New rhenium(V) Complexes with Thiolates: Synthesis, Structures and Monomerization

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Supporting Information

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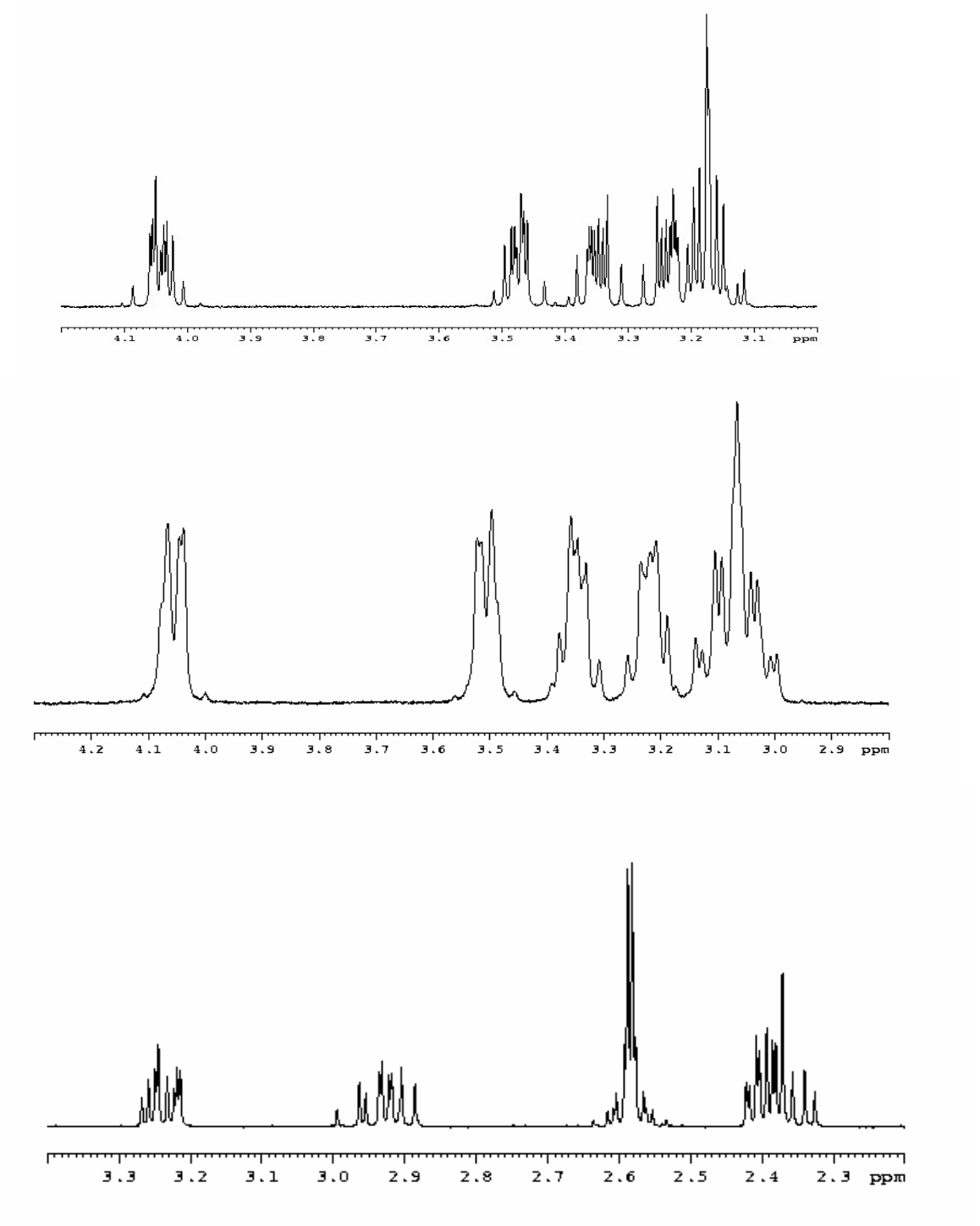

Fig. S-1. ^{1}H-NMR Spectra of $[(ReO)_2(edt)_3]$, (**8**^{edt}) in CD_2Cl_2 at 298 K (top), in CD_2Cl_2 at 233 K (middle); and in C_6D_6 at 298 K (bottom).

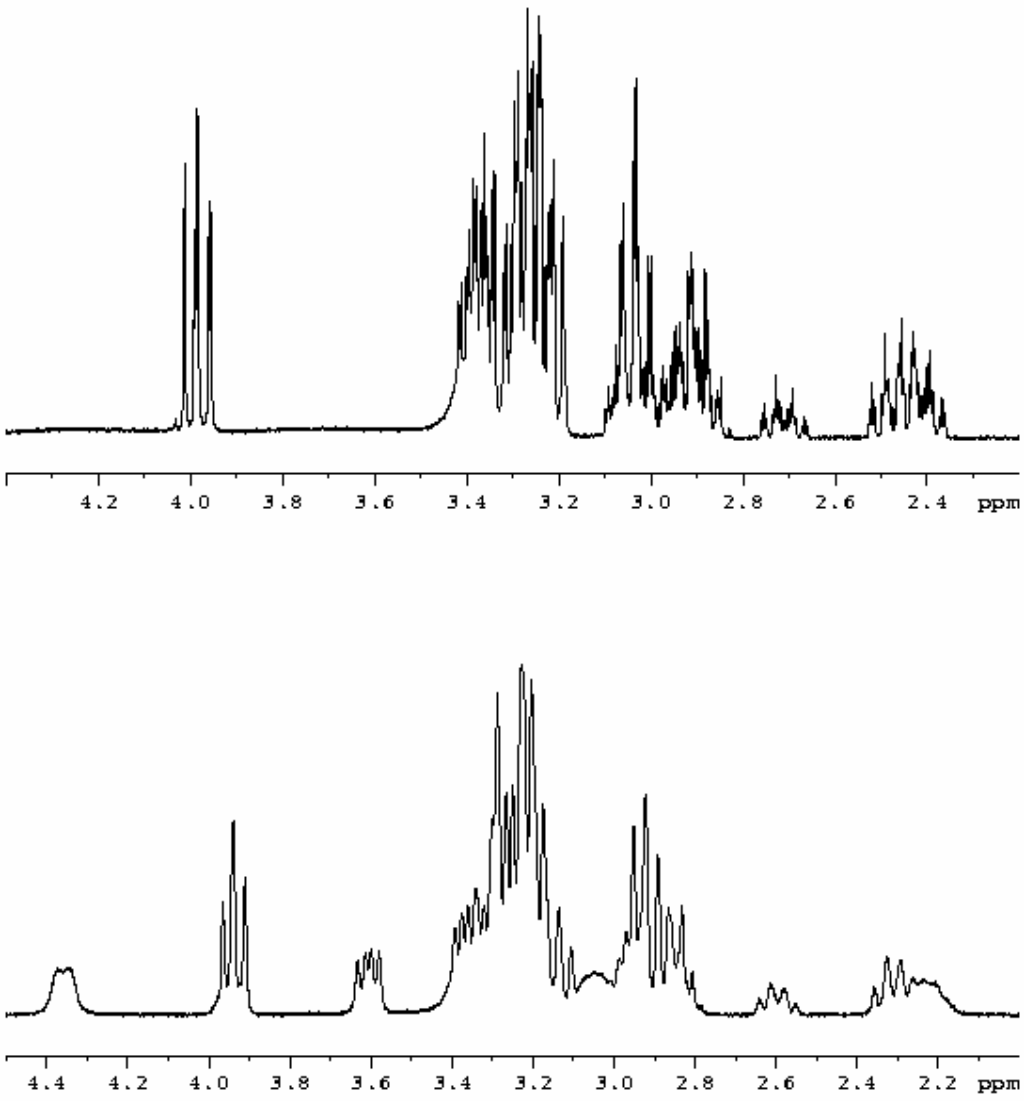

Fig. S-2. ^{1}H-NMR Spectra of $[(ReO)_2(pdt)_3]$ (**8**^{pdt}) in CD_2Cl_2, top: at 298K; bottom: 233K

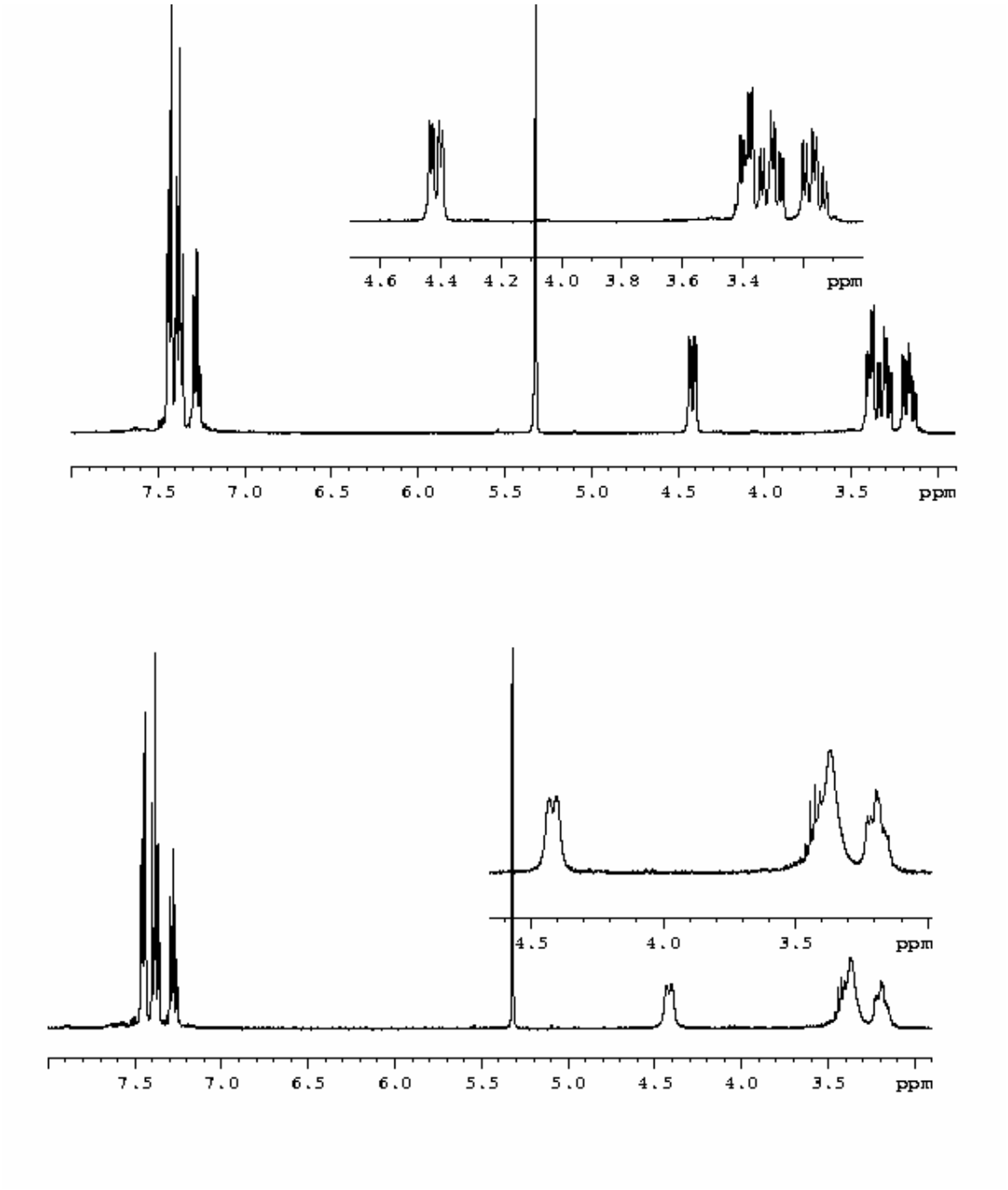

Fig. S-3. ^{1}H-NMR Spectra of $\{(PhS)(ReO)(edt)\}_2$ (**2**) in CD_2Cl_2. at 252 K (top) and at 298 K (bottom).

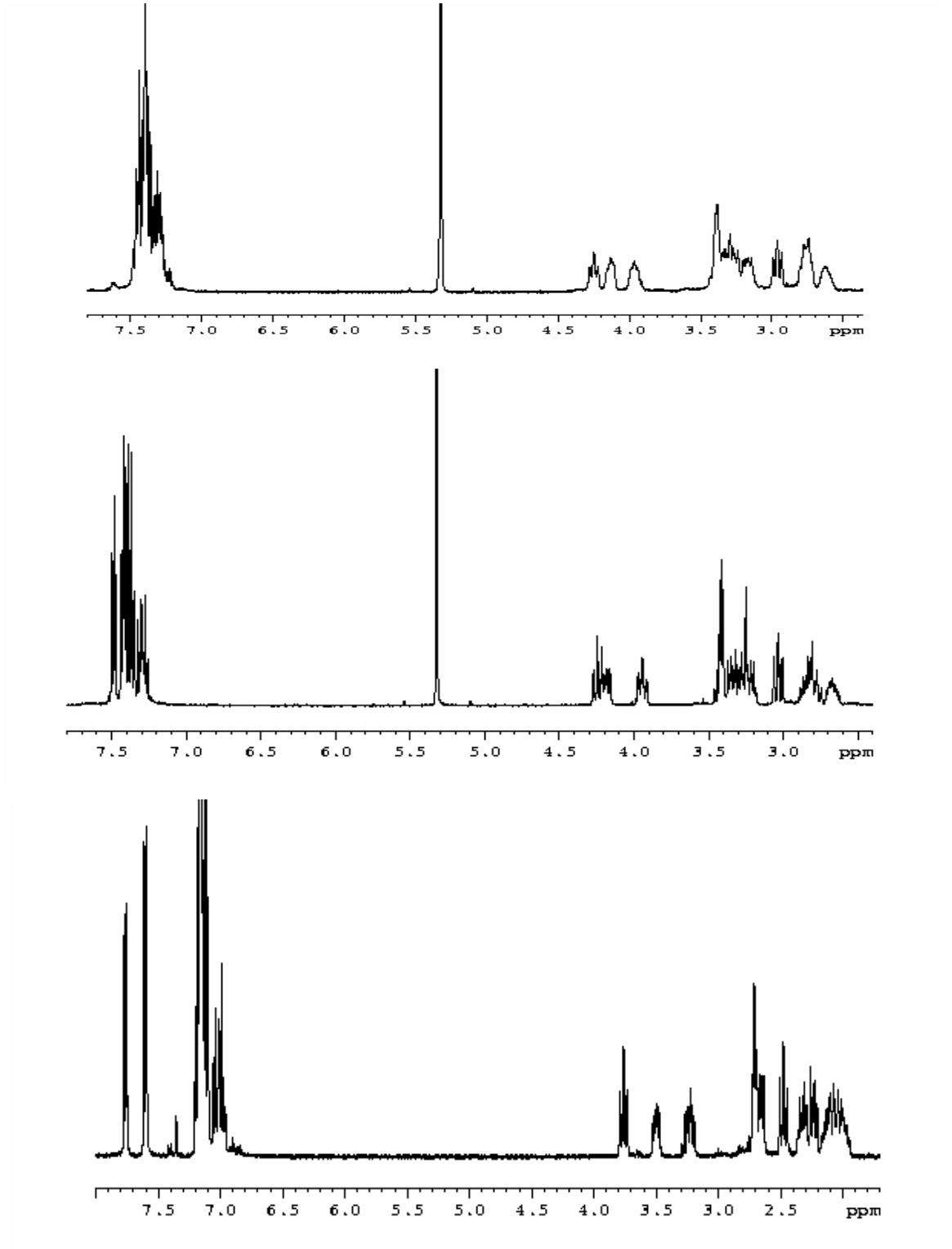

Fig. S-4. ^{1}H-NMR Spectra of {(PhS)(ReO)(pdt)}$_2$ (**3a**) in CD_2Cl_2 at 233 K (top); in CD_2Cl_2 at 298 K (middle); and in C_6D_6 at 298 K (bottom).

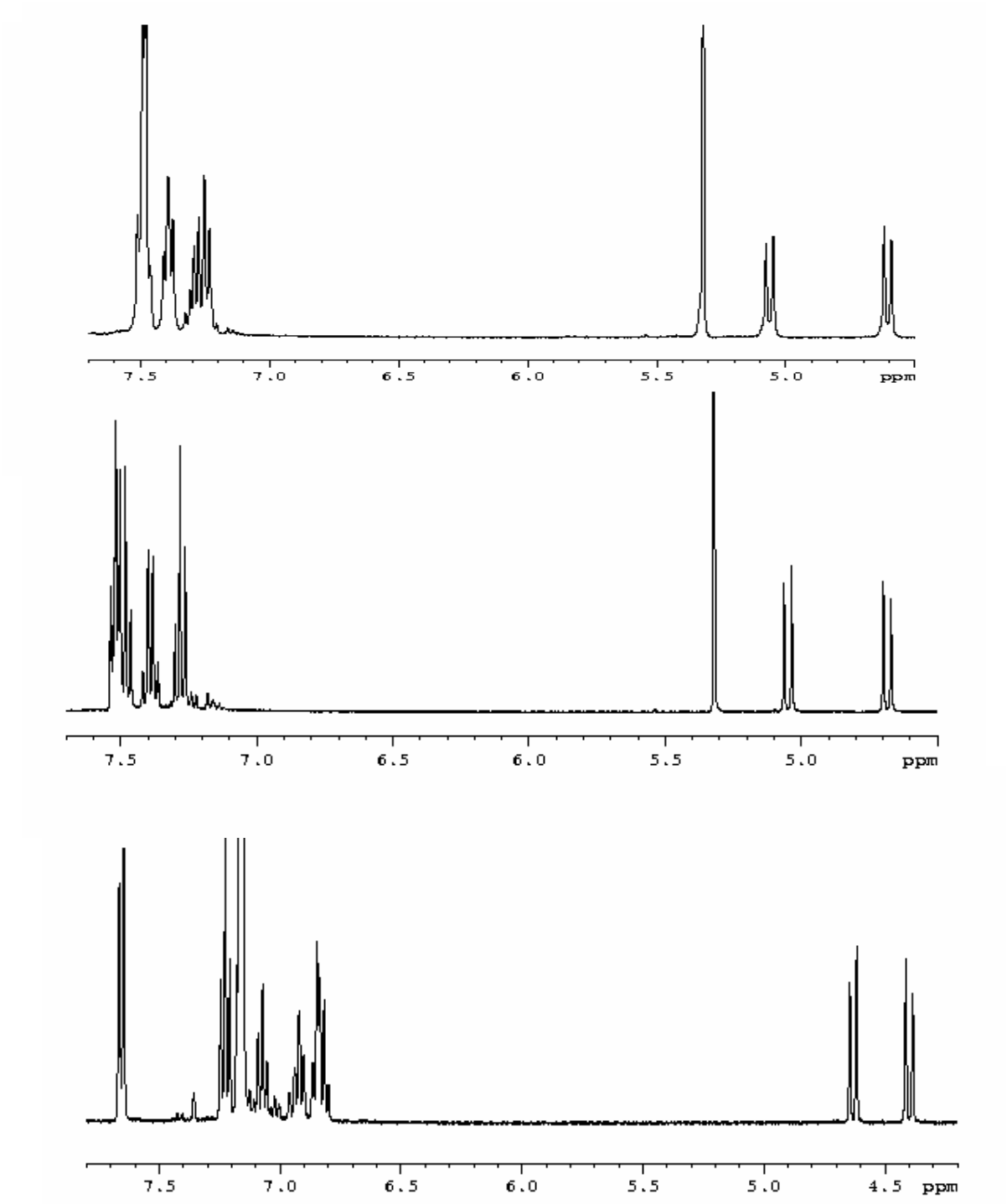

Fig. S-5. ^{1}H-NMR Spectra of {(PhS)(ReO)(mtp)}$_2$ (**4**) in CD_2Cl_2 at 233 K (top), at 298 K (middle), and in C_6D_6 at 323 K (bottom)

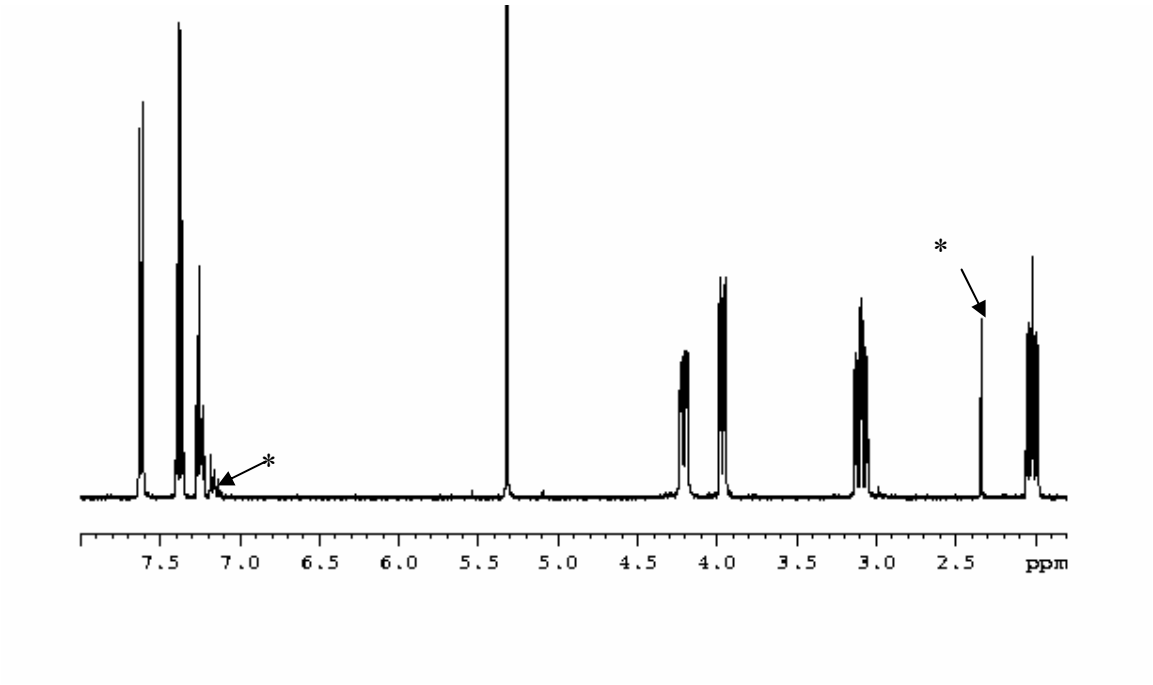

Fig. S-6. ^{1}H-NMR Spectrum of [(ReO)(SPh)(mes)] (**6**) in CD_2Cl_2 at 298K. * toluene

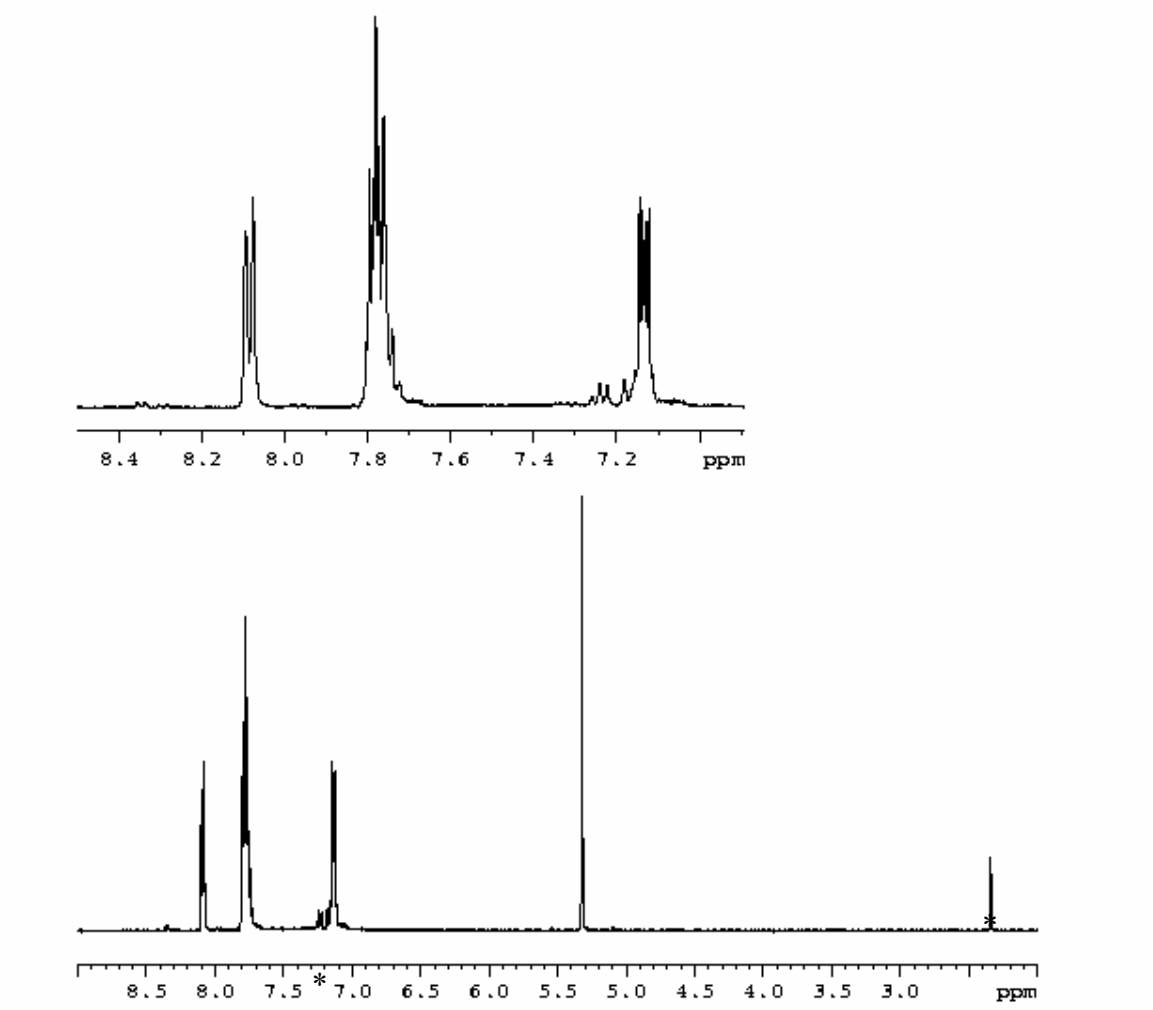

Fig. S-7. ^{1}H-NMR Spectra of {(PhS)(ReO)(bdt)]$_2$ (**5**) in CD_2Cl_2, at 298K. * from toluene

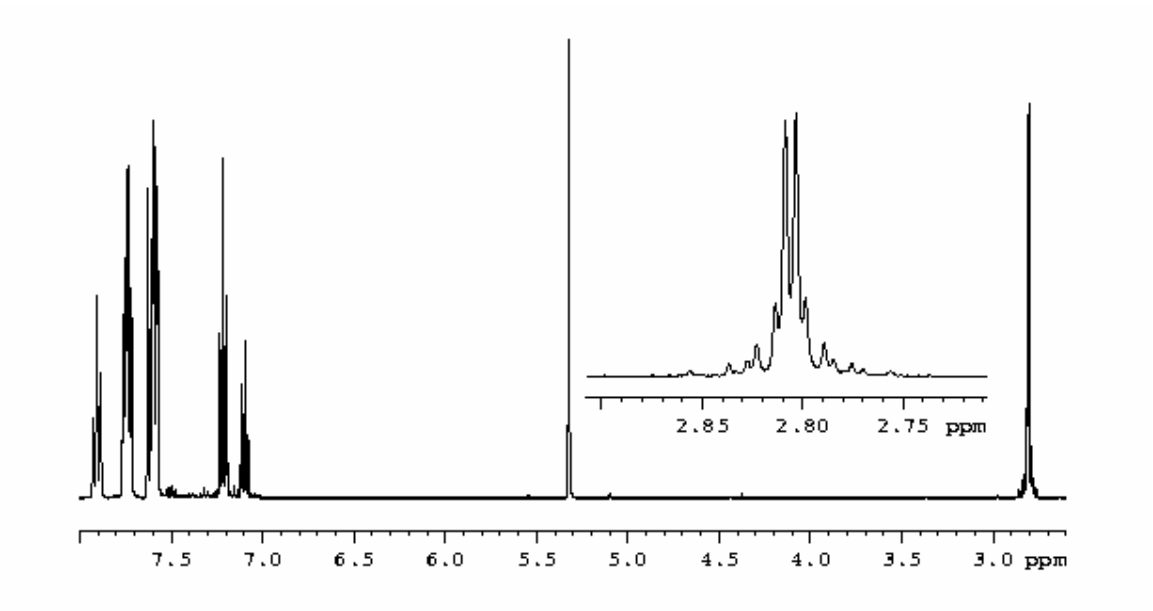

Fig. S-8. ^{1}H-NMR Spectrum of $[Ph_4P][(PhS)_2(ReO)(edt)]$ (**7**) in CD_2Cl_2 at 298 K.

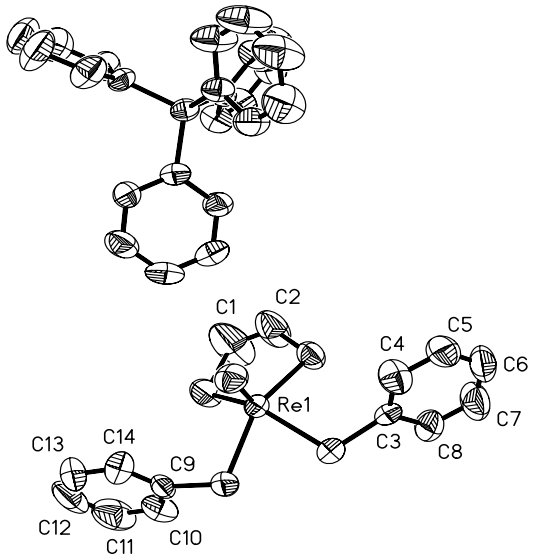

Fig. S-9. ORTEP diagrams with thermal ellipsoids drawn to 50% probability for $[PPh_4]$ $[(PhS)_2(ReO)(edt)]$, **7**.

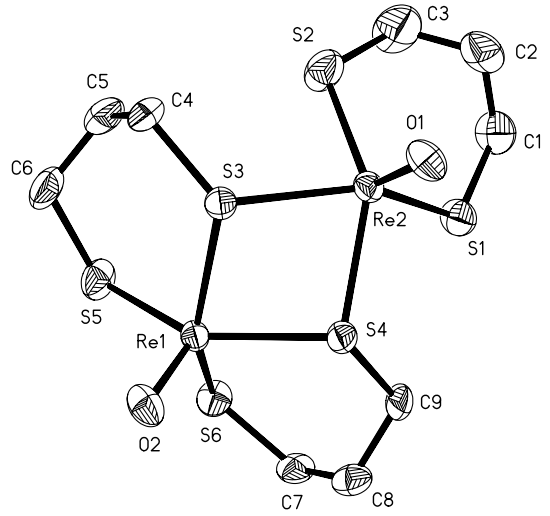

Fig. S-10. ORTEP diagrams with thermal ellipsoids drawn to 50% probability for $\{(ReO)_2(pdt)_3\}$, $\mathbf{8}^{\mathbf{pdt}}$.

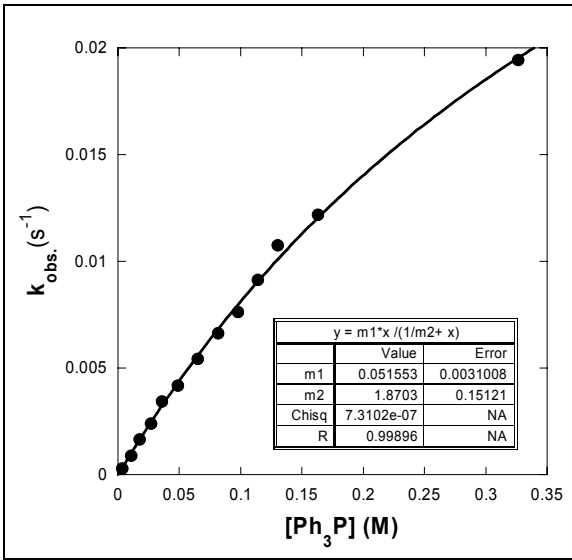

Fig. S-11. Plot of k_{obs} *vs* [PPh_3] for reaction of {PhS(ReO)(mtp)}$_2$ (**4**).

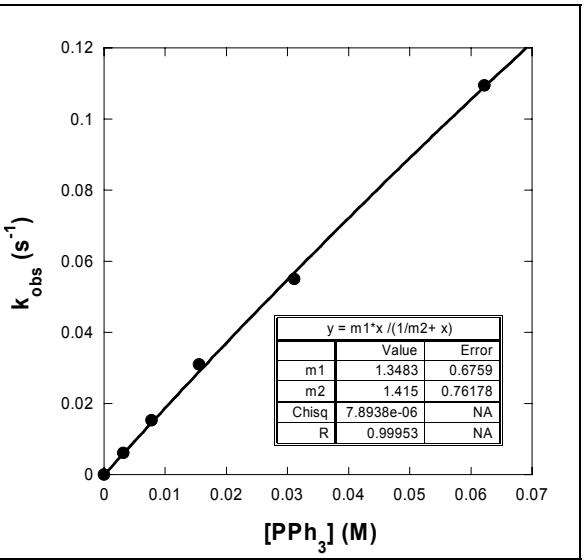

Fig. S-12. Plot of k_{obs} *vs* [PPh_3] for reaction of {PhS(ReO)(edt)}$_2$ (**2**).

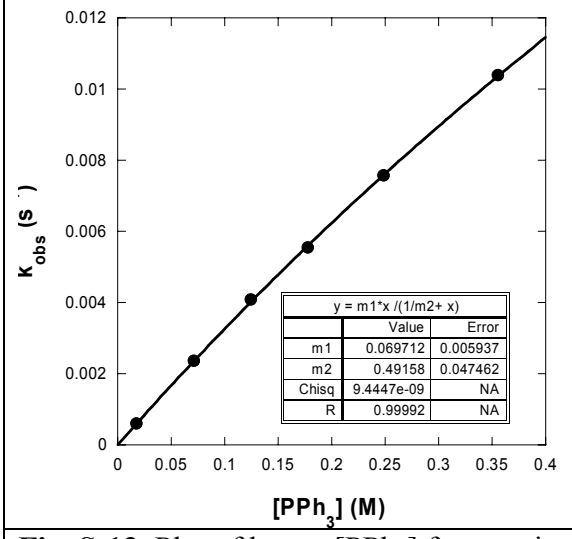

Fig. S-13. Plot of k_{obs} *vs* [PPh_3] for reaction of {PhS(ReO)(pdt)}$_2$ (**3a**).

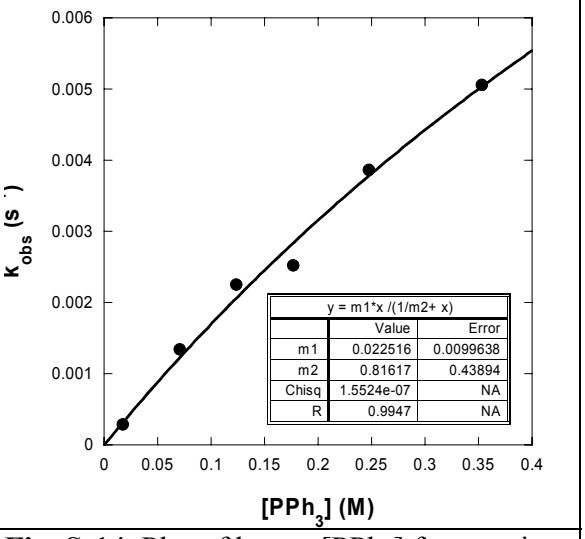

Fig. S-14. Plot of k_{obs} *vs* [PPh_3] for reaction of {PhS(ReO)(pdtMe)}$_2$ (**3b-c**).

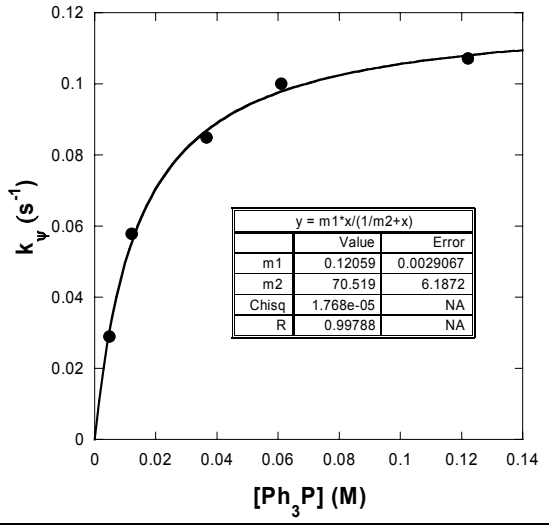

Fig. S-15. Plot of k_{obs} *vs* [PPh_3] for reaction of {PhS(ReO)(bdt)}$_2$ (**5**).

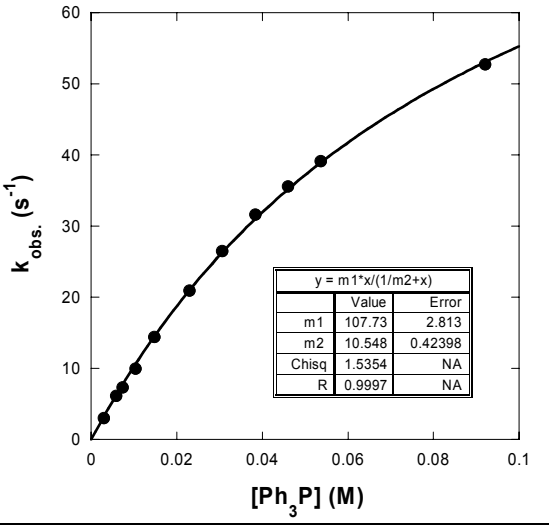

Fig. S-16. Plot of k_{obs} *vs* [PPh_3] for reaction of {$(PhS)_2$(ReO)(μ-SPh)}$_2$ (**1**).

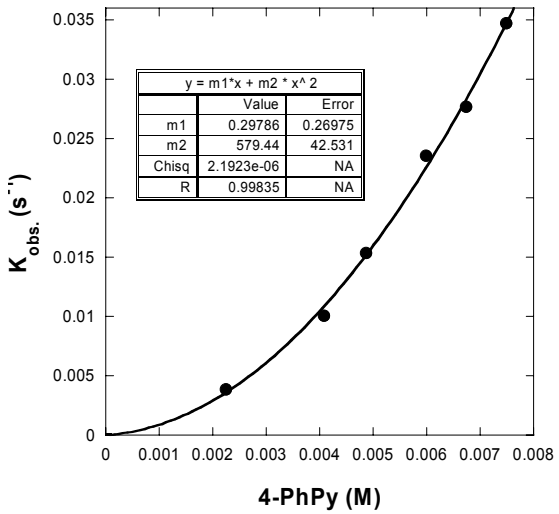

Fig. S-17. Plot of k_{obs} *vs* [4-PhPy] for {PhS(ReO)(mtp)}$_2$ (**4**).

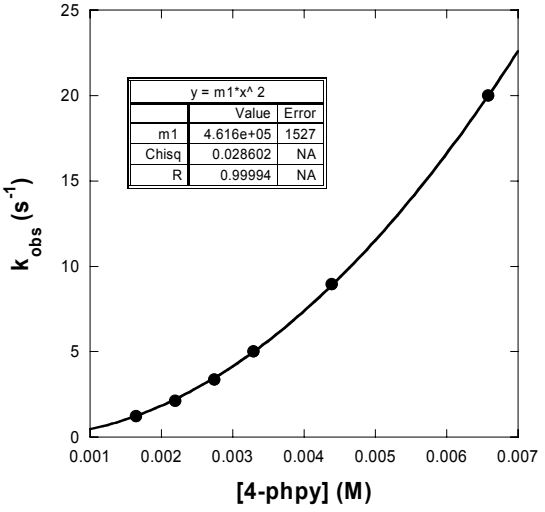

Fig. S-18. Plot of k_{obs} *vs* [4-PhPy] for reaction of {PhS(ReO)(edt)}$_2$ (**2**).

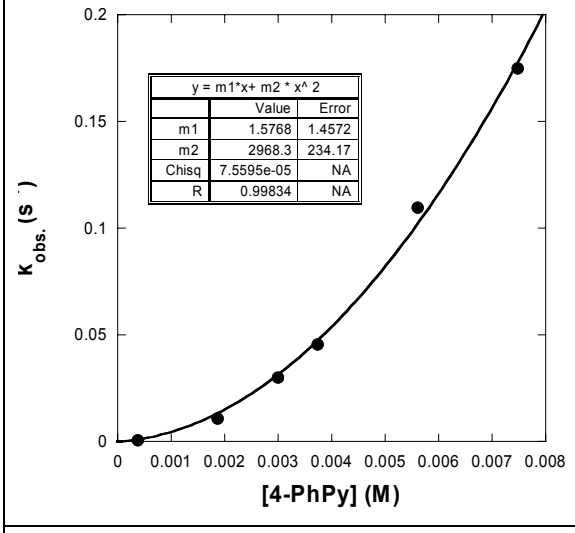

Fig. S-19. Plot of k_{obs} *vs* [4-PhPy] for reaction of $\{PhS(ReO)(pdt)\}_2$ (**3a**).

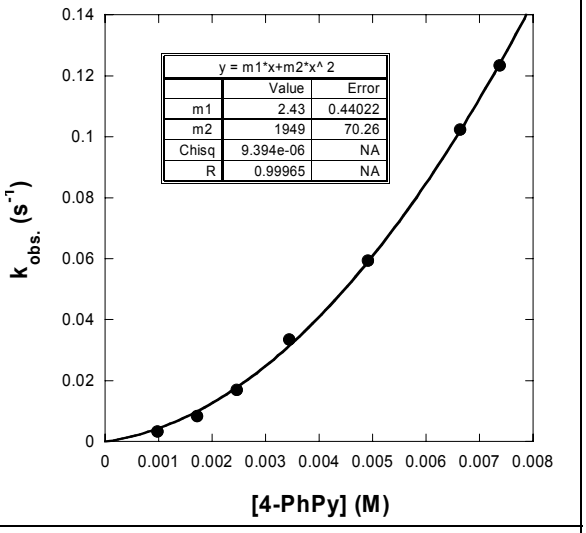

Fig. S-20. Plot of k_{obs} *vs* [4-PhPy] for reaction of $\{PhS(ReO)(pdtMe)\}_2$ (**3b-c**).

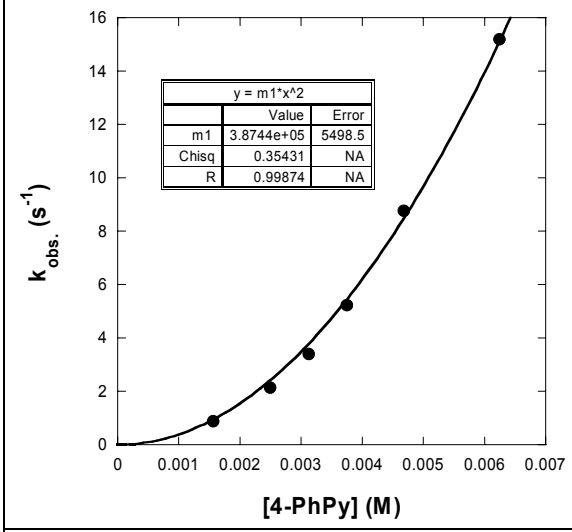

Fig. S-21. Plot of k_{obs} *vs* [4-PhPy] for reaction of $\{PhS(ReO)(bdt)\}_2$ (**5**).

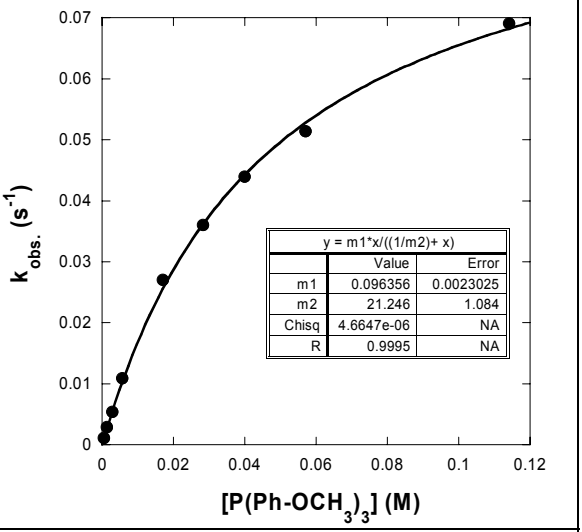

Fig. S-22. Plot of k_{obs} *vs* $[P(Ar\text{-}p\text{-}OCH_3)_3]$ for reaction of $\{PhS(ReO)(mtp)\}_2$ (**4**).

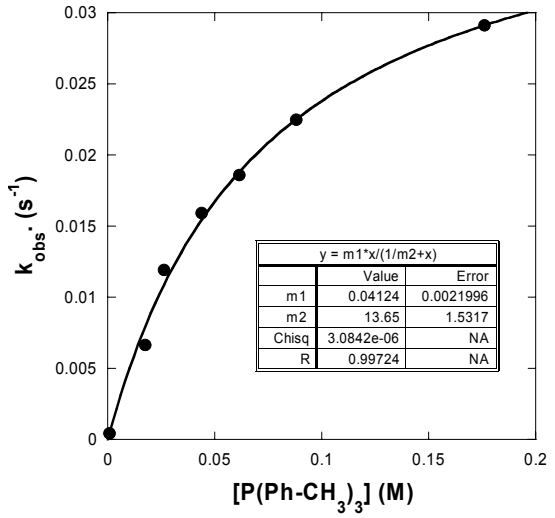

Fig. S-23. Plot of k_{obs} *vs* [P(Ar-*p*-CH_3)$_3$] for reaction of {PhS(ReO)(mtp)}$_2$ (**4**).

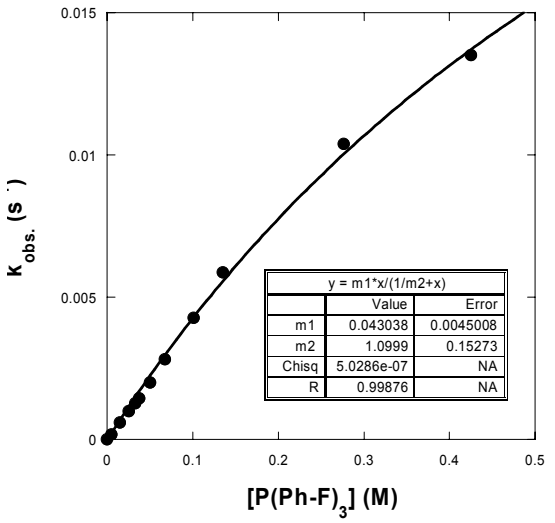

Fig. S-24. Plot of k_{obs} *vs* [P(Ar-*p*-F)$_3$] for reaction of {PhS(ReO)(mtp)}$_2$ (**4**).

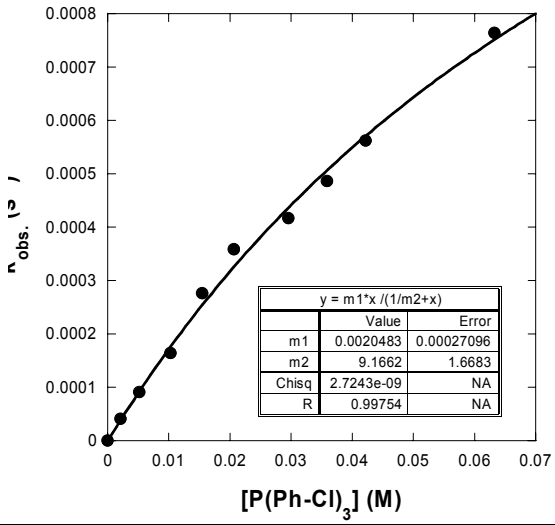

Fig. S-25. Plot of k_{obs} *vs* [P(Ar-*p*-Cl)$_3$] for reaction of {PhS(ReO)(mtp)}$_2$ (**4**).

Table S-1. Crystal data and structure refinement for **1**.

Empirical formula	C36 H30 O2 Re2 S6	
Formula weight	1059.36	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.464(2) Å	α= 78.763(4)°.
	b = 11.820(2) Å	β= 74.363(3)°.
	c = 13.959(3) Å	γ = 86.875(4)°.
Volume	1786.6(6) $Å^3$	
Z	2	
Density (calculated)	1.969 Mg/m^3	
Absorption coefficient	7.152 mm^{-1}	
F(000)	1016	
Crystal size	0.30 x 0.10 x 0.05 mm^3	
Theta range for data collection	1.76 to 28.30°.	
Index ranges	-15<=h<=15, -15<=k<=12, -17<=l<=18	
Reflections collected	12851	
Independent reflections	7586 [R(int) = 0.0367]	
Completeness to theta = 28.30°	85.3 %	
Absorption correction	Numerical	
Max. and min. transmission	0.64 and 0.36	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7586 / 0 / 435	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.0701	
R indices (all data)	R1 = 0.0634, wR2 = 0.0774	
Largest diff. peak and hole	1.118 and -1.249 $e.Å^{-3}$	

$R1 = \Sigma \, | \, |F_o| - |F_c| \, | \, / \, \Sigma \, |F_o|$ and $wR2 = \{ \, \Sigma \, [\, w(F_o^2 - F_c^2)^2 \,] \, / \, \Sigma \, [\, w(F_o^2)^2 \,] \, \}^{1/2}$

Table S-2. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. 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}
e(1)		3494(1)	3414(1)	5376(1)		18(1)
Re(2)		3078(1)	2154(1)	3315(1)		16(1)
Re(1A)		3503(5)	2333(7)	5335(5)		38(3)
Re(2A)		3133(2)	3267(3)	2808(2)		25(1)
S(1)		4040(2)	2427(2)	1622(1)		32(1)
S(2)		1342(1)	2158(2)	2818(1)		25(1)
S(3)		4560(1)	3300(2)	3649(1)		21(1)
S(4)		1973(1)	3292(2)	4514(1)		21(1)
S(5)		5092(2)	2392(2)	5798(1)		31(1)
S(6)		2343(2)	2494(2)	6925(1)		31(1)
C(1)		5560(6)	2949(6)	1267(5)		28(2)
C(2)		6531(6)	2191(7)	1134(5)		35(2)
C(3)		7709(7)	2615(8)	711(6)		48(2)
C(4)		7888(8)	3774(10)	453(7)		60(3)
C(5)		6937(8)	4522(8)	583(7)		52(2)
C(6)		5764(7)	4110(7)	978(6)		40(2)
C(7)		1890(6)	708(7)	1419(5)		34(2)
C(8)		1953(8)	447(8)	483(6)		51(2)
C(9)		1684(8)	1256(9)	-276(6)		54(3)
C(10)		1308(8)	2345(9)	-90(6)		52(2)
C(11)		1234(7)	2613(7)	834(6)		41(2)
C(12)		1530(6)	1806(6)	1589(5)		27(2)
C(13)		5981(5)	2547(6)	3478(5)		22(2)
C(14)		6049(6)	1356(6)	3681(5)		28(2)
C(15)		7167(7)	826(7)	3528(6)		39(2)
C(16)		8215(6)	1467(8)	3207(6)		40(2)
C(17)		8141(6)	2661(8)	3010(6)		41(2)
C(18)		7018(6)	3229(7)	3145(5)		30(2)
C(19)		504(5)	2646(6)	5091(5)		19(1)
C(20)		387(5)	1486(6)	5422(5)		21(1)
C(21)		-761(5)	1010(6)	5785(5)		26(2)

C(22)	-1749(7)	1675(7)	5828(6)	37(2)
C(23)	-1654(6)	2870(6)	5494(6)	31(2)
C(24)	-497(6)	3363(6)	5121(5)	26(2)
C(25)	4984(6)	2122(6)	7111(5)	26(2)
C(26)	5101(6)	1005(6)	7598(5)	32(2)
C(27)	5205(7)	800(7)	8577(6)	40(2)
C(28)	5177(7)	1686(7)	9075(6)	39(2)
C(29)	5016(8)	2804(7)	8620(6)	47(2)
C(30)	4939(8)	3012(7)	7622(6)	43(2)
C(31)	837(6)	3048(6)	7176(5)	26(2)
C(32)	-144(6)	2274(7)	7649(5)	36(2)
C(33)	-1302(7)	2706(9)	7952(6)	48(2)
C(34)	-1501(7)	3877(9)	7784(6)	51(2)
C(35)	-548(7)	4634(8)	7337(6)	40(2)
C(36)	615(6)	4222(6)	7026(5)	31(2)
O(1)	3664(4)	4776(4)	5456(4)	32(1)
O(2)	3253(4)	823(4)	3923(4)	32(1)

Table S-3. Bond lengths [Å] and angles [°] for **1**.

Re(1)-Re(1A)	1.290(8)	C(4)-H(4)	0.9500
Re(1)-O(1)	1.661(5)	C(5)-C(6)	1.385(10)
Re(1)-S(5)	2.2859(18)	C(5)-H(5)	0.9500
Re(1)-S(6)	2.3027(18)	C(6)-H(6)	0.9500
Re(1)-S(4)	2.3952(16)	C(7)-C(8)	1.382(10)
Re(1)-S(3)	2.4173(16)	C(7)-C(12)	1.386(10)
Re(2)-Re(2A)	1.364(3)	C(7)-H(7)	0.9500
Re(2)-O(2)	1.664(5)	C(8)-C(9)	1.372(13)
Re(2)-S(2)	2.2774(17)	C(8)-H(8)	0.9500
Re(2)-S(1)	2.2894(18)	C(9)-C(10)	1.385(13)
Re(2)-S(4)	2.4007(16)	C(9)-H(9)	0.9500
Re(2)-S(3)	2.4212(16)	C(10)-C(11)	1.368(11)
Re(2)-Re(1A)	3.035(8)	C(10)-H(10)	0.9500
Re(1A)-S(5)	2.100(7)	C(11)-C(12)	1.378(10)
Re(1A)-S(6)	2.297(7)	C(11)-H(11)	0.9500
Re(1A)-S(3)	2.425(7)	C(13)-C(14)	1.383(9)
Re(1A)-S(4)	2.456(7)	C(13)-C(18)	1.393(8)
Re(2A)-S(1)	2.099(3)	C(14)-C(15)	1.377(10)
Re(2A)-S(3)	2.262(3)	C(14)-H(14)	0.9500
Re(2A)-S(4)	2.399(3)	C(15)-C(16)	1.377(10)
Re(2A)-S(2)	2.491(3)	C(15)-H(15)	0.9500
S(1)-C(1)	1.789(7)	C(16)-C(17)	1.386(11)
S(2)-C(12)	1.799(7)	C(16)-H(16)	0.9500
S(3)-C(13)	1.794(6)	C(17)-C(18)	1.403(10)
S(4)-C(19)	1.799(6)	C(17)-H(17)	0.9500
S(5)-C(25)	1.769(7)	C(18)-H(18)	0.9500
S(6)-C(31)	1.781(7)	C(19)-C(20)	1.361(9)
C(1)-C(6)	1.366(10)	C(19)-C(24)	1.385(9)
C(1)-C(2)	1.386(10)	C(20)-C(21)	1.385(8)
C(2)-C(3)	1.397(10)	C(20)-H(20)	0.9500
C(2)-H(2)	0.9500	C(21)-C(22)	1.338(10)
C(3)-C(4)	1.359(12)	C(21)-H(21)	0.9500
C(3)-H(3)	0.9500	C(22)-C(23)	1.399(10)
C(4)-C(5)	1.361(13)	C(22)-H(22)	0.9500

C(23)-C(24)	1.401(8)	C(30)-H(30)	0.9500
C(23)-H(23)	0.9500	C(31)-C(36)	1.382(9)
C(24)-H(24)	0.9500	C(31)-C(32)	1.420(9)
C(25)-C(30)	1.373(10)	C(32)-C(33)	1.382(11)
C(25)-C(26)	1.380(10)	C(32)-H(32)	0.9500
C(26)-C(27)	1.378(10)	C(33)-C(34)	1.375(12)
C(26)-H(26)	0.9500	C(33)-H(33)	0.9500
C(27)-C(28)	1.360(10)	C(34)-C(35)	1.380(11)
C(27)-H(27)	0.9500	C(34)-H(34)	0.9500
C(28)-C(29)	1.376(11)	C(35)-C(36)	1.380(10)
C(28)-H(28)	0.9500	C(35)-H(35)	0.9500
C(29)-C(30)	1.393(10)	C(36)-H(36)	0.9500
C(29)-H(29)	0.9500		

Re(1A)-Re(1)-O(1)	172.4(3)	O(2)-Re(2)-S(4)	109.25(17)
Re(1A)-Re(1)-S(5)	65.1(3)	S(2)-Re(2)-S(4)	86.01(6)
O(1)-Re(1)-S(5)	107.33(17)	S(1)-Re(2)-S(4)	137.74(7)
Re(1A)-Re(1)-S(6)	73.5(3)	Re(2A)-Re(2)-S(3)	66.74(12)
O(1)-Re(1)-S(6)	107.76(17)	O(2)-Re(2)-S(3)	104.83(16)
S(5)-Re(1)-S(6)	85.95(7)	S(2)-Re(2)-S(3)	146.43(6)
Re(1A)-Re(1)-S(4)	77.2(3)	S(1)-Re(2)-S(3)	92.24(6)
O(1)-Re(1)-S(4)	109.94(17)	S(4)-Re(2)-S(3)	73.49(5)
S(5)-Re(1)-S(4)	140.64(6)	Re(2A)-Re(2)-Re(1A)	104.02(18)
S(6)-Re(1)-S(4)	94.38(6)	O(2)-Re(2)-Re(1A)	72.1(2)
Re(1A)-Re(1)-S(3)	74.9(3)	S(2)-Re(2)-Re(1A)	131.46(12)
O(1)-Re(1)-S(3)	104.29(17)	S(1)-Re(2)-Re(1A)	141.36(12)
S(5)-Re(1)-S(3)	85.42(6)	S(4)-Re(2)-Re(1A)	52.15(14)
S(6)-Re(1)-S(3)	147.95(6)	S(3)-Re(2)-Re(1A)	51.27(12)
S(4)-Re(1)-S(3)	73.66(5)	Re(1)-Re(1A)-S(5)	81.0(3)
Re(2A)-Re(2)-O(12)	170.44(18)	Re(1)-Re(1A)-S(6)	74.0(3)
Re(2A)-Re(2)-S(2)	82.23(12)	S(5)-Re(1A)-S(6)	90.6(3)
O(2)-Re(2)-S(2)	106.95(15)	Re(1)-Re(1A)-S(3)	74.2(3)
Re(2A)-Re(2)-S(1)	64.43(13)	S(5)-Re(1A)-S(3)	89.4(2)
O(2)-Re(2)-S(1)	112.85(17)	S(6)-Re(1A)-S(3)	147.8(4)
S(2)-Re(2)-S(1)	85.29(6)	Re(1)-Re(1A)-S(4)	72.0(3)
Re(2A)-Re(2)-S(4)	73.44(12)	S(5)-Re(1A)-S(4)	150.6(4)

S(6)-Re(1A)-S(4)	92.9(2)	C(19)-S(4)-Re(2)	107.7(2)
S(3)-Re(1A)-S(4)	72.5(2)	Re(1)-S(4)-Re(2)	98.54(6)
Re(1)-Re(1A)-Re(2)	107.3(4)	Re(2A)-S(4)-Re(2)	33.02(7)
S(5)-Re(1A)-Re(2)	132.2(3)	C(19)-S(4)-Re(1A)	111.5(3)
S(6)-Re(1A)-Re(2)	137.2(3)	Re(1)-S(4)-Re(1A)	30.79(19)
S(3)-Re(1A)-Re(2)	51.17(14)	Re(2A)-S(4)-Re(1A)	96.27(18)
S(4)-Re(1A)-Re(2)	50.51(14)	Re(2)-S(4)-Re(1A)	77.34(19)
Re(2)-Re(2A)-S(1)	79.68(15)	C(25)-S(5)-Re(1A)	118.4(3)
Re(2)-Re(2A)-S(3)	79.61(13)	C(25)-S(5)-Re(1)	113.8(2)
S(1)-Re(2A)-S(3)	102.26(13)	Re(1A)-S(5)-Re(1)	33.9(2)
Re(2)-Re(2A)-S(4)	73.54(12)	C(31)-S(6)-Re(1A)	123.7(3)
S(1)-Re(2A)-S(4)	153.02(16)	C(31)-S(6)-Re(1)	110.7(2)
S(3)-Re(2A)-S(4)	76.41(10)	Re(1A)-S(6)-Re(1)	32.56(19)
Re(2)-Re(2A)-S(2)	64.92(11)	C(6)-C(1)-C(2)	119.6(7)
S(1)-Re(2A)-S(2)	84.29(11)	C(6)-C(1)-S(1)	119.1(6)
S(3)-Re(2A)-S(2)	142.29(14)	C(2)-C(1)-S(1)	120.5(6)
S(4)-Re(2A)-S(2)	81.46(9)	C(1)-C(2)-C(3)	120.0(8)
C(1)-S(1)-Re(2A)	104.5(2)	C(1)-C(2)-H(2)	120.0
C(1)-S(1)-Re(2)	115.9(2)	C(3)-C(2)-H(2)	120.0
Re(2A)-S(1)-Re(2)	35.88(8)	C(4)-C(3)-C(2)	119.2(8)
C(12)-S(2)-Re(2)	115.1(2)	C(4)-C(3)-H(3)	120.4
C(12)-S(2)-Re(2A)	109.5(2)	C(2)-C(3)-H(3)	120.4
Re(2)-S(2)-Re(2A)	32.85(7)	C(3)-C(4)-C(5)	121.0(8)
C(13)-S(3)-Re(2A)	127.7(2)	C(3)-C(4)-H(4)	119.5
C(13)-S(3)-Re(1)	116.0(2)	C(5)-C(4)-H(4)	119.5
Re(2A)-S(3)-Re(1)	106.72(9)	C(4)-C(5)-C(6)	120.2(8)
C(13)-S(3)-Re(2)	109.3(2)	C(4)-C(5)-H(5)	119.9
Re(2A)-S(3)-Re(2)	33.65(8)	C(6)-C(5)-H(5)	119.9
Re(1)-S(3)-Re(2)	97.38(5)	C(1)-C(6)-C(5)	119.9(8)
C(13)-S(3)-Re(1A)	100.6(3)	C(1)-C(6)-H(6)	120.0
Re(2A)-S(3)-Re(1A)	100.96(18)	C(5)-C(6)-H(6)	120.0
Re(1)-S(3)-Re(1A)	30.89(19)	C(8)-C(7)-C(12)	118.8(8)
Re(2)-S(3)-Re(1A)	77.56(18)	C(8)-C(7)-H(7)	120.6
C(19)-S(4)-Re(1)	125.3(2)	C(12)-C(7)-H(7)	120.6
C(19)-S(4)-Re(2A)	124.9(2)	C(9)-C(8)-C(7)	121.3(9)
Re(1)-S(4)-Re(2A)	103.11(8)	C(9)-C(8)-H(8)	119.4

C(7)-C(8)-H(8)	119.4	C(21)-C(20)-H(20)	120.5
C(8)-C(9)-C(10)	119.3(8)	C(22)-C(21)-C(20)	121.0(7)
C(8)-C(9)-H(9)	120.4	C(22)-C(21)-H(21)	119.5
C(10)-C(9)-H(9)	120.4	C(20)-C(21)-H(21)	119.5
C(11)-C(10)-C(9)	120.1(8)	C(21)-C(22)-C(23)	121.1(6)
C(11)-C(10)-H(10)	119.9	C(21)-C(22)-H(22)	119.5
C(9)-C(10)-H(10)	119.9	C(23)-C(22)-H(22)	119.5
C(10)-C(11)-C(12)	120.5(8)	C(22)-C(23)-C(24)	118.6(7)
C(10)-C(11)-H(11)	119.8	C(22)-C(23)-H(23)	120.7
C(12)-C(11)-H(11)	119.8	C(24)-C(23)-H(23)	120.7
C(11)-C(12)-C(7)	120.0(7)	C(19)-C(24)-C(23)	118.6(6)
C(11)-C(12)-S(2)	119.4(6)	C(19)-C(24)-H(24)	120.7
C(7)-C(12)-S(2)	120.4(5)	C(23)-C(24)-H(24)	120.7
C(14)-C(13)-C(18)	121.5(6)	C(30)-C(25)-C(26)	119.3(7)
C(14)-C(13)-S(3)	122.2(5)	C(30)-C(25)-S(5)	121.1(6)
C(18)-C(13)-S(3)	116.3(5)	C(26)-C(25)-S(5)	119.1(5)
C(15)-C(14)-C(13)	119.5(6)	C(27)-C(26)-C(25)	119.7(7)
C(15)-C(14)-H(14)	120.2	C(27)-C(26)-H(26)	120.1
C(13)-C(14)-H(14)	120.2	C(25)-C(26)-H(26)	120.1
C(14)-C(15)-C(16)	120.8(8)	C(28)-C(27)-C(26)	120.7(7)
C(14)-C(15)-H(15)	119.6	C(28)-C(27)-H(27)	119.6
C(16)-C(15)-H(15)	119.6	C(26)-C(27)-H(27)	119.6
C(15)-C(16)-C(17)	119.5(7)	C(27)-C(28)-C(29)	120.7(7)
C(15)-C(16)-H(16)	120.3	C(27)-C(28)-H(28)	119.6
C(17)-C(16)-H(16)	120.3	C(29)-C(28)-H(28)	119.6
C(16)-C(17)-C(18)	121.2(7)	C(28)-C(29)-C(30)	118.4(7)
C(16)-C(17)-H(17)	119.4	C(28)-C(29)-H(29)	120.8
C(18)-C(17)-H(17)	119.4	C(30)-C(29)-H(29)	120.8
C(13)-C(18)-C(17)	117.4(7)	C(25)-C(30)-C(29)	121.0(7)
C(13)-C(18)-H(18)	121.3	C(25)-C(30)-H(30)	119.5
C(17)-C(18)-H(18)	121.3	C(29)-C(30)-H(30)	119.5
C(20)-C(19)-C(24)	121.7(6)	C(36)-C(31)-C(32)	119.3(7)
C(20)-C(19)-S(4)	120.8(5)	C(36)-C(31)-S(6)	121.2(5)
C(24)-C(19)-S(4)	117.4(5)	C(32)-C(31)-S(6)	119.0(6)
C(19)-C(20)-C(21)	119.1(6)	C(33)-C(32)-C(31)	119.5(8)
C(19)-C(20)-H(20)	120.5	C(33)-C(32)-H(32)	120.3

C(31)-C(32)-H(32)	120.3
C(34)-C(33)-C(32)	120.1(8)
C(34)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9
C(33)-C(34)-C(35)	120.6(8)
C(33)-C(34)-H(34)	119.7
C(35)-C(34)-H(34)	119.7
C(34)-C(35)-C(36)	120.3(8)
C(34)-C(35)-H(35)	119.9
C(36)-C(35)-H(35)	119.9
C(31)-C(36)-C(35)	120.2(7)
C(31)-C(36)-H(36)	119.9
C(35)-C(36)-H(36)	119.9

Table S-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. 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}
Re(1)	16(1)	21(1)	17(1)	-6(1)	-5(1)	-1(1)
Re(2)	15(1)	18(1)	18(1)	-5(1)	-5(1)	0(1)
Re(1A)	22(3)	49(6)	34(4)	10(3)	-3(3)	-3(3)
Re(2A)	21(1)	32(2)	22(2)	-4(1)	-7(1)	-4(1)
S(1)	34(1)	41(1)	22(1)	-12(1)	-3(1)	-10(1)
S(2)	24(1)	30(1)	24(1)	-9(1)	-10(1)	0(1)
S(3)	18(1)	26(1)	20(1)	-8(1)	-5(1)	0(1)
S(4)	17(1)	28(1)	20(1)	-9(1)	-5(1)	0(1)
S(5)	27(1)	48(1)	22(1)	-8(1)	-11(1)	9(1)
S(6)	30(1)	38(1)	22(1)	0(1)	-5(1)	1(1)
C(1)	36(4)	32(4)	15(3)	-1(3)	-6(3)	-5(3)
C(2)	36(4)	49(5)	29(4)	-21(4)	-10(3)	-2(4)
C(3)	34(4)	68(7)	45(5)	-25(5)	-9(4)	2(4)
C(4)	39(5)	89(8)	40(5)	-1(5)	4(4)	-19(5)
C(5)	51(5)	51(6)	51(6)	5(5)	-14(4)	-18(5)
C(6)	37(4)	33(5)	41(5)	7(4)	-3(4)	-8(4)
C(7)	42(4)	34(5)	27(4)	-6(3)	-10(3)	-8(3)
C(8)	61(6)	57(6)	36(5)	-25(5)	-3(4)	-12(5)
C(9)	73(6)	65(7)	30(5)	-12(5)	-16(4)	-19(5)
C(10)	62(6)	75(7)	26(5)	-1(4)	-27(4)	-5(5)
C(11)	46(5)	40(5)	36(5)	-4(4)	-15(4)	6(4)
C(12)	23(3)	41(5)	20(4)	-6(3)	-7(3)	-6(3)
C(13)	16(3)	30(4)	25(4)	-15(3)	-7(3)	0(3)
C(14)	25(3)	32(4)	32(4)	-11(3)	-14(3)	4(3)
C(15)	39(4)	36(5)	47(5)	-13(4)	-18(4)	11(4)
C(16)	23(4)	55(6)	51(5)	-27(4)	-14(3)	15(4)
C(17)	19(4)	60(6)	49(5)	-21(4)	-10(3)	-2(4)
C(18)	28(4)	38(5)	25(4)	-18(3)	-5(3)	1(3)
C(19)	19(3)	25(4)	19(3)	-12(3)	-7(2)	0(3)
C(20)	14(3)	21(4)	25(4)	-3(3)	-4(3)	1(3)
C(21)	19(3)	25(4)	37(4)	-6(3)	-10(3)	-3(3)

C(22)	30(4)	39(5)	40(5)	-1(4)	-6(3)	-11(4)
C(23)	20(3)	30(4)	42(5)	-9(3)	-7(3)	4(3)
C(24)	24(3)	25(4)	30(4)	-7(3)	-7(3)	-3(3)
C(25)	24(3)	35(4)	21(4)	-7(3)	-8(3)	1(3)
C(26)	42(4)	28(4)	28(4)	-7(3)	-10(3)	-3(3)
C(27)	65(5)	26(4)	27(4)	2(3)	-14(4)	3(4)
C(28)	53(5)	45(5)	23(4)	-4(4)	-19(4)	-1(4)
C(29)	69(6)	40(5)	43(5)	-24(4)	-24(4)	7(4)
C(30)	72(6)	28(5)	34(5)	-7(4)	-25(4)	13(4)
C(31)	25(3)	38(5)	16(3)	1(3)	-10(3)	-2(3)
C(32)	36(4)	54(5)	19(4)	0(4)	-11(3)	-10(4)
C(33)	34(4)	77(7)	30(5)	-10(4)	-3(3)	-11(5)
C(34)	27(4)	80(8)	44(5)	-20(5)	-2(4)	5(4)
C(35)	37(4)	49(5)	39(5)	-24(4)	-8(4)	10(4)
C(36)	30(4)	30(4)	35(4)	-11(3)	-9(3)	-1(3)
O(1)	32(3)	30(3)	36(3)	-14(2)	-7(2)	-6(2)
O(2)	27(2)	32(3)	39(3)	-8(2)	-13(2)	-3(2)

Table S-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(2)	6396	1383	1330	43
H(3)	8377	2100	605	57
H(4)	8689	4067	177	71
H(5)	7079	5330	403	62
H(6)	5101	4633	1048	48
H(7)	2090	144	1936	41
H(8)	2187	-307	363	61
H(9)	1755	1072	-923	65
H(10)	1100	2906	-605	63
H(11)	977	3362	957	49
H(14)	5331	907	3924	34
H(15)	7215	7	3644	47
H(16)	8982	1095	3121	48
H(17)	8865	3103	2780	49
H(18)	6968	4047	3014	35
H(20)	1084	1009	5403	25
H(21)	-849	199	6008	31
H(22)	-2528	1330	6089	45
H(23)	-2359	3338	5519	37
H(24)	-401	4173	4895	31
H(26)	5109	380	7259	39
H(27)	5298	31	8908	48
H(28)	5269	1531	9745	47
H(29)	4959	3420	8978	56
H(30)	4853	3781	7290	51
H(32)	-6	1465	7758	43
H(33)	-1962	2194	8276	57
H(34)	-2302	4168	7977	61
H(35)	-694	5442	7244	49
H(36)	1266	4747	6709	37

Table S-6. Crystal data and structure refinement for **2**.

Empirical formula	C16 H18 O2 Re2 S6	
Formula weight	807.06	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.240(2) Å	α= 90°.
	b = 14.422(2) Å	β= 101.408(4)°.
	c = 8.0202(11) Å	γ = 90°.
Volume	2181.6(5) $Å^3$	
Z	4	
Density (calculated)	2.457 Mg/m^3	
Absorption coefficient	11.671 mm^{-1}	
F(000)	1504	
Crystal size	0.15 x 0.15 x 0.08 mm^3	
Theta range for data collection	2.16 to 28.30°.	
Index ranges	-25<=h<=24, -19<=k<=19, -10<=l<=10	
Reflections collected	10796	
Independent reflections	2704 [R(int) = 0.0592]	
Completeness to theta = 28.30°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.4	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2704 / 0 / 118	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0349, wR2 = 0.0970	
R indices (all data)	R1 = 0.0418, wR2 = 0.1065	
Largest diff. peak and hole	2.531 and -1.389 $e.Å^{-3}$	

$R1 = \Sigma \, | \, |F_o| - |F_c| \, | \, / \, \Sigma \, |F_o|$ and $wR2 = \{ \, \Sigma \, [\, w(F_o^2 - F_c^2)^2 \,] \, / \, \Sigma \, [\, w(F_o^2)^2 \,] \, \}^{1/2}$

Table S-7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) For **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	5816(1)	3473(1)	1903(1)	34(1)
S(1)	5582(1)	2238(1)	107(2)	49(1)
S(2)	6521(1)	2553(1)	3830(2)	44(1)
S(3)	5377(1)	4009(1)	4264(2)	40(1)
C(1)	6158(3)	1279(5)	665(8)	41(1)
C(2)	6863(4)	1297(6)	535(10)	54(2)
C(3)	7274(4)	488(6)	873(10)	61(2)
C(4)	6980(5)	-300(6)	1296(11)	62(2)
C(5)	6283(5)	-322(6)	1429(11)	67(2)
C(6)	5871(4)	472(5)	1125(10)	52(2)
C(7)	6608(4)	3200(6)	5825(9)	53(2)
C(8)	5890(4)	3447(5)	6163(10)	51(2)
O(1)	6341(3)	4257(4)	1201(7)	59(1)

Table S-8. Bond lengths [Å] and angles [°] for **2**.

Re(1)-O(1)	1.686(5)	S(3)-Re(1)#1	2.4258(14)
Re(1)-S(2)	2.2729(15)	C(1)-C(6)	1.369(10)
Re(1)-S(1)	2.2790(17)	C(1)-C(2)	1.382(9)
Re(1)-S(3)	2.3514(15)	C(2)-C(3)	1.405(11)
Re(1)-S(3)#1	2.4258(14)	C(3)-C(4)	1.343(13)
S(1)-C(1)	1.774(7)	C(4)-C(5)	1.366(12)
S(2)-C(7)	1.831(7)	C(5)-C(6)	1.386(11)
S(3)-C(8)	1.832(8)	C(7)-C(8)	1.503(11)

O(1)-Re(1)-S(2)	107.57(18)
O(1)-Re(1)-S(1)	111.7(2)
S(2)-Re(1)-S(1)	89.41(6)
O(1)-Re(1)-S(3)	112.5(2)
S(2)-Re(1)-S(3)	84.59(6)
S(1)-Re(1)-S(3)	135.11(6)
O(1)-Re(1)-S(3)#1	103.95(18)
S(2)-Re(1)-S(3)#1	147.21(6)
S(1)-Re(1)-S(3)#1	87.24(6)
S(3)-Re(1)-S(3)#1	75.14(6)
C(1)-S(1)-Re(1)	114.5(2)
C(7)-S(2)-Re(1)	103.6(3)
C(8)-S(3)-Re(1)	107.7(3)
C(8)-S(3)-Re(1)#1	119.5(3)
Re(1)-S(3)-Re(1)#1	92.71(5)
C(6)-C(1)-C(2)	119.3(7)
C(6)-C(1)-S(1)	117.8(5)
C(2)-C(1)-S(1)	122.7(6)
C(1)-C(2)-C(3)	119.5(8)
C(4)-C(3)-C(2)	120.2(7)
C(3)-C(4)-C(5)	120.5(8)
C(4)-C(5)-C(6)	120.2(8)
C(1)-C(6)-C(5)	120.2(7)
C(8)-C(7)-S(2)	110.5(5)
C(7)-C(8)-S(3)	108.6(6)

Symmetry transformations used to generate equivalent atoms:

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

Table S-9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. 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}
Re(1)	31(1)	32(1)	41(1)	5(1)	8(1)	0(1)
S(1)	53(1)	49(1)	42(1)	-5(1)	0(1)	11(1)

S(2)	45(1)	43(1)	41(1)	-1(1)	1(1)	12(1)
S(3)	35(1)	35(1)	48(1)	-11(1)	5(1)	-1(1)
C(1)	41(3)	43(3)	37(3)	-9(2)	6(2)	7(3)
C(2)	49(4)	56(4)	59(4)	-7(3)	16(3)	-3(3)
C(3)	45(4)	78(6)	60(4)	-19(4)	8(3)	12(3)
C(4)	65(5)	53(5)	65(5)	-7(3)	6(4)	16(4)
C(5)	76(6)	55(5)	68(5)	8(4)	12(4)	1(4)
C(6)	46(4)	55(4)	54(4)	0(3)	10(3)	-1(3)
C(7)	43(4)	63(4)	48(4)	-8(3)	-3(3)	1(3)
C(8)	48(4)	57(5)	44(4)	-9(3)	0(3)	-3(3)
O(1)	46(3)	52(3)	82(4)	17(3)	20(2)	-5(2)

Table S-10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2**.

	x	y	z	U(eq)
H(2)	7065	1840	225	65
H(3)	7751	499	805	73
H(4)	7253	-836	1500	74
H(5)	6085	-871	1723	80
H(6)	5399	456	1235	62
H(7A)	6862	2827	6756	64
H(7B)	6878	3762	5758	64
H(8A)	5940	3864	7129	61
H(8B)	5647	2892	6425	61

Table S-11. Crystal data and structure refinement for **4**.

Empirical formula	C26 H22 O2 Re2 S6	
Formula weight	931.20	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 28.735(8) Å	α= 90°.
	b = 8.509(2) Å	β= 99.344(8)°.
	c = 23.838(6) Å	γ = 90°.
Volume	5751(3) $Å^3$	
Z	8	
Density (calculated)	2.151 Mg/m^3	
Absorption coefficient	8.871 mm^{-1}	
F(000)	3520	
Crystal size	0.50 x 0.15 x 0.15 mm^3	
Theta range for data collection	1.73 to 28.25°.	
Index ranges	-34<=h<=37, -11<=k<=11, -31<=l<=31	
Reflections collected	20696	
Independent reflections	6403 [R(int) = 0.0688]	
Completeness to theta = 28.25°	90.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.55	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6403 / 0 / 325	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0455, wR2 = 0.1022	
R indices (all data)	R1 = 0.0773, wR2 = 0.1160	
Largest diff. peak and hole	2.504 and -1.880 $e.Å^{-3}$	

$R1 = \Sigma \, | \, |F_o| - |F_c| \, | \, / \, \Sigma \, |F_o|$ and $wR2 = \{ \, \Sigma \, [\, w(F_o^2 - F_c^2)^2 \,] \, / \, \Sigma \, [\, w(F_o^2)^2 \,] \, \}^{1/2}$

Table S-12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	854(1)	3579(1)	4170(1)	27(1)
Re(2)	852(1)	1855(1)	2771(1)	28(1)
S(1)	625(1)	4235(2)	3176(1)	35(1)
S(2)	1450(1)	5373(3)	4195(1)	38(1)
S(3)	1331(1)	2221(2)	4880(1)	37(1)
S(4)	641(1)	1180(2)	3686(1)	34(1)
S(5)	1460(1)	110(3)	2973(1)	42(1)
S(6)	1313(1)	3274(3)	2243(1)	43(1)
C(1)	920(4)	5951(10)	2908(4)	44(3)
C(2)	786(4)	6000(10)	2296(4)	35(2)
C(3)	491(4)	7199(10)	2041(5)	45(3)
C(4)	371(4)	7281(12)	1455(5)	50(3)
C(5)	540(4)	6144(12)	1120(4)	52(3)
C(6)	823(4)	4964(11)	1373(4)	46(3)
C(7)	949(3)	4861(9)	1949(4)	37(2)
C(8)	1838(3)	5439(10)	4865(4)	35(2)
C(9)	1699(4)	6239(13)	5300(5)	59(3)
C(10)	2003(5)	6431(16)	5816(6)	76(4)
C(11)	2441(5)	5824(18)	5882(7)	76(4)
C(12)	2573(5)	5040(20)	5447(8)	112(7)
C(13)	2279(4)	4827(18)	4917(7)	83(5)
C(14)	1004(3)	552(9)	5048(4)	32(2)
C(15)	917(4)	387(10)	5591(4)	44(3)
C(16)	647(4)	-841(12)	5750(5)	58(3)
C(17)	465(4)	-1914(12)	5347(5)	55(3)
C(18)	549(4)	-1812(10)	4798(5)	45(3)
C(19)	827(3)	-602(9)	4645(4)	30(2)
C(20)	956(4)	-482(10)	4063(4)	40(2)
C(21)	1860(4)	193(11)	2479(5)	44(3)
C(22)	1759(4)	-627(15)	1966(5)	63(3)
C(23)	2079(6)	-669(19)	1600(7)	88(5)

C(24)	2492(5)	154(15)	1731(6)	66(4)
C(25)	2602(5)	917(15)	2218(7)	73(4)
C(26)	2287(4)	916(12)	2611(6)	61(3)
O(1)	422(2)	4373(6)	4480(3)	39(2)
O(2)	432(2)	1045(7)	2284(3)	42(2)

Table S-13. Bond lengths [Å] and angles [°] for **4**.

Re(1)-O(1)	1.685(6)	C(5)-C(6)	1.368(14)
Re(1)-S(2)	2.288(2)	C(6)-C(7)	1.365(14)
Re(1)-S(3)	2.309(2)	C(8)-C(9)	1.355(15)
Re(1)-S(4)	2.375(2)	C(8)-C(13)	1.357(14)
Re(1)-S(1)	2.419(2)	C(9)-C(10)	1.397(15)
Re(2)-O(2)	1.681(6)	C(10)-C(11)	1.345(19)
Re(2)-S(5)	2.283(2)	C(11)-C(12)	1.34(2)
Re(2)-S(6)	2.310(3)	C(12)-C(13)	1.412(18)
Re(2)-S(1)	2.379(2)	C(14)-C(15)	1.364(13)
Re(2)-S(4)	2.425(2)	C(14)-C(19)	1.409(12)
S(1)-C(1)	1.853(9)	C(15)-C(16)	1.390(14)
S(2)-C(8)	1.794(9)	C(16)-C(17)	1.366(16)
S(3)-C(14)	1.784(9)	C(17)-C(18)	1.371(16)
S(4)-C(20)	1.833(9)	C(18)-C(19)	1.387(13)
S(5)-C(21)	1.775(11)	C(19)-C(20)	1.498(13)
S(6)-C(7)	1.781(9)	C(21)-C(26)	1.364(14)
C(1)-C(2)	1.449(13)	C(21)-C(22)	1.397(16)
C(2)-C(3)	1.401(13)	C(22)-C(23)	1.37(2)
C(2)-C(7)	1.403(13)	C(23)-C(24)	1.369(19)
C(3)-C(4)	1.385(15)	C(24)-C(25)	1.321(19)
C(4)-C(5)	1.390(16)	C(25)-C(26)	1.404(19)

O(1)-Re(1)-S(2)	108.8(2)	S(2)-Re(1)-S(4)	135.96(9)
O(1)-Re(1)-S(3)	105.7(2)	S(3)-Re(1)-S(4)	90.09(8)
S(2)-Re(1)-S(3)	87.82(8)	O(1)-Re(1)-S(1)	103.6(2)
O(1)-Re(1)-S(4)	114.1(2)	S(2)-Re(1)-S(1)	87.42(8)

S(3)-Re(1)-S(1)	150.33(9)	C(8)-C(9)-C(10)	120.9(12)
S(4)-Re(1)-S(1)	73.46(7)	C(11)-C(10)-C(9)	119.8(14)
O(2)-Re(2)-S(5)	108.5(2)	C(12)-C(11)-C(10)	118.6(14)
O(2)-Re(2)-S(6)	104.4(3)	C(11)-C(12)-C(13)	123.7(14)
S(5)-Re(2)-S(6)	88.16(9)	C(8)-C(13)-C(12)	116.5(13)
O(2)-Re(2)-S(1)	114.6(2)	C(15)-C(14)-C(19)	118.2(8)
S(5)-Re(2)-S(1)	135.96(9)	C(15)-C(14)-S(3)	118.6(7)
S(6)-Re(2)-S(1)	89.72(9)	C(19)-C(14)-S(3)	123.2(7)
O(2)-Re(2)-S(4)	105.5(3)	C(14)-C(15)-C(16)	122.2(10)
S(5)-Re(2)-S(4)	87.19(9)	C(17)-C(16)-C(15)	118.5(11)
S(6)-Re(2)-S(4)	149.62(9)	C(16)-C(17)-C(18)	121.5(10)
S(1)-Re(2)-S(4)	73.27(8)	C(17)-C(18)-C(19)	119.7(10)
C(1)-S(1)-Re(2)	111.1(3)	C(18)-C(19)-C(14)	119.9(9)
C(1)-S(1)-Re(1)	116.9(3)	C(18)-C(19)-C(20)	122.2(9)
Re(2)-S(1)-Re(1)	98.73(8)	C(14)-C(19)-C(20)	117.9(8)
C(8)-S(2)-Re(1)	113.5(3)	C(19)-C(20)-S(4)	109.3(6)
C(14)-S(3)-Re(1)	106.9(3)	C(26)-C(21)-C(22)	118.5(12)
C(20)-S(4)-Re(1)	111.0(3)	C(26)-C(21)-S(5)	121.4(10)
C(20)-S(4)-Re(2)	116.6(3)	C(22)-C(21)-S(5)	119.8(9)
Re(1)-S(4)-Re(2)	98.67(8)	C(23)-C(22)-C(21)	120.5(13)
C(21)-S(5)-Re(2)	113.0(3)	C(22)-C(23)-C(24)	119.3(14)
C(7)-S(6)-Re(2)	105.0(4)	C(25)-C(24)-C(23)	121.7(14)
C(2)-C(1)-S(1)	107.9(6)	C(24)-C(25)-C(26)	119.9(13)
C(3)-C(2)-C(7)	118.9(9)	C(21)-C(26)-C(25)	119.9(14)
C(3)-C(2)-C(1)	120.1(9)		
C(7)-C(2)-C(1)	121.0(9)		
C(4)-C(3)-C(2)	120.5(10)		
C(3)-C(4)-C(5)	119.4(9)		
C(6)-C(5)-C(4)	119.7(10)		
C(7)-C(6)-C(5)	122.1(10)		
C(6)-C(7)-C(2)	119.3(9)		
C(6)-C(7)-S(6)	119.2(8)		
C(2)-C(7)-S(6)	121.5(8)		
C(9)-C(8)-C(13)	120.6(10)		
C(9)-C(8)-S(2)	118.7(8)		
C(13)-C(8)-S(2)	120.4(9)		

Table S-14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4.** 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}
Re(1)	30(1)	24(1)	26(1)	-1(1)	4(1)	-1(1)
Re(2)	29(1)	27(1)	27(1)	-1(1)	1(1)	-1(1)
S(1)	47(2)	28(1)	30(1)	0(1)	4(1)	1(1)
S(2)	44(2)	39(1)	30(1)	2(1)	4(1)	-10(1)
S(3)	41(2)	34(1)	33(1)	2(1)	-3(1)	-6(1)
S(4)	44(2)	27(1)	29(1)	-1(1)	2(1)	-4(1)
S(5)	40(2)	43(1)	44(2)	8(1)	9(1)	9(1)
S(6)	41(2)	40(1)	48(2)	7(1)	13(1)	3(1)
C(1)	67(8)	28(4)	36(6)	-5(4)	11(5)	-11(4)
C(2)	52(6)	39(4)	16(5)	2(3)	11(4)	-7(4)
C(3)	51(7)	33(5)	52(7)	2(4)	13(6)	-5(4)
C(4)	39(6)	45(6)	64(8)	19(5)	2(6)	-1(4)
C(5)	78(9)	62(7)	13(5)	9(4)	2(5)	-2(6)
C(6)	59(7)	46(5)	32(6)	-6(4)	6(5)	-6(5)
C(7)	42(6)	21(4)	45(6)	-2(3)	-1(5)	-3(3)
C(8)	34(6)	39(5)	31(6)	-4(4)	1(4)	-8(4)
C(9)	48(7)	84(8)	42(7)	-10(6)	-4(6)	10(6)
C(10)	58(9)	121(11)	43(8)	-24(7)	-7(7)	5(8)
C(11)	51(9)	106(11)	63(10)	15(8)	-16(8)	-2(7)
C(12)	33(8)	200(19)	92(14)	-42(13)	-24(9)	26(10)
C(13)	27(7)	136(12)	81(11)	-41(9)	-2(7)	16(7)
C(14)	27(5)	31(4)	38(6)	10(4)	4(4)	1(3)
C(15)	70(8)	36(5)	31(6)	1(4)	23(5)	6(5)
C(16)	83(9)	55(6)	39(7)	15(5)	22(7)	0(6)
C(17)	54(7)	45(5)	68(9)	37(5)	17(6)	1(5)
C(18)	39(6)	38(5)	55(8)	6(4)	-6(5)	0(4)
C(19)	39(5)	28(4)	27(5)	5(3)	12(4)	4(3)
C(20)	56(7)	32(4)	33(6)	-3(4)	10(5)	4(4)
C(21)	37(6)	45(5)	52(7)	14(4)	14(5)	15(4)
C(22)	38(7)	103(10)	51(8)	-3(7)	12(6)	17(6)
C(23)	71(11)	124(13)	73(11)	-20(9)	21(9)	8(9)

C(24)	59(9)	78(8)	70(10)	1(7)	36(8)	15(7)
C(25)	48(8)	71(8)	110(14)	5(8)	38(8)	-1(6)
C(26)	44(7)	49(6)	92(11)	12(6)	20(7)	-6(5)
O(1)	32(4)	35(3)	54(5)	-8(3)	15(3)	4(3)
O(2)	41(4)	47(4)	34(4)	-3(3)	-7(3)	-7(3)

Table S-15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(1A)	823	6912	3076	52
H(1B)	1260	5852	3009	52
H(3)	374	7946	2266	54
H(4)	180	8089	1286	60
H(5)	462	6186	727	62
H(6)	932	4207	1145	55
H(9)	1398	6667	5255	71
H(10)	1903	6977	6113	91
H(11)	2647	5944	6222	91
H(12)	2875	4622	5495	135
H(13)	2382	4292	4620	99
H(15)	1043	1119	5863	53
H(16)	591	-929	6122	69
H(17)	281	-2733	5447	66
H(18)	420	-2550	4529	54
H(20A)	871	-1447	3854	48
H(20B)	1293	-330	4091	48
H(22)	1473	-1147	1872	76
H(23)	2018	-1251	1266	106
H(24)	2701	176	1472	79
H(25)	2886	1455	2299	88
H(26)	2370	1408	2962	73

Table S-16. Crystal data and structure refinement for **5**.

Empirical formula	C24 H18 O2 Re2 S6	
Formula weight	903.14	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.4847(19) Å	α= 88.154(4)°.
	b = 9.689(2) Å	β= 89.503(4)°.
	c = 15.028(3) Å	γ = 72.307(3)°.
Volume	1315.0(5) $Å^3$	
Z	2	
Density (calculated)	2.281 Mg/m^3	
Absorption coefficient	9.695 mm^{-1}	
F(000)	848	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.36 to 26.33°.	
Index ranges	-11<=h<=11, -12<=k<=10, -17<=l<=18	
Reflections collected	9731	
Independent reflections	5282 [R(int) = 0.0351]	
Completeness to theta = 26.33°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.46	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5282 / 0 / 307	
Goodness-of-fit on F^2	0.991	
Final R indices [I>2sigma(I)]	R1 = 0.0411, wR2 = 0.0961	
R indices (all data)	R1 = 0.0613, wR2 = 0.1073	
Largest diff. peak and hole	3.280 and -1.982 $e.Å^{-3}$	

$$R1 = \Sigma \, | \, |F_O| - |F_c| \, | \, / \, \Sigma \, |F_o| \quad \text{and} \quad wR2 = \{ \, \Sigma \, [\, w(F_o^2 - F_c^2)^2 \,] \, / \, \Sigma \, [\, w(F_o^2)^2 \,] \, \}^{1/2}$$

Table S-17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For **5**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	8114(1)	4829(1)	3505(1)	27(1)
Re(2)	8854(1)	6413(1)	1581(1)	27(1)
C(1)	8596(11)	2771(10)	5279(6)	36(2)
C(2)	8876(12)	1536(11)	5835(7)	44(2)
C(3)	8308(13)	1647(13)	6696(7)	52(3)
C(4)	7450(13)	2975(12)	6997(7)	50(3)
C(5)	7201(12)	4211(12)	6456(7)	47(3)
C(6)	7771(11)	4094(10)	5620(6)	39(2)
C(7)	10542(9)	2593(9)	2016(6)	29(2)
C(8)	9477(10)	1935(10)	1848(7)	37(2)
C(9)	9865(12)	649(11)	1395(7)	45(2)
C(10)	11333(13)	-4(11)	1144(7)	48(3)
C(11)	12390(13)	637(12)	1350(8)	54(3)
C(12)	12024(10)	1926(10)	1779(7)	39(2)
C(13)	6949(9)	8680(9)	3362(6)	29(2)
C(14)	5561(11)	8609(11)	3560(7)	46(3)
C(15)	4477(12)	9862(12)	3780(8)	53(3)
C(16)	4797(13)	11136(13)	3786(9)	59(3)
C(17)	6186(13)	11215(11)	3583(9)	56(3)
C(18)	7280(11)	9954(10)	3361(7)	45(3)
C(19)	6832(10)	5870(10)	-15(6)	33(2)
C(20)	6413(11)	5291(11)	-756(7)	40(2)
C(21)	5202(12)	6097(13)	-1257(8)	55(3)
C(22)	4455(11)	7491(13)	-1013(7)	48(3)
C(23)	4841(11)	8050(11)	-286(7)	44(2)
C(24)	6050(10)	7246(10)	244(6)	31(2)
O(1)	6628(7)	4690(7)	2971(4)	40(2)
O(2)	10114(7)	7124(7)	1141(4)	39(2)
S(1)	9302(3)	2683(2)	4200(2)	36(1)
S(2)	7464(3)	5649(3)	4891(2)	42(1)
S(3)	10150(2)	4330(2)	2490(2)	30(1)

S(4)	8444(2)	7105(2)	3099(2)	30(1)
S(5)	8364(2)	4859(2)	629(2)	32(1)
S(6)	6555(3)	7917(3)	1227(2)	37(1)

Table S-18. Bond lengths [Å] and angles [°] for **5**.

Re(1)-O(1)	1.670(6)	C(5)-H(5)	0.9400	C(15)-H(15)	0.9400
Re(1)-S(2)	2.267(2)	C(6)-S(2)	1.785(10)	C(16)-C(17)	1.374(16)
Re(1)-S(1)	2.267(2)	C(7)-C(8)	1.377(12)	C(16)-H(16)	0.9400
Re(1)-S(4)	2.380(2)	C(7)-C(12)	1.405(12)	C(17)-C(18)	1.389(13)
Re(1)-S(3)	2.392(2)	C(7)-S(3)	1.780(9)	C(17)-H(17)	0.9400
Re(2)-O(2)	1.672(6)	C(8)-C(9)	1.387(13)	C(18)-H(18)	0.9400
Re(2)-S(5)	2.260(2)	C(8)-H(8)	0.9400	C(19)-C(20)	1.378(12)
Re(2)-S(6)	2.281(2)	C(9)-C(10)	1.397(15)	C(19)-C(24)	1.380(12)
Re(2)-S(4)	2.394(2)	C(9)-H(9)	0.9400	C(19)-S(5)	1.762(9)
Re(2)-S(3)	2.407(2)	C(10)-C(11)	1.372(16)	C(20)-C(21)	1.388(14)
C(1)-C(6)	1.395(13)	C(10)-H(10)	0.9400	C(20)-H(20)	0.9400
C(1)-C(2)	1.395(13)	C(11)-C(12)	1.371(14)	C(21)-C(22)	1.381(15)
C(1)-S(1)	1.743(9)	C(11)-H(11)	0.9400	C(21)-H(21)	0.9400
C(2)-C(3)	1.392(15)	C(12)-H(12)	0.9400	C(22)-C(23)	1.335(14)
C(2)-H(2)	0.9400	C(13)-C(18)	1.364(12)	C(22)-H(22)	0.9400
C(3)-C(4)	1.385(15)	C(13)-C(14)	1.368(13)	C(23)-C(24)	1.410(13)
C(3)-H(3)	0.9400	C(13)-S(4)	1.791(8)	C(23)-H(23)	0.9400
C(4)-C(5)	1.385(15)	C(14)-C(15)	1.379(13)	C(24)-S(6)	1.760(9)
C(4)-H(4)	0.9400	C(14)-H(14)	0.9400		
C(5)-C(6)	1.358(13)	C(15)-C(16)	1.359(15)		
O(1)-Re(1)-S(2)	109.7(2)	S(1)-Re(1)-S(3)	86.93(8)	O(2)-Re(2)-S(3)	107.7(2)
O(1)-Re(1)-S(1)	109.7(2)	S(4)-Re(1)-S(3)	73.63(7)	S(5)-Re(2)-S(3)	87.45(8)
S(2)-Re(1)-S(1)	85.61(9)	O(2)-Re(2)-S(5)	110.1(2)	S(6)-Re(2)-S(3)	143.25(9)
O(1)-Re(1)-S(4)	108.4(2)	O(2)-Re(2)-S(6)	108.5(2)	S(4)-Re(2)-S(3)	73.12(7)
S(2)-Re(1)-S(4)	89.00(8)	S(5)-Re(2)-S(6)	85.97(8)	C(6)-C(1)-C(2)	118.0(9)
S(1)-Re(1)-S(4)	141.10(8)	O(2)-Re(2)-S(4)	108.8(2)	C(6)-C(1)-S(1)	120.6(7)
O(1)-Re(1)-S(3)	108.7(2)	S(5)-Re(2)-S(4)	140.21(8)	C(2)-C(1)-S(1)	121.3(8)
S(2)-Re(1)-S(3)	141.18(9)	S(6)-Re(2)-S(4)	89.49(8)	C(3)-C(2)-C(1)	119.9(10)

C(3)-C(2)-H(2)	120.1	C(13)-C(14)-H(14)	120.6	Re(1)-S(3)-Re(2)	90.14(7)
C(1)-C(2)-H(2)	120.1	C(15)-C(14)-H(14)	120.6	C(13)-S(4)-Re(1)	116.2(3)
C(4)-C(3)-C(2)	120.2(10)	C(16)-C(15)-C(14)	119.7(11)	C(13)-S(4)-Re(2)	119.3(3)
C(4)-C(3)-H(3)	119.9	C(16)-C(15)-H(15)	120.1	Re(1)-S(4)-Re(2)	90.73(7)
C(2)-C(3)-H(3)	119.9	C(14)-C(15)-H(15)	120.1	C(19)-S(5)-Re(2)	106.6(3)
C(3)-C(4)-C(5)	120.2(10)	C(15)-C(16)-C(17)	121.7(11)	C(24)-S(6)-Re(2)	105.5(3)
C(3)-C(4)-H(4)	119.9	C(15)-C(16)-H(16)	119.1		
C(5)-C(4)-H(4)	119.9	C(17)-C(16)-H(16)	119.1		
C(6)-C(5)-C(4)	119.2(10)	C(16)-C(17)-C(18)	118.6(10)		
C(6)-C(5)-H(5)	120.4	C(16)-C(17)-H(17)	120.7		
C(4)-C(5)-H(5)	120.4	C(18)-C(17)-H(17)	120.7		
C(5)-C(6)-C(1)	122.5(9)	C(13)-C(18)-C(17)	119.2(10)		
C(5)-C(6)-S(2)	121.0(8)	C(13)-C(18)-H(18)	120.4		
C(1)-C(6)-S(2)	116.5(7)	C(17)-C(18)-H(18)	120.4		
C(8)-C(7)-C(12)	120.4(8)	C(20)-C(19)-C(24)	120.7(9)		
C(8)-C(7)-S(3)	123.6(7)	C(20)-C(19)-S(5)	120.6(7)		
C(12)-C(7)-S(3)	116.0(7)	C(24)-C(19)-S(5)	118.8(7)		
C(7)-C(8)-C(9)	119.3(9)	C(19)-C(20)-C(21)	120.1(10)		
C(7)-C(8)-H(8)	120.3	C(19)-C(20)-H(20)	120.0		
C(9)-C(8)-H(8)	120.3	C(21)-C(20)-H(20)	120.0		
C(8)-C(9)-C(10)	120.3(10)	C(22)-C(21)-C(20)	119.0(10)		
C(8)-C(9)-H(9)	119.8	C(22)-C(21)-H(21)	120.5		
C(10)-C(9)-H(9)	119.8	C(20)-C(21)-H(21)	120.5		
C(11)-C(10)-C(9)	119.5(10)	C(23)-C(22)-C(21)	121.2(10)		
C(11)-C(10)-H(10)	120.3	C(23)-C(22)-H(22)	119.4		
C(9)-C(10)-H(10)	120.3	C(21)-C(22)-H(22)	119.4		
C(12)-C(11)-C(10)	121.1(10)	C(22)-C(23)-C(24)	121.0(10)		
C(12)-C(11)-H(11)	119.4	C(22)-C(23)-H(23)	119.5		
C(10)-C(11)-H(11)	119.4	C(24)-C(23)-H(23)	119.5		
C(11)-C(12)-C(7)	119.3(10)	C(19)-C(24)-C(23)	118.1(8)		
C(11)-C(12)-H(12)	120.4	C(19)-C(24)-S(6)	119.5(7)		
C(7)-C(12)-H(12)	120.4	C(23)-C(24)-S(6)	122.4(7)		
C(18)-C(13)-C(14)	121.9(9)	C(1)-S(1)-Re(1)	106.4(3)		
C(18)-C(13)-S(4)	116.0(7)	C(6)-S(2)-Re(1)	107.0(3)		
C(14)-C(13)-S(4)	122.2(7)	C(7)-S(3)-Re(1)	112.8(3)		
C(13)-C(14)-C(15)	118.8(10)	C(7)-S(3)-Re(2)	117.7(3)		

Table S-19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. 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}
Re(1)	32(1)	24(1)	25(1)	-8(1)	5(1)	-8(1)
Re(2)	30(1)	24(1)	27(1)	-8(1)	8(1)	-9(1)
C(1)	50(6)	45(5)	16(4)	-9(4)	5(4)	-17(5)
C(2)	53(6)	47(6)	32(5)	0(5)	5(5)	-16(5)
C(3)	66(7)	56(7)	37(6)	4(5)	2(5)	-25(6)
C(4)	65(7)	63(7)	31(6)	-9(5)	12(5)	-33(6)
C(5)	61(7)	49(6)	32(6)	-16(5)	16(5)	-18(5)
C(6)	49(6)	38(5)	30(5)	-3(4)	-2(4)	-13(5)
C(7)	32(5)	26(4)	30(5)	-3(4)	6(4)	-8(4)
C(8)	34(5)	33(5)	45(6)	-16(4)	3(4)	-10(4)
C(9)	65(7)	45(6)	33(5)	-6(4)	2(5)	-26(5)
C(10)	71(8)	35(6)	36(6)	-9(4)	20(5)	-14(5)
C(11)	48(6)	43(6)	68(8)	-10(6)	27(6)	-8(5)
C(12)	36(5)	34(5)	46(6)	-10(4)	26(4)	-6(4)
C(13)	34(5)	25(4)	26(5)	-11(4)	7(4)	-6(4)
C(14)	48(6)	34(5)	57(7)	-16(5)	17(5)	-12(5)
C(15)	46(6)	51(7)	61(8)	-14(6)	15(5)	-13(5)
C(16)	52(7)	47(7)	70(9)	-24(6)	5(6)	0(6)
C(17)	61(7)	27(5)	81(9)	-10(5)	-4(6)	-12(5)
C(18)	47(6)	23(5)	64(7)	0(5)	6(5)	-10(4)
C(19)	34(5)	41(5)	29(5)	-7(4)	12(4)	-20(4)
C(20)	39(5)	42(6)	42(6)	-11(4)	2(4)	-17(4)
C(21)	47(6)	75(8)	50(7)	-6(6)	-11(5)	-28(6)
C(22)	34(5)	67(7)	41(6)	-2(5)	-11(5)	-12(5)
C(23)	39(6)	52(6)	39(6)	-6(5)	14(4)	-10(5)
C(24)	37(5)	40(5)	19(4)	-4(4)	13(4)	-15(4)
O(1)	40(4)	44(4)	37(4)	-7(3)	7(3)	-14(3)
O(2)	46(4)	35(4)	42(4)	-1(3)	13(3)	-20(3)
S(1)	45(1)	29(1)	30(1)	-6(1)	6(1)	-6(1)
S(2)	63(2)	31(1)	32(1)	-12(1)	12(1)	-11(1)
S(3)	32(1)	26(1)	32(1)	-9(1)	6(1)	-9(1)

S(4)	37(1)	25(1)	27(1)	-11(1)	6(1)	-7(1)
S(5)	37(1)	30(1)	29(1)	-10(1)	6(1)	-9(1)
S(6)	39(1)	33(1)	32(1)	-10(1)	4(1)	-2(1)

Table S-20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **5**.

	x	y	z	U(eq)
H(2)	9447	632	5629	53
H(3)	8507	818	7074	62
H(4)	7035	3039	7571	60
H(5)	6644	5119	6665	56
H(8)	8497	2353	2038	44
H(9)	9136	214	1256	54
H(10)	11594	-876	837	57
H(11)	13381	185	1195	65
H(12)	12756	2359	1912	47
H(14)	5351	7723	3547	55
H(15)	3520	9834	3925	63
H(16)	4049	11986	3933	71
H(17)	6392	12104	3594	68
H(18)	8237	9980	3212	54
H(20)	6947	4349	-923	48
H(21)	4896	5700	-1756	66
H(22)	3661	8057	-1363	57
H(23)	4300	8993	-126	53

Table S-21. Crystal data and structure refinement for **6**.

Empirical formula	C10 H13 O Re S4	
Formula weight	463.64	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.161(2) Å	α= 90°.
	b = 14.542(4) Å	β= 92.611(5)°.
	c = 10.279(3) Å	γ = 90°.
Volume	1368.0(6) $Å^3$	
Z	4	
Density (calculated)	2.251 Mg/m^3	
Absorption coefficient	9.469 mm^{-1}	
F(000)	880	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.23 to 26.37°.	
Index ranges	-11<=h<=11, -18<=k<=18, -12<=l<=12	
Reflections collected	11106	
Independent reflections	2804 [R(int) = 0.0848]	
Completeness to theta = 26.37°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.45	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2804 / 0 / 145	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0421, wR2 = 0.0982	
R indices (all data)	R1 = 0.0565, wR2 = 0.1072	
Largest diff. peak and hole	3.203 and -1.014 $e.Å^{-3}$	

$R1 = \Sigma \, | \, |F_o| - |F_c| \, | \, / \, \Sigma \, |F_o|$ and $wR2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$

Table S-22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	3812(1)	5866(1)	2368(1)	33(1)
S(1)	4442(3)	4392(2)	2891(3)	51(1)
S(2)	3783(3)	6572(2)	382(2)	51(1)
S(3)	6361(2)	6106(2)	2358(2)	49(1)
S(4)	1594(2)	5310(1)	1540(2)	41(1)
C(1)	6367(12)	4398(9)	3369(13)	75(3)
C(2)	7212(11)	4993(7)	2475(12)	65(3)
C(3)	6773(11)	6489(6)	749(10)	55(2)
C(4)	5561(11)	7096(6)	233(11)	62(3)
C(5)	965(9)	4355(6)	2449(8)	37(2)
C(6)	1030(11)	4346(6)	3796(9)	49(2)
C(7)	393(11)	3634(7)	4429(10)	60(3)
C(8)	-291(10)	2938(6)	3777(11)	56(2)
C(9)	-361(11)	2946(6)	2439(11)	59(3)
C(10)	266(10)	3643(6)	1762(9)	50(2)
O(1)	3383(8)	6539(4)	3614(6)	57(2)

Table S-23. Bond lengths [Å] and angles [°] for **6**.

Re(1)-O(1)	1.672(6)	S(4)-C(5)	1.783(8)
Re(1)-S(1)	2.278(2)	C(1)-C(2)	1.502(16)
Re(1)-S(2)	2.284(2)	C(3)-C(4)	1.497(13)
Re(1)-S(4)	2.313(2)	C(5)-C(6)	1.383(12)
Re(1)-S(3)	2.362(2)	C(5)-C(10)	1.393(11)
S(1)-C(1)	1.809(12)	C(6)-C(7)	1.367(13)
S(2)-C(4)	1.811(10)	C(7)-C(8)	1.352(13)
S(3)-C(2)	1.799(10)	C(8)-C(9)	1.374(14)
S(3)-C(3)	1.802(10)	C(9)-C(10)	1.370(13)
O(1)-Re(1)-S(1)	115.9(2)	C(8)-C(7)-C(6)	122.0(10)
O(1)-Re(1)-S(2)	115.3(3)	C(7)-C(8)-C(9)	119.2(9)
S(1)-Re(1)-S(2)	128.77(9)	C(10)-C(9)-C(8)	120.9(8)
O(1)-Re(1)-S(4)	104.7(2)	C(9)-C(10)-C(5)	119.1(9)
S(1)-Re(1)-S(4)	88.05(8)		
S(2)-Re(1)-S(4)	81.61(8)		
O(1)-Re(1)-S(3)	100.6(2)		
S(1)-Re(1)-S(3)	84.27(9)		
S(2)-Re(1)-S(3)	84.32(9)		
S(4)-Re(1)-S(3)	154.44(8)		
C(1)-S(1)-Re(1)	107.0(4)		
C(4)-S(2)-Re(1)	106.9(4)		
C(2)-S(3)-C(3)	103.4(5)		
C(2)-S(3)-Re(1)	107.0(4)		
C(3)-S(3)-Re(1)	107.4(3)		
C(5)-S(4)-Re(1)	112.3(3)		
C(2)-C(1)-S(1)	111.1(8)		
C(1)-C(2)-S(3)	109.0(8)		
C(4)-C(3)-S(3)	108.9(7)		
C(3)-C(4)-S(2)	112.2(6)		
C(6)-C(5)-C(10)	119.9(8)		
C(6)-C(5)-S(4)	122.2(6)		
C(10)-C(5)-S(4)	117.7(6)		
C(7)-C(6)-C(5)	118.9(9)		

Table S-24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. 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}
Re(1)	31(1)	32(1)	37(1)	-5(1)	1(1)	2(1)
S(1)	40(1)	46(1)	68(2)	16(1)	0(1)	11(1)
S(2)	52(2)	45(1)	55(1)	14(1)	1(1)	0(1)
S(3)	35(1)	61(1)	51(1)	-16(1)	0(1)	-6(1)
S(4)	34(1)	42(1)	48(1)	7(1)	-6(1)	-1(1)
C(1)	50(7)	88(8)	87(9)	21(7)	-9(6)	20(6)
C(2)	39(6)	68(6)	87(8)	-1(5)	1(5)	10(5)
C(3)	42(6)	59(5)	66(6)	-5(5)	16(5)	-11(4)
C(4)	62(7)	35(4)	89(8)	6(4)	20(6)	-11(4)
C(5)	30(4)	35(4)	46(5)	2(3)	3(3)	2(3)
C(6)	45(6)	49(5)	53(6)	-7(4)	0(4)	-4(4)
C(7)	50(6)	74(7)	54(6)	16(5)	1(5)	-13(5)
C(8)	46(6)	48(5)	75(7)	15(5)	10(5)	-5(4)
C(9)	48(6)	45(5)	85(8)	-14(5)	8(5)	-19(5)
C(10)	44(6)	54(5)	52(6)	-12(4)	6(4)	-14(4)
O(1)	61(4)	60(4)	52(4)	-26(3)	10(3)	-2(3)

Table S-25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6**.

	x	y	z	U(eq)
H(1A)	6496	4627	4254	90
H(1B)	6742	3775	3351	90
H(2A)	7223	4712	1619	78
H(2B)	8213	5054	2812	78
H(3A)	7688	6826	782	66
H(3B)	6874	5963	179	66
H(4A)	5704	7230	-676	74
H(4B)	5592	7674	706	74
H(6)	1498	4816	4264	59
H(7)	432	3628	5334	72
H(8)	-710	2458	4229	67
H(9)	-839	2472	1987	71
H(10)	224	3641	857	60

Table S-26. Crystal data and structure refinement for **7**.

Empirical formula	C59 H58 O P Re S4	
Formula weight	1128.46	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 12.891(2) Å	α= 90°.
	b = 14.463(3) Å	β= 90°.
	c = 29.123(5) Å	γ = 90°.
Volume	5429.7(17) $Å^3$	
Z	4	
Density (calculated)	1.380 Mg/m^3	
Absorption coefficient	2.459 mm^{-1}	
F(000)	2296	
Crystal size	0.40 x 0.30 x 0.10 mm^3	
Theta range for data collection	1.40 to 26.37°.	
Index ranges	-16<=h<=15, -18<=k<=15, -36<=l<=35	
Reflections collected	41564	
Independent reflections	11046 [R(int) = 0.0395]	
Completeness to theta = 26.37°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.66	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11046 / 0 / 559	
Goodness-of-fit on F^2	1.128	
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.1073	
R indices (all data)	R1 = 0.0576, wR2 = 0.1103	
Absolute structure parameter	0.022(8)	
Largest diff. peak and hole	2.002 and -1.909 $e.Å^{-3}$	

$R1 = \Sigma \, | \, |F_o| - |F_c| \, | \, / \, \Sigma \, |F_o|$ and $wR2 = \{ \, \Sigma \, [\, w(F_o^2 - F_c^2)^2 \,] \, / \, \Sigma \, [\, w(F_o^2)^2 \,] \, \}^{1/2}$

Table S-27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	9711(1)	2805(1)	8299(1)	46(1)
C(1)	7461(8)	3592(9)	8681(7)	181(8)
C(2)	7282(8)	2746(8)	8656(5)	116(4)
C(3)	10154(5)	509(4)	8526(2)	52(2)
C(4)	9816(8)	109(6)	8115(3)	78(2)
C(5)	9385(7)	-764(6)	8122(3)	83(3)
C(6)	9313(8)	-1253(6)	8521(4)	89(3)
C(7)	9692(10)	-873(7)	8913(4)	101(3)
C(8)	10097(7)	-4(6)	8924(3)	83(3)
C(9)	10993(5)	4824(4)	8571(3)	57(2)
C(10)	11039(7)	5244(7)	8982(3)	83(2)
C(11)	10988(9)	6197(9)	9007(5)	117(4)
C(12)	10857(8)	6711(7)	8603(7)	132(6)
C(13)	10777(9)	6274(8)	8212(5)	117(4)
C(14)	10834(8)	5340(6)	8185(3)	86(3)
C(15)	5854(5)	3059(4)	6662(2)	51(2)
C(16)	6380(5)	3846(5)	6528(3)	62(2)
C(17)	7274(6)	4112(6)	6748(3)	75(2)
C(18)	7652(6)	3603(7)	7109(3)	75(2)
C(20)	6239(6)	2557(5)	7035(2)	62(2)
C(21)	3766(4)	2253(5)	6743(2)	51(1)
C(22)	3619(6)	2709(6)	7159(2)	66(2)
C(23)	2794(7)	2461(6)	7436(3)	79(2)
C(24)	2145(7)	1763(7)	7311(3)	85(3)
C(19)	7142(6)	2831(7)	7248(3)	74(2)
C(25)	2293(7)	1299(6)	6900(3)	83(3)
C(26)	3090(6)	1539(5)	6616(3)	70(2)
C(27)	5139(5)	1713(5)	5978(2)	52(2)
C(28)	4536(6)	1478(7)	5596(3)	84(3)
C(29)	4801(9)	729(8)	5325(4)	107(4)
C(30)	5645(8)	221(8)	5431(4)	106(4)

C(31)	6241(8)	410(7)	5803(4)	104(3)
C(32)	5997(6)	1182(5)	6078(3)	71(2)
C(33)	4219(5)	3548(5)	6001(2)	51(2)
C(34)	3371(6)	4049(5)	6164(3)	65(2)
C(35)	2991(8)	4781(6)	5896(4)	89(3)
C(36)	3434(9)	4983(8)	5482(4)	102(3)
C(37)	4297(8)	4497(8)	5326(4)	109(4)
C(38)	4668(7)	3767(6)	5585(3)	77(2)
C(39)	5478(9)	9690(5)	7136(3)	136(6)
C(40)	4687(5)	10046(7)	7408(4)	123(4)
C(41)	4925(10)	10569(7)	7794(4)	162(7)
C(42)	5955(13)	10736(5)	7909(3)	144(6)
C(43)	6746(7)	10381(6)	7637(4)	121(5)
C(44)	6508(7)	9858(5)	7250(4)	114(4)
C(45)	5254(16)	9091(15)	6754(7)	214(9)
C(46)	4047(13)	2342(10)	9306(3)	186(8)
C(47)	3129(9)	2652(9)	9503(6)	163(6)
C(48)	3116(14)	2930(7)	9960(7)	199(10)
C(49)	4020(20)	2897(9)	10220(4)	206(12)
C(50)	4938(14)	2587(10)	10022(6)	265(19)
C(51)	4952(9)	2309(10)	9565(7)	249(14)
C(52)	4090(30)	1870(20)	8894(9)	340(20)
C(53)	2126(10)	574(8)	4978(7)	216(14)
C(54)	2477(8)	1183(17)	4643(4)	218(16)
C(55)	2404(9)	2131(14)	4713(6)	280(20)
C(56)	1979(10)	2470(8)	5118(8)	208(12)
C(57)	1628(7)	1861(16)	5453(4)	176(9)
C(58)	1701(8)	913(14)	5383(5)	153(7)
C(59)	2212(15)	-288(12)	4899(9)	310(20)
O(1)	9705(4)	2823(4)	7719(1)	69(1)
P(1)	4748(1)	2641(1)	6351(1)	46(1)
S(1)	8772(2)	4029(1)	8585(1)	80(1)
S(2)	8331(2)	1926(1)	8539(1)	68(1)
S(3)	10804(1)	1596(1)	8540(1)	60(1)
S(4)	11198(1)	3601(1)	8544(1)	64(1)

Table S-28. Bond lengths [Å] and angles [°] for **7**.

Re(1)-O(1)	1.690(4)	C(24)-C(25)	1.384(12)
Re(1)-S(2)	2.2950(19)	C(25)-C(26)	1.364(11)
Re(1)-S(1)	2.300(2)	C(27)-C(32)	1.377(10)
Re(1)-S(4)	2.3476(19)	C(27)-C(28)	1.400(10)
Re(1)-S(3)	2.3520(18)	C(27)-P(1)	1.798(6)
C(1)-C(2)	1.248(15)	C(28)-C(29)	1.382(13)
C(1)-S(1)	1.825(11)	C(29)-C(30)	1.348(16)
C(2)-S(2)	1.831(10)	C(30)-C(31)	1.356(15)
C(3)-C(8)	1.378(10)	C(31)-C(32)	1.410(12)
C(3)-C(4)	1.399(10)	C(33)-C(38)	1.378(10)
C(3)-S(3)	1.782(7)	C(33)-C(34)	1.394(10)
C(4)-C(5)	1.380(12)	C(33)-P(1)	1.798(6)
C(5)-C(6)	1.364(13)	C(34)-C(35)	1.403(12)
C(6)-C(7)	1.357(14)	C(35)-C(36)	1.367(14)
C(7)-C(8)	1.362(13)	C(36)-C(37)	1.391(15)
C(9)-C(10)	1.345(11)	C(37)-C(38)	1.383(12)
C(9)-C(14)	1.363(11)	C(39)-C(40)	1.3900
C(9)-S(4)	1.790(6)	C(39)-C(44)	1.3900
C(10)-C(11)	1.382(16)	C(39)-C(45)	1.44(2)
C(11)-C(12)	1.403(18)	C(40)-C(41)	1.3900
C(12)-C(13)	1.306(19)	C(41)-C(42)	1.3900
C(13)-C(14)	1.356(15)	C(42)-C(43)	1.3900
C(15)-C(16)	1.382(9)	C(43)-C(44)	1.3900
C(15)-C(20)	1.398(9)	C(46)-C(52)	1.38(2)
C(15)-P(1)	1.794(6)	C(46)-C(47)	1.3900
C(16)-C(17)	1.374(10)	C(46)-C(51)	1.3900
C(17)-C(18)	1.372(12)	C(47)-C(48)	1.3900
C(18)-C(19)	1.357(13)	C(48)-C(49)	1.3900
C(20)-C(19)	1.378(10)	C(49)-C(50)	1.3900
C(21)-C(22)	1.393(9)	C(50)-C(51)	1.3900
C(21)-C(26)	1.401(10)	C(53)-C(59)	1.272(17)
C(21)-P(1)	1.794(6)	C(53)-C(54)	1.3900
C(22)-C(23)	1.382(11)	C(53)-C(58)	1.3900
C(23)-C(24)	1.361(12)	C(54)-C(55)	1.3900

C(55)-C(56)	1.3900	C(57)-C(58)	1.3900
C(56)-C(57)	1.3900		

O(1)-Re(1)-S(2)	108.00(18)	C(19)-C(18)-C(17)	119.9(7)
O(1)-Re(1)-S(1)	110.31(19)	C(19)-C(20)-C(15)	120.1(7)
S(2)-Re(1)-S(1)	84.73(8)	C(22)-C(21)-C(26)	119.6(6)
O(1)-Re(1)-S(4)	107.45(18)	C(22)-C(21)-P(1)	120.1(5)
S(2)-Re(1)-S(4)	144.33(8)	C(26)-C(21)-P(1)	120.1(5)
S(1)-Re(1)-S(4)	86.67(8)	C(23)-C(22)-C(21)	119.3(8)
O(1)-Re(1)-S(3)	108.20(18)	C(24)-C(23)-C(22)	120.6(8)
S(2)-Re(1)-S(3)	87.85(7)	C(23)-C(24)-C(25)	120.4(7)
S(1)-Re(1)-S(3)	141.21(9)	C(18)-C(19)-C(20)	120.8(8)
S(4)-Re(1)-S(3)	77.59(7)	C(26)-C(25)-C(24)	120.3(8)
C(2)-C(1)-S(1)	120.1(9)	C(25)-C(26)-C(21)	119.8(7)
C(1)-C(2)-S(2)	120.6(8)	C(32)-C(27)-C(28)	118.6(6)
C(8)-C(3)-C(4)	118.8(7)	C(32)-C(27)-P(1)	120.9(5)
C(8)-C(3)-S(3)	118.7(6)	C(28)-C(27)-P(1)	120.4(5)
C(4)-C(3)-S(3)	122.0(5)	C(29)-C(28)-C(27)	120.4(8)
C(5)-C(4)-C(3)	119.4(8)	C(30)-C(29)-C(28)	119.8(9)
C(6)-C(5)-C(4)	120.9(8)	C(29)-C(30)-C(31)	121.9(9)
C(7)-C(6)-C(5)	118.9(8)	C(30)-C(31)-C(32)	119.2(9)
C(6)-C(7)-C(8)	122.0(9)	C(27)-C(32)-C(31)	120.0(8)
C(7)-C(8)-C(3)	119.9(9)	C(38)-C(33)-C(34)	120.7(7)
C(10)-C(9)-C(14)	119.5(8)	C(38)-C(33)-P(1)	120.4(5)
C(10)-C(9)-S(4)	118.6(6)	C(34)-C(33)-P(1)	118.9(5)
C(14)-C(9)-S(4)	121.8(6)	C(33)-C(34)-C(35)	118.4(8)
C(9)-C(10)-C(11)	119.7(11)	C(36)-C(35)-C(34)	120.4(9)
C(10)-C(11)-C(12)	119.3(11)	C(35)-C(36)-C(37)	120.9(9)
C(13)-C(12)-C(11)	119.0(10)	C(38)-C(37)-C(36)	119.0(9)
C(12)-C(13)-C(14)	121.9(12)	C(33)-C(38)-C(37)	120.5(8)
C(13)-C(14)-C(9)	120.4(11)	C(40)-C(39)-C(44)	120.0
C(16)-C(15)-C(20)	118.3(6)	C(40)-C(39)-C(45)	121.0(13)
C(16)-C(15)-P(1)	121.7(5)	C(44)-C(39)-C(45)	118.8(13)
C(20)-C(15)-P(1)	120.0(5)	C(41)-C(40)-C(39)	120.0
C(17)-C(16)-C(15)	120.6(7)	C(40)-C(41)-C(42)	120.0
C(18)-C(17)-C(16)	120.4(7)	C(41)-C(42)-C(43)	120.0

C(44)-C(43)-C(42)	120.0
C(43)-C(44)-C(39)	120.0
C(52)-C(46)-C(47)	123.6(19)
C(52)-C(46)-C(51)	115(2)
C(47)-C(46)-C(51)	120.0
C(46)-C(47)-C(48)	120.0
C(47)-C(48)-C(49)	120.0
C(50)-C(49)-C(48)	120.0
C(49)-C(50)-C(51)	120.0
C(50)-C(51)-C(46)	120.0
C(59)-C(53)-C(54)	118(2)
C(59)-C(53)-C(58)	122(2)
C(54)-C(53)-C(58)	120.0
C(53)-C(54)-C(55)	120.0
C(56)-C(55)-C(54)	120.0
C(55)-C(56)-C(57)	120.0
C(56)-C(57)-C(58)	120.0
C(57)-C(58)-C(53)	120.0
C(15)-P(1)-C(21)	110.2(3)
C(15)-P(1)-C(33)	110.0(3)
C(21)-P(1)-C(33)	108.7(3)
C(15)-P(1)-C(27)	109.5(3)
C(21)-P(1)-C(27)	110.4(3)
C(33)-P(1)-C(27)	108.0(3)
C(1)-S(1)-Re(1)	106.1(4)
C(2)-S(2)-Re(1)	105.7(3)
C(3)-S(3)-Re(1)	111.6(2)
C(9)-S(4)-Re(1)	112.2(2)

Table S-29. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7**. 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}
Re(1)	47(1)	47(1)	44(1)	4(1)	-3(1)	-1(1)
C(1)	59(6)	97(9)	390(30)	-43(12)	50(10)	8(6)
C(2)	71(6)	77(7)	200(12)	-6(8)	36(7)	-9(6)
C(3)	40(3)	54(4)	61(4)	4(3)	-11(3)	8(3)
C(4)	104(6)	69(5)	60(4)	-11(4)	9(5)	-8(5)
C(5)	90(6)	66(5)	93(6)	-20(5)	-13(5)	-1(4)
C(6)	89(6)	47(4)	133(8)	13(5)	10(6)	0(4)
C(7)	135(8)	70(6)	98(7)	28(5)	1(7)	-24(7)
C(8)	102(7)	70(5)	76(5)	22(4)	-18(5)	-5(5)
C(9)	44(3)	37(3)	90(5)	0(3)	-3(3)	-6(3)
C(10)	74(5)	86(6)	88(6)	-20(5)	-4(5)	-18(5)
C(11)	97(8)	96(9)	159(12)	-56(8)	-11(8)	-8(7)
C(12)	60(5)	47(6)	290(20)	-10(9)	-2(9)	-11(5)
C(13)	106(8)	69(7)	175(13)	50(7)	-28(8)	-22(6)
C(14)	96(6)	72(5)	90(6)	21(5)	-11(5)	3(5)
C(15)	40(3)	64(4)	48(3)	-2(3)	-5(3)	-1(3)
C(16)	54(4)	65(4)	67(4)	17(3)	-5(3)	-11(3)
C(17)	57(4)	82(5)	86(5)	5(5)	1(4)	-24(4)
C(18)	45(4)	96(6)	83(5)	-15(5)	-14(4)	-9(4)
C(20)	64(4)	71(5)	51(4)	6(3)	-11(3)	-12(3)
C(21)	46(3)	53(3)	53(3)	-2(4)	4(3)	-4(3)
C(22)	63(4)	76(5)	59(4)	-10(4)	14(3)	-8(4)
C(23)	86(5)	81(6)	71(5)	-10(4)	24(4)	-8(5)
C(24)	65(5)	94(6)	95(6)	10(5)	32(5)	-13(5)
C(19)	68(4)	88(5)	66(4)	7(5)	-21(4)	8(5)
C(25)	71(5)	76(6)	103(7)	-9(5)	13(5)	-23(4)
C(26)	61(4)	66(4)	81(6)	-13(4)	6(4)	-6(4)
C(27)	38(3)	62(4)	57(3)	-11(3)	0(3)	6(3)
C(28)	52(4)	109(6)	90(6)	-44(5)	-11(4)	19(4)
C(29)	77(6)	140(9)	105(7)	-66(7)	-17(6)	1(7)
C(30)	85(7)	107(8)	128(9)	-71(7)	-1(6)	16(6)

C(31)	85(6)	83(6)	143(10)	-34(6)	6(7)	27(5)
C(32)	63(4)	69(5)	80(5)	-17(4)	-11(4)	9(4)
C(33)	42(3)	57(4)	55(4)	10(3)	-11(3)	4(3)
C(34)	56(4)	59(4)	81(5)	1(4)	2(4)	11(3)
C(35)	82(6)	65(5)	121(8)	-6(5)	-5(6)	26(5)
C(36)	105(8)	94(7)	107(8)	38(6)	-20(7)	20(6)
C(37)	78(6)	134(9)	114(8)	68(7)	3(6)	22(6)
C(38)	54(4)	105(6)	73(5)	22(4)	9(4)	15(5)
C(39)	182(15)	110(9)	116(9)	42(8)	-43(10)	-68(10)
C(40)	85(7)	132(10)	151(12)	61(9)	-1(9)	-22(8)
C(41)	162(16)	122(12)	202(19)	56(12)	10(14)	-24(12)
C(42)	220(19)	95(9)	117(10)	40(8)	-1(13)	-19(12)
C(43)	123(10)	83(8)	157(12)	41(8)	-54(10)	-20(7)
C(44)	85(7)	76(7)	181(13)	47(8)	29(8)	1(6)
C(45)	220(20)	200(18)	220(20)	38(16)	-70(19)	-75(17)
C(46)	220(20)	201(17)	138(12)	-2(12)	101(15)	-27(18)
C(47)	151(14)	111(11)	230(20)	31(13)	20(14)	4(10)
C(48)	280(30)	96(9)	220(30)	-36(14)	40(20)	-22(14)
C(49)	340(30)	148(15)	128(13)	-9(11)	107(19)	-80(20)
C(50)	500(60)	144(15)	150(17)	21(13)	20(30)	0(20)
C(51)	116(12)	320(30)	310(40)	-20(30)	-54(17)	-31(17)
C(52)	340(40)	450(50)	240(30)	-110(30)	110(30)	-30(40)
C(53)	101(13)	194(19)	350(40)	-100(30)	-112(18)	51(14)
C(54)	82(9)	400(50)	175(17)	140(20)	-52(10)	-68(16)
C(55)	113(16)	520(70)	190(20)	180(30)	-70(15)	-110(30)
C(56)	124(17)	170(15)	330(30)	30(20)	-130(20)	-13(14)
C(57)	69(7)	280(30)	183(16)	48(17)	-49(9)	-14(13)
C(58)	92(9)	171(15)	197(18)	76(14)	-37(10)	-16(11)
C(59)	170(17)	166(15)	590(50)	-220(30)	-190(30)	56(14)
O(1)	77(3)	81(3)	50(2)	4(2)	-4(2)	-1(4)
P(1)	37(1)	54(1)	46(1)	-3(1)	-1(1)	4(1)
S(1)	55(1)	58(1)	127(2)	-15(1)	4(1)	2(1)
S(2)	57(1)	58(1)	90(1)	4(1)	7(1)	-10(1)
S(3)	57(1)	57(1)	66(1)	7(1)	-11(1)	3(1)
S(4)	50(1)	54(1)	88(1)	6(1)	-9(1)	-1(1)

Table S-30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7**.

	x	y	z	U(eq)
H(1A)	7248	3795	8985	217
H(1C)	7010	3899	8463	217
H(2A)	6762	2661	8419	139
H(2B)	6964	2563	8944	139
H(4A)	9881	429	7839	93
H(5A)	9140	-1023	7850	99
H(6A)	9010	-1836	8525	107
H(7A)	9675	-1218	9183	121
H(8A)	10334	244	9199	99
H(10A)	11105	4895	9249	99
H(11A)	11040	6495	9289	141
H(12A)	10827	7354	8613	159
H(13A)	10677	6613	7944	140
H(14A)	10765	5049	7902	103
H(16A)	6127	4199	6285	74
H(17A)	7625	4639	6652	90
H(18A)	8256	3787	7258	89
H(20A)	5885	2038	7140	74
H(22A)	4071	3176	7249	79
H(23A)	2682	2774	7710	95
H(24A)	1598	1598	7502	102
H(19A)	7406	2484	7490	89
H(25A)	1847	822	6818	100
H(26A)	3185	1228	6340	83
H(28A)	3953	1828	5523	101
H(29A)	4399	575	5072	129
H(30A)	5823	-274	5243	128
H(31A)	6803	35	5875	124
H(32A)	6416	1333	6327	85
H(34A)	3065	3901	6444	78

H(35A)	2434	5130	6001	107
H(36A)	3155	5451	5301	122
H(37A)	4618	4661	5052	131
H(38A)	5226	3420	5478	93
H(40A)	3998	9933	7332	147
H(41A)	4395	10806	7976	195
H(42A)	6114	11086	8167	173
H(43A)	7435	10493	7713	145
H(44A)	7037	9620	7069	137
H(45A)	4516	9039	6717	322
H(45B)	5544	8490	6811	322
H(45C)	5553	9344	6479	322
H(47A)	2524	2674	9330	195
H(48A)	2502	3138	10092	239
H(49A)	4012	3083	10525	248
H(50A)	5543	2565	10196	317
H(51A)	5566	2101	9433	298
H(52A)	3436	1921	8738	515
H(52B)	4232	1225	8953	515
H(52C)	4629	2120	8705	515
H(54A)	2762	956	4372	261
H(55A)	2639	2539	4489	330
H(56A)	1930	3105	5165	249
H(57A)	1344	2088	5724	211
H(58A)	1466	505	5607	184
H(59A)	2517	-380	4602	464
H(59B)	1539	-570	4907	464
H(59C)	2646	-564	5130	464

Table S-31. Crystal data and structure refinement for **8**^{pdt}.

Empirical formula	C9 H18 O2 Re2 S6	
Formula weight	722.99	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.1533(17) Å	α= 90°.
	b = 12.383(2) Å	β= 90°.
	c = 15.641(3) Å	γ = 90°.
Volume	1772.8(6) Å^3	
Z	4	
Density (calculated)	2.709 Mg/m^3	
Absorption coefficient	14.344 mm^{-1}	
F(000)	1336	
Crystal size	0.17 x 0.14 x 0.05 mm^3	
Theta range for data collection	2.10 to 28.31°.	
Index ranges	-12<=h<=11, -15<=k<=16, -20<=l<=20	
Reflections collected	14538	
Independent reflections	4150 [R(int) = 0.0615]	
Completeness to theta = 28.31°	95.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.52 and 0.18	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4150 / 0 / 172	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0795	
R indices (all data)	R1 = 0.0391, wR2 = 0.0811	
Absolute structure parameter	0.044(11)	
Largest diff. peak and hole	2.839 and -1.746 e.Å^{-3}	

$R1 = \Sigma \, | \, |F_o| - |F_c| \, | \, / \, \Sigma \, |F_o|$ and $wR2 = \{ \, \Sigma \, [\, w(F_o^2 - F_c^2)^2 \,] \, / \, \Sigma \, [\, w(F_o^2)^2 \,] \, \}^{1/2}$

Table S-32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**^{pdt}. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Re(1)	6955(1)	4330(1)	8055(1)	24(1)
Re(2)	9335(1)	6693(1)	8050(1)	25(1)
S(1)	7941(2)	8177(2)	8318(2)	39(1)
S(2)	10423(3)	6717(2)	9354(2)	50(1)
S(3)	9486(2)	4762(2)	8154(1)	27(1)
S(4)	7243(2)	5998(2)	7324(1)	28(1)
S(5)	6915(3)	3488(2)	9364(2)	41(1)
S(6)	4676(2)	4766(2)	8554(2)	36(1)
C(1)	8750(11)	9137(9)	9050(8)	49(3)
C(2)	10279(12)	8986(9)	9284(7)	52(3)
C(3)	10489(17)	8046(9)	9873(8)	78(4)
C(4)	10588(9)	4146(7)	8977(6)	37(2)
C(5)	9850(10)	3859(8)	9802(6)	42(2)
C(6)	8705(10)	2986(8)	9701(7)	47(3)
C(7)	3595(8)	5635(8)	7841(6)	37(2)
C(8)	4308(9)	6057(7)	7054(6)	36(2)
C(9)	5618(9)	6788(7)	7221(7)	42(2)
O(1)	10541(6)	7010(5)	7293(4)	37(1)
O(2)	6783(6)	3386(5)	7305(4)	37(1)

Table S-33. Bond lengths [Å] and angles [°] for **8**^{pdt}.

Re(1)-O(2)	1.663(6)	S(2)-C(3)	1.836(12)
Re(1)-S(6)	2.292(2)	S(3)-C(4)	1.804(8)
Re(1)-S(5)	2.298(2)	S(4)-C(9)	1.788(8)
Re(1)-S(4)	2.374(2)	S(5)-C(6)	1.830(9)
Re(1)-S(3)	2.3825(19)	S(6)-C(7)	1.839(9)
Re(2)-O(1)	1.666(6)	C(1)-C(2)	1.458(14)
Re(2)-S(2)	2.271(3)	C(2)-C(3)	1.498(16)
Re(2)-S(1)	2.277(2)	C(4)-C(5)	1.500(13)
Re(2)-S(4)	2.387(2)	C(5)-C(6)	1.514(14)
Re(2)-S(3)	2.400(2)	C(7)-C(8)	1.488(12)
S(1)-C(1)	1.809(10)	C(8)-C(9)	1.525(12)

O(2)-Re(1)-S(6)	108.6(2)	C(4)-S(3)-Re(1)	119.7(3)
O(2)-Re(1)-S(5)	107.9(2)	C(4)-S(3)-Re(2)	120.1(3)
S(6)-Re(1)-S(5)	77.80(8)	Re(1)-S(3)-Re(2)	99.39(7)
O(2)-Re(1)-S(4)	106.4(2)	C(9)-S(4)-Re(1)	115.3(3)
S(6)-Re(1)-S(4)	93.46(8)	C(9)-S(4)-Re(2)	120.9(3)
S(5)-Re(1)-S(4)	145.62(9)	Re(1)-S(4)-Re(2)	100.01(8)
O(2)-Re(1)-S(3)	107.2(2)	C(6)-S(5)-Re(1)	113.3(3)
S(6)-Re(1)-S(3)	144.10(8)	C(7)-S(6)-Re(1)	114.9(3)
S(5)-Re(1)-S(3)	93.41(8)	C(2)-C(1)-S(1)	117.9(8)
S(4)-Re(1)-S(3)	74.24(7)	C(1)-C(2)-C(3)	112.1(11)
O(1)-Re(2)-S(2)	110.2(2)	C(2)-C(3)-S(2)	114.9(8)
O(1)-Re(2)-S(1)	108.2(2)	C(5)-C(4)-S(3)	117.5(6)
S(2)-Re(2)-S(1)	93.97(9)	C(4)-C(5)-C(6)	113.0(8)
O(1)-Re(2)-S(4)	106.2(2)	C(5)-C(6)-S(5)	114.0(7)
S(2)-Re(2)-S(4)	141.62(10)	C(8)-C(7)-S(6)	118.1(6)
S(1)-Re(2)-S(4)	85.95(8)	C(7)-C(8)-C(9)	114.3(8)
O(1)-Re(2)-S(3)	104.2(2)	C(8)-C(9)-S(4)	110.2(6)
S(2)-Re(2)-S(3)	85.81(8)		
S(1)-Re(2)-S(3)	145.48(8)		
S(4)-Re(2)-S(3)	73.69(7)		
C(1)-S(1)-Re(2)	114.7(3)		
C(3)-S(2)-Re(2)	115.1(4)		

Table S-34. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**^{pdt}. 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}
Re(1)	21(1)	21(1)	30(1)	1(1)	1(1)	0(1)
Re(2)	22(1)	25(1)	29(1)	2(1)	2(1)	-2(1)
S(1)	36(1)	30(1)	50(2)	-6(1)	-1(1)	5(1)
S(2)	69(2)	39(1)	43(2)	-5(1)	-20(1)	9(1)
S(3)	22(1)	26(1)	34(1)	3(1)	0(1)	0(1)
S(4)	22(1)	25(1)	37(1)	4(1)	-1(1)	1(1)
S(5)	40(1)	43(1)	42(1)	17(1)	6(1)	0(1)
S(6)	26(1)	41(1)	41(1)	4(1)	6(1)	3(1)
C(1)	55(6)	36(5)	56(7)	-13(5)	2(5)	9(5)
C(2)	66(7)	48(6)	41(6)	-16(5)	-5(5)	-15(5)
C(3)	113(11)	55(7)	64(9)	-19(7)	-42(8)	7(7)
C(4)	32(4)	36(5)	42(5)	4(4)	-11(4)	7(4)
C(5)	46(5)	49(6)	32(5)	4(4)	-12(4)	10(4)
C(6)	50(5)	44(6)	46(6)	21(5)	-7(5)	8(4)
C(7)	19(3)	45(5)	46(6)	-1(4)	-5(3)	2(3)
C(8)	28(4)	43(5)	38(5)	-5(4)	-6(4)	7(3)
C(9)	34(4)	23(4)	68(7)	14(4)	-15(4)	3(4)
O(1)	31(3)	37(3)	41(4)	-2(3)	9(3)	-9(3)
O(2)	35(3)	28(3)	49(4)	-7(3)	7(3)	-2(3)

Table S-35. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for $\mathbf{8^{pdt}}$.

	x	y	z	U(eq)
H(1A)	8652	9851	8801	59
H(1B)	8178	9131	9572	59
H(2A)	10636	9636	9559	62
H(2B)	10851	8872	8769	62
H(3A)	9738	8072	10311	93
H(3B)	11426	8123	10156	93
H(4A)	11012	3492	8742	44
H(4B)	11388	4633	9106	44
H(5A)	9392	4501	10035	51
H(5B)	10581	3617	10208	51
H(6A)	8596	2612	10242	56
H(6B)	9048	2466	9283	56
H(7A)	2734	5233	7669	44
H(7B)	3260	6250	8173	44
H(8A)	3590	6456	6726	44
H(8B)	4624	5450	6709	44
H(9A)	5459	7198	7741	50
H(9B)	5728	7294	6752	50