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Supporting information for article:

Synthesis and structural characterization of a dumbbell-like phenylphosphonate-stabilized Ti7–oxide cluster

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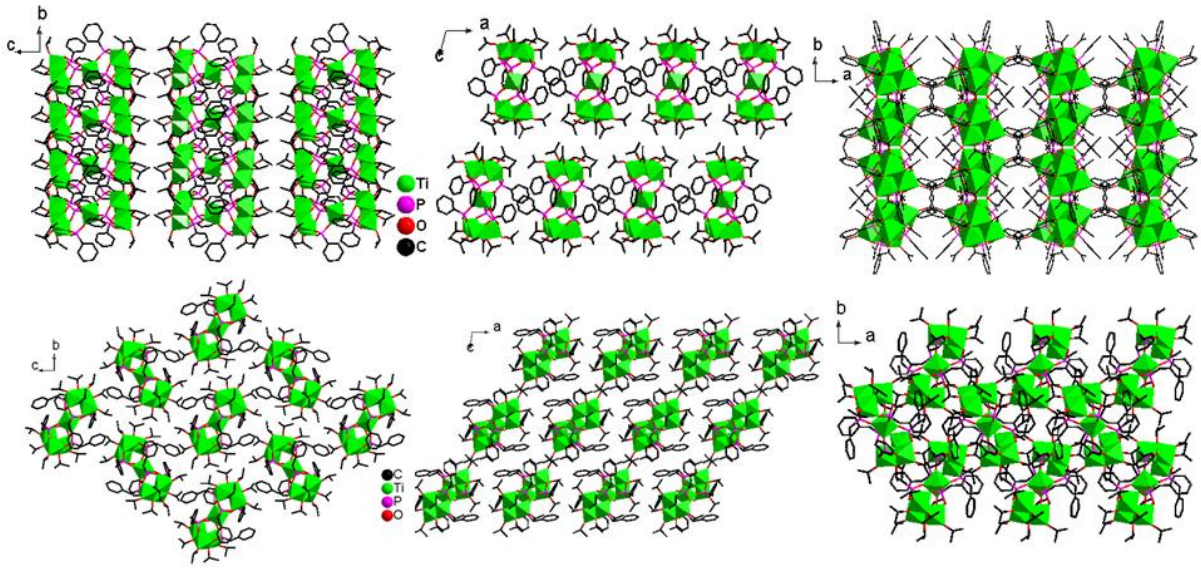

Figure S1 Comparative crystal packing view of **PTC-54** (above) and TMS-BzPP substituted Ti_7-oxo cluster (below; Schubert, U. *Eur J Inorg Chem*. **2013**, 5790) along with the [100], [010], and [001] direction.

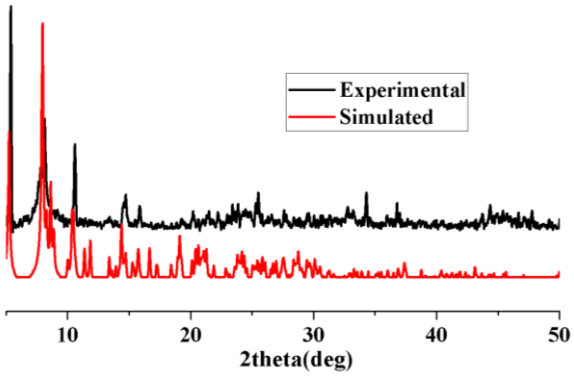

Figure S2 The powder X-ray diffraction (PXRD) pattern for **PTC-54**.

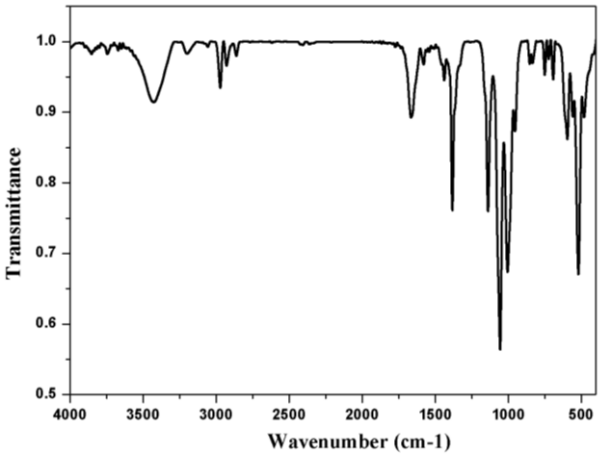

Figure S3 The FT-IR spectrum of **PTC-54**.

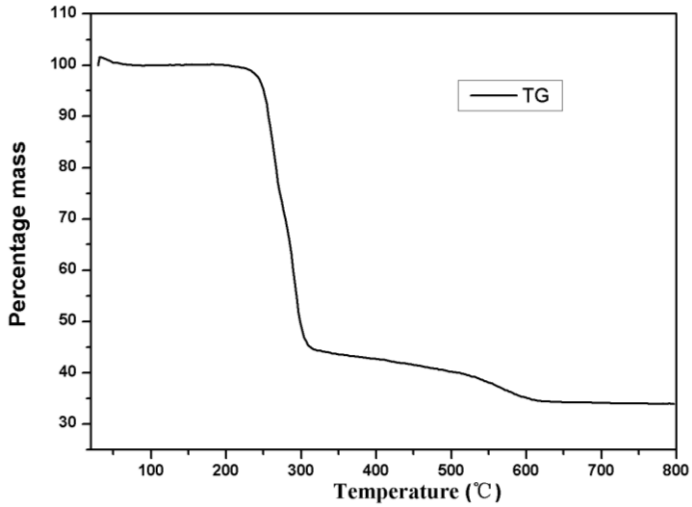

Figure S4 The TGA curve of **PTC-54**.

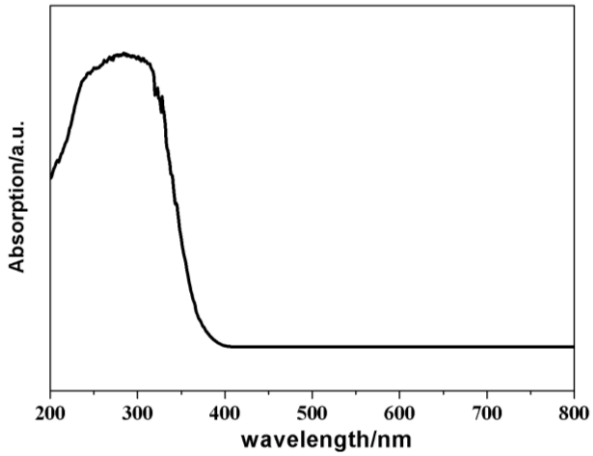

Figure S5 The solid state UV-vis absorption spectrum of commercial TiO_2 (P25).

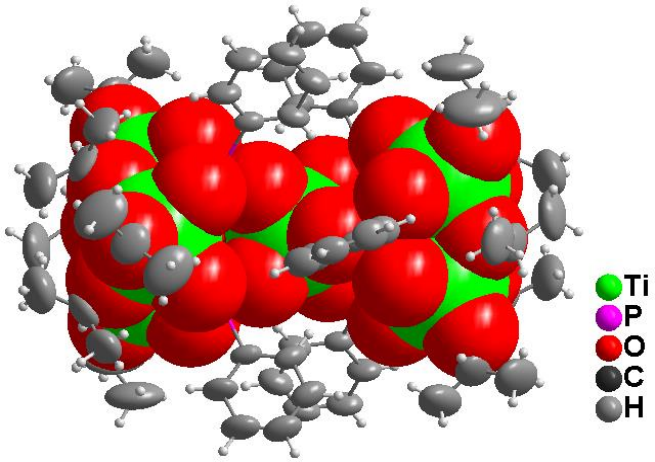

Figure S6 Space filling model of titanium-oxo inorganic core with ORTEP hydrocarbon outer shell.

Table S1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Ti1	2500	7500	0	39.25(18)
Ti2	3594.5(3)	6630.4(5)	1319.7(2)	56.53(19)
Ti3	2251.4(3)	6025.9(5)	1195.9(2)	58.3(2)
Ti4	2652.8(3)	8306.9(5)	1359.7(2)	56.53(19)
P5	3480.1(4)	8594.3(6)	789.9(2)	46.4(2)
P6	1605.4(4)	7761.8(6)	624.6(2)	47.2(2)
P7	2932.4(4)	5388.6(6)	572.3(2)	46.8(2)
O1	2775.8(10)	7084.3(16)	1065.5(6)	46.6(5)
O2	2742.6(10)	6225.9(16)	265.0(6)	48.5(5)
O3	1902.3(11)	8547.2(17)	943.4(7)	54.1(5)
O4	3520.7(10)	5646.4(17)	879.8(7)	54.8(5)
O5	3094.8(10)	8236.1(17)	393.0(6)	48.9(5)
O6	1579.7(11)	6696.7(18)	811.0(8)	55.9(5)
O7	2435.5(11)	5155.8(17)	782.7(7)	56.2(5)
O8	3110.3(11)	9087.0(17)	1052.0(7)	53.4(5)
O9	2215.1(14)	7191(2)	1581.0(7)	70.3(7)
O10	3874.7(10)	7722.3(17)	1015.5(7)	53.7(5)
O11	1906.0(10)	7706.2(17)	288.8(6)	49.8(5)

O12	2566.1(15)	9367(2)	1659.3(8)	77.3(8)
O13	3074.4(14)	5668(2)	1548.8(7)	68.8(7)
O14	3447.3(13)	7739(2)	1692.3(7)	68.1(7)
C0AA	3967.6(16)	9562(3)	680.1(13)	63.5(9)
O16	4322.3(13)	6211(2)	1586.0(8)	73.6(7)
C17	3055.1(16)	4268(3)	306.1(13)	60.2(8)
O18	1803.9(14)	5103(2)	1359.9(9)	78.0(8)
C1AA	853.8(15)	8191(3)	402.5(13)	60.3(8)
C2AA	505(2)	8643(4)	622.1(18)	83.9(11)
C21	2944.0(19)	4290(3)	-98.3(14)	75.0(10)
C23	3269(2)	3351(3)	503.8(17)	79.4(11)
C24	3035(2)	3384(4)	-302.1(18)	92.5(13)
C27	3349(2)	2488(3)	297.8(19)	86.9(12)
C29	603(2)	8048(4)	7.0(16)	81.4(11)
C31	4403(2)	10415(4)	211.7(19)	92.9(12)
C33	4012(2)	9691(3)	297.0(16)	77.9(10)
C36	4300(2)	10176(4)	970.6(19)	99.4(14)
C3AA	-76(2)	8935(4)	458(2)	95.6(13)
C2	3235(2)	2515(4)	-93.6(19)	89.2(12)
C3	-323(2)	8787(4)	78(2)	93.2(13)
C6AA	-1(2)	8340(4)	-156(2)	100.9(15)
C6	3853(3)	8185(6)	2031.8(16)	126(2)
C7AA	1851(3)	7216(6)	1853.0(16)	118(2)
C8	2512(4)	10376(5)	1791(3)	165(3)
C9	4695(3)	10923(5)	867(2)	114.2(17)
C11	3256(4)	4837(5)	1817.1(17)	132(2)
C12	3366(5)	3874(5)	1626(2)	160(3)
C4AA	1246(4)	7678(8)	1673(2)	158(3)
C5AA	1371(5)	4389(8)	1326(3)	181(3)
C15	4324(4)	8841(7)	1946(2)	171(4)
C16	2205(5)	7590(9)	2250.5(19)	193(4)
C18	4910(3)	5924(7)	1632(3)	143(2)
C19	1239(6)	3753(9)	979(3)	226(5)
C1	4736(2)	11006(4)	506(2)	103.2(14)

C4	1868(4)	10715(8)	1643(4)	220(4)
C7	5223(5)	6416(10)	1352(4)	219(4)
C8AA	1101(6)	4293(10)	1661(3)	230(5)
C10	2880(5)	11087(7)	1641(4)	222(5)
C14	5125(5)	5001(9)	1861(4)	228(5)
C5	3830(6)	7620(10)	2391(2)	232(4)
C9AA	3425(6)	5150(8)	2229(2)	214(4)

Table S2 Bond lengths [A] and angles [deg] for **PTC-54**.

Ti(1)-O(2)#1	1.907(3)	P(7)-C(17)	1.795(4)
Ti(1)-O(2)	1.907(3)	O(9)-C(7AA)	1.425(7)
Ti(1)-O(11)#1	1.924(3)	O(12)-C(8)	1.398(7)
Ti(1)-O(11)	1.924(3)	O(13)-C(11)	1.417(6)
Ti(1)-O(5)#1	1.924(3)	O(14)-C(6)	1.437(7)
Ti(1)-O(5)	1.924(3)	C(0AA)-C(36)	1.358(8)
Ti(2)-O(16)	1.782(3)	C(0AA)-C(33)	1.384(8)
Ti(2)-O(1)	1.952(3)	O(16)-C(18)	1.374(9)
Ti(2)-O(4)	1.973(3)	C(17)-C(21)	1.361(7)
Ti(2)-O(10)	1.978(3)	C(17)-C(23)	1.405(7)
Ti(2)-O(14)	2.028(3)	O(18)-C(5AA)	1.349(10)
Ti(2)-O(13)	2.033(3)	C(1AA)-C(29)	1.361(8)
Ti(2)-Ti(4)	3.1035(12)	C(1AA)-C(2AA)	1.386(7)
Ti(2)-Ti(3)	3.1140(13)	C(2AA)-C(3AA)	1.366(8)
Ti(3)-O(18)	1.774(3)	C(21)-C(24)	1.411(7)
Ti(3)-O(1)	1.964(3)	C(23)-C(27)	1.370(8)
Ti(3)-O(7)	1.965(3)	C(24)-C(2)	1.362(9)
Ti(3)-O(6)	1.973(3)	C(27)-C(2)	1.319(9)
Ti(3)-O(13)	2.032(4)	C(29)-C(6AA)	1.413(8)
Ti(3)-O(9)	2.038(3)	C(31)-C(1)	1.348(10)
Ti(3)-Ti(4)	3.1124(12)	C(31)-C(33)	1.383(7)
Ti(4)-O(12)	1.779(3)	C(36)-C(9)	1.424(9)
Ti(4)-O(1)	1.953(3)	C(3AA)-C(3)	1.325(10)
Ti(4)-O(8)	1.971(3)	C(3)-C(6AA)	1.384(10)
Ti(4)-O(3)	1.978(3)	C(6)-C(5)	1.509(9)
Ti(4)-O(14)	2.032(3)	C(6)-C(15)	1.517(9)
Ti(4)-O(9)	2.037(3)	C(7AA)-C(16)	1.505(8)

P(5)-O(5)	1.513(3)	C(7AA)-C(4AA)	1.505(8)
P(5)-O(10)	1.540(3)	C(8)-C(10)	1.465(15)
P(5)-O(8)	1.545(3)	C(8)-C(4)	1.502(9)
P(5)-C(0AA)	1.799(4)	C(9)-C(1)	1.310(11)
P(6)-O(11)	1.514(3)	C(11)-C(9AA)	1.478(9)
P(6)-O(3)	1.534(3)	C(11)-C(12)	1.494(8)
P(6)-O(6)	1.535(3)	C(5AA)-C(19)	1.444(13)
P(6)-C(1AA)	1.789(5)	C(5AA)-C(8AA)	1.476(8)
P(7)-O(2)	1.512(3)	C(18)-C(14)	1.483(9)
P(7)-O(4)	1.534(3)	C(18)-C(7)	1.526(9)
P(7)-O(7)	1.544(3)		
O(2)#1-Ti(1)-O(2)	180.00(15)	O(12)-Ti(4)-Ti(3)	140.71(14)
O(2)#1-Ti(1)-O(11)#1	91.45(12)	O(1)-Ti(4)-Ti(3)	37.50(8)
O(2)-Ti(1)-O(11)#1	88.55(12)	O(8)-Ti(4)-Ti(3)	124.29(9)
O(2)#1-Ti(1)-O(11)	88.55(12)	O(3)-Ti(4)-Ti(3)	81.59(9)
O(2)-Ti(1)-O(11)	91.45(12)	O(14)-Ti(4)-Ti(3)	86.44(11)
O(11)#1-Ti(1)-O(11)	180.00(12)	O(9)-Ti(4)-Ti(3)	40.22(9)
O(2)#1-Ti(1)-O(5)#1	91.14(12)	Ti(2)-Ti(4)-Ti(3)	60.13(3)
O(2)-Ti(1)-O(5)#1	88.86(12)	O(5)-P(5)-O(10)	111.86(16)
O(11)#1-Ti(1)-O(5)#1	91.53(12)	O(5)-P(5)-O(8)	112.83(16)
O(11)-Ti(1)-O(5)#1	88.47(12)	O(10)-P(5)-O(8)	110.14(17)
O(2)#1-Ti(1)-O(5)	88.86(12)	O(5)-P(5)-C(0AA)	105.8(2)
O(2)-Ti(1)-O(5)	91.14(12)	O(10)-P(5)-C(0AA)	107.72(19)
O(11)#1-Ti(1)-O(5)	88.47(12)	O(8)-P(5)-C(0AA)	108.2(2)
O(11)-Ti(1)-O(5)	91.53(12)	O(11)-P(6)-O(3)	112.68(16)
O(5)#1-Ti(1)-O(5)	180.00(14)	O(11)-P(6)-O(6)	111.41(17)
O(16)-Ti(2)-O(1)	175.62(15)	O(3)-P(6)-O(6)	110.57(17)
O(16)-Ti(2)-O(4)	94.89(15)	O(11)-P(6)-C(1AA)	105.3(2)
O(1)-Ti(2)-O(4)	88.04(11)	O(3)-P(6)-C(1AA)	107.6(2)
O(16)-Ti(2)-O(10)	95.85(15)	O(6)-P(6)-C(1AA)	109.01(18)
O(1)-Ti(2)-O(10)	87.34(11)	O(2)-P(7)-O(4)	112.42(16)
O(4)-Ti(2)-O(10)	91.02(12)	O(2)-P(7)-O(7)	111.37(16)
O(16)-Ti(2)-O(14)	100.20(16)	O(4)-P(7)-O(7)	109.81(17)
O(1)-Ti(2)-O(14)	76.84(12)	O(2)-P(7)-C(17)	105.5(2)
O(4)-Ti(2)-O(14)	164.88(13)	O(4)-P(7)-C(17)	108.15(19)
O(10)-Ti(2)-O(14)	88.45(14)	O(7)-P(7)-C(17)	109.37(19)

O(16)-Ti(2)-O(13)	100.25(16)	Ti(2)-O(1)-Ti(4)	105.29(12)
O(1)-Ti(2)-O(13)	76.54(13)	Ti(2)-O(1)-Ti(3)	105.37(12)
O(4)-Ti(2)-O(13)	88.42(14)	Ti(4)-O(1)-Ti(3)	105.25(13)
O(10)-Ti(2)-O(13)	163.88(13)	P(7)-O(2)-Ti(1)	164.51(18)
O(14)-Ti(2)-O(13)	87.91(15)	P(6)-O(3)-Ti(4)	124.64(17)
O(16)-Ti(2)-Ti(4)	140.11(13)	P(7)-O(4)-Ti(2)	124.65(18)
O(1)-Ti(2)-Ti(4)	37.37(8)	P(5)-O(5)-Ti(1)	161.35(18)
O(4)-Ti(2)-Ti(4)	124.86(9)	P(6)-O(6)-Ti(3)	125.22(18)
O(10)-Ti(2)-Ti(4)	81.62(9)	P(7)-O(7)-Ti(3)	124.73(17)
O(14)-Ti(2)-Ti(4)	40.18(9)	P(5)-O(8)-Ti(4)	124.73(17)
O(13)-Ti(2)-Ti(4)	85.49(11)	C(7AA)-O(9)-Ti(4)	133.1(5)
O(16)-Ti(2)-Ti(3)	139.83(13)	C(7AA)-O(9)-Ti(3)	125.5(5)
O(1)-Ti(2)-Ti(3)	37.45(8)	Ti(4)-O(9)-Ti(3)	99.60(13)
O(4)-Ti(2)-Ti(3)	81.32(9)	P(5)-O(10)-Ti(2)	124.73(18)
O(10)-Ti(2)-Ti(3)	124.07(9)	P(6)-O(11)-Ti(1)	161.44(19)
O(14)-Ti(2)-Ti(3)	86.46(11)	C(8)-O(12)-Ti(4)	161.8(6)
O(13)-Ti(2)-Ti(3)	40.00(10)	C(11)-O(13)-Ti(3)	130.0(5)
Ti(4)-Ti(2)-Ti(3)	60.08(3)	C(11)-O(13)-Ti(2)	128.7(5)
O(18)-Ti(3)-O(1)	174.57(16)	Ti(3)-O(13)-Ti(2)	99.98(13)
O(18)-Ti(3)-O(7)	96.19(16)	C(6)-O(14)-Ti(2)	129.7(5)
O(1)-Ti(3)-O(7)	88.05(11)	C(6)-O(14)-Ti(4)	128.6(5)
O(18)-Ti(3)-O(6)	95.77(16)	Ti(2)-O(14)-Ti(4)	99.73(13)
O(1)-Ti(3)-O(6)	87.45(11)	C(36)-C(0AA)-C(33)	119.3(5)
O(7)-Ti(3)-O(6)	91.90(13)	C(36)-C(0AA)-P(5)	120.9(5)
O(18)-Ti(3)-O(13)	100.38(16)	C(33)-C(0AA)-P(5)	119.8(4)
O(1)-Ti(3)-O(13)	76.30(12)	C(18)-O(16)-Ti(2)	155.4(5)
O(7)-Ti(3)-O(13)	88.30(14)	C(21)-C(17)-C(23)	118.4(5)
O(6)-Ti(3)-O(13)	163.74(13)	C(21)-C(17)-P(7)	120.8(4)
O(18)-Ti(3)-O(9)	99.02(16)	C(23)-C(17)-P(7)	120.8(4)
O(1)-Ti(3)-O(9)	76.67(13)	C(5AA)-O(18)-Ti(3)	156.7(6)
O(7)-Ti(3)-O(9)	164.71(13)	C(29)-C(1AA)-C(2AA)	118.1(5)
O(6)-Ti(3)-O(9)	88.11(14)	C(29)-C(1AA)-P(6)	120.1(4)
O(13)-Ti(3)-O(9)	87.47(15)	C(2AA)-C(1AA)-P(6)	121.7(4)
O(18)-Ti(3)-Ti(4)	138.93(13)	C(3AA)-C(2AA)-C(1AA)	122.4(7)
O(1)-Ti(3)-Ti(4)	37.25(8)	C(17)-C(21)-C(24)	119.5(6)
O(7)-Ti(3)-Ti(4)	124.77(8)	C(27)-C(23)-C(17)	120.8(6)

O(6)-Ti(3)-Ti(4)	81.27(9)	C(2)-C(24)-C(21)	119.3(7)
O(13)-Ti(3)-Ti(4)	85.27(10)	C(2)-C(27)-C(23)	119.9(6)
O(9)-Ti(3)-Ti(4)	40.19(9)	C(1AA)-C(29)-C(6AA)	119.4(6)
O(18)-Ti(3)-Ti(2)	140.14(14)	C(1)-C(31)-C(33)	120.3(7)
O(1)-Ti(3)-Ti(2)	37.18(8)	C(31)-C(33)-C(0AA)	119.8(6)
O(7)-Ti(3)-Ti(2)	81.28(9)	C(0AA)-C(36)-C(9)	118.5(7)
O(6)-Ti(3)-Ti(2)	124.01(9)	C(3)-C(3AA)-C(2AA)	119.7(6)
O(13)-Ti(3)-Ti(2)	40.02(9)	C(27)-C(2)-C(24)	122.0(6)
O(9)-Ti(3)-Ti(2)	86.04(11)	C(3AA)-C(3)-C(6AA)	120.6(6)
Ti(4)-Ti(3)-Ti(2)	59.79(3)	C(3)-C(6AA)-C(29)	119.7(7)
O(12)-Ti(4)-O(1)	175.77(15)	O(14)-C(6)-C(5)	106.8(7)
O(12)-Ti(4)-O(8)	94.79(16)	O(14)-C(6)-C(15)	113.7(6)
O(1)-Ti(4)-O(8)	87.52(11)	C(5)-C(6)-C(15)	137.7(8)
O(12)-Ti(4)-O(3)	95.70(15)	O(9)-C(7AA)-C(16)	109.9(7)
O(1)-Ti(4)-O(3)	87.81(11)	O(9)-C(7AA)-C(4AA)	112.2(6)
O(8)-Ti(4)-O(3)	90.34(12)	C(16)-C(7AA)-C(4AA)	119.0(9)
O(12)-Ti(4)-O(14)	99.77(16)	O(12)-C(8)-C(10)	110.8(9)
O(1)-Ti(4)-O(14)	76.73(12)	O(12)-C(8)-C(4)	107.7(8)
O(8)-Ti(4)-O(14)	88.32(14)	C(10)-C(8)-C(4)	108.7(12)
O(3)-Ti(4)-O(14)	164.53(13)	C(1)-C(9)-C(36)	121.2(7)
O(12)-Ti(4)-O(9)	100.76(16)	O(13)-C(11)-C(9AA)	111.1(7)
O(1)-Ti(4)-O(9)	76.95(13)	O(13)-C(11)-C(12)	113.1(6)
O(8)-Ti(4)-O(9)	164.44(13)	C(9AA)-C(11)-C(12)	134.0(8)
O(3)-Ti(4)-O(9)	88.31(14)	O(18)-C(5AA)-C(19)	118.8(8)
O(14)-Ti(4)-O(9)	88.87(15)	O(18)-C(5AA)-C(8AA)	117.6(9)
O(12)-Ti(4)-Ti(2)	139.51(14)	C(19)-C(5AA)-C(8AA)	123.6(9)
O(1)-Ti(4)-Ti(2)	37.34(8)	O(16)-C(18)-C(14)	117.6(8)
O(8)-Ti(4)-Ti(2)	81.66(9)	O(16)-C(18)-C(7)	114.3(8)
O(3)-Ti(4)-Ti(2)	124.50(9)	C(14)-C(18)-C(7)	126.9(10)
O(14)-Ti(4)-Ti(2)	40.09(9)	C(9)-C(1)-C(31)	120.7(6)
O(9)-Ti(4)-Ti(2)	86.35(11)		

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

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for **PTC-54**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**

Ti1	34.0(4)	37.0(3)	46.9(4)	0.5(3)	10.7(3)	-2.6(3)
Ti2	54.8(4)	54.5(4)	53.5(3)	6.4(2)	2.1(3)	2.7(3)
Ti3	65.8(4)	51.0(3)	64.0(4)	11.3(3)	27.3(3)	-3.4(3)
Ti4	63.6(4)	54.3(4)	53.3(3)	-7.3(2)	18.1(3)	-2.2(3)
P5	39.5(4)	41.4(4)	55.0(4)	-2.7(3)	6.4(3)	-6.8(3)
P6	41.2(4)	42.9(4)	61.9(5)	-0.7(3)	21.5(4)	-2.6(3)
P7	44.2(4)	35.2(4)	60.1(4)	4.0(3)	12.3(3)	0.4(3)
O1	48.5(12)	42.8(10)	49.3(10)	2.5(8)	14.2(9)	-1.0(9)
O2	50.0(12)	39.9(10)	55.0(11)	4.1(8)	12.6(10)	1.2(9)
O3	53.6(13)	48.7(12)	63.1(13)	-5.2(10)	20.7(11)	-0.1(10)
O4	49.2(13)	46.8(11)	63.9(13)	5.3(10)	6.7(10)	2.2(9)
O5	42.6(11)	49.3(11)	52.5(11)	-0.9(9)	8.1(9)	-8.2(9)
O6	52.9(13)	48.6(12)	71.5(14)	4.8(10)	26.0(11)	-5.2(10)
O7	59.3(14)	41.6(11)	70.0(13)	7.8(10)	21.2(11)	-5.0(10)
O8	53.8(13)	45.9(11)	59.4(12)	-5.8(9)	12.6(10)	-5.2(9)
O9	88(2)	73.3(17)	60.7(13)	3.3(12)	38.1(14)	-2.4(14)
O10	43.9(12)	49.6(12)	62.4(12)	1.2(10)	4.6(10)	-2.1(9)
O11	40.9(11)	54.7(12)	56.4(11)	0.6(9)	17.5(9)	0.7(9)
O12	95(2)	70.7(17)	69.4(15)	-21.4(13)	27.5(15)	0.1(15)
O13	83.3(19)	62.6(15)	59.4(13)	19.3(12)	17.0(13)	6.0(13)
O14	73.1(18)	76.3(17)	49.1(12)	-3.5(11)	5.4(12)	1.5(14)
C0AA	44.3(17)	46.3(16)	98(2)	5.1(16)	15.9(17)	-7.9(13)
O16	65.5(15)	72.4(16)	70.4(15)	11.2(13)	-4.6(13)	8.8(13)
C17	45.4(17)	42.9(15)	94(2)	-3.7(15)	21.7(16)	-0.3(13)
O18	87(2)	67.3(17)	91.4(19)	19.2(14)	43.6(17)	-8.7(15)
C1AA	40.0(16)	48.8(16)	95(2)	1.4(16)	23.4(16)	-4.5(13)
C2AA	55(2)	86(2)	118(3)	-6(2)	36(2)	6.1(19)
C21	69(2)	56.1(19)	100(2)	-19.4(19)	22(2)	3.0(17)
C23	65(2)	49.1(18)	122(3)	-1.2(19)	22(2)	8.5(16)
C24	82(3)	81(2)	115(3)	-31(2)	26(2)	3(2)
C27	70(2)	51.9(19)	138(3)	-9(2)	24(2)	10.0(17)
C29	54(2)	76(2)	110(3)	2(2)	14(2)	10.5(18)
C31	83(3)	73(2)	136(3)	19(2)	52(2)	-2(2)
C33	74(2)	57.0(19)	117(3)	3.3(19)	49(2)	-5.9(17)

C36	79(3)	82(3)	126(3)	1(2)	6(3)	-37(2)
C3AA	59(2)	97(3)	138(3)	3(3)	39(2)	13(2)
C2	71(2)	60(2)	139(3)	-30(2)	32(2)	4.4(18)
C3	48(2)	82(3)	147(3)	8(3)	20(2)	4.4(19)
C6AA	70(3)	93(3)	126(3)	5(3)	1(3)	0(2)
C6	136(5)	148(5)	73(3)	-34(3)	-10(3)	-11(4)
C7AA	140(5)	149(5)	93(3)	10(3)	80(4)	5(4)
C8	167(7)	82(4)	267(9)	-69(5)	96(7)	1(4)
C9	89(3)	85(3)	152(4)	5(3)	1(3)	-36(2)
C11	186(7)	103(4)	108(3)	65(3)	40(4)	29(4)
C12	236(9)	87(4)	147(6)	48(4)	30(6)	38(5)
C4AA	145(6)	220(8)	143(5)	25(6)	97(5)	38(6)
C5AA	212(7)	188(6)	175(6)	-18(5)	105(5)	-119(5)
C15	187(7)	175(7)	111(5)	-15(5)	-31(5)	-72(6)
C16	239(8)	266(9)	94(4)	-5(5)	78(5)	26(7)
C18	81(3)	167(5)	176(5)	41(4)	25(3)	41(3)
C19	297(10)	209(9)	205(8)	-65(7)	121(8)	-163(8)
C1	72(3)	82(3)	160(4)	16(3)	37(3)	-19(2)
C4	176(8)	120(6)	375(12)	-39(8)	96(9)	30(6)
C7	130(7)	257(10)	293(10)	73(9)	97(7)	38(7)
C8AA	286(10)	241(9)	219(8)	-35(7)	163(8)	-143(8)
C10	207(9)	86(5)	374(12)	-31(7)	76(9)	-40(5)
C14	141(7)	223(9)	318(11)	102(8)	59(8)	85(7)
C5	293(8)	263(8)	106(5)	5(5)	-9(6)	-57(7)
C9AA	315(9)	195(7)	109(3)	53(5)	10(6)	25(7)

Table S4 Hydrogen-bond geometry (Å, º).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O12	0.98	2.54	3.294 (8)	133
C11—H11···O18	0.98	2.58	3.332 (9)	133
C21—H21···O2	0.93	2.50	2.909 (5)	107
C29—H29···O11	0.93	2.57	2.942 (5)	105
C33—H33···O5	0.93	2.51	2.921 (5)	107