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

Identification code	complex 5
Empirical formula	C26 H34 Ni P2 S Si
Formula weight	527.33
Temperature	373(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.589(2) A alpha = 104.41(3) deg.
	b = 11.128(2) A beta = 104.69(3) deg.
	c = 12.139(2) A gamma = 90.20(3) deg.
Volume	1336.7(5) A^3
Z, Calculated density	2, 1.310 Mg/m^3
Absorption coefficient	0.980 mm^-1
F(000)	556
Crystal size	? x ? x ? mm
Theta range for data collection	1.89 to 27.10 deg.
Limiting indices	-13<=h<=9, -14<=k<=14, -13<=l<=15
Reflections collected / unique	7761 / 5223 [R(int) = 0.0678]
Completeness to theta = 27.10	88.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5223 / 0 / 416
Goodness-of-fit on F^2	0.817
Final R indices [I>2sigma(I)]	R1 = 0.0437, wR2 = 0.1121
R indices (all data)	R1 = 0.0546, wR2 = 0.1183
Largest diff. peak and hole	0.490 and -0.953 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^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)
Si(1)	1515(1)	1814(1)	4038(1)	28(1)
S(1)	1341(1)	5610(1)	2590(1)	29(1)
Ni(1)	1141(1)	3576(1)	2347(1)	25(1)
P(1)	-981(1)	3609(1)	2013(1)	29(1)
P(2)	2978(1)	3395(1)	1882(1)	25(1)
C(1)	-1583(4)	3961(4)	592(3)	45(1)
C(2)	-1592(3)	4825(3)	3010(4)	41(1)
C(3)	-2035(3)	2244(3)	1830(3)	40(1)
C(4)	2749(3)	2444(2)	369(2)	29(1)
C(5)	1631(3)	2625(3)	-454(3)	33(1)
C(6)	1377(3)	1967(3)	-1634(3)	38(1)
C(7)	2237(4)	1108(3)	-1985(3)	40(1)
C(8)	3332(3)	913(3)	-1180(3)	36(1)
C(9)	3612(3)	1590(3)	0(3)	31(1)
C(10)	3561(3)	4919(2)	1852(2)	27(1)
C(11)	2817(3)	5900(2)	2241(2)	28(1)
C(12)	3260(3)	7115(3)	2321(3)	32(1)
C(13)	4377(3)	7332(3)	1991(3)	34(1)
C(14)	5091(3)	6352(3)	1564(3)	32(1)
C(15)	4676(3)	5150(3)	1497(2)	29(1)
C(16)	4380(3)	2850(2)	2804(2)	27(1)
C(17)	5303(3)	3730(3)	3654(2)	29(1)
C(18)	6293(3)	3365(3)	4475(3)	32(1)
C(19)	6372(3)	2112(3)	4456(3)	33(1)
C(20)	5459(3)	1228(3)	3618(3)	33(1)
C(21)	4460(3)	1590(3)	2795(3)	30(1)
C(22)	1142(3)	1892(2)	2455(2)	28(1)
C(23)	923(3)	852(3)	1578(3)	34(1)
C(24)	2017(4)	228(3)	4168(3)	39(1)
C(25)	41(3)	2093(3)	4638(3)	38(1)
C(26)	2857(3)	2975(3)	5025(3)	34(1)

Table 3. Bond lengths [A] and angles [deg] for complex 5.

Si(1)-C(26)	1.864(3)
Si(1)-C(24)	1.877(3)
Si(1)-C(25)	1.879(3)
Si(1)-C(22)	1.886(3)
S(1)-C(11)	1.769(3)
S(1)-Ni(1)	2.2117(9)
Ni(1)-C(22)	1.911(3)
Ni(1)-P(2)	2.1546(8)
Ni(1)-P(1)	2.1819(9)
P(1)-C(3)	1.816(3)
P(1)-C(2)	1.818(3)
P(1)-C(1)	1.821(4)
P(2)-C(10)	1.815(3)
P(2)-C(16)	1.824(3)
P(2)-C(4)	1.833(3)
C(4)-C(5)	1.393(4)
C(4)-C(9)	1.393(4)
C(5)-C(6)	1.393(4)
C(6)-C(7)	1.388(5)
C(7)-C(8)	1.371(5)
C(8)-C(9)	1.397(4)
C(10)-C(15)	1.399(4)
C(10)-C(11)	1.405(4)
C(11)-C(12)	1.402(4)
C(12)-C(13)	1.380(4)
C(13)-C(14)	1.397(4)
C(14)-C(15)	1.383(4)
C(16)-C(17)	1.400(4)
C(16)-C(21)	1.402(4)
C(17)-C(18)	1.389(4)
C(18)-C(19)	1.391(4)
C(19)-C(20)	1.390(5)
C(20)-C(21)	1.395(4)
C(22)-C(23)	1.336(4)
C(26)-Si(1)-C(24)	107.87(16)
C(26)-Si(1)-C(25)	107.51(15)
C(24)-Si(1)-C(25)	106.52(15)
C(26)-Si(1)-C(22)	112.48(13)
C(24)-Si(1)-C(22)	110.50(14)

C(25)-Si(1)-C(22)	111.69(14)
C(11)-S(1)-Ni(1)	105.47(9)
C(22)-Ni(1)-P(2)	90.06(8)
C(22)-Ni(1)-P(1)	93.51(9)
P(2)-Ni(1)-P(1)	155.77(3)
C(22)-Ni(1)-S(1)	168.86(9)
P(2)-Ni(1)-S(1)	90.10(4)
P(1)-Ni(1)-S(1)	90.90(4)
C(3)-P(1)-C(2)	103.33(16)
C(3)-P(1)-C(1)	101.45(18)
C(2)-P(1)-C(1)	103.35(19)
C(3)-P(1)-Ni(1)	122.65(12)
C(2)-P(1)-Ni(1)	116.58(12)
C(1)-P(1)-Ni(1)	106.94(12)
C(10)-P(2)-C(16)	103.99(13)
C(10)-P(2)-C(4)	104.28(12)
C(16)-P(2)-C(4)	107.26(13)
C(10)-P(2)-Ni(1)	108.09(9)
C(16)-P(2)-Ni(1)	120.82(9)
C(4)-P(2)-Ni(1)	111.00(10)
C(5)-C(4)-C(9)	119.2(3)
C(5)-C(4)-P(2)	116.1(2)
C(9)-C(4)-P(2)	124.7(2)
C(6)-C(5)-C(4)	120.7(3)
C(7)-C(6)-C(5)	119.4(3)
C(8)-C(7)-C(6)	120.3(3)
C(7)-C(8)-C(9)	120.6(3)
C(4)-C(9)-C(8)	119.7(3)
C(15)-C(10)-C(11)	120.5(2)
C(15)-C(10)-P(2)	124.5(2)
C(11)-C(10)-P(2)	115.02(19)
C(12)-C(11)-C(10)	118.3(2)
C(12)-C(11)-S(1)	120.7(2)
C(10)-C(11)-S(1)	121.0(2)
C(13)-C(12)-C(11)	120.5(3)
C(12)-C(13)-C(14)	121.2(3)
C(15)-C(14)-C(13)	118.9(3)
C(14)-C(15)-C(10)	120.5(2)
C(17)-C(16)-C(21)	119.1(3)
C(17)-C(16)-P(2)	118.7(2)
C(21)-C(16)-P(2)	121.6(2)
C(18)-C(17)-C(16)	120.7(3)
C(17)-C(18)-C(19)	120.0(3)
C(20)-C(19)-C(18)	120.0(3)

C(19)-C(20)-C(21)	120.3(3)
C(20)-C(21)-C(16)	120.0(3)
C(23)-C(22)-Si(1)	120.7(2)
C(23)-C(22)-Ni(1)	128.1(2)
Si(1)-C(22)-Ni(1)	111.20(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 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
Si(1)	30(1)	30(1)	28(1)	9(1)	12(1)	3(1)
S(1)	27(1)	29(1)	32(1)	6(1)	13(1)	3(1)
Ni(1)	23(1)	28(1)	25(1)	6(1)	9(1)	2(1)
P(1)	24(1)	33(1)	30(1)	8(1)	9(1)	2(1)
P(2)	24(1)	28(1)	25(1)	6(1)	10(1)	3(1)
C(1)	32(2)	60(2)	43(2)	21(2)	3(2)	1(2)
C(2)	27(2)	43(2)	51(2)	2(2)	15(2)	4(1)
C(3)	30(2)	45(2)	46(2)	15(1)	9(2)	0(1)
C(4)	30(1)	31(1)	29(1)	9(1)	12(1)	0(1)
C(5)	32(2)	38(2)	31(2)	8(1)	10(1)	-2(1)
C(6)	37(2)	48(2)	27(2)	8(1)	5(2)	-7(1)
C(7)	57(2)	35(2)	28(2)	1(1)	18(2)	-11(1)
C(8)	46(2)	32(2)	35(2)	6(1)	21(2)	0(1)
C(9)	35(2)	30(1)	31(2)	9(1)	15(1)	1(1)
C(10)	26(1)	29(1)	25(1)	7(1)	7(1)	1(1)
C(11)	30(1)	29(1)	24(1)	5(1)	8(1)	1(1)
C(12)	35(2)	29(1)	32(2)	6(1)	11(1)	2(1)
C(13)	38(2)	29(1)	35(2)	7(1)	11(1)	-4(1)
C(14)	28(1)	38(2)	33(2)	11(1)	10(1)	-2(1)
C(15)	27(1)	34(1)	27(1)	9(1)	9(1)	3(1)
C(16)	28(1)	31(1)	26(1)	8(1)	11(1)	3(1)
C(17)	30(1)	31(1)	27(1)	7(1)	10(1)	3(1)
C(18)	27(1)	41(2)	28(1)	9(1)	7(1)	1(1)
C(19)	28(1)	42(2)	31(2)	13(1)	9(1)	7(1)
C(20)	35(2)	36(2)	33(2)	11(1)	15(1)	9(1)
C(21)	30(1)	32(1)	31(1)	7(1)	12(1)	4(1)
C(22)	24(1)	32(1)	29(1)	8(1)	9(1)	1(1)
C(23)	37(2)	33(2)	34(2)	7(1)	12(1)	-1(1)
C(24)	50(2)	36(2)	38(2)	14(1)	17(2)	6(1)
C(25)	34(2)	50(2)	35(2)	13(1)	14(2)	3(1)
C(26)	36(2)	39(2)	30(2)	7(1)	14(1)	2(1)

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

	x	y	z	U(eq)
H(211)	-2500(40)	4830(30)	2680(40)	49(10)
H(212)	-1410(40)	4710(40)	3760(40)	56(12)
H(213)	-1070(40)	5640(40)	3090(40)	53(11)
H(311)	-1790(30)	1450(30)	1240(30)	39(9)
H(312)	-2890(40)	2390(30)	1560(40)	48(10)
H(313)	-1950(40)	2090(40)	2600(40)	58(11)
H(5)	1000(30)	3190(30)	-230(30)	32(8)
H(6)	580(30)	2090(30)	-2230(30)	35(8)
H(7)	2060(30)	620(30)	-2770(30)	31(8)
H(8)	3920(40)	360(30)	-1390(40)	52(10)
H(9)	4390(30)	1420(30)	550(30)	35(9)
H(12)	2740(30)	7820(30)	2600(30)	35(8)
H(13)	4600(30)	8160(30)	2050(30)	36(9)
H(14)	5880(30)	6510(30)	1360(30)	26(7)
H(15)	5170(30)	4440(30)	1190(30)	28(8)
H(17)	5210(30)	4600(30)	3690(30)	40(9)
H(18)	6950(40)	3990(30)	5070(30)	39(9)
H(19)	7060(30)	1890(30)	5040(30)	34(8)
H(20)	5440(30)	360(30)	3580(30)	41(9)
H(21)	3830(30)	1000(30)	2210(30)	27(8)
H(231)	980(30)	10(30)	1680(30)	34(8)
H(232)	720(30)	880(30)	780(30)	34(8)
H(241)	2740(40)	-10(40)	3900(40)	58(12)
H(242)	1330(40)	-470(30)	3700(30)	41(9)
H(243)	2180(40)	260(30)	5000(40)	49(10)
H(251)	300(40)	2050(30)	5420(40)	48(10)
H(252)	-680(40)	1450(30)	4210(30)	39(9)
H(253)	-330(40)	2870(40)	4570(40)	52(11)
H(261)	2920(40)	3000(30)	5810(40)	40(9)
H(262)	3720(50)	2760(40)	4850(40)	65(12)
H(263)	2700(40)	3730(40)	4930(30)	47(10)
H(111)	-1400(40)	3290(40)	20(40)	60(12)
H(112)	-2510(40)	4030(30)	430(40)	51(10)
H(113)	-1100(40)	4810(40)	650(40)	60(12)

Table 6. Torsion angles [deg] for sun3.