)
B(6')	50(3)	30(2)	22(18)	1(16)	6(19)	-18(19)
B(7')	120(4)	39(19)	27(17)	16(15)	70(2)	40(2)

B(8')	170(6)	80(3)	0(2)	-20(2)	30(3)	60(4)
B(9')	110(3)	70(3)	0(13)	21(17)	50(19)	20(3)
B(10')	14(19)	50(3)	140(5)	30(3)	20(2)	16(18)
B(11')	70(3)	0(17)	380(9)	50(3)	140(5)	8(19)
B(12')	90(4)	170(5)	80(3)	100(4)	90(3)	110(4)

Table 4. Bond lengths [A] for compound **2**.

Co(1)-C(7)	1.99(4)	Co(1)-C(3)	2.03(4)
Co(1)-C(6)	2.04(3)	Co(1)-C(4)	2.08(3)
Co(1)-C(5)	2.18(5)	Co(1)-S(1)	2.129(8)
Co(1)-S(2)	2.139(8)	S(1)-C(1)	1.81(3)
S(2)-C(2)	1.69(2)	C(1)-B(5)	1.58(4)
C(1)-B(4)	1.60(4)	C(1)-B(6)	1.75(4)
C(1)-B(3)	1.77(4)	C(1)-C(2)	1.87(4)
C(2)-B(7)	1.63(4)	C(2)-B(3)	1.67(4)
C(2)-B(11)	1.86(6)	C(2)-B(6)	1.92(4)
C(3)-C(7)	0.99(5)	C(3)-C(4)	1.52(5)
C(4)-C(5)	1.47(5)	C(5)-C(6)	1.50(6)
C(6)-C(7)	1.81(5)	B(3)-B(7)	1.77(5)
B(3)-B(4)	1.78(4)	B(3)-B(8)	1.87(5)
B(4)-B(9)	1.74(4)	B(4)-B(5)	1.79(4)
B(4)-B(8)	1.81(4)	B(5)-B(6)	1.64(5)
B(5)-B(10)	1.80(5)	B(5)-B(9)	1.89(5)
B(6)-B(10)	1.65(5)	B(6)-B(11)	1.74(6)
B(7)-B(11)	1.79(6)	B(7)-B(8)	1.84(5)
B(7)-B(12)	1.85(5)	B(8)-B(9)	1.59(5)
B(8)-B(12)	1.62(5)	B(9)-B(12)	1.51(5)
B(9)-B(10)	1.87(5)	B(10)-B(11)	1.71(7)
B(10)-B(12)	1.79(5)	B(11)-B(12)	1.81(6)
Co(1')-C(5')	2.02(4)	Co(1')-C(3')	2.05(3)
Co(1')-C(4')	2.05(4)	Co(1')-C(6')	2.03(4)
Co(1')-C(7')	2.04(4)	Co(1')-S(2')	2.111(11)

Co(1')-S(1')	2.114(10)	S(1')-C(1')	1.89(3)
S(2')-C(2')	1.74(3)	C(1')-C(2')	1.41(4)
C(1')-B(3')	1.52(4)	C(1')-B(4')	1.57(4)
C(1')-B(5')	1.80(4)	C(1')-B(6')	1.85(5)
C(2')-B(3')	1.65(4)	C(2')-B(6')	1.72(5)
C(2')-B(7')	1.80(5)	C(3')-C(4')	1.65(5)
C(3')-C(7')	1.74(5)	C(4')-C(5')	1.11(4)
C(5')-C(6')	1.53(5)	C(6')-C(7')	0.97(4)
B(3')-B(4')	1.72(4)	B(3')-B(8')	1.83(6)
B(3')-B(7')	1.90(5)	B(4')-B(9')	1.78(4)
B(4')-B(8')	1.79(6)	B(4')-B(5')	1.81(4)
B(5')-B(10')	1.66(5)	B(5')-B(9')	1.73(4)
B(5')-B(6')	1.79(5)	B(6')-B(10')	1.62(6)
B(6')-B(11')	1.90(9)	B(7')-B(12')	1.58(6)
B(7')-B(8')	1.78(6)	B(7')-B(11')	1.90(8)
B(8')-B(12')	1.65(6)	B(8')-B(9')	1.84(5)
B(9')-B(10')	1.98(5)	B(9')-B(12')	2.13(6)
B(10')-B(11')	1.82(8)	B(11')-B(12')	2.06(8)

Table 5. Bond angles [deg] for complex **2**.

C(7)-Co(1)-C(3)	28.4(13)	C(7)-Co(1)-C(6)	53.5(14)
C(3)-Co(1)-C(6)	70.0(14)	C(7)-Co(1)-C(4)	63.6(14)
C(3)-Co(1)-C(4)	43.5(14)	C(6)-Co(1)-C(4)	67.1(13)
C(7)-Co(1)-C(5)	75.9(17)	C(3)-Co(1)-C(5)	72.6(16)
C(6)-Co(1)-C(5)	41.4(16)	C(4)-Co(1)-C(5)	40.2(14)
C(7)-Co(1)-S(1)	96.4(12)	C(3)-Co(1)-S(1)	111.8(12)
C(6)-Co(1)-S(1)	114.9(11)	C(4)-Co(1)-S(1)	154.6(8)
C(5)-Co(1)-S(1)	154.7(13)	C(7)-Co(1)-S(2)	162.1(12)
C(3)-Co(1)-S(2)	133.9(12)	C(6)-Co(1)-S(2)	129.4(11)
C(4)-Co(1)-S(2)	100.1(8)	C(5)-Co(1)-S(2)	96.6(13)
S(1)-Co(1)-S(2)	96.9(3)	C(1)-S(1)-Co(1)	109.3(10)
B(5)-C(1)-B(4)	68.6(18)	B(5)-C(1)-B(6)	58.9(19)
B(4)-C(1)-B(6)	113(2)	B(5)-C(1)-B(3)	118(2)
B(4)-C(1)-B(3)	63.3(17)	B(6)-C(1)-B(3)	109(2)
B(5)-C(1)-S(1)	125(2)	B(4)-C(1)-S(1)	128.1(19)
B(6)-C(1)-S(1)	115.7(19)	B(3)-C(1)-S(1)	114.6(19)
B(5)-C(1)-C(2)	113(2)	B(4)-C(1)-C(2)	108.1(18)
B(6)-C(1)-C(2)	64.0(17)	B(3)-C(1)-C(2)	54.3(15)
S(1)-C(1)-C(2)	108.6(16)	B(7)-C(2)-B(3)	64.9(19)
B(7)-C(2)-S(2)	134(2)	B(3)-C(2)-S(2)	123.2(18)
B(7)-C(2)-B(11)	61(2)	B(3)-C(2)-B(11)	111(2)
S(2)-C(2)-B(11)	125(2)	B(7)-C(2)-C(1)	107(2)
B(3)-C(2)-C(1)	59.7(16)	S(2)-C(2)-C(1)	115.6(15)
B(11)-C(2)-C(1)	99(2)	B(7)-C(2)-B(6)	105(2)
B(3)-C(2)-B(6)	106(2)	S(2)-C(2)-B(6)	114.1(16)

B(11)-C(2)-B(6)	55(2)	C(1)-C(2)-B(6)	54.8(15)
C(7)-C(3)-C(4)	116(4)	C(7)-C(3)-Co(1)	73(3)
C(4)-C(3)-Co(1)	70.0(18)	C(5)-C(4)-C(3)	113(3)
C(5)-C(4)-Co(1)	73(2)	C(3)-C(4)-Co(1)	66.6(19)
C(4)-C(5)-C(6)	100(3)	C(4)-C(5)-Co(1)	66(2)
C(6)-C(5)-Co(1)	64(2)	C(5)-C(6)-C(7)	101(3)
C(5)-C(6)-Co(1)	74(2)	C(7)-C(6)-Co(1)	62.0(16)
C(3)-C(7)-C(6)	109(4)	C(3)-C(7)-Co(1)	78(3)
C(6)-C(7)-Co(1)	64.5(16)	C(2)-B(3)-B(7)	56.6(17)
C(2)-B(3)-C(1)	66.0(16)	B(7)-B(3)-C(1)	106(2)
C(2)-B(3)-B(4)	110(2)	B(7)-B(3)-B(4)	108(2)
C(1)-B(3)-B(4)	53.7(15)	C(2)-B(3)-B(8)	106(2)
B(7)-B(3)-B(8)	60.6(19)	C(1)-B(3)-B(8)	101(2)
B(4)-B(3)-B(8)	59.3(17)	C(1)-B(4)-B(9)	106.2(19)
C(1)-B(4)-B(5)	55.1(16)	B(9)-B(4)-B(5)	64.5(17)
C(1)-B(4)-B(3)	62.9(17)	B(9)-B(4)-B(3)	105(2)
B(5)-B(4)-B(3)	108(2)	C(1)-B(4)-B(8)	110(2)
B(9)-B(4)-B(8)	53.2(17)	B(5)-B(4)-B(8)	107.6(19)
B(3)-B(4)-B(8)	63.0(18)	C(1)-B(5)-B(6)	66(2)
C(1)-B(5)-B(4)	56.3(16)	B(6)-B(5)-B(4)	109(2)
C(1)-B(5)-B(10)	110(3)	B(6)-B(5)-B(10)	57(2)
B(4)-B(5)-B(10)	108(2)	C(1)-B(5)-B(9)	101(2)
B(6)-B(5)-B(9)	103(2)	B(4)-B(5)-B(9)	56.5(15)
B(10)-B(5)-B(9)	60.9(19)	B(5)-B(6)-B(10)	66(2)
B(5)-B(6)-C(1)	55.5(18)	B(10)-B(6)-C(1)	109(3)
B(5)-B(6)-B(11)	113(3)	B(10)-B(6)-B(11)	60(3)
C(1)-B(6)-B(11)	109(3)	B(5)-B(6)-C(2)	108(2)

B(10)-B(6)-C(2)	110(2)	C(1)-B(6)-C(2)	61.2(15)
C(2)-B(7)-B(3)	58.5(18)	C(2)-B(7)-B(11)	66(2)
B(3)-B(7)-B(11)	109(3)	C(2)-B(7)-B(8)	110(2)
B(3)-B(7)-B(8)	63(2)	B(11)-B(7)-B(8)	104(3)
C(2)-B(7)-B(12)	110(2)	B(3)-B(7)-B(12)	103(2)
B(11)-B(7)-B(12)	60(2)	B(8)-B(7)-B(12)	51.9(18)
B(9)-B(8)-B(12)	56(2)	B(9)-B(8)-B(4)	61.4(18)
B(12)-B(8)-B(4)	105(2)	B(9)-B(8)-B(7)	108(2)
B(12)-B(8)-B(7)	64(2)	B(4)-B(8)-B(7)	104(2)
B(9)-B(8)-B(3)	107(2)	B(12)-B(8)-B(3)	108(2)
B(4)-B(8)-B(3)	57.7(17)	B(7)-B(8)-B(3)	56.9(18)
B(12)-B(9)-B(8)	63(2)	B(12)-B(9)-B(4)	113(3)
B(8)-B(9)-B(4)	65.4(19)	B(12)-B(9)-B(10)	63(2)
B(8)-B(9)-B(10)	114(3)	B(4)-B(9)-B(10)	108(2)
B(12)-B(9)-B(5)	109(3)	B(8)-B(9)-B(5)	113(2)
B(4)-B(9)-B(5)	59.0(16)	B(10)-B(9)-B(5)	57.3(18)
B(6)-B(10)-B(11)	62(3)	B(6)-B(10)-B(12)	107(3)
B(11)-B(10)-B(12)	62(3)	B(6)-B(10)-B(5)	57(2)
B(11)-B(10)-B(5)	107(3)	B(12)-B(10)-B(5)	101(2)
B(6)-B(10)-B(9)	104(3)	B(11)-B(10)-B(9)	101(3)
B(12)-B(10)-B(9)	48.6(19)	B(5)-B(10)-B(9)	61.8(19)
B(10)-B(11)-B(6)	57(3)	B(10)-B(11)-B(7)	113(3)
B(6)-B(11)-B(7)	106(3)	B(10)-B(11)-B(12)	61(3)
B(6)-B(11)-B(12)	102(3)	B(7)-B(11)-B(12)	62(2)
B(10)-B(11)-C(2)	111(3)	B(6)-B(11)-C(2)	64(2)
B(7)-B(11)-C(2)	53.0(19)	B(12)-B(11)-C(2)	102(3)

B(9)-B(12)-B(8) 61(2) B(9)-B(12)-B(10) 69(2)

B(8)-B(12)-B(10) 117(3) B(9)-B(12)-B(11) 113(3)

B(8)-B(12)-B(11) 113(3) B(10)-B(12)-B(11) 57(2)

B(9)-B(12)-B(7) 111(3) B(8)-B(12)-B(7) 64(2)

B(10)-B(12)-B(7) 107(3) B(11)-B(12)-B(7) 59(2)

C(5')-Co(1')-C(3') 68.1(13) C(5')-Co(1')-C(4') 31.5(12)

C(3')-Co(1')-C(4') 47.5(14) C(5')-Co(1')-C(6') 44.4(14)

C(3')-Co(1')-C(6') 68.6(13) C(4')-Co(1')-C(6') 66.0(14)

C(5')-Co(1')-C(7') 62.8(14) C(3')-Co(1')-C(7') 50.4(14)

C(4')-Co(1')-C(7') 71.0(15) C(6')-Co(1')-C(7') 27.6(11)

C(5')-Co(1')-S(2') 140.9(11) C(3')-Co(1')-S(2') 122.0(11)

C(4')-Co(1')-S(2') 164.7(11) C(6')-Co(1')-S(2') 100.7(11)

C(7')-Co(1')-S(2') 93.7(11) C(5')-Co(1')-S(1') 108.3(11)

C(3')-Co(1')-S(1') 122.4(10) C(4')-Co(1')-S(1') 98.4(10)

C(6')-Co(1')-S(1') 148.1(11) C(7')-Co(1')-S(1') 169.5(11)

S(2')-Co(1')-S(1') 96.9(4) C(1')-S(1')-Co(1') 102.7(10)

C(2')-S(2')-Co(1') 102.3(10) C(2')-C(1')-B(3') 68(2)

C(2')-C(1')-B(4') 122(3) B(3')-C(1')-B(4') 68(2)

C(2')-C(1')-B(5') 112(2) B(3')-C(1')-B(5') 121(2)

B(4')-C(1')-B(5') 64.5(18) C(2')-C(1')-B(6') 61.7(19)

B(3')-C(1')-B(6') 121(3) B(4')-C(1')-B(6') 116(2)

B(5')-C(1')-B(6') 58.8(18) C(2')-C(1')-S(1') 113(2)

B(3')-C(1')-S(1') 119(2) B(4')-C(1')-S(1') 121(2)

B(5')-C(1')-S(1') 114.4(19) B(6')-C(1')-S(1') 108(2)

C(1')-C(2')-B(3') 59.1(18) C(1')-C(2')-S(2') 125(2)

B(3')-C(2')-S(2') 119.5(18) C(1')-C(2')-B(6') 72(2)

B(3')-C(2')-B(6') 122(2) S(2')-C(2')-B(6') 112.9(19)

C(1')-C(2')-B(7') 110(2) B(3')-C(2')-B(7') 67(2)

S(2')-C(2')-B(7') 120(2) B(6')-C(2')-B(7') 107(2)

C(4')-C(3')-C(7') 89(2) C(4')-C(3')-Co(1') 66.4(17)

C(7')-C(3')-Co(1') 64.5(16) C(5')-C(4')-C(3') 110(4)

C(5')-C(4')-Co(1') 73(3) C(3')-C(4')-Co(1') 66.1(18)

C(4')-C(5')-C(6') 114(4) C(4')-C(5')-Co(1') 76(3)

C(6')-C(5')-Co(1') 68.1(19) C(7')-C(6')-C(5') 114(4)

C(7')-C(6')-Co(1') 76(3) C(5')-C(6')-Co(1') 67.6(19)

C(6')-C(7')-C(3') 113(4) C(6')-C(7')-Co(1') 76(3)

C(3')-C(7')-Co(1') 65.1(17) C(1')-B(3')-C(2') 52.7(17)

C(1')-B(3')-B(4') 57.5(18) C(2')-B(3')-B(4') 101(2)

C(1')-B(3')-B(8') 102(2) C(2')-B(3')-B(8') 104(2)

B(4')-B(3')-B(8') 60(2) C(1')-B(3')-B(7') 100(2)

C(2')-B(3')-B(7') 60.4(18) B(4')-B(3')-B(7') 105(2)

B(8')-B(3')-B(7') 57(2) C(1')-B(4')-B(3') 54.7(17)

C(1')-B(4')-B(9') 110(2) B(3')-B(4')-B(9') 116(2)

C(1')-B(4')-B(8') 102(2) B(3')-B(4')-B(8') 63(2)

B(9')-B(4')-B(8') 61.9(19) C(1')-B(4')-B(5') 63.8(18)

B(3')-B(4')-B(5') 110(2) B(9')-B(4')-B(5') 57.6(16)

B(8')-B(4')-B(5') 104(2) B(10')-B(5')-B(9') 71(2)

B(10')-B(5')-B(6') 56(2) B(9')-B(5')-B(6') 117(3)

B(10')-B(5')-C(1') 102(2) B(9')-B(5')-C(1') 102(2)

B(6')-B(5')-C(1') 62.2(19) B(10')-B(5')-B(4') 112(2)

B(9')-B(5')-B(4') 60.5(17) B(6')-B(5')-B(4') 108(2)

C(1')-B(5')-B(4') 51.7(15) B(10')-B(6')-C(2') 107(3)

B(10')-B(6')-B(5') 58(2) C(2')-B(6')-B(5') 99(2)

B(10')-B(6')-C(1') 101(3) C(2')-B(6')-C(1') 46.3(15)

B(5')-B(6')-C(1') 59.0(18) B(10')-B(6')-B(11') 62(3)

C(2')-B(6')-B(11') 70(3) B(5')-B(6')-B(11') 111(3)

C(1')-B(6')-B(11') 107(3) B(12')-B(7')-B(8') 59(3)

B(12')-B(7')-C(2') 118(3) B(8')-B(7')-C(2') 100(3)

B(12')-B(7')-B(3') 113(3) B(8')-B(7')-B(3') 59(2)

C(2')-B(7')-B(3') 52.7(17) B(12')-B(7')-B(11') 72(3)

B(8')-B(7')-B(11') 116(3) C(2')-B(7')-B(11') 69(3)

B(3')-B(7')-B(11') 116(3) B(12')-B(8')-B(7') 55(2)

B(12')-B(8')-B(4') 120(3) B(7')-B(8')-B(4') 107(3)

B(12')-B(8')-B(9') 75(2) B(7')-B(8')-B(9') 111(3)

B(4')-B(8')-B(9') 58.9(19) B(12')-B(8')-B(3') 113(3)

B(7')-B(8')-B(3') 64(2) B(4')-B(8')-B(3') 57(2)

B(9')-B(8')-B(3') 108(3) B(5')-B(9')-B(4') 61.9(17)

B(5')-B(9')-B(8') 105(2) B(4')-B(9')-B(8') 59.2(19)

B(5')-B(9')-B(10') 52.8(19) B(4')-B(9')-B(10') 100(2)

B(8')-B(9')-B(10') 98(2) B(5')-B(9')-B(12') 104(2)

B(4')-B(9')-B(12') 99(2) B(8')-B(9')-B(12') 48.6(19)

B(10')-B(9')-B(12') 62.6(19) B(6')-B(10')-B(5') 66(3)

B(6')-B(10')-B(11') 67(3) B(5')-B(10')-B(11') 122(3)

B(6')-B(10')-B(9') 112(3) B(5')-B(10')-B(9') 55.9(19)

B(11')-B(10')-B(9') 119(3) B(10')-B(11')-B(7') 96(4)

B(10')-B(11')-B(6') 52(3) B(7')-B(11')-B(6') 96(4)

B(10')-B(11')-B(12') 66(3) B(7')-B(11')-B(12') 47(2)

B(6')-B(11')-B(12') 103(4) B(7')-B(12')-B(8') 67(3)

B(7')-B(12')-B(11') 61(3) B(8')-B(12')-B(11') 113(4)

B(7')-B(12')-B(9') 106(3) B(8')-B(12')-B(9') 56(2)

B(11')-B(12')-B(9') 102(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 (58) Co1

* 0.0000 (58) S1

* 0.0000 (2) S2

Angle to previous plane (with approximate esd) = 10.80 (92)

* -0.0292 (60) S1

* 0.0589 (18) C1

* -0.0672 (55) C2

* 0.0375 (65) S2

* -0.0818 (61) Co1

* 0.0510 (53) S1

* 0.0125 (64) C1

* -0.0981 (5) C2

* 0.1165 (40) S2

Angle to previous plane (with approximate esd) = 88.12 (90)

* -0.0221 (79) C3

* 0.0079 (53) C4

* 0.0050 (74) C5

* -0.0135 (27) C6

* 0.0228 (77) C7

* 0.0000 (61) Co1'

* 0.0000 (63) S1'

* 0.0000 (2) S2'

Angle to previous plane (with approximate esd) = 8.51 (9)

* 0.0100 (65) S1'

* -0.0247 (11) C1'

* 0.0279 (2) C2'

* -0.0131 (77) S2'

* -0.0623 (66) Co1'

* 0.0723 (4) S1'

* -0.0638 (16) C1'

* 0.0015 (48) C2'

* 0.0522 (54) S2'

Angle to previous plane (with approximate esd) = 89.08 (76)

* -0.0287 (1) C3'

* 0.0302 (23) C4'

* -0.0133 (29) C5'

* -0.0246 (49) C6'

* 0.0363 (30) C7'

Table 7. Special angles [deg] for complex **2**.

(Q1 means center of C3 C4 C5 C6 and C7

Q2 means center of C3' C4' C5' C6' and C7)

Q1-Co(1)-S(1)	135.7(13)
Q1-Co(1)-S(2)	127.4(13)
S(1)-Co(1)-S(2)	96.9(3)
total : 360.0	
Q2-Co(1')-S(1')	133.2(13)
Q2-Co(1')-S(2')	129.8(13)
S(2')-Co(1')-S(1')	96.9(4)
total : 359.9	

Experimental (KOR113, complex **3**)

A crystal size was 0.2 x 0.3 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 11.34 deg ≤ theta ≤ 13.74 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 $-17 \le h \le 19$, $-68 \le k \le 68$, $0 \le l \le 14$. 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 0.063 with 9948 (I>2sigmaI) observed reflections and 1171 parameters.

Table 1. Crystal data and structure refinement for complex **3**.

Identification code	KOR113
Empirical formula	C12 B10 H20 S2 Co2
Formula weight	454.40
Temperature	293(2) K
Wavelength	0.71070 A
Crystal system, space group	MONOCLINIC , Cc
Unit cell dimensions	a = 15.981(4) Å
	b = 55.478(17) Å beta = 115.063(16) deg.
	c = 12.0562(17) Å
Volume	9683(4) $Å^3$
Z, Calculated density	4, 1.555 Mg/m^3
Absorption coefficient	1.921 mm^{-1}
F(000)	4540
Crystal size	0.2 x 0.3 x 0.2 mm
Theta range for data collection	1.45 to 25.97 deg.
Index ranges	$-17 \le h \le 19, -68 \le k \le 68, 0 \le l \le 14$
Reflections collected / unique	19719 / 9948 [R(int) = 0.0675]
Completeness to 2theta = 25.97	49.9%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9948 / 2 / 1171
Goodness-of-fit on F^2	1.289
Final R indices [I>2sigma(I)]	R1 = 0.0630, wR2 = 0.1685
R indices (all data)	R1 = 0.1158, wR2 = 0.2015
Absolute structure parameter	0.14(4)
Largest diff. peak and hole	1.475 and -0.946 $e.Å^{-3}$

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

	x	y	z	U(eq)
Co(1)	3490(1)	83(1)	7570(2)	32(1)
Co(2)	1873(2)	24(1)	6712(2)	39(1)
S(1)	2761(3)	-146(1)	5932(4)	38(1)
S(2)	2823(3)	-151(1)	8443(3)	31(1)
C(1)	2980(12)	-454(4)	7976(15)	40(4)
C(2)	2947(10)	-449(3)	6591(12)	29(3)
C(3)	580(2)	39(7)	5190(3)	129(13)
C(4)	525(15)	9(5)	6360(3)	102(10)
C(5)	1017(18)	210(6)	7180(3)	96(10)
C(6)	1327(15)	383(4)	6500(2)	83(7)
C(7)	1076(15)	260(5)	5270(2)	75(7)
C(8)	3747(15)	425(4)	8297(17)	61(6)
C(9)	3709(13)	427(4)	7035(19)	62(6)
C(10)	4447(13)	272(3)	7110(2)	54(5)
C(11)	4930(2)	153(5)	8240(3)	79(11)
C(12)	4590(3)	231(8)	8860(4)	150(3)
B(3)	4018(17)	-493(5)	7780(2)	63(7)
B(4)	3710(16)	-663(4)	8859(17)	45(5)
B(5)	2470(17)	-704(4)	8204(19)	51(5)
B(6)	1948(18)	-561(5)	6700(2)	55(7)
B(7)	3717(16)	-659(4)	6439(19)	54(5)
B(8)	4209(16)	-801(4)	7920(2)	60(6)
B(9)	3228(17)	-942(3)	8125(18)	60(6)

B(10)	2183(19)	-871(4)	6820(2)	77(8)
B(11)	2442(18)	-709(4)	5823(17)	64(6)
B(12)	3205(19)	-934(4)	6639(19)	67(7)

Table 3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **3**. 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)	32(1)	31(1)	27(1)	6(1)	7(1)	4(1)
Co(2)	31(1)	45(2)	36(1)	5(1)	8(1)	10(1)
S(1)	58(3)	35(2)	22(2)	6(2)	17(2)	5(2)
S(2)	40(2)	39(3)	17(2)	-3(2)	15(2)	6(2)
C(1)	61(10)	49(10)	22(8)	3(7)	29(7)	-6(7)
C(2)	53(8)	26(7)	17(6)	8(5)	24(6)	8(5)
C(3)	86(16)	170(3)	80(2)	9(18)	-12(15)	92(17)
C(4)	36(11)	98(18)	160(3)	-24(18)	30(14)	-4(11)
C(5)	55(14)	120(2)	110(2)	-30(18)	38(15)	31(14)
C(6)	62(11)	57(12)	108(17)	0(11)	16(11)	37(9)
C(7)	57(10)	73(14)	72(13)	34(11)	4(9)	20(9)
C(8)	74(12)	33(10)	47(10)	-10(8)	-4(9)	-8(8)
C(9)	49(9)	52(11)	55(11)	7(8)	-7(8)	-18(7)
C(10)	41(8)	36(10)	81(13)	11(8)	22(8)	-14(7)
C(11)	55(14)	55(14)	100(2)	36(15)	3(14)	-20(11)
C(12)	90(3)	140(4)	150(4)	50(3)	-30(2)	-80(3)
B(3)	79(14)	91(17)	29(10)	22(10)	31(10)	33(11)
B(4)	76(13)	46(11)	19(8)	13(7)	26(8)	10(9)
B(5)	92(14)	38(10)	31(9)	7(7)	33(9)	-11(9)
B(6)	81(16)	42(13)	43(12)	-3(9)	26(11)	-17(10)
B(7)	99(15)	30(10)	37(10)	3(8)	33(10)	19(9)
B(8)	75(13)	62(13)	43(11)	15(9)	26(10)	33(10)
B(9)	108(16)	29(9)	38(9)	11(7)	26(10)	11(9)

B(10)	130(2)	46(12)	48(12)	5(9)	29(12)	-31(12)
B(11)	124(18)	47(11)	27(9)	-1(8)	37(11)	-13(11)
B(12)	140(2)	32(10)	42(11)	11(8)	50(12)	13(11)

Table 4. Bond lengths [Å] for complex **3**.

Co(1)-C(12) 1.96(3) Co(1)-C(8) 2.06(2)

Co(1)-C(9) 2.09(2) Co(1)-C(11) 2.13(3)

Co(1)-C(10) 2.115(17) Co(1)-S(2) 2.208(5)

Co(1)-S(1) 2.217(5) Co(1)-Co(2) 2.365(3)

Co(2)-C(5) 1.97(2) Co(2)-C(4) 2.01(2)

Co(2)-C(7) 2.12(2) Co(2)-C(3) 2.10(3)

Co(2)-C(6) 2.15(2) Co(2)-S(2) 2.217(5)

Co(2)-S(1) 2.218(5) S(1)-C(2) 1.832(16)

S(2)-C(1) 1.82(2) C(1)-C(2) 1.65(2)

C(1)-B(4) 1.67(3) C(1)-B(5) 1.69(3)

C(1)-B(6) 1.81(3) C(1)-B(3) 1.79(3)

C(2)-B(11) 1.72(3) C(2)-B(3) 1.72(3)

C(2)-B(7) 1.76(2) C(2)-B(6) 1.77(3)

C(3)-C(4) 1.46(5) C(3)-C(7) 1.44(4)

C(4)-C(5) 1.48(4) C(5)-C(6) 1.48(4)

C(6)-C(7) 1.52(3) C(8)-C(9) 1.50(3)

C(8)-C(12) 1.63(5) C(9)-C(10) 1.43(3)

C(10)-C(11) 1.41(4) C(10)-C(12) 2.04(6)

C(11)-C(12) 1.19(6) B(3)-B(7) 1.74(3)

B(3)-B(8) 1.73(3) B(3)-B(4) 1.83(3)

B(4)-B(9) 1.79(3) B(4)-B(5) 1.81(3)

B(4)-B(8) 1.81(3) B(5)-B(10) 1.79(3)

B(5)-B(6) 1.82(3) B(5)-B(9) 1.82(3)

B(6)-B(10) 1.75(4) B(6)-B(11) 1.77(4)

B(7)-B(8) 1.79(3) B(7)-B(12) 1.80(3)

B(7)-B(11) 1.87(3) B(8)-B(12) 1.84(3)

B(8)-B(9) 1.86(3) B(9)-B(12) 1.78(3)

B(9)-B(10) 1.79(3) B(10)-B(11) 1.68(3)

B(10)-B(12) 1.77(4) B(11)-B(12) 1.73(3)

Table 5. Bond angles [deg] for complex **3**.

C(12)-Co(1)-C(8) 47.6(15) C(12)-Co(1)-C(9) 69.7(14)
C(8)-Co(1)-C(9) 42.3(9) C(12)-Co(1)-C(11) 33.4(18)
C(8)-Co(1)-C(11) 71.4(12) C(9)-Co(1)-C(11) 69.8(9)
C(12)-Co(1)-C(10) 60.0(16) C(8)-Co(1)-C(10) 67.5(9)
C(9)-Co(1)-C(10) 39.8(8) C(11)-Co(1)-C(10) 38.9(10)
C(12)-Co(1)-S(2) 108.4(14) C(8)-Co(1)-S(2) 112.8(7)
C(9)-Co(1)-S(2) 149.4(7) C(11)-Co(1)-S(2) 126.1(8)
C(10)-Co(1)-S(2) 165.0(6) C(12)-Co(1)-S(1) 154.4(16)
C(8)-Co(1)-S(1) 147.3(5) C(9)-Co(1)-S(1) 109.9(6)
C(11)-Co(1)-S(1) 121.2(11) C(10)-Co(1)-S(1) 102.5(6)
S(2)-Co(1)-S(1) 84.91(19) C(12)-Co(1)-Co(2) 147.8(16)
C(8)-Co(1)-Co(2) 107.3(6) C(9)-Co(1)-Co(2) 106.6(5)
C(11)-Co(1)-Co(2) 176.0(8) C(10)-Co(1)-Co(2) 137.0(6)
S(2)-Co(1)-Co(2) 57.89(14) S(1)-Co(1)-Co(2) 57.80(16)
C(5)-Co(2)-C(4) 43.5(12) C(5)-Co(2)-C(7) 70.3(12)
C(4)-Co(2)-C(7) 68.6(12) C(5)-Co(2)-C(3) 71.6(13)
C(4)-Co(2)-C(3) 41.3(13) C(7)-Co(2)-C(3) 39.9(11)
C(5)-Co(2)-C(6) 41.8(11) C(4)-Co(2)-C(6) 70.7(11)
C(7)-Co(2)-C(6) 41.8(9) C(3)-Co(2)-C(6) 70.0(11)
C(5)-Co(2)-S(2) 104.0(10) C(4)-Co(2)-S(2) 115.2(11)
C(7)-Co(2)-S(2) 167.7(8) C(3)-Co(2)-S(2) 150.0(12)
C(6)-Co(2)-S(2) 126.9(7) C(5)-Co(2)-S(1) 170.8(10)
C(4)-Co(2)-S(1) 135.4(9) C(7)-Co(2)-S(1) 100.6(7)
C(3)-Co(2)-S(1) 102.5(10) C(6)-Co(2)-S(1) 130.0(8)
S(2)-Co(2)-S(1) 84.66(17) C(5)-Co(2)-Co(1) 124.3(9)

C(4)-Co(2)-Co(1) 166.4(10) C(7)-Co(2)-Co(1) 116.0(7)

C(3)-Co(2)-Co(1) 149.7(12) C(6)-Co(2)-Co(1) 103.8(7)

S(2)-Co(2)-Co(1) 57.50(15) S(1)-Co(2)-Co(1) 57.75(15)

C(2)-S(1)-Co(2) 102.8(5) C(2)-S(1)-Co(1) 102.3(5)

Co(2)-S(1)-Co(1) 64.45(16) C(1)-S(2)-Co(1) 103.7(5)

C(1)-S(2)-Co(2) 104.0(6) Co(1)-S(2)-Co(2) 64.61(15)

C(2)-C(1)-B(4) 111.7(14) C(2)-C(1)-B(5) 111.4(14)

B(4)-C(1)-B(5) 65.2(14) C(2)-C(1)-B(6) 61.3(11)

B(4)-C(1)-B(6) 116.8(17) B(5)-C(1)-B(6) 62.5(12)

C(2)-C(1)-B(3) 60.0(10) B(4)-C(1)-B(3) 64.0(12)

B(5)-C(1)-B(3) 117.3(17) B(6)-C(1)-B(3) 114.2(15)

C(2)-C(1)-S(2) 110.5(12) B(4)-C(1)-S(2) 126.4(13)

B(5)-C(1)-S(2) 124.6(13) B(6)-C(1)-S(2) 111.7(14)

B(3)-C(1)-S(2) 114.3(14) C(1)-C(2)-B(11) 109.9(13)

C(1)-C(2)-B(3) 64.0(11) B(11)-C(2)-B(3) 113.9(16)

C(1)-C(2)-B(7) 111.9(13) B(11)-C(2)-B(7) 65.1(13)

B(3)-C(2)-B(7) 60.0(12) C(1)-C(2)-B(6) 63.9(11)

B(11)-C(2)-B(6) 61.0(13) B(3)-C(2)-B(6) 119.9(13)

B(7)-C(2)-B(6) 118.1(15) C(1)-C(2)-S(1) 112.5(11)

B(11)-C(2)-S(1) 125.8(11) B(3)-C(2)-S(1) 114.3(13)

B(7)-C(2)-S(1) 123.7(11) B(6)-C(2)-S(1) 111.7(12)

C(4)-C(3)-C(7) 107(3) C(4)-C(3)-Co(2) 65.9(13)

C(7)-C(3)-Co(2) 70.6(15) C(3)-C(4)-C(5) 109(3)

C(3)-C(4)-Co(2) 72.7(16) C(5)-C(4)-Co(2) 66.9(12)

C(6)-C(5)-C(4) 109(3) C(6)-C(5)-Co(2) 75.3(13)

C(4)-C(5)-Co(2) 69.6(14) C(5)-C(6)-C(7) 104(2)

C(5)-C(6)-Co(2) 62.9(12) C(7)-C(6)-Co(2) 68.2(11)

C(3)-C(7)-C(6) 111(2) C(3)-C(7)-Co(2) 69.5(13)

C(6)-C(7)-Co(2) 70.0(11) C(9)-C(8)-C(12) 96(2)

C(9)-C(8)-Co(1) 70.0(11) C(12)-C(8)-Co(1) 63.2(15)

C(10)-C(9)-C(8) 104.8(18) C(10)-C(9)-Co(1) 71.1(11)

C(8)-C(9)-Co(1) 67.7(11) C(11)-C(10)-C(9) 116(2)

C(11)-C(10)-C(12) 34(2) C(9)-C(10)-C(12) 82(2)

C(11)-C(10)-Co(1) 71.1(14) C(9)-C(10)-Co(1) 69.2(11)

C(12)-C(10)-Co(1) 56.3(12) C(12)-C(11)-C(10) 103(4)

C(12)-C(11)-Co(1) 66(3) C(10)-C(11)-Co(1) 70.0(14)

C(11)-C(12)-C(8) 120(4) C(11)-C(12)-Co(1) 81(3)

C(8)-C(12)-Co(1) 69.2(15) C(11)-C(12)-C(10) 42(2)

C(8)-C(12)-C(10) 77(2) Co(1)-C(12)-C(10) 63.7(14)

C(2)-B(3)-B(7) 61.1(12) C(2)-B(3)-B(8) 107.0(18)

B(7)-B(3)-B(8) 62.3(14) C(2)-B(3)-C(1) 56.0(10)

B(7)-B(3)-C(1) 106.4(17) B(8)-B(3)-C(1) 104.2(18)

C(2)-B(3)-B(4) 101.0(16) B(7)-B(3)-B(4) 109.7(18)

B(8)-B(3)-B(4) 61.0(13) C(1)-B(3)-B(4) 54.9(11)

C(1)-B(4)-B(9) 104.4(15) C(1)-B(4)-B(5) 58.0(11)

B(9)-B(4)-B(5) 60.8(13) C(1)-B(4)-B(8) 105.6(13)

B(9)-B(4)-B(8) 62.3(13) B(5)-B(4)-B(8) 111.3(15)

C(1)-B(4)-B(3) 61.1(11) B(9)-B(4)-B(3) 106.3(14)

B(5)-B(4)-B(3) 109.2(14) B(8)-B(4)-B(3) 56.6(12)

C(1)-B(5)-B(10) 102.9(14) C(1)-B(5)-B(6) 62.0(12)

B(10)-B(5)-B(6) 58.0(13) C(1)-B(5)-B(4) 56.8(12)

B(10)-B(5)-B(4) 105.8(16) B(6)-B(5)-B(4) 109.5(15)

C(1)-B(5)-B(9) 102.1(15) B(10)-B(5)-B(9) 59.3(13)

B(6)-B(5)-B(9) 107.4(15) B(4)-B(5)-B(9) 59.1(13)

B(10)-B(6)-C(2) 100.3(18) B(10)-B(6)-B(11) 57.1(14)

C(2)-B(6)-B(11) 58.0(12) B(10)-B(6)-B(5) 60.1(14)

C(2)-B(6)-B(5) 100.4(16) B(11)-B(6)-B(5) 105.1(18)

B(10)-B(6)-C(1) 99.7(17) C(2)-B(6)-C(1) 54.8(10)

B(11)-B(6)-C(1) 100.5(17) B(5)-B(6)-C(1) 55.5(11)

B(3)-B(7)-C(2) 58.9(11) B(3)-B(7)-B(8) 58.5(13)

C(2)-B(7)-B(8) 102.6(13) B(3)-B(7)-B(12) 106.7(15)

C(2)-B(7)-B(12) 99.7(14) B(8)-B(7)-B(12) 61.8(13)

B(3)-B(7)-B(11) 105.8(15) C(2)-B(7)-B(11) 56.3(11)

B(8)-B(7)-B(11) 105.9(15) B(12)-B(7)-B(11) 56.3(12)

B(3)-B(8)-B(7) 59.2(12) B(3)-B(8)-B(4) 62.4(12)

B(7)-B(8)-B(4) 108.3(13) B(3)-B(8)-B(12) 105.1(15)

B(7)-B(8)-B(12) 59.1(12) B(4)-B(8)-B(12) 103.6(15)

B(3)-B(8)-B(9) 107.7(15) B(7)-B(8)-B(9) 106.2(15)

B(4)-B(8)-B(9) 58.3(12) B(12)-B(8)-B(9) 57.3(11)

B(12)-B(9)-B(10) 59.5(13) B(12)-B(9)-B(4) 107.3(14)

B(10)-B(9)-B(4) 106.8(14) B(12)-B(9)-B(5) 107.7(14)

B(10)-B(9)-B(5) 59.5(13) B(4)-B(9)-B(5) 60.2(12)

B(12)-B(9)-B(8) 60.8(13) B(10)-B(9)-B(8) 108.2(14)

B(4)-B(9)-B(8) 59.4(12) B(5)-B(9)-B(8) 108.6(13)

B(11)-B(10)-B(6) 62.0(14) B(11)-B(10)-B(5) 110.2(16)

B(6)-B(10)-B(5) 61.8(14) B(11)-B(10)-B(12) 60.1(14)

B(6)-B(10)-B(12) 111.3(16) B(5)-B(10)-B(12) 109.3(17)

B(11)-B(10)-B(9) 109.0(18) B(6)-B(10)-B(9) 112.0(16)

B(5)-B(10)-B(9) 61.2(13) B(12)-B(10)-B(9) 59.9(13)

C(2)-B(11)-B(10) 105.4(13) C(2)-B(11)-B(12) 104.0(15)

B(10)-B(11)-B(12)	62.4(14)	C(2)-B(11)-B(6)	61.0(12)		
B(10)-B(11)-B(6)	60.9(14)	B(12)-B(11)-B(6)	112.3(15)		
C(2)-B(11)-B(7)	58.5(11)	B(10)-B(11)-B(7)	110.6(16)		
B(12)-B(11)-B(7)	59.6(13)	B(6)-B(11)-B(7)	112.4(15)		
B(11)-B(12)-B(9)	107.5(16)	B(11)-B(12)-B(10)	57.5(13)		
B(9)-B(12)-B(10)	60.6(13)	B(11)-B(12)-B(7)	64.0(12)		
B(9)-B(12)-B(7)	110.0(16)	B(10)-B(12)-B(7)	110.2(15)		
B(11)-B(12)-B(8)	109.8(15)	B(9)-B(12)-B(8)	61.9(13)		
B(10)-B(12)-B(8)	109.9(15)	B(7)-B(12)-B(8)	59.1(12)		

Experimental (KOR086, complex **4a**)

A crystal size was 0.2 x 0.15 x 0.3 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 11.37 deg < theta < 13.82 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 $0 \leq h \leq 12$, $-14 \leq k \leq 13$, $-14 \leq l \leq 14$. 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 0.048 with 4325 (I>2sigmal) observed reflections and 288 parameters.

Table 1. Crystal data and structure refinement for complex **4a**.

Identification code	kor086
Empirical formula	C13 H21 B10 Co O4 S2
Formula weight	472.45
Temperature	293(2) K
Wavelength	0.71070 Å
Crystal system, space group	TRICLINIC , P-1
Unit cell dimensions	a = 10.0447(7) Å alpha = 115.980(3) deg.
	b = 11.5109(6) Å beta = 106.281(5) deg.
	c = 12.0399(5) Å gamma = 102.960(5) deg.
Volume	1099.78(11) $Å^3$
Z, Calculated density	2, 1.427 Mg/m^3
Absorption coefficient	0.988 mm^{-1}
F(000)	480
Crystal size	0.2 x 0.15 x 0.3 mm
Theta range for data collection	2.04 to 25.97 deg.
Index ranges	$0 \le h \le 12, -14 \le k \le 13, -14 \le l \le 14$
Reflections collected / unique	4661 / 4325 [R(int) = 0.0195]
Completeness to 2theta = 25.97	100.0%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4325 / 0 / 288
Goodness-of-fit on F^2	0.877
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1205
R indices (all data)	R1 = 0.1329, wR2 = 0.1571
Largest diff. peak and hole	0.297 and -0.337 $e.Å^{-3}$

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

	x	y	z	U(eq)
Co(1)	3876(1)	2469(1)	2269(1)	39(1)
S(1)	5589(2)	4716(1)	3550(1)	48(1)
S(2)	5311(1)	1660(1)	1248(1)	38(1)
O(1)	7613(5)	474(5)	2111(4)	68(1)
O(2)	7149(5)	633(4)	3873(4)	63(1)
O(3)	3941(5)	936(5)	4365(5)	76(1)
O(4)	6210(4)	2748(4)	5643(4)	54(1)
C(1)	6801(5)	4725(5)	2722(5)	38(1)
C(2)	6774(5)	3194(5)	1639(4)	34(1)
C(3)	1874(9)	1575(18)	554(8)	158(7)
C(4)	2067(7)	2879(11)	1439(12)	96(3)
C(5)	2163(8)	2925(11)	2607(8)	92(3)
C(6)	1967(10)	1710(2)	2421(18)	149(6)
C(7)	1834(11)	869(10)	1190(2)	193(11)
C(8)	8185(8)	15(7)	4160(7)	71(2)
C(9)	6988(6)	806(5)	2842(5)	45(1)
C(10)	5916(5)	1476(5)	2675(5)	38(1)
C(11)	5075(5)	1917(5)	3323(5)	39(1)
C(12)	4997(6)	1797(6)	4485(5)	47(1)
C(13)	6280(8)	2665(8)	6818(6)	75(2)
B(3)	5992(8)	4066(7)	976(6)	46(1)
B(4)	7194(8)	5865(7)	2186(7)	57(2)

B(5)	8602(8)	5968(7)	3552(7)	58(2)
B(6)	8299(6)	4263(6)	3209(6)	43(1)
B(7)	7092(8)	3189(7)	320(6)	52(2)
B(8)	7415(9)	4918(8)	674(7)	61(2)
B(9)	9027(9)	6099(8)	2278(8)	64(2)
B(10)	9702(8)	5110(7)	2902(7)	57(2)
B(11)	8506(7)	3306(7)	1676(6)	46(1)
B(12)	8971(9)	4461(8)	1128(7)	62(2)

Table 3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **4a**. 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)	28(1)	40(1)	42(1)	16(1)	15(1)	14(1)
S(1)	48(1)	38(1)	47(1)	11(1)	29(1)	15(1)
S(2)	35(1)	34(1)	35(1)	12(1)	13(1)	15(1)
O(1)	82(3)	92(3)	78(3)	57(3)	55(3)	64(3)
O(2)	77(3)	76(3)	81(3)	58(2)	48(2)	52(2)
O(3)	55(3)	89(3)	84(3)	57(3)	28(2)	6(2)
O(4)	55(2)	61(2)	48(2)	30(2)	26(2)	22(2)
C(1)	41(3)	35(3)	37(3)	15(2)	21(2)	19(2)
C(2)	34(3)	39(3)	31(2)	18(2)	15(2)	19(2)
C(3)	36(4)	257(16)	35(4)	-17(7)	3(3)	39(8)
C(4)	31(4)	147(8)	159(9)	128(8)	29(5)	38(4)
C(5)	41(4)	124(7)	71(5)	17(5)	25(4)	43(5)
C(6)	41(5)	281(18)	252(16)	235(16)	70(8)	68(9)
C(7)	26(4)	50(5)	360(3)	34(9)	38(11)	4(4)
C(8)	79(5)	74(4)	93(5)	62(4)	36(4)	48(4)
C(9)	43(3)	39(3)	52(3)	25(3)	21(3)	15(2)
C(10)	36(3)	35(2)	45(3)	23(2)	18(2)	15(2)
C(11)	31(3)	33(3)	43(3)	16(2)	14(2)	8(2)
C(12)	43(3)	49(3)	51(3)	27(3)	24(3)	18(3)
C(13)	85(5)	94(5)	53(4)	43(4)	32(4)	36(4)
B(3)	56(4)	52(4)	47(3)	32(3)	24(3)	32(3)
B(4)	66(5)	48(4)	74(5)	40(4)	38(4)	26(3)
B(5)	45(4)	48(4)	61(4)	20(3)	23(3)	4(3)

B(6)	31(3)	47(3)	35(3)	19(3)	8(2)	4(3)
B(7)	65(4)	60(4)	41(3)	27(3)	31(3)	32(3)
B(8)	80(5)	70(5)	63(4)	48(4)	42(4)	41(4)
B(9)	65(5)	66(5)	83(5)	51(4)	43(4)	24(4)
B(10)	43(4)	69(4)	58(4)	33(4)	27(3)	17(3)
B(11)	41(3)	56(4)	51(4)	29(3)	27(3)	29(3)
B(12)	70(5)	86(5)	67(4)	53(4)	48(4)	44(4)

Table 4. Bond lengths [Å] for **4a**.

Co(1)-C(11)	1.912(5)	Co(1)-C(7)	2.000(9)
Co(1)-C(5)	2.003(6)	Co(1)-C(6)	2.016(8)
Co(1)-C(3)	2.061(8)	Co(1)-C(4)	2.075(6)
Co(1)-S(2)	2.2462(13)	Co(1)-S(1)	2.2474(15)
S(1)-C(1)	1.778(5)	S(2)-C(10)	1.777(5)
S(2)-C(2)	1.794(5)	O(1)-C(9)	1.200(6)
O(2)-C(9)	1.313(6)	O(2)-C(8)	1.433(6)
O(3)-C(12)	1.202(6)	O(4)-C(12)	1.318(6)
O(4)-C(13)	1.444(7)	C(1)-C(2)	1.659(6)
C(1)-B(5)	1.700(8)	C(1)-B(4)	1.717(8)
C(1)-B(3)	1.739(7)	C(1)-B(6)	1.740(8)
C(2)-B(11)	1.702(7)	C(2)-B(7)	1.703(7)
C(2)-B(6)	1.711(7)	C(2)-B(3)	1.722(7)
C(3)-C(4)	1.334(14)	C(3)-C(7)	1.34(2)
C(4)-C(5)	1.359(11)	C(5)-C(6)	1.276(15)
C(6)-C(7)	1.315(19)	C(9)-C(10)	1.477(7)
C(10)-C(11)	1.340(7)	C(11)-C(12)	1.487(7)
B(3)-B(8)	1.764(10)	B(3)-B(4)	1.765(9)
B(3)-B(7)	1.777(8)	B(4)-B(9)	1.764(10)
B(4)-B(8)	1.774(9)	B(4)-B(5)	1.780(10)
B(5)-B(6)	1.751(9)	B(5)-B(9)	1.760(10)
B(5)-B(10)	1.763(10)	B(6)-B(10)	1.751(9)
B(6)-B(11)	1.789(8)	B(7)-B(11)	1.767(9)
B(7)-B(12)	1.771(10)	B(7)-B(8)	1.772(10)
B(8)-B(9)	1.777(11)	B(8)-B(12)	1.778(10)
B(9)-B(12)	1.760(10)	B(9)-B(10)	1.769(10)

B(10)-B(11) 1.770(9) B(10)-B(12) 1.771(9)

B(11)-B(12) 1.756(10)