Numerical data for Complex 1

Table 2. Atomic coordinates [× 10^4] and equivalent isotropic displacement parameters [Å^2 × 10^3] for 06mz171m. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1A)	5922(3)	3236(3)	793(2)	28(1)
C(2A)	5077(3)	3529(3)	659(2)	26(1)
C(3A)	4888(3)	3940(3)	177(2)	38(1)
C(4A)	4103(3)	4195(3)	42(3)	49(2)
C(5A)	3508(3)	4017(3)	369(3)	53(2)
C(6A)	3683(3)	3599(3)	844(3)	48(1)
C(7A)	4471(3)	3362(3)	992(2)	37(1)
C(8A)	8356(6)	4101(5)	1418(6)	18(2)
C(9A)	7998(5)	4444(4)	857(3)	29(2)
C(10A)	9044(5)	3985(5)	219(5)	32(2)
C(11A)	7658(6)	4144(5)	-282(4)	32(2)
C(8Z)	8107(12)	4101(8)	1454(9)	18(2)
C(9Z)	8600(7)	4365(7)	996(4)	33(3)
C(10Z)	9014(8)	3696(9)	40(7)	32(2)
C(11Z)	7744(9)	4397(8)	-32(6)	32(2)
C(1B)	6434(3)	426(3)	935(2)	29(1)
C(2B)	5814(3)	-286(3)	783(2)	32(1)
C(3B)	5026(3)	-200(3)	884(3)	60(2)
C(4B)	4448(4)	-843(4)	765(3)	68(2)
C(5B)	4655(3)	-1600(4)	539(2)	49(2)
C(6B)	5437(4)	-1696(4)	429(3)	70(2)
C(7B)	6008(3)	-1036(3)	542(3)	56(2)
C(8B)	7993(3)	1700(3)	2371(2)	32(1)
C(9B)	7650(3)	2349(3)	2795(2)	37(1)
C(10B)	6921(3)	3512(3)	2643(2)	45(1)
C(11B)	6135(3)	2250(3)	2513(2)	41(1)
C(1)	7673(9)	1784(9)	-813(6)	35(2)
C(2)	7504(13)	1609(8)	-1500(7)	40(2)
C(3)	6752(12)	1783(10)	-1818(10)	57(2)
C(4)	6574(11)	1596(11)	-2478(10)	73(4)
C(5)	7148(15)	1235(11)	-2821(7)	88(5)
C(6)	7901(14)	1061(11)	-2504(9)	70(3)
C(7)	8079(12)	1247(11)	-1843(9)	40(2)
C(1C)	7853(6)	2127(5)	-886(4)	35(2)
C(2C)	7519(8)	1710(5)	-1582(4)	40(2)
C(3C)	6669(7)	1588(6)	-1798(6)	57(2)
C(4C)	6359(7)	1210(7)	-2426(6)	73(4)
C(5C)	6900(9)	954(6)	-2838(4)	88(5)
C(6C)	7750(8)	1076(6)	-2622(5)	70(3)
C(7C)	8060(7)	1453(6)	-1994(5)	40(2)
C(8C)	9527(3)	1465(3)	566(2)	34(1)
C(9C)	9640(3)	724(3)	826(2)	33(1)
C(10C)	8801(3)	-138(3)	1283(2)	46(1)

C(11C)	8611(3)	-299(3)	132(2)	39(1)
C(1D)	9137(3)	5426(3)	2958(2)	24(1)
C(2D)	8384(3)	5850(3)	3072(2)	32(1)
C(3D)	8314(4)	6603(4)	2935(3)	76(2)
C(4D)	7674(5)	7049(5)	3081(4)	110(3)
C(5D)	7058(5)	6738(5)	3352(4)	97(3)
C(6D)	7119(3)	5988(4)	3471(3)	53(2)
C(7D)	7793(3)	5577(3)	3361(2)	32(1)
C(8D)	11263(3)	5289(3)	1405(2)	40(1)
C(9D)	11135(4)	6154(3)	1686(2)	47(1)
C(10D)	12226(3)	6396(3)	2637(2)	42(1)
C(11D)	10945(3)	7012(3)	2685(3)	45(1)
C(1E)	10038(3)	1064(3)	3374(2)	29(1)
C(2E)	9805(3)	217(3)	3365(2)	41(1)
C(3E)	9476(4)	29(4)	3870(3)	71(2)
C(4E)	9292(6)	-750(5)	3880(4)	111(3)
C(5E)	9419(6)	-1366(4)	3387(4)	107(3)
C(6E)	9723(4)	-1175(4)	2878(3)	72(2)
C(7E)	9937(3)	-387(3)	2879(3)	42(1)
C(8E)	9255(3)	3931(3)	4411(2)	28(1)
C(9E)	9371(3)	3367(3)	4863(2)	37(1)
C(10E)	10839(3)	3753(3)	5256(2)	42(1)
C(11E)	10303(4)	2433(3)	5227(2)	50(2)
C(1F)	11594(3)	2801(3)	662(2)	30(1)
C(2F)	11604(3)	2814(3)	-23(2)	41(1)
C(3F)	12091(5)	2289(3)	-363(3)	71(2)
C(4F)	12149(6)	2295(4)	-974(3)	93(3)
C(5F)	11706(6)	2819(5)	-1265(3)	90(3)
C(6F)	11216(4)	3351(4)	-953(3)	69(2)
C(7F)	11184(3)	3351(4)	-319(2)	49(2)
C(8F)	11836(3)	680(3)	2132(2)	36(1)
C(9F)	12481(3)	592(3)	1696(2)	43(1)
C(10F)	13607(4)	1499(4)	2386(3)	74(2)
C(11F)	13395(4)	1357(4)	1237(3)	66(2)
C(1G)	11319(3)	5181(3)	3890(2)	23(1)
C(2G)	12056(2)	5386(3)	4427(2)	26(1)
C(3G)	12400(3)	6166(3)	4641(2)	35(1)
C(4G)	13081(3)	6343(4)	5137(2)	45(1)
C(5G)	13425(3)	5754(4)	5393(3)	55(2)
C(6G)	13106(3)	4976(4)	5161(2)	53(2)
C(7G)	12405(3)	4793(3)	4685(2)	38(1)
C(1H)	12051(3)	2457(3)	3864(2)	27(1)
C(2H)	12947(3)	2661(3)	4194(2)	30(1)
C(3H)	13173(3)	2651(3)	4827(2)	37(1)
C(4H)	14002(3)	2834(4)	5128(2)	49(2)
C(5H)	14577(3)	3055(4)	4790(2)	53(2)
C(6H)	14351(3)	3078(3)	4157(2)	49(2)
C(7H)	13526(3)	2874(3)	3864(2)	42(1)
C(1I)	12856(3)	3824(3)	2337(2)	31(1)
C(2I)	13559(3)	4320(3)	2799(2)	30(1)
C(3I)	13393(3)	4927(3)	3280(2)	34(1)
C(4I)	14038(3)	5369(3)	3722(2)	44(1)
C(5I)	14843(3)	5226(3)	3682(2)	46(1)
C(6I)	15009(3)	4641(3)	3204(2)	44(1)

C(7I)	14374(3)	4166(3)	2769(2)	40(1)
Cu(1)	7714(1)	2848(1)	371(1)	27(1)
Cu(2)	7010(1)	2336(1)	1488(1)	25(1)
Cu(3)	7971(1)	1101(1)	767(1)	27(1)
Cu(4)	12147(1)	2187(1)	1872(1)	27(1)
Cu(5)	10827(1)	5292(1)	2581(1)	24(1)
Cu(6)	10377(1)	2829(1)	3998(1)	23(1)
N(1)	8206(2)	3906(2)	281(2)	40(1)
N(2)	6915(2)	2635(2)	2429(2)	31(1)
N(3)	8821(2)	283(2)	759(2)	28(1)
N(4)	11315(2)	6296(2)	2398(2)	32(1)
N(5)	10210(2)	3087(2)	4899(2)	28(1)
N(6)	12978(2)	1359(3)	1796(2)	41(1)
O(1)	7222(2)	1926(2)	614(1)	25(1)
O(2)	8171(2)	3247(2)	1284(1)	28(1)
O(3)	8063(2)	1933(2)	1793(1)	24(1)
O(4)	8885(2)	1876(2)	815(1)	26(1)
O(5)	10814(2)	4797(2)	1687(1)	28(1)
O(6)	9488(2)	3534(2)	3836(1)	21(1)
O(7)	11413(2)	1355(2)	2027(1)	25(1)
O(8)	6425(2)	3348(2)	446(2)	35(1)
O(9)	6049(2)	2891(2)	1251(1)	31(1)
O(10)	6291(2)	1056(2)	1274(2)	34(1)
O(11)	7094(2)	298(2)	695(2)	39(1)
O(12)	7381(2)	2388(2)	-533(2)	42(1)
O(13)	8606(3)	2210(4)	-727(3)	50(2)
O(14)	9573(2)	5653(2)	2606(1)	28(1)
O(15)	9267(2)	4863(2)	3242(1)	24(1)
O(16)	9796(2)	1602(2)	3762(1)	31(1)
O(17)	10475(2)	1182(2)	2965(1)	27(1)
O(18)	11829(2)	2218(2)	859(1)	36(1)
O(19)	11337(2)	3422(2)	980(1)	29(1)
O(20)	11248(2)	5635(2)	3504(1)	27(1)
O(21)	10843(2)	4579(2)	3874(1)	25(1)
O(22)	11521(2)	2544(2)	4226(1)	31(1)
O(23)	11918(2)	2228(2)	3263(1)	27(1)
O(30)	12985(2)	3109(2)	2116(2)	35(1)
O(31)	12196(2)	4152(2)	2219(1)	26(1)
O(32)	7966(6)	1268(6)	-501(4)	57(3)
O(24)	10492(2)	2943(2)	3169(1)	21(1)
O(25)	11276(2)	2807(2)	2143(1)	22(1)
O(26)	10590(2)	4192(2)	2591(1)	22(1)
O(27)	9108(2)	3359(2)	2470(1)	21(1)
O(28)	9788(2)	1972(2)	2056(1)	23(1)
O(29)	9912(2)	3218(2)	1454(1)	23(1)
Ti(1)	9086(1)	2638(1)	1690(1)	22(1)
Ti(2)	10926(1)	3674(1)	1824(1)	22(1)
Ti(3)	9900(1)	3865(1)	3103(1)	20(1)
Ti(4)	10773(1)	2108(1)	2573(1)	21(1)

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 3. Bond lengths [Å] and angles [deg] for 06mz171m.

C(1A)-O(8)	1.248(5)	C(11Z)-H(11V)	0.9800
C(1A)-O(9)	1.264(5)	C(1B)-O(10)	1.235(5)
C(1A)-C(2A)	1.501(6)	C(1B)-O(11)	1.290(5)
C(2A)-C(7A)	1.384(6)	C(1B)-C(2B)	1.507(6)
C(2A)-C(3A)	1.393(6)	C(2B)-C(3B)	1.360(7)
C(3A)-C(4A)	1.385(6)	C(2B)-C(7B)	1.362(7)
C(3A)-H(3A)	0.9500	C(3B)-C(4B)	1.382(7)
C(4A)-C(5A)	1.365(7)	C(3B)-H(3B)	0.9500
C(4A)-H(4A)	0.9500	C(4B)-C(5B)	1.375(8)
C(5A)-C(6A)	1.386(8)	C(4B)-H(4B)	0.9500
C(5A)-H(5A)	0.9500	C(5B)-C(6B)	1.357(8)
C(6A)-C(7A)	1.382(6)	C(5B)-H(5B)	0.9500
C(6A)-H(6A)	0.9500	C(6B)-C(7B)	1.398(7)
C(7A)-H(7A)	0.9500	C(6B)-H(6B)	0.9500
C(8A)-O(2)	1.450(9)	C(7B)-H(7B)	0.9500
C(8A)-C(9A)	1.516(11)	C(8B)-O(3)	1.428(5)
C(8A)-H(8A1)	0.9900	C(8B)-C(9B)	1.491(6)
C(8A)-H(8A2)	0.9900	C(8B)-H(8B1)	0.9900
C(9A)-N(1)	1.498(7)	C(8B)-H(8B2)	0.9900
C(9A)-H(9A1)	0.9900	C(9B)-N(2)	1.495(6)
C(9A)-H(9A2)	0.9900	C(9B)-H(9B1)	0.9900
C(10A)-N(1)	1.410(8)	C(9B)-H(9B2)	0.9900
C(10A)-H(10A)	0.9800	C(10B)-N(2)	1.486(6)
C(10A)-H(10B)	0.9800	C(10B)-H(10D)	0.9800
C(10A)-H(10C)	0.9800	C(10B)-H(10E)	0.9800
C(11A)-N(1)	1.539(8)	C(10B)-H(10F)	0.9800
C(11A)-H(11A)	0.9800	C(11B)-N(2)	1.474(6)
C(11A)-H(11B)	0.9800	C(11B)-H(11D)	0.9800
C(11A)-H(11C)	0.9800	C(11B)-H(11E)	0.9800
C(8Z)-O(2)	1.455(13)	C(11B)-H(11F)	0.9800
C(8Z)-C(9Z)	1.520(14)	C(1)-O(12)	1.251(16)
C(8Z)-H(8Z1)	0.9900	C(1)-O(32)	1.295(17)
C(8Z)-H(8Z2)	0.9900	C(1)-C(2)	1.445(19)
C(9Z)-N(1)	1.608(10)	C(2)-C(3)	1.3900
C(9Z)-H(9Z1)	0.9900	C(2)-C(7)	1.3900
C(9Z)-H(9Z2)	0.9900	C(3)-C(4)	1.3900
C(10Z)-N(1)	1.539(11)	C(3)-H(3)	0.9500
C(10Z)-H(10T)	0.9800	C(4)-C(5)	1.3900
C(10Z)-H(10U)	0.9800	C(4)-H(4C)	0.9500
C(10Z)-H(10V)	0.9800	C(5)-C(6)	1.3900
C(11Z)-N(1)	1.374(10)	C(5)-H(5)	0.9500
C(11Z)-H(11T)	0.9800	C(6)-C(7)	1.3900
C(11Z)-H(11U)	0.9800	C(6)-H(6)	0.9500

C(7)-H(7)	0.9500	C(10D)-H(10L)	0.9800
C(1C)-O(12)	1.219(10)	C(11D)-N(4)	1.468(6)
C(1C)-O(13)	1.221(11)	C(11D)-H(11J)	0.9800
C(1C)-C(2C)	1.535(12)	C(11D)-H(11K)	0.9800
C(2C)-C(3C)	1.3900	C(11D)-H(11L)	0.9800
C(2C)-C(7C)	1.3900	C(1E)-O(16)	1.245(5)
C(3C)-C(4C)	1.3900	C(1E)-O(17)	1.281(5)
C(3C)-H(3C)	0.9500	C(1E)-C(2E)	1.493(7)
C(4C)-C(5C)	1.3900	C(2E)-C(7E)	1.375(7)
C(4C)-H(4C1)	0.9500	C(2E)-C(3E)	1.399(7)
C(5C)-C(6C)	1.3900	C(3E)-C(4E)	1.373(9)
C(5C)-H(5C)	0.9500	C(3E)-H(3E)	0.9500
C(6C)-C(7C)	1.3900	C(4E)-C(5E)	1.395(10)
C(6C)-H(6C)	0.9500	C(4E)-H(4E)	0.9500
C(7C)-H(7C)	0.9500	C(5E)-C(6E)	1.389(9)
C(8C)-O(4)	1.415(5)	C(5E)-H(5E)	0.9500
C(8C)-C(9C)	1.513(7)	C(6E)-C(7E)	1.392(7)
C(8C)-H(8C1)	0.9900	C(6E)-H(6E)	0.9500
C(8C)-H(8C2)	0.9900	C(7E)-H(7E)	0.9500
C(9C)-N(3)	1.487(6)	C(8E)-O(6)	1.419(5)
C(9C)-H(9C1)	0.9900	C(8E)-C(9E)	1.526(6)
C(9C)-H(9C2)	0.9900	C(8E)-H(8E1)	0.9900
C(10C)-N(3)	1.488(6)	C(8E)-H(8E2)	0.9900
C(10C)-H(10G)	0.9800	C(9E)-N(5)	1.473(5)
C(10C)-H(10H)	0.9800	C(9E)-H(9E1)	0.9900
C(10C)-H(10I)	0.9800	C(9E)-H(9E2)	0.9900
C(11C)-N(3)	1.496(5)	C(10E)-N(5)	1.501(6)
C(11C)-H(11G)	0.9800	C(10E)-H(10M)	0.9800
C(11C)-H(11H)	0.9800	C(10E)-H(10N)	0.9800
C(11C)-H(11I)	0.9800	C(10E)-H(10O)	0.9800
C(1D)-O(14)	1.245(5)	C(11E)-N(5)	1.461(6)
C(1D)-O(15)	1.268(5)	C(11E)-H(11M)	0.9800
C(1D)-C(2D)	1.494(6)	C(11E)-H(11N)	0.9800
C(2D)-C(7D)	1.364(6)	C(11E)-H(11O)	0.9800
C(2D)-C(3D)	1.400(7)	C(1F)-O(18)	1.227(6)
C(3D)-C(4D)	1.370(8)	C(1F)-O(19)	1.278(5)
C(3D)-H(3D)	0.9500	C(1F)-C(2F)	1.506(6)
C(4D)-C(5D)	1.398(10)	C(2F)-C(7F)	1.383(7)
C(4D)-H(4D)	0.9500	C(2F)-C(3F)	1.412(7)
C(5D)-C(6D)	1.378(9)	C(3F)-C(4F)	1.360(8)
C(5D)-H(5D)	0.9500	C(3F)-H(3F)	0.9500
C(6D)-C(7D)	1.366(7)	C(4F)-C(5F)	1.377(10)
C(6D)-H(6D)	0.9500	C(4F)-H(4F)	0.9500
C(7D)-H(7D)	0.9500	C(5F)-C(6F)	1.392(10)
C(8D)-O(5)	1.403(5)	C(5F)-H(5F)	0.9500
C(8D)-C(9D)	1.528(7)	C(6F)-C(7F)	1.399(7)
C(8D)-H(8D1)	0.9900	C(6F)-H(6F)	0.9500
C(8D)-H(8D2)	0.9900	C(7F)-H(7F)	0.9500
C(9D)-N(4)	1.501(6)	C(8F)-O(7)	1.421(5)
C(9D)-H(9D1)	0.9900	C(8F)-C(9F)	1.533(6)
C(9D)-H(9D2)	0.9900	C(8F)-H(8F1)	0.9900
C(10D)-N(4)	1.490(6)	C(8F)-H(8F2)	0.9900
C(10D)-H(10J)	0.9800	C(9F)-N(6)	1.482(6)
C(10D)-H(10K)	0.9800	C(9F)-H(9F1)	0.9900

C(9F)-H(9F2)	0.9900	Cu(1)-N(1)	2.028(4)
C(10F)-N(6)	1.480(7)	Cu(1)-O(8)	2.338(3)
C(10F)-H(10P)	0.9800	Cu(2)-O(9)	1.934(3)
C(10F)-H(10Q)	0.9800	Cu(2)-O(3)	1.956(3)
C(10F)-H(10R)	0.9800	Cu(2)-O(1)	1.988(3)
C(11F)-N(6)	1.499(7)	Cu(2)-N(2)	2.050(4)
C(11F)-H(11P)	0.9800	Cu(2)-O(10)	2.380(3)
C(11F)-H(11Q)	0.9800	Cu(2)-Cu(3)	3.0358(10)
C(11F)-H(11R)	0.9800	Cu(3)-O(11)	1.920(3)
C(1G)-O(20)	1.264(5)	Cu(3)-O(4)	1.945(3)
C(1G)-O(21)	1.265(5)	Cu(3)-O(1)	1.966(3)
C(1G)-C(2G)	1.512(5)	Cu(3)-N(3)	2.026(4)
C(2G)-C(7G)	1.371(6)	Cu(3)-O(3)	2.372(3)
C(2G)-C(3G)	1.391(6)	Cu(4)-O(25)	1.920(3)
C(3G)-C(4G)	1.395(6)	Cu(4)-O(7)	1.958(3)
C(3G)-H(3G)	0.9500	Cu(4)-O(30)	1.981(3)
C(4G)-C(5G)	1.361(8)	Cu(4)-N(6)	2.018(4)
C(4G)-H(4G)	0.9500	Cu(4)-O(18)	2.205(3)
C(5G)-C(6G)	1.379(8)	Cu(4)-Ti(4)	2.9491(12)
C(5G)-H(5G)	0.9500	Cu(5)-O(26)	1.929(3)
C(6G)-C(7G)	1.392(6)	Cu(5)-O(5)	1.960(3)
C(6G)-H(6G)	0.9500	Cu(5)-O(20)	1.975(3)
C(7G)-H(7G)	0.9500	Cu(5)-N(4)	2.023(4)
C(1H)-O(22)	1.266(5)	Cu(5)-O(14)	2.181(3)
C(1H)-O(23)	1.267(5)	Cu(5)-Ti(2)	2.9567(12)
C(1H)-C(2H)	1.518(6)	Cu(6)-O(24)	1.907(3)
C(2H)-C(7H)	1.372(6)	Cu(6)-O(22)	1.970(3)
C(2H)-C(3H)	1.377(6)	Cu(6)-O(6)	1.975(3)
C(3H)-C(4H)	1.400(6)	Cu(6)-N(5)	1.995(3)
C(3H)-H(3H)	0.9500	Cu(6)-O(16)	2.206(3)
C(4H)-C(5H)	1.382(7)	Cu(6)-Ti(3)	2.9567(11)
C(4H)-H(4H)	0.9500	O(1)-H(1)	0.813(19)
C(5H)-C(6H)	1.384(7)	O(2)-Ti(1)	2.057(3)
C(5H)-H(5H)	0.9500	O(3)-Ti(1)	2.105(3)
C(6H)-C(7H)	1.394(6)	O(4)-Ti(1)	2.049(3)
C(6H)-H(6H)	0.9500	O(5)-Ti(2)	2.035(3)
C(7H)-H(7H)	0.9500	O(6)-Ti(3)	2.022(3)
C(1I)-O(31)	1.257(5)	O(7)-Ti(4)	2.025(3)
C(1I)-O(30)	1.268(5)	O(15)-Ti(3)	2.044(3)
C(1I)-C(2I)	1.499(6)	O(17)-Ti(4)	2.047(3)
C(2I)-C(7I)	1.386(6)	O(19)-Ti(2)	2.040(3)
C(2I)-C(3I)	1.391(6)	O(21)-Ti(3)	2.201(3)
C(3I)-C(4I)	1.384(6)	O(23)-Ti(4)	2.176(3)
C(3I)-H(3I)	0.9500	O(31)-Ti(2)	2.174(3)
C(4I)-C(5I)	1.368(6)	O(24)-Ti(4)	1.858(3)
C(4I)-H(4I)	0.9500	O(24)-Ti(3)	1.917(3)
C(5I)-C(6I)	1.365(7)	O(25)-Ti(2)	1.855(3)
C(5I)-H(5I)	0.9500	O(25)-Ti(4)	1.920(3)
C(6I)-C(7I)	1.389(6)	O(26)-Ti(3)	1.872(3)
C(6I)-H(6I)	0.9500	O(26)-Ti(2)	1.908(3)
C(7I)-H(7I)	0.9500	O(27)-Ti(3)	1.779(3)
Cu(1)-O(12)	1.943(3)	O(27)-Ti(1)	1.881(3)
Cu(1)-O(1)	1.969(3)	O(28)-Ti(4)	1.788(3)
Cu(1)-O(2)	1.976(3)	O(28)-Ti(1)	1.865(3)

O(29)-Ti(2)	1.793(3)	C(8Z)-C(9Z)-H(9Z2)	109.8
O(29)-Ti(1)	1.861(3)	N(1)-C(9Z)-H(9Z2)	109.8
Ti(1)-Ti(4)	3.3776(13)	H(9Z1)-C(9Z)-H(9Z2)	108.3
Ti(1)-Ti(3)	3.3812(13)	N(1)-C(10Z)-H(10T)	109.5
Ti(1)-Ti(2)	3.3855(14)	N(1)-C(10Z)-H(10U)	109.5
		N(1)-C(10Z)-H(10V)	109.5
O(8)-C(1A)-O(9)	126.5(4)	N(1)-C(11Z)-H(11T)	109.5
O(8)-C(1A)-C(2A)	117.9(4)	N(1)-C(11Z)-H(11U)	109.5
O(9)-C(1A)-C(2A)	115.6(4)	N(1)-C(11Z)-H(11V)	109.5
C(7A)-C(2A)-C(3A)	119.6(4)	O(10)-C(1B)-O(11)	126.0(4)
C(7A)-C(2A)-C(1A)	120.5(4)	O(10)-C(1B)-C(2B)	119.9(4)
C(3A)-C(2A)-C(1A)	119.8(4)	O(11)-C(1B)-C(2B)	114.1(4)
C(4A)-C(3A)-C(2A)	120.0(5)	C(3B)-C(2B)-C(7B)	117.1(5)
C(4A)-C(3A)-H(3A)	120.0	C(3B)-C(2B)-C(1B)	120.4(4)
C(2A)-C(3A)-H(3A)	120.0	C(7B)-C(2B)-C(1B)	122.5(4)
C(5A)-C(4A)-C(3A)	119.7(5)	C(2B)-C(3B)-C(4B)	121.8(5)
C(5A)-C(4A)-H(4A)	120.1	C(2B)-C(3B)-H(3B)	119.1
C(3A)-C(4A)-H(4A)	120.1	C(4B)-C(3B)-H(3B)	119.1
C(4A)-C(5A)-C(6A)	121.0(5)	C(5B)-C(4B)-C(3B)	120.7(5)
C(4A)-C(5A)-H(5A)	119.5	C(5B)-C(4B)-H(4B)	119.7
C(6A)-C(5A)-H(5A)	119.5	C(3B)-C(4B)-H(4B)	119.7
C(7A)-C(6A)-C(5A)	119.5(5)	C(6B)-C(5B)-C(4B)	118.2(5)
C(7A)-C(6A)-H(6A)	120.3	C(6B)-C(5B)-H(5B)	120.9
C(5A)-C(6A)-H(6A)	120.3	C(4B)-C(5B)-H(5B)	120.9
C(6A)-C(7A)-C(2A)	120.1(5)	C(5B)-C(6B)-C(7B)	120.2(6)
C(6A)-C(7A)-H(7A)	119.9	C(5B)-C(6B)-H(6B)	119.9
C(2A)-C(7A)-H(7A)	119.9	C(7B)-C(6B)-H(6B)	119.9
O(2)-C(8A)-C(9A)	111.4(8)	C(2B)-C(7B)-C(6B)	122.0(5)
O(2)-C(8A)-H(8A1)	109.3	C(2B)-C(7B)-H(7B)	119.0
C(9A)-C(8A)-H(8A1)	109.3	C(6B)-C(7B)-H(7B)	119.0
O(2)-C(8A)-H(8A2)	109.3	O(3)-C(8B)-C(9B)	109.3(4)
C(9A)-C(8A)-H(8A2)	109.3	O(3)-C(8B)-H(8B1)	109.8
H(8A1)-C(8A)-H(8A2)	108.0	C(9B)-C(8B)-H(8B1)	109.8
N(1)-C(9A)-C(8A)	106.1(6)	O(3)-C(8B)-H(8B2)	109.8
N(1)-C(9A)-H(9A1)	110.5	C(9B)-C(8B)-H(8B2)	109.8
C(8A)-C(9A)-H(9A1)	110.5	H(8B1)-C(8B)-H(8B2)	108.3
N(1)-C(9A)-H(9A2)	110.5	C(8B)-C(9B)-N(2)	110.0(4)
C(8A)-C(9A)-H(9A2)	110.5	C(8B)-C(9B)-H(9B1)	109.7
H(9A1)-C(9A)-H(9A2)	108.7	N(2)-C(9B)-H(9B1)	109.7
N(1)-C(10A)-H(10A)	109.5	C(8B)-C(9B)-H(9B2)	109.7
N(1)-C(10A)-H(10B)	109.5	N(2)-C(9B)-H(9B2)	109.7
N(1)-C(10A)-H(10C)	109.5	H(9B1)-C(9B)-H(9B2)	108.2
N(1)-C(11A)-H(11A)	109.5	N(2)-C(10B)-H(10D)	109.5
N(1)-C(11A)-H(11B)	109.5	N(2)-C(10B)-H(10E)	109.5
N(1)-C(11A)-H(11C)	109.5	H(10D)-C(10B)-H(10E)	109.5
O(2)-C(8Z)-C(9Z)	99.8(10)	N(2)-C(10B)-H(10F)	109.5
O(2)-C(8Z)-H(8Z1)	111.8	H(10D)-C(10B)-H(10F)	109.5
C(9Z)-C(8Z)-H(8Z1)	111.8	H(10E)-C(10B)-H(10F)	109.5
O(2)-C(8Z)-H(8Z2)	111.8	N(2)-C(11B)-H(11D)	109.5
C(9Z)-C(8Z)-H(8Z2)	111.8	N(2)-C(11B)-H(11E)	109.5
H(8Z1)-C(8Z)-H(8Z2)	109.5	H(11D)-C(11B)-H(11E)	109.5
C(8Z)-C(9Z)-N(1)	109.3(11)	N(2)-C(11B)-H(11F)	109.5
C(8Z)-C(9Z)-H(9Z1)	109.8	H(11D)-C(11B)-H(11F)	109.5
N(1)-C(9Z)-H(9Z1)	109.8	H(11E)-C(11B)-H(11F)	109.5

O(12)-C(1)-O(32)	119.9(11)	N(3)-C(10C)-H(10G)	109.5
O(12)-C(1)-C(2)	117.0(13)	N(3)-C(10C)-H(10H)	109.5
O(32)-C(1)-C(2)	121.6(13)	H(10G)-C(10C)-H(10H)	109.5
C(3)-C(2)-C(7)	120.0	N(3)-C(10C)-H(10I)	109.5
C(3)-C(2)-C(1)	119.6(15)	H(10G)-C(10C)-H(10I)	109.5
C(7)-C(2)-C(1)	120.4(15)	H(10H)-C(10C)-H(10I)	109.5
C(2)-C(3)-C(4)	120.0	N(3)-C(11C)-H(11G)	109.5
C(2)-C(3)-H(3)	120.0	N(3)-C(11C)-H(11H)	109.5
C(4)-C(3)-H(3)	120.0	H(11G)-C(11C)-H(11H)	109.5
C(3)-C(4)-C(5)	120.0	N(3)-C(11C)-H(11I)	109.5
C(3)-C(4)-H(4C)	120.0	H(11G)-C(11C)-H(11I)	109.5
C(5)-C(4)-H(4C)	120.0	H(11H)-C(11C)-H(11I)	109.5
C(6)-C(5)-C(4)	120.0	O(14)-C(1D)-O(15)	126.6(4)
C(6)-C(5)-H(5)	120.0	O(14)-C(1D)-C(2D)	118.5(4)
C(4)-C(5)-H(5)	120.0	O(15)-C(1D)-C(2D)	115.0(4)
C(5)-C(6)-C(7)	120.0	C(7D)-C(2D)-C(3D)	117.6(5)
C(5)-C(6)-H(6)	120.0	C(7D)-C(2D)-C(1D)	123.3(4)
C(7)-C(6)-H(6)	120.0	C(3D)-C(2D)-C(1D)	118.8(5)
C(6)-C(7)-C(2)	120.0	C(4D)-C(3D)-C(2D)	121.3(6)
C(6)-C(7)-H(7)	120.0	C(4D)-C(3D)-H(3D)	119.3
C(2)-C(7)-H(7)	120.0	C(2D)-C(3D)-H(3D)	119.3
O(12)-C(1C)-O(13)	123.2(7)	C(3D)-C(4D)-C(5D)	119.7(7)
O(12)-C(1C)-C(2C)	120.7(9)	C(3D)-C(4D)-H(4D)	120.2
O(13)-C(1C)-C(2C)	116.1(9)	C(5D)-C(4D)-H(4D)	120.2
C(3C)-C(2C)-C(7C)	120.0	C(6D)-C(5D)-C(4D)	118.6(6)
C(3C)-C(2C)-C(1C)	119.4(9)	C(6D)-C(5D)-H(5D)	120.7
C(7C)-C(2C)-C(1C)	120.6(9)	C(4D)-C(5D)-H(5D)	120.7
C(4C)-C(3C)-C(2C)	120.0	C(7D)-C(6D)-C(5D)	120.5(6)
C(4C)-C(3C)-H(3C)	120.0	C(7D)-C(6D)-H(6D)	119.7
C(2C)-C(3C)-H(3C)	120.0	C(5D)-C(6D)-H(6D)	119.7
C(3C)-C(4C)-C(5C)	120.0	C(2D)-C(7D)-C(6D)	121.9(5)
C(3C)-C(4C)-H(4C1)	120.0	C(2D)-C(7D)-H(7D)	119.1
C(5C)-C(4C)-H(4C1)	120.0	C(6D)-C(7D)-H(7D)	119.1
C(6C)-C(5C)-C(4C)	120.0	O(5)-C(8D)-C(9D)	108.6(4)
C(6C)-C(5C)-H(5C)	120.0	O(5)-C(8D)-H(8D1)	110.0
C(4C)-C(5C)-H(5C)	120.0	C(9D)-C(8D)-H(8D1)	110.0
C(7C)-C(6C)-C(5C)	120.0	O(5)-C(8D)-H(8D2)	110.0
C(7C)-C(6C)-H(6C)	120.0	C(9D)-C(8D)-H(8D2)	110.0
C(5C)-C(6C)-H(6C)	120.0	H(8D1)-C(8D)-H(8D2)	108.4
C(6C)-C(7C)-C(2C)	120.0	N(4)-C(9D)-C(8D)	108.9(4)
C(6C)-C(7C)-H(7C)	120.0	N(4)-C(9D)-H(9D1)	109.9
C(2C)-C(7C)-H(7C)	120.0	C(8D)-C(9D)-H(9D1)	109.9
O(4)-C(8C)-C(9C)	109.3(4)	N(4)-C(9D)-H(9D2)	109.9
O(4)-C(8C)-H(8C1)	109.8	C(8D)-C(9D)-H(9D2)	109.9
C(9C)-C(8C)-H(8C1)	109.8	H(9D1)-C(9D)-H(9D2)	108.3
O(4)-C(8C)-H(8C2)	109.8	N(4)-C(10D)-H(10J)	109.5
C(9C)-C(8C)-H(8C2)	109.8	N(4)-C(10D)-H(10K)	109.5
H(8C1)-C(8C)-H(8C2)	108.3	H(10J)-C(10D)-H(10K)	109.5
N(3)-C(9C)-C(8C)	109.8(4)	N(4)-C(10D)-H(10L)	109.5
N(3)-C(9C)-H(9C1)	109.7	H(10J)-C(10D)-H(10L)	109.5
C(8C)-C(9C)-H(9C1)	109.7	H(10K)-C(10D)-H(10L)	109.5
N(3)-C(9C)-H(9C2)	109.7	N(4)-C(11D)-H(11J)	109.5
C(8C)-C(9C)-H(9C2)	109.7	N(4)-C(11D)-H(11K)	109.5
H(9C1)-C(9C)-H(9C2)	108.2	H(11J)-C(11D)-H(11K)	109.5

N(4)-C(11D)-H(11L)	109.5	C(4F)-C(3F)-C(2F)	121.5(6)
H(11J)-C(11D)-H(11L)	109.5	C(4F)-C(3F)-H(3F)	119.2
H(11K)-C(11D)-H(11L)	109.5	C(2F)-C(3F)-H(3F)	119.2
O(16)-C(1E)-O(17)	124.5(4)	C(3F)-C(4F)-C(5F)	118.5(7)
O(16)-C(1E)-C(2E)	119.4(4)	C(3F)-C(4F)-H(4F)	120.8
O(17)-C(1E)-C(2E)	116.1(4)	C(5F)-C(4F)-H(4F)	120.8
C(7E)-C(2E)-C(3E)	119.4(5)	C(4F)-C(5F)-C(6F)	122.5(6)
C(7E)-C(2E)-C(1E)	121.0(4)	C(4F)-C(5F)-H(5F)	118.7
C(3E)-C(2E)-C(1E)	119.6(5)	C(6F)-C(5F)-H(5F)	118.7
C(4E)-C(3E)-C(2E)	120.2(6)	C(5F)-C(6F)-C(7F)	118.1(6)
C(4E)-C(3E)-H(3E)	119.9	C(5F)-C(6F)-H(6F)	121.0
C(2E)-C(3E)-H(3E)	119.9	C(7F)-C(6F)-H(6F)	121.0
C(3E)-C(4E)-C(5E)	120.8(7)	C(2F)-C(7F)-C(6F)	120.4(6)
C(3E)-C(4E)-H(4E)	119.6	C(2F)-C(7F)-H(7F)	119.8
C(5E)-C(4E)-H(4E)	119.6	C(6F)-C(7F)-H(7F)	119.8
C(6E)-C(5E)-C(4E)	118.7(6)	O(7)-C(8F)-C(9F)	105.8(4)
C(6E)-C(5E)-H(5E)	120.6	O(7)-C(8F)-H(8F1)	110.6
C(4E)-C(5E)-H(5E)	120.6	C(9F)-C(8F)-H(8F1)	110.6
C(5E)-C(6E)-C(7E)	120.4(6)	O(7)-C(8F)-H(8F2)	110.6
C(5E)-C(6E)-H(6E)	119.8	C(9F)-C(8F)-H(8F2)	110.6
C(7E)-C(6E)-H(6E)	119.8	H(8F1)-C(8F)-H(8F2)	108.7
C(2E)-C(7E)-C(6E)	120.4(5)	N(6)-C(9F)-C(8F)	109.8(4)
C(2E)-C(7E)-H(7E)	119.8	N(6)-C(9F)-H(9F1)	109.7
C(6E)-C(7E)-H(7E)	119.8	C(8F)-C(9F)-H(9F1)	109.7
O(6)-C(8E)-C(9E)	106.8(3)	N(6)-C(9F)-H(9F2)	109.7
O(6)-C(8E)-H(8E1)	110.4	C(8F)-C(9F)-H(9F2)	109.7
C(9E)-C(8E)-H(8E1)	110.4	H(9F1)-C(9F)-H(9F2)	108.2
O(6)-C(8E)-H(8E2)	110.4	N(6)-C(10F)-H(10P)	109.5
C(9E)-C(8E)-H(8E2)	110.4	N(6)-C(10F)-H(10Q)	109.5
H(8E1)-C(8E)-H(8E2)	108.6	H(10P)-C(10F)-H(10Q)	109.5
N(5)-C(9E)-C(8E)	109.6(4)	N(6)-C(10F)-H(10R)	109.5
N(5)-C(9E)-H(9E1)	109.7	H(10P)-C(10F)-H(10R)	109.5
C(8E)-C(9E)-H(9E1)	109.7	H(10Q)-C(10F)-H(10R)	109.5
N(5)-C(9E)-H(9E2)	109.7	N(6)-C(11F)-H(11P)	109.5
C(8E)-C(9E)-H(9E2)	109.7	N(6)-C(11F)-H(11Q)	109.5
H(9E1)-C(9E)-H(9E2)	108.2	H(11P)-C(11F)-H(11Q)	109.5
N(5)-C(10E)-H(10M)	109.5	N(6)-C(11F)-H(11R)	109.5
N(5)-C(10E)-H(10N)	109.5	H(11P)-C(11F)-H(11R)	109.5
H(10M)-C(10E)-H(10N)	109.5	H(11Q)-C(11F)-H(11R)	109.5
N(5)-C(10E)-H(10O)	109.5	O(20)-C(1G)-O(21)	127.2(4)
H(10M)-C(10E)-H(10O)	109.5	O(20)-C(1G)-C(2G)	115.7(4)
H(10N)-C(10E)-H(10O)	109.5	O(21)-C(1G)-C(2G)	117.0(4)
N(5)-C(11E)-H(11M)	109.5	C(7G)-C(2G)-C(3G)	120.2(4)
N(5)-C(11E)-H(11N)	109.5	C(7G)-C(2G)-C(1G)	119.6(4)
H(11M)-C(11E)-H(11N)	109.5	C(3G)-C(2G)-C(1G)	120.2(4)
N(5)-C(11E)-H(11O)	109.5	C(2G)-C(3G)-C(4G)	119.3(5)
H(11M)-C(11E)-H(11O)	109.5	C(2G)-C(3G)-H(3G)	120.3
H(11N)-C(11E)-H(11O)	109.5	C(4G)-C(3G)-H(3G)	120.3
O(18)-C(1F)-O(19)	126.8(4)	C(5G)-C(4G)-C(3G)	120.3(5)
O(18)-C(1F)-C(2F)	118.7(4)	C(5G)-C(4G)-H(4G)	119.8
O(19)-C(1F)-C(2F)	114.5(4)	C(3G)-C(4G)-H(4G)	119.8
C(7F)-C(2F)-C(3F)	118.9(5)	C(4G)-C(5G)-C(6G)	120.2(5)
C(7F)-C(2F)-C(1F)	122.1(5)	C(4G)-C(5G)-H(5G)	119.9
C(3F)-C(2F)-C(1F)	118.9(5)	C(6G)-C(5G)-H(5G)	119.9

C(5G)-C(6G)-C(7G)	120.2(5)	O(12)-Cu(1)-O(8)	92.53(13)
C(5G)-C(6G)-H(6G)	119.9	O(1)-Cu(1)-O(8)	83.93(12)
C(7G)-C(6G)-H(6G)	119.9	O(2)-Cu(1)-O(8)	94.12(12)
C(2G)-C(7G)-C(6G)	119.7(5)	N(1)-Cu(1)-O(8)	91.89(14)
C(2G)-C(7G)-H(7G)	120.2	O(9)-Cu(2)-O(3)	171.41(13)
C(6G)-C(7G)-H(7G)	120.2	O(9)-Cu(2)-O(1)	96.95(12)
O(22)-C(1H)-O(23)	127.6(4)	O(3)-Cu(2)-O(1)	86.86(11)
O(22)-C(1H)-C(2H)	115.4(4)	O(9)-Cu(2)-N(2)	91.65(13)
O(23)-C(1H)-C(2H)	117.0(4)	O(3)-Cu(2)-N(2)	84.93(13)
C(7H)-C(2H)-C(3H)	120.1(4)	O(1)-Cu(2)-N(2)	171.11(14)
C(7H)-C(2H)-C(1H)	119.7(4)	O(9)-Cu(2)-O(10)	96.03(12)
C(3H)-C(2H)-C(1H)	120.1(4)	O(3)-Cu(2)-O(10)	92.16(11)
C(2H)-C(3H)-C(4H)	119.8(5)	O(1)-Cu(2)-O(10)	81.14(12)
C(2H)-C(3H)-H(3H)	120.1	N(2)-Cu(2)-O(10)	95.75(14)
C(4H)-C(3H)-H(3H)	120.1	O(9)-Cu(2)-Cu(3)	134.52(9)
C(5H)-C(4H)-C(3H)	119.4(5)	O(3)-Cu(2)-Cu(3)	51.35(8)
C(5H)-C(4H)-H(4H)	120.3	O(1)-Cu(2)-Cu(3)	39.57(8)
C(3H)-C(4H)-H(4H)	120.3	N(2)-Cu(2)-Cu(3)	131.55(11)
C(4H)-C(5H)-C(6H)	121.0(5)	O(10)-Cu(2)-Cu(3)	69.84(8)
C(4H)-C(5H)-H(5H)	119.5	O(11)-Cu(3)-O(4)	177.19(13)
C(6H)-C(5H)-H(5H)	119.5	O(11)-Cu(3)-O(1)	94.56(13)
C(5H)-C(6H)-C(7H)	118.5(5)	O(4)-Cu(3)-O(1)	87.42(12)
C(5H)-C(6H)-H(6H)	120.7	O(11)-Cu(3)-N(3)	91.09(14)
C(7H)-C(6H)-H(6H)	120.7	O(4)-Cu(3)-N(3)	86.61(14)
C(2H)-C(7H)-C(6H)	121.1(5)	O(1)-Cu(3)-N(3)	168.12(13)
C(2H)-C(7H)-H(7H)	119.4	O(11)-Cu(3)-O(3)	105.46(12)
C(6H)-C(7H)-H(7H)	119.4	O(4)-Cu(3)-O(3)	76.92(10)
O(31)-C(1I)-O(30)	126.7(4)	O(1)-Cu(3)-O(3)	76.75(11)
O(31)-C(1I)-C(2I)	117.1(4)	N(3)-Cu(3)-O(3)	111.77(12)
O(30)-C(1I)-C(2I)	116.2(4)	O(11)-Cu(3)-Cu(2)	90.24(10)
C(7I)-C(2I)-C(3I)	119.2(4)	O(4)-Cu(3)-Cu(2)	92.56(9)
C(7I)-C(2I)-C(1I)	121.0(4)	O(1)-Cu(3)-Cu(2)	40.09(8)
C(3I)-C(2I)-C(1I)	119.7(4)	N(3)-Cu(3)-Cu(2)	150.52(10)
C(4I)-C(3I)-C(2I)	120.0(4)	O(3)-Cu(3)-Cu(2)	40.11(7)
C(4I)-C(3I)-H(3I)	120.0	O(25)-Cu(4)-O(7)	79.82(12)
C(2I)-C(3I)-H(3I)	120.0	O(25)-Cu(4)-O(30)	93.78(12)
C(5I)-C(4I)-C(3I)	120.6(5)	O(7)-Cu(4)-O(30)	155.41(13)
C(5I)-C(4I)-H(4I)	119.7	O(25)-Cu(4)-N(6)	162.00(15)
C(3I)-C(4I)-H(4I)	119.7	O(7)-Cu(4)-N(6)	85.63(15)
C(6I)-C(5I)-C(4I)	119.6(4)	O(30)-Cu(4)-N(6)	95.12(15)
C(6I)-C(5I)-H(5I)	120.2	O(25)-Cu(4)-O(18)	96.41(12)
C(4I)-C(5I)-H(5I)	120.2	O(7)-Cu(4)-O(18)	107.93(12)
C(5I)-C(6I)-C(7I)	121.1(4)	O(30)-Cu(4)-O(18)	96.32(13)
C(5I)-C(6I)-H(6I)	119.5	N(6)-Cu(4)-O(18)	98.12(15)
C(7I)-C(6I)-H(6I)	119.5	O(25)-Cu(4)-Ti(4)	39.82(8)
C(2I)-C(7I)-C(6I)	119.4(4)	O(7)-Cu(4)-Ti(4)	43.12(8)
C(2I)-C(7I)-H(7I)	120.3	O(30)-Cu(4)-Ti(4)	120.98(9)
C(6I)-C(7I)-H(7I)	120.3	N(6)-Cu(4)-Ti(4)	122.77(13)
O(12)-Cu(1)-O(1)	93.07(13)	O(18)-Cu(4)-Ti(4)	117.74(9)
O(12)-Cu(1)-O(2)	173.26(13)	O(26)-Cu(5)-O(5)	79.93(12)
O(1)-Cu(1)-O(2)	86.53(12)	O(26)-Cu(5)-O(20)	95.21(11)
O(12)-Cu(1)-N(1)	96.58(15)	O(5)-Cu(5)-O(20)	158.66(13)
O(1)-Cu(1)-N(1)	169.65(14)	O(26)-Cu(5)-N(4)	162.41(14)
O(2)-Cu(1)-N(1)	84.33(14)	O(5)-Cu(5)-N(4)	86.72(14)

O(20)-Cu(5)-N(4)	93.09(14)	C(9C)-N(3)-Cu(3)	106.4(3)
O(26)-Cu(5)-O(14)	96.81(12)	C(10C)-N(3)-Cu(3)	110.8(3)
O(5)-Cu(5)-O(14)	104.62(12)	C(11C)-N(3)-Cu(3)	107.4(3)
O(20)-Cu(5)-O(14)	96.56(12)	C(11D)-N(4)-C(10D)	108.8(4)
N(4)-Cu(5)-O(14)	97.61(14)	C(11D)-N(4)-C(9D)	110.6(4)
O(26)-Cu(5)-Ti(2)	39.33(8)	C(10D)-N(4)-C(9D)	110.4(4)
O(5)-Cu(5)-Ti(2)	43.25(8)	C(11D)-N(4)-Cu(5)	112.9(3)
O(20)-Cu(5)-Ti(2)	124.07(9)	C(10D)-N(4)-Cu(5)	110.1(3)
N(4)-Cu(5)-Ti(2)	124.14(11)	C(9D)-N(4)-Cu(5)	104.0(3)
O(14)-Cu(5)-Ti(2)	115.06(8)	C(11E)-N(5)-C(9E)	111.9(4)
O(24)-Cu(6)-O(22)	94.75(12)	C(11E)-N(5)-C(10E)	107.8(4)
O(24)-Cu(6)-O(6)	79.89(11)	C(9E)-N(5)-C(10E)	109.8(4)
O(22)-Cu(6)-O(6)	156.71(13)	C(11E)-N(5)-Cu(6)	115.2(3)
O(24)-Cu(6)-N(5)	161.23(14)	C(9E)-N(5)-Cu(6)	104.4(2)
O(22)-Cu(6)-N(5)	93.45(13)	C(10E)-N(5)-Cu(6)	107.6(3)
O(6)-Cu(6)-N(5)	85.93(12)	C(10F)-N(6)-C(9F)	111.1(4)
O(24)-Cu(6)-O(16)	99.67(11)	C(10F)-N(6)-C(11F)	109.8(4)
O(22)-Cu(6)-O(16)	95.96(13)	C(9F)-N(6)-C(11F)	109.3(4)
O(6)-Cu(6)-O(16)	107.26(12)	C(10F)-N(6)-Cu(4)	110.2(3)
N(5)-Cu(6)-O(16)	96.23(13)	C(9F)-N(6)-Cu(4)	104.7(3)
O(24)-Cu(6)-Ti(3)	39.47(8)	C(11F)-N(6)-Cu(4)	111.6(3)
O(22)-Cu(6)-Ti(3)	123.17(9)	Cu(3)-O(1)-Cu(1)	115.96(14)
O(6)-Cu(6)-Ti(3)	42.90(8)	Cu(3)-O(1)-Cu(2)	100.34(13)
N(5)-Cu(6)-Ti(3)	122.97(11)	Cu(1)-O(1)-Cu(2)	105.22(14)
O(16)-Cu(6)-Ti(3)	118.34(8)	Cu(3)-O(1)-H(1)	116(3)
C(11Z)-N(1)-C(10A)	111.0(9)	Cu(1)-O(1)-H(1)	103(3)
C(11Z)-N(1)-C(9A)	82.9(6)	Cu(2)-O(1)-H(1)	116(3)
C(10A)-N(1)-C(9A)	114.5(5)	C(8A)-O(2)-C(8Z)	17.0(9)
C(11Z)-N(1)-C(11A)	23.5(6)	C(8A)-O(2)-Cu(1)	109.7(5)
C(10A)-N(1)-C(11A)	109.4(6)	C(8Z)-O(2)-Cu(1)	109.2(8)
C(9A)-N(1)-C(11A)	104.4(5)	C(8A)-O(2)-Ti(1)	114.7(4)
C(11Z)-N(1)-C(10Z)	114.7(9)	C(8Z)-O(2)-Ti(1)	125.8(9)
C(9A)-N(1)-C(10Z)	134.8(6)	Cu(1)-O(2)-Ti(1)	117.37(14)
C(11A)-N(1)-C(10Z)	104.3(8)	C(8B)-O(3)-Cu(2)	107.5(2)
C(11Z)-N(1)-C(9Z)	110.7(7)	C(8B)-O(3)-Ti(1)	123.1(3)
C(10A)-N(1)-C(9Z)	80.7(6)	Cu(2)-O(3)-Ti(1)	111.97(14)
C(9A)-N(1)-C(9Z)	37.6(4)	C(8B)-O(3)-Cu(3)	127.8(3)
C(11A)-N(1)-C(9Z)	134.1(5)	Cu(2)-O(3)-Cu(3)	88.54(10)
C(10Z)-N(1)-C(9Z)	98.6(6)	Ti(1)-O(3)-Cu(3)	92.88(10)
C(11Z)-N(1)-Cu(1)	121.8(7)	C(8C)-O(4)-Cu(3)	108.0(3)
C(10A)-N(1)-Cu(1)	119.4(4)	C(8C)-O(4)-Ti(1)	122.3(2)
C(9A)-N(1)-Cu(1)	100.1(3)	Cu(3)-O(4)-Ti(1)	108.89(13)
C(11A)-N(1)-Cu(1)	107.7(4)	C(8D)-O(5)-Cu(5)	110.8(3)
C(10Z)-N(1)-Cu(1)	103.6(6)	C(8D)-O(5)-Ti(2)	133.6(3)
C(9Z)-N(1)-Cu(1)	104.6(5)	Cu(5)-O(5)-Ti(2)	95.46(12)
C(11B)-N(2)-C(10B)	109.8(4)	C(8E)-O(6)-Cu(6)	111.3(2)
C(11B)-N(2)-C(9B)	111.2(4)	C(8E)-O(6)-Ti(3)	136.0(3)
C(10B)-N(2)-C(9B)	109.4(4)	Cu(6)-O(6)-Ti(3)	95.42(11)
C(11B)-N(2)-Cu(2)	108.9(3)	C(8F)-O(7)-Cu(4)	112.4(3)
C(10B)-N(2)-Cu(2)	110.1(3)	C(8F)-O(7)-Ti(4)	131.9(3)
C(9B)-N(2)-Cu(2)	107.3(3)	Cu(4)-O(7)-Ti(4)	95.52(13)
C(9C)-N(3)-C(10C)	111.5(4)	C(1A)-O(8)-Cu(1)	130.1(3)
C(9C)-N(3)-C(11C)	110.9(3)	C(1A)-O(9)-Cu(2)	126.4(3)
C(10C)-N(3)-C(11C)	109.7(4)	C(1B)-O(10)-Cu(2)	129.2(3)

C(1B)-O(11)-Cu(3)	123.9(3)	O(3)-Ti(1)-Ti(3)	109.69(8)
C(1C)-O(12)-C(1)	33.4(6)	Ti(4)-Ti(1)-Ti(3)	61.74(3)
C(1C)-O(12)-Cu(1)	124.7(4)	O(29)-Ti(1)-Ti(2)	21.68(8)
C(1)-O(12)-Cu(1)	123.3(6)	O(28)-Ti(1)-Ti(2)	80.68(9)
C(1D)-O(14)-Cu(5)	121.9(3)	O(27)-Ti(1)-Ti(2)	80.22(9)
C(1D)-O(15)-Ti(3)	134.9(3)	O(4)-Ti(1)-Ti(2)	106.08(8)
C(1E)-O(16)-Cu(6)	121.6(3)	O(2)-Ti(1)-Ti(2)	107.90(9)
C(1E)-O(17)-Ti(4)	136.8(3)	O(3)-Ti(1)-Ti(2)	167.59(8)
C(1F)-O(18)-Cu(4)	124.4(3)	Ti(4)-Ti(1)-Ti(2)	61.73(3)
C(1F)-O(19)-Ti(2)	133.8(3)	Ti(3)-Ti(1)-Ti(2)	61.68(2)
C(1G)-O(20)-Cu(5)	125.0(3)	O(29)-Ti(2)-O(25)	95.03(13)
C(1G)-O(21)-Ti(3)	131.2(3)	O(29)-Ti(2)-O(26)	94.55(12)
C(1H)-O(22)-Cu(6)	125.7(3)	O(25)-Ti(2)-O(26)	93.81(12)
C(1H)-O(23)-Ti(4)	130.4(3)	O(29)-Ti(2)-O(5)	100.70(13)
C(1I)-O(30)-Cu(4)	126.1(3)	O(25)-Ti(2)-O(5)	162.96(12)
C(1I)-O(31)-Ti(2)	132.4(3)	O(26)-Ti(2)-O(5)	78.53(12)
Ti(4)-O(24)-Cu(6)	121.59(15)	O(29)-Ti(2)-O(19)	91.59(12)
Ti(4)-O(24)-Ti(3)	133.51(15)	O(25)-Ti(2)-O(19)	99.46(12)
Cu(6)-O(24)-Ti(3)	101.29(12)	O(26)-Ti(2)-O(19)	164.83(13)
Ti(2)-O(25)-Ti(4)	133.55(15)	O(5)-Ti(2)-O(19)	86.71(12)
Ti(2)-O(25)-Cu(4)	123.79(14)	O(29)-Ti(2)-O(31)	175.22(13)
Ti(4)-O(25)-Cu(4)	100.35(13)	O(25)-Ti(2)-O(31)	82.90(12)
Ti(3)-O(26)-Ti(2)	133.21(15)	O(26)-Ti(2)-O(31)	89.89(11)
Ti(3)-O(26)-Cu(5)	123.14(14)	O(5)-Ti(2)-O(31)	81.89(12)
Ti(2)-O(26)-Cu(5)	100.83(13)	O(19)-Ti(2)-O(31)	84.52(11)
Ti(3)-O(27)-Ti(1)	134.99(15)	O(29)-Ti(2)-Cu(5)	110.84(10)
Ti(4)-O(28)-Ti(1)	135.22(16)	O(25)-Ti(2)-Cu(5)	126.01(9)
Ti(2)-O(29)-Ti(1)	135.78(15)	O(26)-Ti(2)-Cu(5)	39.84(8)
O(29)-Ti(1)-O(28)	96.01(12)	O(5)-Ti(2)-Cu(5)	41.28(8)
O(29)-Ti(1)-O(27)	94.46(12)	O(19)-Ti(2)-Cu(5)	125.02(9)
O(28)-Ti(1)-O(27)	93.51(12)	O(31)-Ti(2)-Cu(5)	73.76(8)
O(29)-Ti(1)-O(4)	90.17(12)	O(29)-Ti(2)-Ti(1)	22.54(9)
O(28)-Ti(1)-O(4)	92.76(12)	O(25)-Ti(2)-Ti(1)	79.40(9)
O(27)-Ti(1)-O(4)	171.78(11)	O(26)-Ti(2)-Ti(1)	79.55(8)
O(29)-Ti(1)-O(2)	92.18(12)	O(5)-Ti(2)-Ti(1)	113.58(9)
O(28)-Ti(1)-O(2)	171.42(12)	O(19)-Ti(2)-Ti(1)	110.01(9)
O(27)-Ti(1)-O(2)	88.40(12)	O(31)-Ti(2)-Ti(1)	158.66(8)
O(4)-Ti(1)-O(2)	84.64(11)	Cu(5)-Ti(2)-Ti(1)	107.54(3)
O(29)-Ti(1)-O(3)	170.25(11)	O(27)-Ti(3)-O(26)	96.31(12)
O(28)-Ti(1)-O(3)	89.09(12)	O(27)-Ti(3)-O(24)	95.18(12)
O(27)-Ti(1)-O(3)	93.51(11)	O(26)-Ti(3)-O(24)	92.39(12)
O(4)-Ti(1)-O(3)	81.27(11)	O(27)-Ti(3)-O(6)	99.21(12)
O(2)-Ti(1)-O(3)	82.43(12)	O(26)-Ti(3)-O(6)	162.62(11)
O(29)-Ti(1)-Ti(4)	80.21(9)	O(24)-Ti(3)-O(6)	78.50(11)
O(28)-Ti(1)-Ti(4)	21.89(8)	O(27)-Ti(3)-O(15)	92.06(12)
O(27)-Ti(1)-Ti(4)	79.77(8)	O(26)-Ti(3)-O(15)	97.26(12)
O(4)-Ti(1)-Ti(4)	107.75(8)	O(24)-Ti(3)-O(15)	167.24(11)
O(2)-Ti(1)-Ti(4)	165.32(9)	O(6)-Ti(3)-O(15)	89.98(11)
O(3)-Ti(1)-Ti(4)	106.78(8)	O(27)-Ti(3)-O(21)	175.48(12)
O(29)-Ti(1)-Ti(3)	79.49(9)	O(26)-Ti(3)-O(21)	82.65(11)
O(28)-Ti(1)-Ti(3)	79.42(9)	O(24)-Ti(3)-O(21)	89.27(11)
O(27)-Ti(1)-Ti(3)	21.84(8)	O(6)-Ti(3)-O(21)	82.47(11)
O(4)-Ti(1)-Ti(3)	166.22(8)	O(15)-Ti(3)-O(21)	83.73(11)
O(2)-Ti(1)-Ti(3)	104.68(9)	O(27)-Ti(3)-Cu(6)	109.92(10)

O(26)-Ti(3)-Cu(6)	124.62(9)	O(25)-Ti(4)-O(17)	165.12(12)
O(24)-Ti(3)-Cu(6)	39.24(8)	O(7)-Ti(4)-O(17)	87.79(12)
O(6)-Ti(3)-Cu(6)	41.68(8)	O(28)-Ti(4)-O(23)	174.78(12)
O(15)-Ti(3)-Cu(6)	128.12(8)	O(24)-Ti(4)-O(23)	83.28(11)
O(21)-Ti(3)-Cu(6)	74.13(8)	O(25)-Ti(4)-O(23)	89.71(11)
O(27)-Ti(3)-Ti(1)	23.17(8)	O(7)-Ti(4)-O(23)	82.57(11)
O(26)-Ti(3)-Ti(1)	80.09(9)	O(17)-Ti(4)-O(23)	83.57(12)
O(24)-Ti(3)-Ti(1)	79.46(8)	O(28)-Ti(4)-Cu(4)	111.65(9)
O(6)-Ti(3)-Ti(1)	112.20(8)	O(24)-Ti(4)-Cu(4)	125.24(9)
O(15)-Ti(3)-Ti(1)	110.37(8)	O(25)-Ti(4)-Cu(4)	39.83(8)
O(21)-Ti(3)-Ti(1)	158.91(8)	O(7)-Ti(4)-Cu(4)	41.37(8)
Cu(6)-Ti(3)-Ti(1)	106.20(4)	O(17)-Ti(4)-Cu(4)	125.29(9)
O(28)-Ti(4)-O(24)	95.08(12)	O(23)-Ti(4)-Cu(4)	73.18(8)
O(28)-Ti(4)-O(25)	95.33(12)	O(28)-Ti(4)-Ti(1)	22.89(9)
O(24)-Ti(4)-O(25)	93.14(12)	O(24)-Ti(4)-Ti(1)	80.25(9)
O(28)-Ti(4)-O(7)	99.75(12)	O(25)-Ti(4)-Ti(1)	78.88(8)
O(24)-Ti(4)-O(7)	163.39(12)	O(7)-Ti(4)-Ti(1)	111.35(9)
O(25)-Ti(4)-O(7)	78.16(12)	O(17)-Ti(4)-Ti(1)	111.27(9)
O(28)-Ti(4)-O(17)	91.83(12)	O(23)-Ti(4)-Ti(1)	159.34(8)
O(24)-Ti(4)-O(17)	99.21(12)	Cu(4)-Ti(4)-Ti(1)	106.67(4)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 06mz171m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(h\,a^*)^2 U11 + ... + 2\,h\,k\,a^*\,b^*\,U12]$

	U11	U22	U33	U23	U13	U12
C(1A)	26(2)	23(3)	33(3)	3(2)	4(2)	1(2)
C(2A)	18(2)	29(3)	31(2)	5(2)	4(2)	-2(2)
C(3A)	25(3)	32(3)	56(3)	11(2)	7(2)	-4(2)
C(4A)	27(3)	41(3)	85(4)	38(3)	-4(3)	-5(2)
C(5A)	24(3)	39(3)	96(5)	25(3)	2(3)	2(2)
C(6A)	22(3)	45(3)	77(4)	8(3)	16(3)	0(2)
C(7A)	35(3)	34(3)	41(3)	10(2)	1(2)	-1(2)
C(8A)	11(7)	20(3)	23(3)	6(2)	2(4)	0(3)
C(9A)	31(5)	28(4)	36(4)	17(4)	15(4)	8(4)
C(10A)	32(2)	21(4)	40(4)	5(3)	4(3)	-5(3)
C(11A)	32(2)	21(4)	40(4)	5(3)	4(3)	-5(3)
C(8Z)	11(7)	20(3)	23(3)	6(2)	2(4)	0(3)
C(9Z)	33(7)	35(7)	42(7)	28(6)	4(6)	18(6)
C(10Z)	32(2)	21(4)	40(4)	5(3)	4(3)	-5(3)
C(11Z)	32(2)	21(4)	40(4)	5(3)	4(3)	-5(3)
C(1B)	23(2)	24(3)	37(3)	3(2)	2(2)	-2(2)
C(2B)	32(3)	25(3)	35(3)	3(2)	2(2)	-3(2)
C(3B)	34(3)	31(3)	107(5)	2(3)	8(3)	-1(3)
C(4B)	37(3)	51(4)	117(6)	20(4)	18(4)	-5(3)
C(5B)	47(3)	50(4)	42(3)	5(3)	1(3)	-29(3)

C(6B)	82(5)	42(4)	72(4)	-30(3)	42(4)	-34(3)
C(7B)	51(3)	46(4)	65(4)	-15(3)	35(3)	-18(3)
C(8B)	33(3)	40(3)	29(2)	17(2)	9(2)	2(2)
C(9B)	37(3)	51(3)	26(2)	12(2)	9(2)	1(2)
C(10B)	60(3)	39(3)	34(3)	-4(2)	16(3)	4(3)
C(11B)	36(3)	54(4)	35(3)	10(2)	17(2)	-2(3)
C(1)	33(5)	21(6)	40(4)	-9(4)	-4(3)	-10(4)
C(2)	54(3)	28(4)	37(4)	10(3)	6(3)	-4(3)
C(3)	66(5)	74(7)	28(3)	12(4)	-4(3)	0(5)
C(4)	73(8)	93(13)	41(5)	3(8)	-5(5)	-3(7)
C(5)	163(13)	80(11)	28(4)	28(5)	11(6)	20(10)
C(6)	146(9)	36(4)	40(6)	13(4)	39(6)	18(5)
C(7)	76(5)	22(7)	33(7)	18(3)	22(4)	6(4)
C(1C)	33(5)	21(6)	40(4)	-9(4)	-4(3)	-10(4)
C(2C)	54(3)	28(4)	37(4)	10(3)	6(3)	-4(3)
C(3C)	66(5)	74(7)	28(3)	12(4)	-4(3)	0(5)
C(4C)	73(8)	93(13)	41(5)	3(8)	-5(5)	-3(7)
C(5C)	163(13)	80(11)	28(4)	28(5)	11(6)	20(10)
C(6C)	146(9)	36(4)	40(6)	13(4)	39(6)	18(5)
C(7C)	76(5)	22(7)	33(7)	18(3)	22(4)	6(4)
C(8C)	20(2)	46(3)	31(3)	-2(2)	6(2)	-4(2)
C(9C)	27(2)	36(3)	29(2)	-5(2)	2(2)	5(2)
C(10C)	61(4)	41(3)	36(3)	8(2)	12(3)	5(3)
C(11C)	37(3)	37(3)	35(3)	-13(2)	10(2)	-4(2)
C(1D)	24(2)	23(2)	22(2)	0(2)	1(2)	1(2)
C(2D)	36(3)	37(3)	26(2)	13(2)	6(2)	12(2)
C(3D)	86(5)	91(5)	92(5)	63(4)	60(4)	60(4)
C(4D)	144(8)	101(7)	141(8)	87(6)	87(7)	85(6)
C(5D)	94(6)	140(8)	102(6)	80(6)	59(5)	79(6)
C(6D)	41(3)	72(4)	55(4)	25(3)	17(3)	20(3)
C(7D)	25(2)	35(3)	32(3)	0(2)	1(2)	-3(2)
C(8D)	53(3)	37(3)	28(3)	10(2)	5(2)	-16(2)
C(9D)	74(4)	36(3)	31(3)	15(2)	4(3)	-9(3)
C(10D)	49(3)	39(3)	39(3)	12(2)	10(2)	-13(3)
C(11D)	51(3)	26(3)	57(3)	13(3)	10(3)	-1(2)
C(1E)	27(2)	32(3)	29(2)	12(2)	4(2)	3(2)
C(2E)	50(3)	28(3)	49(3)	14(2)	16(3)	5(2)
C(3E)	112(6)	37(4)	86(5)	27(3)	58(4)	20(4)
C(4E)	197(10)	55(5)	115(7)	47(5)	91(7)	10(6)
C(5E)	173(9)	32(4)	142(8)	31(5)	82(7)	12(5)
C(6E)	106(6)	28(3)	88(5)	10(3)	38(4)	12(3)
C(7E)	50(3)	25(3)	55(3)	13(2)	18(3)	5(2)
C(8E)	29(2)	33(3)	21(2)	4(2)	6(2)	4(2)
C(9E)	38(3)	51(3)	26(2)	8(2)	15(2)	10(2)
C(10E)	40(3)	55(4)	25(3)	-5(2)	5(2)	6(3)
C(11E)	76(4)	52(4)	34(3)	25(3)	20(3)	21(3)
C(1F)	30(3)	30(3)	25(2)	-2(2)	8(2)	-19(2)
C(2F)	66(4)	32(3)	22(2)	-1(2)	16(2)	-19(3)
C(3F)	149(7)	33(3)	45(3)	7(3)	56(4)	12(4)
C(4F)	205(9)	35(4)	57(4)	8(3)	80(5)	2(5)
C(5F)	174(8)	67(5)	29(3)	-7(3)	43(4)	-30(5)
C(6F)	101(5)	64(5)	37(3)	16(3)	-1(3)	-28(4)
C(7F)	57(4)	63(4)	24(3)	9(3)	6(2)	-20(3)
C(8F)	40(3)	34(3)	38(3)	8(2)	13(2)	15(2)
C(9F)	48(3)	41(3)	42(3)	4(2)	17(2)	17(3)
C(10F)	54(4)	66(5)	82(5)	-9(4)	-16(3)	25(3)
C(11F)	61(4)	55(4)	88(5)	2(4)	45(4)	19(3)

C(1G)	25(2)	22(2)	20(2)	-3(2)	7(2)	4(2)
C(2G)	17(2)	42(3)	16(2)	4(2)	3(2)	-5(2)
C(3G)	26(2)	44(3)	31(3)	0(2)	13(2)	-4(2)
C(4G)	34(3)	56(4)	36(3)	-12(3)	12(2)	-20(3)
C(5G)	36(3)	83(5)	37(3)	12(3)	-9(2)	-19(3)
C(6G)	38(3)	76(5)	47(3)	34(3)	-6(3)	-12(3)
C(7G)	30(3)	50(3)	32(3)	12(2)	-2(2)	-6(2)
C(1H)	28(2)	28(3)	28(2)	11(2)	2(2)	6(2)
C(2H)	29(2)	36(3)	21(2)	4(2)	0(2)	5(2)
C(3H)	31(3)	51(3)	29(3)	6(2)	7(2)	8(2)
C(4H)	35(3)	81(4)	28(3)	10(3)	-6(2)	12(3)
C(5H)	31(3)	79(5)	41(3)	6(3)	-7(2)	-9(3)
C(6H)	34(3)	72(4)	36(3)	5(3)	5(2)	-16(3)
C(7H)	38(3)	52(4)	29(3)	-1(2)	-3(2)	-3(3)
C(1I)	27(3)	38(3)	25(2)	-1(2)	9(2)	-8(2)
C(2I)	26(2)	30(3)	30(2)	0(2)	7(2)	-1(2)
C(3I)	22(2)	42(3)	32(3)	-4(2)	8(2)	-3(2)
C(4I)	34(3)	56(4)	34(3)	-12(3)	9(2)	3(3)
C(5I)	25(3)	56(4)	42(3)	-16(3)	-1(2)	-2(2)
C(6I)	17(2)	56(4)	51(3)	-7(3)	5(2)	1(2)
C(7I)	26(3)	49(3)	38(3)	-6(2)	8(2)	1(2)
Cu(1)	26(1)	30(1)	25(1)	7(1)	4(1)	-1(1)
Cu(2)	24(1)	27(1)	24(1)	5(1)	4(1)	1(1)
Cu(3)	25(1)	23(1)	31(1)	-2(1)	8(1)	-3(1)
Cu(4)	25(1)	27(1)	26(1)	-2(1)	8(1)	0(1)
Cu(5)	27(1)	21(1)	22(1)	5(1)	3(1)	-3(1)
Cu(6)	26(1)	24(1)	18(1)	4(1)	6(1)	3(1)
N(1)	56(3)	34(3)	34(2)	8(2)	23(2)	-8(2)
N(2)	32(2)	35(2)	25(2)	3(2)	7(2)	6(2)
N(3)	35(2)	24(2)	21(2)	-3(2)	6(2)	-5(2)
N(4)	37(2)	25(2)	32(2)	6(2)	4(2)	-6(2)
N(5)	29(2)	34(2)	20(2)	7(2)	4(2)	8(2)
N(6)	31(2)	40(3)	50(3)	-3(2)	15(2)	5(2)
O(1)	23(2)	28(2)	20(2)	3(1)	-3(1)	-5(1)
O(2)	29(2)	22(2)	28(2)	5(1)	-2(1)	-1(1)
O(3)	22(2)	25(2)	24(2)	1(1)	5(1)	-5(1)
O(4)	22(2)	29(2)	24(2)	0(1)	6(1)	0(1)
O(5)	40(2)	23(2)	20(2)	7(1)	5(1)	-5(1)
O(6)	22(2)	21(2)	17(1)	1(1)	5(1)	1(1)
O(7)	28(2)	24(2)	24(2)	3(1)	11(1)	6(1)
O(8)	28(2)	41(2)	43(2)	17(2)	12(2)	6(2)
O(9)	32(2)	32(2)	31(2)	9(2)	6(1)	5(1)
O(10)	27(2)	23(2)	47(2)	-3(2)	11(2)	-5(1)
O(11)	32(2)	29(2)	52(2)	-3(2)	14(2)	-2(2)
O(12)	56(2)	47(2)	25(2)	8(2)	13(2)	11(2)
O(13)	42(4)	65(5)	34(3)	-8(3)	4(3)	10(3)
O(14)	30(2)	30(2)	27(2)	12(1)	6(1)	3(1)
O(15)	26(2)	23(2)	24(2)	4(1)	6(1)	1(1)
O(16)	42(2)	22(2)	32(2)	5(1)	16(2)	2(2)
O(17)	33(2)	22(2)	26(2)	5(1)	7(1)	2(1)
O(18)	50(2)	33(2)	26(2)	1(2)	16(2)	-8(2)
O(19)	34(2)	30(2)	21(2)	2(1)	5(1)	-7(1)
O(20)	38(2)	21(2)	20(2)	4(1)	1(1)	-5(1)
O(21)	29(2)	24(2)	19(2)	3(1)	2(1)	-5(1)
O(22)	29(2)	42(2)	25(2)	11(2)	8(1)	5(2)
O(23)	25(2)	30(2)	23(2)	1(1)	3(1)	4(1)
O(30)	26(2)	31(2)	44(2)	-7(2)	13(2)	-3(1)

O(31)	26(2)	25(2)	25(2)	3(1)	3(1)	-5(1)
O(32)	84(8)	56(7)	19(5)	-12(4)	-3(4)	31(6)
O(24)	22(2)	22(2)	20(1)	3(1)	7(1)	-2(1)
O(25)	23(2)	24(2)	17(1)	1(1)	7(1)	0(1)
O(26)	25(2)	19(2)	20(1)	4(1)	4(1)	-3(1)
O(27)	19(1)	21(2)	21(1)	2(1)	4(1)	1(1)
O(28)	25(2)	23(2)	21(2)	1(1)	6(1)	-2(1)
O(29)	26(2)	21(2)	20(1)	6(1)	0(1)	-4(1)
Ti(1)	21(1)	21(1)	22(1)	3(1)	0(1)	-2(1)
Ti(2)	24(1)	23(1)	18(1)	3(1)	4(1)	-4(1)
Ti(3)	22(1)	19(1)	19(1)	3(1)	5(1)	0(1)
Ti(4)	23(1)	22(1)	18(1)	2(1)	5(1)	2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for 06mz171m.

	x	y	z	U(eq)
H(3A)	5298	4045	-60	46
H(4A)	3979	4492	-276	59
H(5A)	2967	4183	269	63
H(6A)	3263	3476	1066	58
H(7A)	4598	3084	1323	44
H(8A1)	8964	4224	1520	22
H(8A2)	8123	4353	1794	22
H(9A1)	7390	4458	821	35
H(9A2)	8246	4991	907	35
H(10A)	9116	3662	-191	48
H(10B)	9391	3805	563	48
H(10C)	9207	4544	241	48
H(11A)	7841	4683	-304	48
H(11B)	7080	4128	-222	48
H(11C)	7704	3771	-678	48
H(8Z1)	8362	4331	1902	22
H(8Z2)	7524	4237	1376	22
H(9Z1)	9185	4246	1099	40
H(9Z2)	8586	4946	1035	40
H(10T)	8883	3356	-389	48
H(10U)	9344	3414	326	48
H(10V)	9331	4185	29	48
H(11T)	8091	4875	-26	48
H(11U)	7276	4549	180	48
H(11V)	7536	4117	-473	48
H(3B)	4868	318	1042	72
H(4B)	3901	-761	839	81
H(5B)	4262	-2044	463	59
H(6B)	5597	-2214	274	84
H(7B)	6547	-1112	449	67
H(8B1)	8545	1595	2584	39
H(8B2)	7623	1206	2279	39

H(9B1)	8080	2796	2975	44
H(9B2)	7485	2150	3152	44
H(10D)	6432	3698	2410	67
H(10E)	7424	3765	2562	67
H(10F)	6909	3650	3099	67
H(11D)	6063	2423	2955	61
H(11E)	6156	1672	2408	61
H(11F)	5669	2401	2231	61
H(3)	6359	2030	-1583	69
H(4C)	6059	1716	-2695	88
H(5)	7027	1108	-3273	106
H(6)	8294	814	-2738	85
H(7)	8593	1128	-1626	48
H(3C)	6299	1763	-1516	69
H(4C1)	5777	1127	-2574	88
H(5C)	6688	696	-3267	106
H(6C)	8120	900	-2903	85
H(7C)	8642	1536	-1846	48
H(8C1)	10049	1812	686	41
H(8C2)	9384	1317	96	41
H(9C1)	10005	380	592	39
H(9C2)	9905	873	1280	39
H(10G)	8250	-410	1232	69
H(10H)	8922	247	1692	69
H(10I)	9217	-530	1271	69
H(11G)	8975	-735	130	59
H(11H)	8686	-32	-209	59
H(11I)	8033	-513	66	59
H(3D)	8720	6809	2737	91
H(4D)	7648	7567	2999	132
H(5D)	6607	7037	3451	116
H(6D)	6690	5755	3631	63
H(7D)	7851	5087	3489	39
H(8D1)	11067	5164	939	48
H(8D2)	11859	5200	1489	48
H(9D1)	11510	6514	1543	56
H(9D2)	10557	6266	1541	56
H(10J)	12467	6847	2501	63
H(10K)	12477	5911	2464	63
H(10L)	12335	6498	3102	63
H(11J)	11067	7093	3149	67
H(11K)	10343	6948	2538	67
H(11L)	11177	7474	2559	67
H(3E)	9380	442	4207	85
H(4E)	9075	-872	4228	133
H(5E)	9299	-1905	3399	129
H(6E)	9786	-1585	2528	86
H(7E)	10176	-264	2541	50
H(8E1)	8670	4058	4331	33
H(8E2)	9608	4432	4595	33
H(9E1)	9294	3646	5291	45
H(9E2)	8952	2907	4710	45
H(10M)	10711	3957	5679	63
H(10N)	10826	4180	5024	63
H(10O)	11392	3555	5299	63
H(11M)	10207	2613	5662	75
H(11N)	10865	2260	5236	75

H(11O)	9899	1988	5001	75
H(3F)	12385	1923	-160	85
H(4F)	12488	1945	-1196	112
H(5F)	11736	2818	-1695	109
H(6F)	10913	3704	-1165	83
H(7F)	10872	3723	-90	59
H(8F1)	11444	199	2023	44
H(8F2)	12108	762	2582	44
H(9F1)	12850	177	1791	51
H(9F2)	12200	426	1247	51
H(10P)	13331	1506	2750	111
H(10Q)	13923	2011	2443	111
H(10R)	13984	1073	2356	111
H(11P)	13762	923	1195	99
H(11Q)	13720	1865	1301	99
H(11R)	12974	1281	850	99
H(3G)	12172	6575	4452	41
H(4G)	13306	6878	5296	55
H(5G)	13887	5879	5732	66
H(6G)	13365	4563	5327	63
H(7G)	12170	4260	4539	46
H(3H)	12768	2520	5059	45
H(4H)	14167	2807	5559	59
H(5H)	15137	3193	4997	64
H(6H)	14749	3229	3927	59
H(7H)	13363	2884	3428	51
H(3I)	12836	5039	3305	40
H(4I)	13921	5774	4057	53
H(5I)	15283	5532	3986	55
H(6I)	15569	4557	3167	53
H(7I)	14498	3740	2454	48
H(1)	6814(18)	1780(30)	338(16)	30

Numerical data for Complex 2

Table 2. Atomic coordinates [× 10^4] and equivalent isotropic displacement parameters [Å^2 × 10^3] for 06mz069m. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	7850(2)	5005(2)	6580(1)	40(1)
C(2)	7379(2)	5432(2)	6570(1)	46(1)
C(3)	6239(2)	5354(3)	6791(1)	61(1)
C(4)	7488(2)	5998(2)	7010(1)	48(1)
C(5)	6796(2)	5877(2)	5762(1)	36(1)
C(6)	7562(2)	6578(2)	5671(1)	40(1)
C(7)	8804(2)	6932(2)	5457(1)	47(1)
C(8)	7589(2)	6126(2)	5223(1)	42(1)
C(9)	5559(2)	3858(2)	5293(1)	28(1)
C(10)	5703(2)	4105(2)	5007(1)	32(1)
C(11)	6436(2)	4300(2)	4901(1)	42(1)
C(12)	6605(3)	4496(3)	4637(1)	60(1)
C(13)	6043(3)	4529(2)	4479(1)	63(1)
C(14)	5334(3)	4363(2)	4582(1)	56(1)
C(15)	5136(2)	4132(2)	4848(1)	41(1)
C(16)	4346(2)	3950(2)	4956(1)	57(1)
C(10B)	5459(8)	4150(7)	5049(1)	32(1)
C(11B)	4826(10)	4184(8)	4942(1)	42(1)
C(12B)	4877(13)	4479(11)	4688(1)	60(1)
C(13B)	5561(14)	4740(11)	4541(1)	63(1)
C(14B)	6194(12)	4706(10)	4648(2)	56(1)
C(15B)	6143(10)	4411(8)	4902(2)	41(1)
C(16B)	6806(8)	4306(8)	5006(2)	57(1)
C(17)	4603(2)	3789(2)	5958(1)	31(1)
C(18)	4196(1)	4167(2)	6097(1)	38(1)
C(19)	4606(2)	4692(2)	6297(1)	70(1)
C(20)	4268(5)	5044(4)	6445(1)	103(2)
C(21)	3517(4)	4871(4)	6384(1)	99(2)
C(22)	3117(3)	4375(3)	6179(1)	76(2)
C(23)	3443(2)	4005(2)	6030(1)	48(1)
C(24)	2992(2)	3513(2)	5808(1)	64(1)
Cu(1)	6802(1)	4320(1)	6988(1)	32(1)
C(25)	5451(3)	3862(3)	7306(1)	51(1)
O(11)	6149(2)	4386(2)	7260(1)	49(1)
O(12)	5097(2)	3170(2)	7216(1)	51(1)
C(26)	5030(2)	4117(2)	7489(1)	57(1)
C(27)	5269(2)	4290(2)	7751(1)	71(2)
C(28)	4886(2)	4543(2)	7921(1)	78(2)
C(29)	4263(2)	4622(2)	7829(1)	77(2)
C(30)	4024(2)	4448(2)	7567(1)	65(1)
C(31)	4407(2)	4196(2)	7397(1)	63(1)
C(32)	4101(4)	3963(5)	7115(1)	80(2)
Cu(1B)	6538(3)	4209(2)	6874(1)	32(1)
C(25B)	5230(20)	3820(30)	7219(6)	51(1)
O(11B)	5795(14)	4294(14)	7093(5)	49(1)
O(12B)	5200(20)	3110(20)	7281(7)	51(1)

C(26B)	4689(16)	4084(17)	7303(6)	57(1)
C(27B)	4210(20)	4040(20)	7094(5)	71(2)
C(28B)	3669(19)	4300(20)	7130(6)	78(2)
C(29B)	3608(16)	4585(19)	7374(7)	77(2)
C(30B)	4090(20)	4620(20)	7582(5)	65(1)
C(31B)	4627(17)	4374(18)	7547(5)	63(1)
C(32B)	5140(40)	4400(40)	7776(8)	80(2)
O(3)	6667	3333	7115(1)	33(1)
Ti(2)	6292(1)	4110(1)	5868(1)	23(1)
Ti(1)	6667	3333	6408(1)	28(1)
Cu(2)	7814(1)	5299(1)	5646(1)	27(1)
N(1)	6995(2)	5350(2)	6830(1)	40(1)
N(2)	7974(2)	6315(1)	5486(1)	35(1)
O(1)	7338(1)	4226(1)	6674(1)	31(1)
O(2)	6966(1)	5298(1)	5853(1)	28(1)
O(5)	6376(1)	3955(1)	6214(1)	26(1)
O(6)	7295(1)	4239(1)	5777(1)	23(1)
O(7)	8317(1)	5080(1)	5345(1)	33(1)
O(8)	8872(1)	5786(1)	5896(1)	35(1)
O(9)	6095(1)	4274(1)	5453(1)	28(1)
O(10)	5340(1)	4236(1)	5925(1)	33(1)

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 3. Bond lengths [Å] and angles [deg] for 06mz069m.

C(1)-O(1)	1.431(4)	C(5)-H(5B)	0.9900
C(1)-C(2)	1.532(5)	C(6)-N(2)	1.487(4)
C(1)-H(1A)	0.9900	C(6)-H(6A)	0.9900
C(1)-H(1B)	0.9900	C(6)-H(6B)	0.9900
C(2)-N(1)	1.484(4)	C(7)-N(2)	1.475(4)
C(2)-H(2A)	0.9900	C(7)-H(7A)	0.9800
C(2)-H(2B)	0.9900	C(7)-H(7B)	0.9800
C(3)-N(1)	1.503(5)	C(7)-H(7C)	0.9800
C(3)-H(3A)	0.9800	C(8)-N(2)	1.484(4)
C(3)-H(3B)	0.9800	C(8)-H(8A)	0.9800
C(3)-H(3C)	0.9800	C(8)-H(8B)	0.9800
C(4)-N(1)	1.469(4)	C(8)-H(8C)	0.9800
C(4)-H(4A)	0.9800	C(9)-O(9)	1.254(3)
C(4)-H(4B)	0.9800	C(9)-O(7)#1	1.267(3)
C(4)-H(4C)	0.9800	C(9)-C(10B)	1.417(9)
C(5)-O(2)	1.415(3)	C(9)-C(10)	1.508(4)
C(5)-C(6)	1.520(4)	C(10)-C(15)	1.396(4)
C(5)-H(5A)	0.9900	C(10)-C(11)	1.399(5)

C(11)-C(12)	1.384(5)	C(28)-C(29)	1.3900
C(11)-H(11)	0.9500	C(28)-H(28)	0.9500
C(12)-C(13)	1.391(7)	C(29)-C(30)	1.3900
C(12)-H(12)	0.9500	C(29)-H(29)	0.9500
C(13)-C(14)	1.368(7)	C(30)-C(31)	1.3900
C(13)-H(13)	0.9500	C(30)-H(30)	0.9500
C(14)-C(15)	1.405(5)	C(31)-C(32)	1.523(5)
C(14)-H(14)	0.9500	C(32)-H(32A)	0.9800
C(15)-C(16)	1.515(5)	C(32)-H(32B)	0.9800
C(16)-H(16A)	0.9800	C(32)-H(32C)	0.9800
C(16)-H(16B)	0.9800	Cu(1B)-O(1)	1.857(4)
C(16)-H(16C)	0.9800	Cu(1B)-O(11B)	1.905(15)
C(10B)-C(11B)	1.3900	Cu(1B)-N(1)	1.971(5)
C(10B)-C(15B)	1.3900	Cu(1B)-O(1)#1	2.165(5)
C(11B)-C(12B)	1.3900	Cu(1B)-O(3)	2.225(5)
C(11B)-H(11B)	0.9500	Cu(1B)-Ti(1)	3.002(4)
C(12B)-C(13B)	1.3900	C(25B)-O(11B)	1.21(5)
C(12B)-H(12B)	0.9500	C(25B)-O(12B)	1.40(6)
C(13B)-C(14B)	1.3900	C(25B)-C(26B)	1.470(16)
C(13B)-H(13B)	0.9500	C(26B)-C(27B)	1.3900
C(14B)-C(15B)	1.3900	C(26B)-C(31B)	1.3900
C(14B)-H(14B)	0.9500	C(27B)-C(28B)	1.3900
C(15B)-C(16B)	1.5120	C(27B)-H(27B)	0.9500
C(16B)-H(16D)	0.9800	C(28B)-C(29B)	1.3900
C(16B)-H(16E)	0.9800	C(28B)-H(28B)	0.9500
C(16B)-H(16F)	0.9800	C(29B)-C(30B)	1.3900
C(17)-O(8)#1	1.241(3)	C(29B)-H(29B)	0.9500
C(17)-O(10)	1.277(3)	C(30B)-C(31B)	1.3900
C(17)-C(18)	1.5109	C(30B)-H(30B)	0.9500
C(18)-C(19)	1.3830	C(31B)-C(32B)	1.515(8)
C(18)-C(23)	1.393(4)	C(32B)-H(32D)	0.9800
C(19)-C(20)	1.392(6)	C(32B)-H(32E)	0.9800
C(19)-H(19)	0.9500	C(32B)-H(32F)	0.9800
C(20)-C(21)	1.375(10)	O(3)-Cu(1)#2	1.9320(12)
C(20)-H(20)	0.9500	O(3)-Cu(1)#1	1.9320(12)
C(21)-C(22)	1.368(9)	O(3)-Cu(1B)#2	2.225(5)
C(21)-H(21)	0.9500	O(3)-Cu(1B)#1	2.225(5)
C(22)-C(23)	1.406(6)	O(3)-H(3)	0.83(2)
C(22)-H(22)	0.9500	Ti(2)-O(5)	1.7958(19)
C(23)-C(24)	1.457(6)	Ti(2)-O(6)#1	1.8554(18)
C(24)-H(24A)	0.9800	Ti(2)-O(6)	1.9150(18)
C(24)-H(24B)	0.9800	Ti(2)-O(10)	2.029(2)
C(24)-H(24C)	0.9800	Ti(2)-O(2)	2.0319(19)
Cu(1)-O(11)	1.931(3)	Ti(2)-O(9)	2.1840(19)
Cu(1)-O(3)	1.9320(12)	Ti(2)-Cu(2)	2.9499(6)
Cu(1)-O(1)	1.962(2)	Ti(2)-Ti(1)	3.3835(8)
Cu(1)-N(1)	2.032(3)	Ti(1)-O(5)#2	1.8677(19)
C(25)-O(11)	1.259(6)	Ti(1)-O(5)#1	1.8677(19)
C(25)-O(12)	1.263(6)	Ti(1)-O(5)	1.8677(19)
C(25)-C(26)	1.488(4)	Ti(1)-O(1)#2	2.078(2)
C(26)-C(27)	1.3900	Ti(1)-O(1)	2.078(2)
C(26)-C(31)	1.3900	Ti(1)-O(1)#1	2.078(2)
C(27)-C(28)	1.3900	Ti(1)-Cu(1B)#2	3.002(4)
C(27)-H(27)	0.9500	Ti(1)-Cu(1B)#1	3.002(4)

Ti(1)-Ti(2)#1	3.3835(8)	N(2)-C(8)-H(8A)	109.5
Ti(1)-Ti(2)#2	3.3835(8)	N(2)-C(8)-H(8B)	109.5
Cu(2)-O(6)	1.9242(17)	H(8A)-C(8)-H(8B)	109.5
Cu(2)-O(2)	1.9688(19)	N(2)-C(8)-H(8C)	109.5
Cu(2)-O(7)	1.976(2)	H(8A)-C(8)-H(8C)	109.5
Cu(2)-N(2)	2.029(2)	H(8B)-C(8)-H(8C)	109.5
Cu(2)-O(8)	2.203(2)	O(9)-C(9)-O(7)#1	127.0(3)
O(1)-Cu(1B)#2	2.165(5)	O(9)-C(9)-C(10B)	122.7(6)
O(6)-Ti(2)#2	1.8554(17)	O(7)#1-C(9)-C(10B)	107.4(6)
O(7)-C(9)#2	1.267(3)	O(9)-C(9)-C(10)	116.6(2)
O(8)-C(17)#2	1.24(2)	O(7)#1-C(9)-C(10)	116.4(2)
		C(15)-C(10)-C(11)	120.3(3)
O(1)-C(1)-C(2)	107.8(3)	C(15)-C(10)-C(9)	122.6(3)
O(1)-C(1)-H(1A)	110.2	C(11)-C(10)-C(9)	117.1(3)
C(2)-C(1)-H(1A)	110.2	C(12)-C(11)-C(10)	120.9(4)
O(1)-C(1)-H(1B)	110.2	C(12)-C(11)-H(11)	119.5
C(2)-C(1)-H(1B)	110.2	C(10)-C(11)-H(11)	119.5
H(1A)-C(1)-H(1B)	108.5	C(11)-C(12)-C(13)	118.7(4)
N(1)-C(2)-C(1)	109.0(3)	C(11)-C(12)-H(12)	120.6
N(1)-C(2)-H(2A)	109.9	C(13)-C(12)-H(12)	120.6
C(1)-C(2)-H(2A)	109.9	C(14)-C(13)-C(12)	120.6(4)
N(1)-C(2)-H(2B)	109.9	C(14)-C(13)-H(13)	119.7
C(1)-C(2)-H(2B)	109.9	C(12)-C(13)-H(13)	119.7
H(2A)-C(2)-H(2B)	108.3	C(13)-C(14)-C(15)	121.7(4)
N(1)-C(3)-H(3A)	109.5	C(13)-C(14)-H(14)	119.1
N(1)-C(3)-H(3B)	109.5	C(15)-C(14)-H(14)	119.1
H(3A)-C(3)-H(3B)	109.5	C(10)-C(15)-C(14)	117.6(4)
N(1)-C(3)-H(3C)	109.5	C(10)-C(15)-C(16)	121.9(3)
H(3A)-C(3)-H(3C)	109.5	C(14)-C(15)-C(16)	120.5(3)
H(3B)-C(3)-H(3C)	109.5	C(11B)-C(10B)-C(15B)	120.0
N(1)-C(4)-H(4A)	109.5	C(11B)-C(10B)-C(9)	131.9(3)
N(1)-C(4)-H(4B)	109.5	C(15B)-C(10B)-C(9)	108.1(3)
H(4A)-C(4)-H(4B)	109.5	C(10B)-C(11B)-C(12B)	120.0
N(1)-C(4)-H(4C)	109.5	C(10B)-C(11B)-H(11B)	120.0
H(4A)-C(4)-H(4C)	109.5	C(12B)-C(11B)-H(11B)	120.0
H(4B)-C(4)-H(4C)	109.5	C(13B)-C(12B)-C(11B)	120.0
O(2)-C(5)-C(6)	107.6(2)	C(13B)-C(12B)-H(12B)	120.0
O(2)-C(5)-H(5A)	110.2	C(11B)-C(12B)-H(12B)	120.0
C(6)-C(5)-H(5A)	110.2	C(14B)-C(13B)-C(12B)	120.0
O(2)-C(5)-H(5B)	110.2	C(14B)-C(13B)-H(13B)	120.0
C(6)-C(5)-H(5B)	110.2	C(12B)-C(13B)-H(13B)	120.0
H(5A)-C(5)-H(5B)	108.5	C(13B)-C(14B)-C(15B)	120.0
N(2)-C(6)-C(5)	110.0(2)	C(13B)-C(14B)-H(14B)	120.0
N(2)-C(6)-H(6A)	109.7	C(15B)-C(14B)-H(14B)	120.0
C(5)-C(6)-H(6A)	109.7	C(14B)-C(15B)-C(10B)	120.0
N(2)-C(6)-H(6B)	109.7	C(14B)-C(15B)-C(16B)	119.4
C(5)-C(6)-H(6B)	109.7	C(10B)-C(15B)-C(16B)	120.4
H(6A)-C(6)-H(6B)	108.2	C(15B)-C(16B)-H(16D)	109.5
N(2)-C(7)-H(7A)	109.5	C(15B)-C(16B)-H(16E)	109.5
N(2)-C(7)-H(7B)	109.5	H(16D)-C(16B)-H(16E)	109.5
H(7A)-C(7)-H(7B)	109.5	C(15B)-C(16B)-H(16F)	109.5
N(2)-C(7)-H(7C)	109.5	H(16D)-C(16B)-H(16F)	109.5
H(7A)-C(7)-H(7C)	109.5	H(16E)-C(16B)-H(16F)	109.5
H(7B)-C(7)-H(7C)	109.5	O(8)#1-C(17)-O(10)	126.1(2)

O(8)#1-C(17)-C(18)	118.9(2)	O(1)-Cu(1B)-O(11B)	174.2(9)
O(10)-C(17)-C(18)	114.91(19)	O(1)-Cu(1B)-N(1)	91.04(19)
C(19)-C(18)-C(23)	120.4(2)	O(11B)-Cu(1B)-N(1)	84.2(7)
C(19)-C(18)-C(17)	116.9	O(1)-Cu(1B)-O(1)#1	85.66(19)
C(23)-C(18)-C(17)	122.7(2)	O(11B)-Cu(1B)-O(1)#1	100.2(8)
C(18)-C(19)-C(20)	121.3(4)	N(1)-Cu(1B)-O(1)#1	140.9(3)
C(18)-C(19)-H(19)	119.4	O(1)-Cu(1B)-O(3)	83.49(18)
C(20)-C(19)-H(19)	119.4	O(11B)-Cu(1B)-O(3)	98.1(9)
C(21)-C(20)-C(19)	118.5(6)	N(1)-Cu(1B)-O(3)	141.4(3)
C(21)-C(20)-H(20)	120.7	O(1)#1-Cu(1B)-O(3)	76.95(14)
C(19)-C(20)-H(20)	120.7	O(1)-Cu(1B)-Ti(1)	43.09(11)
C(22)-C(21)-C(20)	120.7(4)	O(11B)-Cu(1B)-Ti(1)	142.5(9)
C(22)-C(21)-H(21)	119.7	N(1)-Cu(1B)-Ti(1)	116.33(19)
C(20)-C(21)-H(21)	119.7	O(1)#1-Cu(1B)-Ti(1)	43.81(9)
C(21)-C(22)-C(23)	121.7(5)	O(3)-Cu(1B)-Ti(1)	84.78(13)
C(21)-C(22)-H(22)	119.1	O(11B)-C(25B)-O(12B)	117(3)
C(23)-C(22)-H(22)	119.1	O(11B)-C(25B)-C(26B)	115(4)
C(18)-C(23)-C(22)	117.3(4)	O(12B)-C(25B)-C(26B)	128(4)
C(18)-C(23)-C(24)	124.3(3)	C(25B)-O(11B)-Cu(1B)	133(2)
C(22)-C(23)-C(24)	118.3(4)	C(27B)-C(26B)-C(31B)	120.0
C(23)-C(24)-H(24A)	109.5	C(27B)-C(26B)-C(25B)	110.9(19)
C(23)-C(24)-H(24B)	109.5	C(31B)-C(26B)-C(25B)	129.0(19)
H(24A)-C(24)-H(24B)	109.5	C(26B)-C(27B)-C(28B)	120.0
C(23)-C(24)-H(24C)	109.5	C(26B)-C(27B)-H(27B)	120.0
H(24A)-C(24)-H(24C)	109.5	C(28B)-C(27B)-H(27B)	120.0
H(24B)-C(24)-H(24C)	109.5	C(27B)-C(28B)-C(29B)	120.0
O(11)-Cu(1)-O(3)	93.98(12)	C(27B)-C(28B)-H(28B)	120.0
O(11)-Cu(1)-O(1)	171.29(12)	C(29B)-C(28B)-H(28B)	120.0
O(3)-Cu(1)-O(1)	89.10(10)	C(30B)-C(29B)-C(28B)	120.0
O(11)-Cu(1)-N(1)	90.60(12)	C(30B)-C(29B)-H(29B)	120.0
O(3)-Cu(1)-N(1)	175.41(12)	C(28B)-C(29B)-H(29B)	120.0
O(1)-Cu(1)-N(1)	86.32(10)	C(31B)-C(30B)-C(29B)	120.0
O(11)-C(25)-O(12)	127.3(4)	C(31B)-C(30B)-H(30B)	120.0
O(11)-C(25)-C(26)	113.6(4)	C(29B)-C(30B)-H(30B)	120.0
O(12)-C(25)-C(26)	119.1(4)	C(30B)-C(31B)-C(26B)	120.0
C(25)-O(11)-Cu(1)	124.4(3)	C(30B)-C(31B)-C(32B)	120.0(8)
C(27)-C(26)-C(31)	120.0	C(26B)-C(31B)-C(32B)	120.0(8)
C(27)-C(26)-C(25)	119.8(3)	C(31B)-C(32B)-H(32D)	109.5
C(31)-C(26)-C(25)	120.2(3)	C(31B)-C(32B)-H(32E)	109.5
C(26)-C(27)-C(28)	120.0	H(32D)-C(32B)-H(32E)	109.5
C(26)-C(27)-H(27)	120.0	C(31B)-C(32B)-H(32F)	109.5
C(28)-C(27)-H(27)	120.0	H(32D)-C(32B)-H(32F)	109.5
C(29)-C(28)-C(27)	120.0	H(32E)-C(32B)-H(32F)	109.5
C(29)-C(28)-H(28)	120.0	Cu(1)#2-O(3)-Cu(1)#1	109.55(10)
C(27)-C(28)-H(28)	120.0	Cu(1)#2-O(3)-Cu(1)	109.55(10)
C(30)-C(29)-C(28)	120.0	Cu(1)#1-O(3)-Cu(1)	109.55(10)
C(30)-C(29)-H(29)	120.0	Cu(1)#1-O(3)-Cu(1B)#2	111.57(16)
C(28)-C(29)-H(29)	120.0	Cu(1)-O(3)-Cu(1B)#2	92.02(15)
C(31)-C(30)-C(29)	120.0	Cu(1)#2-O(3)-Cu(1B)#1	92.02(15)
C(31)-C(30)-H(30)	120.0	Cu(1)-O(3)-Cu(1B)#1	111.57(16)
C(29)-C(30)-H(30)	120.0	Cu(1B)#2-O(3)-Cu(1B)#1	92.95(18)
C(30)-C(31)-C(26)	120.0	Cu(1)#2-O(3)-Cu(1B)	111.57(16)
C(30)-C(31)-C(32)	118.9(3)	Cu(1)#1-O(3)-Cu(1B)	92.02(15)
C(26)-C(31)-C(32)	121.0(3)	Cu(1B)#2-O(3)-Cu(1B)	92.95(18)

Cu(1B)#1-O(3)-Cu(1B)	92.95(18)	O(1)-Ti(1)-Cu(1B)#2	46.17(10)
Cu(1)#2-O(3)-H(3)	109.40(10)	O(1)#1-Ti(1)-Cu(1B)#2	87.84(11)
Cu(1)#1-O(3)-H(3)	109.40(10)	O(5)#2-Ti(1)-Cu(1B)#1	139.55(10)
Cu(1)-O(3)-H(3)	109.40(10)	O(5)#1-Ti(1)-Cu(1B)#1	83.89(11)
Cu(1B)#2-O(3)-H(3)	123.15(13)	O(5)-Ti(1)-Cu(1B)#1	125.44(10)
Cu(1B)#1-O(3)-H(3)	123.15(13)	O(1)#2-Ti(1)-Cu(1B)#1	46.17(10)
Cu(1B)-O(3)-H(3)	123.15(13)	O(1)-Ti(1)-Cu(1B)#1	87.84(11)
O(5)-Ti(2)-O(6)#1	95.75(8)	O(1)#1-Ti(1)-Cu(1B)#1	37.64(10)
O(5)-Ti(2)-O(6)	94.65(8)	Cu(1B)#2-Ti(1)-Cu(1B)#1	65.03(14)
O(6)#1-Ti(2)-O(6)	93.22(10)	O(5)#2-Ti(1)-Cu(1B)	125.44(10)
O(5)-Ti(2)-O(10)	92.97(9)	O(5)#1-Ti(1)-Cu(1B)	139.55(10)
O(6)#1-Ti(2)-O(10)	97.66(8)	O(5)-Ti(1)-Cu(1B)	83.89(11)
O(6)-Ti(2)-O(10)	166.03(8)	O(1)#2-Ti(1)-Cu(1B)	87.84(11)
O(5)-Ti(2)-O(2)	99.76(8)	O(1)-Ti(1)-Cu(1B)	37.64(10)
O(6)#1-Ti(2)-O(2)	162.93(8)	O(1)#1-Ti(1)-Cu(1B)	46.17(10)
O(6)-Ti(2)-O(2)	78.54(8)	Cu(1B)#2-Ti(1)-Cu(1B)	65.03(14)
O(10)-Ti(2)-O(2)	88.64(8)	Cu(1B)#1-Ti(1)-Cu(1B)	65.03(14)
O(5)-Ti(2)-O(9)	175.49(8)	O(5)#2-Ti(1)-Ti(2)#1	79.95(6)
O(6)#1-Ti(2)-O(9)	83.38(7)	O(5)#1-Ti(1)-Ti(2)#1	22.08(6)
O(6)-Ti(2)-O(9)	89.82(8)	O(5)-Ti(1)-Ti(2)#1	80.32(6)
O(10)-Ti(2)-O(9)	82.77(8)	O(1)#2-Ti(1)-Ti(2)#1	105.30(6)
O(2)-Ti(2)-O(9)	81.69(8)	O(1)-Ti(1)-Ti(2)#1	166.19(6)
O(5)-Ti(2)-Cu(2)	111.27(6)	O(1)#1-Ti(1)-Ti(2)#1	109.28(6)
O(6)#1-Ti(2)-Cu(2)	125.00(6)	Cu(1B)#2-Ti(1)-Ti(2)#1	138.30(7)
O(6)-Ti(2)-Cu(2)	39.91(5)	Cu(1B)#1-Ti(1)-Ti(2)#1	105.84(9)
O(10)-Ti(2)-Cu(2)	126.16(6)	Cu(1B)-Ti(1)-Ti(2)#1	151.29(9)
O(2)-Ti(2)-Cu(2)	41.67(5)	O(5)#2-Ti(1)-Ti(2)#2	22.08(6)
O(9)-Ti(2)-Cu(2)	72.67(5)	O(5)#1-Ti(1)-Ti(2)#2	80.32(6)
O(5)-Ti(2)-Ti(1)	23.02(6)	O(5)-Ti(1)-Ti(2)#2	79.95(6)
O(6)#1-Ti(2)-Ti(1)	79.81(6)	O(1)#2-Ti(1)-Ti(2)#2	109.28(6)
O(6)-Ti(2)-Ti(1)	79.12(5)	O(1)-Ti(1)-Ti(2)#2	105.30(6)
O(10)-Ti(2)-Ti(1)	111.38(6)	O(1)#1-Ti(1)-Ti(2)#2	166.19(6)
O(2)-Ti(2)-Ti(1)	112.71(6)	Cu(1B)#2-Ti(1)-Ti(2)#2	105.84(9)
O(9)-Ti(2)-Ti(1)	159.25(5)	Cu(1B)#1-Ti(1)-Ti(2)#2	151.29(9)
Cu(2)-Ti(2)-Ti(1)	107.546(15)	Cu(1B)-Ti(1)-Ti(2)#2	138.30(7)
O(5)#2-Ti(1)-O(5)#1	94.99(8)	Ti(2)#1-Ti(1)-Ti(2)#2	61.631(18)
O(5)#2-Ti(1)-O(5)	94.99(8)	O(5)#2-Ti(1)-Ti(2)	80.32(6)
O(5)#1-Ti(1)-O(5)	94.99(8)	O(5)#1-Ti(1)-Ti(2)	79.95(6)
O(5)#2-Ti(1)-O(1)#2	93.42(8)	O(5)-Ti(1)-Ti(2)	22.08(6)
O(5)#1-Ti(1)-O(1)#2	88.42(8)	O(1)#2-Ti(1)-Ti(2)	166.19(6)
O(5)-Ti(1)-O(1)#2	170.62(9)	O(1)-Ti(1)-Ti(2)	109.28(6)
O(5)#2-Ti(1)-O(1)	88.42(8)	O(1)#1-Ti(1)-Ti(2)	105.30(6)
O(5)#1-Ti(1)-O(1)	170.62(9)	Cu(1B)#2-Ti(1)-Ti(2)	151.29(10)
O(5)-Ti(1)-O(1)	93.42(8)	Cu(1B)#1-Ti(1)-Ti(2)	138.30(7)
O(1)#2-Ti(1)-O(1)	82.64(9)	Cu(1B)-Ti(1)-Ti(2)	105.84(9)
O(5)#2-Ti(1)-O(1)#1	170.62(9)	Ti(2)#1-Ti(1)-Ti(2)	61.631(18)
O(5)#1-Ti(1)-O(1)#1	93.42(8)	Ti(2)#2-Ti(1)-Ti(2)	61.631(18)
O(5)-Ti(1)-O(1)#1	88.42(8)	O(6)-Cu(2)-O(2)	79.89(8)
O(1)#2-Ti(1)-O(1)#1	82.64(9)	O(6)-Cu(2)-O(7)	94.67(8)
O(1)-Ti(1)-O(1)#1	82.64(9)	O(2)-Cu(2)-O(7)	157.78(9)
O(5)#2-Ti(1)-Cu(1B)#2	83.89(11)	O(6)-Cu(2)-N(2)	160.35(9)
O(5)#1-Ti(1)-Cu(1B)#2	125.44(10)	O(2)-Cu(2)-N(2)	85.77(9)
O(5)-Ti(1)-Cu(1B)#2	139.55(10)	O(7)-Cu(2)-N(2)	93.57(10)
O(1)#2-Ti(1)-Cu(1B)#2	37.64(10)	O(6)-Cu(2)-O(8)	98.51(8)

O(2)-Cu(2)-O(8)	108.17(8)	C(6)-N(2)-Cu(2)	104.52(18)
O(7)-Cu(2)-O(8)	93.90(9)	C(1)-O(1)-Cu(1B)	109.6(2)
N(2)-Cu(2)-O(8)	98.69(9)	C(1)-O(1)-Cu(1)	106.90(17)
O(6)-Cu(2)-Ti(2)	39.68(5)	C(1)-O(1)-Ti(1)	120.00(17)
O(2)-Cu(2)-Ti(2)	43.33(5)	Cu(1B)-O(1)-Ti(1)	99.27(18)
O(7)-Cu(2)-Ti(2)	122.75(6)	Cu(1)-O(1)-Ti(1)	117.21(10)
N(2)-Cu(2)-Ti(2)	121.94(8)	C(1)-O(1)-Cu(1B)#2	127.1(2)
O(8)-Cu(2)-Ti(2)	119.37(6)	Cu(1B)-O(1)-Cu(1B)#2	106.4(3)
C(4)-N(1)-C(2)	112.0(3)	Cu(1)-O(1)-Cu(1B)#2	93.01(15)
C(4)-N(1)-C(3)	107.6(3)	Ti(1)-O(1)-Cu(1B)#2	90.02(12)
C(2)-N(1)-C(3)	109.7(3)	C(5)-O(2)-Cu(2)	111.63(17)
C(4)-N(1)-Cu(1B)	130.2(3)	C(5)-O(2)-Ti(2)	131.14(18)
C(2)-N(1)-Cu(1B)	98.1(2)	Cu(2)-O(2)-Ti(2)	95.00(8)
C(3)-N(1)-Cu(1B)	97.5(3)	Ti(2)-O(5)-Ti(1)	134.90(11)
C(4)-N(1)-Cu(1)	109.5(2)	Ti(2)#2-O(6)-Ti(2)	133.68(10)
C(2)-N(1)-Cu(1)	106.7(2)	Ti(2)#2-O(6)-Cu(2)	123.55(9)
C(3)-N(1)-Cu(1)	111.3(2)	Ti(2)-O(6)-Cu(2)	100.42(8)
C(7)-N(2)-C(8)	109.5(3)	C(9)#2-O(7)-Cu(2)	127.34(17)
C(7)-N(2)-C(6)	110.4(3)	C(17)#2-O(8)-Cu(2)	122.1(5)
C(8)-N(2)-C(6)	110.5(3)	C(9)-O(9)-Ti(2)	132.55(18)
C(7)-N(2)-Cu(2)	114.4(2)	C(17)-O(10)-Ti(2)	137.28(16)
C(8)-N(2)-Cu(2)	107.48(18)		

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y,z #2 -x+y+1,-x+1,z

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 06mz069m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(h a^*)^2 U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
C(1)	36(2)	32(2)	36(2)	-3(1)	7(1)	6(1)
C(2)	56(2)	31(2)	39(2)	0(1)	-2(2)	12(2)
C(3)	49(2)	57(2)	79(3)	1(2)	-11(2)	29(2)
C(4)	51(2)	39(2)	47(2)	-11(1)	-1(2)	18(2)
C(5)	39(2)	26(1)	50(2)	1(1)	1(1)	21(1)
C(6)	46(2)	24(1)	52(2)	-1(1)	2(1)	19(1)
C(7)	41(2)	27(2)	64(2)	11(1)	3(2)	10(1)
C(8)	50(2)	35(2)	44(2)	7(1)	-2(1)	23(2)
C(9)	29(1)	26(1)	33(1)	-1(1)	-5(1)	16(1)
C(10)	36(2)	21(1)	34(2)	-1(1)	-8(1)	11(1)
C(11)	43(2)	37(2)	37(2)	5(1)	1(1)	14(2)
C(12)	64(3)	52(2)	47(2)	10(2)	13(2)	17(2)
C(13)	85(3)	43(2)	37(2)	8(2)	-5(2)	13(2)
C(14)	74(3)	38(2)	43(2)	3(2)	-25(2)	17(2)

C(15)	48(2)	27(1)	41(2)	-2(1)	-18(2)	14(1)
C(16)	51(2)	50(2)	75(3)	0(2)	-27(2)	29(2)
C(10B)	36(2)	21(1)	34(2)	-1(1)	-8(1)	11(1)
C(11B)	43(2)	37(2)	37(2)	5(1)	1(1)	14(2)
C(12B)	64(3)	52(2)	47(2)	10(2)	13(2)	17(2)
C(13B)	85(3)	43(2)	37(2)	8(2)	-5(2)	13(2)
C(14B)	74(3)	38(2)	43(2)	3(2)	-25(2)	17(2)
C(15B)	48(2)	27(1)	41(2)	-2(1)	-18(2)	14(1)
C(16B)	51(2)	50(2)	75(3)	0(2)	-27(2)	29(2)
C(17)	28(1)	38(2)	32(1)	0(1)	0(1)	21(1)
C(18)	40(2)	46(2)	39(2)	3(1)	7(1)	29(1)
C(19)	86(3)	90(3)	58(2)	-25(2)	-8(2)	63(3)
C(20)	155(6)	132(6)	71(3)	-29(3)	6(4)	108(5)
C(21)	118(5)	107(5)	107(5)	2(4)	50(4)	83(4)
C(22)	54(2)	73(3)	119(4)	30(3)	43(3)	45(2)
C(23)	37(2)	47(2)	68(2)	20(2)	20(2)	26(2)
C(24)	33(2)	48(2)	113(4)	12(2)	-5(2)	23(2)
Cu(1)	34(1)	29(1)	31(1)	0(1)	5(1)	15(1)
C(25)	63(3)	42(2)	53(3)	8(2)	21(2)	29(2)
O(11)	52(2)	36(1)	56(2)	-1(1)	21(1)	19(1)
O(12)	51(1)	51(1)	51(1)	-4(1)	3(1)	26(1)
C(26)	55(2)	30(2)	74(3)	-2(2)	33(2)	11(2)
C(27)	54(3)	54(3)	88(4)	-9(3)	9(3)	16(2)
C(28)	67(3)	66(3)	86(4)	-27(3)	13(3)	22(3)
C(29)	63(3)	48(3)	107(4)	-16(3)	34(3)	18(2)
C(30)	49(2)	40(3)	93(3)	5(2)	25(2)	14(2)
C(31)	60(3)	34(2)	82(4)	13(2)	22(3)	13(2)
C(32)	74(4)	88(4)	84(4)	18(3)	19(3)	44(4)
Cu(1B)	34(1)	29(1)	31(1)	0(1)	5(1)	15(1)
C(25B)	63(3)	42(2)	53(3)	8(2)	21(2)	29(2)
O(11B)	52(2)	36(1)	56(2)	-1(1)	21(1)	19(1)
O(12B)	51(1)	51(1)	51(1)	-4(1)	3(1)	26(1)
C(26B)	55(2)	30(2)	74(3)	-2(2)	33(2)	11(2)
C(27B)	54(3)	54(3)	88(4)	-9(3)	9(3)	16(2)
C(28B)	67(3)	66(3)	86(4)	-27(3)	13(3)	22(3)
C(29B)	63(3)	48(3)	107(4)	-16(3)	34(3)	18(2)
C(30B)	49(2)	40(3)	93(3)	5(2)	25(2)	14(2)
C(31B)	60(3)	34(2)	82(4)	13(2)	22(3)	13(2)
C(32B)	74(4)	88(4)	84(4)	18(3)	19(3)	44(4)
O(3)	37(1)	37(1)	26(2)	0	0	18(1)
Ti(2)	21(1)	20(1)	28(1)	-2(1)	-2(1)	11(1)
Ti(1)	29(1)	29(1)	25(1)	0	0	14(1)
Cu(2)	26(1)	20(1)	33(1)	2(1)	0(1)	11(1)
N(1)	40(1)	31(1)	45(2)	-5(1)	-1(1)	15(1)
N(2)	35(1)	24(1)	45(1)	3(1)	1(1)	14(1)
O(1)	30(1)	29(1)	29(1)	-2(1)	1(1)	11(1)
O(2)	29(1)	22(1)	36(1)	-3(1)	-3(1)	14(1)
O(5)	27(1)	26(1)	27(1)	-2(1)	0(1)	14(1)
O(6)	21(1)	20(1)	29(1)	1(1)	0(1)	10(1)
O(7)	34(1)	27(1)	37(1)	7(1)	8(1)	15(1)
O(8)	28(1)	27(1)	44(1)	-1(1)	-4(1)	11(1)
O(9)	29(1)	24(1)	32(1)	-1(1)	-6(1)	13(1)
O(10)	28(1)	31(1)	43(1)	-6(1)	-3(1)	18(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for 06mz069m.

	x	y	z	U(eq)
H(1A)	8048	4988	6402	48
H(1B)	8304	5283	6701	48
H(2A)	7733	5994	6529	55
H(2B)	6978	5203	6429	55
H(3A)	6344	5832	6697	91
H(3B)	6006	5337	6964	91
H(3C)	5875	4894	6687	91
H(4A)	7529	6485	6944	72
H(4B)	8013	6057	7019	72
H(4C)	7252	5883	7187	72
H(5A)	6563	6034	5907	43
H(5B)	6417	5669	5614	43
H(6A)	7453	6960	5580	48
H(6B)	7900	6841	5826	48
H(7A)	8833	7391	5370	71
H(7B)	9081	6732	5350	71
H(7C)	9048	7082	5633	71
H(8A)	7867	5954	5104	63
H(8B)	7603	6594	5149	63
H(8C)	7042	5706	5241	63
H(11)	6823	4297	5013	50
H(12)	7095	4606	4565	71
H(13)	6153	4668	4298	76
H(14)	4966	4405	4472	68
H(16A)	4405	4119	5141	85
H(16B)	3979	3385	4945	85
H(16C)	4143	4230	4852	85
H(11B)	4359	4005	5042	50
H(12B)	4444	4502	4615	71
H(13B)	5595	4942	4368	76
H(14B)	6661	4885	4548	68
H(16D)	6600	3757	5057	85
H(16E)	7043	4645	5160	85
H(16F)	7203	4449	4867	85
H(19)	5127	4814	6335	84
H(20)	4550	5396	6585	124
H(21)	3273	5097	6485	119
H(22)	2606	4279	6137	91
H(24A)	2725	2961	5862	95
H(24B)	3347	3592	5660	95
H(24C)	2603	3656	5752	95
H(27)	5695	4236	7814	85
H(28)	5049	4661	8100	94
H(29)	4001	4795	7946	92
H(30)	3598	4503	7505	77
H(32A)	3715	4126	7078	120

H(32B)	3853	3392	7096	120
H(32C)	4539	4220	6990	120
H(27B)	4252	3846	6927	85
H(28B)	3342	4268	6987	94
H(29B)	3238	4756	7398	92
H(30B)	4045	4823	7749	77
H(32D)	5602	4399	7708	120
H(32E)	4836	3936	7889	120
H(32F)	5296	4874	7881	120
H(3)	6667	3333	7280(4)	40