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atom	x	y	z	B(eq)
Mo	0.30723(7)	0.46931(6)	0.2005(1)	2.77(4)
Ti	0.2586(1)	0.6977(1)	0.2366(2)	2.62(8)
O(1)	0.2830(5)	0.5848(4)	0.2196(7)	3.5(3)
O(2)	0.2629(5)	0.3877(4)	0.0357(6)	3.4(3)
O(3)	0.2626(5)	0.4241(5)	0.3304(7)	3.7(3)
N(1)	0.3256(5)	0.7849(5)	0.3915(7)	2.5(3)
N(2)	0.1311(6)	0.6924(6)	0.2503(9)	3.5(4)
N(3)	0.2926(6)	0.7364(5)	0.0888(7)	3.1(3)
N(4)	0.4207(6)	0.4826(6)	0.217(1)	5.0(5)
C(1)	0.299(1)	0.3299(8)	-0.074(1)	5.0(6)
C(2)	0.378(1)	0.387(1)	-0.113(1)	7.8(8)
C(3)	0.325(1)	0.256(1)	-0.034(2)	11(1)
C(4)	0.221(1)	0.296(1)	-0.178(1)	9.0(9)
C(11)	0.2858(7)	0.8541(7)	0.472(1)	2.7(4)
C(12)	0.2940(7)	0.9388(7)	0.450(1)	2.9(4)
C(13)	0.2566(7)	1.0077(7)	0.525(1)	3.7(5)
C(14)	0.2080(8)	0.9923(8)	0.627(1)	4.0(5)
C(15)	0.2001(8)	0.9138(8)	0.656(1)	4.0(5)
C(16)	0.2382(8)	0.8442(7)	0.576(1)	3.2(4)
C(17)	0.4194(7)	0.7848(7)	0.448(1)	3.0(4)
C(18)	0.4787(8)	0.8808(8)	0.487(1)	4.8(5)
C(19)	0.4136(8)	0.7523(8)	0.568(1)	4.8(6)
C(21)	0.0872(8)	0.7477(8)	0.194(1)	4.4(5)
C(22)	0.0851(8)	0.8363(9)	0.268(1)	4.8(6)
C(23)	0.0453(9)	0.893(1)	0.220(2)	6.0(7)
C(24)	0.006(1)	0.862(1)	0.094(2)	7.3(8)
C(25)	0.0035(9)	0.772(1)	0.017(2)	6.8(8)
C(26)	0.0453(8)	0.7144(8)	0.066(1)	5.0(6)
C(27)	0.0706(9)	0.6347(9)	0.313(1)	4.9(6)
C(28)	0.1253(8)	0.5981(8)	0.397(1)	5.3(6)
C(29)	0.008(1)	0.560(1)	0.212(2)	11(1)
C(31)	0.3349(8)	0.8312(7)	0.108(1)	3.0(4)
C(32)	0.2801(8)	0.8927(7)	0.104(1)	3.7(5)
C(33)	0.319(1)	0.9850(8)	0.126(1)	4.1(5)
C(34)	0.410(1)	1.0123(8)	0.147(1)	5.1(6)
C(35)	0.4644(9)	0.9535(8)	0.151(1)	4.4(5)
C(36)	0.4259(8)	0.8614(7)	0.129(1)	3.6(5)
C(37)	0.2910(8)	0.6762(7)	-0.053(1)	3.8(5)
C(38)	0.382(1)	0.660(1)	-0.084(1)	7.5(7)
C(39)	0.2244(9)	0.5870(7)	-0.067(1)	4.8(5)
C(110)	0.4633(7)	0.7224(7)	0.348(1)	3.6(4)
C(131)	0.2693(9)	1.1000(8)	0.501(1)	5.6(6)
C(151)	0.150(1)	0.897(1)	0.767(1)	7.2(8)
C(210)	0.011(1)	0.692(1)	0.399(2)	9(1)
C(231)	0.042(1)	0.989(1)	0.302(2)	9(1)
C(251)	-0.043(1)	0.733(1)	-0.123(2)	8.6(9)
C(310)	0.253(1)	0.7180(8)	-0.146(1)	5.6(3)
C(331)	0.260(1)	1.0491(9)	0.117(1)	5.7(3)
C(351)	0.567(1)	0.9827(9)	0.173(1)	5.7(3)

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atom	x	y	z	B(eq)
H(1)	0.4299	0.4146	-0.0456	7.9
H(2)	0.4085	0.3520	-0.1890	7.9
H(3)	0.3654	0.4365	-0.1423	7.9
H(4)	0.2720	0.2200	-0.0168	9.0
H(5)	0.3509	0.2164	-0.1040	9.0
H(6)	0.3675	0.2788	0.0397	9.0
H(7)	0.1979	0.3450	-0.1976	9.0
H(8)	0.2315	0.2563	-0.2602	9.0
H(9)	0.1693	0.2615	-0.1489	9.0
H(10)	0.3925	0.4668	0.6160	15.9
H(11)	0.4157	0.5066	0.5030	15.9
H(12)	0.3386	0.5344	0.5859	15.9
H(13)	0.3602	0.3102	0.4669	16.0
H(14)	0.3107	0.2898	0.3290	16.0
H(15)	0.4007	0.3613	0.3728	16.0
H(16)	0.1783	0.4060	0.5123	18.5
H(17)	0.1869	0.3108	0.4248	18.5
H(18)	0.2311	0.3476	0.5681	18.5
H(19)	0.3247	0.9461	0.3746	3.3
H(20)	0.1816	1.0415	0.6785	4.8
H(21)	0.2316	0.7865	0.5929	3.9
H(22)	0.5352	0.8796	0.5164	5.4
H(23)	0.4797	0.8980	0.4062	5.4
H(24)	0.4495	0.9195	0.5457	5.4
H(25)	0.3815	0.7885	0.6331	5.3
H(26)	0.3694	0.6888	0.5443	5.3
H(27)	0.4652	0.7451	0.6040	5.3
H(28)	0.1148	0.8607	0.3623	6.0
H(29)	-0.0230	0.8925	0.0447	8.7
H(30)	0.0415	0.6467	0.0077	6.4
H(31)	0.0914	0.5603	0.4413	5.7
H(32)	0.1673	0.5637	0.3498	5.7
H(33)	0.1651	0.6482	0.4673	5.7
H(34)	-0.0309	0.5150	0.2337	9.6
H(35)	-0.0238	0.5767	0.1444	9.6
H(36)	0.0481	0.5188	0.1475	9.6
H(37)	0.2136	0.8732	0.0932	4.2
H(38)	0.4349	1.0732	0.1597	5.0
H(39)	0.4636	0.8159	0.1279	4.0
H(40)	0.4073	0.6290	-0.0257	7.5
H(41)	0.3833	0.6179	-0.1718	7.5
H(42)	0.4262	0.7130	-0.0753	7.5
H(43)	0.1664	0.6010	-0.0457	5.0
H(44)	0.2145	0.5465	-0.1565	5.0
H(45)	0.2426	0.5552	-0.0125	5.0
H(46)	0.4313	0.6585	0.3169	3.8
H(47)	0.4681	0.7398	0.2670	3.8
H(48)	0.5243	0.7216	0.3767	3.8
H(49)	0.2943	1.1456	0.5695	6.5
H(50)	0.2969	1.0968	0.4224	6.5

Positional parameters and B(eq) for 95025 Peters/CCC 4

atom	x	y	z	B(eq)
H(51)	0.2051	1.1076	0.4768	6.5
H(52)	0.1297	0.9493	0.8062	7.0
H(53)	0.1021	0.8466	0.7288	7.0
H(54)	0.1910	0.8837	0.8221	7.0
H(55)	0.0516	0.7418	0.4712	8.9
H(56)	-0.0221	0.7219	0.3559	8.9
H(57)	-0.0286	0.6592	0.4439	8.9
H(58)	0.1114	1.0277	0.3426	9.6
H(59)	0.0226	1.0325	0.2702	9.6
H(60)	0.0190	0.9939	0.3871	9.6
H(61)	-0.0758	0.7717	-0.1543	9.3
H(62)	-0.0091	0.7071	-0.1941	9.3
H(63)	-0.0977	0.6753	-0.1388	9.3
H(64)	0.2961	0.7735	-0.1498	6.9
H(65)	0.2471	0.6783	-0.2402	6.9
H(66)	0.1984	0.7325	-0.1298	6.9
H(67)	0.2912	1.1096	0.1329	6.1
H(68)	0.2244	1.0293	0.0329	6.1
H(69)	0.2147	1.0506	0.1810	6.1
H(70)	0.5934	0.9694	0.2475	6.0
H(71)	0.5972	0.9507	0.0986	6.0
H(72)	0.5897	1.0464	0.1860	6.0
C(5A)	0.2952(8)	0.3960(7)	0.435(1)	5.5(3)
C(6A)	0.345(1)	0.318(1)	0.385(2)	14.6(8)
C(7A)	0.359(1)	0.4753(9)	0.539(2)	14.6(7)
C(8A)	0.2104(9)	0.363(1)	0.495(2)	22(1)

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Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 95146. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	3500(1)	7371(1)	2197(1)	41(1)
Ti(1)	5554(1)	7981(1)	2470(2)	24(1)
Ti(2)	1843(1)	8263(1)	2394(2)	22(1)
O(1)	4504(5)	7716(4)	2384(5)	25(2)
O(2)	2784(5)	8068(4)	2205(5)	27(3)
O(3)	3568(6)	6747(5)	2875(7)	73(4)
O(4)	3156(6)	6952(6)	1346(7)	78(4)
N(1)	5844(6)	8862(6)	3035(6)	23(3)
N(2)	2041(6)	8620(6)	3409(6)	25(3)
N(3)	5570(6)	8129(6)	1482(6)	23(3)
N(4)	1124(6)	8924(6)	1660(6)	23(3)
N(5)	6338(6)	7267(5)	2952(6)	23(3)
N(6)	1315(6)	7345(5)	2232(6)	20(3)
C(11)	6676(9)	8998(7)	3490(9)	16(4)
C(12)	7025(9)	8814(7)	4246(9)	31(4)
C(13)	7839(12)	8950(9)	4696(10)	57(5)
C(14)	8292(10)	9308(9)	4369(11)	42(5)
C(15)	7966(10)	9495(8)	3607(11)	40(5)
C(16)	7189(10)	9346(7)	3200(9)	29(4)
C(17)	5299(9)	9445(8)	3094(10)	35(4)
C(18)	5244(10)	9449(9)	3865(11)	68(6)
C(19)	5621(10)	10185(8)	2968(11)	72(6)
C(21)	1424(9)	9047(9)	3544(8)	25(4)
C(22)	1364(9)	9786(9)	3421(7)	20(4)
C(23)	760(11)	10173(9)	3505(9)	42(5)
C(24)	202(10)	9834(10)	3726(9)	42(5)
C(25)	261(11)	9116(11)	3848(9)	44(5)
C(26)	858(11)	8736(8)	3773(8)	30(4)
C(27)	2779(9)	8556(8)	4121(9)	34(4)
C(28)	3164(9)	9290(8)	4397(9)	70(6)
C(29)	2602(9)	8188(8)	4767(9)	53(5)
C(31)	5911(11)	8771(9)	1300(7)	24(4)
C(32)	5457(9)	9397(10)	1065(8)	39(4)
C(33)	5807(13)	10021(9)	913(9)	57(5)
C(34)	6576(12)	10028(10)	992(10)	54(5)
C(35)	7043(10)	9431(10)	1203(9)	42(5)
C(36)	6702(10)	8805(9)	1380(8)	31(4)
C(37)	5202(9)	7653(8)	794(9)	32(4)
C(38)	4481(10)	7989(8)	200(8)	55(5)
C(39)	5819(9)	7437(8)	458(8)	44(4)
C(41)	277(10)	8808(7)	1330(10)	21(4)
C(42)	-166(10)	8682(7)	541(9)	35(4)
C(43)	-994(12)	8543(7)	270(10)	47(5)
C(44)	-1397(10)	8532(8)	758(12)	45(5)
C(45)	-962(10)	8630(8)	1517(11)	41(5)
C(46)	-143(9)	8795(7)	1785(9)	33(4)
C(47)	1429(9)	9568(7)	1398(9)	26(4)
C(48)	1499(10)	9432(8)	615(9)	60(5)

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C(49)	896(9)	10213(7)	1343(9)	49(5)
C(51)	6989(8)	7109(7)	2702(8)	16(4)
C(52)	6995(10)	6548(7)	2239(9)	41(5)
C(53)	7632(12)	6441(9)	2017(10)	53(5)
C(54)	8273(11)	6869(11)	2252(11)	59(5)
C(55)	8307(9)	7420(10)	2722(11)	48(5)
C(56)	7679(9)	7553(7)	2970(8)	31(4)
C(57)	6349(9)	6796(8)	3603(8)	28(4)
C(58)	5723(10)	7071(8)	3899(8)	53(5)
C(59)	7188(8)	6821(8)	4271(8)	43(5)
C(61)	1235(8)	6986(7)	2863(8)	19(4)
C(62)	516(8)	7017(7)	3006(9)	26(4)
C(63)	417(10)	6652(8)	3594(10)	37(4)
C(64)	1041(12)	6220(8)	4062(9)	41(5)
C(65)	1760(11)	6193(8)	3963(10)	38(4)
C(66)	1845(8)	6560(7)	3379(9)	20(4)
C(67)	1004(9)	6914(7)	1512(8)	23(4)
C(68)	79(8)	6836(7)	1216(7)	28(4)
C(69)	1220(8)	7283(7)	901(7)	30(4)
C(110)	4451(9)	9356(7)	2468(10)	51(5)
C(210)	3413(8)	8096(7)	3955(8)	44(5)
C(310)	4920(8)	6967(8)	1063(8)	41(5)
C(410)	2292(9)	9729(7)	1959(8)	38(5)
C(510)	6146(9)	6020(8)	3360(9)	45(5)
C(610)	1409(9)	6168(7)	1646(9)	46(5)