

Structure, Substitution and Hydrolysis of Bis(trifluorobenzoylacetato-O,O')dichloro titanium(IV): an Experimental and Computational Study.

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Figure S1. The ten possible isomers of $[\{\text{Ti}(\text{CF}_3\text{COCHCOPh})_2\text{Cl}\}_2(\mu\text{-O})]$.

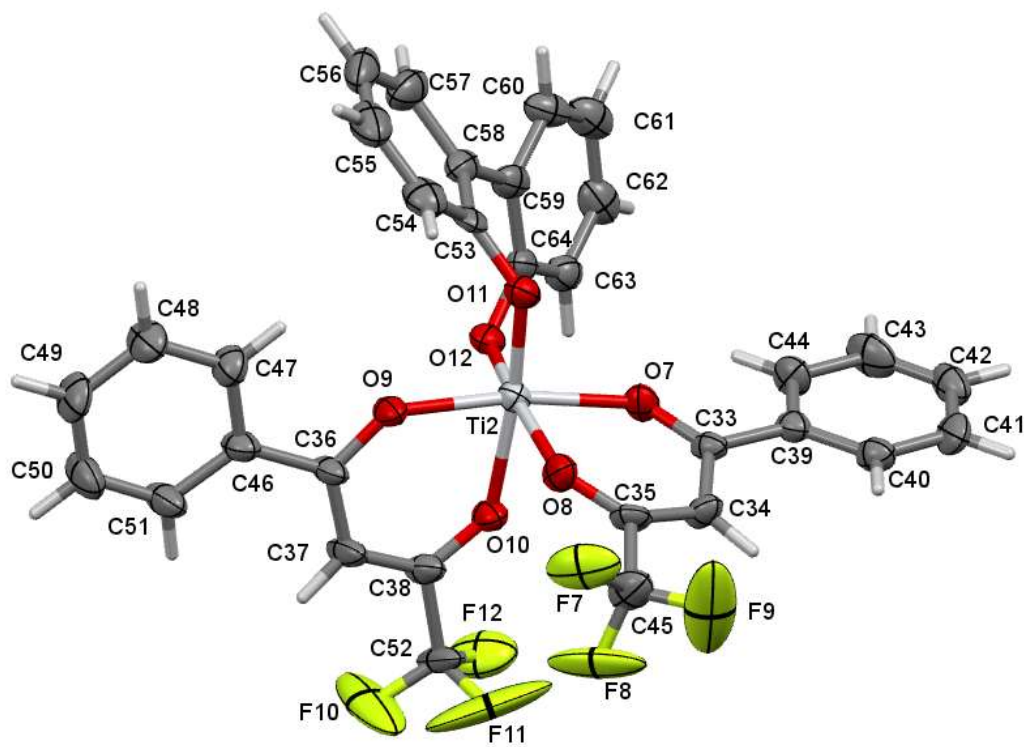
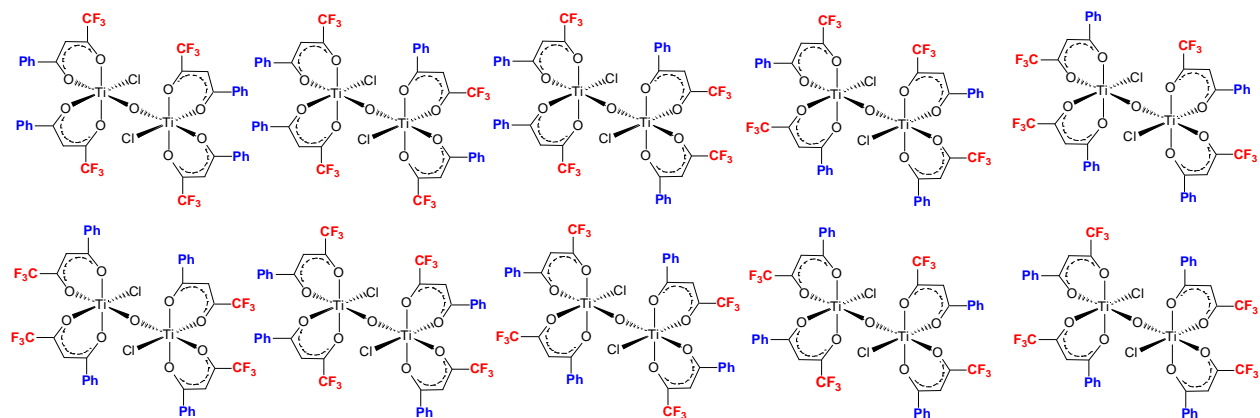


Figure S2. One of the isomeric molecular structures (50% probability displacement ellipsoids) of $[\text{Ti}(\text{tfba}_2)\text{biphen}]$ (2) showing the numbering scheme.

Crystal data

[Ti(tfba₂)biphen] (2)

Table 1. Crystal data and structure refinement for mo_mljc03x2_0m_a.

Identification code	shelx	
Empirical formula	C ₃₂ H ₂₀ F ₆ O ₆ Ti	
Formula weight	662.38	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2	
Unit cell dimensions	a = 53.4099(19) Å	α = 90°.
	b = 9.1895(3) Å	β = 99.190(2)°.
	c = 17.9050(6) Å	γ = 90°.
Volume	8675.2(5) Å ³	
Z	12	
Density (calculated)	1.521 Mg/m ³	
Absorption coefficient	0.380 mm ⁻¹	
F(000)	4032	
Crystal size	0.406 x 0.208 x 0.206 mm ³	
Theta range for data collection	2.070 to 26.373°.	
Index ranges	-66<=h<=66, -11<=k<=11, -22<=l<=22	
Reflections collected	146277	
Independent reflections	17751 [R(int) = 0.0871]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	17751 / 1 / 1217	
Goodness-of-fit on F ²	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0729, wR2 = 0.1740	
R indices (all data)	R1 = 0.1081, wR2 = 0.1947	
Absolute structure parameter	0.5	
Largest diff. peak and hole	1.291 and -0.590 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_mljc03x2_0m_a. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ti(1)	6693(1)	4914(2)	840(1)	30(1)
Ti(2)	8318(1)	5012(2)	4261(1)	30(1)
Ti(3)	5000	2663(2)	5000	29(1)
Ti(4)	5000	7628(2)	0	30(1)
O(1)	6714(1)	5198(6)	-258(3)	33(1)
O(2)	6970(1)	3423(6)	765(3)	34(1)
O(3)	6725(1)	4636(6)	1962(3)	37(1)
O(4)	6992(1)	6280(6)	1133(3)	36(1)
O(5)	6442(1)	3547(6)	713(3)	33(1)
O(6)	6468(1)	6419(6)	786(3)	31(1)
O(7)	8302(1)	5286(6)	3139(3)	33(1)
O(8)	8033(1)	3564(6)	3927(3)	37(1)
O(9)	8274(1)	4759(6)	5337(3)	35(1)
O(10)	8030(1)	6452(6)	4257(3)	36(1)
O(11)	8567(1)	3628(6)	4390(3)	32(1)
O(12)	8549(1)	6480(6)	4418(3)	32(1)
O(13)	5219(1)	9185(5)	-368(3)	31(1)
O(14)	5251(1)	7836(6)	952(3)	36(1)
O(15)	4837(1)	6240(5)	481(3)	33(1)
O(16)	5220(1)	4237(5)	5575(3)	31(1)
O(17)	5249(1)	2886(5)	4287(3)	35(1)
O(18)	4839(1)	1277(5)	4362(3)	33(1)
F(1)	7488(1)	3061(11)	1154(6)	145(4)
F(2)	7517(2)	2440(16)	112(5)	195(7)
F(3)	7313(1)	1222(8)	761(6)	126(4)
F(4)	7536(1)	6545(8)	1498(5)	93(3)
F(5)	7471(2)	7909(14)	2393(3)	172(6)
F(6)	7326(1)	8457(6)	1270(3)	59(1)
F(7)	7678(1)	1601(7)	3807(4)	75(2)
F(8)	7469(1)	3447(8)	3462(5)	106(3)
F(9)	7565(2)	1954(13)	2660(4)	158(5)

F(10)	7559(2)	8237(17)	4980(5)	224(8)
F(11)	7490(1)	6900(9)	4075(7)	172(6)
F(12)	7714(1)	8685(7)	4029(4)	81(2)
F(13)	5850(1)	3336(8)	3899(3)	65(2)
F(14)	5538(1)	2121(5)	3313(3)	50(1)
F(15)	5555(1)	4435(6)	3186(3)	56(1)
F(16)	5559(1)	9428(5)	2343(3)	57(1)
F(17)	5534(1)	7109(5)	2205(2)	49(1)
F(18)	5850(1)	8281(7)	1899(3)	64(2)
C(1)	6869(1)	4790(8)	-695(4)	28(2)
C(2)	7090(1)	3981(9)	-414(4)	38(2)
C(3)	7121(1)	3374(9)	290(4)	34(2)
C(4)	6863(1)	5158(9)	2529(4)	33(2)
C(5)	7077(1)	5982(10)	2468(4)	41(2)
C(6)	7126(1)	6495(9)	1781(4)	38(2)
C(7)	6802(1)	5203(8)	-1495(4)	30(2)
C(8)	6606(1)	6160(9)	-1718(4)	35(2)
C(9)	6535(2)	6532(10)	-2479(4)	45(2)
C(10)	6659(2)	5921(10)	-3016(5)	45(2)
C(11)	6852(2)	4968(11)	-2808(5)	51(2)
C(12)	6925(2)	4601(10)	-2051(4)	42(2)
C(13)	7361(2)	2500(11)	555(4)	46(2)
C(14)	6792(1)	4799(9)	3289(4)	32(2)
C(15)	6601(1)	3796(9)	3323(4)	40(2)
C(16)	6524(2)	3504(10)	4016(5)	47(2)
C(17)	6641(2)	4201(10)	4663(5)	46(2)
C(18)	6824(2)	5264(11)	4628(5)	46(2)
C(19)	6903(1)	5538(10)	3935(4)	40(2)
C(20)	7364(2)	7337(13)	1745(5)	58(3)
C(21)	6230(1)	3449(9)	1053(4)	36(2)
C(22)	6211(2)	2246(10)	1528(4)	46(2)
C(23)	6001(2)	2096(12)	1874(5)	58(3)
C(24)	5807(2)	3078(12)	1747(5)	59(3)
C(25)	5823(2)	4235(10)	1285(5)	49(2)
C(26)	6035(1)	4480(8)	915(4)	35(2)
C(27)	6033(1)	5733(9)	394(4)	35(2)

C(28)	5805(2)	6063(10)	-83(5)	46(2)
C(29)	5788(2)	7253(10)	-574(5)	52(2)
C(30)	5993(2)	8123(9)	-604(5)	47(2)
C(31)	6220(1)	7801(9)	-144(4)	39(2)
C(32)	6243(1)	6638(9)	344(4)	31(2)
C(33)	8153(1)	4867(8)	2559(4)	28(2)
C(34)	7930(1)	4061(9)	2616(4)	34(2)
C(35)	7893(1)	3491(9)	3287(4)	32(2)
C(36)	8126(1)	5278(9)	5764(4)	33(2)
C(37)	7923(1)	6183(11)	5476(4)	47(2)
C(38)	7888(1)	6683(10)	4752(4)	37(2)
C(39)	8221(1)	5270(8)	1817(4)	30(2)
C(40)	8105(1)	4611(9)	1140(4)	36(2)
C(41)	8177(2)	4981(11)	461(4)	46(2)
C(42)	8363(2)	5999(10)	438(5)	45(2)
C(43)	8481(2)	6656(11)	1089(5)	53(2)
C(44)	8411(1)	6299(10)	1784(4)	39(2)
C(45)	7646(2)	2606(12)	3302(5)	50(2)
C(46)	8188(1)	4884(9)	6580(4)	36(2)
C(47)	8383(2)	3896(9)	6819(4)	40(2)
C(48)	8446(2)	3539(10)	7580(4)	46(2)
C(49)	8315(2)	4201(10)	8107(4)	48(2)
C(50)	8125(2)	5206(11)	7867(5)	53(2)
C(51)	8063(2)	5558(11)	7127(5)	47(2)
C(52)	7662(1)	7678(13)	4466(5)	56(3)
C(53)	8781(1)	3526(8)	4908(4)	31(2)
C(54)	8799(2)	2315(10)	5413(5)	46(2)
C(55)	9012(2)	2170(12)	5951(5)	60(3)
C(56)	9209(2)	3139(12)	5987(5)	58(3)
C(57)	9196(2)	4292(11)	5489(5)	53(2)
C(58)	8978(1)	4538(9)	4936(4)	35(2)
C(59)	8979(1)	5765(9)	4405(4)	35(2)
C(60)	9201(1)	6097(9)	4122(5)	41(2)
C(61)	9220(2)	7242(10)	3656(5)	50(2)
C(62)	9012(2)	8172(10)	3434(5)	44(2)
C(63)	8792(1)	7860(9)	3704(4)	36(2)

C(64)	8772(1)	6693(9)	4166(4)	33(2)
C(65)	5430(1)	4833(8)	5514(4)	29(2)
C(66)	5556(1)	4557(9)	4892(4)	37(2)
C(67)	5459(1)	3594(7)	4338(4)	27(2)
C(68)	5545(1)	5791(8)	6136(4)	29(2)
C(69)	5732(2)	6778(9)	6049(4)	42(2)
C(70)	5854(2)	7583(10)	6660(4)	47(2)
C(71)	5791(2)	7373(12)	7359(5)	58(3)
C(72)	5602(2)	6328(13)	7459(5)	63(3)
C(73)	5483(2)	5579(10)	6860(5)	47(2)
C(74)	5599(1)	3370(9)	3686(4)	38(2)
C(75)	4928(1)	41(8)	4103(4)	31(2)
C(76)	5007(1)	-1144(8)	4586(4)	32(2)
C(77)	5092(1)	-2389(9)	4262(4)	42(2)
C(78)	5098(2)	-2510(10)	3497(5)	46(2)
C(79)	5021(2)	-1328(10)	3028(5)	46(2)
C(80)	4937(1)	-82(10)	3333(4)	40(2)
C(81)	5430(1)	9800(7)	-100(4)	29(2)
C(82)	5549(1)	9521(8)	639(4)	35(2)
C(83)	5456(1)	8563(8)	1100(4)	29(2)
C(84)	5542(1)	10766(8)	-622(4)	30(2)
C(85)	5482(2)	10532(10)	-1395(5)	46(2)
C(86)	5601(2)	11259(14)	-1891(5)	71(3)
C(87)	5782(2)	12337(12)	-1604(5)	60(3)
C(88)	5846(2)	12566(10)	-848(5)	46(2)
C(89)	5727(2)	11785(9)	-348(5)	42(2)
C(90)	5604(1)	8318(9)	1887(4)	36(2)
C(91)	4929(1)	5004(8)	827(4)	32(2)
C(92)	5006(1)	3817(8)	424(4)	32(2)
C(93)	5095(2)	2584(10)	829(5)	46(2)
C(94)	5102(2)	2476(10)	1599(5)	46(2)
C(95)	5023(2)	3648(9)	1992(5)	45(2)
C(96)	4939(1)	4910(9)	1620(4)	39(2)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for mo_mljc03x2_0m_a.

Ti(1)-O(6)	1.825(5)
Ti(1)-O(5)	1.828(5)
Ti(1)-O(1)	2.004(5)
Ti(1)-O(3)	2.005(5)
Ti(1)-O(4)	2.033(5)
Ti(1)-O(2)	2.033(5)
Ti(2)-O(12)	1.816(5)
Ti(2)-O(11)	1.828(5)
Ti(2)-O(9)	1.990(5)
Ti(2)-O(7)	2.014(5)
Ti(2)-O(10)	2.028(5)
Ti(2)-O(8)	2.039(5)
Ti(3)-O(18)	1.831(5)
Ti(3)-O(18)#1	1.831(5)
Ti(3)-O(17)#1	1.995(5)
Ti(3)-O(17)	1.995(5)
Ti(3)-O(16)	2.036(5)
Ti(3)-O(16)#1	2.036(5)
Ti(4)-O(15)	1.834(5)
Ti(4)-O(15)#2	1.834(5)
Ti(4)-O(14)	2.001(5)
Ti(4)-O(14)#2	2.002(5)
Ti(4)-O(13)	2.023(5)
Ti(4)-O(13)#2	2.023(5)
O(1)-C(1)	1.281(8)
O(2)-C(3)	1.267(8)
O(3)-C(4)	1.251(8)
O(4)-C(6)	1.276(9)
O(5)-C(21)	1.368(8)
O(6)-C(32)	1.345(8)
O(7)-C(33)	1.266(8)
O(8)-C(35)	1.267(8)
O(9)-C(36)	1.278(8)
O(10)-C(38)	1.275(8)

O(11)-C(53)	1.356(8)
O(12)-C(64)	1.357(8)
O(13)-C(81)	1.286(8)
O(14)-C(83)	1.276(8)
O(15)-C(91)	1.347(9)
O(16)-C(65)	1.268(8)
O(17)-C(67)	1.287(8)
O(18)-C(75)	1.342(9)
F(1)-C(13)	1.280(11)
F(2)-C(13)	1.238(10)
F(3)-C(13)	1.270(11)
F(4)-C(20)	1.305(12)
F(5)-C(20)	1.319(11)
F(6)-C(20)	1.331(11)
F(7)-C(45)	1.285(10)
F(8)-C(45)	1.290(12)
F(9)-C(45)	1.306(11)
F(10)-C(52)	1.254(12)
F(11)-C(52)	1.279(13)
F(12)-C(52)	1.272(11)
F(13)-C(74)	1.338(9)
F(14)-C(74)	1.341(9)
F(15)-C(74)	1.321(9)
F(16)-C(90)	1.351(9)
F(17)-C(90)	1.327(9)
F(18)-C(90)	1.316(9)
C(1)-C(2)	1.419(10)
C(1)-C(7)	1.469(9)
C(2)-C(3)	1.365(10)
C(2)-H(2)	0.9500
C(3)-C(13)	1.522(11)
C(4)-C(5)	1.393(10)
C(4)-C(14)	1.503(9)
C(5)-C(6)	1.381(10)
C(5)-H(5)	0.9500
C(6)-C(20)	1.498(11)

C(7)-C(8)	1.375(10)
C(7)-C(12)	1.393(10)
C(8)-C(9)	1.397(10)
C(8)-H(8)	0.9500
C(9)-C(10)	1.371(12)
C(9)-H(9)	0.9500
C(10)-C(11)	1.358(12)
C(10)-H(10)	0.9500
C(11)-C(12)	1.391(11)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(14)-C(15)	1.384(10)
C(14)-C(19)	1.390(11)
C(15)-C(16)	1.394(10)
C(15)-H(15)	0.9500
C(16)-C(17)	1.382(12)
C(16)-H(16)	0.9500
C(17)-C(18)	1.390(12)
C(17)-H(17)	0.9500
C(18)-C(19)	1.397(11)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(21)-C(26)	1.401(11)
C(21)-C(22)	1.408(11)
C(22)-C(23)	1.373(12)
C(22)-H(22)	0.9500
C(23)-C(24)	1.365(14)
C(23)-H(23)	0.9500
C(24)-C(25)	1.358(14)
C(24)-H(24)	0.9500
C(25)-C(26)	1.419(10)
C(25)-H(25)	0.9500
C(26)-C(27)	1.481(11)
C(27)-C(28)	1.403(11)
C(27)-C(32)	1.411(10)
C(28)-C(29)	1.397(13)

C(28)-H(28)	0.9500
C(29)-C(30)	1.363(12)
C(29)-H(29)	0.9500
C(30)-C(31)	1.388(11)
C(30)-H(30)	0.9500
C(31)-C(32)	1.373(11)
C(31)-H(31)	0.9500
C(33)-C(34)	1.417(9)
C(33)-C(39)	1.481(9)
C(34)-C(35)	1.354(10)
C(34)-H(34)	0.9500
C(35)-C(45)	1.553(10)
C(36)-C(37)	1.400(10)
C(36)-C(46)	1.492(10)
C(37)-C(38)	1.360(10)
C(37)-H(37)	0.9500
C(38)-C(52)	1.535(11)
C(39)-C(44)	1.393(10)
C(39)-C(40)	1.408(10)
C(40)-C(41)	1.376(10)
C(40)-H(40)	0.9500
C(41)-C(42)	1.371(12)
C(41)-H(41)	0.9500
C(42)-C(43)	1.372(13)
C(42)-H(42)	0.9500
C(43)-C(44)	1.393(10)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(46)-C(47)	1.396(11)
C(46)-C(51)	1.415(11)
C(47)-C(48)	1.390(10)
C(47)-H(47)	0.9500
C(48)-C(49)	1.401(12)
C(48)-H(48)	0.9500
C(49)-C(50)	1.388(12)
C(49)-H(49)	0.9500

C(50)-C(51)	1.354(11)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(53)-C(58)	1.398(11)
C(53)-C(54)	1.426(11)
C(54)-C(55)	1.376(12)
C(54)-H(54)	0.9500
C(55)-C(56)	1.372(14)
C(55)-H(55)	0.9500
C(56)-C(57)	1.379(14)
C(56)-H(56)	0.9500
C(57)-C(58)	1.418(10)
C(57)-H(57)	0.9500
C(58)-C(59)	1.475(11)
C(59)-C(60)	1.397(10)
C(59)-C(64)	1.407(11)
C(60)-C(61)	1.357(13)
C(60)-H(60)	0.9500
C(61)-C(62)	1.405(12)
C(61)-H(61)	0.9500
C(62)-C(63)	1.373(10)
C(62)-H(62)	0.9500
C(63)-C(64)	1.368(11)
C(63)-H(63)	0.9500
C(65)-C(66)	1.413(10)
C(65)-C(68)	1.474(10)
C(66)-C(67)	1.370(10)
C(66)-H(66)	0.9500
C(67)-C(74)	1.497(10)
C(68)-C(69)	1.379(10)
C(68)-C(73)	1.403(11)
C(69)-C(70)	1.393(11)
C(69)-H(69)	0.9500
C(70)-C(71)	1.362(12)
C(70)-H(70)	0.9500
C(71)-C(72)	1.423(13)

C(71)-H(71)	0.9500
C(72)-C(73)	1.347(12)
C(72)-H(72)	0.9500
C(73)-H(73)	0.9500
C(75)-C(80)	1.392(10)
C(75)-C(76)	1.412(11)
C(76)-C(77)	1.392(11)
C(76)-C(76)#1	1.495(15)
C(77)-C(78)	1.380(11)
C(77)-H(77)	0.9500
C(78)-C(79)	1.394(12)
C(78)-H(78)	0.9500
C(79)-C(80)	1.374(12)
C(79)-H(79)	0.9500
C(80)-H(80)	0.9500
C(81)-C(82)	1.396(10)
C(81)-C(84)	1.481(10)
C(82)-C(83)	1.354(10)
C(82)-H(82)	0.9500
C(83)-C(90)	1.518(10)
C(84)-C(85)	1.387(11)
C(84)-C(89)	1.395(10)
C(85)-C(86)	1.349(12)
C(85)-H(85)	0.9500
C(86)-C(87)	1.421(14)
C(86)-H(86)	0.9500
C(87)-C(88)	1.359(12)
C(87)-H(87)	0.9500
C(88)-C(89)	1.378(11)
C(88)-H(88)	0.9500
C(89)-H(89)	0.9500
C(91)-C(92)	1.405(11)
C(91)-C(96)	1.415(11)
C(92)-C(93)	1.388(11)
C(92)-C(92)#2	1.510(15)
C(93)-C(94)	1.378(11)

C(93)-H(93)	0.9500
C(94)-C(95)	1.386(12)
C(94)-H(94)	0.9500
C(95)-C(96)	1.377(12)
C(95)-H(95)	0.9500
C(96)-H(96)	0.9500

O(6)-Ti(1)-O(5)	92.8(2)
O(6)-Ti(1)-O(1)	89.3(2)
O(5)-Ti(1)-O(1)	97.1(2)
O(6)-Ti(1)-O(3)	95.7(2)
O(5)-Ti(1)-O(3)	88.8(2)
O(1)-Ti(1)-O(3)	172.1(2)
O(6)-Ti(1)-O(4)	91.6(2)
O(5)-Ti(1)-O(4)	171.3(2)
O(1)-Ti(1)-O(4)	90.5(2)
O(3)-Ti(1)-O(4)	83.28(19)
O(6)-Ti(1)-O(2)	170.4(2)
O(5)-Ti(1)-O(2)	93.2(2)
O(1)-Ti(1)-O(2)	82.47(19)
O(3)-Ti(1)-O(2)	92.0(2)
O(4)-Ti(1)-O(2)	83.4(2)
O(12)-Ti(2)-O(11)	92.1(2)
O(12)-Ti(2)-O(9)	96.9(2)
O(11)-Ti(2)-O(9)	89.6(2)
O(12)-Ti(2)-O(7)	88.9(2)
O(11)-Ti(2)-O(7)	97.3(2)
O(9)-Ti(2)-O(7)	170.89(19)
O(12)-Ti(2)-O(10)	90.6(2)
O(11)-Ti(2)-O(10)	172.1(2)
O(9)-Ti(2)-O(10)	82.71(19)
O(7)-Ti(2)-O(10)	90.2(2)
O(12)-Ti(2)-O(8)	170.2(2)
O(11)-Ti(2)-O(8)	94.4(2)
O(9)-Ti(2)-O(8)	90.5(2)
O(7)-Ti(2)-O(8)	82.99(19)

O(10)-Ti(2)-O(8)	83.9(2)
O(18)-Ti(3)-O(18)#1	91.8(3)
O(18)-Ti(3)-O(17)#1	100.2(2)
O(18)#1-Ti(3)-O(17)#1	88.1(2)
O(18)-Ti(3)-O(17)	88.1(2)
O(18)#1-Ti(3)-O(17)	100.2(2)
O(17)#1-Ti(3)-O(17)	168.2(3)
O(18)-Ti(3)-O(16)	170.1(2)
O(18)#1-Ti(3)-O(16)	90.2(2)
O(17)#1-Ti(3)-O(16)	89.6(2)
O(17)-Ti(3)-O(16)	81.99(19)
O(18)-Ti(3)-O(16)#1	90.2(2)
O(18)#1-Ti(3)-O(16)#1	170.1(2)
O(17)#1-Ti(3)-O(16)#1	82.00(19)
O(17)-Ti(3)-O(16)#1	89.6(2)
O(16)-Ti(3)-O(16)#1	89.5(3)
O(15)-Ti(4)-O(15)#2	91.9(3)
O(15)-Ti(4)-O(14)	88.2(2)
O(15)#2-Ti(4)-O(14)	99.5(2)
O(15)-Ti(4)-O(14)#2	99.5(2)
O(15)#2-Ti(4)-O(14)#2	88.2(2)
O(14)-Ti(4)-O(14)#2	169.0(3)
O(15)-Ti(4)-O(13)	170.6(2)
O(15)#2-Ti(4)-O(13)	89.87(19)
O(14)-Ti(4)-O(13)	82.40(19)
O(14)#2-Ti(4)-O(13)	89.8(2)
O(15)-Ti(4)-O(13)#2	89.87(19)
O(15)#2-Ti(4)-O(13)#2	170.6(2)
O(14)-Ti(4)-O(13)#2	89.8(2)
O(14)#2-Ti(4)-O(13)#2	82.39(19)
O(13)-Ti(4)-O(13)#2	89.9(3)
C(1)-O(1)-Ti(1)	134.8(4)
C(3)-O(2)-Ti(1)	128.1(5)
C(4)-O(3)-Ti(1)	135.2(5)
C(6)-O(4)-Ti(1)	129.2(5)
C(21)-O(5)-Ti(1)	129.3(5)

C(32)-O(6)-Ti(1)	131.6(4)
C(33)-O(7)-Ti(2)	134.5(4)
C(35)-O(8)-Ti(2)	127.3(5)
C(36)-O(9)-Ti(2)	135.7(5)
C(38)-O(10)-Ti(2)	130.0(5)
C(53)-O(11)-Ti(2)	130.6(5)
C(64)-O(12)-Ti(2)	131.8(5)
C(81)-O(13)-Ti(4)	135.1(4)
C(83)-O(14)-Ti(4)	131.5(4)
C(91)-O(15)-Ti(4)	129.6(4)
C(65)-O(16)-Ti(3)	135.3(4)
C(67)-O(17)-Ti(3)	132.0(4)
C(75)-O(18)-Ti(3)	130.4(4)
O(1)-C(1)-C(2)	121.2(6)
O(1)-C(1)-C(7)	116.2(6)
C(2)-C(1)-C(7)	122.7(6)
C(3)-C(2)-C(1)	121.0(7)
C(3)-C(2)-H(2)	119.5
C(1)-C(2)-H(2)	119.5
O(2)-C(3)-C(2)	127.5(7)
O(2)-C(3)-C(13)	114.0(6)
C(2)-C(3)-C(13)	118.5(7)
O(3)-C(4)-C(5)	121.9(6)
O(3)-C(4)-C(14)	116.9(6)
C(5)-C(4)-C(14)	121.2(6)
C(6)-C(5)-C(4)	122.0(7)
C(6)-C(5)-H(5)	119.0
C(4)-C(5)-H(5)	119.0
O(4)-C(6)-C(5)	126.9(7)
O(4)-C(6)-C(20)	113.3(6)
C(5)-C(6)-C(20)	119.7(7)
C(8)-C(7)-C(12)	118.0(7)
C(8)-C(7)-C(1)	120.2(6)
C(12)-C(7)-C(1)	121.7(7)
C(7)-C(8)-C(9)	121.0(7)
C(7)-C(8)-H(8)	119.5

C(9)-C(8)-H(8)	119.5
C(10)-C(9)-C(8)	119.8(8)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(11)-C(10)-C(9)	120.1(8)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	120.4(8)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(11)-C(12)-C(7)	120.6(8)
C(11)-C(12)-H(12)	119.7
C(7)-C(12)-H(12)	119.7
F(2)-C(13)-F(3)	109.5(11)
F(2)-C(13)-F(1)	103.8(10)
F(3)-C(13)-F(1)	103.5(9)
F(2)-C(13)-C(3)	116.1(7)
F(3)-C(13)-C(3)	112.2(7)
F(1)-C(13)-C(3)	110.7(8)
C(15)-C(14)-C(19)	120.5(6)
C(15)-C(14)-C(4)	118.6(6)
C(19)-C(14)-C(4)	120.7(7)
C(14)-C(15)-C(16)	119.5(7)
C(14)-C(15)-H(15)	120.3
C(16)-C(15)-H(15)	120.3
C(17)-C(16)-C(15)	119.9(8)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	121.0(7)
C(16)-C(17)-H(17)	119.5
C(18)-C(17)-H(17)	119.5
C(17)-C(18)-C(19)	118.7(8)
C(17)-C(18)-H(18)	120.6
C(19)-C(18)-H(18)	120.6
C(14)-C(19)-C(18)	120.2(7)
C(14)-C(19)-H(19)	119.9

C(18)-C(19)-H(19)	119.9
F(4)-C(20)-F(5)	106.9(9)
F(4)-C(20)-F(6)	104.9(6)
F(5)-C(20)-F(6)	104.8(10)
F(4)-C(20)-C(6)	112.0(9)
F(5)-C(20)-C(6)	114.9(7)
F(6)-C(20)-C(6)	112.6(7)
O(5)-C(21)-C(26)	121.4(7)
O(5)-C(21)-C(22)	117.6(8)
C(26)-C(21)-C(22)	121.0(7)
C(23)-C(22)-C(21)	119.6(9)
C(23)-C(22)-H(22)	120.2
C(21)-C(22)-H(22)	120.2
C(24)-C(23)-C(22)	120.8(9)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	120.0(8)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	122.7(9)
C(24)-C(25)-H(25)	118.6
C(26)-C(25)-H(25)	118.6
C(21)-C(26)-C(25)	115.9(8)
C(21)-C(26)-C(27)	124.6(6)
C(25)-C(26)-C(27)	119.4(8)
C(28)-C(27)-C(32)	117.1(8)
C(28)-C(27)-C(26)	118.0(7)
C(32)-C(27)-C(26)	124.9(7)
C(29)-C(28)-C(27)	121.1(8)
C(29)-C(28)-H(28)	119.4
C(27)-C(28)-H(28)	119.4
C(30)-C(29)-C(28)	120.7(8)
C(30)-C(29)-H(29)	119.7
C(28)-C(29)-H(29)	119.7
C(29)-C(30)-C(31)	119.0(8)
C(29)-C(30)-H(30)	120.5

C(31)-C(30)-H(30)	120.5
C(32)-C(31)-C(30)	121.6(8)
C(32)-C(31)-H(31)	119.2
C(30)-C(31)-H(31)	119.2
O(6)-C(32)-C(31)	118.1(7)
O(6)-C(32)-C(27)	121.3(7)
C(31)-C(32)-C(27)	120.5(7)
O(7)-C(33)-C(34)	121.9(6)
O(7)-C(33)-C(39)	116.4(6)
C(34)-C(33)-C(39)	121.7(6)
C(35)-C(34)-C(33)	120.5(6)
C(35)-C(34)-H(34)	119.7
C(33)-C(34)-H(34)	119.7
O(8)-C(35)-C(34)	129.4(6)
O(8)-C(35)-C(45)	113.1(6)
C(34)-C(35)-C(45)	117.5(6)
O(9)-C(36)-C(37)	121.4(6)
O(9)-C(36)-C(46)	115.7(6)
C(37)-C(36)-C(46)	122.9(6)
C(38)-C(37)-C(36)	122.1(7)
C(38)-C(37)-H(37)	118.9
C(36)-C(37)-H(37)	118.9
O(10)-C(38)-C(37)	126.8(7)
O(10)-C(38)-C(52)	113.2(6)
C(37)-C(38)-C(52)	120.0(6)
C(44)-C(39)-C(40)	118.6(7)
C(44)-C(39)-C(33)	119.6(7)
C(40)-C(39)-C(33)	121.7(7)
C(41)-C(40)-C(39)	120.5(8)
C(41)-C(40)-H(40)	119.7
C(39)-C(40)-H(40)	119.7
C(42)-C(41)-C(40)	120.1(8)
C(42)-C(41)-H(41)	120.0
C(40)-C(41)-H(41)	120.0
C(41)-C(42)-C(43)	120.7(7)
C(41)-C(42)-H(42)	119.7

C(43)-C(42)-H(42)	119.7
C(42)-C(43)-C(44)	120.3(8)
C(42)-C(43)-H(43)	119.9
C(44)-C(43)-H(43)	119.9
C(39)-C(44)-C(43)	119.8(8)
C(39)-C(44)-H(44)	120.1
C(43)-C(44)-H(44)	120.1
F(7)-C(45)-F(8)	106.9(7)
F(7)-C(45)-F(9)	106.1(10)
F(8)-C(45)-F(9)	108.4(8)
F(7)-C(45)-C(35)	112.0(6)
F(8)-C(45)-C(35)	110.2(9)
F(9)-C(45)-C(35)	113.0(7)
C(47)-C(46)-C(51)	119.2(7)
C(47)-C(46)-C(36)	119.7(6)
C(51)-C(46)-C(36)	121.0(7)
C(48)-C(47)-C(46)	120.3(7)
C(48)-C(47)-H(47)	119.9
C(46)-C(47)-H(47)	119.9
C(47)-C(48)-C(49)	119.4(8)
C(47)-C(48)-H(48)	120.3
C(49)-C(48)-H(48)	120.3
C(50)-C(49)-C(48)	119.9(7)
C(50)-C(49)-H(49)	120.0
C(48)-C(49)-H(49)	120.0
C(51)-C(50)-C(49)	121.1(8)
C(51)-C(50)-H(50)	119.4
C(49)-C(50)-H(50)	119.4
C(50)-C(51)-C(46)	120.1(8)
C(50)-C(51)-H(51)	120.0
C(46)-C(51)-H(51)	120.0
F(10)-C(52)-F(12)	108.6(12)
F(10)-C(52)-F(11)	105.8(11)
F(12)-C(52)-F(11)	106.1(8)
F(10)-C(52)-C(38)	114.3(7)
F(12)-C(52)-C(38)	113.5(6)

F(11)-C(52)-C(38)	107.8(10)
O(11)-C(53)-C(58)	121.7(7)
O(11)-C(53)-C(54)	116.7(7)
C(58)-C(53)-C(54)	121.6(7)
C(55)-C(54)-C(53)	118.8(9)
C(55)-C(54)-H(54)	120.6
C(53)-C(54)-H(54)	120.6
C(56)-C(55)-C(54)	120.9(9)
C(56)-C(55)-H(55)	119.6
C(54)-C(55)-H(55)	119.6
C(55)-C(56)-C(57)	120.5(8)
C(55)-C(56)-H(56)	119.8
C(57)-C(56)-H(56)	119.8
C(56)-C(57)-C(58)	121.7(9)
C(56)-C(57)-H(57)	119.1
C(58)-C(57)-H(57)	119.1
C(53)-C(58)-C(57)	116.5(8)
C(53)-C(58)-C(59)	124.4(6)
C(57)-C(58)-C(59)	119.0(7)
C(60)-C(59)-C(64)	115.3(8)
C(60)-C(59)-C(58)	119.4(7)
C(64)-C(59)-C(58)	125.2(6)
C(61)-C(60)-C(59)	122.9(8)
C(61)-C(60)-H(60)	118.5
C(59)-C(60)-H(60)	118.5
C(60)-C(61)-C(62)	120.9(8)
C(60)-C(61)-H(61)	119.6
C(62)-C(61)-H(61)	119.6
C(63)-C(62)-C(61)	117.1(8)
C(63)-C(62)-H(62)	121.5
C(61)-C(62)-H(62)	121.5
C(64)-C(63)-C(62)	122.0(8)
C(64)-C(63)-H(63)	119.0
C(62)-C(63)-H(63)	119.0
O(12)-C(64)-C(63)	118.1(7)
O(12)-C(64)-C(59)	120.1(7)

C(63)-C(64)-C(59)	121.8(7)
O(16)-C(65)-C(66)	122.0(7)
O(16)-C(65)-C(68)	117.4(6)
C(66)-C(65)-C(68)	120.6(6)
C(67)-C(66)-C(65)	120.8(7)
C(67)-C(66)-H(66)	119.6
C(65)-C(66)-H(66)	119.6
O(17)-C(67)-C(66)	127.2(6)
O(17)-C(67)-C(74)	114.4(6)
C(66)-C(67)-C(74)	118.3(6)
C(69)-C(68)-C(73)	118.6(7)
C(69)-C(68)-C(65)	122.0(6)
C(73)-C(68)-C(65)	119.0(7)
C(68)-C(69)-C(70)	121.2(7)
C(68)-C(69)-H(69)	119.4
C(70)-C(69)-H(69)	119.4
C(71)-C(70)-C(69)	119.5(8)
C(71)-C(70)-H(70)	120.2
C(69)-C(70)-H(70)	120.2
C(70)-C(71)-C(72)	119.8(8)
C(70)-C(71)-H(71)	120.1
C(72)-C(71)-H(71)	120.1
C(73)-C(72)-C(71)	120.0(8)
C(73)-C(72)-H(72)	120.0
C(71)-C(72)-H(72)	120.0
C(72)-C(73)-C(68)	120.9(8)
C(72)-C(73)-H(73)	119.5
C(68)-C(73)-H(73)	119.5
F(15)-C(74)-F(13)	105.6(6)
F(15)-C(74)-F(14)	107.1(6)
F(13)-C(74)-F(14)	106.0(7)
F(15)-C(74)-C(67)	111.8(7)
F(13)-C(74)-C(67)	112.6(6)
F(14)-C(74)-C(67)	113.2(6)
O(18)-C(75)-C(80)	118.7(7)
O(18)-C(75)-C(76)	121.9(6)

C(80)-C(75)-C(76)	119.4(7)
C(77)-C(76)-C(75)	117.6(7)
C(77)-C(76)-C(76)#1	118.9(5)
C(75)-C(76)-C(76)#1	123.4(5)
C(78)-C(77)-C(76)	122.7(8)
C(78)-C(77)-H(77)	118.7
C(76)-C(77)-H(77)	118.7
C(77)-C(78)-C(79)	118.9(8)
C(77)-C(78)-H(78)	120.5
C(79)-C(78)-H(78)	120.5
C(80)-C(79)-C(78)	119.6(7)
C(80)-C(79)-H(79)	120.2
C(78)-C(79)-H(79)	120.2
C(79)-C(80)-C(75)	121.7(8)
C(79)-C(80)-H(80)	119.2
C(75)-C(80)-H(80)	119.2
O(13)-C(81)-C(82)	120.7(6)
O(13)-C(81)-C(84)	116.5(6)
C(82)-C(81)-C(84)	122.8(6)
C(83)-C(82)-C(81)	122.9(7)
C(83)-C(82)-H(82)	118.6
C(81)-C(82)-H(82)	118.6
O(14)-C(83)-C(82)	126.9(7)
O(14)-C(83)-C(90)	114.6(6)
C(82)-C(83)-C(90)	118.5(6)
C(85)-C(84)-C(89)	119.5(7)
C(85)-C(84)-C(81)	119.0(7)
C(89)-C(84)-C(81)	121.0(7)
C(86)-C(85)-C(84)	121.5(8)
C(86)-C(85)-H(85)	119.2
C(84)-C(85)-H(85)	119.2
C(85)-C(86)-C(87)	118.1(8)
C(85)-C(86)-H(86)	120.9
C(87)-C(86)-H(86)	120.9
C(88)-C(87)-C(86)	121.2(8)
C(88)-C(87)-H(87)	119.4

C(86)-C(87)-H(87)	119.4
C(87)-C(88)-C(89)	119.7(8)
C(87)-C(88)-H(88)	120.1
C(89)-C(88)-H(88)	120.1
C(88)-C(89)-C(84)	119.8(7)
C(88)-C(89)-H(89)	120.1
C(84)-C(89)-H(89)	120.1
F(18)-C(90)-F(17)	108.5(7)
F(18)-C(90)-F(16)	106.4(6)
F(17)-C(90)-F(16)	106.6(5)
F(18)-C(90)-C(83)	112.9(6)
F(17)-C(90)-C(83)	112.6(6)
F(16)-C(90)-C(83)	109.5(6)
O(15)-C(91)-C(92)	122.2(6)
O(15)-C(91)-C(96)	117.7(7)
C(92)-C(91)-C(96)	120.0(7)
C(93)-C(92)-C(91)	118.1(7)
C(93)-C(92)-C(92)#2	118.7(5)
C(91)-C(92)-C(92)#2	123.2(5)
C(94)-C(93)-C(92)	122.2(8)
C(94)-C(93)-H(93)	118.9
C(92)-C(93)-H(93)	118.9
C(93)-C(94)-C(95)	119.4(8)
C(93)-C(94)-H(94)	120.3
C(95)-C(94)-H(94)	120.3
C(96)-C(95)-C(94)	120.7(8)
C(96)-C(95)-H(95)	119.6
C(94)-C(95)-H(95)	119.6
C(95)-C(96)-C(91)	119.6(8)
C(95)-C(96)-H(96)	120.2
C(91)-C(96)-H(96)	120.2

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_mljc03x2_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ti(1)	25(1)	41(1)	25(1)	-1(1)	5(1)	-7(1)
Ti(2)	23(1)	41(1)	27(1)	1(1)	6(1)	2(1)
Ti(3)	24(1)	27(1)	37(1)	0	5(1)	0
Ti(4)	24(1)	27(1)	38(1)	0	4(1)	0
O(1)	33(3)	41(3)	26(2)	2(2)	5(2)	7(2)
O(2)	32(3)	44(3)	26(3)	10(2)	6(2)	0(2)
O(3)	32(3)	51(4)	28(3)	4(2)	6(2)	-19(3)
O(4)	26(2)	57(4)	26(3)	5(2)	5(2)	-12(3)
O(5)	31(3)	36(3)	30(3)	-1(2)	4(2)	-8(2)
O(6)	29(2)	34(3)	32(3)	-9(2)	8(2)	-7(2)
O(7)	29(3)	39(3)	31(3)	-4(2)	9(2)	-11(2)
O(8)	32(3)	55(4)	26(3)	11(2)	8(2)	-4(3)
O(9)	28(2)	51(3)	26(2)	10(2)	5(2)	15(3)
O(10)	28(2)	50(3)	29(3)	9(2)	5(2)	12(2)
O(11)	26(2)	37(3)	35(3)	-3(2)	8(2)	1(2)
O(12)	26(2)	37(3)	34(3)	-5(2)	5(2)	8(2)
O(13)	29(3)	27(3)	36(3)	4(2)	4(2)	-3(2)
O(14)	33(3)	35(3)	38(3)	4(2)	3(2)	-4(2)
O(15)	22(2)	31(3)	46(3)	0(2)	7(2)	0(2)
O(16)	31(3)	26(3)	37(3)	-3(2)	8(2)	1(2)
O(17)	34(3)	31(3)	39(3)	-8(2)	8(2)	-6(2)
O(18)	24(2)	31(3)	43(3)	1(2)	3(2)	0(2)
F(1)	82(5)	136(8)	183(9)	-19(7)	-88(6)	20(5)
F(2)	109(5)	364(17)	130(7)	160(9)	76(5)	168(9)
F(3)	37(3)	60(4)	266(11)	58(6)	-24(4)	12(3)
F(4)	27(3)	89(5)	167(7)	70(5)	28(3)	8(3)
F(5)	139(7)	325(15)	51(4)	-8(6)	13(4)	-185(9)
F(6)	51(3)	44(3)	90(4)	12(3)	30(3)	-14(2)
F(7)	43(3)	67(4)	116(5)	46(4)	16(3)	-14(3)
F(8)	24(3)	92(5)	208(8)	83(5)	37(4)	10(3)
F(9)	122(6)	288(14)	71(4)	-45(6)	34(4)	-165(8)

F(10)	204(10)	396(19)	88(5)	105(8)	76(6)	263(13)
F(11)	49(4)	94(6)	333(15)	79(8)	-95(6)	-10(4)
F(12)	62(4)	70(4)	107(5)	37(4)	3(3)	19(3)
F(13)	37(3)	105(5)	57(3)	-19(3)	16(2)	-4(3)
F(14)	75(3)	35(3)	46(3)	-10(2)	26(2)	-14(2)
F(15)	84(4)	46(3)	45(3)	12(2)	28(3)	-1(3)
F(16)	88(4)	45(3)	35(2)	-13(2)	-2(2)	2(3)
F(17)	70(3)	39(3)	34(2)	9(2)	-3(2)	-10(2)
F(18)	38(3)	102(5)	50(3)	17(3)	-5(2)	-2(3)
C(1)	22(3)	37(4)	25(3)	8(3)	5(3)	-3(3)
C(2)	28(4)	53(5)	33(4)	17(4)	7(3)	5(4)
C(3)	27(4)	45(5)	30(4)	12(3)	3(3)	-4(3)
C(4)	26(4)	41(5)	30(4)	1(3)	2(3)	-8(3)
C(5)	31(4)	66(6)	25(4)	11(4)	3(3)	-20(4)
C(6)	34(4)	45(5)	34(4)	9(4)	6(3)	-11(4)
C(7)	27(4)	32(4)	33(4)	4(3)	9(3)	-6(3)
C(8)	34(4)	37(5)	34(4)	8(3)	3(3)	3(3)
C(9)	43(4)	53(5)	35(4)	12(4)	-6(3)	10(4)
C(10)	52(5)	47(5)	32(4)	13(4)	0(4)	-8(4)
C(11)	58(5)	63(6)	36(4)	15(5)	24(4)	3(5)
C(12)	43(4)	53(5)	36(4)	10(4)	18(3)	11(4)
C(13)	43(5)	57(6)	38(4)	23(4)	3(4)	5(4)
C(14)	28(4)	43(5)	26(3)	7(3)	6(3)	-7(4)
C(15)	43(5)	45(5)	32(4)	8(4)	5(3)	-12(4)
C(16)	49(5)	50(5)	46(5)	15(4)	19(4)	-17(4)
C(17)	50(5)	55(6)	34(4)	11(4)	15(4)	-4(4)
C(18)	39(4)	60(6)	38(4)	8(4)	1(3)	-4(4)
C(19)	38(4)	53(5)	30(4)	6(4)	3(3)	-16(4)
C(20)	45(5)	94(8)	37(5)	6(5)	9(4)	-38(6)
C(21)	32(4)	44(5)	32(4)	-8(4)	6(3)	-16(4)
C(22)	49(5)	49(5)	39(4)	2(4)	1(4)	-27(4)
C(23)	71(6)	70(7)	36(5)	-12(5)	13(4)	-42(6)
C(24)	64(6)	71(7)	50(5)	-20(5)	31(5)	-36(6)
C(25)	50(5)	51(5)	52(5)	-27(5)	27(4)	-16(4)
C(26)	40(4)	31(4)	37(4)	-9(3)	13(3)	-14(3)
C(27)	32(4)	34(4)	40(4)	-14(3)	10(3)	-3(3)

C(28)	33(4)	47(5)	60(6)	-21(5)	9(4)	4(4)
C(29)	43(5)	43(5)	67(6)	-16(5)	-6(4)	14(4)
C(30)	62(6)	35(5)	44(5)	-8(4)	8(4)	12(4)
C(31)	39(4)	37(5)	44(4)	-5(4)	13(3)	-4(4)
C(32)	27(4)	37(4)	30(4)	-8(3)	9(3)	1(3)
C(33)	21(3)	34(4)	30(3)	11(3)	7(3)	3(3)
C(34)	22(3)	47(5)	30(4)	8(3)	-1(3)	-8(3)
C(35)	15(3)	41(5)	42(4)	2(4)	7(3)	-4(3)
C(36)	26(4)	42(5)	34(4)	10(3)	13(3)	15(3)
C(37)	28(4)	83(7)	35(4)	25(4)	17(3)	22(4)
C(38)	22(3)	51(5)	38(4)	15(4)	8(3)	6(3)
C(39)	26(3)	36(4)	30(4)	5(3)	7(3)	7(3)
C(40)	29(4)	44(5)	36(4)	10(4)	8(3)	1(3)
C(41)	48(5)	64(6)	25(4)	13(4)	2(3)	13(5)
C(42)	51(5)	53(6)	35(5)	16(4)	20(4)	18(5)
C(43)	50(5)	59(6)	57(6)	20(5)	30(4)	1(5)
C(44)	35(4)	49(5)	34(4)	8(4)	13(3)	-9(4)
C(45)	33(4)	76(7)	42(5)	18(5)	7(3)	-12(5)
C(46)	28(4)	44(5)	36(4)	9(4)	9(3)	13(4)
C(47)	47(5)	42(5)	29(4)	7(3)	5(3)	9(4)
C(48)	52(5)	49(5)	37(4)	17(4)	9(4)	16(4)
C(49)	63(5)	55(6)	25(4)	16(4)	6(4)	5(5)
C(50)	64(6)	66(6)	36(4)	14(4)	27(4)	21(5)
C(51)	41(5)	63(6)	42(5)	17(4)	21(4)	23(4)
C(52)	20(4)	111(8)	40(4)	39(6)	10(3)	20(5)
C(53)	26(4)	36(4)	33(4)	-2(3)	12(3)	15(3)
C(54)	49(5)	41(5)	49(5)	5(4)	15(4)	17(4)
C(55)	68(6)	71(7)	42(5)	10(5)	15(4)	36(6)
C(56)	64(6)	74(7)	32(5)	-14(5)	-6(4)	31(6)
C(57)	43(5)	60(6)	49(5)	-19(5)	-10(4)	7(4)
C(58)	31(4)	37(5)	34(4)	-11(3)	0(3)	8(3)
C(59)	25(4)	34(4)	43(4)	-17(4)	2(3)	-5(3)
C(60)	28(4)	34(5)	61(5)	-16(4)	10(3)	-3(3)
C(61)	39(5)	51(6)	64(6)	-24(5)	17(4)	-14(4)
C(62)	44(5)	41(5)	50(5)	-15(4)	16(4)	-17(4)
C(63)	30(4)	40(5)	38(4)	-7(4)	4(3)	-1(3)

C(64)	26(4)	42(5)	29(4)	-11(3)	3(3)	1(3)
C(65)	37(4)	21(4)	29(3)	8(3)	2(3)	5(3)
C(66)	42(4)	45(5)	24(4)	3(3)	6(3)	-11(4)
C(67)	32(4)	21(4)	29(4)	5(3)	8(3)	2(3)
C(68)	32(4)	24(4)	28(4)	0(3)	1(3)	-2(3)
C(69)	61(5)	32(4)	30(4)	3(3)	-5(3)	-15(4)
C(70)	53(5)	45(5)	38(5)	1(4)	-5(4)	-10(4)
C(71)	53(5)	74(7)	44(5)	-13(5)	0(4)	-11(5)
C(72)	57(6)	99(9)	36(5)	-23(5)	20(4)	-20(6)
C(73)	37(4)	56(6)	51(5)	-19(4)	15(4)	-7(4)
C(74)	40(4)	40(5)	32(4)	-1(4)	5(3)	-5(4)
C(75)	20(3)	30(4)	41(4)	0(3)	0(3)	-2(3)
C(76)	28(4)	26(4)	41(4)	2(3)	5(3)	-3(3)
C(77)	42(4)	35(4)	47(5)	3(4)	0(3)	13(4)
C(78)	43(5)	45(5)	52(5)	-11(4)	7(4)	7(4)
C(79)	47(5)	57(6)	34(4)	-2(4)	8(3)	4(4)
C(80)	32(4)	44(5)	42(4)	1(4)	4(3)	0(4)
C(81)	39(4)	15(3)	33(4)	1(3)	11(3)	3(3)
C(82)	40(4)	36(4)	33(4)	-13(3)	15(3)	-19(3)
C(83)	30(4)	20(4)	35(4)	-6(3)	6(3)	2(3)
C(84)	35(4)	22(4)	35(4)	-4(3)	11(3)	-2(3)
C(85)	43(5)	52(5)	40(5)	11(4)	-4(4)	-11(4)
C(86)	67(6)	113(10)	30(5)	11(6)	-1(4)	-19(7)
C(87)	60(6)	75(7)	50(5)	5(5)	19(4)	-15(5)
C(88)	55(5)	43(5)	45(5)	-7(4)	20(4)	-14(4)
C(89)	57(5)	33(4)	39(4)	-10(4)	18(4)	-12(4)
C(90)	40(4)	34(4)	34(4)	-1(4)	8(3)	-13(4)
C(91)	22(3)	30(4)	43(4)	3(3)	7(3)	1(3)
C(92)	28(4)	24(4)	43(4)	0(3)	7(3)	-3(3)
C(93)	46(5)	45(5)	48(5)	-5(4)	5(4)	11(4)
C(94)	43(4)	44(5)	49(5)	11(4)	6(4)	9(4)
C(95)	51(5)	43(5)	40(5)	3(4)	2(4)	0(4)
C(96)	40(4)	40(5)	40(4)	-1(4)	12(3)	4(4)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_mljc03x2_0m_a.

	x	y	z	U(eq)
H(2)	7218	3860	-721	45
H(5)	7194	6197	2913	49
H(8)	6518	6574	-1350	42
H(9)	6402	7206	-2625	54
H(10)	6610	6165	-3534	53
H(11)	6938	4549	-3182	61
H(12)	7061	3934	-1911	51
H(15)	6523	3310	2878	48
H(16)	6391	2828	4044	57
H(17)	6596	3949	5139	55
H(18)	6894	5795	5068	55
H(19)	7033	6232	3905	49
H(22)	6343	1543	1609	56
H(23)	5990	1298	2205	70
H(24)	5661	2952	1982	71
H(25)	5687	4909	1207	59
H(28)	5661	5466	-73	56
H(29)	5631	7459	-890	63
H(30)	5980	8937	-934	56
H(31)	6364	8399	-168	47
H(34)	7806	3921	2179	40
H(37)	7805	6456	5797	57
H(40)	7976	3905	1153	43
H(41)	8097	4530	6	56
H(42)	8412	6252	-33	54
H(43)	8610	7357	1066	64
H(44)	8492	6756	2234	46
H(47)	8474	3466	6459	47
H(48)	8576	2852	7741	55
H(49)	8356	3962	8629	57

H(50)	8038	5655	8229	64
H(51)	7934	6259	6974	57
H(54)	8665	1623	5378	55
H(55)	9023	1389	6302	72
H(56)	9356	3014	6357	70
H(57)	9335	4940	5517	63
H(60)	9345	5493	4261	49
H(61)	9375	7419	3478	61
H(62)	9024	8980	3110	53
H(63)	8649	8473	3567	43
H(66)	5711	5045	4859	44
H(69)	5779	6912	5564	50
H(70)	5981	8273	6590	56
H(71)	5872	7922	7779	69
H(72)	5561	6157	7949	75
H(73)	5354	4899	6929	56
H(77)	5149	-3188	4582	51
H(78)	5153	-3385	3293	56
H(79)	5026	-1383	2502	55
H(80)	4883	716	3009	48
H(82)	5701	10026	826	42
H(85)	5354	9842	-1579	56
H(86)	5565	11057	-2418	85
H(87)	5859	12908	-1947	72
H(88)	5973	13261	-664	56
H(89)	5772	11941	181	50
H(93)	5154	1787	566	56
H(94)	5160	1608	1859	55
H(95)	5028	3578	2523	54
H(96)	4888	5713	1894	47

Table 6. Torsion angles [°] for mo_mljc03x2_0m_a.

O(6)-Ti(1)-O(5)-C(21)	-45.6(6)
O(1)-Ti(1)-O(5)-C(21)	-135.3(6)
O(3)-Ti(1)-O(5)-C(21)	50.1(6)
O(2)-Ti(1)-O(5)-C(21)	141.9(6)
O(5)-Ti(1)-O(6)-C(32)	-39.9(6)
O(1)-Ti(1)-O(6)-C(32)	57.2(6)
O(3)-Ti(1)-O(6)-C(32)	-128.9(6)
O(4)-Ti(1)-O(6)-C(32)	147.7(6)
O(12)-Ti(2)-O(11)-C(53)	43.1(6)
O(9)-Ti(2)-O(11)-C(53)	-53.8(6)
O(7)-Ti(2)-O(11)-C(53)	132.2(6)
O(8)-Ti(2)-O(11)-C(53)	-144.3(6)
O(11)-Ti(2)-O(12)-C(64)	43.2(6)
O(9)-Ti(2)-O(12)-C(64)	133.0(6)
O(7)-Ti(2)-O(12)-C(64)	-54.0(6)
O(10)-Ti(2)-O(12)-C(64)	-144.2(6)
O(15)#2-Ti(4)-O(15)-C(91)	43.8(5)
O(14)-Ti(4)-O(15)-C(91)	-55.6(6)
O(14)#2-Ti(4)-O(15)-C(91)	132.3(6)
O(13)#2-Ti(4)-O(15)-C(91)	-145.4(6)
O(18)#1-Ti(3)-O(18)-C(75)	-43.7(5)
O(17)#1-Ti(3)-O(18)-C(75)	-132.1(6)
O(17)-Ti(3)-O(18)-C(75)	56.4(6)
O(16)#1-Ti(3)-O(18)-C(75)	146.0(6)
Ti(1)-O(1)-C(1)-C(2)	-2.7(11)
Ti(1)-O(1)-C(1)-C(7)	177.1(5)
O(1)-C(1)-C(2)-C(3)	12.7(12)
C(7)-C(1)-C(2)-C(3)	-167.0(8)
Ti(1)-O(2)-C(3)-C(2)	-23.1(12)
Ti(1)-O(2)-C(3)-C(13)	158.2(6)
C(1)-C(2)-C(3)-O(2)	0.5(14)
C(1)-C(2)-C(3)-C(13)	179.1(8)
Ti(1)-O(3)-C(4)-C(5)	-12.2(12)
Ti(1)-O(3)-C(4)-C(14)	170.6(5)

O(3)-C(4)-C(5)-C(6)	12.1(13)
C(14)-C(4)-C(5)-C(6)	-170.7(8)
Ti(1)-O(4)-C(6)-C(5)	-9.5(13)
Ti(1)-O(4)-C(6)-C(20)	167.3(6)
C(4)-C(5)-C(6)-O(4)	-1.5(15)
C(4)-C(5)-C(6)-C(20)	-178.1(9)
O(1)-C(1)-C(7)-C(8)	9.6(10)
C(2)-C(1)-C(7)-C(8)	-170.6(7)
O(1)-C(1)-C(7)-C(12)	-167.6(7)
C(2)-C(1)-C(7)-C(12)	12.1(11)
C(12)-C(7)-C(8)-C(9)	-0.7(11)
C(1)-C(7)-C(8)-C(9)	-178.1(7)
C(7)-C(8)-C(9)-C(10)	1.0(12)
C(8)-C(9)-C(10)-C(11)	-0.6(13)
C(9)-C(10)-C(11)-C(12)	0.1(14)
C(10)-C(11)-C(12)-C(7)	0.1(14)
C(8)-C(7)-C(12)-C(11)	0.2(12)
C(1)-C(7)-C(12)-C(11)	177.6(8)
O(2)-C(3)-C(13)-F(2)	-179.1(11)
C(2)-C(3)-C(13)-F(2)	2.1(15)
O(2)-C(3)-C(13)-F(3)	53.9(11)
C(2)-C(3)-C(13)-F(3)	-124.9(9)
O(2)-C(3)-C(13)-F(1)	-61.2(11)
C(2)-C(3)-C(13)-F(1)	120.0(10)
O(3)-C(4)-C(14)-C(15)	7.2(11)
C(5)-C(4)-C(14)-C(15)	-170.1(8)
O(3)-C(4)-C(14)-C(19)	-168.0(8)
C(5)-C(4)-C(14)-C(19)	14.8(12)
C(19)-C(14)-C(15)-C(16)	-1.5(12)
C(4)-C(14)-C(15)-C(16)	-176.7(8)
C(14)-C(15)-C(16)-C(17)	-0.9(13)
C(15)-C(16)-C(17)-C(18)	4.3(14)
C(16)-C(17)-C(18)-C(19)	-5.1(13)
C(15)-C(14)-C(19)-C(18)	0.6(13)
C(4)-C(14)-C(19)-C(18)	175.7(8)
C(17)-C(18)-C(19)-C(14)	2.7(13)

O(4)-C(6)-C(20)-F(4)	-74.9(10)
C(5)-C(6)-C(20)-F(4)	102.1(10)
O(4)-C(6)-C(20)-F(5)	162.9(10)
C(5)-C(6)-C(20)-F(5)	-20.1(16)
O(4)-C(6)-C(20)-F(6)	43.0(12)
C(5)-C(6)-C(20)-F(6)	-139.9(8)
Ti(1)-O(5)-C(21)-C(26)	66.7(9)
Ti(1)-O(5)-C(21)-C(22)	-115.3(7)
O(5)-C(21)-C(22)-C(23)	-179.3(7)
C(26)-C(21)-C(22)-C(23)	-1.3(11)
C(21)-C(22)-C(23)-C(24)	1.7(12)
C(22)-C(23)-C(24)-C(25)	-1.2(13)
C(23)-C(24)-C(25)-C(26)	0.4(13)
O(5)-C(21)-C(26)-C(25)	178.4(7)
C(22)-C(21)-C(26)-C(25)	0.5(10)
O(5)-C(21)-C(26)-C(27)	1.2(11)
C(22)-C(21)-C(26)-C(27)	-176.7(7)
C(24)-C(25)-C(26)-C(21)	0.0(12)
C(24)-C(25)-C(26)-C(27)	177.3(7)
C(21)-C(26)-C(27)-C(28)	137.3(8)
C(25)-C(26)-C(27)-C(28)	-39.8(10)
C(21)-C(26)-C(27)-C(32)	-43.2(11)
C(25)-C(26)-C(27)-C(32)	139.7(8)
C(32)-C(27)-C(28)-C(29)	-1.3(11)
C(26)-C(27)-C(28)-C(29)	178.2(7)
C(27)-C(28)-C(29)-C(30)	0.4(12)
C(28)-C(29)-C(30)-C(31)	0.6(12)
C(29)-C(30)-C(31)-C(32)	-0.7(12)
Ti(1)-O(6)-C(32)-C(31)	-117.2(7)
Ti(1)-O(6)-C(32)-C(27)	64.9(8)
C(30)-C(31)-C(32)-O(6)	-178.2(7)
C(30)-C(31)-C(32)-C(27)	-0.3(11)
C(28)-C(27)-C(32)-O(6)	179.1(6)
C(26)-C(27)-C(32)-O(6)	-0.4(11)
C(28)-C(27)-C(32)-C(31)	1.2(10)
C(26)-C(27)-C(32)-C(31)	-178.2(7)

Ti(2)-O(7)-C(33)-C(34)	3.4(11)
Ti(2)-O(7)-C(33)-C(39)	-177.0(5)
O(7)-C(33)-C(34)-C(35)	-11.8(12)
C(39)-C(33)-C(34)-C(35)	168.5(7)
Ti(2)-O(8)-C(35)-C(34)	18.4(12)
Ti(2)-O(8)-C(35)-C(45)	-161.8(6)
C(33)-C(34)-C(35)-O(8)	0.5(14)
C(33)-C(34)-C(35)-C(45)	-179.2(8)
Ti(2)-O(9)-C(36)-C(37)	6.1(13)
Ti(2)-O(9)-C(36)-C(46)	-172.6(5)
O(9)-C(36)-C(37)-C(38)	-7.2(14)
C(46)-C(36)-C(37)-C(38)	171.3(9)
Ti(2)-O(10)-C(38)-C(37)	12.6(13)
Ti(2)-O(10)-C(38)-C(52)	-169.5(6)
C(36)-C(37)-C(38)-O(10)	-2.0(15)
C(36)-C(37)-C(38)-C(52)	-179.7(9)
O(7)-C(33)-C(39)-C(44)	-12.6(10)
C(34)-C(33)-C(39)-C(44)	167.1(7)
O(7)-C(33)-C(39)-C(40)	165.6(7)
C(34)-C(33)-C(39)-C(40)	-14.7(11)
C(44)-C(39)-C(40)-C(41)	-0.2(11)
C(33)-C(39)-C(40)-C(41)	-178.4(7)
C(39)-C(40)-C(41)-C(42)	0.0(12)
C(40)-C(41)-C(42)-C(43)	0.2(13)
C(41)-C(42)-C(43)-C(44)	-0.2(13)
C(40)-C(39)-C(44)-C(43)	0.2(12)
C(33)-C(39)-C(44)-C(43)	178.4(7)
C(42)-C(43)-C(44)-C(39)	0.0(13)
O(8)-C(35)-C(45)-F(7)	-30.1(11)
C(34)-C(35)-C(45)-F(7)	149.7(8)
O(8)-C(35)-C(45)-F(8)	88.7(9)
C(34)-C(35)-C(45)-F(8)	-91.5(9)
O(8)-C(35)-C(45)-F(9)	-149.9(10)
C(34)-C(35)-C(45)-F(9)	29.9(13)
O(9)-C(36)-C(46)-C(47)	-5.8(12)
C(37)-C(36)-C(46)-C(47)	175.6(8)

O(9)-C(36)-C(46)-C(51)	170.6(8)
C(37)-C(36)-C(46)-C(51)	-8.1(13)
C(51)-C(46)-C(47)-C(48)	2.5(13)
C(36)-C(46)-C(47)-C(48)	178.9(8)
C(46)-C(47)-C(48)-C(49)	-1.3(13)
C(47)-C(48)-C(49)-C(50)	-0.2(14)
C(48)-C(49)-C(50)-C(51)	0.4(15)
C(49)-C(50)-C(51)-C(46)	0.9(15)
C(47)-C(46)-C(51)-C(50)	-2.3(14)
C(36)-C(46)-C(51)-C(50)	-178.7(9)
O(10)-C(38)-C(52)-F(10)	-161.7(12)
C(37)-C(38)-C(52)-F(10)	16.3(17)
O(10)-C(38)-C(52)-F(12)	-36.4(12)
C(37)-C(38)-C(52)-F(12)	141.7(9)
O(10)-C(38)-C(52)-F(11)	80.9(10)
C(37)-C(38)-C(52)-F(11)	-101.0(11)
Ti(2)-O(11)-C(53)-C(58)	-65.0(8)
Ti(2)-O(11)-C(53)-C(54)	116.4(7)
O(11)-C(53)-C(54)-C(55)	-179.7(7)
C(58)-C(53)-C(54)-C(55)	1.7(11)
C(53)-C(54)-C(55)-C(56)	-2.3(12)
C(54)-C(55)-C(56)-C(57)	0.9(13)
C(55)-C(56)-C(57)-C(58)	1.2(13)
O(11)-C(53)-C(58)-C(57)	-178.2(7)
C(54)-C(53)-C(58)-C(57)	0.3(10)
O(11)-C(53)-C(58)-C(59)	-2.1(11)
C(54)-C(53)-C(58)-C(59)	176.4(7)
C(56)-C(57)-C(58)-C(53)	-1.8(12)
C(56)-C(57)-C(58)-C(59)	-178.1(7)
C(53)-C(58)-C(59)-C(60)	-137.7(7)
C(57)-C(58)-C(59)-C(60)	38.3(10)
C(53)-C(58)-C(59)-C(64)	44.4(11)
C(57)-C(58)-C(59)-C(64)	-139.6(8)
C(64)-C(59)-C(60)-C(61)	0.8(11)
C(58)-C(59)-C(60)-C(61)	-177.3(7)
C(59)-C(60)-C(61)-C(62)	0.2(12)

C(60)-C(61)-C(62)-C(63)	-0.4(12)
C(61)-C(62)-C(63)-C(64)	-0.5(11)
Ti(2)-O(12)-C(64)-C(63)	116.2(7)
Ti(2)-O(12)-C(64)-C(59)	-66.4(8)
C(62)-C(63)-C(64)-O(12)	178.9(7)
C(62)-C(63)-C(64)-C(59)	1.6(11)
C(60)-C(59)-C(64)-O(12)	-179.0(6)
C(58)-C(59)-C(64)-O(12)	-1.0(11)
C(60)-C(59)-C(64)-C(63)	-1.7(10)
C(58)-C(59)-C(64)-C(63)	176.3(7)
Ti(3)-O(16)-C(65)-C(66)	7.2(10)
Ti(3)-O(16)-C(65)-C(68)	-170.4(5)
O(16)-C(65)-C(66)-C(67)	-1.8(11)
C(68)-C(65)-C(66)-C(67)	175.7(6)
Ti(3)-O(17)-C(67)-C(66)	-8.2(11)
Ti(3)-O(17)-C(67)-C(74)	175.3(5)
C(65)-C(66)-C(67)-O(17)	2.5(12)
C(65)-C(66)-C(67)-C(74)	178.8(7)
O(16)-C(65)-C(68)-C(69)	-162.7(7)
C(66)-C(65)-C(68)-C(69)	19.7(11)
O(16)-C(65)-C(68)-C(73)	24.9(10)
C(66)-C(65)-C(68)-C(73)	-152.7(7)
C(73)-C(68)-C(69)-C(70)	-1.8(12)
C(65)-C(68)-C(69)-C(70)	-174.2(8)
C(68)-C(69)-C(70)-C(71)	1.3(14)
C(69)-C(70)-C(71)-C(72)	0.5(15)
C(70)-C(71)-C(72)-C(73)	-1.8(16)
C(71)-C(72)-C(73)-C(68)	1.4(15)
C(69)-C(68)-C(73)-C(72)	0.4(13)
C(65)-C(68)-C(73)-C(72)	173.1(8)
O(17)-C(67)-C(74)-F(15)	98.0(7)
C(66)-C(67)-C(74)-F(15)	-78.8(8)
O(17)-C(67)-C(74)-F(13)	-143.3(7)
C(66)-C(67)-C(74)-F(13)	39.9(10)
O(17)-C(67)-C(74)-F(14)	-23.2(9)
C(66)-C(67)-C(74)-F(14)	160.1(7)

Ti(3)-O(18)-C(75)-C(80)	-114.5(7)
Ti(3)-O(18)-C(75)-C(76)	67.2(9)
O(18)-C(75)-C(76)-C(77)	178.9(6)
C(80)-C(75)-C(76)-C(77)	0.6(10)
O(18)-C(75)-C(76)-C(76)#1	1.2(12)
C(80)-C(75)-C(76)-C(76)#1	-177.1(8)
C(75)-C(76)-C(77)-C(78)	-1.3(12)
C(76)#1-C(76)-C(77)-C(78)	176.5(8)
C(76)-C(77)-C(78)-C(79)	1.7(12)
C(77)-C(78)-C(79)-C(80)	-1.3(12)
C(78)-C(79)-C(80)-C(75)	0.7(12)
O(18)-C(75)-C(80)-C(79)	-178.7(7)
C(76)-C(75)-C(80)-C(79)	-0.3(11)
Ti(4)-O(13)-C(81)-C(82)	-6.8(10)
Ti(4)-O(13)-C(81)-C(84)	171.4(5)
O(13)-C(81)-C(82)-C(83)	2.7(11)
C(84)-C(81)-C(82)-C(83)	-175.4(7)
Ti(4)-O(14)-C(83)-C(82)	6.3(11)
Ti(4)-O(14)-C(83)-C(90)	-175.0(5)
C(81)-C(82)-C(83)-O(14)	-2.7(12)
C(81)-C(82)-C(83)-C(90)	178.6(7)
O(13)-C(81)-C(84)-C(85)	-25.7(10)
C(82)-C(81)-C(84)-C(85)	152.5(8)
O(13)-C(81)-C(84)-C(89)	162.0(7)
C(82)-C(81)-C(84)-C(89)	-19.8(11)
C(89)-C(84)-C(85)-C(86)	0.5(13)
C(81)-C(84)-C(85)-C(86)	-171.9(9)
C(84)-C(85)-C(86)-C(87)	-3.1(15)
C(85)-C(86)-C(87)-C(88)	4.3(16)
C(86)-C(87)-C(88)-C(89)	-2.8(15)
C(87)-C(88)-C(89)-C(84)	0.1(13)
C(85)-C(84)-C(89)-C(88)	1.1(12)
C(81)-C(84)-C(89)-C(88)	173.4(7)
O(14)-C(83)-C(90)-F(18)	141.3(7)
C(82)-C(83)-C(90)-F(18)	-39.8(10)
O(14)-C(83)-C(90)-F(17)	18.0(9)

C(82)-C(83)-C(90)-F(17)	-163.1(6)
O(14)-C(83)-C(90)-F(16)	-100.3(7)
C(82)-C(83)-C(90)-F(16)	78.6(8)
Ti(4)-O(15)-C(91)-C(92)	-68.5(8)
Ti(4)-O(15)-C(91)-C(96)	113.6(7)
O(15)-C(91)-C(92)-C(93)	-179.3(6)
C(96)-C(91)-C(92)-C(93)	-1.4(11)
O(15)-C(91)-C(92)-C(92)#2	0.4(12)
C(96)-C(91)-C(92)-C(92)#2	178.3(8)
C(91)-C(92)-C(93)-C(94)	2.5(12)
C(92)#2-C(92)-C(93)-C(94)	-177.3(8)
C(92)-C(93)-C(94)-C(95)	-1.8(13)
C(93)-C(94)-C(95)-C(96)	0.0(13)
C(94)-C(95)-C(96)-C(91)	0.9(12)
O(15)-C(91)-C(96)-C(95)	177.7(7)
C(92)-C(91)-C(96)-C(95)	-0.2(11)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for mo_mljc03x2_0m_a [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
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[Ti(tfba)₂(μ-O)]₄ (4)

Table 1. Crystal data and structure refinement for mo_jcti.

Identification code	shelx	
Empirical formula	C ₈₀ H ₄₈ F ₂₄ O ₂₀ Ti ₄	
Formula weight	1976.78	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c c n	
Unit cell dimensions	a = 38.492(6) Å	α = 90°.
	b = 20.574(11) Å	β = 90°.
	c = 21.340(13) Å	γ = 90°.
Volume	16900(14) Å ³	
Z	8	
Density (calculated)	1.554 Mg/m ³	
Absorption coefficient	0.486 mm ⁻¹	
F(000)	7936	
Crystal size	0.251 x 0.181 x 0.135 mm ³	
Theta range for data collection	2.182 to 25.349°.	
Index ranges	-46 ≤ h ≤ 46, -24 ≤ k ≤ 24, -25 ≤ l ≤ 25	
Reflections collected	360658	
Independent reflections	15473 [R(int) = 0.1270]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	15473 / 0 / 1153	
Goodness-of-fit on F ²	1.080	
Final R indices [I > 2σ(I)]	R1 = 0.0726, wR2 = 0.1530	
R indices (all data)	R1 = 0.1120, wR2 = 0.1706	
Largest diff. peak and hole	0.968 and -0.475 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_jcti. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ti(1)	5970(1)	4035(1)	7116(1)	32(1)
Ti(2)	6061(1)	4577(1)	8666(1)	32(1)
Ti(3)	6307(1)	6008(1)	7914(1)	37(1)
Ti(4)	6684(1)	5002(1)	6812(1)	37(1)
O(1)	6100(1)	3141(1)	7371(1)	35(1)
O(2)	6010(1)	3636(2)	6196(1)	37(1)
O(3)	5760(1)	4771(1)	6647(1)	32(1)
O(4)	5480(1)	3655(1)	7032(1)	36(1)
O(5)	5655(1)	5056(1)	8950(2)	37(1)
O(6)	5758(1)	3774(2)	8966(2)	41(1)
O(7)	6439(1)	3932(2)	8670(2)	42(1)
O(8)	6213(1)	4693(2)	9585(2)	46(1)
O(9)	5801(1)	5962(2)	7787(2)	38(1)
O(10)	6242(1)	6919(2)	7534(2)	51(1)
O(11)	6786(1)	6281(2)	8096(2)	44(1)
O(12)	6210(1)	6509(2)	8760(2)	49(1)
O(13)	6996(1)	4946(2)	7549(2)	41(1)
O(14)	7054(1)	4393(2)	6416(2)	45(1)
O(15)	6491(1)	5084(2)	5953(2)	40(1)
O(16)	7020(1)	5739(2)	6481(2)	49(1)
O(17)	5895(1)	4323(1)	7876(1)	33(1)
O(18)	6293(1)	5265(1)	8422(1)	33(1)
O(19)	6430(1)	5667(2)	7185(1)	38(1)
O(20)	6418(1)	4332(2)	6992(1)	37(1)
F(1)	6110(1)	2341(2)	5166(1)	74(1)
F(2)	5807(1)	3200(2)	5063(1)	62(1)
F(3)	6358(1)	3276(2)	5097(2)	74(1)
F(4)	4750(1)	3382(2)	6134(2)	90(1)
F(5)	5040(1)	2734(2)	6699(2)	85(1)
F(6)	4739(1)	3448(2)	7117(2)	114(2)
F(7)	5330(1)	2884(2)	8304(2)	99(1)

F(8)	5420(1)	2655(2)	9253(2)	80(1)
F(9)	4941(1)	3066(2)	8990(2)	92(1)
F(10)	6189(1)	4733(4)	10862(2)	149(3)
F(11)	6681(2)	4325(3)	10917(2)	142(2)
F(12)	6614(1)	5239(2)	10556(2)	115(2)
F(13)	6049(1)	6528(3)	10017(2)	137(2)
F(14)	6073(3)	7415(3)	9658(3)	215(4)
F(15)	6473(2)	7112(5)	10185(3)	236(5)
F(16)	7176(1)	7063(2)	5499(2)	116(2)
F(17)	7218(3)	7007(3)	6464(3)	216(5)
F(18)	7538(1)	6460(4)	5914(5)	234(5)
F(19)	5763(1)	8154(2)	6834(2)	99(1)
F(20)	6281(1)	7892(2)	6706(3)	123(2)
F(21)	6117(1)	8282(2)	7569(2)	98(1)
F(22)	7297(1)	3166(2)	6136(3)	117(2)
F(23)	7569(1)	3907(2)	5667(2)	103(2)
F(24)	7801(1)	3438(2)	6454(2)	87(1)
C(1)	6153(1)	2604(2)	7090(2)	31(1)
C(2)	6136(1)	2539(2)	6436(2)	44(1)
C(3)	6076(1)	3061(2)	6048(2)	35(1)
C(4)	5489(1)	4847(2)	6311(2)	31(1)
C(5)	5237(1)	4351(2)	6258(2)	36(1)
C(6)	5248(1)	3811(2)	6644(2)	36(1)
C(7)	5333(1)	4928(2)	9052(2)	38(1)
C(8)	5210(1)	4298(2)	9014(2)	47(1)
C(9)	5428(1)	3771(2)	8965(2)	43(1)
C(10)	6621(1)	3645(2)	9099(3)	45(1)
C(11)	6625(1)	3866(3)	9713(3)	48(1)
C(12)	6433(1)	4382(3)	9906(3)	49(1)
C(13)	5563(1)	6327(2)	7578(2)	35(1)
C(14)	5634(1)	6963(2)	7372(2)	46(1)
C(15)	5964(2)	7203(2)	7365(2)	45(1)
C(16)	6952(1)	6484(2)	8578(3)	46(1)
C(17)	6784(2)	6645(3)	9130(3)	59(2)
C(18)	6427(2)	6662(3)	9171(3)	54(1)
C(19)	7291(1)	4694(2)	7674(2)	37(1)

C(20)	7467(1)	4309(3)	7230(2)	48(1)
C(21)	7330(1)	4172(2)	6654(2)	44(1)
C(22)	6508(1)	5505(2)	5512(2)	39(1)
C(23)	6733(2)	6025(3)	5536(3)	62(2)
C(24)	6972(1)	6100(3)	6009(3)	57(2)
C(25)	6228(1)	2031(2)	7497(2)	31(1)
C(26)	6168(1)	2077(2)	8135(2)	35(1)
C(27)	6226(1)	1548(3)	8516(2)	46(1)
C(28)	6343(1)	970(3)	8263(3)	48(1)
C(29)	6407(1)	923(2)	7634(3)	48(1)
C(30)	6349(1)	1451(2)	7248(2)	42(1)
C(31)	6084(2)	2959(3)	5342(3)	51(1)
C(32)	5449(1)	5485(2)	6006(2)	29(1)
C(33)	5152(1)	5649(2)	5662(2)	45(1)
C(34)	5123(2)	6250(3)	5391(3)	56(2)
C(35)	5389(2)	6697(3)	5446(2)	50(1)
C(36)	5682(1)	6547(2)	5782(2)	44(1)
C(37)	5708(1)	5947(2)	6067(2)	33(1)
C(38)	4946(1)	3339(3)	6635(3)	54(1)
C(39)	6821(1)	3085(2)	8878(3)	50(1)
C(40)	6875(1)	3001(3)	8232(3)	54(2)
C(41)	7050(1)	2457(3)	8018(4)	72(2)
C(42)	7164(2)	1994(3)	8421(5)	86(3)
C(43)	7112(2)	2071(3)	9052(5)	92(3)
C(44)	6944(1)	2608(3)	9289(3)	65(2)
C(45)	6480(2)	4664(4)	10568(3)	62(2)
C(46)	5117(1)	5507(2)	9196(2)	39(1)
C(47)	4758(1)	5456(3)	9292(3)	60(2)
C(48)	4571(2)	6022(4)	9402(3)	71(2)
C(49)	4723(2)	6609(4)	9423(3)	73(2)
C(50)	5076(2)	6660(3)	9357(3)	61(2)
C(51)	5273(1)	6106(3)	9234(2)	48(1)
C(52)	5276(2)	3089(3)	8887(3)	57(2)
C(53)	5215(1)	6039(2)	7537(2)	36(1)
C(54)	5171(1)	5382(3)	7635(2)	39(1)
C(55)	4851(1)	5086(3)	7613(2)	49(1)

C(56)	4566(1)	5458(3)	7499(3)	65(2)
C(57)	4598(1)	6107(4)	7394(4)	81(2)
C(58)	4919(2)	6414(3)	7411(3)	67(2)
C(59)	6032(2)	7887(3)	7108(3)	62(2)
C(60)	7331(1)	6559(2)	8492(3)	47(1)
C(61)	7465(1)	6523(3)	7898(3)	65(2)
C(62)	7816(2)	6616(4)	7791(3)	80(2)
C(63)	8030(2)	6729(3)	8291(4)	79(2)
C(64)	7901(2)	6755(3)	8880(4)	72(2)
C(65)	7552(1)	6674(3)	8994(3)	59(2)
C(66)	6267(2)	6916(4)	9767(4)	87(2)
C(67)	7419(1)	4793(2)	8318(2)	37(1)
C(68)	7774(1)	4754(3)	8462(3)	56(2)
C(69)	7884(1)	4846(3)	9065(3)	64(2)
C(70)	7653(2)	4961(3)	9539(3)	56(2)
C(71)	7304(1)	5009(3)	9402(3)	52(1)
C(72)	7191(1)	4931(2)	8792(2)	42(1)
C(73)	7505(2)	3671(3)	6216(3)	65(2)
C(74)	6267(1)	5404(2)	4980(2)	37(1)
C(75)	6065(1)	4854(2)	4973(2)	40(1)
C(76)	5827(1)	4753(3)	4491(2)	48(1)
C(77)	5790(1)	5203(3)	4025(2)	55(2)
C(78)	5990(2)	5748(3)	4024(3)	61(2)
C(79)	6230(1)	5851(3)	4492(3)	55(1)
C(80)	7232(3)	6652(5)	5960(4)	110(3)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for mo_jcti.

Ti(1)-O(17)	1.750(3)
Ti(1)-O(20)	1.849(3)
Ti(1)-O(1)	1.982(3)
Ti(1)-O(3)	1.989(3)
Ti(1)-O(4)	2.050(3)
Ti(1)-O(2)	2.133(3)
Ti(2)-O(18)	1.752(3)
Ti(2)-O(17)	1.878(3)
Ti(2)-O(5)	1.946(3)
Ti(2)-O(7)	1.968(3)
Ti(2)-O(8)	2.060(4)
Ti(2)-O(6)	2.123(3)
Ti(3)-O(19)	1.770(3)
Ti(3)-O(18)	1.875(3)
Ti(3)-O(11)	1.963(3)
Ti(3)-O(9)	1.971(3)
Ti(3)-O(10)	2.058(4)
Ti(3)-O(12)	2.112(4)
Ti(4)-O(20)	1.760(3)
Ti(4)-O(19)	1.861(3)
Ti(4)-O(13)	1.982(3)
Ti(4)-O(15)	1.986(3)
Ti(4)-O(14)	2.077(3)
Ti(4)-O(16)	2.115(3)
O(1)-C(1)	1.273(5)
O(2)-C(3)	1.250(5)
O(3)-C(4)	1.275(5)
O(4)-C(6)	1.259(5)
O(5)-C(7)	1.284(5)
O(6)-C(9)	1.269(6)
O(7)-C(10)	1.295(6)
O(8)-C(12)	1.262(6)
O(9)-C(13)	1.265(5)
O(10)-C(15)	1.272(6)

O(11)-C(16)	1.283(6)
O(12)-C(18)	1.250(6)
O(13)-C(19)	1.276(5)
O(14)-C(21)	1.263(6)
O(15)-C(22)	1.280(5)
O(16)-C(24)	1.264(6)
F(1)-C(31)	1.329(6)
F(2)-C(31)	1.317(6)
F(3)-C(31)	1.344(6)
F(4)-C(38)	1.312(6)
F(5)-C(38)	1.302(6)
F(6)-C(38)	1.321(7)
F(7)-C(52)	1.330(7)
F(8)-C(52)	1.309(6)
F(9)-C(52)	1.309(7)
F(10)-C(45)	1.291(7)
F(11)-C(45)	1.281(7)
F(12)-C(45)	1.290(7)
F(13)-C(66)	1.275(8)
F(14)-C(66)	1.291(11)
F(15)-C(66)	1.257(9)
F(16)-C(80)	1.315(9)
F(17)-C(80)	1.299(11)
F(18)-C(80)	1.246(13)
F(19)-C(59)	1.310(7)
F(20)-C(59)	1.285(7)
F(21)-C(59)	1.317(7)
F(22)-C(73)	1.322(8)
F(23)-C(73)	1.293(7)
F(24)-C(73)	1.336(7)
C(1)-C(2)	1.402(6)
C(1)-C(25)	1.494(6)
C(2)-C(3)	1.376(7)
C(2)-H(2)	0.9500
C(3)-C(31)	1.523(7)
C(4)-C(5)	1.410(6)

C(4)-C(32)	1.474(6)
C(5)-C(6)	1.382(6)
C(5)-H(5)	0.9500
C(6)-C(38)	1.516(7)
C(7)-C(8)	1.382(7)
C(7)-C(46)	1.486(7)
C(8)-C(9)	1.376(7)
C(8)-H(8)	0.9500
C(9)-C(52)	1.532(7)
C(10)-C(11)	1.387(8)
C(10)-C(39)	1.464(7)
C(11)-C(12)	1.359(8)
C(11)-H(11)	0.9500
C(12)-C(45)	1.538(8)
C(13)-C(14)	1.408(7)
C(13)-C(53)	1.467(6)
C(14)-C(15)	1.364(7)
C(14)-H(14)	0.9500
C(15)-C(59)	1.532(7)
C(16)-C(17)	1.384(8)
C(16)-C(60)	1.477(7)
C(17)-C(18)	1.381(8)
C(17)-H(17)	0.9500
C(18)-C(66)	1.505(8)
C(19)-C(20)	1.408(7)
C(19)-C(67)	1.476(7)
C(20)-C(21)	1.365(7)
C(20)-H(20)	0.9500
C(21)-C(73)	1.544(8)
C(22)-C(23)	1.377(7)
C(22)-C(74)	1.481(7)
C(23)-C(24)	1.374(8)
C(23)-H(23)	0.9500
C(24)-C(80)	1.517(8)
C(25)-C(26)	1.383(6)
C(25)-C(30)	1.389(6)

C(26)-C(27)	1.376(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.379(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.369(8)
C(28)-H(28)	0.9500
C(29)-C(30)	1.380(7)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(32)-C(37)	1.385(6)
C(32)-C(33)	1.397(6)
C(33)-C(34)	1.371(7)
C(33)-H(33)	0.9500
C(34)-C(35)	1.379(8)
C(34)-H(34)	0.9500
C(35)-C(36)	1.371(7)
C(35)-H(35)	0.9500
C(36)-C(37)	1.379(6)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
C(39)-C(44)	1.399(8)
C(39)-C(40)	1.406(8)
C(40)-C(41)	1.384(8)
C(40)-H(40)	0.9500
C(41)-C(42)	1.356(10)
C(41)-H(41)	0.9500
C(42)-C(43)	1.369(11)
C(42)-H(42)	0.9500
C(43)-C(44)	1.379(10)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(46)-C(51)	1.374(7)
C(46)-C(47)	1.402(7)
C(47)-C(48)	1.389(8)
C(47)-H(47)	0.9500
C(48)-C(49)	1.345(9)

C(48)-H(48)	0.9500
C(49)-C(50)	1.369(9)
C(49)-H(49)	0.9500
C(50)-C(51)	1.393(7)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(53)-C(54)	1.379(7)
C(53)-C(58)	1.401(6)
C(54)-C(55)	1.374(7)
C(54)-H(54)	0.9500
C(55)-C(56)	1.361(7)
C(55)-H(55)	0.9500
C(56)-C(57)	1.360(9)
C(56)-H(56)	0.9500
C(57)-C(58)	1.389(8)
C(57)-H(57)	0.9500
C(58)-H(58)	0.9500
C(60)-C(61)	1.371(8)
C(60)-C(65)	1.389(7)
C(61)-C(62)	1.386(8)
C(61)-H(61)	0.9500
C(62)-C(63)	1.368(9)
C(62)-H(62)	0.9500
C(63)-C(64)	1.353(10)
C(63)-H(63)	0.9500
C(64)-C(65)	1.375(8)
C(64)-H(64)	0.9500
C(65)-H(65)	0.9500
C(67)-C(72)	1.367(7)
C(67)-C(68)	1.401(6)
C(68)-C(69)	1.368(8)
C(68)-H(68)	0.9500
C(69)-C(70)	1.368(8)
C(69)-H(69)	0.9500
C(70)-C(71)	1.375(7)
C(70)-H(70)	0.9500

C(71)-C(72)	1.383(7)
C(71)-H(71)	0.9500
C(72)-H(72)	0.9500
C(74)-C(75)	1.374(7)
C(74)-C(79)	1.397(7)
C(75)-C(76)	1.392(7)
C(75)-H(75)	0.9500
C(76)-C(77)	1.365(7)
C(76)-H(76)	0.9500
C(77)-C(78)	1.360(8)
C(77)-H(77)	0.9500
C(78)-C(79)	1.378(8)
C(78)-H(78)	0.9500
C(79)-H(79)	0.9500

O(17)-Ti(1)-O(20)	100.02(14)
O(17)-Ti(1)-O(1)	95.87(13)
O(20)-Ti(1)-O(1)	96.34(13)
O(17)-Ti(1)-O(3)	98.10(13)
O(20)-Ti(1)-O(3)	93.24(13)
O(1)-Ti(1)-O(3)	161.42(13)
O(17)-Ti(1)-O(4)	93.37(13)
O(20)-Ti(1)-O(4)	166.42(14)
O(1)-Ti(1)-O(4)	84.42(12)
O(3)-Ti(1)-O(4)	82.59(12)
O(17)-Ti(1)-O(2)	174.09(13)
O(20)-Ti(1)-O(2)	85.87(13)
O(1)-Ti(1)-O(2)	83.00(12)
O(3)-Ti(1)-O(2)	81.86(13)
O(4)-Ti(1)-O(2)	80.76(12)
O(18)-Ti(2)-O(17)	97.58(14)
O(18)-Ti(2)-O(5)	95.36(14)
O(17)-Ti(2)-O(5)	98.43(13)
O(18)-Ti(2)-O(7)	99.75(14)
O(17)-Ti(2)-O(7)	93.88(13)
O(5)-Ti(2)-O(7)	159.06(14)

O(18)-Ti(2)-O(8)	92.62(14)
O(17)-Ti(2)-O(8)	169.58(14)
O(5)-Ti(2)-O(8)	82.64(14)
O(7)-Ti(2)-O(8)	82.27(14)
O(18)-Ti(2)-O(6)	177.13(13)
O(17)-Ti(2)-O(6)	82.36(13)
O(5)-Ti(2)-O(6)	81.82(13)
O(7)-Ti(2)-O(6)	83.11(13)
O(8)-Ti(2)-O(6)	87.56(14)
O(19)-Ti(3)-O(18)	101.13(15)
O(19)-Ti(3)-O(11)	92.10(14)
O(18)-Ti(3)-O(11)	98.36(13)
O(19)-Ti(3)-O(9)	97.15(14)
O(18)-Ti(3)-O(9)	90.72(13)
O(11)-Ti(3)-O(9)	165.58(14)
O(19)-Ti(3)-O(10)	92.73(16)
O(18)-Ti(3)-O(10)	165.22(15)
O(11)-Ti(3)-O(10)	86.12(14)
O(9)-Ti(3)-O(10)	82.42(13)
O(19)-Ti(3)-O(12)	172.47(15)
O(18)-Ti(3)-O(12)	84.18(14)
O(11)-Ti(3)-O(12)	81.79(14)
O(9)-Ti(3)-O(12)	88.05(14)
O(10)-Ti(3)-O(12)	82.52(15)
O(20)-Ti(4)-O(19)	100.20(14)
O(20)-Ti(4)-O(13)	97.68(14)
O(19)-Ti(4)-O(13)	91.25(13)
O(20)-Ti(4)-O(15)	92.90(14)
O(19)-Ti(4)-O(15)	97.86(14)
O(13)-Ti(4)-O(15)	164.61(13)
O(20)-Ti(4)-O(14)	90.86(14)
O(19)-Ti(4)-O(14)	168.01(14)
O(13)-Ti(4)-O(14)	82.62(13)
O(15)-Ti(4)-O(14)	86.10(14)
O(20)-Ti(4)-O(16)	172.12(15)
O(19)-Ti(4)-O(16)	86.43(14)

O(13)-Ti(4)-O(16)	86.33(14)
O(15)-Ti(4)-O(16)	81.91(14)
O(14)-Ti(4)-O(16)	82.91(14)
C(1)-O(1)-Ti(1)	135.7(3)
C(3)-O(2)-Ti(1)	127.6(3)
C(4)-O(3)-Ti(1)	135.2(3)
C(6)-O(4)-Ti(1)	127.8(3)
C(7)-O(5)-Ti(2)	136.4(3)
C(9)-O(6)-Ti(2)	123.5(3)
C(10)-O(7)-Ti(2)	135.2(3)
C(12)-O(8)-Ti(2)	130.3(4)
C(13)-O(9)-Ti(3)	137.5(3)
C(15)-O(10)-Ti(3)	129.3(3)
C(16)-O(11)-Ti(3)	136.1(3)
C(18)-O(12)-Ti(3)	127.3(3)
C(19)-O(13)-Ti(4)	136.8(3)
C(21)-O(14)-Ti(4)	129.1(3)
C(22)-O(15)-Ti(4)	135.8(3)
C(24)-O(16)-Ti(4)	126.7(3)
Ti(1)-O(17)-Ti(2)	150.45(17)
Ti(2)-O(18)-Ti(3)	147.62(16)
Ti(3)-O(19)-Ti(4)	143.88(18)
Ti(4)-O(20)-Ti(1)	146.37(17)
O(1)-C(1)-C(2)	123.0(4)
O(1)-C(1)-C(25)	116.1(4)
C(2)-C(1)-C(25)	120.8(4)
C(3)-C(2)-C(1)	122.1(4)
C(3)-C(2)-H(2)	119.0
C(1)-C(2)-H(2)	119.0
O(2)-C(3)-C(2)	128.4(4)
O(2)-C(3)-C(31)	112.6(4)
C(2)-C(3)-C(31)	119.0(4)
O(3)-C(4)-C(5)	121.2(4)
O(3)-C(4)-C(32)	116.3(4)
C(5)-C(4)-C(32)	122.5(4)
C(6)-C(5)-C(4)	120.9(4)

C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
O(4)-C(6)-C(5)	128.2(4)
O(4)-C(6)-C(38)	112.8(4)
C(5)-C(6)-C(38)	119.0(4)
O(5)-C(7)-C(8)	121.0(4)
O(5)-C(7)-C(46)	114.2(4)
C(8)-C(7)-C(46)	124.8(4)
C(9)-C(8)-C(7)	122.1(5)
C(9)-C(8)-H(8)	118.9
C(7)-C(8)-H(8)	118.9
O(6)-C(9)-C(8)	127.5(5)
O(6)-C(9)-C(52)	112.8(5)
C(8)-C(9)-C(52)	119.7(5)
O(7)-C(10)-C(11)	121.7(5)
O(7)-C(10)-C(39)	114.6(5)
C(11)-C(10)-C(39)	123.7(5)
C(12)-C(11)-C(10)	122.3(5)
C(12)-C(11)-H(11)	118.8
C(10)-C(11)-H(11)	118.8
O(8)-C(12)-C(11)	126.7(5)
O(8)-C(12)-C(45)	112.7(5)
C(11)-C(12)-C(45)	120.6(5)
O(9)-C(13)-C(14)	121.4(4)
O(9)-C(13)-C(53)	116.3(4)
C(14)-C(13)-C(53)	122.2(4)
C(15)-C(14)-C(13)	121.4(5)
C(15)-C(14)-H(14)	119.3
C(13)-C(14)-H(14)	119.3
O(10)-C(15)-C(14)	127.9(5)
O(10)-C(15)-C(59)	112.3(5)
C(14)-C(15)-C(59)	119.7(5)
O(11)-C(16)-C(17)	121.8(5)
O(11)-C(16)-C(60)	115.3(5)
C(17)-C(16)-C(60)	122.8(5)
C(18)-C(17)-C(16)	121.8(5)

C(18)-C(17)-H(17)	119.1
C(16)-C(17)-H(17)	119.1
O(12)-C(18)-C(17)	127.7(5)
O(12)-C(18)-C(66)	114.2(5)
C(17)-C(18)-C(66)	118.0(6)
O(13)-C(19)-C(20)	121.1(4)
O(13)-C(19)-C(67)	115.8(4)
C(20)-C(19)-C(67)	123.0(4)
C(21)-C(20)-C(19)	122.4(4)
C(21)-C(20)-H(20)	118.8
C(19)-C(20)-H(20)	118.8
O(14)-C(21)-C(20)	127.7(5)
O(14)-C(21)-C(73)	111.2(5)
C(20)-C(21)-C(73)	121.0(5)
O(15)-C(22)-C(23)	122.0(5)
O(15)-C(22)-C(74)	115.8(4)
C(23)-C(22)-C(74)	122.2(5)
C(24)-C(23)-C(22)	122.4(5)
C(24)-C(23)-H(23)	118.8
C(22)-C(23)-H(23)	118.8
O(16)-C(24)-C(23)	128.0(5)
O(16)-C(24)-C(80)	113.4(5)
C(23)-C(24)-C(80)	118.4(6)
C(26)-C(25)-C(30)	119.4(4)
C(26)-C(25)-C(1)	119.2(4)
C(30)-C(25)-C(1)	121.4(4)
C(27)-C(26)-C(25)	120.0(5)
C(27)-C(26)-H(26)	120.0
C(25)-C(26)-H(26)	120.0
C(26)-C(27)-C(28)	120.2(5)
C(26)-C(27)-H(27)	119.9
C(28)-C(27)-H(27)	119.9
C(29)-C(28)-C(27)	120.2(5)
C(29)-C(28)-H(28)	119.9
C(27)-C(28)-H(28)	119.9
C(28)-C(29)-C(30)	120.0(5)

C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(29)-C(30)-C(25)	120.2(5)
C(29)-C(30)-H(30)	119.9
C(25)-C(30)-H(30)	119.9
F(2)-C(31)-F(1)	107.0(5)
F(2)-C(31)-F(3)	106.1(4)
F(1)-C(31)-F(3)	107.3(4)
F(2)-C(31)-C(3)	112.1(4)
F(1)-C(31)-C(3)	114.4(4)
F(3)-C(31)-C(3)	109.6(5)
C(37)-C(32)-C(33)	118.2(4)
C(37)-C(32)-C(4)	119.7(4)
C(33)-C(32)-C(4)	122.1(4)
C(34)-C(33)-C(32)	120.3(5)
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(33)-C(34)-C(35)	120.3(5)
C(33)-C(34)-H(34)	119.8
C(35)-C(34)-H(34)	119.8
C(36)-C(35)-C(34)	120.3(5)
C(36)-C(35)-H(35)	119.8
C(34)-C(35)-H(35)	119.8
C(35)-C(36)-C(37)	119.4(5)
C(35)-C(36)-H(36)	120.3
C(37)-C(36)-H(36)	120.3
C(36)-C(37)-C(32)	121.4(4)
C(36)-C(37)-H(37)	119.3
C(32)-C(37)-H(37)	119.3
F(5)-C(38)-F(4)	108.1(5)
F(5)-C(38)-F(6)	104.5(5)
F(4)-C(38)-F(6)	106.0(5)
F(5)-C(38)-C(6)	113.4(4)
F(4)-C(38)-C(6)	114.0(5)
F(6)-C(38)-C(6)	110.2(4)
C(44)-C(39)-C(40)	118.6(5)

C(44)-C(39)-C(10)	121.9(6)
C(40)-C(39)-C(10)	119.4(5)
C(41)-C(40)-C(39)	119.7(6)
C(41)-C(40)-H(40)	120.1
C(39)-C(40)-H(40)	120.1
C(42)-C(41)-C(40)	121.1(7)
C(42)-C(41)-H(41)	119.5
C(40)-C(41)-H(41)	119.5
C(41)-C(42)-C(43)	119.7(7)
C(41)-C(42)-H(42)	120.1
C(43)-C(42)-H(42)	120.1
C(42)-C(43)-C(44)	121.5(7)
C(42)-C(43)-H(43)	119.3
C(44)-C(43)-H(43)	119.3
C(43)-C(44)-C(39)	119.4(7)
C(43)-C(44)-H(44)	120.3
C(39)-C(44)-H(44)	120.3
F(11)-C(45)-F(12)	105.7(6)
F(11)-C(45)-F(10)	107.5(6)
F(12)-C(45)-F(10)	104.9(7)
F(11)-C(45)-C(12)	113.6(6)
F(12)-C(45)-C(12)	112.0(5)
F(10)-C(45)-C(12)	112.6(5)
C(51)-C(46)-C(47)	119.3(5)
C(51)-C(46)-C(7)	119.2(4)
C(47)-C(46)-C(7)	121.5(5)
C(48)-C(47)-C(46)	118.2(6)
C(48)-C(47)-H(47)	120.9
C(46)-C(47)-H(47)	120.9
C(49)-C(48)-C(47)	122.2(6)
C(49)-C(48)-H(48)	118.9
C(47)-C(48)-H(48)	118.9
C(48)-C(49)-C(50)	119.8(6)
C(48)-C(49)-H(49)	120.1
C(50)-C(49)-H(49)	120.1
C(49)-C(50)-C(51)	119.8(6)

C(49)-C(50)-H(50)	120.1
C(51)-C(50)-H(50)	120.1
C(46)-C(51)-C(50)	120.5(5)
C(46)-C(51)-H(51)	119.7
C(50)-C(51)-H(51)	119.7
F(9)-C(52)-F(8)	107.0(5)
F(9)-C(52)-F(7)	107.5(5)
F(8)-C(52)-F(7)	106.1(5)
F(9)-C(52)-C(9)	113.1(5)
F(8)-C(52)-C(9)	113.4(5)
F(7)-C(52)-C(9)	109.4(5)
C(54)-C(53)-C(58)	117.9(5)
C(54)-C(53)-C(13)	119.9(4)
C(58)-C(53)-C(13)	122.2(5)
C(55)-C(54)-C(53)	122.7(5)
C(55)-C(54)-H(54)	118.6
C(53)-C(54)-H(54)	118.6
C(56)-C(55)-C(54)	118.6(6)
C(56)-C(55)-H(55)	120.7
C(54)-C(55)-H(55)	120.7
C(57)-C(56)-C(55)	120.6(5)
C(57)-C(56)-H(56)	119.7
C(55)-C(56)-H(56)	119.7
C(56)-C(57)-C(58)	121.5(5)
C(56)-C(57)-H(57)	119.3
C(58)-C(57)-H(57)	119.3
C(57)-C(58)-C(53)	118.7(6)
C(57)-C(58)-H(58)	120.7
C(53)-C(58)-H(58)	120.7
F(20)-C(59)-F(19)	106.7(6)
F(20)-C(59)-F(21)	108.0(6)
F(19)-C(59)-F(21)	105.7(5)
F(20)-C(59)-C(15)	112.0(5)
F(19)-C(59)-C(15)	114.1(5)
F(21)-C(59)-C(15)	109.9(5)
C(61)-C(60)-C(65)	119.5(5)

C(61)-C(60)-C(16)	118.7(5)
C(65)-C(60)-C(16)	121.8(5)
C(60)-C(61)-C(62)	120.8(6)
C(60)-C(61)-H(61)	119.6
C(62)-C(61)-H(61)	119.6
C(63)-C(62)-C(61)	118.9(7)
C(63)-C(62)-H(62)	120.5
C(61)-C(62)-H(62)	120.5
C(64)-C(63)-C(62)	120.6(6)
C(64)-C(63)-H(63)	119.7
C(62)-C(63)-H(63)	119.7
C(63)-C(64)-C(65)	121.2(6)
C(63)-C(64)-H(64)	119.4
C(65)-C(64)-H(64)	119.4
C(64)-C(65)-C(60)	118.9(6)
C(64)-C(65)-H(65)	120.5
C(60)-C(65)-H(65)	120.5
F(15)-C(66)-F(13)	108.5(8)
F(15)-C(66)-F(14)	103.8(8)
F(13)-C(66)-F(14)	101.2(8)
F(15)-C(66)-C(18)	117.0(7)
F(13)-C(66)-C(18)	113.8(6)
F(14)-C(66)-C(18)	111.0(8)
C(72)-C(67)-C(68)	118.4(5)
C(72)-C(67)-C(19)	120.2(4)
C(68)-C(67)-C(19)	121.4(4)
C(69)-C(68)-C(67)	119.9(5)
C(69)-C(68)-H(68)	120.0
C(67)-C(68)-H(68)	120.0
C(70)-C(69)-C(68)	121.2(5)
C(70)-C(69)-H(69)	119.4
C(68)-C(69)-H(69)	119.4
C(69)-C(70)-C(71)	119.4(5)
C(69)-C(70)-H(70)	120.3
C(71)-C(70)-H(70)	120.3
C(70)-C(71)-C(72)	119.8(5)

C(70)-C(71)-H(71)	120.1
C(72)-C(71)-H(71)	120.1
C(67)-C(72)-C(71)	121.2(5)
C(67)-C(72)-H(72)	119.4
C(71)-C(72)-H(72)	119.4
F(23)-C(73)-F(22)	107.1(6)
F(23)-C(73)-F(24)	108.3(5)
F(22)-C(73)-F(24)	106.5(5)
F(23)-C(73)-C(21)	112.4(5)
F(22)-C(73)-C(21)	109.8(5)
F(24)-C(73)-C(21)	112.3(5)
C(75)-C(74)-C(79)	118.5(5)
C(75)-C(74)-C(22)	118.7(4)
C(79)-C(74)-C(22)	122.8(5)
C(74)-C(75)-C(76)	120.2(5)
C(74)-C(75)-H(75)	119.9
C(76)-C(75)-H(75)	119.9
C(77)-C(76)-C(75)	120.4(5)
C(77)-C(76)-H(76)	119.8
C(75)-C(76)-H(76)	119.8
C(78)-C(77)-C(76)	120.1(5)
C(78)-C(77)-H(77)	119.9
C(76)-C(77)-H(77)	119.9
C(77)-C(78)-C(79)	120.4(5)
C(77)-C(78)-H(78)	119.8
C(79)-C(78)-H(78)	119.8
C(78)-C(79)-C(74)	120.4(5)
C(78)-C(79)-H(79)	119.8
C(74)-C(79)-H(79)	119.8
F(18)-C(80)-F(17)	106.4(8)
F(18)-C(80)-F(16)	107.5(9)
F(17)-C(80)-F(16)	104.6(9)
F(18)-C(80)-C(24)	113.0(9)
F(17)-C(80)-C(24)	109.7(8)
F(16)-C(80)-C(24)	115.1(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_jcti. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ti(1)	33(1)	29(1)	34(1)	0(1)	-8(1)	3(1)
Ti(2)	27(1)	34(1)	36(1)	-1(1)	-4(1)	3(1)
Ti(3)	25(1)	35(1)	50(1)	-1(1)	-6(1)	-2(1)
Ti(4)	24(1)	48(1)	37(1)	6(1)	-3(1)	1(1)
O(1)	43(2)	27(2)	35(2)	-2(1)	-6(1)	5(1)
O(2)	49(2)	31(2)	31(2)	0(1)	-5(1)	5(1)
O(3)	29(2)	31(2)	37(2)	4(1)	-7(1)	0(1)
O(4)	37(2)	31(2)	40(2)	5(1)	-12(2)	-6(1)
O(5)	29(2)	37(2)	45(2)	-3(2)	4(1)	3(1)
O(6)	39(2)	36(2)	48(2)	6(2)	-1(2)	0(1)
O(7)	35(2)	42(2)	50(2)	1(2)	-10(2)	9(2)
O(8)	45(2)	60(2)	34(2)	0(2)	-5(2)	5(2)
O(9)	24(2)	37(2)	54(2)	4(2)	-6(1)	3(1)
O(10)	49(2)	33(2)	71(3)	6(2)	-5(2)	-3(2)
O(11)	31(2)	46(2)	54(2)	-6(2)	-10(2)	-10(2)
O(12)	42(2)	41(2)	64(2)	-16(2)	1(2)	-3(2)
O(13)	23(2)	54(2)	45(2)	0(2)	-4(1)	6(2)
O(14)	31(2)	63(2)	42(2)	0(2)	4(2)	6(2)
O(15)	33(2)	50(2)	37(2)	11(2)	-3(1)	-1(2)
O(16)	35(2)	61(2)	51(2)	6(2)	1(2)	-13(2)
O(17)	25(2)	33(2)	41(2)	10(1)	2(1)	6(1)
O(18)	24(2)	32(2)	44(2)	-6(1)	-16(1)	2(1)
O(19)	20(2)	56(2)	38(2)	8(2)	-6(1)	5(1)
O(20)	35(2)	35(2)	41(2)	1(1)	-14(1)	9(1)
F(1)	130(3)	53(2)	39(2)	-11(2)	0(2)	25(2)
F(2)	83(2)	63(2)	38(2)	-4(2)	-21(2)	13(2)
F(3)	79(2)	92(3)	49(2)	7(2)	23(2)	4(2)
F(4)	82(2)	78(3)	111(3)	33(2)	-61(2)	-43(2)
F(5)	83(2)	34(2)	138(4)	11(2)	-47(2)	-18(2)
F(6)	91(3)	120(4)	131(4)	-36(3)	44(3)	-68(3)
F(7)	163(4)	65(2)	68(3)	-8(2)	-2(3)	-46(3)

F(8)	103(3)	37(2)	98(3)	24(2)	-24(2)	-10(2)
F(9)	59(2)	58(2)	160(4)	25(2)	-9(2)	-25(2)
F(10)	84(3)	301(8)	61(3)	-53(4)	22(2)	-39(4)
F(11)	187(5)	181(5)	59(3)	3(3)	-44(3)	54(4)
F(12)	159(4)	127(4)	60(3)	-29(3)	-3(3)	-58(4)
F(13)	135(4)	183(6)	93(3)	-55(3)	57(3)	-67(4)
F(14)	349(11)	128(5)	167(6)	-51(5)	96(7)	82(7)
F(15)	118(4)	446(13)	143(5)	-199(7)	48(4)	-128(6)
F(16)	152(4)	107(3)	89(3)	38(3)	-17(3)	-78(3)
F(17)	381(12)	176(6)	91(4)	22(4)	-47(5)	-213(8)
F(18)	55(3)	212(7)	433(15)	132(9)	-31(5)	-77(4)
F(19)	125(3)	48(2)	125(4)	29(2)	-44(3)	5(2)
F(20)	159(4)	71(3)	141(4)	47(3)	72(4)	13(3)
F(21)	152(4)	40(2)	102(3)	-7(2)	-38(3)	-18(2)
F(22)	112(3)	78(3)	159(5)	-51(3)	6(3)	16(3)
F(23)	109(3)	149(4)	53(2)	13(2)	29(2)	71(3)
F(24)	80(3)	106(3)	76(3)	-3(2)	9(2)	57(2)
C(1)	25(2)	35(3)	34(3)	2(2)	1(2)	-2(2)
C(2)	64(3)	33(3)	34(3)	-2(2)	1(2)	9(2)
C(3)	34(2)	40(3)	30(2)	0(2)	4(2)	1(2)
C(4)	33(2)	31(2)	28(2)	-4(2)	2(2)	6(2)
C(5)	33(2)	34(3)	41(3)	-4(2)	-14(2)	-1(2)
C(6)	35(2)	30(2)	43(3)	-8(2)	-7(2)	-5(2)
C(7)	36(3)	44(3)	33(3)	9(2)	1(2)	-2(2)
C(8)	37(3)	48(3)	54(3)	7(3)	-2(2)	-1(2)
C(9)	49(3)	39(3)	42(3)	12(2)	-2(2)	-7(2)
C(10)	25(2)	36(3)	72(4)	10(3)	-11(2)	-5(2)
C(11)	46(3)	52(3)	47(3)	17(3)	-13(3)	-9(3)
C(12)	40(3)	58(4)	49(3)	13(3)	3(2)	-14(3)
C(13)	36(2)	39(3)	31(3)	-14(2)	-5(2)	10(2)
C(14)	52(3)	34(3)	52(3)	-11(2)	-12(3)	10(2)
C(15)	70(4)	25(2)	40(3)	-4(2)	-6(3)	6(2)
C(16)	43(3)	36(3)	58(4)	5(2)	-11(3)	-15(2)
C(17)	56(4)	70(4)	50(4)	-10(3)	-3(3)	-30(3)
C(18)	59(4)	43(3)	60(4)	-16(3)	4(3)	-17(3)
C(19)	24(2)	37(3)	51(3)	9(2)	2(2)	-2(2)

C(20)	31(3)	59(3)	54(3)	4(3)	-2(2)	15(2)
C(21)	33(3)	49(3)	49(3)	6(3)	11(2)	5(2)
C(22)	39(3)	41(3)	36(3)	1(2)	10(2)	2(2)
C(23)	76(4)	61(4)	48(3)	16(3)	-4(3)	-22(3)
C(24)	51(3)	65(4)	55(4)	11(3)	4(3)	-21(3)
C(25)	28(2)	29(2)	35(3)	4(2)	-6(2)	1(2)
C(26)	31(2)	34(3)	40(3)	2(2)	-1(2)	-3(2)
C(27)	44(3)	50(3)	43(3)	10(3)	0(2)	-4(2)
C(28)	39(3)	46(3)	59(4)	19(3)	-7(3)	-1(2)
C(29)	47(3)	33(3)	64(4)	5(3)	-9(3)	8(2)
C(30)	49(3)	38(3)	37(3)	0(2)	-1(2)	9(2)
C(31)	63(4)	43(3)	47(3)	3(3)	8(3)	10(3)
C(32)	33(2)	30(2)	23(2)	0(2)	1(2)	9(2)
C(33)	45(3)	42(3)	47(3)	6(2)	-8(2)	5(2)
C(34)	65(4)	50(3)	54(4)	10(3)	-15(3)	18(3)
C(35)	67(4)	41(3)	41(3)	9(2)	4(3)	19(3)
C(36)	57(3)	36(3)	38(3)	0(2)	13(2)	1(2)
C(37)	41(3)	30(2)	29(2)	3(2)	6(2)	6(2)
C(38)	50(3)	42(3)	69(4)	1(3)	-20(3)	-8(3)
C(39)	24(2)	37(3)	89(5)	0(3)	-9(3)	-6(2)
C(40)	26(2)	43(3)	94(5)	-14(3)	-15(3)	0(2)
C(41)	29(3)	58(4)	128(6)	-24(4)	-1(3)	0(3)
C(42)	40(3)	44(4)	175(9)	-11(5)	5(5)	1(3)
C(43)	37(3)	47(4)	191(10)	25(5)	-8(5)	1(3)
C(44)	32(3)	46(3)	116(5)	27(3)	-8(3)	-2(3)
C(45)	59(4)	97(5)	30(3)	7(3)	-8(3)	-11(4)
C(46)	35(3)	55(3)	27(2)	-1(2)	6(2)	12(2)
C(47)	42(3)	83(4)	55(4)	0(3)	12(3)	9(3)
C(48)	50(4)	89(5)	74(5)	-5(4)	17(3)	26(4)
C(49)	74(5)	80(5)	64(4)	-10(4)	3(3)	39(4)
C(50)	79(4)	53(4)	52(4)	-8(3)	0(3)	24(3)
C(51)	51(3)	48(3)	43(3)	-5(2)	0(2)	12(3)
C(52)	65(4)	49(3)	57(4)	9(3)	-12(3)	-17(3)
C(53)	30(2)	44(3)	34(3)	-13(2)	-6(2)	14(2)
C(54)	27(2)	59(3)	32(3)	-5(2)	-3(2)	8(2)
C(55)	33(3)	70(4)	43(3)	-11(3)	-3(2)	1(3)

C(56)	33(3)	87(5)	76(4)	-33(4)	-12(3)	7(3)
C(57)	31(3)	85(5)	128(6)	-36(4)	-39(3)	22(3)
C(58)	59(4)	51(3)	92(5)	-25(3)	-31(3)	24(3)
C(59)	88(5)	40(3)	59(4)	1(3)	-4(4)	1(3)
C(60)	38(3)	42(3)	62(4)	11(3)	-13(3)	-16(2)
C(61)	37(3)	87(5)	70(4)	12(4)	-14(3)	-22(3)
C(62)	38(3)	122(6)	80(5)	20(4)	-2(3)	-22(3)
C(63)	35(3)	89(5)	113(6)	35(5)	-21(4)	-18(3)
C(64)	51(4)	68(4)	98(6)	22(4)	-36(4)	-21(3)
C(65)	47(3)	57(4)	73(4)	7(3)	-21(3)	-17(3)
C(66)	86(5)	95(6)	82(5)	-49(5)	30(4)	-31(5)
C(67)	28(2)	38(3)	45(3)	4(2)	-7(2)	-1(2)
C(68)	36(3)	73(4)	59(4)	-7(3)	-5(3)	11(3)
C(69)	37(3)	75(4)	79(5)	-16(3)	-21(3)	11(3)
C(70)	60(4)	49(3)	59(4)	4(3)	-24(3)	-12(3)
C(71)	50(3)	59(4)	47(3)	3(3)	0(3)	-18(3)
C(72)	32(2)	46(3)	48(3)	5(2)	-2(2)	-7(2)
C(73)	64(4)	64(4)	67(4)	2(3)	10(3)	21(3)
C(74)	33(2)	51(3)	26(2)	4(2)	7(2)	10(2)
C(75)	41(3)	46(3)	32(3)	-2(2)	0(2)	13(2)
C(76)	52(3)	54(3)	39(3)	-8(3)	-8(2)	11(3)
C(77)	47(3)	81(4)	36(3)	0(3)	-7(2)	15(3)
C(78)	63(4)	87(5)	33(3)	25(3)	-2(3)	15(3)
C(79)	55(3)	62(4)	48(3)	14(3)	5(3)	-3(3)
C(80)	133(8)	115(7)	82(6)	30(5)	-33(5)	-89(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_jcti.

	x	y	z	U(eq)
H(2)	6168	2121	6256	52
H(5)	5058	4389	5955	43
H(8)	4966	4227	9022	56
H(11)	6768	3649	10009	58
H(14)	5447	7231	7236	55
H(17)	6919	6746	9490	71
H(20)	7689	4138	7335	58
H(23)	6722	6343	5215	74
H(26)	6087	2473	8311	42
H(27)	6186	1581	8954	55
H(28)	6379	604	8527	58
H(29)	6491	527	7462	58
H(30)	6393	1417	6812	50
H(33)	4970	5341	5615	53
H(34)	4919	6361	5164	67
H(35)	5369	7110	5250	60
H(36)	5866	6853	5818	53
H(37)	5907	5850	6311	40
H(40)	6792	3316	7943	65
H(41)	7091	2406	7582	86
H(42)	7280	1619	8267	104
H(43)	7195	1746	9332	110
H(44)	6911	2654	9728	78
H(47)	4645	5045	9281	72
H(48)	4327	5993	9465	85
H(49)	4586	6989	9484	87
H(50)	5186	7071	9395	74
H(51)	5517	6143	9176	57
H(54)	5369	5124	7720	47
H(55)	4830	4631	7677	58

H(56)	4342	5262	7492	78
H(57)	4395	6357	7307	97
H(58)	4937	6868	7340	81
H(61)	7315	6434	7555	78
H(62)	7907	6601	7377	96
H(63)	8272	6790	8223	95
H(64)	8055	6830	9221	87
H(65)	7464	6697	9409	70
H(68)	7938	4664	8140	67
H(69)	8125	4830	9156	76
H(70)	7732	5007	9958	67
H(71)	7142	5096	9727	62
H(72)	6951	4973	8699	50
H(75)	6087	4541	5298	48
H(76)	5690	4369	4486	58
H(77)	5624	5135	3702	66
H(78)	5964	6059	3698	73
H(79)	6372	6229	4484	66

Table 6. Torsion angles [°] for mo_jcti.

O(20)-Ti(1)-O(17)-Ti(2)	-27.0(4)
O(1)-Ti(1)-O(17)-Ti(2)	70.5(4)
O(3)-Ti(1)-O(17)-Ti(2)	-121.8(3)
O(4)-Ti(1)-O(17)-Ti(2)	155.3(3)
O(18)-Ti(2)-O(17)-Ti(1)	65.9(4)
O(5)-Ti(2)-O(17)-Ti(1)	162.5(3)
O(7)-Ti(2)-O(17)-Ti(1)	-34.4(4)
O(8)-Ti(2)-O(17)-Ti(1)	-102.3(8)
O(6)-Ti(2)-O(17)-Ti(1)	-117.0(4)
O(17)-Ti(2)-O(18)-Ti(3)	42.0(4)
O(5)-Ti(2)-O(18)-Ti(3)	-57.3(4)
O(7)-Ti(2)-O(18)-Ti(3)	137.3(3)
O(8)-Ti(2)-O(18)-Ti(3)	-140.1(3)
O(19)-Ti(3)-O(18)-Ti(2)	-80.5(4)
O(11)-Ti(3)-O(18)-Ti(2)	-174.3(3)
O(9)-Ti(3)-O(18)-Ti(2)	16.9(4)
O(10)-Ti(3)-O(18)-Ti(2)	78.9(7)
O(12)-Ti(3)-O(18)-Ti(2)	104.9(3)
O(18)-Ti(3)-O(19)-Ti(4)	-31.7(3)
O(11)-Ti(3)-O(19)-Ti(4)	67.3(3)
O(9)-Ti(3)-O(19)-Ti(4)	-123.8(3)
O(10)-Ti(3)-O(19)-Ti(4)	153.5(3)
O(20)-Ti(4)-O(19)-Ti(3)	72.0(3)
O(13)-Ti(4)-O(19)-Ti(3)	-26.1(3)
O(15)-Ti(4)-O(19)-Ti(3)	166.4(3)
O(14)-Ti(4)-O(19)-Ti(3)	-85.0(7)
O(16)-Ti(4)-O(19)-Ti(3)	-112.3(3)
O(19)-Ti(4)-O(20)-Ti(1)	33.2(4)
O(13)-Ti(4)-O(20)-Ti(1)	125.9(3)
O(15)-Ti(4)-O(20)-Ti(1)	-65.3(3)
O(14)-Ti(4)-O(20)-Ti(1)	-151.4(3)
O(17)-Ti(1)-O(20)-Ti(4)	-78.1(3)
O(1)-Ti(1)-O(20)-Ti(4)	-175.2(3)
O(3)-Ti(1)-O(20)-Ti(4)	20.8(3)

O(4)-Ti(1)-O(20)-Ti(4)	92.4(6)
O(2)-Ti(1)-O(20)-Ti(4)	102.3(3)
Ti(1)-O(1)-C(1)-C(2)	2.5(7)
Ti(1)-O(1)-C(1)-C(25)	-176.4(3)
O(1)-C(1)-C(2)-C(3)	2.7(7)
C(25)-C(1)-C(2)-C(3)	-178.5(4)
Ti(1)-O(2)-C(3)-C(2)	0.4(7)
Ti(1)-O(2)-C(3)-C(31)	-179.8(3)
C(1)-C(2)-C(3)-O(2)	-4.0(8)
C(1)-C(2)-C(3)-C(31)	176.1(5)
Ti(1)-O(3)-C(4)-C(5)	7.0(6)
Ti(1)-O(3)-C(4)-C(32)	-175.3(3)
O(3)-C(4)-C(5)-C(6)	10.3(7)
C(32)-C(4)-C(5)-C(6)	-167.2(4)
Ti(1)-O(4)-C(6)-C(5)	-13.4(7)
Ti(1)-O(4)-C(6)-C(38)	168.6(3)
C(4)-C(5)-C(6)-O(4)	-6.5(8)
C(4)-C(5)-C(6)-C(38)	171.4(4)
Ti(2)-O(5)-C(7)-C(8)	6.3(7)
Ti(2)-O(5)-C(7)-C(46)	-172.6(3)
O(5)-C(7)-C(8)-C(9)	10.3(8)
C(46)-C(7)-C(8)-C(9)	-170.8(5)
Ti(2)-O(6)-C(9)-C(8)	-26.9(7)
Ti(2)-O(6)-C(9)-C(52)	151.9(3)
C(7)-C(8)-C(9)-O(6)	2.3(9)
C(7)-C(8)-C(9)-C(52)	-176.5(5)
Ti(2)-O(7)-C(10)-C(11)	-14.6(7)
Ti(2)-O(7)-C(10)-C(39)	166.4(3)
O(7)-C(10)-C(11)-C(12)	2.0(8)
C(39)-C(10)-C(11)-C(12)	-179.0(5)
Ti(2)-O(8)-C(12)-C(11)	-1.6(8)
Ti(2)-O(8)-C(12)-C(45)	176.3(3)
C(10)-C(11)-C(12)-O(8)	5.5(8)
C(10)-C(11)-C(12)-C(45)	-172.2(5)
Ti(3)-O(9)-C(13)-C(14)	-2.0(7)
Ti(3)-O(9)-C(13)-C(53)	175.5(3)

O(9)-C(13)-C(14)-C(15)	3.0(7)
C(53)-C(13)-C(14)-C(15)	-174.4(4)
Ti(3)-O(10)-C(15)-C(14)	-2.5(8)
Ti(3)-O(10)-C(15)-C(59)	179.6(3)
C(13)-C(14)-C(15)-O(10)	-0.7(9)
C(13)-C(14)-C(15)-C(59)	177.0(5)
Ti(3)-O(11)-C(16)-C(17)	-9.2(8)
Ti(3)-O(11)-C(16)-C(60)	173.2(3)
O(11)-C(16)-C(17)-C(18)	-7.1(9)
C(60)-C(16)-C(17)-C(18)	170.3(5)
Ti(3)-O(12)-C(18)-C(17)	12.2(9)
Ti(3)-O(12)-C(18)-C(66)	-170.2(5)
C(16)-C(17)-C(18)-O(12)	4.4(10)
C(16)-C(17)-C(18)-C(66)	-173.1(6)
Ti(4)-O(13)-C(19)-C(20)	-4.3(7)
Ti(4)-O(13)-C(19)-C(67)	179.8(3)
O(13)-C(19)-C(20)-C(21)	-1.7(8)
C(67)-C(19)-C(20)-C(21)	173.9(5)
Ti(4)-O(14)-C(21)-C(20)	-4.2(8)
Ti(4)-O(14)-C(21)-C(73)	173.1(4)
C(19)-C(20)-C(21)-O(14)	5.9(9)
C(19)-C(20)-C(21)-C(73)	-171.2(5)
Ti(4)-O(15)-C(22)-C(23)	9.0(7)
Ti(4)-O(15)-C(22)-C(74)	-169.8(3)
O(15)-C(22)-C(23)-C(24)	5.3(9)
C(74)-C(22)-C(23)-C(24)	-176.0(5)
Ti(4)-O(16)-C(24)-C(23)	-13.7(9)
Ti(4)-O(16)-C(24)-C(80)	170.3(6)
C(22)-C(23)-C(24)-O(16)	-1.7(11)
C(22)-C(23)-C(24)-C(80)	174.0(7)
O(1)-C(1)-C(25)-C(26)	12.9(6)
C(2)-C(1)-C(25)-C(26)	-166.0(4)
O(1)-C(1)-C(25)-C(30)	-168.3(4)
C(2)-C(1)-C(25)-C(30)	12.8(7)
C(30)-C(25)-C(26)-C(27)	-0.6(7)
C(1)-C(25)-C(26)-C(27)	178.2(4)

C(25)-C(26)-C(27)-C(28)	-0.3(7)
C(26)-C(27)-C(28)-C(29)	1.1(7)
C(27)-C(28)-C(29)-C(30)	-1.1(8)
C(28)-C(29)-C(30)-C(25)	0.2(7)
C(26)-C(25)-C(30)-C(29)	0.7(7)
C(1)-C(25)-C(30)-C(29)	-178.1(4)
O(2)-C(3)-C(31)-F(2)	-49.9(6)
C(2)-C(3)-C(31)-F(2)	129.9(5)
O(2)-C(3)-C(31)-F(1)	-172.0(4)
C(2)-C(3)-C(31)-F(1)	7.9(7)
O(2)-C(3)-C(31)-F(3)	67.6(5)
C(2)-C(3)-C(31)-F(3)	-112.6(5)
O(3)-C(4)-C(32)-C(37)	3.4(6)
C(5)-C(4)-C(32)-C(37)	-178.9(4)
O(3)-C(4)-C(32)-C(33)	-175.4(4)
C(5)-C(4)-C(32)-C(33)	2.2(7)
C(37)-C(32)-C(33)-C(34)	0.4(7)
C(4)-C(32)-C(33)-C(34)	179.3(5)
C(32)-C(33)-C(34)-C(35)	1.2(8)
C(33)-C(34)-C(35)-C(36)	-1.2(8)
C(34)-C(35)-C(36)-C(37)	-0.4(7)
C(35)-C(36)-C(37)-C(32)	2.0(7)
C(33)-C(32)-C(37)-C(36)	-2.0(6)
C(4)-C(32)-C(37)-C(36)	179.1(4)
O(4)-C(6)-C(38)-F(5)	-38.3(7)
C(5)-C(6)-C(38)-F(5)	143.5(5)
O(4)-C(6)-C(38)-F(4)	-162.6(5)
C(5)-C(6)-C(38)-F(4)	19.2(7)
O(4)-C(6)-C(38)-F(6)	78.4(6)
C(5)-C(6)-C(38)-F(6)	-99.8(6)
O(7)-C(10)-C(39)-C(44)	-160.2(4)
C(11)-C(10)-C(39)-C(44)	20.8(7)
O(7)-C(10)-C(39)-C(40)	16.1(6)
C(11)-C(10)-C(39)-C(40)	-163.0(5)
C(44)-C(39)-C(40)-C(41)	-0.6(7)
C(10)-C(39)-C(40)-C(41)	-177.0(4)

C(39)-C(40)-C(41)-C(42)	1.4(8)
C(40)-C(41)-C(42)-C(43)	-1.3(9)
C(41)-C(42)-C(43)-C(44)	0.5(10)
C(42)-C(43)-C(44)-C(39)	0.3(9)
C(40)-C(39)-C(44)-C(43)	-0.2(7)
C(10)-C(39)-C(44)-C(43)	176.1(5)
O(8)-C(12)-C(45)-F(11)	174.6(5)
C(11)-C(12)-C(45)-F(11)	-7.4(8)
O(8)-C(12)-C(45)-F(12)	-65.8(7)
C(11)-C(12)-C(45)-F(12)	112.2(6)
O(8)-C(12)-C(45)-F(10)	52.1(8)
C(11)-C(12)-C(45)-F(10)	-129.9(6)
O(5)-C(7)-C(46)-C(51)	-2.6(6)
C(8)-C(7)-C(46)-C(51)	178.5(5)
O(5)-C(7)-C(46)-C(47)	177.2(4)
C(8)-C(7)-C(46)-C(47)	-1.7(7)
C(51)-C(46)-C(47)-C(48)	2.1(8)
C(7)-C(46)-C(47)-C(48)	-177.7(5)
C(46)-C(47)-C(48)-C(49)	-0.4(10)
C(47)-C(48)-C(49)-C(50)	-2.5(10)
C(48)-C(49)-C(50)-C(51)	3.5(10)
C(47)-C(46)-C(51)-C(50)	-1.0(8)
C(7)-C(46)-C(51)-C(50)	178.8(5)
C(49)-C(50)-C(51)-C(46)	-1.8(8)
O(6)-C(9)-C(52)-F(9)	169.2(5)
C(8)-C(9)-C(52)-F(9)	-11.9(7)
O(6)-C(9)-C(52)-F(8)	47.1(7)
C(8)-C(9)-C(52)-F(8)	-134.0(6)
O(6)-C(9)-C(52)-F(7)	-71.1(6)
C(8)-C(9)-C(52)-F(7)	107.9(6)
O(9)-C(13)-C(53)-C(54)	-9.3(6)
C(14)-C(13)-C(53)-C(54)	168.1(4)
O(9)-C(13)-C(53)-C(58)	169.4(5)
C(14)-C(13)-C(53)-C(58)	-13.1(7)
C(58)-C(53)-C(54)-C(55)	0.1(7)
C(13)-C(53)-C(54)-C(55)	178.9(4)

C(53)-C(54)-C(55)-C(56)	-0.9(8)
C(54)-C(55)-C(56)-C(57)	1.5(9)
C(55)-C(56)-C(57)-C(58)	-1.2(11)
C(56)-C(57)-C(58)-C(53)	0.3(10)
C(54)-C(53)-C(58)-C(57)	0.2(8)
C(13)-C(53)-C(58)-C(57)	-178.6(5)
O(10)-C(15)-C(59)-F(20)	47.9(7)
C(14)-C(15)-C(59)-F(20)	-130.1(6)
O(10)-C(15)-C(59)-F(19)	169.3(5)
C(14)-C(15)-C(59)-F(19)	-8.8(8)
O(10)-C(15)-C(59)-F(21)	-72.1(7)
C(14)-C(15)-C(59)-F(21)	109.8(6)
O(11)-C(16)-C(60)-C(61)	11.5(7)
C(17)-C(16)-C(60)-C(61)	-166.1(6)
O(11)-C(16)-C(60)-C(65)	-169.6(5)
C(17)-C(16)-C(60)-C(65)	12.8(8)
C(65)-C(60)-C(61)-C(62)	-1.5(9)
C(16)-C(60)-C(61)-C(62)	177.4(6)
C(60)-C(61)-C(62)-C(63)	1.5(11)
C(61)-C(62)-C(63)-C(64)	-0.5(11)
C(62)-C(63)-C(64)-C(65)	-0.6(11)
C(63)-C(64)-C(65)-C(60)	0.5(9)
C(61)-C(60)-C(65)-C(64)	0.5(8)
C(16)-C(60)-C(65)-C(64)	-178.4(5)
O(12)-C(18)-C(66)-F(15)	-176.2(9)
C(17)-C(18)-C(66)-F(15)	1.7(12)
O(12)-C(18)-C(66)-F(13)	56.0(10)
C(17)-C(18)-C(66)-F(13)	-126.2(8)
O(12)-C(18)-C(66)-F(14)	-57.4(9)
C(17)-C(18)-C(66)-F(14)	120.5(8)
O(13)-C(19)-C(67)-C(72)	22.5(6)
C(20)-C(19)-C(67)-C(72)	-153.3(5)
O(13)-C(19)-C(67)-C(68)	-157.2(5)
C(20)-C(19)-C(67)-C(68)	27.0(7)
C(72)-C(67)-C(68)-C(69)	0.7(8)
C(19)-C(67)-C(68)-C(69)	-179.7(5)

C(67)-C(68)-C(69)-C(70)	1.6(9)
C(68)-C(69)-C(70)-C(71)	-2.4(9)
C(69)-C(70)-C(71)-C(72)	1.0(8)
C(68)-C(67)-C(72)-C(71)	-2.1(8)
C(19)-C(67)-C(72)-C(71)	178.3(5)
C(70)-C(71)-C(72)-C(67)	1.3(8)
O(14)-C(21)-C(73)-F(23)	56.4(7)
C(20)-C(21)-C(73)-F(23)	-126.1(6)
O(14)-C(21)-C(73)-F(22)	-62.8(6)
C(20)-C(21)-C(73)-F(22)	114.7(6)
O(14)-C(21)-C(73)-F(24)	178.8(5)
C(20)-C(21)-C(73)-F(24)	-3.7(8)
O(15)-C(22)-C(74)-C(75)	-4.8(6)
C(23)-C(22)-C(74)-C(75)	176.4(5)
O(15)-C(22)-C(74)-C(79)	173.8(4)
C(23)-C(22)-C(74)-C(79)	-5.1(7)
C(79)-C(74)-C(75)-C(76)	-0.7(7)
C(22)-C(74)-C(75)-C(76)	178.0(4)
C(74)-C(75)-C(76)-C(77)	-0.7(7)
C(75)-C(76)-C(77)-C(78)	1.2(8)
C(76)-C(77)-C(78)-C(79)	-0.3(9)
C(77)-C(78)-C(79)-C(74)	-1.1(9)
C(75)-C(74)-C(79)-C(78)	1.6(8)
C(22)-C(74)-C(79)-C(78)	-177.0(5)
O(16)-C(24)-C(80)-F(18)	60.4(11)
C(23)-C(24)-C(80)-F(18)	-115.9(9)
O(16)-C(24)-C(80)-F(17)	-58.1(11)
C(23)-C(24)-C(80)-F(17)	125.6(9)
O(16)-C(24)-C(80)-F(16)	-175.6(8)
C(23)-C(24)-C(80)-F(16)	8.0(13)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_jcti [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
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DFT calculated optimized coordinates.

REACTANT

C	-6.367519	-1.245509	1.257693
C	-5.393733	-1.436563	0.260159
C	-5.749603	-2.093600	-0.933110
C	-7.048654	-2.540815	-1.124202
C	-8.007834	-2.344694	-0.128627
C	-7.664398	-1.698637	1.060617
C	-4.014196	-0.973215	0.419724
O	-3.175660	-1.340860	-0.493384
Ti	-1.407496	-0.853569	-1.054472
Cl	-1.770038	-1.413137	-3.227604
O	0.285579	0.061753	-1.326485
C	0.713339	1.276844	-1.290245
C	-0.193880	2.339609	-1.062723
C	-1.550473	2.112202	-1.092954
C	-2.529962	3.268720	-0.876480
F	-3.458942	3.302728	-1.843457
C	2.136802	1.486919	-1.551376
C	2.762501	2.724266	-1.314878
C	4.112119	2.885282	-1.595510
C	4.847741	1.824148	-2.125579
C	4.236883	0.590745	-2.357227
C	2.892791	0.418513	-2.068817
O	-2.144336	0.991829	-1.271183
O	-1.280666	-0.195811	0.882880
C	-2.239713	0.121499	1.657095
C	-1.772706	0.936164	2.869455
F	-1.172543	2.068571	2.445730
O	2.742976	-1.711689	0.269414
C	2.974355	-0.632212	1.091993
C	4.311604	-0.252139	1.303703
C	4.528592	0.869143	2.122326
C	3.481327	1.581788	2.696619
C	2.167835	1.174902	2.471373
C	1.916661	0.063829	1.673612
C	5.477777	-0.939827	0.684960
C	5.647994	-2.342679	0.667839
C	6.822404	-2.902637	0.153379
C	7.834488	-2.099885	-0.356960
C	7.676629	-0.713510	-0.369342
C	6.513452	-0.156057	0.146549
O	4.735114	-3.214266	1.189401
F	-3.167251	3.090479	0.301198
F	-1.922171	4.465159	-0.836400
C	-3.580025	-0.175827	1.498245
F	-2.776199	1.282281	3.688412
F	-0.869113	0.241183	3.583472
Cl	-0.303234	-2.773743	-0.371579
H	0.899895	-0.257018	1.489144
H	1.337024	1.711594	2.911578

H	3.691215	2.440232	3.323416
H	5.549722	1.173787	2.318716
H	6.386140	0.919262	0.126075
H	8.448562	-0.073521	-0.780103
H	8.735194	-2.554836	-0.753326
H	6.913557	-3.982421	0.167390
H	1.792806	-1.883505	0.167931
H	3.842185	-2.888101	0.974898
H	0.158222	3.352223	-0.967347
H	-4.277235	0.170541	2.241268
H	2.416064	-0.537895	-2.228639
H	4.815698	-0.236552	-2.747569
H	5.900712	1.954027	-2.345071
H	4.592267	3.836021	-1.399859
H	2.210752	3.553227	-0.892802
H	-4.999986	-2.238033	-1.699746
H	-7.316880	-3.040736	-2.046826
H	-9.022180	-2.695410	-0.278443
H	-8.408267	-1.551883	1.833912
H	-6.118592	-0.757392	2.190299

INTER1

C	5.899926	0.537960	0.425760
C	4.720862	1.246050	0.140635
C	4.804358	2.490881	-0.507245
C	6.040732	3.020201	-0.848435
C	7.208225	2.309234	-0.561639
C	7.134814	1.067646	0.070016
C	3.387082	0.714737	0.472565
O	2.392838	1.295698	-0.046643
Ti	0.402991	0.838670	-0.159783
Cl	0.602718	3.006374	1.075730
O	-0.996671	-0.503958	-0.708270
C	-1.012324	-1.747944	-0.997239
C	0.171488	-2.454237	-1.304847
C	1.315366	-1.722295	-1.531511
C	2.557538	-2.389386	-2.133309
F	2.831783	-1.865357	-3.341749
C	-2.333971	-2.392949	-1.081745
C	-2.491773	-3.770874	-0.866057
C	-3.756067	-4.343647	-0.934017
C	-4.865663	-3.555125	-1.242826
C	-4.711369	-2.186835	-1.467856
C	-3.454987	-1.604071	-1.375606
O	1.480904	-0.477148	-1.336658
O	0.848422	-0.379161	1.294418
C	1.980908	-0.831357	1.721312
C	1.803179	-1.996918	2.691495
F	1.270500	-3.053914	2.044230
O	-1.413834	1.160111	1.056812
C	-2.521510	0.375692	1.379304
C	-3.804222	0.787140	0.990351
C	-4.876471	-0.038116	1.362006

C	-4.674529	-1.222278	2.061827
C	-3.383446	-1.609929	2.418012
C	-2.302944	-0.801162	2.083124
C	-4.042026	1.989536	0.150931
C	-3.488818	3.248488	0.439607
C	-3.721786	4.348880	-0.381998
C	-4.528226	4.216311	-1.508097
C	-5.104727	2.984011	-1.809682
C	-4.860009	1.891621	-0.984250
O	-2.718289	3.356262	1.579210
Cl	-0.088622	2.048145	-2.071687
F	3.630709	-2.178346	-1.345181
F	2.412549	-3.717568	-2.280788
C	3.222724	-0.390993	1.371527
F	2.958065	-2.393488	3.248690
F	0.954871	-1.664384	3.683685
H	-1.287411	-1.065888	2.343054
H	-3.216332	-2.534071	2.958079
H	-5.522880	-1.842656	2.324599
H	-5.881263	0.260137	1.086990
H	-5.297659	0.930573	-1.225477
H	-5.732430	2.871021	-2.685072
H	-4.702940	5.075842	-2.144119
H	-3.276377	5.305710	-0.132220
H	-1.564803	2.079064	1.379428
H	-2.304664	4.227509	1.629245
H	0.149090	-3.504089	-1.542049
H	4.081366	-0.856049	1.824343
H	-3.322935	-0.542537	-1.532672
H	-5.574263	-1.576474	-1.705733
H	-5.849151	-4.006224	-1.303677
H	-3.877160	-5.403622	-0.746150
H	-1.639576	-4.387935	-0.610450
H	3.892418	3.029529	-0.728595
H	6.098229	3.984365	-1.338951
H	8.173274	2.721368	-0.832500
H	8.039312	0.511442	0.283909
H	5.863462	-0.433115	0.900912

Tsdissociation

C	2.624231	3.853429	-0.704045
C	2.471359	2.472673	-0.914076
C	3.607337	1.659468	-1.045039
C	4.874900	2.219140	-0.979724
C	5.021968	3.589668	-0.760981
C	3.896685	4.403341	-0.616453
C	1.144021	1.850641	-0.978590
O	1.077508	0.599460	-0.717559
Ti	-0.392460	-0.664433	-0.297056
O	-1.376344	0.640335	-1.461155
C	-1.155899	1.882607	-1.666733
C	-2.348979	2.584298	-2.321509
F	-3.445097	2.447938	-1.550453

O	-0.755552	0.663595	1.170829
C	-1.871851	1.120221	1.599604
C	-3.127437	0.640667	1.312656
C	-3.277416	-0.529875	0.525261
C	-4.571940	-1.179963	0.299068
C	-1.691649	2.336004	2.512287
O	-2.254976	-1.105059	0.015378
O	1.161966	-1.238815	1.028723
C	2.351217	-0.608559	1.428640
C	3.583540	-1.136443	1.018889
C	4.735697	-0.467747	1.457300
C	4.656441	0.676860	2.243648
C	3.412819	1.180317	2.620456
C	2.251521	0.528777	2.216452
C	3.689339	-2.298731	0.100441
C	2.994618	-3.498290	0.324239
C	3.075205	-4.559088	-0.574634
C	3.868077	-4.443797	-1.712429
C	4.588912	-3.273530	-1.945006
C	4.497787	-2.219164	-1.042015
O	2.246935	-3.587582	1.478793
Cl	0.150672	-1.943612	-2.102104
C	-0.003429	2.574458	-1.382827
F	-2.135328	3.897289	-2.506351
F	-2.618551	2.032930	-3.517468
Cl	-0.797515	-3.432681	0.884189
H	1.269800	0.892778	2.484251
H	3.342748	2.074817	3.227359
H	5.564888	1.176686	2.557366
H	5.704023	-0.857279	1.166262
H	5.045404	-1.303532	-1.230869
H	5.210155	-3.178117	-2.827107
H	3.923264	-5.270198	-2.411012
H	2.523333	-5.470509	-0.374282
H	1.187458	-2.189365	1.303942
H	1.556957	-4.263240	1.385584
H	0.058240	3.622994	-1.618812
H	-3.983505	1.112415	1.764012
H	3.476549	0.597734	-1.199196
H	5.749461	1.589437	-1.086513
H	6.012908	4.023995	-0.699484
H	4.012583	5.464770	-0.434558
H	1.758347	4.489482	-0.572253
C	-4.580493	-2.498141	-0.191919
C	-5.785797	-3.147730	-0.417149
C	-6.991859	-2.487865	-0.170952
C	-6.991240	-1.176322	0.306921
C	-5.789251	-0.523608	0.548240
H	-3.636013	-2.996745	-0.369348
H	-5.789055	-4.167072	-0.783641
H	-7.932325	-2.994998	-0.352240
H	-7.927601	-0.663406	0.489210
H	-5.804753	0.498095	0.904264
F	-2.841711	2.743442	3.071371

F	-0.822962	2.057409	3.502949
F	-1.185163	3.366323	1.806248

INTER2

C	-5.556859	0.772176	0.914593
C	-4.463416	0.021116	0.442462
C	-4.690239	-1.227851	-0.167383
C	-5.983463	-1.714657	-0.290388
C	-7.062689	-0.960654	0.174149
C	-6.847151	0.283178	0.772855
C	-3.091221	0.503497	0.564839
O	-2.196832	-0.111670	-0.148324
Ti	-0.355071	0.018076	-0.591113
Cl	-0.386279	-1.552081	-2.209573
O	1.530323	0.512190	-0.659123
C	2.159057	1.609693	-0.888551
C	1.466787	2.714326	-1.462704
C	0.166313	2.590313	-1.871357
C	-0.555727	3.747390	-2.561203
F	-1.047271	3.356745	-3.748012
C	3.582147	1.644452	-0.562671
C	4.370932	2.794021	-0.765111
C	5.714763	2.784434	-0.421221
C	6.290912	1.634182	0.122817
C	5.518826	0.488152	0.324404
C	4.175192	0.490469	-0.014505
O	-0.588291	1.550605	-1.732489
O	-0.377860	1.398028	0.922109
C	-1.369855	1.898724	1.541594
C	-0.946991	2.991131	2.532028
F	-0.302427	3.975890	1.882763
O	0.229042	-1.323136	0.851708
C	1.436219	-1.432770	1.552470
C	2.317598	-2.476948	1.233282
C	3.507842	-2.538920	1.979210
C	3.807093	-1.596756	2.956532
C	2.913906	-0.560446	3.226613
C	1.714952	-0.484030	2.526885
C	2.080430	-3.443611	0.128010
C	0.838353	-4.057886	-0.114070
C	0.671295	-4.978843	-1.146148
C	1.745890	-5.297877	-1.968205
C	2.985991	-4.693709	-1.763245
C	3.142806	-3.782151	-0.726461
O	-0.221486	-3.718109	0.703423
F	-1.588796	4.153350	-1.799319
F	0.247863	4.802498	-2.767013
C	-2.703452	1.552716	1.418221
F	-1.984784	3.532486	3.187747
F	-0.099498	2.479197	3.447027
Cl	-2.895382	-4.526756	-0.245576
H	1.004106	0.309615	2.706572
H	3.144017	0.182181	3.980602

H	4.737192	-1.671947	3.506631
H	4.203411	-3.345413	1.782311
H	4.101613	-3.299023	-0.580899
H	3.822978	-4.924612	-2.410936
H	1.609356	-6.010148	-2.773376
H	-0.303970	-5.424222	-1.298051
H	-0.165223	-2.286942	0.799672
H	-1.108926	-4.064536	0.363662
H	1.976710	3.642558	-1.653508
H	-3.430182	2.058325	2.030929
H	3.570852	-0.390137	0.143634
H	5.962689	-0.402455	0.751492
H	7.340955	1.633043	0.390725
H	6.315223	3.672237	-0.575582
H	3.946093	3.695796	-1.184158
H	-3.853344	-1.822585	-0.509756
H	-6.149961	-2.683496	-0.745025
H	-8.072330	-1.340840	0.071230
H	-7.686528	0.869381	1.125898
H	-5.407324	1.743883	1.366345

TSproton1

C	-3.650502	3.474356	-0.603617
C	-2.532181	3.206499	0.203728
C	-1.366712	3.939758	-0.070232
C	-1.310869	4.902158	-1.070776
C	-2.441952	5.151626	-1.840403
C	-3.613187	4.430763	-1.610917
C	-2.634579	2.196604	1.290469
C	-1.621965	1.262877	1.571173
C	-1.769232	0.274979	2.539333
C	-2.953487	0.198782	3.262736
C	-3.972375	1.121623	3.025631
C	-3.809379	2.104645	2.056802
O	-0.437716	1.323526	0.848807
Ti	0.323468	0.107607	-0.519301
O	0.536139	-1.290306	0.966740
C	1.611078	-1.777527	1.440804
C	2.901757	-1.320366	1.246507
C	3.140508	-0.155006	0.492956
O	2.157366	0.437756	-0.109785
O	-0.236068	3.673848	0.704333
C	4.455053	0.471541	0.364977
C	5.633548	-0.182749	0.771244
C	6.862195	0.445087	0.625828
C	6.931718	1.732464	0.088058
C	5.767451	2.391169	-0.311087
C	4.535397	1.766316	-0.182304
Cl	0.201075	1.627041	-2.192005
O	-1.484392	-0.638485	-0.647009
C	-1.964411	-1.801581	-0.903857
C	-3.394223	-1.998895	-0.664594
C	-4.058722	-3.185068	-1.030534

C	-5.415001	-3.330069	-0.774899
C	-6.124953	-2.301226	-0.152124
C	-5.475839	-1.119881	0.212499
C	-4.122188	-0.965859	-0.043645
O	0.784266	-1.417331	-1.646356
C	0.182770	-2.552139	-1.748691
C	1.100945	-3.655618	-2.273558
F	0.449616	-4.807885	-2.495974
C	-1.114311	-2.827595	-1.402321
F	1.698858	-3.283729	-3.415373
F	2.065636	-3.894645	-1.360352
C	1.356527	-3.013362	2.311996
F	0.458989	-2.732948	3.274237
F	0.848152	-4.002229	1.550857
F	2.468705	-3.476488	2.903420
Cl	2.261273	4.792156	-0.210272
H	-0.966466	-0.432977	2.689787
H	-3.077088	-0.575702	4.009864
H	-4.892929	1.076454	3.594630
H	-4.601586	2.823370	1.887091
H	-4.556022	2.901917	-0.443830
H	-4.491817	4.606278	-2.219577
H	-2.401030	5.898964	-2.623591
H	-0.384163	5.434919	-1.241147
H	-0.167796	2.464737	0.792704
H	0.635648	4.111819	0.355737
H	-1.487358	-3.825103	-1.556927
H	3.709722	-1.824997	1.747703
H	-3.613566	-0.056817	0.240010
H	-6.023495	-0.322607	0.699713
H	-7.183189	-2.421309	0.048162
H	-5.921053	-4.243672	-1.061185
H	-3.530067	-3.991148	-1.520878
H	3.631643	2.283275	-0.477964
H	5.820414	3.392668	-0.720218
H	7.893482	2.220518	-0.018459
H	7.766834	-0.066862	0.929899
H	5.600034	-1.184027	1.179540

INTER3

C	-3.761329	-1.536958	0.139374
C	-2.898507	-2.292783	-0.673835
C	-3.369235	-3.479946	-1.260209
C	-4.674678	-3.898877	-1.034445
C	-5.520931	-3.146580	-0.217922
C	-5.060897	-1.966303	0.369175
C	-1.526479	-1.805552	-0.886489
C	-0.495971	-2.637626	-1.387213
C	0.743942	-2.114310	-1.682924
C	1.852833	-3.026008	-2.216641
F	2.836204	-3.117165	-1.295269
O	-1.302359	-0.581216	-0.583510
Ti	0.315540	0.548283	-0.387595

O	1.130432	-0.907602	-1.531756
O	-0.627076	1.460972	0.885612
C	-1.714155	1.265882	1.682019
C	-2.926794	1.898729	1.352663
C	-4.027310	1.643532	2.186897
C	-3.932275	0.793105	3.283466
C	-2.718019	0.171168	3.579369
C	-1.606728	0.410108	2.780848
C	-3.093357	2.742721	0.141604
C	-4.202003	2.514543	-0.690683
C	-4.469769	3.313668	-1.795578
C	-3.619883	4.380616	-2.089898
C	-2.504323	4.615346	-1.296179
C	-2.224327	3.801926	-0.195708
O	-1.115485	4.122846	0.537707
O	0.830790	-0.840496	1.063466
C	1.997254	-1.170271	1.434880
C	2.008217	-2.473049	2.244717
F	3.224063	-2.789321	2.721213
O	2.105208	1.187568	-0.028573
C	3.192134	0.715623	0.482730
C	4.405309	1.521973	0.289698
C	5.601533	1.252124	0.977498
C	6.724567	2.039282	0.758910
C	6.671751	3.099863	-0.147154
C	5.488034	3.377222	-0.833234
C	4.360342	2.598083	-0.614757
Cl	-0.017263	1.900403	-2.208537
C	3.186233	-0.506349	1.182373
F	1.425691	-4.272098	-2.482690
F	2.391715	-2.522886	-3.339498
F	1.164254	-2.385161	3.289441
F	1.592221	-3.493433	1.467406
H	-0.659924	-0.080406	2.962100
H	-2.638036	-0.501633	4.424998
H	-4.802268	0.616240	3.904479
H	-4.971171	2.125952	1.961955
H	-4.856956	1.681890	-0.460724
H	-5.330299	3.105776	-2.420277
H	-3.814921	5.017729	-2.945048
H	-1.816131	5.422592	-1.516638
H	-0.696792	3.302453	0.843495
H	-0.675509	-3.683731	-1.567421
H	4.100781	-0.919143	1.571521
H	-3.397957	-0.626204	0.592969
H	-5.713492	-1.382082	1.006812
H	-6.537001	-3.479707	-0.041095
H	-5.034363	-4.809710	-1.497432
H	-2.731970	-4.065152	-1.910232
H	3.438709	2.803263	-1.143066
H	5.447292	4.199545	-1.537199
H	7.551476	3.709664	-0.316604
H	7.640926	1.828854	1.296723
H	5.658707	0.443312	1.693796

TSinterchange

C	-4.399481	0.877934	-0.610627
C	-4.199268	-0.499319	-0.816083
C	-5.282235	-1.297003	-1.222761
C	-6.534251	-0.727336	-1.419616
C	-6.722075	0.640289	-1.214294
C	-5.652378	1.440829	-0.809247
C	-2.851271	-1.050845	-0.595590
C	-2.524937	-2.411090	-0.817036
C	-1.244229	-2.853203	-0.583150
C	-0.882854	-4.324620	-0.803817
F	-0.419788	-4.869232	0.337172
O	-1.965392	-0.229104	-0.180923
Ti	-0.008629	-0.214350	0.167155
O	-0.244504	-2.164781	-0.183187
O	-0.411217	0.988116	1.471466
C	-1.384359	1.908795	1.671806
C	-1.238727	3.209470	1.150622
C	-2.261445	4.132697	1.403706
C	-3.391009	3.781195	2.138351
C	-3.513545	2.487707	2.647494
C	-2.509905	1.554017	2.417999
C	-0.031852	3.603152	0.383218
C	0.657028	4.786239	0.681892
C	1.778717	5.177950	-0.044593
C	2.239634	4.383987	-1.092988
C	1.576828	3.201279	-1.409936
C	0.455592	2.829403	-0.678930
O	-0.236646	1.667364	-0.997692
O	0.973063	-1.101032	1.711524
C	2.208709	-1.307958	1.912974
C	2.472990	-2.084206	3.210064
F	3.781392	-2.303799	3.425690
O	1.820565	0.076491	-0.444000
C	3.018443	-0.222300	-0.084388
C	4.087801	0.183176	-1.007991
C	5.417157	0.339696	-0.584880
C	6.391483	0.741377	-1.491116
C	6.053812	0.973574	-2.825363
C	4.735226	0.809594	-3.254534
C	3.753134	0.424336	-2.351683
C	3.267190	-0.923974	1.109562
F	-1.929053	-5.061686	-1.216706
F	0.087593	-4.432218	-1.730097
F	1.989336	-1.403732	4.265286
F	1.854423	-3.278287	3.173354
Cl	-0.075928	-0.522268	-2.816899
H	-2.578605	0.540947	2.793755
H	-4.391803	2.204114	3.215339
H	-4.172902	4.511621	2.308058
H	-2.171324	5.134247	0.998943
H	0.305683	5.397849	1.504669

H	2.293330	6.096100	0.211931
H	3.114583	4.675411	-1.661477
H	1.922316	2.568818	-2.217145
H	-0.082036	1.346160	-1.919479
H	-3.264841	-3.114403	-1.157843
H	4.270343	-1.195760	1.391387
H	-3.566427	1.487940	-0.289674
H	-5.796836	2.502117	-0.646614
H	-7.700461	1.080248	-1.368819
H	-7.364087	-1.349163	-1.732755
H	-5.159837	-2.359424	-1.385482
H	2.727483	0.283400	-2.671033
H	4.475638	0.982008	-4.292138
H	6.817853	1.281644	-3.529552
H	7.413185	0.876167	-1.157395
H	5.687738	0.179294	0.451017

INTER4

C	-4.451251	1.107793	-0.013113
C	-4.233464	-0.226967	-0.402814
C	-5.315746	-1.125215	-0.418237
C	-6.582457	-0.695178	-0.045710
C	-6.788419	0.632110	0.334240
C	-5.720904	1.532620	0.348058
C	-2.873292	-0.634419	-0.767989
C	-2.587175	-1.882557	-1.392911
C	-1.331830	-2.155485	-1.871472
C	-1.056073	-3.445796	-2.644542
F	-0.145331	-4.186792	-1.985596
O	-0.282221	-1.413990	-1.759395
Ti	0.032024	0.068045	-0.542829
Cl	0.864679	0.970470	3.635719
O	1.923206	-0.355436	-0.282993
C	2.633159	-1.130615	0.462612
C	2.025325	-1.973614	1.416355
C	0.659256	-1.943932	1.609164
O	-0.189173	-1.213515	0.999444
C	4.088695	-1.055624	0.278065
C	4.618526	0.024938	-0.450125
C	5.989022	0.137233	-0.637089
C	6.847440	-0.830843	-0.112325
C	6.330500	-1.911287	0.604658
C	4.960764	-2.023785	0.805470
C	0.008068	-2.898511	2.616353
F	-0.866644	-2.255582	3.402053
F	-0.670466	-3.854594	1.946036
F	0.907087	-3.511988	3.405396
O	0.449233	1.425905	-1.644416
C	1.296177	2.486336	-1.637972
C	1.020104	3.607187	-0.830752
C	1.940786	4.663355	-0.860566
C	3.084608	4.613457	-1.652737
C	3.331096	3.495196	-2.448790

C	2.434164	2.432443	-2.444524
C	-0.210470	3.714672	-0.005072
C	-0.980645	4.887547	-0.048636
C	-2.111365	5.049097	0.745954
C	-2.505981	4.030426	1.611719
C	-1.769543	2.850990	1.666467
C	-0.643747	2.704825	0.864829
O	0.068926	1.506827	0.945023
O	-1.932924	0.205120	-0.543299
F	-2.158448	-4.195294	-2.808532
F	-0.556601	-3.167774	-3.861104
H	2.595382	1.548730	-3.049091
H	4.219195	3.446164	-3.067581
H	3.781508	5.442749	-1.644490
H	1.759386	5.528985	-0.234402
H	-0.682049	5.679034	-0.725703
H	-2.684625	5.966325	0.684898
H	-3.386444	4.144238	2.232432
H	-2.056799	2.033958	2.315682
H	0.325949	1.275503	1.930648
H	2.621868	-2.615976	2.041161
H	-3.375525	-2.588094	-1.590769
H	3.946544	0.773145	-0.848816
H	6.389591	0.978575	-1.189671
H	7.917361	-0.744418	-0.261666
H	6.995901	-2.666185	1.005360
H	4.577541	-2.875723	1.351395
H	-3.618283	1.796981	-0.000015
H	-5.880052	2.562840	0.642628
H	-7.779663	0.963401	0.620804
H	-7.409746	-1.394080	-0.049932
H	-5.175818	-2.160558	-0.698455

TSproton2

C	4.947627	-1.979072	0.562497
C	4.067737	-0.952571	0.179366
C	4.587250	0.211484	-0.414767
C	5.954472	0.347224	-0.611723
C	6.820664	-0.679174	-0.230500
C	6.314170	-1.841814	0.352335
C	2.611496	-1.049106	0.375609
C	2.013305	-2.048752	1.174413
C	0.661618	-2.010624	1.455694
C	0.033820	-3.098934	2.333241
F	-0.845627	-3.813732	1.599412
O	1.900332	-0.148922	-0.202016
Ti	-0.016944	0.234351	-0.436959
O	-0.189195	-1.153724	1.055334
O	0.368389	1.550689	-1.617278
C	1.202557	2.620400	-1.562323
C	0.906038	3.712238	-0.720234
C	1.822444	4.773372	-0.697691
C	2.979358	4.759986	-1.471972

C	3.244702	3.673079	-2.304482
C	2.354030	2.606000	-2.351825
C	-0.342040	3.791834	0.083616
C	-0.796471	2.744775	0.906897
C	-1.944769	2.881901	1.685792
C	-2.677494	4.063690	1.650987
C	-2.256296	5.111654	0.833446
C	-1.104603	4.970323	0.065338
O	-0.106294	1.556844	0.987843
O	-1.982993	0.209187	-0.571829
C	-2.850430	-0.706082	-0.799124
C	-4.257521	-0.361126	-0.552666
C	-4.558110	0.931544	-0.084468
C	-5.872583	1.299023	0.163767
C	-6.905744	0.384227	-0.049648
C	-6.619226	-0.900174	-0.514770
C	-5.305638	-1.273537	-0.768125
O	-0.167966	-1.359034	-1.629362
C	-1.142031	-2.192117	-1.678804
C	-0.718664	-3.561475	-2.214473
F	-1.751538	-4.407036	-2.369264
C	-2.442304	-1.976539	-1.286379
F	-0.095777	-3.444652	-3.398897
F	0.149269	-4.126810	-1.348360
F	0.937844	-3.957308	2.836598
F	-0.639382	-2.556300	3.361676
C1	0.933497	1.038577	3.527769
H	2.532694	1.743945	-2.982349
H	4.143063	3.650953	-2.910135
H	3.671008	5.592335	-1.421523
H	1.626016	5.615014	-0.043732
H	-0.785865	5.783667	-0.576120
H	-2.823652	6.033608	0.789151
H	-3.573546	4.160107	2.252662
H	-2.249685	2.044852	2.301505
H	0.377086	1.290301	2.223456
H	2.612612	-2.816214	1.633155
H	-3.156998	-2.769612	-1.421400
H	3.908610	1.001058	-0.708816
H	6.345992	1.251235	-1.062636
H	7.887850	-0.574582	-0.387893
H	6.985049	-2.641283	0.642315
H	4.574899	-2.892498	1.006571
H	-3.752241	1.633398	0.081774
H	-6.093459	2.296303	0.524791
H	-7.932446	0.671005	0.145800
H	-7.420623	-1.609513	-0.681161
H	-5.108508	-2.273306	-1.130551

PRODUCT

C	-0.821970	2.762298	0.921320
C	-0.373533	3.808929	0.090100
C	-1.131339	4.990786	0.079426

C	-2.274185	5.139735	0.859112
C	-2.690024	4.095103	1.684029
C	-1.961565	2.911035	1.714148
C	0.867099	3.727644	-0.725991
C	1.162514	2.632546	-1.565760
C	2.305841	2.625977	-2.368388
C	3.189647	3.699023	-2.336151
C	2.926260	4.787231	-1.504619
C	1.777755	4.794743	-0.718192
O	0.339432	1.554862	-1.609838
Ti	-0.025601	0.267993	-0.380527
O	-1.993377	0.201463	-0.531662
C	-2.846964	-0.717927	-0.790472
C	-2.424145	-1.971508	-1.302698
C	-1.114713	-2.169523	-1.681150
O	-0.148121	-1.335814	-1.599693
O	-0.145054	1.576211	0.995104
C	-4.261459	-0.392417	-0.546817
C	-4.577749	0.881481	-0.040118
C	-5.897983	1.230658	0.205811
C	-6.921628	0.315787	-0.048346
C	-6.619371	-0.950393	-0.551577
C	-5.299848	-1.304981	-0.802566
C	-0.678531	-3.525551	-2.242551
F	-0.046092	-3.379221	-3.419177
F	0.185937	-4.105904	-1.382582
F	-1.704113	-4.375143	-2.425869
O	1.900617	-0.108390	-0.160978
C	2.616812	-1.028966	0.373575
C	4.073190	-0.919584	0.174781
C	4.575305	0.219598	-0.479601
C	5.940277	0.367348	-0.683427
C	6.823490	-0.620364	-0.243780
C	6.335630	-1.755926	0.404479
C	4.970874	-1.906039	0.617555
O	-0.176098	-1.158088	1.088530
C	0.676746	-2.038003	1.430503
C	0.058851	-3.165262	2.265041
F	0.963693	-4.061898	2.695901
C	2.023871	-2.067594	1.127330
F	-0.577086	-2.670274	3.341113
F	-0.851781	-3.828598	1.521119
Cl	0.969873	0.943566	3.632284
H	2.483347	1.762743	-2.997835
H	4.080969	3.680756	-2.952377
H	3.612551	5.624621	-1.464484
H	1.583117	5.637832	-0.065488
H	-0.816840	5.801431	-0.567645
H	-2.838056	6.064019	0.818512
H	-3.578679	4.196807	2.295946
H	-2.262049	2.077408	2.336916
H	0.429986	1.220068	2.423670
H	2.623421	-2.864714	1.531503
H	-3.130876	-2.766749	-1.464110

H	3.884271	0.980536	-0.816764
H	6.316843	1.250992	-1.184692
H	7.889109	-0.506095	-0.405118
H	7.019734	-2.523808	0.744652
H	4.615730	-2.795324	1.120550
H	-3.779270	1.583963	0.157077
H	-6.130552	2.214045	0.596547
H	-7.952666	0.588210	0.144925
H	-7.413031	-1.660333	-0.749802
H	-5.090836	-2.290769	-1.195511