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Table 1. Crystal data and structure refinement for 1383.

Identification code	1383b
Empirical formula	C24 H15 Fe Mo O7 P
Formula weight	598.12
Temperature	293(2) K
Wavelength	0.71069 A
Crystal system	ORTHORHOMBIC
Space group	Pca21
Unit cell dimensions	a = 16.621(3) A alpha = 90 deg. b = 9.048(2) A beta = 90 deg. c = 15.941(3) A gamma = 90 deg.
Volume	2397.3(8) A^3
Z	4
Density (calculated)	1.657 Mg/m^3
Absorption coefficient	1.237 mm^-1
F(000)	1192
Crystal size	0.36 x 0.32 x 0.30 mm
2Theta	45 deg.
Index ranges	-17<=h<=0, -9<=k<=9, 0<=l<=17
Reflections collected	3017
Independent reflections	1639 [R(int) = 0.1371]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1366 / 1 / 307
Goodness-of-fit on F^2	0.913
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0812
R indices (all data)	R1 = 0.0489, wR2 = 0.0875
Weight = 1 / [sigma^2(Fo^2) + (0.0359 * P)^2] where P = (Max (Fo^2, 0) + 2 * Fc^2) / 3	
Absolute structure parameter	0.06(4)
Largest diff. peak and hole	0.691 and -0.746 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1383. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	182(1)	8569(1)	2162(1)	38(1)
Fe	-1153(1)	4764(1)	2865(1)	49(1)
P	4600(1)	3218(3)	3318(2)	38(1)
C(1)	1230(6)	9601(9)	2214(11)	54(3)
O(1)	1829(5)	10228(8)	2265(9)	87(3)
O(3)	1446(4)	6007(7)	2187(10)	82(3)
C(4)	-421(6)	4333(11)	2140(13)	66(3)
C(3)	979(5)	6894(9)	2218(10)	48(2)
C(12)	156(8)	9082(18)	739(9)	68(4)
C(2)	126(7)	9870(14)	3180(8)	57(3)
C(31)	3938(6)	2229(10)	4090(8)	40(2)
O(5)	-2527(5)	6688(7)	2552(8)	81(3)
O(6)	-2042(5)	2195(8)	2333(15)	147(7)
C(36)	3887(7)	2727(11)	4907(9)	53(3)
C(5)	-1995(6)	5969(10)	2668(8)	52(3)
C(25)	6457(7)	5585(13)	4402(10)	70(4)
O(7)	-1160(7)	3580(11)	4597(8)	95(4)
C(21)	5449(6)	3771(11)	4004(8)	48(3)
O(2)	118(7)	10673(10)	3720(8)	91(3)
C(7)	-1136(7)	4078(12)	3941(13)	69(4)
C(26)	5782(7)	5207(11)	3943(8)	58(3)
C(11)	-294(12)	10158(14)	1170(11)	86(6)
C(6)	-1702(6)	3216(11)	2552(13)	91(7)
C(22)	5828(7)	2773(12)	4520(7)	55(3)
O(4)	36(6)	4017(11)	1579(8)	88(3)
C(32)	3439(7)	1129(11)	3826(8)	55(3)
C(34)	2852(7)	966(15)	5180(10)	71(3)
C(23)	6481(7)	3156(17)	4971(10)	73(4)
C(13)	-232(8)	7784(14)	840(9)	69(4)
C(14)	-910(8)	7987(17)	1286(9)	73(4)
C(35)	3329(7)	2152(12)	5446(8)	60(3)
C(24)	-1803(7)	4586(19)	-85(11)	85(5)
C(33)	2880(7)	515(13)	4345(11)	77(4)
C(15)	-970(9)	9463(21)	1526(10)	91(5)

Table 3. Bond lengths [A] and angles [deg] for 1383.

Mo(1)-C(1)	1.978(10)
Mo(1)-C(2)	2.006(13)
Mo(1)-C(3)	2.015(9)
Mo(1)-C(11)	2.278(13)
Mo(1)-C(15)	2.313(12)
Mo(1)-C(12)	2.316(14)
Mo(1)-C(13)	2.328(14)
Mo(1)-C(14)	2.349(12)
Mo(1)-P#1	2.635(3)
Fe-C(4)	1.72(2)
Fe-C(6)	1.745(11)
Fe-C(5)	1.801(10)
Fe-C(7)	1.82(2)
Fe-P#1	2.327(3)
P-C(21)	1.854(11)
P-C(31)	1.877(11)
P-Fe#2	2.327(3)
P-Mo(1)#2	2.635(3)
C(1)-O(1)	1.149(11)
O(3)-C(3)	1.117(10)
C(4)-O(4)	1.21(2)
C(12)-C(13)	1.35(2)
C(12)-C(11)	1.41(2)
C(12)-H(12)	0.930(13)
C(2)-O(2)	1.13(2)
C(31)-C(32)	1.36(2)
C(31)-C(36)	1.38(2)
O(5)-C(5)	1.114(12)
O(6)-C(6)	1.138(14)
C(36)-C(35)	1.37(2)
C(36)-H(36)	0.930(10)
C(25)-C(24)#3	1.35(2)
C(25)-C(26)	1.38(2)
C(25)-H(25)	0.930(11)
O(7)-C(7)	1.14(2)
C(21)-C(22)	1.37(2)
C(21)-C(26)	1.416(14)
C(26)-H(26)	0.930(12)
C(11)-C(15)	1.41(2)
C(11)-H(11)	0.930(13)
C(22)-C(23)	1.35(2)
C(22)-H(22)	0.930(11)
C(32)-C(33)	1.36(2)
C(32)-H(32)	0.930(12)
C(34)-C(35)	1.40(2)
C(34)-C(33)	1.39(2)
C(34)-H(34)	0.930(13)
C(23)-C(24)#3	1.40(2)
C(23)-H(23)	0.93(2)
C(13)-C(14)	1.34(2)
C(13)-H(13)	0.930(12)
C(14)-C(15)	1.39(2)
C(14)-H(14)	0.930(12)
C(35)-H(35)	0.930(12)
C(24)-C(25)#4	1.35(2)
C(24)-C(23)#4	1.40(2)

C(24)-H(24)	0.930(13)
C(33)-H(33)	0.930(13)
C(15)-H(15)	0.930(13)
C(1)-Mo(1)-C(2)	74.4(6)
C(1)-Mo(1)-C(3)	76.9(3)
C(2)-Mo(1)-C(3)	115.8(5)
C(1)-Mo(1)-C(11)	92.1(6)
C(2)-Mo(1)-C(11)	100.1(6)
C(3)-Mo(1)-C(11)	137.2(7)
C(1)-Mo(1)-C(15)	125.6(6)
C(2)-Mo(1)-C(15)	96.4(5)
C(3)-Mo(1)-C(15)	145.8(6)
C(11)-Mo(1)-C(15)	35.7(6)
C(1)-Mo(1)-C(12)	87.8(6)
C(2)-Mo(1)-C(12)	132.3(6)
C(3)-Mo(1)-C(12)	101.9(6)
C(11)-Mo(1)-C(12)	35.7(6)
C(15)-Mo(1)-C(12)	59.0(5)
C(1)-Mo(1)-C(13)	116.2(6)
C(2)-Mo(1)-C(13)	153.8(5)
C(3)-Mo(1)-C(13)	90.3(5)
C(11)-Mo(1)-C(13)	57.4(5)
C(15)-Mo(1)-C(13)	57.6(5)
C(12)-Mo(1)-C(13)	33.8(5)
C(1)-Mo(1)-C(14)	144.2(6)
C(2)-Mo(1)-C(14)	125.2(6)
C(3)-Mo(1)-C(14)	111.5(5)
C(11)-Mo(1)-C(14)	57.4(5)
C(15)-Mo(1)-C(14)	34.8(5)
C(12)-Mo(1)-C(14)	56.5(4)
C(13)-Mo(1)-C(14)	33.4(5)
C(1)-Mo(1)-P#1	125.7(4)
C(2)-Mo(1)-P#1	77.1(3)
C(3)-Mo(1)-P#1	75.5(4)
C(11)-Mo(1)-P#1	138.1(5)
C(15)-Mo(1)-P#1	102.5(5)
C(12)-Mo(1)-P#1	143.2(4)
C(13)-Mo(1)-P#1	109.7(4)
C(14)-Mo(1)-P#1	89.7(3)
C(4)-Fe-C(6)	89.8(6)
C(4)-Fe-C(5)	124.6(7)
C(6)-Fe-C(5)	91.7(4)
C(4)-Fe-C(7)	122.9(7)
C(6)-Fe-C(7)	90.2(7)
C(5)-Fe-C(7)	112.5(6)
C(4)-Fe-P#1	90.3(4)
C(6)-Fe-P#1	178.1(6)
C(5)-Fe-P#1	89.8(3)
C(7)-Fe-P#1	88.1(4)
C(21)-P-C(31)	100.8(5)
C(21)-P-Fe#2	112.4(3)
C(31)-P-Fe#2	105.2(3)
C(21)-P-Mo(1)#2	107.4(3)
C(31)-P-Mo(1)#2	112.4(3)
Fe#2-P-Mo(1)#2	117.51(12)
O(1)-C(1)-Mo(1)	177.7(12)
O(4)-C(4)-Fe	174.0(14)
O(3)-C(3)-Mo(1)	174.1(13)
C(13)-C(12)-C(11)	106.8(12)

C(13)-C(12)-Mo(1)	73.6(8)
C(11)-C(12)-Mo(1)	70.7(8)
C(13)-C(12)-H(12)	127(2)
C(11)-C(12)-H(12)	127(2)
Mo(1)-C(12)-H(12)	120.9(10)
O(2)-C(2)-Mo(1)	175.3(10)
C(32)-C(31)-C(36)	119.5(10)
C(32)-C(31)-P	120.2(9)
C(36)-C(31)-P	119.9(8)
C(35)-C(36)-C(31)	120.7(10)
C(35)-C(36)-H(36)	119.7(14)
C(31)-C(36)-H(36)	119.7(13)
O(5)-C(5)-Fe	178.3(8)
C(24)#3-C(25)-C(26)	120.1(10)
C(24)#3-C(25)-H(25)	119.9(13)
C(26)-C(25)-H(25)	120(2)
C(22)-C(21)-C(26)	117.7(10)
C(22)-C(21)-P	121.7(7)
C(26)-C(21)-P	120.3(10)
O(7)-C(7)-Fe	175.5(13)
C(25)-C(26)-C(21)	120.5(12)
C(25)-C(26)-H(26)	119.7(11)
C(21)-C(26)-H(26)	119.7(11)
C(12)-C(11)-C(15)	108.2(11)
C(12)-C(11)-Mo(1)	73.6(8)
C(15)-C(11)-Mo(1)	73.5(8)
C(12)-C(11)-H(11)	126(2)
C(15)-C(11)-H(11)	126(2)
Mo(1)-C(11)-H(11)	118.9(11)
O(6)-C(6)-Fe	178(2)
C(23)-C(22)-C(21)	121.4(12)
C(23)-C(22)-H(22)	119.3(12)
C(21)-C(22)-H(22)	119.3(10)
C(31)-C(32)-C(33)	121.7(12)
C(31)-C(32)-H(32)	119.1(11)
C(33)-C(32)-H(32)	119.2(12)
C(35)-C(34)-C(33)	119.6(12)
C(35)-C(34)-H(34)	120(2)
C(33)-C(34)-H(34)	120(2)
C(22)-C(23)-C(24)#3	121(2)
C(22)-C(23)-H(23)	120(2)
C(24)#3-C(23)-H(23)	120(2)
C(14)-C(13)-C(12)	110.2(13)
C(14)-C(13)-Mo(1)	74.2(8)
C(12)-C(13)-Mo(1)	72.6(8)
C(14)-C(13)-H(13)	125(2)
C(12)-C(13)-H(13)	125(2)
Mo(1)-C(13)-H(13)	120.0(10)
C(13)-C(14)-C(15)	109.7(13)
C(13)-C(14)-Mo(1)	72.4(7)
C(15)-C(14)-Mo(1)	71.2(8)
C(13)-C(14)-H(14)	125(2)
C(15)-C(14)-H(14)	125(2)
Mo(1)-C(14)-H(14)	122.8(10)
C(36)-C(35)-C(34)	119.1(13)
C(36)-C(35)-H(35)	120.4(12)
C(34)-C(35)-H(35)	120.4(12)
C(25)#4-C(24)-C(23)#4	119.7(13)
C(25)#4-C(24)-H(24)	120(2)
C(23)#4-C(24)-H(24)	120(2)

C(32)-C(33)-C(34)	119.0(12)
C(32)-C(33)-H(33)	121(2)
C(34)-C(33)-H(33)	121(2)
C(14)-C(15)-C(11)	105.1(12)
C(14)-C(15)-Mo(1)	74.1(7)
C(11)-C(15)-Mo(1)	70.8(7)
C(14)-C(15)-H(15)	128(2)
C(11)-C(15)-H(15)	128(2)
Mo(1)-C(15)-H(15)	119.7(12)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+1,z #2 x+1/2,-y+1,z #3 -x+1/2,y,z+1/2
#4 -x+1/2,y,z-1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1383. 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
Mo(1)	42(1)	32(1)	39(1)	2(1)	-1(1)	2(1)
Fe	45(1)	32(1)	70(1)	-2(1)	0(1)	0(1)
P	39(1)	34(1)	40(2)	-3(1)	-1(1)	-4(1)
C(1)	63(6)	35(4)	65(8)	3(7)	-28(9)	1(4)
O(1)	66(5)	65(4)	132(9)	11(7)	-35(7)	-18(4)
O(3)	53(4)	52(4)	142(9)	10(8)	11(7)	14(4)
C(4)	56(6)	43(5)	100(10)	-19(9)	20(11)	-14(4)
C(3)	38(5)	45(5)	62(7)	7(8)	-6(7)	2(4)
C(12)	64(8)	93(10)	48(9)	21(9)	-11(7)	-14(8)
C(2)	59(7)	47(7)	64(9)	-2(7)	16(6)	1(5)
C(31)	39(5)	40(5)	42(6)	9(5)	-2(5)	5(5)
O(5)	49(4)	56(3)	139(10)	1(5)	-15(5)	18(4)
O(6)	65(5)	61(4)	316(23)	-50(10)	-8(10)	-16(4)
C(36)	57(6)	51(6)	52(8)	-9(6)	-9(6)	3(5)
C(5)	50(6)	38(4)	67(8)	0(6)	-4(6)	-10(5)
C(25)	59(7)	61(6)	89(11)	-34(8)	-1(8)	-17(6)
O(7)	100(8)	88(7)	98(9)	57(7)	-1(7)	4(5)
C(21)	36(5)	50(5)	57(7)	-14(6)	8(6)	-8(4)
O(2)	146(9)	59(5)	70(7)	-28(6)	11(7)	-27(6)
C(7)	53(7)	38(6)	115(14)	5(8)	-1(8)	1(5)
C(26)	51(6)	59(6)	64(8)	-19(7)	-8(6)	-8(5)
C(11)	141(16)	37(7)	81(12)	6(7)	-70(12)	1(8)
C(6)	51(6)	37(5)	183(21)	-13(8)	-9(10)	-1(5)
C(22)	51(6)	71(6)	42(7)	-7(7)	-15(6)	1(6)
O(4)	91(7)	92(6)	81(8)	-38(7)	13(6)	-20(5)
C(32)	59(7)	57(6)	50(7)	2(6)	1(6)	-10(6)
C(34)	55(7)	92(8)	68(9)	29(8)	18(7)	8(7)
C(23)	57(8)	99(9)	62(8)	-1(9)	-6(7)	2(8)
C(13)	85(9)	63(8)	58(9)	-25(8)	-12(7)	16(7)
C(14)	69(8)	101(10)	48(8)	17(9)	-24(7)	-35(8)
C(35)	64(7)	67(6)	50(7)	9(7)	15(6)	18(6)
C(24)	39(6)	123(11)	92(12)	-58(11)	-12(8)	12(8)
C(33)	63(7)	67(6)	102(12)	14(9)	3(8)	-18(6)
C(15)	71(8)	146(15)	55(8)	-15(11)	-10(7)	66(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1383.

	x	y	z	U(eq)
H(12)	630	9236	442	82
H(36)	4235	3462	5093	64
H(25)	6672	6530	4357	84
H(26)	5545	5902	3591	70
H(11)	-166	11156	1213	103
H(22)	5630	1814	4558	66
H(32)	3481	787	3277	66
H(34)	2517	482	5559	86
H(23)	6721	2465	5324	87
H(13)	-57	6881	631	82
H(14)	-1281	7253	1415	88
H(35)	3268	2543	5981	72
H(24)	-2252	4843	229	102
H(33)	2523	-194	4145	93
H(15)	-1371	9896	1851	109

Data Collection and Structure Refinement

TITLE,	- ASCI1070 -
Formula ,	C25 H24 Fe Mo O8 P2
FW ,	666.19
Diffractometer used,	Nonius
Space Group,	Monoclinic P 21
a(angstron),	10.8113(8)
b(angstron),	11.5250(17)
c(angstron),	10.9303(7)
beta(deg.),	97.243(6)
V(A**3),	1351.05(24)
Z ,	2
Dcalc(g.cm-3),	1.638
lambda(Angstron),	0.70930
F(000) ,	670.
Unit cell detn: #;(2theta range),	25;(15.04 - 33.98 deg.)
Scan type,	theta/2theta
Scan width (deg),	2(0.65+0.35tan(theta))
Scan Speed (deg/min),	1.18-8.24
2 Theta(max),	50.0
h k l ranges ,	(-12; 12)(-13; 0)(-12; 12)
mu(cm-1),	11.525
Crystal size(mm),	0.38 X 0.19 X 0.34
Transmission,	0.926; 1.000
Temperature,	295.00
# of meas. reflns,	2630
# of obsed relfns (I > 2.5sig(I)),	2413
# of unique reflns,	2497
RF;RW ,	0.018;0.022
GoF,	1.33
Refinement program,	NRCVAX
# of atoms,	61
# of refined params,	334 (2413 out of 2497 reflns.)
Minimize function,	SUM(w|Fo-Fc|**2)
Weights scheme,	(1/sigma**2)(Fo)
The weight modifier K in KFo**2 is,	0.000100

***** No. Refine 2nd. ext. coeff. OR ext. coeff is negative *****

(delta/sigma)max ,	0.0011
(D -map)max.min e/A**3 ,	-0.260; 0.170

NOTE :

RF = Sum(Fo-Fc)/Sum(Fo)

Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)]

GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]

Mo-Fe	2.9295(5)	C8-H8-2	0.998
Mo-P1	2.3824(9)	C8-H8-3	1.000
Mo-C4	1.953(4)	C9-C10	1.417(6)
Mo-C5	1.949(4)	C9-C13	1.374(6)
Mo-C9	2.358(4)	C9-H9	1.000
Mo-C10	2.385(4)	C10-C11	1.409(7)
Mo-C11	2.360(4)	C10-H10	0.996
Mo-C12	2.306(4)	C11-C12	1.403(7)
Mo-C13	2.320(4)	C11-H11	0.999
Fe-P1	2.2638(11)	C12-C13	1.420(6)
Fe-P2	2.1519(9)	C12-H12	0.999
Fe-C1	1.789(4)	C13-H13	0.998
Fe-C2	1.793(4)	C21-C22	1.390(5)
Fe-C3	1.784(4)	C21-C26	1.396(5)
P1-C21	1.840(4)	C22-C23	1.383(6)
P1-C31	1.832(3)	C22-H22	0.998
P2-O6	1.591(3)	C23-C24	1.385(7)
P2-O7	1.597(3)	C23-H23	1.000
P2-O8	1.601(3)	C24-C25	1.367(7)
O1-C1	1.142(5)	C24-H24	1.001
O2-C2	1.137(5)	C25-C26	1.384(6)
O3-C3	1.143(5)	C25-H25	1.000
O4-C4	1.146(6)	C26-H26	0.999
O5-C5	1.155(5)	C31-C32	1.383(5)
O6-C6	1.422(6)	C31-C36	1.376(5)
O7-C7	1.461(5)	C32-C33	1.391(5)
O8-C8	1.441(6)	C32-H32	1.000
C6-H6-1	1.000	C33-C34	1.377(6)
C6-H6-2	0.999	C33-H33	0.998
C6-H6-3	0.999	C34-C35	1.367(6)
C7-H7-1	1.002	C34-H34	1.000
C7-H7-2	0.997	C35-C36	1.384(5)
C7-H7-3	0.995	C35-H35	1.000
C8-H8-1	1.000	C36-H36	1.000

Fe-Mo-P1	49.13(3)	O7-C7-H7-2	109.9
Fe-Mo-C4	123.82(12)	O7-C7-H7-3	110.9
Fe-Mo-C5	85.20(11)	H7-1-C7-H7-2	108.9
Fe-Mo-C9	97.11(10)	H7-1-C7-H7-3	108.2
Fe-Mo-C10	89.98(10)	H7-2-C7-H7-3	107.9
Fe-Mo-C11	115.88(12)	O8-C8-H8-1	109.8
Fe-Mo-C12	147.65(13)	O8-C8-H8-2	111.8
Fe-Mo-C13	129.69(11)	O8-C8-H8-3	110.0
P1-Mo-C4	83.01(12)	H8-1-C8-H8-2	108.8
P1-Mo-C5	104.95(12)	H8-1-C8-H8-3	107.0
P1-Mo-C9	98.73(10)	H8-2-C8-H8-3	109.2
P1-Mo-C10	118.76(11)	Mo-C9-C10	73.65(24)
P1-Mo-C11	153.27(12)	Mo-C9-C13	71.40(25)
P1-Mo-C12	145.77(12)	Mo-C9-H9	127.9(3)
P1-Mo-C13	110.92(11)	C10-C9-C13	108.1(4)
C4-Mo-C5	80.48(18)	C10-C9-H9	115.8
C4-Mo-C9	120.77(17)	C13-C9-H9	135.4
C4-Mo-C10	144.63(16)	Mo-C10-C9	71.58(25)
C4-Mo-C11	119.11(17)	Mo-C10-C11	71.8(3)
C4-Mo-C12	88.28(18)	Mo-C10-H10	135.4
C4-Mo-C13	89.78(18)	C9-C10-C11	108.1(4)
C5-Mo-C9	150.15(16)	C9-C10-H10	137.6
C5-Mo-C10	115.85(16)	C11-C10-H10	111.5
C5-Mo-C11	94.11(16)	Mo-C11-C10	73.67(25)
C5-Mo-C12	106.13(16)	Mo-C11-C12	70.4(3)
C5-Mo-C13	141.31(15)	Mo-C11-H11	121.1
C9-Mo-C10	34.77(15)	C10-C11-C12	107.3(4)
C9-Mo-C11	58.04(15)	C10-C11-H11	125.5
C9-Mo-C12	58.17(15)	C12-C11-H11	127.2

C10-Mo-C11	34.55(16)	Mo-C12-C13	72.65(23)
C10-Mo-C12	57.73(16)	Mo-C12-H12	123.8
C10-Mo-C13	57.39(16)	C11-C12-C13	107.9(4)
C11-Mo-C12	34.98(18)	C11-C12-H12	124.1
C11-Mo-C13	58.38(16)	C13-C12-H12	127.7
C12-Mo-C13	35.74(16)	Mo-C13-C9	74.45(23)
Mo-Fe-P1	52.735(24)	Mo-C13-C12	71.61(24)
Mo-Fe-P2	172.55(3)	Mo-C13-H13	123.7
Mo-Fe-C1	87.34(11)	C9-C13-C12	108.5(4)
Mo-Fe-C2	95.89(12)	C9-C13-H13	127.2
Mo-Fe-C3	80.18(13)	C12-C13-H13	124.1
P1-Fe-P2	121.95(4)	P1-C21-C22	120.5(3)
P1-Fe-C1	87.36(12)	P1-C21-C26	121.4(3)
P1-Fe-C2	88.48(13)	C22-C21-C26	118.1(3)
P1-Fe-C3	132.76(13)	C21-C22-C23	121.4(4)
P2-Fe-C1	87.15(11)	C21-C22-H22	118.5
P2-Fe-C2	88.91(12)	C23-C22-H22	120.1
P2-Fe-C3	105.29(14)	C22-C23-C24	119.2(4)
C1-Fe-C2	171.65(19)	C22-C23-H23	120.3
C1-Fe-C3	94.78(19)	C24-C23-H23	120.5
C2-Fe-C3	93.36(19)	C23-C24-C25	120.5(4)
Mo-P1-Fe	78.13(3)	C23-C24-H24	120.3
Mo-P1-C21	124.48(11)	C25-C24-H24	119.2
Mo-P1-C31	117.23(12)	C24-C25-C26	120.3(4)
Fe-P1-C21	118.14(11)	C24-C25-H25	120.0
Fe-P1-C31	118.24(12)	C26-C25-H25	119.7
C21-P1-C31	101.11(16)	C21-C26-C25	120.5(4)
Fe-P2-O6	121.24(12)	C21-C26-H26	119.1
Fe-P2-O7	112.79(10)	C25-C26-H26	120.3
Fe-P2-O8	117.63(11)	P1-C31-C32	118.3(3)
O6-P2-O7	104.65(16)	P1-C31-C36	123.5(3)
O6-P2-O8	93.04(15)	C32-C31-C36	118.2(3)
O7-P2-O8	104.71(16)	C31-C32-C33	120.9(3)
P2-O6-C6	120.8(3)	C31-C32-H32	120.5
P2-O7-C7	120.6(3)	C33-C32-H32	118.6
P2-O8-C8	119.4(3)	C32-C33-C34	119.4(4)
Fe-C1-O1	176.4(3)	C32-C33-H33	121.3
Fe-C2-O2	178.4(3)	C34-C33-H33	119.3
Fe-C3-O3	177.7(4)	C33-C34-C35	120.3(3)
Mo-C4-O4	178.7(4)	C33-C34-H34	121.3
Mo-C5-O5	175.9(3)	C35-C34-H34	118.4
O6-C6-H6-1	110.8	C34-C35-C36	119.8(3)
O6-C6-H6-2	109.6	C34-C35-H35	121.6
O6-C6-H6-3	110.7	C36-C35-H35	118.6
H6-1-C6-H6-2	108.3	C31-C36-C35	121.3(3)
H6-1-C6-H6-3	109.5	C31-C36-H36	118.3
H6-2-C6-H6-3	107.9	C35-C36-H36	120.5
O7-C7-H7-1	111.0		

Atom	x	y	z	Biso
Mo	0.75681(2)	0.50867	0.04515(2)	2.18(1)
Fe	0.70440(4)	0.52928(8)	0.30075(4)	2.13(2)
P1	0.85600(8)	0.62081(9)	0.21262(8)	2.05(3)
P2	0.69159(8)	0.54183(9)	0.49518(7)	2.37(3)
O1	0.8781(3)	0.3374(3)	0.3652(3)	4.4(1)
O2	0.5513(3)	0.7391(3)	0.2641(3)	5.1(2)
O3	0.4962(3)	0.3791(3)	0.2048(3)	5.3(2)
O4	0.8318(4)	0.7146(4)	-0.1122(3)	6.1(2)
O5	0.4981(3)	0.6219(3)	-0.0302(3)	5.5(2)
O6	0.7888(3)	0.6166(3)	0.5839(2)	3.5(1)
O7	0.5581(2)	0.5857(3)	0.5238(2)	3.8(1)
O8	0.7177(3)	0.4269(2)	0.5765(2)	3.5(1)
C1	0.8129(3)	0.4135(4)	0.3375(3)	2.8(1)
C2	0.6119(4)	0.6584(4)	0.2773(3)	3.2(2)
C3	0.5790(4)	0.4368(4)	0.2406(4)	3.3(2)
C4	0.8048(4)	0.6392(4)	-0.0527(3)	3.6(2)
C5	0.5940(4)	0.5808(4)	0.0025(3)	3.2(2)
C6	0.8008(5)	0.7381(4)	0.5658(5)	5.1(2)
C7	0.5292(5)	0.5925(6)	0.6507(4)	5.6(2)
C8	0.6431(5)	0.3249(5)	0.5455(5)	5.5(2)
C9	0.8823(4)	0.3410(4)	0.0723(4)	3.6(2)
C10	0.7570(4)	0.3025(4)	0.0633(4)	3.9(2)
C11	0.6972(4)	0.3321(4)	-0.0547(4)	4.4(2)
C12	0.7856(4)	0.3883(4)	-0.1174(4)	4.3(2)
C13	0.9000(4)	0.3919(4)	-0.0378(4)	3.9(2)
C21	0.8598(3)	0.7804(3)	0.2164(3)	2.4(1)
C22	0.7699(4)	0.8446(3)	0.1435(4)	3.2(2)
C23	0.7701(4)	0.9646(4)	0.1462(4)	4.2(2)
C24	0.8632(4)	1.0218(4)	0.2217(4)	4.5(2)
C25	0.9530(4)	0.9606(4)	0.2939(4)	3.9(2)
C26	0.9523(3)	0.8405(3)	0.2917(3)	2.8(1)
C31	1.0187(3)	0.5861(3)	0.2684(3)	2.4(1)
C32	1.1036(3)	0.5830(4)	0.1837(3)	3.4(2)
C33	1.2284(4)	0.5569(5)	0.2204(4)	4.4(2)
C34	1.2681(3)	0.5351(4)	0.3429(4)	4.1(2)
C35	1.1855(4)	0.5389(4)	0.4277(4)	3.9(2)
C36	1.0616(3)	0.5654(4)	0.3904(3)	3.0(2)
H6-1	0.866	0.772	0.629	5.7
H6-2	0.826	0.753	0.482	5.7
H6-3	0.720	0.778	0.570	5.7
H7-1	0.443	0.623	0.653	6.3
H7-2	0.536	0.514	0.689	6.3
H7-3	0.589	0.645	0.701	6.3
H8-1	0.671	0.261	0.604	6.3
H8-2	0.553	0.340	0.549	6.3
H8-3	0.655	0.297	0.461	6.3
H9	0.938	0.316	0.148	4.4
H10	0.708	0.244	0.105	4.7
H11	0.608	0.316	-0.086	5.0
H12	0.770	0.412	-0.206	4.9
H13	0.980	0.421	-0.063	4.8
H22	0.704	0.802	0.089	3.9
H23	0.704	1.009	0.094	4.9
H24	0.864	1.109	0.225	5.4
H25	1.020	1.002	0.348	4.6
H26	1.017	0.796	0.345	3.6
H32	1.076	0.598	0.094	4.2
H33	1.290	0.552	0.159	5.1
H34	1.357	0.517	0.372	4.7
H35	1.213	0.525	0.517	4.5
H36	1.001	0.570	0.452	3.8

Mo	2.64(1)	3.21(2)	2.43(1)	-0.04(1)	0.29(1)	-0.19(1)
Fe	2.46(2)	3.12(3)	2.57(2)	0.21(2)	0.55(2)	0.24(2)
P1	2.27(4)	2.93(5)	2.58(4)	0.07(4)	0.22(3)	0.13(4)
P2	3.02(4)	3.36(5)	2.61(4)	0.25(4)	0.33(3)	0.14(4)
O1	6.2(2)	5.1(2)	5.7(2)	2.3(2)	1.5(1)	1.7(2)
O2	6.1(2)	6.8(2)	6.8(2)	3.7(2)	2.4(2)	2.3(2)
O3	4.6(2)	7.5(2)	7.9(2)	-2.1(2)	0.8(2)	-1.9(2)
O4	10.7(3)	7.4(3)	5.4(2)	-3.2(2)	2.0(2)	1.6(2)
O5	4.0(2)	8.0(3)	8.3(2)	1.9(2)	-1.3(2)	0.1(2)
O6	4.9(2)	4.4(2)	3.8(1)	-0.2(1)	-0.7(1)	-0.5(1)
O7	4.0(1)	7.6(2)	3.2(1)	1.6(1)	1.3(1)	0.3(1)
O8	6.2(2)	3.6(2)	3.5(1)	0.3(1)	0.9(1)	0.8(1)
C1	3.7(2)	3.8(2)	3.4(2)	0.3(2)	1.2(2)	0.4(2)
C2	3.4(2)	5.2(3)	3.6(2)	0.9(2)	1.4(2)	0.8(2)
C3	4.0(2)	4.4(2)	4.3(2)	0.1(2)	0.9(2)	-0.4(2)
C4	5.1(3)	5.2(3)	3.2(2)	-0.7(2)	0.3(2)	0.0(2)
C5	3.9(2)	4.6(2)	3.7(2)	-0.4(2)	0.0(2)	-0.4(2)
C6	9.0(4)	4.7(3)	5.4(3)	-2.0(3)	0.6(3)	-1.1(2)
C7	7.1(3)	10.8(4)	3.9(2)	3.0(3)	2.6(2)	0.7(3)
C8	9.8(4)	4.5(3)	7.1(3)	-1.6(3)	3.2(3)	1.0(2)
C9	4.6(2)	4.5(3)	4.7(2)	1.6(2)	0.4(2)	-0.7(2)
C10	5.7(3)	3.0(2)	6.4(3)	0.2(2)	1.6(2)	-0.7(2)
C11	5.6(3)	4.6(3)	6.0(3)	0.0(2)	-0.5(2)	-2.2(2)
C12	7.4(3)	5.5(3)	3.2(2)	0.8(3)	0.2(2)	-1.4(2)
C13	5.1(2)	5.6(3)	4.6(2)	1.2(2)	2.0(2)	-1.0(2)
C21	3.4(2)	2.8(2)	3.1(2)	-0.1(2)	0.9(1)	0.4(1)
C22	3.8(2)	3.6(2)	4.4(2)	0.4(2)	-0.1(2)	0.3(2)
C23	5.9(3)	4.2(2)	5.9(3)	1.4(2)	0.4(2)	0.9(2)
C24	7.7(3)	3.0(2)	6.7(3)	0.1(2)	1.8(2)	-0.1(2)
C25	5.8(3)	4.1(2)	4.8(2)	-0.9(2)	0.9(2)	-1.0(2)
C26	3.7(2)	3.7(2)	3.3(2)	-0.4(2)	0.4(2)	0.0(2)
C31	2.6(2)	2.7(2)	3.7(2)	0.1(1)	0.0(1)	0.0(1)
C32	3.0(2)	5.7(3)	4.1(2)	0.3(2)	0.5(2)	0.1(2)
C33	2.8(2)	7.6(3)	6.3(3)	0.5(2)	0.9(2)	-0.3(2)
C34	2.8(2)	5.3(3)	7.0(3)	0.6(2)	-0.6(2)	-0.3(2)
C35	4.1(2)	5.5(3)	4.6(2)	0.3(2)	-1.1(2)	0.8(2)
C36	3.1(2)	4.8(2)	3.6(2)	0.3(2)	0.2(1)	0.2(2)

H6-1	7.2
H6-2	7.2
H6-3	7.2
H7-1	8.0
H7-2	8.0
H7-3	8.0
H8-1	8.0
H8-2	8.0
H8-3	8.0
H9	5.6
H10	6.0
H11	6.4
H12	6.2
H13	6.1
H22	4.9
H23	6.3
H24	6.9
H25	5.8
H26	4.5
H32	5.3
H33	6.5
H34	6.0
H35	5.7
H36	4.8

Temp=-2(Pi)**2(u11*h*h*astar*astar+---+2*u12*h*k*astar*bstar+---)
The uij values have been multiplied by 100.

Torsion angles - ASCI1070 -

P1	Mo	Fe	P1	0.0(0)	P1	Mo	Fe	P2	-46.3(0)
P1	Mo	Fe	C1	-88.7(1)	P1	Mo	Fe	C2	83.6(1)
P1	Mo	Fe	C3	176.0(1)	C4	Mo	Fe	P1	-39.4(1)
C4	Mo	Fe	P2	-85.7(1)	C4	Mo	Fe	C1	-128.1(2)
C4	Mo	Fe	C2	44.2(2)	C4	Mo	Fe	C3	136.6(2)
C5	Mo	Fe	P1	-114.5(1)	C5	Mo	Fe	P2	-160.8(1)
C5	Mo	Fe	C1	156.8(2)	C5	Mo	Fe	C2	-30.9(2)
C5	Mo	Fe	C3	61.5(2)	C9	Mo	Fe	P1	95.4(1)
C9	Mo	Fe	P2	49.1(1)	C9	Mo	Fe	C1	6.7(2)
C9	Mo	Fe	C2	179.0(2)	C9	Mo	Fe	C3	-88.6(2)
C10	Mo	Fe	P1	129.5(1)	C10	Mo	Fe	P2	83.2(1)
C10	Mo	Fe	C1	40.8(2)	C10	Mo	Fe	C2	-146.9(2)
C10	Mo	Fe	C3	-54.5(2)	C11	Mo	Fe	P1	153.2(1)
C11	Mo	Fe	P2	106.9(1)	C11	Mo	Fe	C1	64.5(2)
C11	Mo	Fe	C2	-123.2(2)	C11	Mo	Fe	C3	-30.8(2)
C12	Mo	Fe	P1	132.6(1)	C12	Mo	Fe	P2	86.3(1)
C12	Mo	Fe	C1	43.9(2)	C12	Mo	Fe	C2	-143.8(2)
C12	Mo	Fe	C3	-51.4(2)	C13	Mo	Fe	P1	84.0(1)
C13	Mo	Fe	P2	37.7(1)	C13	Mo	Fe	C1	-4.7(2)
C13	Mo	Fe	C2	167.6(2)	C13	Mo	Fe	C3	-100.0(2)
Fe	Mo	P1	Fe	0.0(0)	Fe	Mo	P1	C21	-116.1(1)
Fe	Mo	P1	C31	115.8(1)	C4	Mo	P1	Fe	147.9(1)
C4	Mo	P1	C21	31.8(2)	C4	Mo	P1	C31	-96.2(2)
C5	Mo	P1	Fe	69.8(1)	C5	Mo	P1	C21	-46.3(2)
C5	Mo	P1	C31	-174.4(2)	C9	Mo	P1	Fe	-91.9(1)
C9	Mo	P1	C21	152.0(2)	C9	Mo	P1	C31	24.0(1)
C10	Mo	P1	Fe	-61.6(1)	C10	Mo	P1	C21	-177.7(2)
C10	Mo	P1	C31	54.2(1)	C11	Mo	P1	Fe	-64.2(1)
C11	Mo	P1	C21	179.6(2)	C11	Mo	P1	C31	51.6(2)
C12	Mo	P1	Fe	-135.6(1)	C12	Mo	P1	C21	108.3(2)
C12	Mo	P1	C31	-19.8(2)	C13	Mo	P1	Fe	-125.0(1)
C13	Mo	P1	C21	118.9(2)	C13	Mo	P1	C31	-9.1(1)
Fe	Mo	C4	O4	-150.7(3)	P1	Mo	C4	O4	-179.6(4)
C5	Mo	C4	O4	-73.1(3)	C9	Mo	C4	O4	84.4(3)
C10	Mo	C4	O4	48.7(3)	C11	Mo	C4	O4	16.3(2)
C12	Mo	C4	O4	33.6(3)	C13	Mo	C4	O4	69.3(3)
Fe	Mo	C5	O5	-169.0(3)	P1	Mo	C5	O5	145.6(3)
C4	Mo	C5	O5	65.5(3)	C9	Mo	C5	O5	-73.1(3)
C10	Mo	C5	O5	-81.4(3)	C11	Mo	C5	O5	-53.4(3)
C12	Mo	C5	O5	-19.9(2)	C13	Mo	C5	O5	-12.1(2)
Fe	Mo	C9	C10	79.6(2)	Fe	Mo	C9	C13	-164.3(3)
P1	Mo	C9	C10	129.2(3)	P1	Mo	C9	C13	-114.7(3)
C4	Mo	C9	C10	-143.7(3)	C4	Mo	C9	C13	-27.6(2)
C5	Mo	C9	C10	-13.1(2)	C5	Mo	C9	C13	103.0(3)
C10	Mo	C9	C10	0.0(2)	C10	Mo	C9	C13	116.1(3)
C11	Mo	C9	C10	-36.5(2)	C11	Mo	C9	C13	79.6(3)
C12	Mo	C9	C10	-78.0(3)	C12	Mo	C9	C13	38.1(2)
C13	Mo	C9	C10	-116.1(3)	C13	Mo	C9	C13	0.0(2)
Fe	Mo	C10	C9	-102.6(3)	Fe	Mo	C10	C11	140.4(3)
P1	Mo	C10	C9	-60.9(2)	P1	Mo	C10	C11	-177.9(3)
C4	Mo	C10	C9	61.4(3)	C4	Mo	C10	C11	-55.7(3)
C5	Mo	C10	C9	172.8(4)	C5	Mo	C10	C11	55.7(3)
C9	Mo	C10	C9	0.0(2)	C9	Mo	C10	C11	-117.1(3)
C11	Mo	C10	C9	117.1(3)	C11	Mo	C10	C11	0.0(2)
C12	Mo	C10	C9	79.4(3)	C12	Mo	C10	C11	-37.7(2)
C13	Mo	C10	C9	36.8(2)	C13	Mo	C10	C11	-80.3(3)
Fe	Mo	C11	C10	-45.1(2)	Fe	Mo	C11	C12	-160.8(3)
P1	Mo	C11	C10	4.0(2)	P1	Mo	C11	C12	-111.6(3)
C4	Mo	C11	C10	146.8(4)	C4	Mo	C11	C12	31.1(2)
C5	Mo	C11	C10	-131.8(4)	C5	Mo	C11	C12	112.5(3)
C9	Mo	C11	C10	36.8(2)	C9	Mo	C11	C12	-78.9(3)
C10	Mo	C11	C10	0.0(2)	C10	Mo	C11	C12	-115.7(3)
C12	Mo	C11	C10	115.7(3)	C12	Mo	C11	C12	0.0(2)

Fe	Mo	C12	C11	33.5(2)	Fe	Mo	C12	C13	-81.3(3)
P1	Mo	C12	C11	132.0(3)	P1	Mo	C12	C13	17.1(2)
C4	Mo	C12	C11	-153.1(4)	C4	Mo	C12	C13	92.0(3)
C5	Mo	C12	C11	-73.6(3)	C5	Mo	C12	C13	171.6(4)
C9	Mo	C12	C11	78.5(3)	C9	Mo	C12	C13	-36.4(2)
C10	Mo	C12	C11	37.2(2)	C10	Mo	C12	C13	-77.7(3)
C11	Mo	C12	C11	0.0(2)	C11	Mo	C12	C13	-114.9(3)
C13	Mo	C12	C11	114.9(3)	C13	Mo	C12	C13	0.0(2)
Fe	Mo	C13	C9	20.5(2)	Fe	Mo	C13	C12	136.6(3)
P1	Mo	C13	C9	74.1(2)	P1	Mo	C13	C12	-169.8(3)
C4	Mo	C13	C9	156.5(4)	C4	Mo	C13	C12	-87.4(3)
C5	Mo	C13	C9	-129.1(3)	C5	Mo	C13	C12	-13.0(2)
C9	Mo	C13	C9	0.0(2)	C9	Mo	C13	C12	116.1(3)
C10	Mo	C13	C9	-37.4(2)	C10	Mo	C13	C12	78.7(3)
C11	Mo	C13	C9	-78.5(3)	C11	Mo	C13	C12	37.7(2)
C12	Mo	C13	C9	-116.1(3)	C12	Mo	C13	C12	0.0(2)
Mo	Fe	P1	Mo	0.0(0)	Mo	Fe	P1	C21	122.9(1)
Mo	Fe	P1	C31	-114.7(1)	P2	Fe	P1	Mo	173.7(1)
P2	Fe	P1	C21	-63.4(1)	P2	Fe	P1	C31	59.0(1)
C1	Fe	P1	Mo	88.7(1)	C1	Fe	P1	C21	-148.4(2)
C1	Fe	P1	C31	-26.0(2)	C2	Fe	P1	Mo	-98.6(1)
C2	Fe	P1	C21	24.4(2)	C2	Fe	P1	C31	146.7(2)
C3	Fe	P1	Mo	-5.4(1)	C3	Fe	P1	C21	117.5(2)
C3	Fe	P1	C31	-120.1(2)	Mo	Fe	P2	O6	42.8(1)
Mo	Fe	P2	O7	168.0(1)	Mo	Fe	P2	O8	-70.0(1)
P1	Fe	P2	O6	0.1(1)	P1	Fe	P2	O7	125.3(1)
P1	Fe	P2	O8	-112.7(1)	C1	Fe	P2	O6	85.2(2)
C1	Fe	P2	O7	-149.6(2)	C1	Fe	P2	O8	-27.6(2)
C2	Fe	P2	O6	-87.4(2)	C2	Fe	P2	O7	37.7(2)
C2	Fe	P2	O8	159.8(2)	C3	Fe	P2	O6	179.4(2)
C3	Fe	P2	O7	-55.5(2)	C3	Fe	P2	O8	66.6(2)
Mo	Fe	C1	O1	-141.7(3)	P1	Fe	C1	O1	165.5(3)
P2	Fe	C1	O1	43.3(2)	C2	Fe	C1	O1	105.3(3)
C3	Fe	C1	O1	-61.8(3)	Mo	Fe	C2	O2	137.4(3)
P1	Fe	C2	O2	-170.3(3)	P2	Fe	C2	O2	-48.3(2)
C1	Fe	C2	O2	-110.1(3)	C3	Fe	C2	O2	57.0(3)
Mo	Fe	C3	O3	-149.5(3)	P1	Fe	C3	O3	-145.1(3)
P2	Fe	C3	O3	35.7(2)	C1	Fe	C3	O3	124.1(4)
C2	Fe	C3	O3	-54.1(3)	Mo	P1	C21	C22	23.1(2)
Mo	P1	C21	C26	-156.8(3)	Fe	P1	C21	C22	-71.7(2)
Fe	P1	C21	C26	108.4(2)	C31	P1	C21	C22	157.6(3)
C31	P1	C21	C26	-22.3(2)	Mo	P1	C31	C32	52.9(2)
Mo	P1	C31	C36	-128.5(3)	Fe	P1	C31	C32	143.7(3)
Fe	P1	C31	C36	-37.7(2)	C21	P1	C31	C32	-85.7(3)
C21	P1	C31	C36	92.9(3)	Fe	P2	O6	C6	61.0(2)
O7	P2	O6	C6	-67.8(3)	O8	P2	O6	C6	-173.8(3)
Fe	P2	O7	C7	176.0(3)	O6	P2	O7	C7	-50.2(2)
O8	P2	O7	C7	46.9(2)	Fe	P2	O8	C8	-57.9(2)
O6	P2	O8	C8	174.2(3)	O7	P2	O8	C8	68.2(3)
Mo	C9	C10	Mo	0.0(0)	Mo	C9	C10	C11	62.9(3)
C13	C9	C10	Mo	-63.5(3)	C13	C9	C10	C11	-0.7(3)
Mo	C9	C13	Mo	0.0(0)	Mo	C9	C13	C12	-64.0(3)
C10	C9	C13	Mo	65.0(3)	C10	C9	C13	C12	1.0(2)
Mo	C10	C11	Mo	0.0(0)	Mo	C10	C11	C12	62.8(3)
C9	C10	C11	Mo	-62.8(3)	C9	C10	C11	C12	0.0(2)
Mo	C11	C12	Mo	0.0(0)	Mo	C11	C12	C13	65.5(3)
C10	C11	C12	Mo	-64.9(3)	C10	C11	C12	C13	0.6(2)
Mo	C12	C13	Mo	0.0(0)	Mo	C12	C13	C9	65.8(3)
C11	C12	C13	Mo	-66.9(3)	C11	C12	C13	C9	-1.0(2)
P1	C21	C22	C23	179.1(4)	C26	C21	C22	C23	-0.9(2)
P1	C21	C26	C25	-179.5(4)	C22	C21	C26	C25	0.5(2)
C21	C22	C23	C24	1.1(2)	C22	C23	C24	C25	-0.8(2)
C23	C24	C25	C26	0.4(2)	C24	C25	C26	C21	-0.3(2)
P1	C31	C32	C33	-179.8(4)	C36	C31	C32	C33	1.5(2)
P1	C31	C36	C35	179.7(4)	C32	C31	C36	C35	-1.8(2)
C31	C32	C33	C34	-0.7(2)	C32	C33	C34	C35	0.1(2)
C33	C34	C35	C36	-0.3(2)	C34	C35	C36	C31	1.2(2)