Supporting Information For:

Comparison of Thermodynamic and Kinetic Aspects of Oxidative Addition of PhE-EPh (E = S, Se, Te) to $Mo(CO)_3(PR_3)_2$, $W(CO)_3(PR_3)_2$, and $Mo(N[R]Ar)_3$ Complexes. The Role of Oxidation State and Ancillary Ligands in Metal Complex Induced Chalcogenyl Radical Generation.

James E. McDonough, John J. Weir, Kengkaj Sukcharoenphon, Carl D. Hoff*, Olga P. Kryatova, Elena V. Rybak-Akimova*, Brian L. Scott, Gregory J. Kubas*, Arjun Mendriatta, Christopher C. Cummins*

University of Miami, Coral Gables, Florida 33124, Tufts University, Medford, Massachusetts 02155 Massachusetts Institute of Technology, Room 2-227, 77 Massachusetts Ave, Cambridge, Massachusetts 02139, and Los Alamos National Laboratory, Structural Inorganic Chemistry Group, Chemistry Division, MS J514, Los Alamos National Laboratory, Los Alamos, New Mexico 87545.

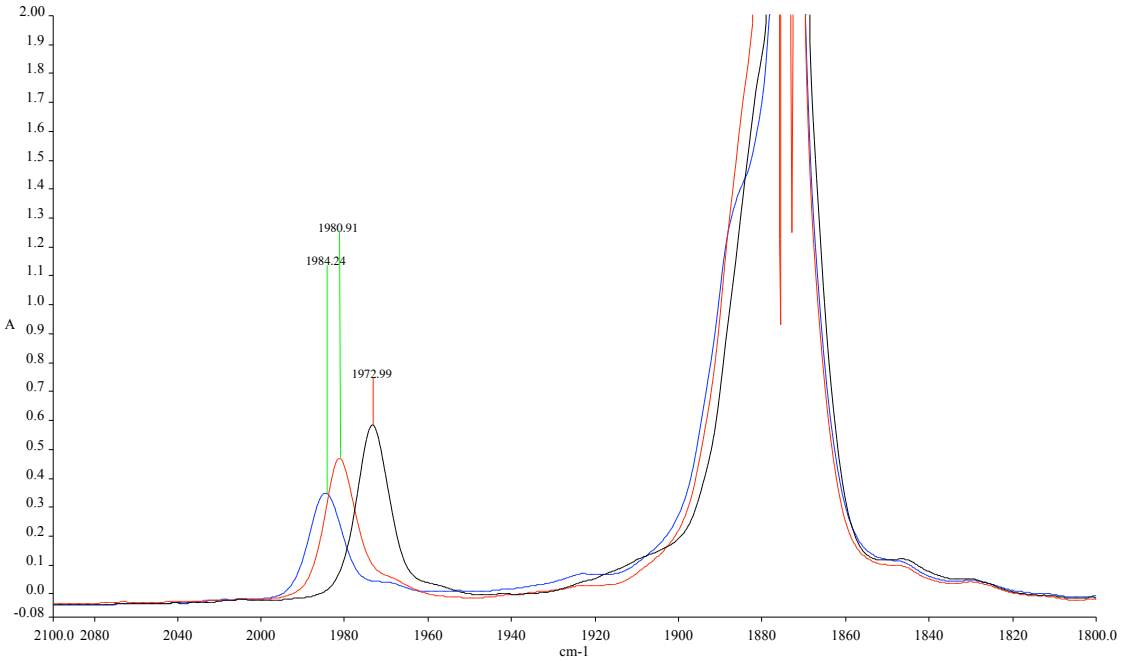

Figure S1. FTIR data (toluene solution, cm^{-1}) for (PhE•)Mo($PiPr_3$)$_2$(CO)$_3$ complexes showing bands at: 1984, 1878 (E = S); 1981, 1878 (E = Se); 1973, 1874 (E = Te). Data for W derivatives are not shown (for clarity) and occur at: 1976, 1875, (E =S); 1973, 1870 (E =Se); 1967, 1869 (E = Te).

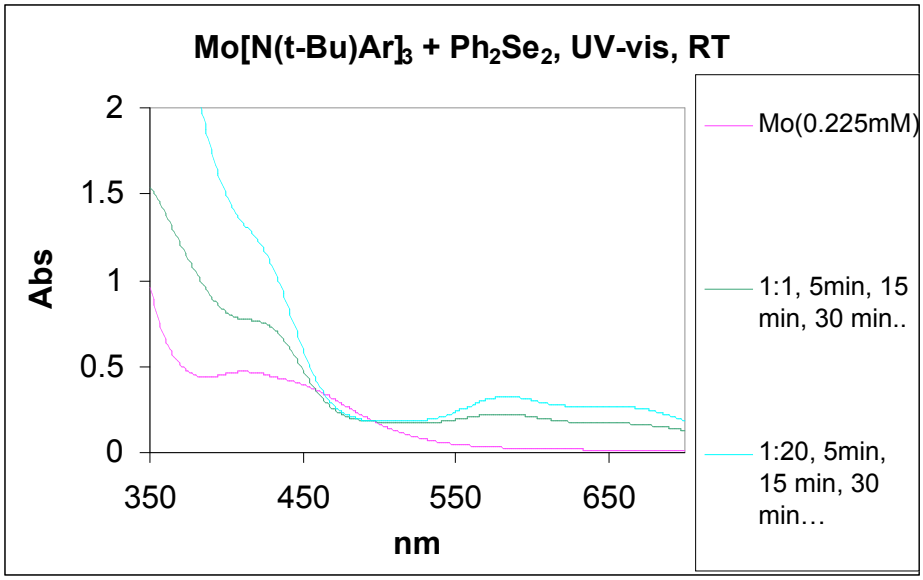

Figure S2. Room temperature UV-Vis study of formation of Mo(NtBuAr)3(SePh) in toluene solution.

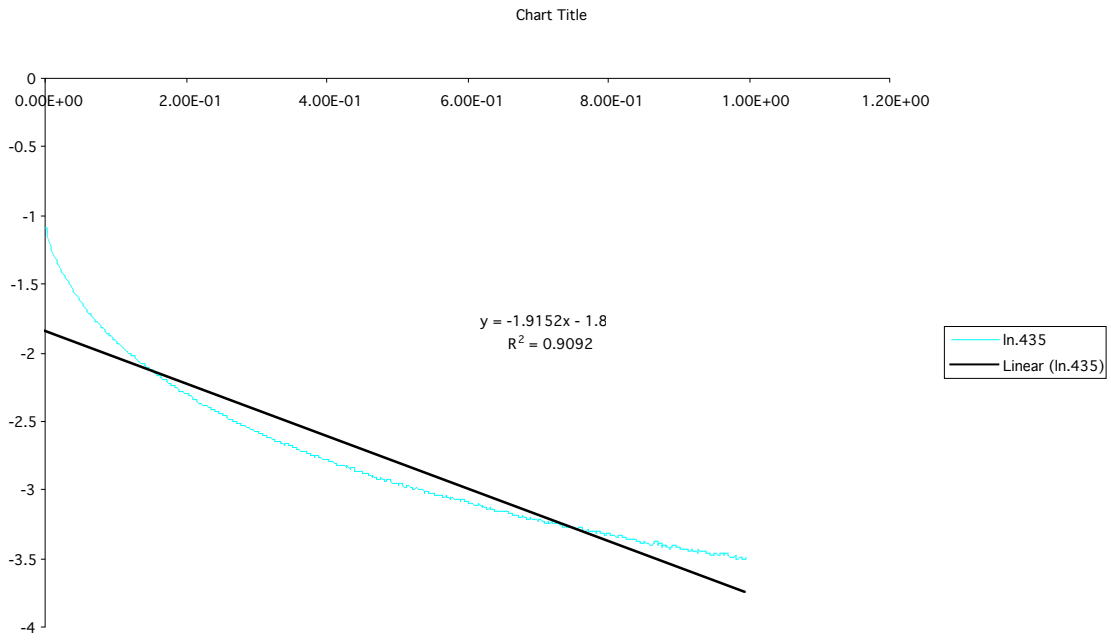

Figure S3. Plot of ln [A∞ -A] versus time for reaction of Ph_2Se_2at -80 C, [Ph_2Se_2] = 1.3 mM, $Mo(PiPr_3)_2(CO)_3$ = 0.225 mM.

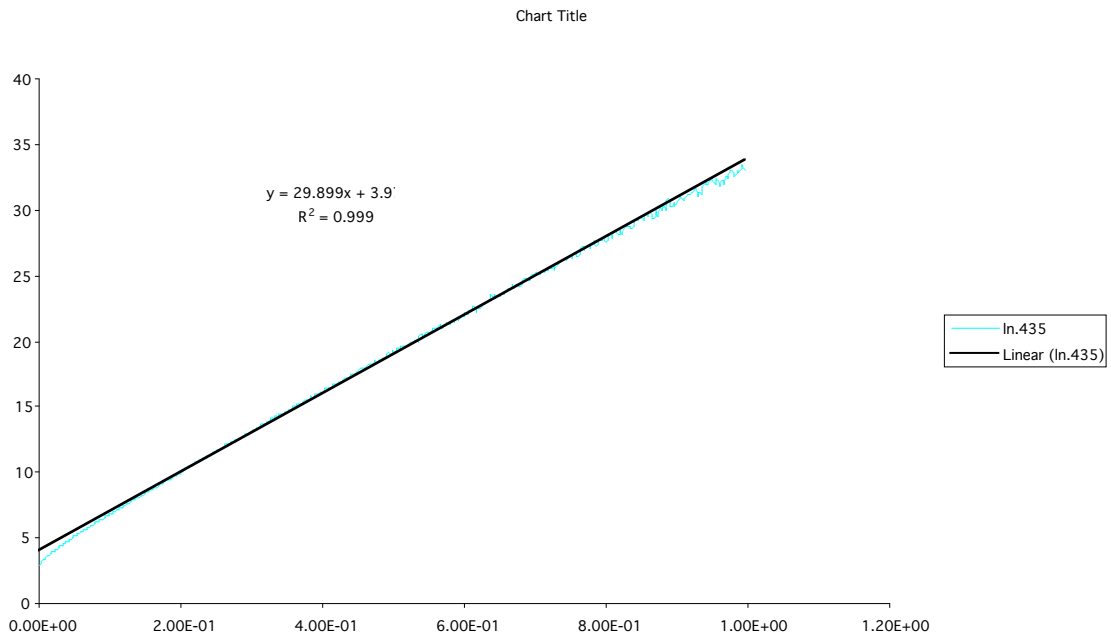

Figure S4. Plot of 1/[A∞ -A] versus time for reaction of Ph_2Se_2 at -80 C, [Ph_2Se_2] = 1.3 mM, $Mo(PiPr_3)_2(CO)_3$ = 0.225 mM.

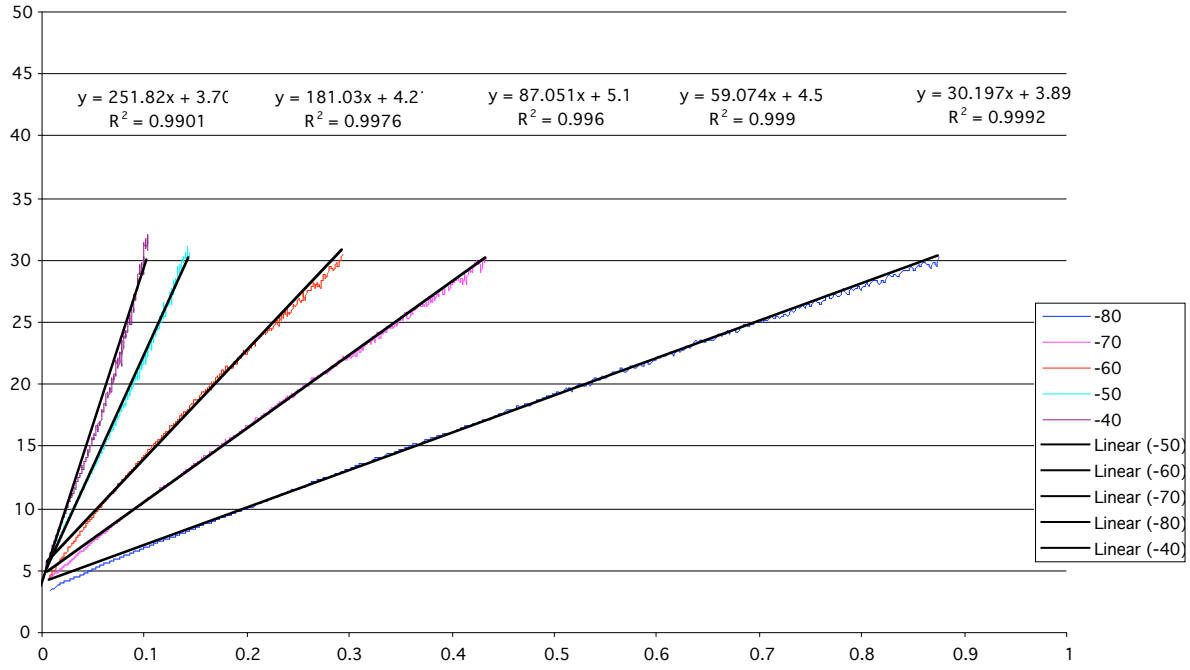

Figure S5. Best fit data from -40 to -80 C for $Mo(CO)_3(PiPr_3)_2 + Ph_2Se_2$ to second order equation. Note that the first five msec of mixing have been deleted, as has the last 12.5 % of reaction--i.e. data are through the first three half lives only. Deviations from apparent second order behavior appeared beyond that range, and appeared to be more serious at higher temperatures.

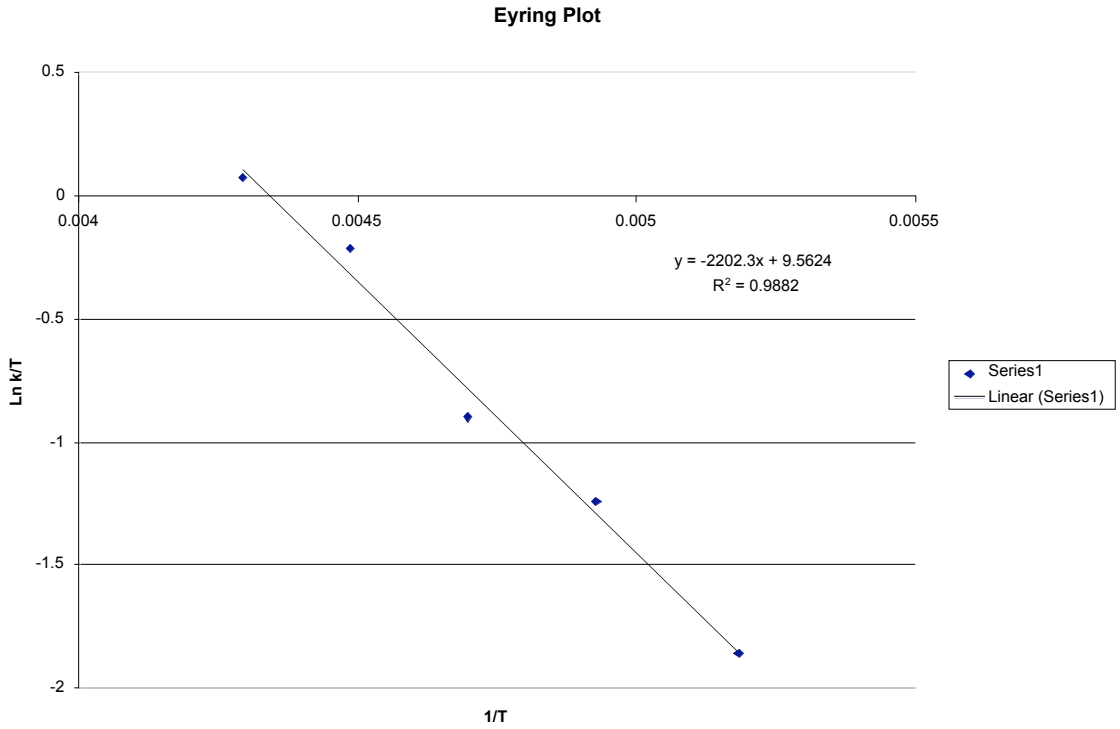

Figure S6. Eyring plot for reaction of $Mo(P^iPr_3)_2(CO)_3$ and Ph_2Se_2 at -40 to -80 ^oC

Values of the rate constant are as follows: -40 ^oC, 252 $M^{-1}s^{-1}$; -50 ^oC, 181 $M^{-1}s^{-1}$; -60 ^oC, 87 $M^{-1}s^{-1}$; -70 ^oC, 59 $M^{-1}s^{-1}$; -80 ^oC, 30 $M^{-1}s^{-1}$.

Table S1. Crystal data and structure refinement for ccd758.

Identification code	ccd758	
Empirical formula	C27 H47 O3 P2 Te W	
Formula weight	793.04	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P –1 (#2)	
Unit cell dimensions	a = 12.154(5) Å	α= 75.872(6)°.
	b = 16.218(7) Å	β= 79.373(8)°.
	c = 16.684(7) Å	γ = 89.993(8)°.
Volume	3131(2) $Å^3$	
Z	4	
Density (calculated)	1.682 Mg/m^3	
Absorption coefficient	4.729 mm^{-1}	
F(000)	1556	
Crystal size	0.32 x 0.20 x 0.16 mm^3	
Theta range for data collection	1.28 to 25.42°.	
Index ranges	-14<=h<=9, -19<=k<=19, -20<=l<=20	
Reflections collected	19754	
Independent reflections	10297 [R(int) = 0.0326]	
Completeness to theta = 25.00°	89.7 %	
Max. and min. transmission	0.5183 and 0.3130	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10297 / 12 / 632	
Goodness-of-fit on F^2	2.549	
Final R indices [I>2sigma(I)]	R1 = 0.0850, wR2 = 0.2160	
R indices (all data)	R1 = 0.1057, wR2 = 0.2236	
Largest diff. peak and hole	2.575 and -2.951 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ccd758. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
W(1)	2998(1)	5656(1)	2390(1)	20(1)
W(2)	1979(1)	9336(1)	7600(1)	21(1)
Te(1)	2696(1)	5367(1)	4114(1)	32(1)
Te(2)	2292(1)	9924(1)	5875(1)	33(1)
P(1)	1156(1)	4928(1)	2346(1)	37(1)
P(2)	4896(1)	6470(1)	2066(1)	34(1)
P(3)	75(1)	9992(1)	7901(1)	35(1)
P(4)	3812(1)	8568(1)	7636(1)	38(1)
O(1)	1653(3)	7300(2)	2533(2)	70(1)
O(2)	3277(3)	6036(3)	433(2)	83(2)
O(3)	4247(3)	3917(2)	2553(2)	59(1)
O(4)	3315(3)	11042(2)	7516(2)	69(1)
O(5)	1668(3)	8733(2)	9564(2)	67(1)
O(6)	719(3)	7704(2)	7413(2)	61(1)
C(1)	2154(4)	6697(3)	2467(3)	49(2)
C(2)	3192(4)	5902(3)	1163(3)	49(2)
C(3)	3798(3)	4555(2)	2482(3)	39(1)
C(4)	66(4)	4796(3)	3315(3)	46(1)
C(5)	-357(5)	5615(3)	3525(3)	69(2)
C(6)	-988(4)	4210(3)	3386(3)	58(2)
C(7)	537(4)	5465(3)	1369(3)	62(2)
C(8)	425(6)	6390(4)	1219(4)	112(3)
C(9)	-516(5)	5023(4)	1262(3)	112(2)
C(10)	1254(4)	3810(2)	2236(3)	48(1)
C(11)	1508(4)	3215(2)	3011(3)	51(1)
C(12)	2023(5)	3778(2)	1427(3)	75(2)
C(13)	4802(4)	7647(2)	1979(3)	41(1)
C(14)	4280(4)	7811(2)	2802(3)	50(2)
C(15)	4285(4)	8084(3)	1210(3)	55(2)

C(16)	5807(4)	6160(2)	2839(3)	51(1)
C(17)	6260(4)	5245(3)	2910(3)	63(2)
C(18)	6769(5)	6753(3)	2871(3)	64(2)
C(19)	5725(4)	6449(3)	1039(3)	50(2)
C(20)	5906(4)	5557(3)	864(3)	55(2)
C(21)	6875(4)	6959(3)	733(3)	57(2)
C(22)	3272(4)	4138(3)	4600(2)	39(1)
C(23)	4389(4)	4053(3)	4697(3)	51(2)
C(24)	4809(5)	3227(3)	5002(3)	62(2)
C(25)	4001(5)	2530(3)	5272(3)	63(2)
C(26)	2876(5)	2637(3)	5183(3)	59(2)
C(27)	2531(4)	3413(2)	4878(3)	47(1)
C(28)	2799(4)	10413(2)	7556(3)	41(1)
C(29)	1776(4)	8942(3)	8835(2)	48(1)
C(30)	1201(4)	8293(2)	7486(3)	38(1)
C(31)	-768(4)	9451(2)	8953(3)	39(1)
C(32)	-886(5)	8484(3)	9111(3)	58(2)
C(33)	-1886(5)	9832(3)	9213(3)	67(2)
C(34)	-814(4)	10078(2)	7090(3)	40(1)
C(35)	-1291(4)	9209(2)	7048(3)	45(1)
C(36)	-1779(4)	10687(3)	7105(3)	48(2)
C(37)	128(4)	11115(2)	7979(3)	40(1)
C(38)	726(3)	11700(2)	7159(3)	37(1)
C(39)	682(4)	11213(3)	8717(3)	53(2)
C(40)	3681(4)	7402(2)	7762(3)	46(1)
C(41)	3367(5)	7190(3)	6999(3)	61(2)
C(42)	2814(5)	6945(3)	8540(3)	64(2)
C(43)	4881(5)	8929(3)	6671(3)	52(2)
C(44)	5957(4)	8385(3)	6579(3)	54(2)
C(45)	5295(5)	9864(3)	6480(3)	65(2)
C(46)	4422(4)	8597(3)	8591(3)	52(2)
C(47)	4601(5)	9456(3)	8727(3)	82(2)
C(48)	5483(5)	8059(4)	8665(4)	81(2)
C(49)	1737(4)	8929(3)	5387(3)	43(1)
C(50)	2455(4)	8348(2)	5125(3)	52(2)
C(51)	2087(5)	7715(3)	4826(3)	61(2)

C(52)	973(6)	7615(3)	4762(3)	76(2)
C(53)	242(4)	8201(3)	5001(3)	50(2)
C(54)	593(4)	8884(3)	5308(3)	57(2)
W(2A)	-3046(2)	9392(1)	7583(1)	65(1)
Te(2A)	-2713(3)	9649(2)	5868(2)	70(1)
Te(1A)	-2337(3)	5062(2)	4102(2)	83(1)
W(1A)	-2021(2)	5627(1)	2385(1)	66(1)

—

Table S3. Bond lengths [Å] and angles [°] for ccd758.

W(1)-C(2)	1.956(5)
W(1)-C(1)	1.994(5)
W(1)-C(3)	2.019(4)
W(1)-P(1)	2.5524(15)
W(1)-P(2)	2.5600(14)
W(1)-Te(1)	2.7535(12)
W(2)-C(29)	1.971(4)
W(2)-C(28)	1.991(4)
W(2)-C(30)	2.004(4)
W(2)-P(4)	2.5557(15)
W(2)-P(3)	2.5636(14)
W(2)-Te(2)	2.7552(11)
Te(1)-C(22)	2.131(4)
Te(1)-Te(1A)#1	2.837(4)
Te(2)-C(49)	2.136(5)
Te(2)-Te(2A)#2	2.769(3)
P(1)-C(4)	1.858(4)
P(1)-C(10)	1.868(4)
P(1)-C(7)	1.934(5)
P(2)-C(19)	1.829(5)
P(2)-C(16)	1.831(5)
P(2)-C(13)	1.883(4)
P(3)-C(37)	1.858(4)
P(3)-C(34)	1.862(5)
P(3)-C(31)	1.866(4)
P(4)-C(43)	1.841(5)
P(4)-C(40)	1.854(4)
P(4)-C(46)	1.887(6)
O(1)-C(1)	1.169(6)
O(2)-C(2)	1.168(6)
O(3)-C(3)	1.160(5)
O(4)-C(28)	1.179(5)
O(5)-C(29)	1.161(5)
O(6)-C(30)	1.163(5)

C(4)-C(5)	1.522(7)
C(4)-C(6)	1.564(7)
C(7)-C(8)	1.469(8)
C(7)-C(9)	1.527(9)
C(10)-C(11)	1.495(6)
C(10)-C(12)	1.506(7)
C(13)-C(14)	1.488(6)
C(13)-C(15)	1.548(7)
C(16)-C(18)	1.529(7)
C(16)-C(17)	1.568(6)
C(19)-C(20)	1.554(7)
C(19)-C(21)	1.558(6)
C(22)-C(23)	1.400(7)
C(22)-C(27)	1.410(6)
C(23)-C(24)	1.440(7)
C(24)-C(25)	1.426(7)
C(25)-C(26)	1.409(8)
C(26)-C(27)	1.336(6)
C(31)-C(33)	1.527(7)
C(31)-C(32)	1.528(6)
C(34)-C(36)	1.534(6)
C(34)-C(35)	1.546(6)
C(37)-C(38)	1.517(5)
C(37)-C(39)	1.548(7)
C(40)-C(41)	1.509(7)
C(40)-C(42)	1.539(6)
C(43)-C(45)	1.536(6)
C(43)-C(44)	1.582(7)
C(46)-C(47)	1.488(7)
C(46)-C(48)	1.564(8)
C(49)-C(50)	1.379(7)
C(49)-C(54)	1.425(7)
C(50)-C(51)	1.355(7)
C(51)-C(52)	1.389(9)
C(52)-C(53)	1.382(8)
C(53)-C(54)	1.424(7)

W(2A)-Te(2A)	2.742(4)
Te(2A)-C(45)#3	2.509(6)
Te(2A)-C(44)#3	2.516(5)
Te(2A)-Te(2)#2	2.769(3)
Te(1A)-W(1A)	2.740(4)
Te(1A)-Te(1)#1	2.837(4)
W(1A)-C(17)#3	2.140(5)
W(1A)-C(18)#3	2.538(5)

C(2)-W(1)-C(1)	93.96(19)
C(2)-W(1)-C(3)	93.66(19)
C(1)-W(1)-C(3)	172.31(18)
C(2)-W(1)-P(1)	83.42(15)
C(1)-W(1)-P(1)	87.90(15)
C(3)-W(1)-P(1)	91.91(13)
C(2)-W(1)-P(2)	83.47(15)
C(1)-W(1)-P(2)	92.56(14)
C(3)-W(1)-P(2)	89.37(12)
P(1)-W(1)-P(2)	166.87(4)
C(2)-W(1)-Te(1)	177.90(14)
C(1)-W(1)-Te(1)	83.98(13)
C(3)-W(1)-Te(1)	88.41(13)
P(1)-W(1)-Te(1)	96.85(3)
P(2)-W(1)-Te(1)	96.24(3)
C(29)-W(2)-C(28)	93.54(19)
C(29)-W(2)-C(30)	93.65(18)
C(28)-W(2)-C(30)	172.77(17)
C(29)-W(2)-P(4)	83.43(14)
C(28)-W(2)-P(4)	89.24(13)
C(30)-W(2)-P(4)	90.77(14)
C(29)-W(2)-P(3)	84.54(14)
C(28)-W(2)-P(3)	91.82(13)
C(30)-W(2)-P(3)	89.68(13)
P(4)-W(2)-P(3)	167.97(4)
C(29)-W(2)-Te(2)	178.53(14)
C(28)-W(2)-Te(2)	84.99(13)

C(30)-W(2)-Te(2)	87.83(11)
P(4)-W(2)-Te(2)	96.53(3)
P(3)-W(2)-Te(2)	95.50(3)
C(22)-Te(1)-W(1)	108.20(11)
C(22)-Te(1)-Te(1A)#1	68.36(13)
W(1)-Te(1)-Te(1A)#1	175.59(8)
C(49)-Te(2)-W(2)	107.75(10)
C(49)-Te(2)-Te(2A)#2	68.19(12)
W(2)-Te(2)-Te(2A)#2	173.84(7)
C(4)-P(1)-C(10)	101.51(19)
C(4)-P(1)-C(7)	109.9(2)
C(10)-P(1)-C(7)	101.1(2)
C(4)-P(1)-W(1)	114.80(17)
C(10)-P(1)-W(1)	115.41(16)
C(7)-P(1)-W(1)	112.77(15)
C(19)-P(2)-C(16)	107.1(2)
C(19)-P(2)-C(13)	102.02(18)
C(16)-P(2)-C(13)	101.9(2)
C(19)-P(2)-W(1)	112.98(17)
C(16)-P(2)-W(1)	116.85(13)
C(13)-P(2)-W(1)	114.35(15)
C(37)-P(3)-C(34)	100.54(19)
C(37)-P(3)-C(31)	101.44(18)
C(34)-P(3)-C(31)	109.0(2)
C(37)-P(3)-W(2)	115.64(16)
C(34)-P(3)-W(2)	116.24(14)
C(31)-P(3)-W(2)	112.40(14)
C(43)-P(4)-C(40)	103.3(2)
C(43)-P(4)-C(46)	110.3(2)
C(40)-P(4)-C(46)	100.3(2)
C(43)-P(4)-W(2)	114.08(16)
C(40)-P(4)-W(2)	115.02(16)
C(46)-P(4)-W(2)	112.73(16)
O(1)-C(1)-W(1)	178.4(4)
O(2)-C(2)-W(1)	177.9(4)
O(3)-C(3)-W(1)	178.5(4)

C(5)-C(4)-C(6)	107.1(4)
C(5)-C(4)-P(1)	115.8(3)
C(6)-C(4)-P(1)	116.6(4)
C(8)-C(7)-C(9)	111.3(5)
C(8)-C(7)-P(1)	115.9(5)
C(9)-C(7)-P(1)	115.8(3)
C(11)-C(10)-C(12)	115.2(4)
C(11)-C(10)-P(1)	111.8(3)
C(12)-C(10)-P(1)	110.7(3)
C(14)-C(13)-C(15)	116.5(4)
C(14)-C(13)-P(2)	110.8(2)
C(15)-C(13)-P(2)	110.8(3)
C(18)-C(16)-C(17)	107.9(4)
C(18)-C(16)-P(2)	121.5(3)
C(17)-C(16)-P(2)	114.3(4)
C(20)-C(19)-C(21)	107.2(4)
C(20)-C(19)-P(2)	116.2(3)
C(21)-C(19)-P(2)	118.9(4)
C(23)-C(22)-C(27)	119.0(4)
C(23)-C(22)-Te(1)	119.7(3)
C(27)-C(22)-Te(1)	121.2(3)
C(22)-C(23)-C(24)	120.8(4)
C(25)-C(24)-C(23)	116.2(5)
C(26)-C(25)-C(24)	121.6(4)
C(27)-C(26)-C(25)	119.9(4)
C(26)-C(27)-C(22)	122.1(5)
O(4)-C(28)-W(2)	177.8(4)
O(5)-C(29)-W(2)	178.0(4)
O(6)-C(30)-W(2)	177.7(4)
C(33)-C(31)-C(32)	111.7(4)
C(33)-C(31)-P(3)	116.3(3)
C(32)-C(31)-P(3)	114.1(3)
C(36)-C(34)-C(35)	107.8(4)
C(36)-C(34)-P(3)	117.8(3)
C(35)-C(34)-P(3)	113.5(3)
C(38)-C(37)-C(39)	110.4(4)

C(38)-C(37)-P(3)	111.2(3)
C(39)-C(37)-P(3)	112.0(3)
C(41)-C(40)-C(42)	108.0(4)
C(41)-C(40)-P(4)	111.7(3)
C(42)-C(40)-P(4)	113.3(3)
C(45)-C(43)-C(44)	107.0(4)
C(45)-C(43)-P(4)	114.8(3)
C(44)-C(43)-P(4)	117.2(3)
C(47)-C(46)-C(48)	111.5(5)
C(47)-C(46)-P(4)	116.0(3)
C(48)-C(46)-P(4)	113.3(4)
C(50)-C(49)-C(54)	119.2(5)
C(50)-C(49)-Te(2)	122.3(4)
C(54)-C(49)-Te(2)	118.5(3)
C(51)-C(50)-C(49)	121.5(5)
C(50)-C(51)-C(52)	122.2(5)
C(53)-C(52)-C(51)	117.4(5)
C(52)-C(53)-C(54)	122.3(5)
C(53)-C(54)-C(49)	117.2(4)
C(45)#3-Te(2A)-C(44)#3	59.85(17)
C(45)#3-Te(2A)-W(2A)	68.27(16)
C(44)#3-Te(2A)-W(2A)	69.55(15)
C(45)#3-Te(2A)-Te(2)#2	112.43(18)
C(44)#3-Te(2A)-Te(2)#2	116.09(18)
W(2A)-Te(2A)-Te(2)#2	174.08(14)
W(1A)-Te(1A)-Te(1)#1	174.78(16)
C(17)#3-W(1A)-C(18)#3	64.08(18)
C(17)#3-W(1A)-Te(1A)	69.13(18)
C(18)#3-W(1A)-Te(1A)	77.75(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x,-y+2,-z+1 #3 x-1,y,z

Table S4. Anisotropic displacement parameters ($Å^2 x 10^3$) for ccd758. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W(1)	20(1)	13(1)	29(1)	-6(1)	-2(1)	-1(1)
W(2)	21(1)	13(1)	29(1)	-8(1)	-4(1)	-1(1)
Te(1)	38(1)	26(1)	31(1)	-10(1)	-1(1)	-1(1)
Te(2)	40(1)	23(1)	32(1)	-4(1)	-3(1)	-2(1)
P(1)	33(1)	30(1)	50(1)	-13(1)	-9(1)	-2(1)
P(2)	34(1)	24(1)	44(1)	-9(1)	-2(1)	-1(1)
P(3)	37(1)	24(1)	43(1)	-10(1)	-6(1)	0(1)
P(4)	39(1)	29(1)	50(1)	-14(1)	-11(1)	3(1)
O(1)	39(2)	35(1)	135(3)	-34(2)	-3(2)	12(1)
O(2)	82(3)	130(3)	27(2)	3(2)	-12(2)	-22(2)
O(3)	51(2)	34(1)	97(2)	-23(1)	-17(2)	11(1)
O(4)	55(2)	32(1)	131(2)	-30(1)	-30(2)	-5(1)
O(5)	44(2)	132(3)	30(1)	-35(1)	-5(2)	17(2)
O(6)	60(2)	30(1)	103(2)	-24(1)	-29(2)	-8(1)
C(1)	54(3)	33(2)	56(3)	-7(2)	-7(2)	-3(2)
C(2)	40(3)	65(3)	47(2)	-19(2)	-12(2)	1(2)
C(3)	16(2)	42(2)	64(2)	-20(2)	-7(2)	2(2)
C(4)	29(2)	44(2)	63(3)	-19(2)	0(2)	-4(2)
C(5)	45(3)	57(2)	109(3)	-45(2)	11(3)	-5(2)
C(6)	55(3)	35(2)	82(3)	-10(2)	-12(3)	-6(2)
C(7)	48(3)	63(3)	79(3)	-13(2)	-29(2)	-5(2)
C(8)	156(5)	65(4)	135(4)	-10(3)	-102(3)	15(4)
C(9)	133(4)	141(5)	60(3)	16(3)	-64(2)	-65(4)
C(10)	43(3)	34(2)	70(3)	-20(2)	-11(2)	-7(2)
C(11)	69(3)	21(2)	75(2)	-11(2)	-47(2)	-1(2)
C(12)	126(5)	29(2)	83(3)	-38(2)	-22(3)	-5(2)
C(13)	48(2)	13(1)	59(2)	-10(1)	-4(2)	-7(2)
C(14)	59(3)	31(2)	67(3)	-22(2)	-17(2)	16(2)
C(15)	51(3)	35(2)	70(3)	7(2)	-13(2)	1(2)
C(16)	40(2)	33(2)	97(3)	-31(2)	-37(2)	16(2)
C(17)	62(3)	42(2)	86(3)	-3(2)	-36(3)	11(2)

C(18)	68(3)	30(2)	93(4)	-16(2)	-17(3)	4(2)
C(19)	40(3)	44(2)	63(3)	-15(2)	-2(2)	0(2)
C(20)	39(3)	63(2)	56(3)	-24(2)	21(2)	5(2)
C(21)	32(3)	63(3)	67(3)	-15(2)	10(2)	-16(2)
C(22)	33(3)	54(2)	30(2)	-20(1)	6(2)	7(2)
C(23)	37(3)	63(2)	60(2)	-27(2)	-10(2)	-2(2)
C(24)	50(3)	71(3)	55(3)	-5(2)	-2(3)	0(3)
C(25)	90(4)	49(2)	58(3)	-13(2)	-34(2)	6(2)
C(26)	77(3)	34(2)	64(3)	-7(2)	-19(3)	-11(2)
C(27)	34(2)	36(2)	72(3)	-14(2)	-8(2)	-9(2)
C(28)	31(2)	30(2)	60(2)	-13(2)	-3(2)	-3(2)
C(29)	28(2)	94(2)	34(2)	-40(2)	-3(2)	22(2)
C(30)	46(3)	25(2)	37(2)	-3(2)	-1(2)	2(2)
C(31)	36(2)	31(2)	51(2)	-13(2)	-4(2)	-1(2)
C(32)	67(4)	43(2)	50(3)	-2(2)	6(3)	-8(2)
C(33)	77(4)	73(3)	50(3)	-18(2)	-6(3)	18(3)
C(34)	41(2)	30(2)	56(2)	-10(2)	-28(2)	11(2)
C(35)	29(2)	47(2)	62(2)	-22(2)	-7(2)	-2(2)
C(36)	43(3)	48(2)	54(2)	-19(2)	-8(2)	1(2)
C(37)	51(3)	21(2)	52(2)	-15(1)	-10(2)	16(2)
C(38)	11(2)	38(2)	64(2)	-13(2)	-11(2)	5(2)
C(39)	74(3)	46(2)	50(2)	-28(2)	-20(2)	5(2)
C(40)	42(2)	18(2)	77(3)	-9(2)	-15(2)	-2(2)
C(41)	59(4)	44(2)	80(3)	-30(2)	8(3)	6(2)
C(42)	65(3)	21(2)	93(4)	8(2)	-15(3)	-1(2)
C(43)	69(3)	51(2)	39(2)	-15(2)	-16(2)	1(2)
C(44)	49(3)	60(3)	49(3)	-13(2)	-3(2)	2(2)
C(45)	62(4)	37(2)	85(3)	-14(2)	9(3)	-13(2)
C(46)	38(3)	60(2)	64(3)	-20(2)	-18(2)	14(2)
C(47)	102(3)	59(3)	100(3)	-12(2)	-64(3)	-19(3)
C(48)	75(4)	104(4)	67(3)	-9(3)	-37(3)	25(3)
C(49)	47(3)	46(2)	32(2)	-6(2)	-2(2)	-14(2)
C(50)	57(3)	34(2)	74(3)	-19(2)	-27(2)	8(2)
C(51)	57(3)	60(3)	73(3)	-28(2)	-16(2)	10(2)
C(52)	119(5)	49(2)	65(3)	-22(2)	-17(3)	5(3)
C(53)	18(2)	72(3)	64(3)	-22(2)	-10(2)	-2(2)

C(54)	63(3)	45(2)	61(3)	-7(2)	-19(2)	-1(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for ccd758.

	x	y	z	U(eq)
H(4)	431	4514	3779	55
H(5A)	269	5990	3494	104
H(5B)	-799	5486	4084	104
H(5C)	-809	5887	3131	104
H(6A)	-753	3690	3245	88
H(6B)	-1450	4497	3006	88
H(6C)	-1408	4085	3952	88
H(7)	1107	5401	892	74
H(8A)	1111	6654	1262	167
H(8B)	-177	6507	1631	167
H(8C)	266	6612	666	167
H(9A)	-405	4425	1334	169
H(9B)	-665	5261	708	169
H(9C)	-1141	5104	1675	169
H(10)	505	3632	2184	58
H(11A)	974	3274	3493	76
H(11B)	2249	3350	3079	76
H(11C)	1465	2640	2958	76
H(12A)	1792	4171	964	112
H(12B)	1992	3212	1347	112
H(12C)	2777	3929	1454	112
H(13)	5576	7878	1858	49
H(14A)	4658	7506	3232	75
H(14B)	3503	7623	2937	75
H(14C)	4340	8409	2766	75
H(15A)	4687	7939	715	83
H(15B)	4334	8690	1133	83
H(15C)	3513	7894	1305	83

H(16)	5300	6110	3380	61
H(17A)	5665	4857	2906	94
H(17B)	6535	5062	3426	94
H(17C)	6857	5255	2442	94
H(18A)	6506	7315	2844	95
H(18B)	7367	6769	2402	95
H(18C)	7037	6546	3386	95
H(19)	5265	6729	636	60
H(20A)	5209	5227	1038	83
H(20B)	6449	5273	1172	83
H(20C)	6171	5619	272	83
H(21A)	6792	7519	828	85
H(21B)	7126	7004	143	85
H(21C)	7415	6669	1041	85
H(23)	4867	4535	4564	62
H(24)	5563	3153	5021	74
H(25)	4222	1992	5513	76
H(26)	2373	2168	5337	70
H(27)	1778	3477	4847	57
H(31)	-315	9542	9355	47
H(32A)	-171	8267	8937	86
H(32B)	-1410	8340	8795	86
H(32C)	-1153	8237	9700	86
H(33A)	-1779	10438	9114	100
H(33B)	-2172	9591	9800	100
H(33C)	-2411	9708	8888	100
H(34)	-309	10300	6548	48
H(35A)	-699	8818	7028	67
H(35B)	-1611	9281	6552	67
H(35C)	-1859	8988	7538	67
H(36A)	-1500	11237	7116	71
H(36B)	-2344	10468	7597	71
H(36C)	-2097	10736	6610	71
H(37)	-645	11291	8088	48
H(38A)	366	11640	6709	56
H(38B)	1494	11552	7044	56

H(38C)	697	12279	7204	56
H(39A)	290	10844	9233	79
H(39B)	649	11792	8760	79
H(39C)	1450	11062	8617	79
H(40)	4412	7169	7827	55
H(41A)	3905	7460	6507	92
H(41B)	2637	7390	6937	92
H(41C)	3360	6584	7069	92
H(42A)	3004	7064	9035	96
H(42B)	2815	6343	8591	96
H(42C)	2083	7144	8478	96
H(43)	4510	8889	6207	62
H(44A)	5731	7796	6681	81
H(44B)	6403	8453	6979	81
H(44C)	6389	8577	6019	81
H(45A)	4662	10217	6521	97
H(45B)	5735	10031	5922	97
H(45C)	5744	9929	6879	97
H(46)	3850	8307	9073	62
H(47A)	3935	9768	8682	124
H(47B)	5216	9756	8310	124
H(47C)	4770	9399	9278	124
H(48A)	5337	7507	8583	121
H(48B)	5659	7998	9214	121
H(48C)	6105	8343	8244	121
H(50)	3208	8391	5154	63
H(51)	2597	7334	4657	73
H(52)	730	7170	4566	92
H(53)	-507	8148	4961	60
H(54)	96	9284	5451	68