Supporting Information for

A base-free terminal thorium phosphinidene metallocene and its reactivity toward selected organic molecules

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1. Crystal parameters

Table S1. Crystal Data and Experimental Parameters for Compounds 3-6

Compound	**3**	**4**	**5**	**6**·0.5C_6H_{14}
Formula	$C_{46}H_{68}Se_2Th$	$C_{49}H_{81}PTh$	$C_{46}H_{68}P_2Th$	$C_{70}H_{109}NPTh$
Fw	1010.96	933.14	914.98	1227.59
crystal system	monoclinic	monoclinic	monoclinic	triclinic
space group	*C*2/*c*	$P2_1/n$	$P2_1/n$	*P*(-1)
a (Å)	22.726(6)	13.809(1)	10.342(1)	12.022(1)
b (Å)	20.038(5)	21.587(1)	19.315(1)	14.940(1)
c (Å)	19.906(5)	15.483(1)	21.267(1)	19.817(1)
α (deg)	90	90	90	68.24(1)
β (deg)	104.79(1)	92.98(1)	102.86(1)	82.48(1)
γ (deg)	90	90	90	80.23(1)
V (Å^3)	8764(4)	4609.1(3)	4141.7(2)	3248.8(2)
Z	8	4	4	2
D_{calc} (g/cm^3)	1.532	1.345	1.467	1.255
μ(Mo/Kα)$_{calc}$ (cm^{-1})	5.093	10.964	3.708	7.905
size (mm)	0.30 × 0.25 × 0.20	0.20 × 0.15 × 0.15	0.08 × 0.07 × 0.05	0.20 × 0.15 × 0.10
F(000)	4016	1920	1856	1282
2θ range (deg)	3.17 to 55.13	7.03 to 147.13	6.58 to 59.65	7.48 to 146.66
no. of reflns, collected	29514	19005	38778	23582
no of obsd reflns	10086	8988	10352	12661
no of variables	460	486	461	692
abscorr (T_{max}, T_{min})	0.75, 0.59	1.00, 0.77	1.00, 0.65	1.00, 0.81
R	0.027	0.077	0.046	0.042
R_w	0.055	0.169	0.070	0.098
R_{all}	0.035	0.088	0.077	0.049
Gof	1.03	1.09	1.13	1.05
CCDC	1883600	1883596	1883601	1883598

Table S2. Crystal Data and Experimental Parameters for Compounds 8, 9 and 11

Compound	**8**	**9**	**11**
Formula	$C_{40}H_{66}OTh$	$C_{37}H_{65}OPTh$	$C_{42}H_{68}N_4Th$
Fw	794.96	788.90	861.04
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/n$	$P2_1/c$	$C2/c$
a (Å)	10.229(1)	12.284(1)	13.450(1)
b (Å)	20.825(1)	18.114(1)	17.076(1)
c (Å)	17.420(1)	16.749(1)	17.676(1)
α (deg)	90	90	90
β (deg)	95.54(1)	92.29(1)	97.63(1)
γ (deg)	90	90	90
V (Å^3)	3693.69(7)	3723.81(17)	4023.7(2)
Z	4	4	4
D_{calc} (g/cm^3)	1.430	1.407	1.421
μ(Mo/Kα)$_{calc}$ (cm^{-1})	13.206	13.487	3.738
size (mm)	0.20 × 0.10 × 0.10	0.25 × 0.20 × 0.20	0.15 × 0.15 × 0.15
F(000)	1616	1600	1752
2θ range (deg)	8.49 to 143.95	7.19 to 147.98	7.17 to 59.38
no. of reflns, collected	15173	24887	11095
no of obsd reflns	7093	7437	4841
no of variables	396	380	223
abscorr (T_{max}, T_{min})	1.00, 0.45	1.00, 0.33	1.00, 0.98
R	0.029	0.061	0.034
R_w	0.071	0.153	0.062
R_{all}	0.033	0.075	0.040
Gof	1.03	1.07	1.13
CCDC	1883599	1883602	1883597