Snapshots of Titanium BINOLate Complexes with Diverse Solid State Structures

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Supplementary Material

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Formula:	$Ti_3C_{79}H_{79}O_{12}Cl_3$
Formula weight:	1470.47
Crystal class:	orthorhombic
Space group:	$P2_12_12_1$ (#19)
Z	4
Cell constants:	
a	18.9384(3)Å
b	22.5807(6)Å
c	17.8197(4)Å
V	7620.5(3)$Å^3$
μ	4.70 cm^{-1}
crystal size, mm	0.32 x 0.22 x 0.08
D_{calc}	1.282 g/cm^3
F(000)	3064
Radiation:	Mo-K_α (λ=0.71069Å)
2θ range	5.06 – 50.7 °
hkl collected:	-22≤ h ≤20; -24≤ k ≤27; -20≤ l ≤21
No. reflections measured:	35081
No. unique reflections:	13430 (R_{int}=0.0687)
No. observed reflections	11300 (F>4σ)
No. reflections used in refinement	13430
No. parameters	839
R indices (F>4σ)	R_1=0.0906
	wR_2=0.2340
R indices (all data)	R_1=0.1046
	wR_2=0.2476
GOF:	1.074
Final Difference Peaks, $e/Å^3$	+0.567, -0.364

Table S2. Refined Positional Parameters for Compound 2.

Atom	x	y	z	U_{eq}, Å^2
Ti1	0.12078(7)	0.15970(6)	0.50263(7)	0.0518(3)
Ti2	0.02870(6)	0.14023(5)	0.66015(7)	0.0455(3)
Ti3	0.00231(7)	0.00943(6)	0.74288(7)	0.0505(3)
O1	0.2183(3)	0.1655(2)	0.5070(3)	0.0590(12)
O2	0.1200(2)	0.1767(2)	0.6196(2)	0.0457(10)
O3	0.0468(2)	0.1093(2)	0.5497(2)	0.0469(11)
O4	0.0734(2)	0.0577(2)	0.6856(3)	0.0466(10)
O5	-0.0483(2)	0.0798(2)	0.6887(3)	0.0481(11)
O6	-0.0814(3)	-0.0323(2)	0.7359(3)	0.0600(13)
O7	0.1155(3)	0.1207(3)	0.4179(3)	0.075(2)
O8	0.0875(3)	0.2307(2)	0.4792(3)	0.067(2)
O9	-0.0333(3)	0.1914(2)	0.6231(3)	0.0536(12)
O10	0.0429(2)	0.1707(2)	0.7508(3)	0.0557(12)
O11	0.0593(3)	-0.0522(3)	0.7398(4)	0.070(2)
O12	0.0021(3)	0.0332(3)	0.8380(3)	0.0698(14)
C1	0.2685(3)	0.1523(3)	0.5575(4)	0.050(2)
C2	0.3208(4)	0.1107(3)	0.5388(5)	0.059(2)
H2	0.3194(4)	0.0932(3)	0.4916(5)	0.078
C3	0.3717(5)	0.0956(4)	0.5852(6)	0.070(2)
H3	0.4073(5)	0.0703(4)	0.5690(6)	0.093
C4	0.3727(4)	0.1171(4)	0.6587(6)	0.070(3)
C5	0.4217(5)	0.0975(5)	0.7167(9)	0.092(4)
H5	0.4567(5)	0.0706(5)	0.7036(9)	0.123
C6	0.4188(6)	0.1167(5)	0.7888(8)	0.096(4)
H6	0.4488(6)	0.1016(5)	0.8254(8)	0.128
C7	0.3691(5)	0.1598(5)	0.8055(5)	0.086(3)
H7	0.3670(5)	0.1741(5)	0.8544(5)	0.114
C8	0.3237(4)	0.1820(4)	0.7549(5)	0.070(2)
H8	0.2922(4)	0.2114(4)	0.7695(5)	0.093
C9	0.3229(4)	0.1616(4)	0.6795(5)	0.058(2)
C10	0.2726(4)	0.1814(3)	0.6254(4)	0.053(2)
C11	0.2244(4)	0.2325(3)	0.6402(4)	0.049(2)
C12	0.2566(4)	0.2888(3)	0.6552(4)	0.055(2)
C13	0.3310(4)	0.2974(4)	0.6491(4)	0.060(2)
H13	0.3603(4)	0.2656(4)	0.6377(4)	0.080
C14	0.3597(5)	0.3533(4)	0.6604(5)	0.075(2)
H14	0.4078(5)	0.3596(4)	0.6529(5)	0.100
C15	0.3156(5)	0.4011(4)	0.6833(5)	0.074(2)
H15	0.3355(5)	0.4377(4)	0.6939(5)	0.098

C16	0.2459(6)	0.3938(4)	0.6896(4)	0.072(2)
H16	0.2181(6)	0.4255(4)	0.7049(4)	0.096
C17	0.2127(5)	0.3379(3)	0.6735(4)	0.061(2)
C18	0.1392(4)	0.3307(4)	0.6768(4)	0.061(2)
H18	0.1107(4)	0.3619(4)	0.6920(4)	0.081
C19	0.1092(4)	0.2768(3)	0.6572(5)	0.059(2)
H19	0.0604(4)	0.2729(3)	0.6556(5)	0.079
C20	0.1527(4)	0.2282(3)	0.6400(4)	0.049(2)
C21	0.0235(4)	0.0550(3)	0.5252(3)	0.045(2)
C22	-0.0378(4)	0.0518(4)	0.4826(4)	0.054(2)
H22	-0.0632(4)	0.0862(4)	0.4731(4)	0.072
C23	-0.0616(4)	-0.0001(4)	0.4545(4)	0.067(2)
H23	-0.1016(4)	-0.0008(4)	0.4242(4)	0.089
C24	-0.0251(4)	-0.0537(4)	0.4714(4)	0.056(2)
C25	-0.0514(5)	-0.1079(5)	0.4437(5)	0.071(2)
H25	-0.0910(5)	-0.1082(5)	0.4128(5)	0.094
C26	-0.0192(6)	-0.1600(5)	0.4619(5)	0.083(3)
H26	-0.0363(6)	-0.1960(5)	0.4444(5)	0.111
C27	0.0414(6)	-0.1573(4)	0.5087(5)	0.077(2)
H27	0.0640(6)	-0.1924(4)	0.5219(5)	0.102
C28	0.0672(5)	-0.1060(3)	0.5344(5)	0.062(2)
H28	0.1068(5)	-0.1063(3)	0.5654(5)	0.082
C29	0.0357(4)	-0.0517(3)	0.5157(4)	0.052(2)
C30	0.0636(4)	0.0048(3)	0.5413(4)	0.046(2)
C31	0.1307(3)	0.0089(3)	0.5825(4)	0.046(2)
C32	0.1946(4)	-0.0143(3)	0.5510(5)	0.053(2)
C33	0.1997(5)	-0.0344(4)	0.4757(5)	0.068(2)
H33	0.1603(5)	-0.0315(4)	0.4447(5)	0.091
C34	0.2599(5)	-0.0576(4)	0.4474(7)	0.084(3)
H34	0.2610(5)	-0.0715(4)	0.3983(7)	0.112
C35	0.3183(6)	-0.0606(5)	0.4901(8)	0.101(4)
H35	0.3601(6)	-0.0745(5)	0.4689(8)	0.135
C36	0.3181(5)	-0.0437(4)	0.5647(7)	0.083(3)
H36	0.3580(5)	-0.0494(4)	0.5943(7)	0.111
C37	0.2560(4)	-0.0173(3)	0.5959(6)	0.063(2)
C38	0.2543(4)	0.0061(4)	0.6677(5)	0.064(2)
H38	0.2949(4)	0.0039(4)	0.6969(5)	0.085
C39	0.1973(4)	0.0315(3)	0.6967(4)	0.057(2)
H39	0.1987(4)	0.0480(3)	0.7445(4)	0.075
C40	0.1333(3)	0.0332(3)	0.6531(4)	0.046(2)
C41	-0.1165(4)	0.0932(3)	0.7110(4)	0.052(2)
C42	-0.1255(4)	0.1461(3)	0.7547(4)	0.058(2)
H42	-0.0865(4)	0.1686(3)	0.7688(4)	0.077

C43	-0.1922(4)	0.1630(5)	0.7754(4)	0.072(2)
H43	-0.1985(4)	0.1977(5)	0.8026(4)	0.096
C44	-0.2523(4)	0.1278(4)	0.7556(5)	0.067(2)
C45	-0.3218(5)	0.1478(5)	0.7787(5)	0.080(3)
H45	-0.3273(5)	0.1834(5)	0.8044(5)	0.106
C46	-0.3792(5)	0.1133(5)	0.7619(5)	0.083(3)
H46	-0.4243(5)	0.1261(5)	0.7746(5)	0.110
C47	-0.3702(5)	0.0596(5)	0.7262(5)	0.077(3)
H47	-0.4094(5)	0.0360(5)	0.7164(5)	0.103
C48	-0.3032(4)	0.0400(4)	0.7044(5)	0.069(2)
H48	-0.2983(4)	0.0032(4)	0.6816(5)	0.092
C49	-0.2425(4)	0.0760(4)	0.7167(4)	0.058(2)
C50	-0.1746(4)	0.0584(4)	0.6898(4)	0.060(2)
C51	-0.1655(4)	0.0026(3)	0.6466(4)	0.055(2)
C52	-0.2032(4)	-0.0083(4)	0.5782(4)	0.065(2)
C53	-0.2412(4)	0.0385(5)	0.5404(5)	0.066(2)
H53	-0.2435(4)	0.0763(5)	0.5611(5)	0.088
C54	-0.2735(4)	0.0264(5)	0.4744(5)	0.073(2)
H54	-0.2993(4)	0.0564(5)	0.4514(5)	0.097
C55	-0.2701(5)	-0.0282(6)	0.4396(6)	0.091(3)
H55	-0.2913(5)	-0.0337(6)	0.3931(6)	0.121
C56	-0.2342(5)	-0.0760(5)	0.4751(5)	0.080(3)
H56	-0.2339(5)	-0.1135(5)	0.4537(5)	0.106
C57	-0.1996(4)	-0.0653(4)	0.5426(5)	0.066(2)
C58	-0.1590(4)	-0.1088(4)	0.5800(5)	0.066(2)
H58	-0.1589(4)	-0.1470(4)	0.5604(5)	0.088
C59	-0.1208(5)	-0.0986(4)	0.6418(5)	0.069(2)
H59	-0.0937(5)	-0.1288(4)	0.6626(5)	0.092
C60	-0.1214(4)	-0.0415(4)	0.6757(4)	0.057(2)
C61	0.1320(11)	0.0936(7)	0.3507(6)	0.165(8)
H61	0.1750(11)	0.0717(7)	0.3636(6)	0.220
C62	0.0870(8)	0.0480(5)	0.3264(6)	0.114(4)
H62a	0.0733(8)	0.0243(5)	0.3686(6)	0.171
H62b	0.1113(8)	0.0237(5)	0.2905(6)	0.171
H62c	0.0458(8)	0.0649(5)	0.3035(6)	0.171
C63	0.1598(9)	0.1392(6)	0.2936(6)	0.132(6)
H63a	0.1886(9)	0.1679(6)	0.3190(6)	0.198
H63b	0.1207(9)	0.1588(6)	0.2700(6)	0.198
H63c	0.1875(9)	0.1193(6)	0.2561(6)	0.198
C64	0.0927(7)	0.2772(6)	0.4286(9)	0.136(6)
H64	0.1241(7)	0.2548(6)	0.3955(9)	0.182
C65	0.0373(9)	0.2782(9)	0.3740(11)	0.200(11)

H65a	0.0107(9)	0.2421(9)	0.3770(11)	0.300
H65b	0.0574(9)	0.2819(9)	0.3247(11)	0.300
H65c	0.0068(9)	0.3113(9)	0.3835(11)	0.300
C66	0.1397(14)	0.3183(9)	0.4397(11)	0.233(14)
H66a	0.1699(14)	0.3070(9)	0.4806(11)	0.350
H66b	0.1165(14)	0.3549(9)	0.4517(11)	0.350
H66c	0.1675(14)	0.3234(9)	0.3951(11)	0.350
C67	-0.0763(5)	0.2106(4)	0.5596(5)	0.070(2)
H67	-0.0523(5)	0.1978(4)	0.5137(5)	0.094
C68	-0.1463(5)	0.1794(5)	0.5624(6)	0.086(3)
H68a	-0.1389(5)	0.1374(5)	0.5619(6)	0.129
H68b	-0.1741(5)	0.1907(5)	0.5196(6)	0.129
H68c	-0.1708(5)	0.1904(5)	0.6075(6)	0.129
C69	-0.0762(7)	0.2755(4)	0.5601(7)	0.104(4)
H69a	-0.0284(7)	0.2896(4)	0.5583(7)	0.157
H69b	-0.0985(7)	0.2895(4)	0.6052(7)	0.157
H69c	-0.1016(7)	0.2899(4)	0.5173(7)	0.157
C70	0.0706(6)	0.1766(5)	0.8208(5)	0.089(3)
H70	0.0594(6)	0.1381(5)	0.8434(5)	0.118
C71	0.1453(6)	0.1776(7)	0.8253(7)	0.123(5)
H71a	0.1646(6)	0.1484(7)	0.7919(7)	0.184
H71b	0.1597(6)	0.1690(7)	0.8758(7)	0.184
H71c	0.1623(6)	0.2161(7)	0.8112(7)	0.184
C72	0.0305(8)	0.2175(6)	0.8685(7)	0.116(4)
H72a	-0.0192(8)	0.2115(6)	0.8606(7)	0.174
H72b	0.0426(8)	0.2576(6)	0.8559(7)	0.174
H72c	0.0417(8)	0.2102(6)	0.9202(7)	0.174
C73	0.1079(4)	-0.0968(4)	0.7507(6)	0.068(2)
H73	0.1423(4)	-0.0941(4)	0.7097(6)	0.090
C74	0.0671(5)	-0.1562(4)	0.7403(6)	0.081(3)
H74a	0.0427(5)	-0.1558(4)	0.6931(6)	0.122
H74b	0.0336(5)	-0.1609(4)	0.7803(6)	0.122
H74c	0.0999(5)	-0.1886(4)	0.7411(6)	0.122
C75	0.1469(5)	-0.0927(5)	0.8201(6)	0.090(3)
H75a	0.1706(5)	-0.0552(5)	0.8225(6)	0.135
H75b	0.1811(5)	-0.1240(5)	0.8223(6)	0.135
H75c	0.1149(5)	-0.0962(5)	0.8617(6)	0.135
C76	-0.0323(13)	0.0219(8)	0.9032(7)	0.185(10)
H76	-0.0801(13)	0.0165(8)	0.8834(7)	0.246
C77	-0.0444(11)	0.0674(9)	0.9493(10)	0.183(9)
H77a	-0.0527(11)	0.1025(9)	0.9203(10)	0.275
H77b	-0.0042(11)	0.0733(9)	0.9811(10)	0.275

H77c	-0.0852(11)	0.0591(9)	0.9795(10)	0.275
C78	-0.0218(8)	-0.0345(7)	0.9338(9)	0.149(7)
H78a	-0.0161(8)	-0.0627(7)	0.8940(9)	0.224
H78b	-0.0619(8)	-0.0452(7)	0.9637(9)	0.224
H78c	0.0198(8)	-0.0342(7)	0.9645(9)	0.224

$U_{eq}={}^{1}/_{3}[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$

Table S3. Bond Distances in Compound 2, Å

Ti1-O7	1.751(6)	Ti1-O8	1.771(5)	Ti1-O1	1.853(5)
Ti1-O3	1.991(5)	Ti1-O2	2.119(4)	Ti1-Ti2	3.334(2)
Ti2-O9	1.776(5)	Ti2-O10	1.776(5)	Ti2-O2	2.046(5)
Ti2-O5	2.061(5)	Ti2-O4	2.096(5)	Ti2-O3	2.117(5)
Ti2-Ti3	3.339(2)	Ti3-O11	1.762(5)	Ti3-O12	1.778(6)
Ti3-O6	1.848(5)	Ti3-O4	2.012(5)	Ti3-O5	2.093(5)
O1-C1	1.343(9)	O2-C20	1.368(8)	O3-C21	1.373(8)
O4-C40	1.388(8)	O5-C41	1.385(8)	O6-C60	1.330(9)
O7-C61	1.381(14)	O8-C64	1.388(11)	O9-C67	1.459(9)
O10-C70	1.359(10)	O11-C73	1.377(9)	O12-C76	1.356(14)
C1-C10	1.379(11)	C1-C2	1.404(10)	C2-C3	1.315(12)
C3-C4	1.396(13)	C4-C9	1.426(12)	C4-C5	1.457(14)
C5-C6	1.36(2)	C6-C7	1.39(2)	C7-C8	1.343(12)
C8-C9	1.421(12)	C9-C10	1.429(10)	C10-C11	1.494(10)
C11-C20	1.361(10)	C11-C12	1.436(10)	C12-C17	1.423(11)
C12-C13	1.427(11)	C13-C14	1.390(12)	C14-C15	1.424(13)
C15-C16	1.336(13)	C16-C17	1.439(12)	C17-C18	1.401(12)
C18-C19	1.386(11)	C19-C20	1.406(10)	C21-C22	1.390(10)
C21-C30	1.394(9)	C22-C23	1.350(11)	C23-C24	1.427(12)
C24-C29	1.396(10)	C24-C25	1.411(12)	C25-C26	1.363(14)
C26-C27	1.419(14)	C27-C28	1.338(12)	C28-C29	1.404(11)
C29-C30	1.455(10)	C30-C31	1.471(9)	C31-C40	1.373(10)
C31-C32	1.432(10)	C32-C37	1.413(11)	C32-C33	1.421(11)
C33-C34	1.352(12)	C34-C35	1.34(2)	C35-C36	1.38(2)
C36-C37	1.431(11)	C37-C38	1.386(12)	C38-C39	1.327(11)
C39-C40	1.441(9)	C41-C50	1.402(11)	C41-C42	1.436(10)
C42-C43	1.370(11)	C43-C44	1.431(13)	C44-C49	1.374(12)
C44-C45	1.452(11)	C45-C46	1.371(14)	C46-C47	1.381(14)
C47-C48	1.398(12)	C48-C49	1.425(12)	C49-C50	1.429(11)
C50-C51	1.487(11)	C51-C60	1.399(11)	C51-C52	1.433(10)
C52-C57	1.438(13)	C52-C53	1.446(12)	C53-C54	1.353(12)
C54-C55	1.38(2)	C55-C56	1.42(2)	C56-C57	1.391(12)
C57-C58	1.413(12)	C58-C59	1.339(12)	C59-C60	1.423(12)
C61-C62	1.40(2)	C61-C63	1.54(2)	C64-C66	1.30(2)
C64-C65	1.43(2)	C67-C69	1.464(14)	C67-C68	1.502(13)
C70-C71	1.42(2)	C70-C72	1.468(14)	C73-C75	1.444(14)
C73-C74	1.560(12)	C76-C77	1.34(2)	C76-C78	1.40(2)

Table S4. Bond Angles in 2, °

O7-Ti1-O8	103.4(3)	O7-Ti1-O1	97.4(3)	O8-Ti1-O1	107.5(3)
O7-Ti1-O3	92.0(2)	O8-Ti1-O3	111.5(2)	O1-Ti1-O3	136.4(2)
O7-Ti1-O2	159.8(3)	O8-Ti1-O2	93.8(2)	O1-Ti1-O2	87.3(2)
O3-Ti1-O2	71.6(2)	O7-Ti1-Ti2	129.0(2)	O8-Ti1-Ti2	97.6(2)
O1-Ti1-Ti2	119.7(2)	O3-Ti1-Ti2	37.05(13)	O2-Ti1-Ti2	36.09(13)
O9-Ti2-O10	100.8(2)	O9-Ti2-O2	99.5(2)	O10-Ti2-O2	92.2(2)
O9-Ti2-O5	93.1(2)	O10-Ti2-O5	97.9(2)	O2-Ti2-O5	162.0(2)
O9-Ti2-O4	157.9(2)	O10-Ti2-O4	94.9(2)	O2-Ti2-O4	95.3(2)
O5-Ti2-O4	69.2(2)	O9-Ti2-O3	88.6(2)	O10-Ti2-O3	161.7(2)
O2-Ti2-O3	70.6(2)	O5-Ti2-O3	97.2(2)	O4-Ti2-O3	80.9(2)
O9-Ti2-Ti1	86.9(2)	O10-Ti2-Ti1	129.5(2)	O2-Ti2-Ti1	37.58(12)
O5-Ti2-Ti1	131.73(14)	O4-Ti2-Ti1	95.04(13)	O3-Ti2-Ti1	34.50(13)
O9-Ti2-Ti3	129.9(2)	O10-Ti2-Ti3	87.9(2)	O2-Ti2-Ti3	129.65(13)
O5-Ti2-Ti3	36.82(13)	O4-Ti2-Ti3	34.79(13)	O3-Ti2-Ti3	98.20(13)
Ti1-Ti2-Ti3	124.52(5)	O11-Ti3-O12	105.7(3)	O11-Ti3-O6	96.9(3)
O12-Ti3-O6	102.5(3)	O11-Ti3-O4	90.1(2)	O12-Ti3-O4	108.8(2)
O6-Ti3-O4	144.7(2)	O11-Ti3-O5	150.0(2)	O12-Ti3-O5	102.1(2)
O6-Ti3-O5	87.9(2)	O4-Ti3-O5	70.2(2)	O11-Ti3-Ti2	126.4(2)
O12-Ti3-Ti2	98.9(2)	O6-Ti3-Ti2	123.3(2)	O4-Ti3-Ti2	36.49(14)
O5-Ti3-Ti2	36.18(13)	C1-O1-Ti1	135.9(5)	C20-O2-Ti2	129.1(4)
C20-O2-Ti1	114.3(4)	Ti2-O2-Ti1	106.3(2)	C21-O3-Ti1	127.1(4)
C21-O3-Ti2	122.5(4)	Ti1-O3-Ti2	108.5(2)	C40-O4-Ti3	122.8(4)
C40-O4-Ti2	126.5(4)	Ti3-O4-Ti2	108.7(2)	C41-O5-Ti2	126.0(4)
C41-O5-Ti3	117.4(4)	Ti2-O5-Ti3	107.0(2)	C60-O6-Ti3	128.5(5)
C61-O7-Ti1	163.4(9)	C64-O8-Ti1	144.4(9)	C67-O9-Ti2	148.3(5)
C70-O10-Ti2	158.5(6)	C73-O11-Ti3	169.0(6)	C76-O12-Ti3	139.5(8)
O1-C1-C10	121.4(6)	O1-C1-C2	119.2(7)	C10-C1-C2	119.2(7)
C3-C2-C1	122.8(8)	C2-C3-C4	120.6(8)	C3-C4-C9	118.6(8)
C3-C4-C5	124.7(9)	C9-C4-C5	116.7(10)	C6-C5-C4	123.4(11)
C5-C6-C7	117.0(10)	C8-C7-C6	123.6(11)	C7-C8-C9	121.3(9)
C10-C9-C4	119.1(8)	C10-C9-C8	122.9(7)	C4-C9-C8	117.9(8)
C1-C10-C9	118.7(7)	C1-C10-C11	119.3(6)	C9-C10-C11	122.0(7)
C20-C11-C12	119.1(7)	C20-C11-C10	123.6(7)	C12-C11-C10	117.2(6)
C11-C12-C17	118.9(7)	C11-C12-C13	121.7(7)	C17-C12-C13	119.3(7)
C14-C13-C12	119.9(8)	C13-C14-C15	120.0(8)	C16-C15-C14	120.8(8)
C15-C16-C17	121.6(9)	C18-C17-C12	120.0(7)	C18-C17-C16	121.8(8)
C12-C17-C16	118.2(8)	C19-C18-C17	119.8(8)	C18-C19-C20	120.0(7)
O2-C20-C11	120.9(6)	O2-C20-C19	117.2(6)	C11-C20-C19	121.8(7)
O3-C21-C22	119.3(6)	O3-C21-C30	119.1(6)	C22-C21-C30	121.6(7)
C23-C22-C21	121.8(7)	C22-C23-C24	119.7(7)	C29-C24-C25	121.1(8)
C29-C24-C23	119.4(7)	C25-C24-C23	119.4(7)	C26-C25-C24	120.4(8)

C25-C26-C27	117.8(9)	C28-C27-C26	122.2(9)	C27-C28-C29	121.2(9)
C24-C29-C28	117.2(7)	C24-C29-C30	120.3(7)	C28-C29-C30	122.4(7)
C21-C30-C29	116.8(6)	C21-C30-C31	121.4(6)	C29-C30-C31	121.8(6)
C40-C31-C32	118.4(6)	C40-C31-C30	120.9(6)	C32-C31-C30	120.7(6)
C37-C32-C33	117.5(7)	C37-C32-C31	119.4(7)	C33-C32-C31	123.1(7)
C34-C33-C32	122.2(10)	C35-C34-C33	120.2(11)	C34-C35-C36	121.8(9)
C35-C36-C37	119.4(10)	C38-C37-C32	119.0(7)	C38-C37-C36	122.5(8)
C32-C37-C36	118.5(9)	C39-C38-C37	122.9(7)	C38-C39-C40	119.1(8)
C31-C40-O4	120.8(6)	C31-C40-C39	120.9(6)	O4-C40-C39	118.2(6)
O5-C41-C50	122.1(7)	O5-C41-C42	116.5(6)	C50-C41-C42	121.3(7)
C43-C42-C41	119.1(7)	C42-C43-C44	120.8(8)	C49-C44-C43	119.4(7)
C49-C44-C45	122.0(9)	C43-C44-C45	118.6(9)	C46-C45-C44	118.7(9)
C45-C46-C47	120.2(8)	C46-C47-C48	121.1(9)	C47-C48-C49	120.6(9)
C44-C49-C50	121.8(7)	C44-C49-C48	117.1(7)	C50-C49-C48	121.2(8)
C41-C50-C49	117.4(7)	C41-C50-C51	121.6(7)	C49-C50-C51	120.8(7)
C60-C51-C52	119.4(7)	C60-C51-C50	118.7(6)	C52-C51-C50	121.9(7)
C51-C52-C57	120.3(8)	C51-C52-C53	121.3(8)	C57-C52-C53	118.2(7)
C54-C53-C52	118.9(9)	C53-C54-C55	123.3(10)	C54-C55-C56	119.9(9)
C57-C56-C55	118.6(10)	C56-C57-C58	122.9(9)	C56-C57-C52	120.9(9)
C58-C57-C52	116.1(8)	C59-C58-C57	124.2(9)	C58-C59-C60	120.1(9)
O6-C60-C51	121.8(7)	O6-C60-C59	118.7(8)	C51-C60-C59	119.5(7)
O7-C61-C62	117.0(12)	O7-C61-C63	110.8(11)	C62-C61-C63	119.6(11)
C66-C64-O8	119.3(12)	C66-C64-C65	126.4(13)	O8-C64-C65	113.8(10)
O9-C67-C69	106.9(8)	O9-C67-C68	109.1(7)	C69-C67-C68	118.0(9)
O10-C70-C71	116.1(9)	O10-C70-C72	113.1(9)	C71-C70-C72	118.3(10)
O11-C73-C75	114.6(8)	O11-C73-C74	106.3(7)	C75-C73-C74	114.2(8)
C77-C76-O12	117.6(13)	C77-C76-C78	119(2)	O12-C76-C78	116(2)

Table S5. Refined Thermal Parameters (U's) for 2.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti1	0.0564(7)	0.0525(7)	0.0464(6)	0.0046(6)	-0.0028(6)	0.0010(6)
Ti2	0.0459(6)	0.0438(6)	0.0468(6)	0.0003(5)	-0.0047(5)	0.0041(5)
Ti3	0.0474(6)	0.0542(7)	0.0499(7)	0.0068(6)	-0.0015(5)	0.0023(6)
O1	0.056(3)	0.065(3)	0.055(3)	-0.008(3)	0.000(2)	0.005(2)
O2	0.051(3)	0.043(3)	0.043(2)	-0.003(2)	-0.005(2)	0.005(2)
O3	0.049(3)	0.047(3)	0.044(2)	0.001(2)	-0.002(2)	0.009(2)
O4	0.044(2)	0.051(3)	0.045(2)	0.004(2)	-0.003(2)	0.000(2)
O5	0.042(2)	0.049(3)	0.054(3)	-0.002(2)	0.000(2)	0.006(2)
O6	0.058(3)	0.055(3)	0.067(3)	0.010(2)	-0.005(3)	0.000(2)
O7	0.079(4)	0.099(5)	0.048(3)	-0.006(3)	0.001(3)	-0.025(4)
O8	0.067(3)	0.055(3)	0.078(4)	0.013(3)	-0.011(3)	0.002(3)
O9	0.050(3)	0.053(3)	0.058(3)	0.003(2)	-0.013(2)	0.007(2)
O10	0.053(3)	0.053(3)	0.060(3)	-0.001(2)	-0.003(2)	0.004(2)
O11	0.060(3)	0.063(3)	0.089(4)	0.024(3)	0.006(3)	0.011(3)
O12	0.063(3)	0.081(4)	0.066(3)	0.007(3)	-0.007(3)	-0.010(3)
C1	0.039(3)	0.057(4)	0.055(4)	-0.006(3)	0.006(3)	-0.003(3)
C2	0.066(5)	0.047(4)	0.064(5)	0.003(3)	0.015(4)	-0.003(4)
C3	0.058(5)	0.053(5)	0.098(7)	-0.003(4)	0.028(5)	-0.001(4)
C4	0.035(4)	0.055(4)	0.119(7)	0.045(5)	0.006(4)	-0.007(3)
C5	0.045(5)	0.076(7)	0.155(12)	0.039(7)	-0.011(6)	-0.013(4)
C6	0.073(7)	0.087(8)	0.130(10)	0.045(7)	-0.023(7)	-0.006(6)
C7	0.081(6)	0.113(8)	0.062(5)	0.026(5)	-0.014(5)	-0.019(6)
C8	0.056(4)	0.081(6)	0.072(5)	0.009(5)	-0.009(4)	-0.011(4)
C9	0.035(3)	0.059(4)	0.078(5)	0.016(4)	-0.006(3)	-0.008(3)
C10	0.044(4)	0.058(4)	0.057(4)	0.020(3)	0.009(3)	0.001(3)
C11	0.051(4)	0.057(4)	0.039(3)	0.002(3)	-0.004(3)	0.003(3)
C12	0.070(5)	0.048(4)	0.048(4)	0.008(3)	0.000(3)	-0.010(3)
C13	0.063(5)	0.070(5)	0.047(4)	0.015(4)	0.002(3)	-0.011(4)
C14	0.085(6)	0.078(6)	0.063(5)	0.010(5)	0.000(4)	-0.026(5)
C15	0.087(6)	0.071(6)	0.063(5)	-0.005(4)	0.006(4)	-0.036(5)
C16	0.108(7)	0.057(5)	0.050(4)	0.005(4)	0.000(4)	-0.001(5)
C17	0.084(6)	0.045(4)	0.055(4)	-0.004(3)	-0.005(4)	-0.006(4)
C18	0.072(5)	0.055(4)	0.056(4)	0.003(3)	-0.003(4)	-0.003(4)
C19	0.064(5)	0.048(4)	0.066(5)	-0.003(3)	-0.013(4)	0.004(3)
C20	0.049(4)	0.045(4)	0.053(4)	-0.001(3)	-0.001(3)	0.002(3)
C21	0.053(4)	0.044(4)	0.037(3)	-0.003(3)	0.008(3)	0.006(3)
C22	0.051(4)	0.060(4)	0.052(4)	-0.004(3)	-0.004(3)	0.002(3)
C23	0.054(4)	0.093(7)	0.054(4)	-0.009(4)	-0.007(3)	-0.016(4)
C24	0.047(4)	0.068(5)	0.054(4)	-0.011(3)	0.008(3)	-0.016(4)

C25	0.072(5)	0.085(6)	0.055(5)	-0.012(4)	-0.006(4)	-0.002(5)
C26	0.108(8)	0.074(6)	0.068(5)	-0.013(5)	0.017(5)	-0.029(6)
C27	0.101(7)	0.058(5)	0.070(5)	0.001(4)	0.024(5)	-0.003(5)
C28	0.069(5)	0.042(4)	0.075(5)	-0.007(4)	0.018(4)	-0.005(4)
C29	0.052(4)	0.060(4)	0.045(4)	-0.003(3)	0.009(3)	0.006(3)
C30	0.049(4)	0.047(4)	0.043(3)	-0.003(3)	0.008(3)	0.007(3)
C31	0.043(3)	0.040(3)	0.056(4)	0.009(3)	-0.005(3)	-0.006(3)
C32	0.046(4)	0.031(3)	0.083(5)	0.012(3)	0.014(3)	0.002(3)
C33	0.076(5)	0.059(5)	0.071(5)	0.001(4)	0.031(4)	0.007(4)
C34	0.072(6)	0.061(5)	0.120(8)	0.002(5)	0.030(6)	0.012(5)
C35	0.071(7)	0.075(6)	0.157(11)	0.012(7)	0.059(7)	0.032(5)
C36	0.059(5)	0.049(5)	0.143(10)	0.008(5)	0.033(6)	0.004(4)
C37	0.038(4)	0.045(4)	0.107(7)	0.011(4)	0.012(4)	-0.010(3)
C38	0.034(3)	0.064(5)	0.093(6)	0.016(5)	-0.002(4)	0.003(3)
C39	0.053(4)	0.057(4)	0.059(4)	0.021(3)	-0.008(3)	0.002(3)
C40	0.037(3)	0.047(4)	0.053(4)	0.003(3)	0.003(3)	0.004(3)
C41	0.041(4)	0.053(4)	0.064(4)	0.000(3)	0.004(3)	0.001(3)
C42	0.061(4)	0.060(4)	0.052(4)	-0.015(3)	-0.001(3)	-0.006(4)
C43	0.062(5)	0.101(7)	0.054(4)	-0.015(4)	-0.003(4)	0.018(5)
C44	0.050(4)	0.088(6)	0.063(5)	0.010(5)	0.011(4)	0.013(4)
C45	0.060(5)	0.114(8)	0.067(5)	-0.005(5)	0.018(4)	0.025(5)
C46	0.046(4)	0.132(9)	0.071(5)	-0.002(6)	0.007(4)	0.029(5)
C47	0.055(5)	0.095(7)	0.083(6)	0.016(5)	0.003(4)	-0.005(5)
C48	0.040(4)	0.088(6)	0.081(6)	0.026(5)	0.005(4)	0.003(4)
C49	0.047(4)	0.076(5)	0.050(4)	0.001(4)	-0.002(3)	0.001(4)
C50	0.049(4)	0.077(5)	0.054(4)	0.004(4)	-0.006(3)	0.007(4)
C51	0.047(4)	0.061(5)	0.056(4)	0.006(3)	0.000(3)	-0.005(3)
C52	0.048(4)	0.093(6)	0.054(4)	0.004(4)	-0.002(3)	-0.003(4)
C53	0.047(4)	0.088(6)	0.064(5)	0.008(4)	-0.002(3)	-0.005(4)
C54	0.051(4)	0.101(7)	0.067(5)	0.013(5)	-0.002(4)	-0.013(5)
C55	0.077(6)	0.131(10)	0.066(6)	-0.005(6)	-0.016(5)	-0.028(6)
C56	0.068(6)	0.112(8)	0.059(5)	-0.004(5)	0.002(4)	-0.014(5)
C57	0.051(4)	0.086(6)	0.062(5)	-0.009(4)	0.000(4)	-0.008(4)
C58	0.058(5)	0.066(5)	0.074(5)	-0.005(4)	0.013(4)	-0.005(4)
C59	0.078(6)	0.062(5)	0.068(5)	-0.003(4)	0.007(4)	-0.009(4)
C60	0.049(4)	0.070(5)	0.053(4)	0.004(4)	0.004(3)	-0.019(4)
C61	0.29(2)	0.154(13)	0.055(6)	-0.019(7)	0.038(9)	-0.122(14)
C62	0.172(12)	0.091(8)	0.079(7)	-0.016(6)	0.026(7)	-0.048(8)
C63	0.22(2)	0.111(10)	0.067(6)	-0.001(6)	0.052(8)	-0.035(11)
C64	0.120(9)	0.096(9)	0.194(14)	0.096(10)	-0.076(10)	-0.048(7)
C65	0.129(12)	0.23(2)	0.24(2)	0.19(2)	-0.034(13)	-0.022(13)
C66	0.36(3)	0.19(2)	0.16(2)	0.081(14)	-0.04(2)	-0.17(2)
C67	0.068(5)	0.087(6)	0.056(5)	-0.001(4)	-0.010(4)	0.036(5)

C68	0.060(5)	0.126(9)	0.071(6)	0.008(6)	-0.025(4)	0.008(5)
C69	0.131(10)	0.066(6)	0.117(9)	-0.010(6)	-0.042(8)	0.037(6)
C70	0.107(8)	0.108(8)	0.052(5)	-0.030(5)	-0.020(5)	0.009(6)
C71	0.077(7)	0.189(14)	0.103(8)	-0.047(9)	-0.041(6)	0.024(8)
C72	0.133(11)	0.126(10)	0.088(7)	-0.024(7)	0.007(7)	0.036(9)
C73	0.065(5)	0.054(4)	0.083(6)	0.004(4)	0.007(5)	0.009(4)
C74	0.100(7)	0.060(5)	0.083(6)	0.007(5)	0.006(5)	0.006(5)
C75	0.077(6)	0.092(7)	0.100(8)	0.028(6)	-0.012(5)	0.001(5)
C76	0.33(3)	0.152(14)	0.068(7)	-0.008(8)	0.060(12)	-0.12(2)
C77	0.23(2)	0.20(2)	0.123(12)	-0.069(13)	0.080(13)	-0.09(2)
C78	0.135(12)	0.165(14)	0.148(13)	0.089(12)	0.044(10)	0.013(11)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

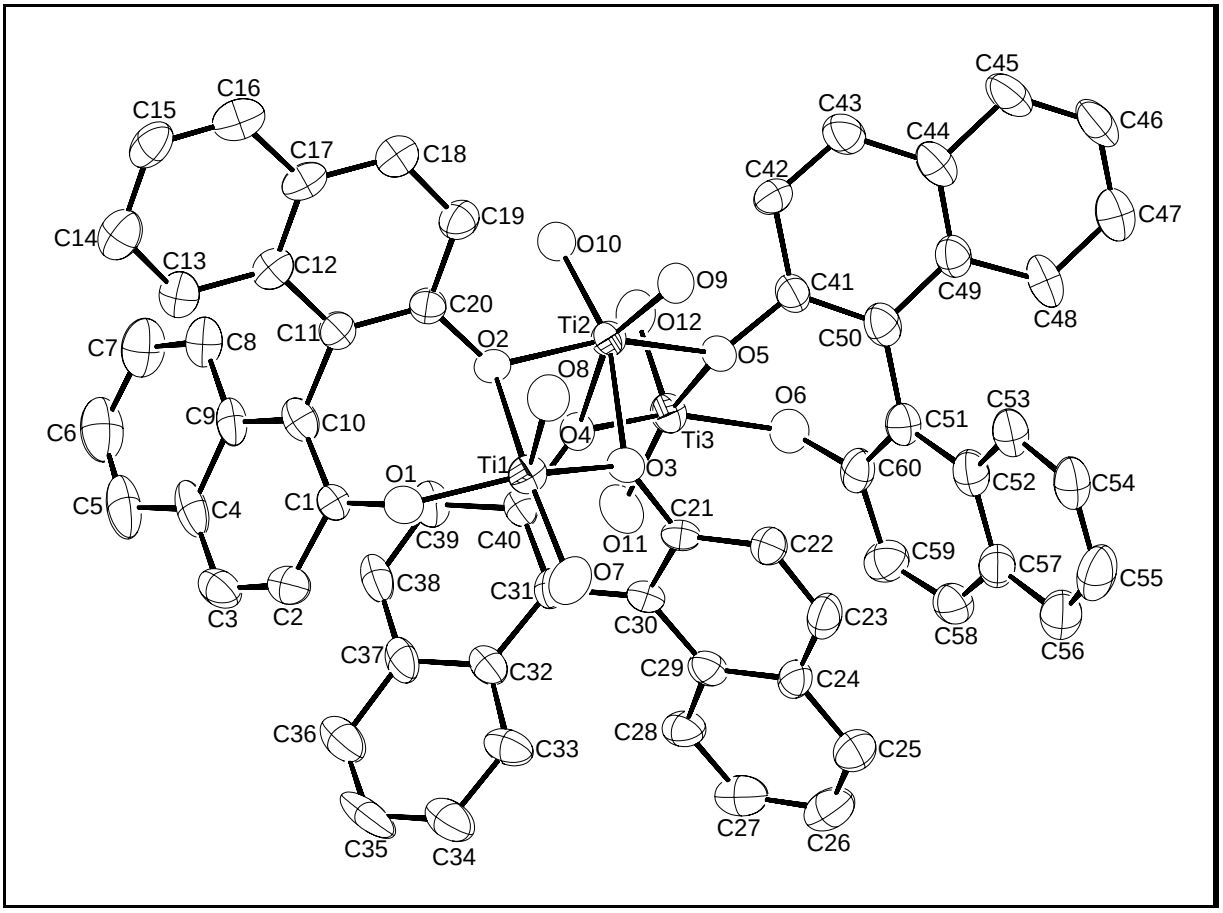


Table S6. Summary of Structure Determination of Compound 3.

Formula:	$Ti_2C_{38}H_{54}O_8$
Formula weight:	734.61
Crystal class:	monoclinic
Space group:	$P2_1/c$ (#14)
Z	4
Cell constants:	
a	18.9125(2)Å
b	12.9863(1)Å
c	17.2672(2)Å
β	109.651(1)°
V	3993.89(7)Å^3
μ	4.46 cm^{-1}
crystal size, mm	0.44 x 0.32 x 0.02
D_{calc}	1.222 g/cm^3
F(000)	1560
Radiation:	Mo-K_α (λ=0.71069Å)
2θ range	5 – 50.7 °
hkl collected:	-22≤ h ≤22; -15≤ k ≤15; -20≤ l ≤20
No. reflections measured:	28478
No. unique reflections:	7178 (R_{int}=0.0546)
No. observed reflections	6334 (F>4σ)
No. reflections used in refinement	7178
No. parameters	445
R indices (F>4σ)	R_1=0.0826
	wR_2=0.1459
R indices (all data)	R_1=0.0966
	wR_2=0.1516
GOF:	1.261
Final Difference Peaks, e/Å^3	+0.467, -0.345

Table S7. Refined Positional Parameters for Compound 3.

Atom	x	y	z	U_{eq}, Å^2
Ti1	0.77650(4)	0.58202(6)	0.25180(4)	0.0356(2)
Ti2	0.79820(4)	0.36407(6)	0.35646(4)	0.0345(2)
O1	0.72751(14)	0.4389(2)	0.2621(2)	0.0345(6)
O2	0.6793(2)	0.6299(2)	0.2326(2)	0.0361(6)
O3	0.8216(2)	0.7044(2)	0.2705(2)	0.0526(8)
O4	0.7892(2)	0.5457(3)	0.1580(2)	0.0545(8)
O5	0.84176(14)	0.5122(2)	0.3472(2)	0.0372(6)
O6	0.8051(2)	0.3929(2)	0.4604(2)	0.0513(8)
O7	0.7400(2)	0.2541(2)	0.3369(2)	0.0496(8)
O8	0.8841(2)	0.3084(2)	0.3516(2)	0.0493(8)
C1	0.6675(2)	0.4056(3)	0.1968(2)	0.0326(8)
C2	0.6819(2)	0.3346(3)	0.1425(3)	0.0395(10)
H2	0.7305(2)	0.3108(3)	0.1523(3)	0.053
C3	0.6253(2)	0.3006(3)	0.0760(3)	0.0427(10)
H3	0.6351(2)	0.2513(3)	0.0418(3)	0.057
C4	0.5522(2)	0.3389(3)	0.0580(2)	0.0365(9)
C5	0.4930(3)	0.3092(3)	-0.0144(2)	0.0432(10)
H5	0.5024(3)	0.2605(3)	-0.0492(2)	0.057
C6	0.4234(3)	0.3500(4)	-0.0337(3)	0.0498(12)
H6	0.3853(3)	0.3290(4)	-0.0810(3)	0.066
C7	0.4093(2)	0.4241(4)	0.0181(3)	0.0459(11)
H7	0.3618(2)	0.4535(4)	0.0040(3)	0.061
C8	0.4640(2)	0.4541(3)	0.0893(2)	0.0376(9)
H8	0.4528(2)	0.5026(3)	0.1230(2)	0.050
C9	0.5375(2)	0.4121(3)	0.1122(2)	0.0303(8)
C10	0.5966(2)	0.4431(3)	0.1850(2)	0.0293(8)
C11	0.5846(2)	0.5156(3)	0.2465(2)	0.0295(8)
C12	0.5326(2)	0.4928(3)	0.2887(2)	0.0310(8)
C13	0.4905(2)	0.4002(3)	0.2761(2)	0.0353(9)
H13	0.4953(2)	0.3525(3)	0.2381(2)	0.047
C14	0.4427(2)	0.3797(3)	0.3189(2)	0.0396(10)
H14	0.4156(2)	0.3185(3)	0.3094(2)	0.053
C15	0.4345(3)	0.4501(4)	0.3771(3)	0.0473(11)
H15	0.4021(3)	0.4356(4)	0.4059(3)	0.063
C16	0.4740(2)	0.5394(4)	0.3910(3)	0.0442(11)
H16	0.4679(2)	0.5860(4)	0.4291(3)	0.059
C17	0.5242(2)	0.5630(3)	0.3487(2)	0.0357(9)
C18	0.5679(2)	0.6543(3)	0.3652(3)	0.0426(10)
H18	0.5619(2)	0.7014(3)	0.4032(3)	0.057
C19	0.6179(2)	0.6739(3)	0.3269(2)	0.0398(10)
H19	0.6466(2)	0.7337(3)	0.3393(2)	0.053
C20	0.6270(2)	0.6043(3)	0.2679(2)	0.0332(9)
C21	0.8133(4)	0.8133(4)	0.2670(4)	0.091(2)
H21	0.7807(4)	0.8296(4)	0.2991(4)	0.122
C22	0.7718(5)	0.8466(5)	0.1822(5)	0.132(3)
H22a	0.802(2)	0.835(5)	0.1481(10)	0.198
H22b	0.760(3)	0.9187(14)	0.1820(8)	0.198
H22c	0.726(2)	0.808(4)	0.161(2)	0.198

C23	0.8833(4)	0.8661(5)	0.3074(6)	0.137(4)
H23a	0.8744(8)	0.9389(7)	0.307(4)	0.206
H23b	0.9180(14)	0.852(4)	0.279(3)	0.206
H23c	0.904(2)	0.843(4)	0.3632(14)	0.206
C24	0.8427(4)	0.5542(7)	0.1191(4)	0.099(2)
H24	0.8800(4)	0.6033(7)	0.1523(4)	0.131
C25	0.8125(5)	0.6010(8)	0.0383(4)	0.136(4)
H25a	0.8526(7)	0.615(5)	0.018(2)	0.203
H25b	0.787(3)	0.664(3)	0.0423(8)	0.203
H25c	0.777(3)	0.555(2)	0.0016(12)	0.203
C26	0.8838(5)	0.4548(7)	0.1255(6)	0.133(3)
H26a	0.924(2)	0.463(2)	0.104(4)	0.200
H26b	0.8499(10)	0.4027(14)	0.095(3)	0.200
H26c	0.904(3)	0.434(3)	0.1821(7)	0.200
C27	0.9121(2)	0.5405(4)	0.4106(3)	0.0498(12)
H27	0.9309(2)	0.4798(4)	0.4451(3)	0.066
C28	0.8972(3)	0.6235(4)	0.4644(3)	0.072(2)
H28a	0.9421(7)	0.636(2)	0.5100(14)	0.108
H28b	0.858(2)	0.6012(13)	0.484(2)	0.108
H28c	0.882(2)	0.6854(10)	0.4329(7)	0.108
C29	0.9698(3)	0.5701(5)	0.3718(3)	0.069(2)
H29a	1.0169(6)	0.584(3)	0.4141(3)	0.104
H29b	0.9533(11)	0.631(2)	0.339(2)	0.104
H29c	0.976(2)	0.5147(13)	0.338(2)	0.104
C30	0.7654(3)	0.3725(4)	0.5156(3)	0.0489(11)
H30	0.7442(3)	0.3030(4)	0.5049(3)	0.065
C31	0.7021(3)	0.4482(5)	0.5004(4)	0.077(2)
H31a	0.677(2)	0.437(2)	0.539(2)	0.116
H31b	0.6673(13)	0.439(2)	0.4456(10)	0.116
H31c	0.7217(4)	0.5170(5)	0.506(3)	0.116
C32	0.8198(3)	0.3762(5)	0.6013(3)	0.071(2)
H32a	0.7938(5)	0.363(3)	0.6394(3)	0.107
H32b	0.843(2)	0.4431(11)	0.6119(9)	0.107
H32c	0.8579(13)	0.325(2)	0.6077(8)	0.107
C33	0.6793(3)	0.1824(5)	0.3079(4)	0.072(2)
H33	0.6544(3)	0.1973(5)	0.2494(4)	0.096
C34	0.7072(4)	0.0778(5)	0.3127(6)	0.126(3)
H34a	0.739(3)	0.0718(13)	0.280(3)	0.188
H34b	0.6657(5)	0.0312(7)	0.292(4)	0.188
H34c	0.735(3)	0.061(2)	0.3689(8)	0.188
C35	0.6238(3)	0.1995(5)	0.3476(5)	0.098(2)
H35a	0.5781(10)	0.165(3)	0.317(2)	0.147
H35b	0.614(2)	0.2720(6)	0.349(3)	0.147
H35c	0.6423(12)	0.173(4)	0.4027(11)	0.147
C36	0.9087(3)	0.2057(4)	0.3464(3)	0.0613(14)
H36	0.8663(3)	0.1659(4)	0.3104(3)	0.082
C37	0.9688(3)	0.2090(6)	0.3085(4)	0.100(2)
H37a	0.984(2)	0.1400(6)	0.301(3)	0.151
H37b	1.0114(12)	0.246(4)	0.344(2)	0.151
H37c	0.9503(10)	0.243(4)	0.256(2)	0.151
C38	0.9340(4)	0.1574(5)	0.4300(4)	0.089(2)
H38a	0.948(3)	0.0871(12)	0.4259(6)	0.134

H38b	0.8938(10)	0.160(3)	0.4522(13)	0.134
H38c	0.976(2)	0.194(2)	0.4656(9)	0.134

$U_{eq}=1/3[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$

Table S8. Bond Distances in Compound 3, Å.

Ti1-O4	1.779(3)	Ti1-O3	1.781(3)	Ti1-O2	1.861(3)
Ti1-O5	1.921(3)	Ti1-O1	2.111(3)	Ti1-Ti2	3.3085(10)
Ti2-O7	1.765(3)	Ti2-O6	1.794(3)	Ti2-O8	1.805(3)
Ti2-O1	1.980(3)	Ti2-O5	2.120(3)	O1-C1	1.373(4)
O2-C20	1.366(5)	O3-C21	1.422(6)	O4-C24	1.395(6)
O5-C27	1.458(5)	O6-C30	1.423(5)	O7-C33	1.431(6)
O8-C36	1.426(5)	C1-C10	1.377(5)	C1-C2	1.405(5)
C2-C3	1.354(6)	C3-C4	1.402(6)	C4-C5	1.422(5)
C4-C9	1.427(5)	C5-C6	1.352(7)	C6-C7	1.400(7)
C7-C8	1.370(6)	C8-C9	1.420(5)	C9-C10	1.431(5)
C10-C11	1.493(5)	C11-C20	1.381(5)	C11-C12	1.438(5)
C12-C13	1.418(5)	C12-C17	1.429(5)	C13-C14	1.371(5)
C14-C15	1.405(6)	C15-C16	1.356(6)	C16-C17	1.412(6)
C17-C18	1.417(6)	C18-C19	1.349(6)	C19-C20	1.415(5)
C21-C23	1.446(9)	C21-C22	1.475(9)	C24-C25	1.450(9)
C24-C26	1.493(10)	C27-C28	1.509(7)	C27-C29	1.509(6)
C30-C32	1.492(6)	C30-C31	1.503(7)	C33-C35	1.450(8)
C33-C34	1.450(8)	C36-C37	1.491(8)	C36-C38	1.498(8)

Table S9. Bond Angles in Compound 3, °

O4-Ti1-O3	101.4(2)	O4-Ti1-O2	110.76(14)	O3-Ti1-O2	96.79(13)
O4-Ti1-O5	114.27(14)	O3-Ti1-O5	97.74(13)	O2-Ti1-O5	128.41(12)
O4-Ti1-O1	92.35(13)	O3-Ti1-O1	165.32(14)	O2-Ti1-O1	82.78(11)
O5-Ti1-O1	71.69(10)	O4-Ti1-Ti2	103.92(12)	O3-Ti1-Ti2	134.44(10)
O2-Ti1-Ti2	108.47(9)	O5-Ti1-Ti2	37.08(8)	O1-Ti1-Ti2	34.71(7)
O7-Ti2-O6	101.0(2)	O7-Ti2-O8	100.4(2)	O6-Ti2-O8	111.5(2)
O7-Ti2-O1	91.96(13)	O6-Ti2-O1	121.51(13)	O8-Ti2-O1	121.81(13)
O7-Ti2-O5	162.37(13)	O6-Ti2-O5	89.22(13)	O8-Ti2-O5	88.93(13)
O1-Ti2-O5	70.42(10)	O7-Ti2-Ti1	129.25(10)	O6-Ti2-Ti1	108.78(11)
O8-Ti2-Ti1	105.38(10)	O1-Ti2-Ti1	37.39(7)	O5-Ti2-Ti1	33.12(7)
C1-O1-Ti2	131.6(2)	C1-O1-Ti1	118.2(2)	Ti2-O1-Ti1	107.90(11)
C20-O2-Ti1	131.2(2)	C21-O3-Ti1	147.1(4)	C24-O4-Ti1	139.5(4)
C27-O5-Ti1	133.3(3)	C27-O5-Ti2	116.9(2)	Ti1-O5-Ti2	109.80(12)
C30-O6-Ti2	138.9(3)	C33-O7-Ti2	165.6(3)	C36-O8-Ti2	134.1(3)
O1-C1-C10	120.3(3)	O1-C1-C2	117.6(3)	C10-C1-C2	122.1(4)
C3-C2-C1	120.3(4)	C2-C3-C4	120.8(4)	C3-C4-C5	121.7(4)
C3-C4-C9	119.1(4)	C5-C4-C9	119.2(4)	C6-C5-C4	121.6(4)
C5-C6-C7	119.4(4)	C8-C7-C6	121.3(4)	C7-C8-C9	121.0(4)
C8-C9-C4	117.5(3)	C8-C9-C10	122.7(3)	C4-C9-C10	119.8(3)
C1-C10-C9	117.8(3)	C1-C10-C11	119.5(3)	C9-C10-C11	122.8(3)
C20-C11-C12	118.1(3)	C20-C11-C10	120.1(3)	C12-C11-C10	121.6(3)
C13-C12-C17	117.3(4)	C13-C12-C11	122.8(3)	C17-C12-C11	119.9(3)
C14-C13-C12	121.3(4)	C13-C14-C15	120.6(4)	C16-C15-C14	119.8(4)
C15-C16-C17	121.4(4)	C16-C17-C18	121.7(4)	C16-C17-C12	119.6(4)
C18-C17-C12	118.7(4)	C19-C18-C17	121.1(4)	C18-C19-C20	120.5(4)
O2-C20-C11	121.8(3)	O2-C20-C19	116.5(3)	C11-C20-C19	121.7(4)
O3-C21-C23	112.4(6)	O3-C21-C22	110.5(6)	C23-C21-C22	115.8(6)
O4-C24-C25	112.4(6)	O4-C24-C26	109.9(6)	C25-C24-C26	117.5(7)
O5-C27-C28	109.2(4)	O5-C27-C29	110.1(4)	C28-C27-C29	113.9(4)
O6-C30-C32	108.4(4)	O6-C30-C31	109.3(4)	C32-C30-C31	113.3(5)
O7-C33-C35	111.0(5)	O7-C33-C34	110.9(5)	C35-C33-C34	115.1(6)
O8-C36-C37	108.3(5)	O8-C36-C38	109.7(4)	C37-C36-C38	113.0(5)

Table S10. Refined Thermal Parameters (U's) for Compound 3.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti1	0.0344(4)	0.0360(4)	0.0333(4)	0.0026(3)	0.0075(3)	-0.0040(3)
Ti2	0.0335(4)	0.0339(4)	0.0365(4)	0.0023(3)	0.0121(3)	-0.0002(3)
O1	0.0300(14)	0.0313(14)	0.038(2)	-0.0029(12)	0.0065(12)	-0.0015(12)
O2	0.040(2)	0.0301(14)	0.036(2)	0.0034(12)	0.0107(12)	-0.0007(12)
O3	0.047(2)	0.036(2)	0.064(2)	0.010(2)	0.004(2)	-0.0092(14)
O4	0.053(2)	0.072(2)	0.044(2)	-0.001(2)	0.024(2)	-0.009(2)
O5	0.0306(14)	0.038(2)	0.037(2)	0.0032(12)	0.0030(12)	-0.0062(12)
O6	0.061(2)	0.057(2)	0.042(2)	-0.001(2)	0.025(2)	-0.009(2)
O7	0.045(2)	0.040(2)	0.059(2)	0.004(2)	0.011(2)	-0.0111(14)
O8	0.044(2)	0.042(2)	0.064(2)	-0.001(2)	0.021(2)	0.0084(14)
C1	0.034(2)	0.030(2)	0.033(2)	-0.003(2)	0.009(2)	-0.002(2)
C2	0.036(2)	0.038(2)	0.047(2)	-0.007(2)	0.018(2)	0.000(2)
C3	0.053(3)	0.040(2)	0.041(2)	-0.011(2)	0.024(2)	-0.003(2)
C4	0.052(2)	0.032(2)	0.026(2)	-0.003(2)	0.015(2)	-0.009(2)
C5	0.059(3)	0.041(2)	0.028(2)	-0.005(2)	0.012(2)	-0.017(2)
C6	0.064(3)	0.046(3)	0.027(2)	0.004(2)	0.000(2)	-0.023(2)
C7	0.040(2)	0.047(3)	0.039(2)	0.016(2)	-0.001(2)	-0.004(2)
C8	0.037(2)	0.037(2)	0.035(2)	0.001(2)	0.007(2)	-0.001(2)
C9	0.037(2)	0.029(2)	0.025(2)	0.002(2)	0.010(2)	-0.004(2)
C10	0.034(2)	0.028(2)	0.025(2)	0.002(2)	0.009(2)	0.000(2)
C11	0.033(2)	0.028(2)	0.025(2)	-0.002(2)	0.006(2)	0.003(2)
C12	0.034(2)	0.032(2)	0.025(2)	0.001(2)	0.007(2)	0.005(2)
C13	0.043(2)	0.033(2)	0.030(2)	0.001(2)	0.012(2)	0.000(2)
C14	0.040(2)	0.039(2)	0.039(2)	0.003(2)	0.012(2)	0.000(2)
C15	0.053(3)	0.054(3)	0.042(2)	0.002(2)	0.025(2)	0.003(2)
C16	0.053(3)	0.047(3)	0.037(2)	-0.005(2)	0.020(2)	0.012(2)
C17	0.041(2)	0.035(2)	0.030(2)	-0.002(2)	0.010(2)	0.006(2)
C18	0.055(3)	0.036(2)	0.037(2)	-0.008(2)	0.016(2)	0.006(2)
C19	0.046(2)	0.030(2)	0.038(2)	-0.007(2)	0.008(2)	-0.002(2)
C20	0.039(2)	0.029(2)	0.029(2)	0.000(2)	0.009(2)	0.002(2)
C21	0.105(5)	0.043(3)	0.109(5)	0.017(3)	0.012(4)	-0.008(3)
C22	0.129(7)	0.070(5)	0.150(8)	0.053(5)	-0.015(6)	-0.010(5)
C23	0.121(6)	0.056(4)	0.180(9)	0.000(5)	-0.022(6)	-0.040(4)
C24	0.081(4)	0.147(7)	0.086(5)	0.017(5)	0.051(4)	0.012(5)
C25	0.132(7)	0.223(11)	0.068(5)	0.030(6)	0.055(5)	-0.033(7)
C26	0.120(7)	0.143(8)	0.160(8)	-0.029(6)	0.077(6)	0.034(6)
C27	0.037(2)	0.056(3)	0.044(3)	0.004(2)	-0.003(2)	-0.010(2)
C28	0.085(4)	0.066(4)	0.051(3)	-0.009(3)	0.005(3)	-0.020(3)
C29	0.038(3)	0.090(4)	0.071(4)	0.020(3)	0.005(2)	-0.015(3)
C30	0.053(3)	0.054(3)	0.045(3)	0.000(2)	0.023(2)	-0.005(2)
C31	0.063(3)	0.077(4)	0.092(4)	-0.008(3)	0.027(3)	0.011(3)
C32	0.076(4)	0.096(4)	0.043(3)	0.006(3)	0.020(3)	-0.012(3)
C33	0.078(4)	0.074(4)	0.064(3)	-0.004(3)	0.023(3)	-0.040(3)
C34	0.104(6)	0.050(4)	0.241(10)	-0.049(5)	0.080(6)	-0.022(4)
C35	0.062(4)	0.062(4)	0.179(8)	-0.006(4)	0.052(5)	-0.021(3)
C36	0.053(3)	0.052(3)	0.073(4)	-0.012(3)	0.013(3)	0.013(2)

C37	0.073(4)	0.129(6)	0.103(5)	-0.024(5)	0.035(4)	0.038(4)
C38	0.098(5)	0.058(4)	0.097(5)	0.018(3)	0.013(4)	0.014(3)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

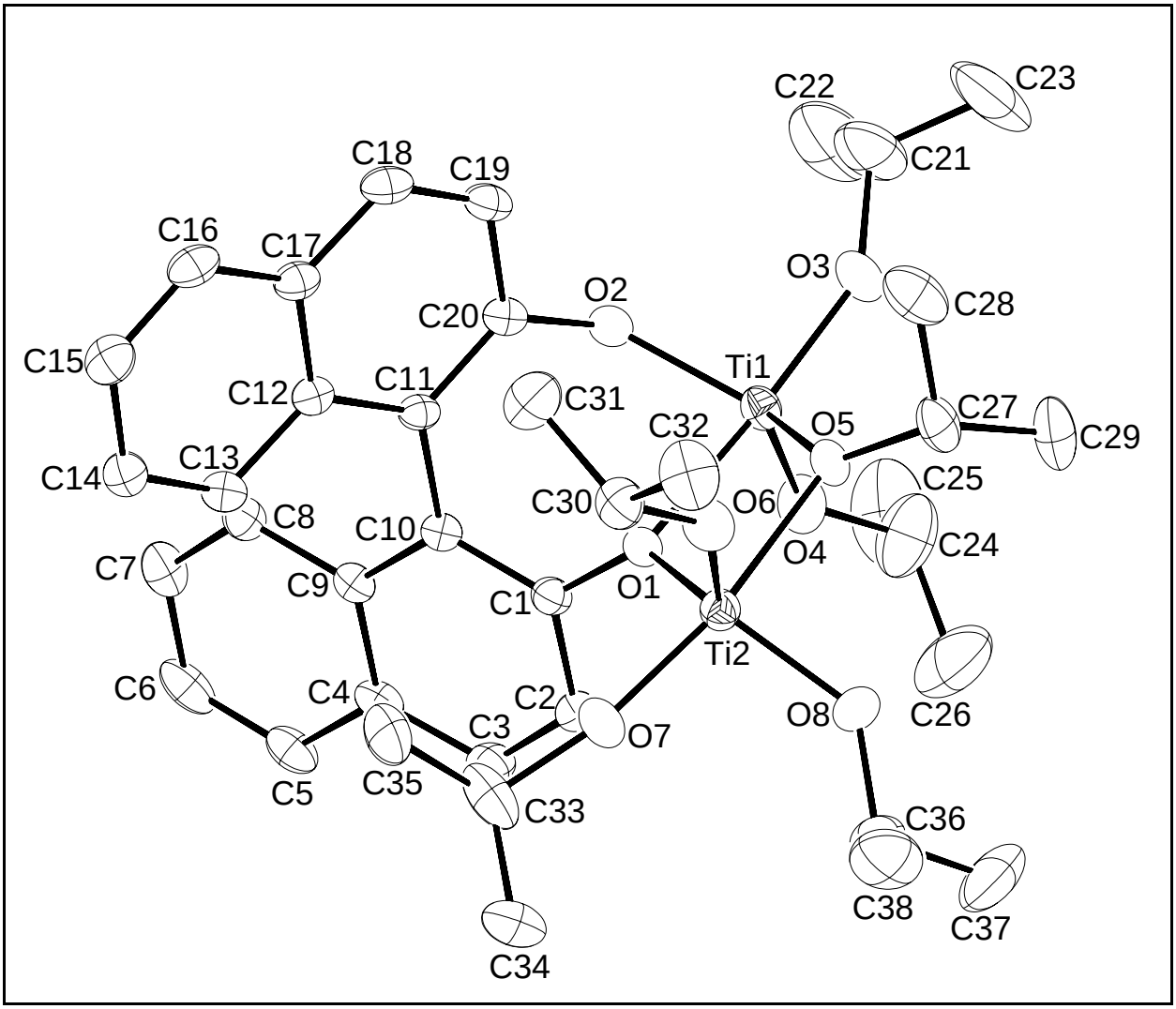


Table S11. Summary of Structure Determination of Compound 4.

Formula:	$Ti_2C_{38}H_{54}O_8$
Formula weight:	734.61
Crystal class:	monoclinic
Space group:	$P2_1/c$ (#14)
Z	4
Cell constants:	
a	18.9125(2)Å
b	12.9863(1)Å
c	17.2672(2)Å
β	109.651(1)°
V	3993.89(7)Å^3
μ	4.46 cm^{-1}
crystal size, mm	0.44 x 0.32 x 0.02
D_{calc}	1.222 g/cm^3
F(000)	1560
Radiation:	Mo-K_α (λ=0.71069Å)
2θ range	5 – 50.7 °
hkl collected:	-22≤ h ≤22; -15≤ k ≤15; -20≤ l ≤20
No. reflections measured:	28478
No. unique reflections:	7178 (R_{int}=0.0546)
No. observed reflections	6334 (F>4σ)
No. reflections used in refinement	7178
No. parameters	445
R indices (F>4σ)	R_1=0.0826
	wR_2=0.1459
R indices (all data)	R_1=0.0966
	wR_2=0.1516
GOF:	1.261
Final Difference Peaks, e/Å^3	+0.467, -0.345

Table S12. Refined Positional Parameters for Compound 4.

Atom	x	y	z	U_{eq}, Å^2
Ti1	0.46726(2)	0.65959(2)	0.09989(5)	0.03355(13)
Ti2	0.61623(2)	0.68489(2)	0.11051(5)	0.03497(13)
Ti3	0.42452(3)	0.52956(2)	0.16061(6)	0.03774(14)
O1	0.55437(9)	0.63037(8)	0.0379(2)	0.0301(4)
O2	0.48179(8)	0.58890(8)	0.2233(2)	0.0321(4)
O3	0.53181(10)	0.70479(8)	0.1850(2)	0.0380(5)
O4	0.42307(10)	0.59456(9)	0.0276(2)	0.0389(5)
O5	0.45972(11)	0.70219(9)	-0.0398(2)	0.0458(6)
O6	0.40774(10)	0.68305(10)	0.2024(2)	0.0460(6)
O7	0.67733(10)	0.64540(10)	0.0470(2)	0.0456(6)
O8	0.64926(11)	0.69986(11)	0.2666(2)	0.0528(6)
O9	0.62013(11)	0.74512(10)	0.0100(3)	0.0517(6)
O10	0.44932(13)	0.48589(10)	0.2891(2)	0.0560(7)
O11	0.42866(12)	0.48055(10)	0.0305(2)	0.0520(6)
O12	0.34636(11)	0.53923(11)	0.2021(3)	0.0617(7)
C1	0.56744(13)	0.57703(11)	0.0047(3)	0.0284(6)
C2	0.56769(14)	0.56297(13)	-0.1275(3)	0.0352(7)
H2	0.55852(14)	0.58973(13)	-0.1892(3)	0.047
C3	0.58114(14)	0.51083(13)	-0.1666(3)	0.0396(7)
H3	0.58216(14)	0.50243(13)	-0.2547(3)	0.053
C4	0.59359(13)	0.46932(13)	-0.0740(3)	0.0363(7)
C5	0.6059(2)	0.41417(14)	-0.1121(4)	0.0485(8)
H5	0.6065(2)	0.40519(14)	-0.1999(4)	0.064
C6	0.6168(2)	0.3743(2)	-0.0224(4)	0.0558(10)
H6	0.6247(2)	0.3383(2)	-0.0489(4)	0.074
C7	0.6161(2)	0.38744(14)	0.1108(4)	0.0510(8)
H7	0.6236(2)	0.36005(14)	0.1720(4)	0.068
C8	0.60456(14)	0.44009(12)	0.1505(3)	0.0402(7)
H8	0.60422(14)	0.44804(12)	0.2389(3)	0.053
C9	0.59308(13)	0.48289(12)	0.0605(3)	0.0312(6)
C10	0.58137(12)	0.53883(11)	0.0998(3)	0.0284(6)
C11	0.58332(13)	0.55630(12)	0.2382(3)	0.0292(6)
C12	0.63701(13)	0.55053(12)	0.3153(3)	0.0322(6)
C13	0.69287(14)	0.53234(14)	0.2628(3)	0.0399(7)
H13	0.69488(14)	0.52281(14)	0.1754(3)	0.053
C14	0.7437(2)	0.5285(2)	0.3372(4)	0.0480(8)
H14	0.7799(2)	0.5169(2)	0.3000(4)	0.064
C15	0.7417(2)	0.5419(2)	0.4694(4)	0.0527(9)
H15	0.7765(2)	0.5390(2)	0.5198(4)	0.070
C16	0.6890(2)	0.5591(2)	0.5243(3)	0.0516(9)
H16	0.6879(2)	0.5669(2)	0.6127(3)	0.069
C17	0.6355(2)	0.56534(13)	0.4494(3)	0.0384(7)
C18	0.5820(2)	0.58774(14)	0.5009(3)	0.0445(8)
H18	0.5805(2)	0.59711(14)	0.5884(3)	0.059
C19	0.5328(2)	0.59593(13)	0.4264(3)	0.0370(7)
H19	0.4984(2)	0.61207(13)	0.4621(3)	0.049
C20	0.53313(14)	0.58012(12)	0.2943(3)	0.0308(6)
C21	0.5274(2)	0.7548(2)	0.2617(4)	0.0628(11)

H21	0.5693(2)	0.7680(2)	0.2646(4)	0.084
C22	0.5140(2)	0.7420(2)	0.4000(4)	0.0594(10)
H22a	0.5468(6)	0.7211(11)	0.4364(9)	0.089
H22b	0.4773(8)	0.7208(11)	0.4053(4)	0.089
H22c	0.5092(14)	0.7758(2)	0.4477(7)	0.089
C23	0.4968(3)	0.7981(2)	0.2012(5)	0.106(2)
H23a	0.499(2)	0.8304(6)	0.255(2)	0.159
H23b	0.4553(6)	0.7879(8)	0.188(4)	0.159
H23c	0.5155(14)	0.8058(13)	0.119(2)	0.159
C24	0.3797(2)	0.5899(2)	-0.0786(4)	0.0507(9)
H24	0.3575(2)	0.5552(2)	-0.0663(4)	0.067
C25	0.4125(2)	0.5858(2)	-0.2059(4)	0.0646(11)
H25a	0.3839(2)	0.5791(13)	-0.2742(5)	0.097
H25b	0.4411(10)	0.5560(8)	-0.2022(11)	0.097
H25c	0.4336(11)	0.6198(5)	-0.222(2)	0.097
C26	0.3338(2)	0.6362(2)	-0.0745(4)	0.0661(12)
H26a	0.3049(9)	0.6312(8)	-0.143(2)	0.099
H26b	0.3541(3)	0.6709(2)	-0.086(3)	0.099
H26c	0.3133(10)	0.6358(9)	0.0077(13)	0.099
C27	0.4752(2)	0.7468(2)	-0.1212(4)	0.0764(14)
H27	0.5093(2)	0.7663(2)	-0.0812(4)	0.102
C28	0.4970(5)	0.7230(3)	-0.2509(6)	0.192(5)
H28a	0.520(4)	0.690(2)	-0.2353(8)	0.288
H28b	0.522(4)	0.750(2)	-0.295(4)	0.288
H28c	0.4626(6)	0.714(4)	-0.304(4)	0.288
C29	0.4232(3)	0.7858(3)	-0.1271(12)	0.205(5)
H29a	0.392(2)	0.771(2)	-0.183(8)	0.308
H29b	0.4367(11)	0.8206(14)	-0.161(9)	0.308
H29c	0.407(3)	0.791(3)	-0.041(2)	0.308
C30	0.3511(2)	0.6805(2)	0.2678(4)	0.0552(9)
H30	0.3264(2)	0.6521(2)	0.2251(4)	0.073
C31	0.3200(2)	0.7344(2)	0.2512(7)	0.100(2)
H31a	0.3397(13)	0.7618(5)	0.304(3)	0.150
H31b	0.2785(6)	0.7310(5)	0.278(4)	0.150
H31c	0.322(2)	0.7452(9)	0.1616(10)	0.150
C32	0.3599(2)	0.6633(3)	0.4074(5)	0.099(2)
H32a	0.3212(3)	0.656(2)	0.4462(13)	0.149
H32b	0.380(2)	0.6926(7)	0.4542(11)	0.149
H32c	0.384(2)	0.6307(11)	0.4108(5)	0.149
C33	0.7172(2)	0.61497(14)	-0.0321(4)	0.0462(8)
H33	0.7026(2)	0.57679(14)	-0.0360(4)	0.061
C34	0.7179(2)	0.6375(2)	-0.1664(4)	0.0665(11)
H34a	0.7435(12)	0.6151(8)	-0.2200(8)	0.100
H34b	0.7330(14)	0.6747(5)	-0.1649(6)	0.100
H34c	0.6775(3)	0.6374(12)	-0.2008(12)	0.100
C35	0.7801(2)	0.6147(2)	0.0281(5)	0.0725(13)
H35a	0.7964(7)	0.6515(3)	0.027(3)	0.109
H35b	0.8061(4)	0.5907(11)	-0.021(2)	0.109
H35c	0.7776(3)	0.6018(14)	0.1160(12)	0.109
C36	0.7052(2)	0.6961(2)	0.3340(4)	0.0607(10)
H36	0.7207(2)	0.6583(2)	0.3255(4)	0.081
C37	0.6944(3)	0.7080(2)	0.4762(4)	0.079(2)

H37a	0.679(2)	0.7450(6)	0.4858(5)	0.119
H37b	0.7318(4)	0.704(2)	0.5230(7)	0.119
H37c	0.6652(13)	0.6824(10)	0.5100(10)	0.119
C38	0.7506(2)	0.7354(3)	0.2757(6)	0.098(2)
H38a	0.7879(7)	0.7334(14)	0.324(3)	0.147
H38b	0.7350(9)	0.7723(4)	0.280(4)	0.147
H38c	0.758(2)	0.7254(12)	0.187(2)	0.147
C39	0.6630(2)	0.7812(2)	-0.0470(6)	0.078(2)
H39	0.7030(2)	0.7639(2)	-0.0404(6)	0.103
C40	0.6474(3)	0.7866(4)	-0.1889(7)	0.156(4)
H40a	0.679(2)	0.807(3)	-0.233(2)	0.234
H40b	0.610(2)	0.806(3)	-0.1978(7)	0.234
H40c	0.644(3)	0.7505(4)	-0.227(2)	0.234
C41	0.6644(3)	0.8337(2)	0.0275(9)	0.136(3)
H41a	0.696(2)	0.8568(11)	-0.005(4)	0.203
H41b	0.672(3)	0.8259(3)	0.1176(13)	0.203
H41c	0.6263(11)	0.8523(12)	0.019(5)	0.203
C42	0.4466(2)	0.4563(2)	0.4074(4)	0.0601(10)
H42	0.4235(2)	0.4224(2)	0.3916(4)	0.080
C43	0.5086(2)	0.4399(2)	0.4520(5)	0.0695(12)
H43a	0.5057(3)	0.4213(12)	0.534(2)	0.104
H43b	0.5333(5)	0.4723(2)	0.461(3)	0.104
H43c	0.5266(6)	0.4156(11)	0.389(2)	0.104
C44	0.4136(3)	0.4888(2)	0.5082(5)	0.089(2)
H44a	0.4366(9)	0.5212(9)	0.530(3)	0.134
H44b	0.408(2)	0.4666(6)	0.585(2)	0.134
H44c	0.3747(8)	0.500(2)	0.475(2)	0.134
C45	0.4400(2)	0.42365(14)	0.0046(4)	0.0574(10)
H45	0.4795(2)	0.41372(14)	0.0414(4)	0.076
C46	0.4426(2)	0.4163(2)	-0.1408(5)	0.0751(13)
H46a	0.456(2)	0.3797(5)	-0.1607(5)	0.113
H46b	0.4699(12)	0.4428(10)	-0.1774(6)	0.113
H46c	0.4029(4)	0.4216(14)	-0.1768(6)	0.113
C47	0.3921(2)	0.3884(2)	0.0671(6)	0.087(2)
H47a	0.3975(11)	0.3507(3)	0.041(3)	0.131
H47b	0.3528(2)	0.4009(11)	0.040(3)	0.131
H47c	0.3953(11)	0.3911(13)	0.1598(6)	0.131
C48	0.2922(2)	0.5157(2)	0.2423(8)	0.105(2)
H48	0.3037(2)	0.4822(2)	0.2897(8)	0.140
C49	0.2591(5)	0.4956(6)	0.1224(14)	0.121(5)
H49a	0.2864(5)	0.4747(6)	0.0690(14)	0.182
H49b	0.2442(5)	0.5267(6)	0.0744(14)	0.182
H49c	0.2258(5)	0.4726(6)	0.1479(14)	0.182
C50	0.2568(5)	0.5486(5)	0.335(2)	0.117(4)
H50a	0.2822(5)	0.5593(5)	0.406(2)	0.175
H50b	0.2235(5)	0.5270(5)	0.367(2)	0.175
H50c	0.2416(5)	0.5810(5)	0.292(2)	0.175
C49'	0.2404(4)	0.5538(6)	0.205(2)	0.112(7)
H49a'	0.2548(4)	0.5912(6)	0.202(2)	0.168
H49b'	0.2088(4)	0.5509(6)	0.269(2)	0.168
H49c'	0.2250(4)	0.5434(6)	0.122(2)	0.168
C50'	0.2825(5)	0.4602(5)	0.254(2)	0.099(5)

H50a'	0.3197(5)	0.4423(5)	0.278(2)	0.149
H50b'	0.2685(5)	0.4458(5)	0.172(2)	0.149
H50c'	0.2526(5)	0.4537(5)	0.320(2)	0.149

$U_{eq}=1/3[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$

Table S13 Bond Distances in Compound 4, Å.

Ti1-O5	1.778(2)	Ti1-O6	1.779(2)	Ti1-O4	1.997(2)
Ti1-O3	2.000(2)	Ti1-O1	2.147(2)	Ti1-O2	2.156(2)
Ti1-Ti3	3.3468(8)	Ti1-Ti2	3.3488(8)	Ti2-O7	1.779(2)
Ti2-O9	1.791(2)	Ti2-O8	1.802(2)	Ti2-O1	2.042(2)
Ti2-O3	2.073(2)	Ti3-O10	1.780(2)	Ti3-O11	1.792(2)
Ti3-O12	1.794(3)	Ti3-O2	2.021(2)	Ti3-O4	2.087(2)
O1-C1	1.367(3)	O2-C20	1.366(3)	O3-C21	1.450(4)
O4-C24	1.458(4)	O5-C27	1.409(4)	O6-C30	1.423(4)
O7-C33	1.408(4)	O8-C36	1.421(5)	O9-C39	1.416(4)
O10-C42	1.415(4)	O11-C45	1.426(4)	O12-C48	1.389(5)
C1-C10	1.382(4)	C1-C2	1.404(4)	C2-C3	1.358(4)
C3-C4	1.413(5)	C4-C5	1.418(4)	C4-C9	1.423(4)
C5-C6	1.358(5)	C6-C7	1.408(6)	C7-C8	1.363(4)
C8-C9	1.414(4)	C9-C10	1.438(4)	C10-C11	1.487(4)
C11-C20	1.376(4)	C11-C12	1.434(4)	C12-C13	1.417(4)
C12-C17	1.427(4)	C13-C14	1.362(5)	C14-C15	1.401(5)
C15-C16	1.360(6)	C16-C17	1.418(5)	C17-C18	1.405(5)
C18-C19	1.344(5)	C19-C20	1.414(4)	C21-C23	1.394(6)
C21-C22	1.488(5)	C24-C25	1.502(5)	C24-C26	1.512(5)
C27-C29	1.487(8)	C27-C28	1.532(9)	C30-C31	1.486(6)
C30-C32	1.509(6)	C33-C34	1.486(6)	C33-C35	1.522(5)
C36-C38	1.507(6)	C36-C37	1.511(6)	C39-C41	1.486(8)
C39-C40	1.507(9)	C42-C44	1.493(6)	C42-C43	1.498(6)
C45-C47	1.505(6)	C45-C46	1.509(6)	C48-C50'	1.364(11)
C48-C50	1.468(11)	C48-C49	1.514(13)	C48-C49'	1.519(11)

Table S14 Bond Angles in Compound 4, °

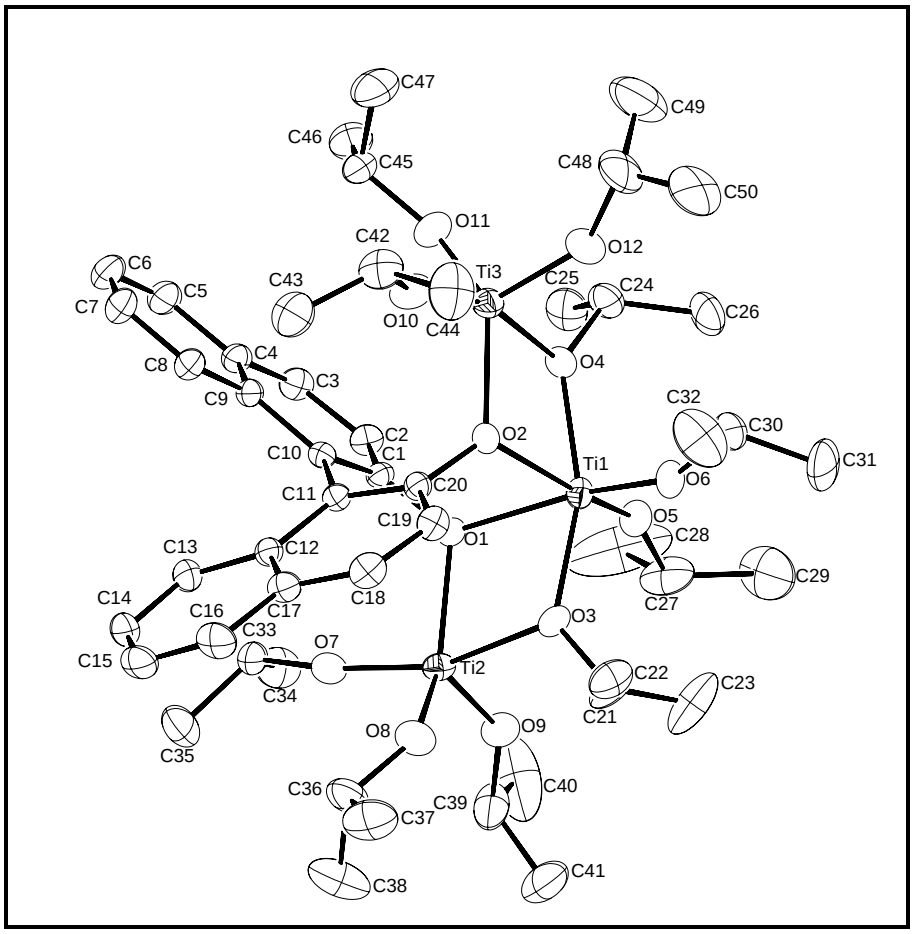
O5-Ti1-O6	103.02(11)	O5-Ti1-O4	96.34(10)	O6-Ti1-O4	96.42(11)
O5-Ti1-O3	95.94(10)	O6-Ti1-O3	95.29(10)	O4-Ti1-O3	160.67(9)
O5-Ti1-O1	91.99(9)	O6-Ti1-O1	160.70(10)	O4-Ti1-O1	93.87(9)
O3-Ti1-O1	70.83(8)	O5-Ti1-O2	162.08(10)	O6-Ti1-O2	90.81(9)
O4-Ti1-O2	70.49(8)	O3-Ti1-O2	94.04(8)	O1-Ti1-O2	77.29(7)
O5-Ti1-Ti3	132.13(8)	O6-Ti1-Ti3	88.93(8)	O4-Ti1-Ti3	35.85(6)
O3-Ti1-Ti3	129.38(6)	O1-Ti1-Ti3	89.90(5)	O2-Ti1-Ti3	35.38(5)
O5-Ti1-Ti2	90.70(8)	O6-Ti1-Ti2	130.41(9)	O4-Ti1-Ti2	129.56(7)
O3-Ti1-Ti2	35.41(6)	O1-Ti1-Ti2	35.85(5)	O2-Ti1-Ti2	88.84(5)
Ti3-Ti1-Ti2	116.31(2)	O7-Ti2-O9	100.89(12)	O7-Ti2-O8	97.39(12)
O9-Ti2-O8	109.40(12)	O7-Ti2-O1	91.46(9)	O9-Ti2-O1	110.32(10)
O8-Ti2-O1	136.69(10)	O7-Ti2-O3	160.65(10)	O9-Ti2-O3	93.89(10)
O8-Ti2-O3	89.29(10)	O1-Ti2-O3	71.57(8)	O7-Ti2-Ti1	129.43(8)
O9-Ti2-Ti1	100.23(9)	O8-Ti2-Ti1	117.64(8)	O1-Ti2-Ti1	38.02(5)
O3-Ti2-Ti1	33.98(6)	O10-Ti3-O11	98.42(12)	O10-Ti3-O12	101.34(13)
O11-Ti3-O12	108.28(13)	O10-Ti3-O2	89.58(10)	O11-Ti3-O2	132.67(11)
O12-Ti3-O2	115.70(11)	O10-Ti3-O4	160.15(11)	O11-Ti3-O4	90.58(10)
O12-Ti3-O4	92.47(11)	O2-Ti3-O4	71.48(8)	O10-Ti3-Ti1	127.67(9)
O11-Ti3-Ti1	117.99(8)	O12-Ti3-Ti1	101.14(9)	O2-Ti3-Ti1	38.15(6)
O4-Ti3-Ti1	34.08(6)	C1-O1-Ti2	124.1(2)	C1-O1-Ti1	125.1(2)
Ti2-O1-Ti1	106.13(9)	C20-O2-Ti3	125.4(2)	C20-O2-Ti1	124.2(2)
Ti3-O2-Ti1	106.47(9)	C21-O3-Ti1	130.4(3)	C21-O3-Ti2	117.2(2)
Ti1-O3-Ti2	110.61(9)	C24-O4-Ti1	131.4(2)	C24-O4-Ti3	116.3(2)
Ti1-O4-Ti3	110.07(10)	C27-O5-Ti1	154.6(3)	C30-O6-Ti1	156.5(2)
C33-O7-Ti2	165.6(2)	C36-O8-Ti2	140.8(2)	C39-O9-Ti2	140.7(3)
C42-O10-Ti3	158.1(3)	C45-O11-Ti3	142.1(3)	C48-O12-Ti3	147.8(3)
O1-C1-C10	120.2(2)	O1-C1-C2	118.2(3)	C10-C1-C2	121.6(3)
C3-C2-C1	120.9(3)	C2-C3-C4	120.3(3)	C3-C4-C5	121.4(3)
C3-C4-C9	119.4(3)	C5-C4-C9	119.2(3)	C6-C5-C4	121.0(3)
C5-C6-C7	120.0(3)	C8-C7-C6	120.4(3)	C7-C8-C9	121.5(3)
C8-C9-C4	117.9(3)	C8-C9-C10	122.6(3)	C4-C9-C10	119.6(3)
C1-C10-C9	118.1(3)	C1-C10-C11	119.7(2)	C9-C10-C11	122.2(2)
C20-C11-C12	118.4(3)	C20-C11-C10	119.8(3)	C12-C11-C10	121.8(3)
C13-C12-C17	117.8(3)	C13-C12-C11	122.7(3)	C17-C12-C11	119.5(3)
C14-C13-C12	121.7(3)	C13-C14-C15	120.2(4)	C16-C15-C14	120.2(3)
C15-C16-C17	121.3(3)	C18-C17-C16	122.5(3)	C18-C17-C12	118.8(3)
C16-C17-C12	118.7(3)	C19-C18-C17	121.5(3)	C18-C19-C20	120.3(3)
O2-C20-C11	120.6(3)	O2-C20-C19	118.0(3)	C11-C20-C19	121.4(3)
C23-C21-O3	114.7(4)	C23-C21-C22	119.2(4)	O3-C21-C22	111.2(3)
O4-C24-C25	110.0(3)	O4-C24-C26	111.3(3)	C25-C24-C26	113.4(3)
O5-C27-C29	108.9(5)	O5-C27-C28	107.9(4)	C29-C27-C28	116.5(7)
O6-C30-C31	108.3(4)	O6-C30-C32	110.5(3)	C31-C30-C32	114.3(5)
O7-C33-C34	110.6(3)	O7-C33-C35	109.7(3)	C34-C33-C35	111.8(4)
O8-C36-C38	110.1(4)	O8-C36-C37	108.9(4)	C38-C36-C37	111.7(4)
O9-C39-C41	109.1(4)	O9-C39-C40	107.6(5)	C41-C39-C40	115.5(6)
O10-C42-C44	110.6(4)	O10-C42-C43	111.1(3)	C44-C42-C43	111.9(4)
O11-C45-C47	110.1(4)	O11-C45-C46	107.9(3)	C47-C45-C46	112.5(4)
C50'-C48-O12	124.4(6)	O12-C48-C50	115.4(6)	O12-C48-C49	107.7(7)
C50-C48-C49	116.6(8)	C50'-C48-C49'	120.2(8)	O12-C48-C49'	108.9(7)

Table S15. Refined Thermal Parameters (U's) for Compound 4.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti1	0.0332(3)	0.0324(3)	0.0351(3)	0.0030(2)	0.0015(2)	0.0047(2)
Ti2	0.0379(3)	0.0337(3)	0.0333(3)	-0.0020(2)	0.0032(3)	-0.0069(2)
Ti3	0.0354(3)	0.0363(3)	0.0415(3)	0.0047(2)	0.0006(3)	-0.0036(2)
O1	0.0340(10)	0.0279(10)	0.0283(10)	-0.0008(8)	0.0027(9)	0.0005(8)
O2	0.0296(10)	0.0347(11)	0.0319(11)	0.0035(9)	0.0020(8)	0.0028(8)
O3	0.0491(12)	0.0288(11)	0.0361(11)	-0.0059(9)	0.0062(10)	0.0004(9)
O4	0.0357(11)	0.0414(12)	0.0394(12)	0.0051(9)	-0.0099(10)	-0.0004(9)
O5	0.0505(13)	0.0400(13)	0.0468(12)	0.0121(10)	-0.0038(12)	0.0052(10)
O6	0.0398(12)	0.0429(12)	0.0553(14)	0.0034(11)	0.0107(11)	0.0100(10)
O7	0.0390(12)	0.0482(14)	0.0497(13)	-0.0080(11)	0.0040(11)	-0.0060(10)
O8	0.0504(14)	0.066(2)	0.0421(13)	-0.0111(12)	-0.0046(12)	-0.0072(12)
O9	0.0541(14)	0.0425(13)	0.058(2)	0.0101(11)	0.0112(13)	-0.0082(11)
O10	0.074(2)	0.0445(14)	0.0490(14)	0.0154(11)	-0.0051(13)	-0.0128(12)
O11	0.067(2)	0.0360(13)	0.0526(14)	0.0002(11)	-0.0049(13)	-0.0007(12)
O12	0.0404(13)	0.063(2)	0.082(2)	0.007(2)	0.0122(13)	-0.0115(12)
C1	0.029(2)	0.0257(14)	0.030(2)	-0.0034(11)	0.0036(12)	-0.0023(11)
C2	0.042(2)	0.039(2)	0.0253(14)	-0.0021(12)	0.0012(13)	-0.0022(13)
C3	0.042(2)	0.046(2)	0.031(2)	-0.0100(14)	0.005(2)	-0.0025(14)
C4	0.0343(14)	0.035(2)	0.039(2)	-0.0088(13)	0.0043(13)	-0.0015(13)
C5	0.048(2)	0.043(2)	0.054(2)	-0.016(2)	0.004(2)	0.001(2)
C6	0.056(2)	0.035(2)	0.077(3)	-0.013(2)	0.008(2)	0.002(2)
C7	0.052(2)	0.034(2)	0.067(2)	0.003(2)	0.000(2)	0.005(2)
C8	0.042(2)	0.032(2)	0.047(2)	0.0013(14)	0.001(2)	0.0012(13)
C9	0.0282(14)	0.030(2)	0.036(2)	-0.0042(12)	0.0037(12)	0.0001(11)
C10	0.0265(13)	0.0300(14)	0.0287(13)	0.0002(12)	-0.0019(12)	-0.0020(11)
C11	0.032(2)	0.0293(14)	0.0267(14)	-0.0007(11)	-0.0008(12)	-0.0004(12)
C12	0.034(2)	0.0288(14)	0.033(2)	0.0015(12)	-0.0064(13)	0.0009(12)
C13	0.037(2)	0.038(2)	0.045(2)	-0.001(2)	-0.0064(14)	0.0042(14)
C14	0.037(2)	0.042(2)	0.065(2)	0.005(2)	-0.013(2)	0.0045(14)
C15	0.050(2)	0.051(2)	0.057(2)	0.009(2)	-0.026(2)	-0.005(2)
C16	0.057(2)	0.061(2)	0.037(2)	0.007(2)	-0.019(2)	-0.005(2)
C17	0.046(2)	0.037(2)	0.032(2)	0.0030(13)	-0.0092(14)	-0.0031(13)
C18	0.059(2)	0.047(2)	0.028(2)	-0.0012(14)	0.000(2)	0.000(2)
C19	0.044(2)	0.041(2)	0.0257(14)	-0.0007(12)	0.0083(14)	0.0028(14)
C20	0.0330(14)	0.030(2)	0.0299(14)	0.0007(11)	-0.0048(13)	0.0016(12)
C21	0.107(3)	0.032(2)	0.049(2)	-0.011(2)	0.011(2)	0.001(2)
C22	0.082(3)	0.051(2)	0.045(2)	-0.013(2)	0.015(2)	-0.005(2)
C23	0.193(7)	0.048(3)	0.076(3)	-0.004(2)	0.019(4)	0.035(3)
C24	0.046(2)	0.055(2)	0.051(2)	0.002(2)	-0.016(2)	-0.001(2)
C25	0.068(3)	0.078(3)	0.047(2)	-0.010(2)	-0.019(2)	0.005(2)
C26	0.050(2)	0.078(3)	0.071(3)	0.001(2)	-0.023(2)	0.014(2)
C27	0.115(4)	0.056(2)	0.058(2)	0.033(2)	-0.026(3)	-0.027(2)
C28	0.383(13)	0.151(6)	0.044(3)	0.003(3)	0.031(5)	-0.149(8)
C29	0.136(6)	0.088(4)	0.39(2)	0.123(7)	-0.137(8)	-0.012(4)
C30	0.037(2)	0.060(2)	0.069(2)	-0.009(2)	0.014(2)	0.003(2)
C31	0.065(3)	0.071(3)	0.163(6)	-0.012(4)	0.035(4)	0.029(2)
C32	0.073(3)	0.160(5)	0.065(3)	0.013(4)	0.028(3)	-0.001(3)
C33	0.038(2)	0.038(2)	0.063(2)	-0.008(2)	0.009(2)	0.0034(14)

C34	0.066(3)	0.078(3)	0.056(2)	-0.012(2)	0.016(2)	-0.009(2)
C35	0.039(2)	0.080(3)	0.098(4)	0.006(3)	0.002(2)	0.001(2)
C36	0.047(2)	0.076(3)	0.060(2)	-0.013(2)	-0.013(2)	-0.009(2)
C37	0.107(4)	0.082(3)	0.049(2)	-0.003(2)	-0.025(3)	-0.022(3)
C38	0.070(3)	0.145(5)	0.079(3)	-0.009(3)	0.002(3)	-0.047(3)
C39	0.059(2)	0.050(2)	0.124(4)	0.033(3)	0.042(3)	0.008(2)
C40	0.118(5)	0.214(8)	0.135(5)	0.130(6)	0.060(5)	0.062(5)
C41	0.095(4)	0.045(3)	0.266(8)	-0.020(4)	0.030(5)	-0.009(3)
C42	0.076(3)	0.057(2)	0.048(2)	0.018(2)	0.003(2)	-0.010(2)
C43	0.084(3)	0.060(3)	0.064(3)	0.018(2)	0.000(2)	0.003(2)
C44	0.096(4)	0.103(4)	0.069(3)	0.012(3)	0.021(3)	0.021(3)
C45	0.054(2)	0.034(2)	0.084(3)	-0.003(2)	-0.017(2)	-0.001(2)
C46	0.075(3)	0.065(3)	0.086(3)	-0.035(2)	-0.015(2)	-0.002(2)
C47	0.095(3)	0.049(2)	0.118(4)	0.016(3)	-0.011(3)	-0.016(2)
C48	0.040(2)	0.087(4)	0.188(6)	0.035(4)	0.018(3)	-0.015(2)
C49	0.071(6)	0.146(12)	0.147(9)	-0.007(9)	-0.033(7)	-0.028(7)
C50	0.052(6)	0.136(10)	0.162(10)	-0.031(9)	0.066(7)	-0.016(6)
C49'	0.032(5)	0.088(8)	0.22(2)	0.021(11)	-0.022(8)	0.009(5)
C50'	0.062(7)	0.071(6)	0.165(14)	0.017(8)	0.029(8)	-0.023(6)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.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C4
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C8
C3
C9
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C17
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O7
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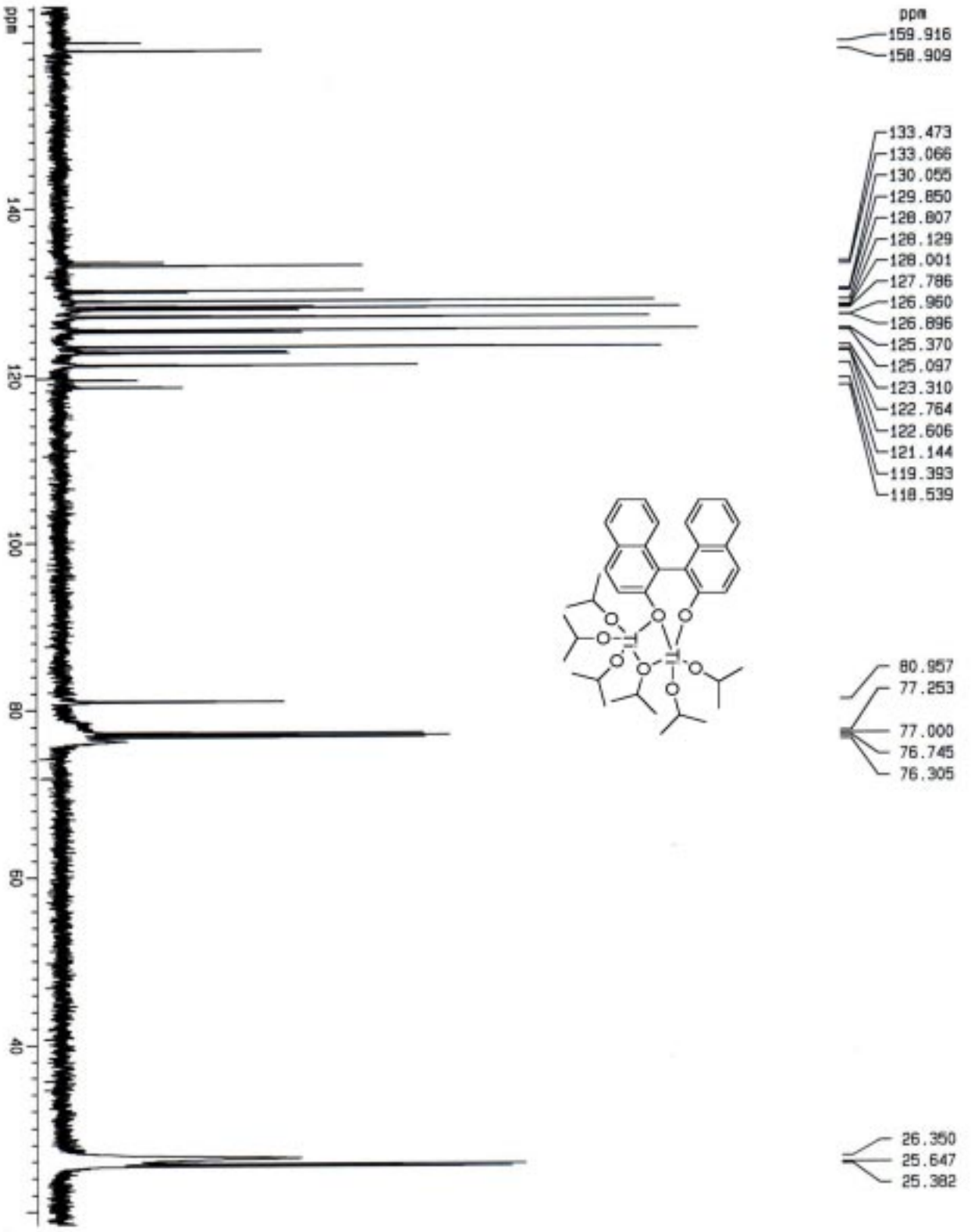
C38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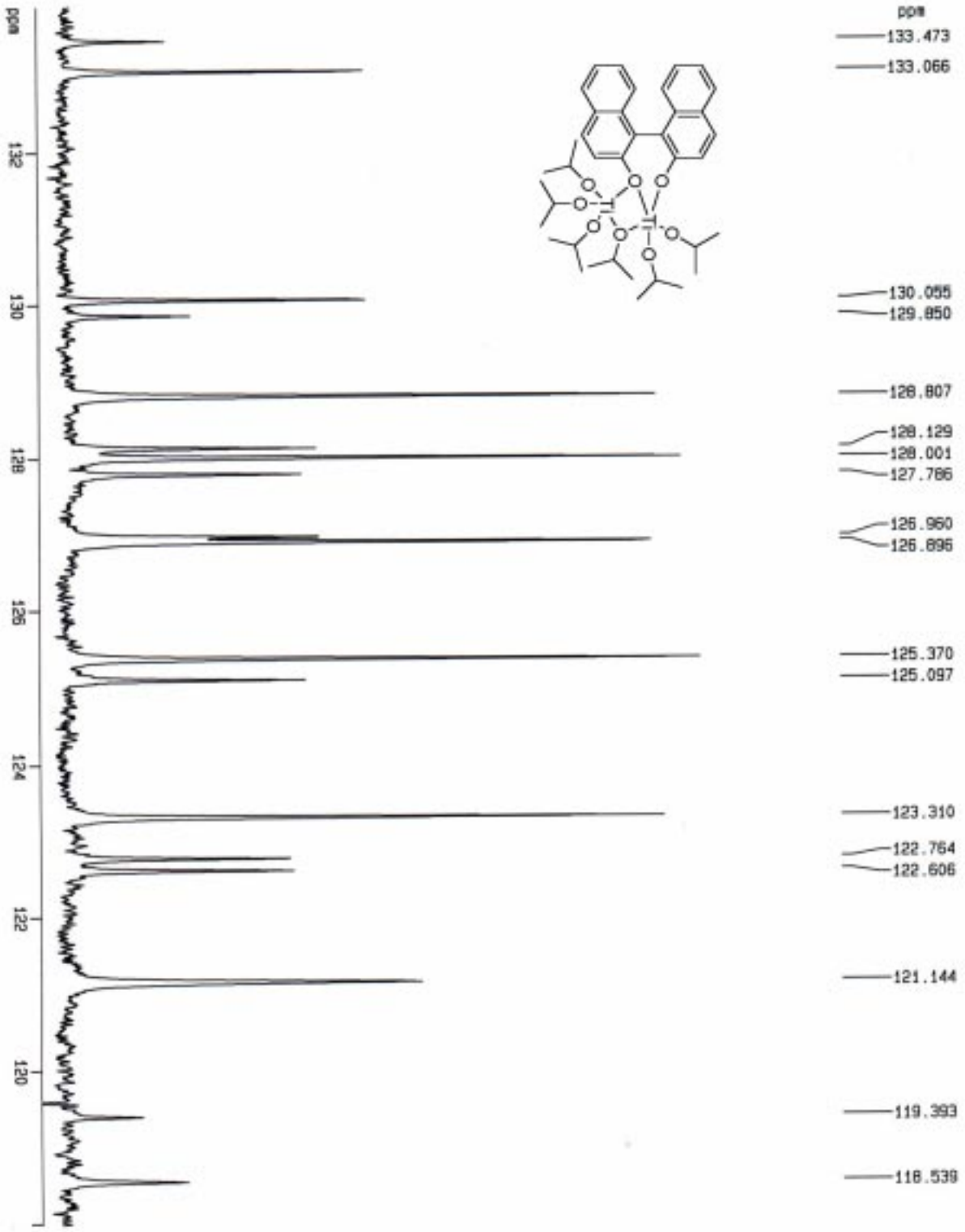
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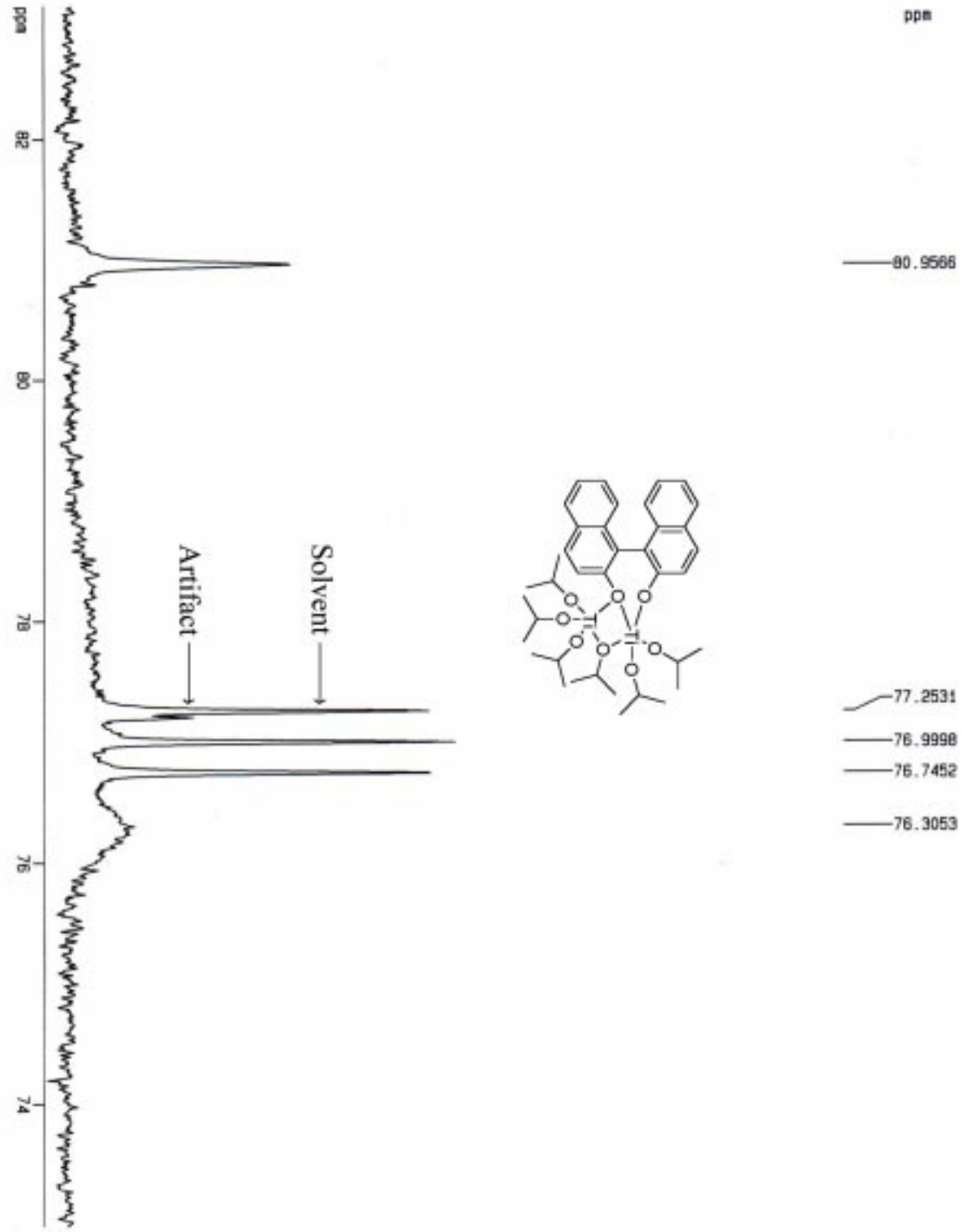
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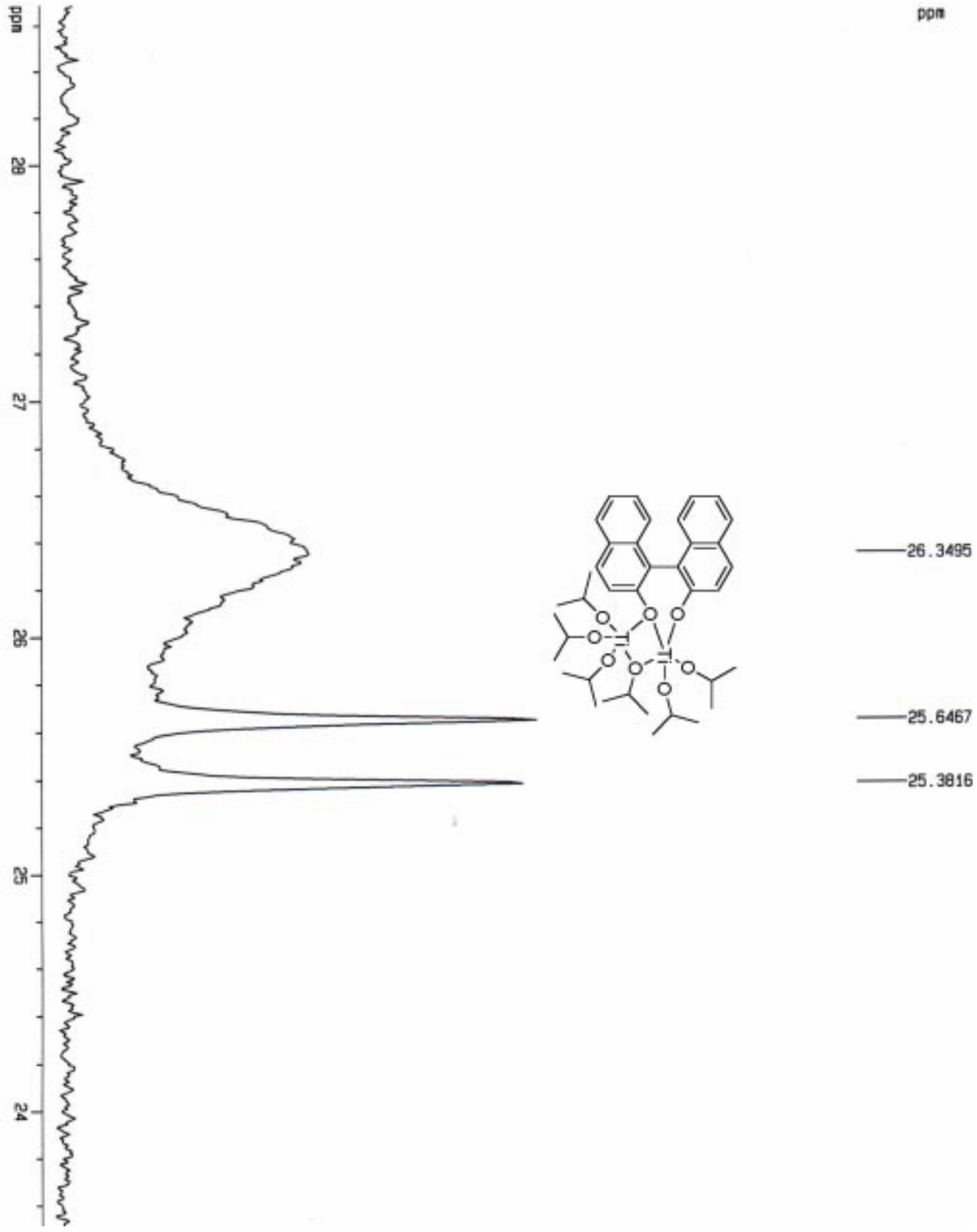
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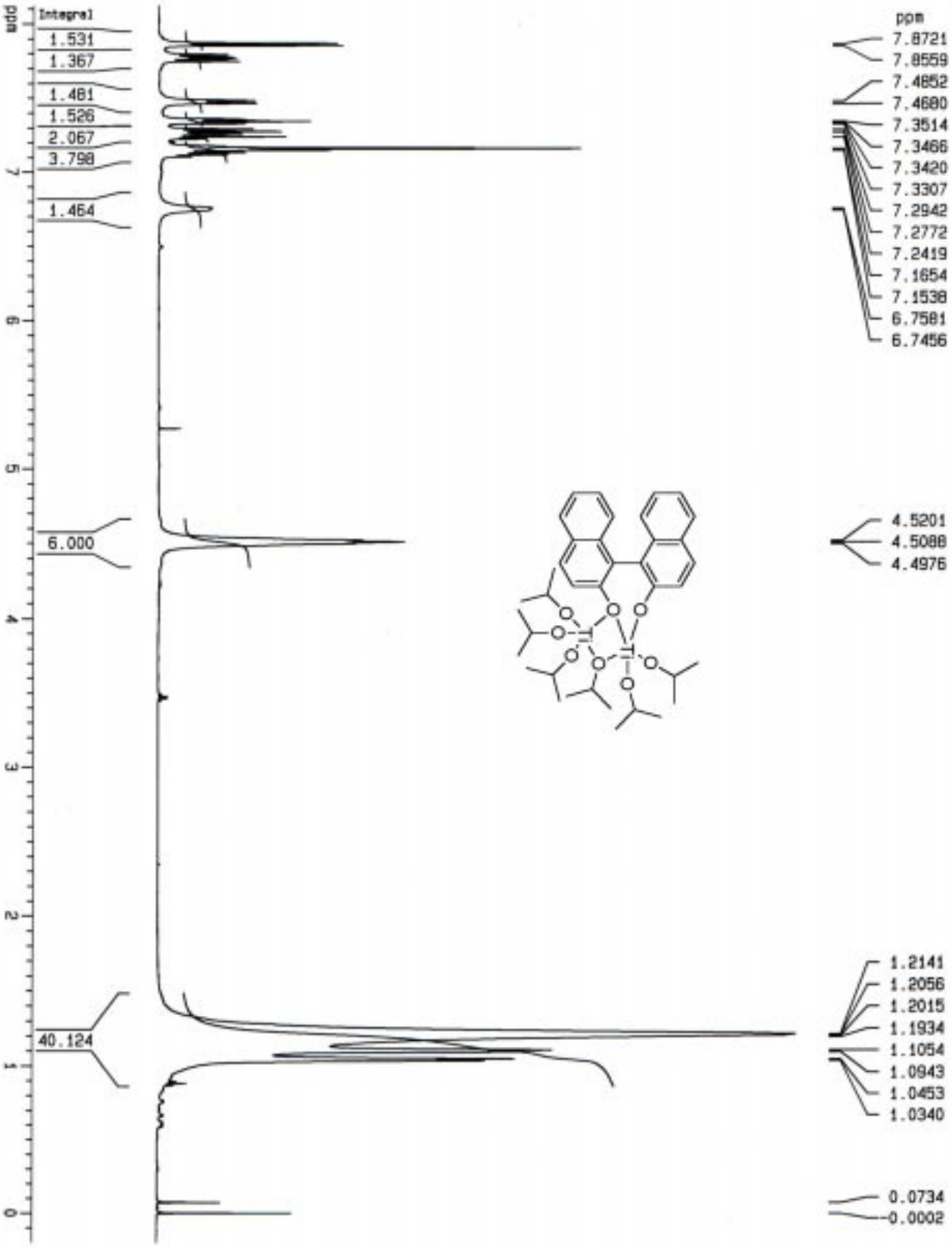
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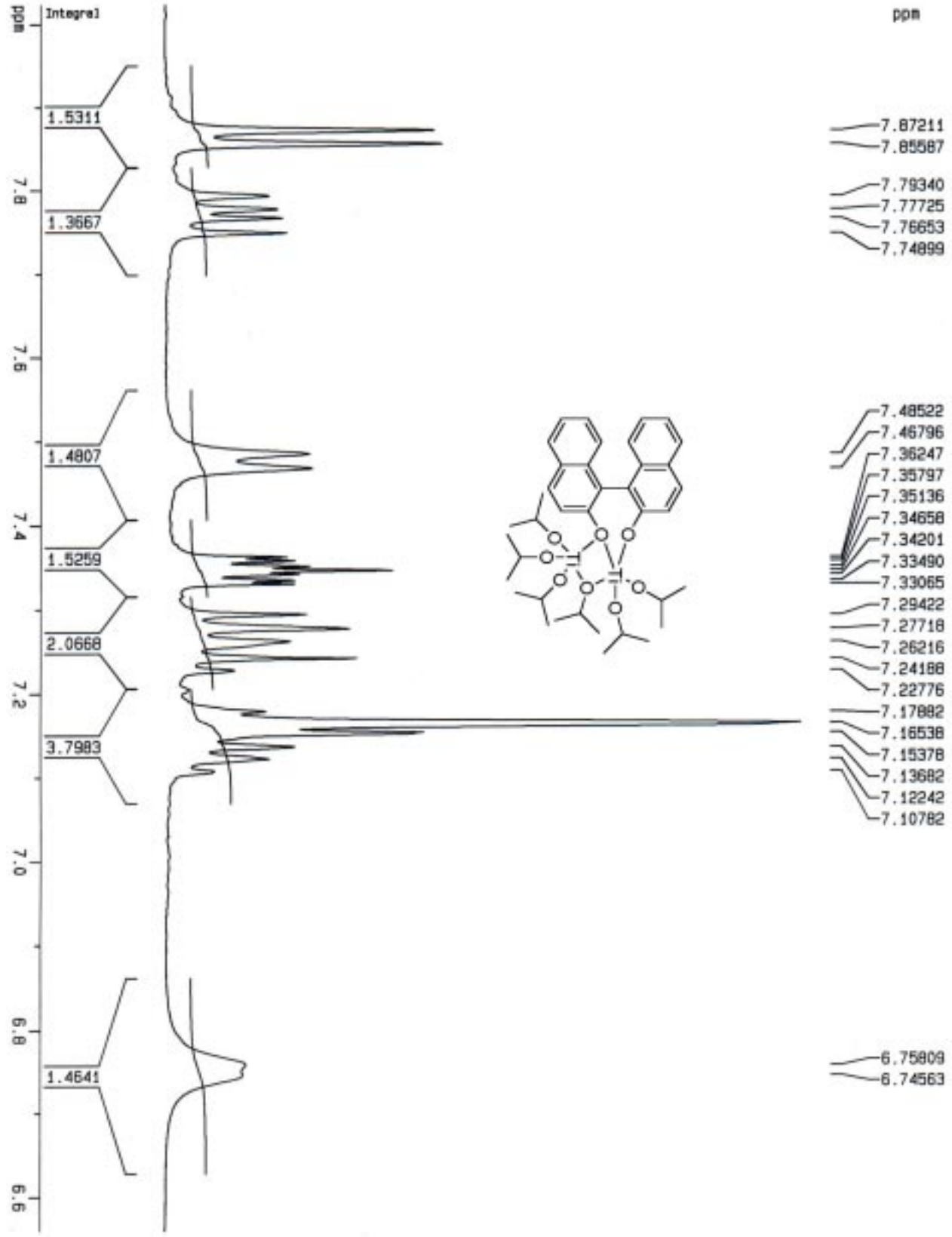
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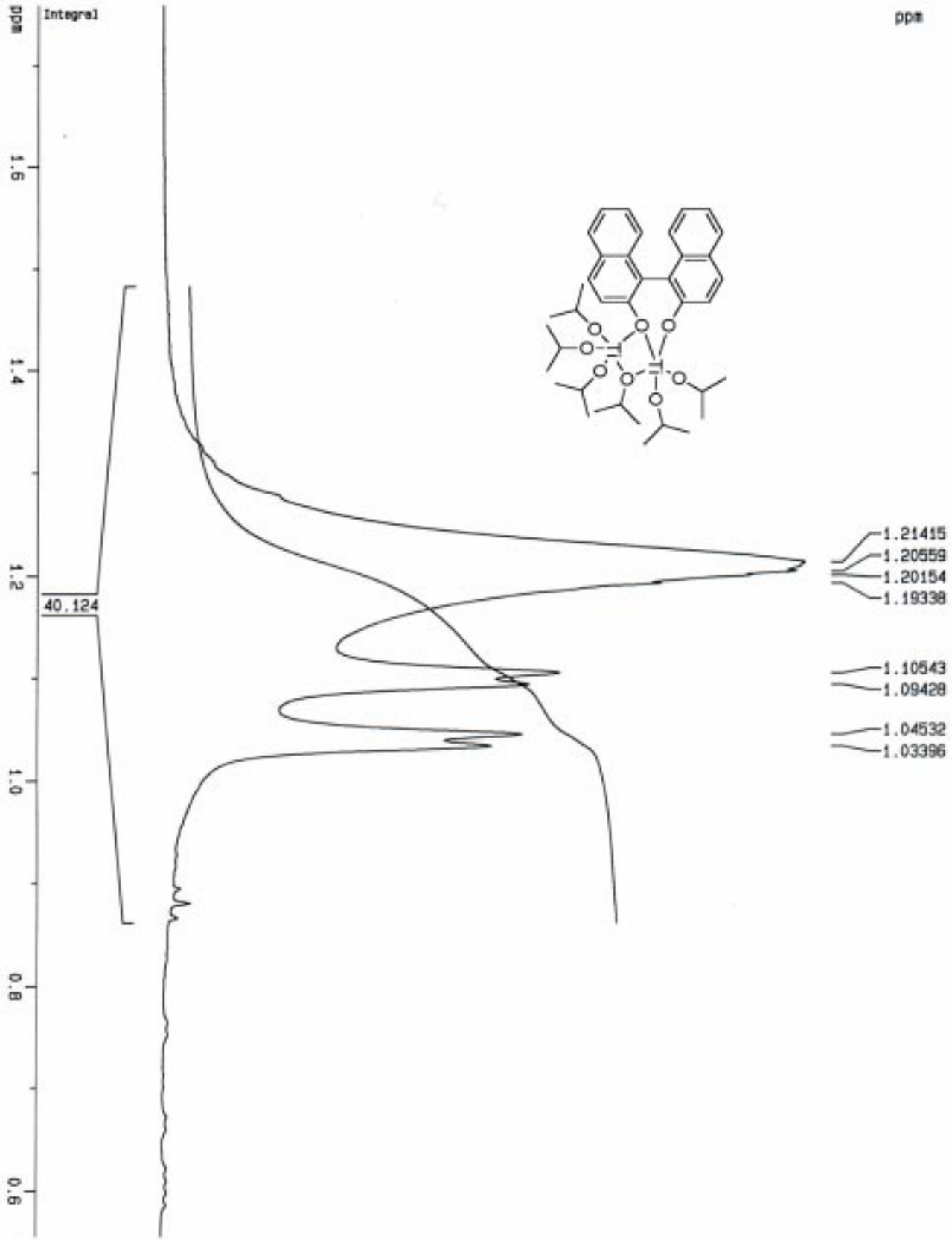
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Ti
O