Table 1. Crystal data and structure refinement for bay01.

Identification code	bay01
Measurement device	Nonius KappaCCD
Empirical formula	C26 H38 As Fe Mo O4 P Si2
Formula weight	728.42
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic P 21/n
Unit cell dimensions	a = 12.96200(10) A alpha = 90 deg. b = 18.3280(2) A beta = 104.2460(8) deg. c = 13.7430(2) A gamma = 90 deg.
Volume	3164.49(6) A^3
Z, Calculated density	4, 1.529 Mg/m^3
Absorption coefficient	2.047 mm^-1
F(000)	1480
Crystal size, colour and habit	0.25 x 0.25 x 0.24 mm^3, red fragment
Theta range for data collection	2.95 to 30.00 deg.
Index ranges	-18<=h<=18, -25<=k<=25, -19<=l<=19
Reflections collected / unique	18141 / 9224 [R(int) = 0.0186]
Completeness to theta = 30.00	99.7%
Absorption correction	multi-scan
Max. and min. transmission	0.6394 and 0.6286
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9224 / 0 / 336
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0318, wR2 = 0.0722 [7859]
R indices (all data)	R1 = 0.0409, wR2 = 0.0757
Largest diff. peak and hole	0.970 and -0.829 e.A^-3
remarks	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for bay01.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
As(1)	4802(1)	1584(1)	2891(1)	28(1)
Mo(1)	5781(1)	1271(1)	1366(1)	24(1)
Fe(1)	3858(1)	2728(1)	2732(1)	25(1)
P(1)	6525(1)	1857(1)	3029(1)	30(1)
Si(1)	6710(1)	182(1)	3730(1)	27(1)
Si(2)	8477(1)	1024(1)	2905(1)	43(1)
O(1)	2712(2)	2338(1)	701(1)	51(1)
O(2)	5512(2)	3564(1)	2153(2)	55(1)
O(3)	3573(2)	522(1)	1069(2)	45(1)
O(4)	6424(2)	-363(1)	1312(1)	47(1)
C(1)	2438(2)	3075(1)	3058(2)	29(1)
C(2)	2787(2)	2410(1)	3586(2)	29(1)
C(3)	3800(2)	2552(1)	4257(2)	28(1)
C(4)	4088(2)	3284(1)	4117(2)	29(1)
C(5)	3231(2)	3616(1)	3380(2)	30(1)
C(6)	1379(2)	3174(2)	2325(2)	41(1)
C(7)	2176(2)	1711(2)	3517(2)	41(1)
C(8)	4410(2)	2030(2)	5027(2)	38(1)
C(9)	5072(2)	3665(2)	4694(2)	43(1)
C(10)	3165(2)	4401(1)	3061(2)	41(1)
C(11)	3189(2)	2476(1)	1498(2)	36(1)
C(12)	4875(2)	3214(1)	2376(2)	37(1)
C(13)	7025(2)	956(1)	2932(2)	26(1)
C(14)	5336(2)	-219(2)	3369(2)	43(1)
C(15)	6934(3)	505(2)	5057(2)	50(1)
C(16)	7572(2)	-642(1)	3722(2)	34(1)
C(17)	9345(3)	885(2)	4209(3)	82(1)
C(18)	8860(3)	352(2)	2034(3)	68(1)
C(19)	8874(2)	1956(2)	2538(3)	59(1)
C(20)	4396(2)	816(1)	1261(2)	32(1)
C(21)	6203(2)	244(1)	1372(2)	32(1)
C(22)	6458(2)	2313(1)	708(2)	42(1)
C(23)	6830(2)	1678(2)	318(2)	44(1)
C(24)	5939(3)	1312(1)	-276(2)	43(1)
C(25)	5023(3)	1711(1)	-258(2)	41(1)
C(26)	5342(2)	2325(1)	356(2)	39(1)

Table 3. Bond lengths [A] and angles [deg] for bay01.

As(1)-P(1)	2.2507(7)
As(1)-Fe(1)	2.4098(4)
As(1)-Mo(1)	2.7644(3)
Mo(1)-C(20)	1.953(2)
Mo(1)-C(21)	1.959(2)
Mo(1)-C(24)	2.316(2)
Mo(1)-C(23)	2.332(2)
Mo(1)-C(25)	2.349(3)
Mo(1)-C(26)	2.365(2)
Mo(1)-C(22)	2.371(2)
Mo(1)-C(13)	2.420(2)
Mo(1)-P(1)	2.4940(6)
Fe(1)-C(12)	1.757(3)
Fe(1)-C(11)	1.766(2)
Fe(1)-C(1)	2.097(2)
Fe(1)-C(2)	2.108(2)
Fe(1)-C(5)	2.112(2)
Fe(1)-C(4)	2.114(2)
Fe(1)-C(3)	2.140(2)
P(1)-C(13)	1.791(2)
Si(1)-C(15)	1.872(3)
Si(1)-C(14)	1.877(3)
Si(1)-C(16)	1.878(2)
Si(1)-C(13)	1.898(2)
Si(2)-C(18)	1.868(4)
Si(2)-C(17)	1.884(4)
Si(2)-C(19)	1.889(3)
Si(2)-C(13)	1.895(2)
O(1)-C(11)	1.146(3)
O(2)-C(12)	1.146(3)
O(3)-C(20)	1.167(3)
O(4)-C(21)	1.157(3)
C(1)-C(5)	1.418(3)
C(1)-C(2)	1.434(3)
C(1)-C(6)	1.501(3)
C(2)-C(3)	1.430(3)
C(2)-C(7)	1.497(4)
C(3)-C(4)	1.418(3)
C(3)-C(8)	1.500(3)
C(4)-C(5)	1.441(3)
C(4)-C(9)	1.499(3)
C(5)-C(10)	1.500(3)
C(22)-C(26)	1.408(4)
C(22)-C(23)	1.415(4)
C(23)-C(24)	1.410(4)
C(24)-C(25)	1.399(4)
C(25)-C(26)	1.407(4)

P(1)-As(1)-Fe(1)	106.587(19)
P(1)-As(1)-Mo(1)	58.577(16)
Fe(1)-As(1)-Mo(1)	115.444(11)
C(20)-Mo(1)-C(21)	80.83(11)
C(20)-Mo(1)-C(24)	104.00(10)
C(21)-Mo(1)-C(24)	86.77(9)
C(20)-Mo(1)-C(23)	139.12(10)
C(21)-Mo(1)-C(23)	96.03(10)
C(24)-Mo(1)-C(23)	35.30(11)
C(20)-Mo(1)-C(25)	85.09(10)
C(21)-Mo(1)-C(25)	112.60(9)
C(24)-Mo(1)-C(25)	34.90(10)
C(23)-Mo(1)-C(25)	58.32(11)
C(20)-Mo(1)-C(26)	102.80(10)
C(21)-Mo(1)-C(26)	144.44(9)

C(24)-Mo(1)-C(26)	57.86(9)
C(23)-Mo(1)-C(26)	57.94(10)
C(25)-Mo(1)-C(26)	34.73(9)
C(20)-Mo(1)-C(22)	137.37(11)
C(21)-Mo(1)-C(22)	130.23(10)
C(24)-Mo(1)-C(22)	58.21(9)
C(23)-Mo(1)-C(22)	34.99(9)
C(25)-Mo(1)-C(22)	57.95(10)
C(26)-Mo(1)-C(22)	34.60(10)
C(20)-Mo(1)-C(13)	111.27(9)
C(21)-Mo(1)-C(13)	69.07(9)
C(24)-Mo(1)-C(13)	132.44(9)
C(23)-Mo(1)-C(13)	105.27(10)
C(25)-Mo(1)-C(13)	163.40(9)
C(26)-Mo(1)-C(13)	136.75(9)
C(22)-Mo(1)-C(13)	107.64(9)
C(20)-Mo(1)-P(1)	113.10(7)
C(21)-Mo(1)-P(1)	111.41(7)
C(24)-Mo(1)-P(1)	140.53(7)
C(23)-Mo(1)-P(1)	106.00(8)
C(25)-Mo(1)-P(1)	134.44(7)
C(26)-Mo(1)-P(1)	99.75(7)
C(22)-Mo(1)-P(1)	84.65(7)
C(13)-Mo(1)-P(1)	42.71(5)
C(20)-Mo(1)-As(1)	63.83(7)
C(21)-Mo(1)-As(1)	112.09(7)
C(24)-Mo(1)-As(1)	154.00(8)
C(23)-Mo(1)-As(1)	147.97(7)
C(25)-Mo(1)-As(1)	119.10(7)
C(26)-Mo(1)-As(1)	100.74(6)
C(22)-Mo(1)-As(1)	113.82(6)
C(13)-Mo(1)-As(1)	72.85(5)
P(1)-Mo(1)-As(1)	50.362(16)
C(12)-Fe(1)-C(11)	95.15(12)
C(12)-Fe(1)-C(1)	131.60(11)
C(11)-Fe(1)-C(1)	91.99(10)
C(12)-Fe(1)-C(2)	159.57(10)
C(11)-Fe(1)-C(2)	103.12(11)
C(1)-Fe(1)-C(2)	39.88(9)
C(12)-Fe(1)-C(5)	96.90(10)
C(11)-Fe(1)-C(5)	117.21(11)
C(1)-Fe(1)-C(5)	39.38(9)
C(2)-Fe(1)-C(5)	66.69(9)
C(12)-Fe(1)-C(4)	93.31(10)
C(11)-Fe(1)-C(4)	156.60(10)
C(1)-Fe(1)-C(4)	66.32(9)
C(2)-Fe(1)-C(4)	66.33(9)
C(5)-Fe(1)-C(4)	39.89(9)
C(12)-Fe(1)-C(3)	123.99(11)
C(11)-Fe(1)-C(3)	140.69(11)
C(1)-Fe(1)-C(3)	65.94(8)
C(2)-Fe(1)-C(3)	39.33(9)
C(5)-Fe(1)-C(3)	66.00(9)
C(4)-Fe(1)-C(3)	38.93(9)
C(12)-Fe(1)-As(1)	93.84(8)
C(11)-Fe(1)-As(1)	88.70(8)
C(1)-Fe(1)-As(1)	134.19(7)
C(2)-Fe(1)-As(1)	95.62(7)
C(5)-Fe(1)-As(1)	150.71(6)
C(4)-Fe(1)-As(1)	112.47(7)
C(3)-Fe(1)-As(1)	85.42(6)
C(13)-P(1)-As(1)	99.15(7)
C(13)-P(1)-Mo(1)	66.45(7)
As(1)-P(1)-Mo(1)	71.061(18)
C(15)-Si(1)-C(14)	106.90(15)
C(15)-Si(1)-C(16)	108.08(13)
C(14)-Si(1)-C(16)	102.20(12)

C(15)-Si(1)-C(13)	108.80(12)
C(14)-Si(1)-C(13)	117.68(11)
C(16)-Si(1)-C(13)	112.63(10)
C(18)-Si(2)-C(17)	109.2(2)
C(18)-Si(2)-C(19)	106.97(16)
C(17)-Si(2)-C(19)	103.79(16)
C(18)-Si(2)-C(13)	112.99(14)
C(17)-Si(2)-C(13)	109.66(15)
C(19)-Si(2)-C(13)	113.71(13)
C(5)-C(1)-C(2)	108.8(2)
C(5)-C(1)-C(6)	126.7(2)
C(2)-C(1)-C(6)	124.4(2)
C(5)-C(1)-Fe(1)	70.87(12)
C(2)-C(1)-Fe(1)	70.49(12)
C(6)-C(1)-Fe(1)	126.86(16)
C(3)-C(2)-C(1)	107.2(2)
C(3)-C(2)-C(7)	125.8(2)
C(1)-C(2)-C(7)	126.8(2)
C(3)-C(2)-Fe(1)	71.53(12)
C(1)-C(2)-Fe(1)	69.64(12)
C(7)-C(2)-Fe(1)	127.76(17)
C(4)-C(3)-C(2)	108.4(2)
C(4)-C(3)-C(8)	126.1(2)
C(2)-C(3)-C(8)	125.4(2)
C(4)-C(3)-Fe(1)	69.53(12)
C(2)-C(3)-Fe(1)	69.14(12)
C(8)-C(3)-Fe(1)	130.33(15)
C(3)-C(4)-C(5)	108.2(2)
C(3)-C(4)-C(9)	125.9(2)
C(5)-C(4)-C(9)	125.7(2)
C(3)-C(4)-Fe(1)	71.54(12)
C(5)-C(4)-Fe(1)	69.98(12)
C(9)-C(4)-Fe(1)	127.84(16)
C(1)-C(5)-C(4)	107.3(2)
C(1)-C(5)-C(10)	126.5(2)
C(4)-C(5)-C(10)	126.1(2)
C(1)-C(5)-Fe(1)	69.75(13)
C(4)-C(5)-Fe(1)	70.13(12)
C(10)-C(5)-Fe(1)	128.05(16)
O(1)-C(11)-Fe(1)	176.3(2)
O(2)-C(12)-Fe(1)	176.3(2)
P(1)-C(13)-Si(2)	108.67(11)
P(1)-C(13)-Si(1)	120.88(12)
Si(2)-C(13)-Si(1)	114.58(12)
P(1)-C(13)-Mo(1)	70.85(8)
Si(2)-C(13)-Mo(1)	114.49(10)
Si(1)-C(13)-Mo(1)	120.09(10)
O(3)-C(20)-Mo(1)	170.9(2)
O(4)-C(21)-Mo(1)	175.7(2)
C(26)-C(22)-C(23)	107.4(2)
C(26)-C(22)-Mo(1)	72.45(14)
C(23)-C(22)-Mo(1)	71.00(14)
C(24)-C(23)-C(22)	107.7(3)
C(24)-C(23)-Mo(1)	71.73(14)
C(22)-C(23)-Mo(1)	74.01(14)
C(25)-C(24)-C(23)	108.6(2)
C(25)-C(24)-Mo(1)	73.83(14)
C(23)-C(24)-Mo(1)	72.97(14)
C(24)-C(25)-C(26)	107.6(3)
C(24)-C(25)-Mo(1)	71.28(15)
C(26)-C(25)-Mo(1)	73.25(14)
C(25)-C(26)-C(22)	108.6(2)
C(25)-C(26)-Mo(1)	72.02(14)
C(22)-C(26)-Mo(1)	72.96(15)

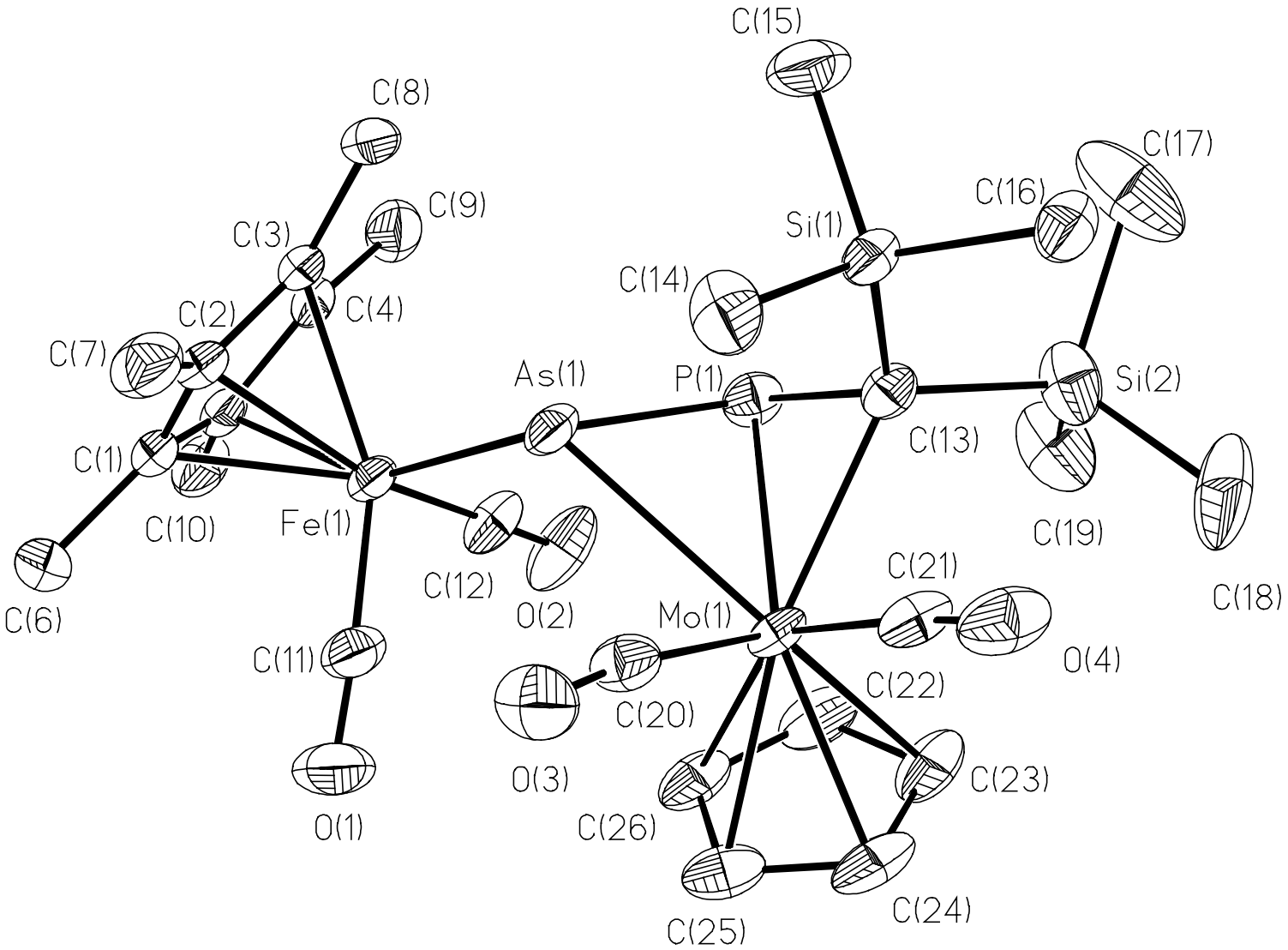
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for bay01. 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
As(1)	35(1)	31(1)	23(1)	3(1)	16(1)	5(1)
Mo(1)	33(1)	23(1)	20(1)	-3(1)	15(1)	-7(1)
Fe(1)	29(1)	31(1)	19(1)	1(1)	12(1)	3(1)
P(1)	37(1)	25(1)	27(1)	-7(1)	8(1)	-2(1)
Si(1)	31(1)	28(1)	24(1)	0(1)	14(1)	0(1)
Si(2)	27(1)	37(1)	66(1)	10(1)	15(1)	-6(1)
O(1)	63(1)	64(1)	24(1)	-3(1)	4(1)	7(1)
O(2)	75(2)	35(1)	74(2)	-11(1)	53(1)	-15(1)
O(3)	40(1)	52(1)	43(1)	2(1)	8(1)	-18(1)
O(4)	79(1)	29(1)	33(1)	-6(1)	14(1)	2(1)
C(1)	26(1)	43(1)	21(1)	3(1)	11(1)	7(1)
C(2)	29(1)	39(1)	21(1)	4(1)	12(1)	3(1)
C(3)	26(1)	41(1)	19(1)	1(1)	10(1)	8(1)
C(4)	25(1)	41(1)	24(1)	-6(1)	11(1)	4(1)
C(5)	31(1)	37(1)	24(1)	0(1)	14(1)	8(1)
C(6)	30(1)	64(2)	28(1)	8(1)	5(1)	7(1)
C(7)	45(2)	48(2)	35(1)	4(1)	17(1)	-8(1)
C(8)	42(1)	54(2)	21(1)	7(1)	11(1)	18(1)
C(9)	34(1)	58(2)	38(1)	-16(1)	9(1)	-3(1)
C(10)	50(2)	37(1)	43(1)	2(1)	24(1)	10(1)
C(11)	46(1)	40(1)	24(1)	3(1)	13(1)	7(1)
C(12)	50(2)	30(1)	38(1)	-4(1)	27(1)	1(1)
C(13)	29(1)	25(1)	26(1)	-5(1)	10(1)	-4(1)
C(14)	34(1)	41(1)	56(2)	19(1)	19(1)	-4(1)
C(15)	75(2)	50(2)	25(1)	0(1)	15(1)	15(2)
C(16)	39(1)	31(1)	38(1)	3(1)	19(1)	3(1)
C(17)	44(2)	70(2)	108(3)	37(2)	-24(2)	-24(2)
C(18)	61(2)	53(2)	114(3)	19(2)	65(2)	14(2)
C(19)	36(2)	51(2)	87(2)	19(2)	8(2)	-18(1)
C(20)	38(1)	34(1)	26(1)	1(1)	10(1)	-7(1)
C(21)	49(1)	28(1)	23(1)	-3(1)	15(1)	-4(1)
C(22)	64(2)	33(1)	37(1)	-2(1)	27(1)	-19(1)
C(23)	57(2)	44(2)	44(2)	6(1)	37(1)	-5(1)
C(24)	78(2)	31(1)	28(1)	-1(1)	30(1)	-4(1)
C(25)	63(2)	36(1)	25(1)	5(1)	14(1)	-8(1)
C(26)	64(2)	30(1)	31(1)	5(1)	27(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for bay01.

	x	y	z	U(eq)
H(6A)	844	3309	2688	61
H(6B)	1168	2716	1961	61
H(6C)	1432	3560	1847	61
H(7A)	2673	1299	3645	62
H(7B)	1703	1664	2844	62
H(7C)	1752	1712	4017	62
H(8A)	4209	2102	5663	57
H(8B)	5175	2118	5128	57
H(8C)	4245	1528	4794	57
H(9A)	5259	4055	4281	65
H(9B)	5660	3314	4869	65
H(9C)	4942	3874	5309	65
H(10A)	2703	4445	2382	62
H(10B)	3879	4580	3066	62
H(10C)	2871	4691	3528	62
H(14A)	5180	-384	2670	64
H(14B)	4816	153	3441	64
H(14C)	5294	-634	3807	64
H(15A)	6780	108	5478	74
H(15B)	6462	919	5084	74
H(15C)	7677	659	5306	74
H(16A)	8322	-498	3925	51
H(16B)	7415	-850	3045	51
H(16C)	7427	-1006	4193	51
H(17A)	9260	385	4428	122
H(17B)	9136	1230	4671	122
H(17C)	10091	969	4205	122
H(18A)	8405	420	1356	102
H(18B)	8770	-144	2265	102
H(18C)	9605	429	2024	102
H(19A)	9651	1983	2666	89
H(19B)	8622	2330	2934	89
H(19C)	8556	2039	1822	89
H(22)	6883	2666	1131	50
H(23)	7551	1526	436	53
H(24)	5957	869	-629	51
H(25)	4314	1589	-599	49
H(26)	4882	2687	507	47


C(15)
C(8)
C(17)
C(16)
C(9)
Si(1)
C(3)
C(14)
C(2)
C(4)
C(7)
As(1)
P(1)
Si(2)
C(1)
C(13)
C(10)
Fe(1)
C(19)
C(12)
C(18)
C(6)
O(2)
C(21)
Mo(1)
O(4)
C(11)
C(22)
C(20)
O(3)
C(23)
C(26)
O(1)
C(24)
C(25)