Supporting Information

Chalcogen centered spirocyclic mixed metal carbonyl complexes: Synthesis and molecular structures of $(CO)_8(\mu\text{-}PCy_2)Re_2(\mu_4\text{-}E)Fe_2(\mu\text{-}ER)(CO)_6$ and $[(CO)_8(\mu\text{-}PCy_2)Re_2(\mu_4\text{-}E)Fe_2(CO)_6]_2(\mu_4\text{-}E_2)$ (E = S, Se, Te; R =org. residue)

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The supporting information contains tables of atomic coordinates, bond lenghts and angles, anisotropic displacement factors and hydrogen coordinates of the following compounds:

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	-9188(1)	3741(1)	3821(1)	20(1)
Re(2)	-5615(1)	3774(1)	3063(1)	19(1)
Fe(1)	-6968(2)	1710(1)	3911(1)	26(1)
Fe(2)	-5880(2)	2539(1)	4812(1)	26(1)
S(1)	-6974(3)	3001(1)	3867(1)	20(1)
S(2)	-4717(3)	1984(1)	4023(1)	28(1)
P(1)	-7960(3)	4364(1)	2917(1)	18(1)
O(1)	-7912(9)	4740(4)	4972(3)	55(2)
C(1)	-8356(10)	4398(5)	4542(5)	27(2)
O(2)	-11710(7)	4748(4)	3565(3)	39(2)
C(2)	-10788(10)	4376(5)	3678(4)	26(2)
O(3)	-10079(8)	2543(4)	2768(3)	45(2)
C(3)	-9805(10)	2976(6)	3149(5)	29(3)
O(4)	-10897(8)	2923(4)	4836(3)	55(2)
C(4)	-10209(10)	3204(6)	4477(5)	27(2)
C(5)	-4739(10)	4382(6)	2433(5)	30(3)
O(5)	-4191(8)	4715(4)	2051(3)	42(2)
O(6)	-6386(8)	2646(4)	1932(3)	42(2)
C(6)	-6132(10)	3051(5)	2347(5)	27(2)
O(7)	-2700(7)	3114(4)	3302(4)	46(2)
C(7)	-3807(10)	3309(5)	3243(5)	27(2)
O(8)	-4895(8)	4951(4)	4179(4)	48(2)
C(8)	-5171(10)	4534(5)	3780(5)	27(2)
O(9)	-9826(8)	1551(4)	4208(4)	55(2)
C(9)	-8696(11)	1644(6)	4097(6)	41(3)
O(10)	-7416(10)	1211(5)	2530(3)	75(3)
C(10)	-7202(12)	1421(5)	3051(5)	40(3)
O(11)	-6432(8)	243(4)	4496(4)	52(2)
C(11)	-6650(11)	820(6)	4258(5)	33(3)
O(12)	-5029(8)	1427(4)	5806(3)	56(2)
C(12)	-5359(11)	1858(5)	5409(5)	34(3)

O(13)	-3807(8)	3703(4)	5101(4)	55(2)
C(13)	-4649(11)	3269(6)	5002(5)	36(3)
O(14)	-8052(8)	3013(5)	5645(3)	62(3)
C(14)	-7221(11)	2836(6)	5306(5)	37(3)
C(21)	-8825(8)	4129(5)	2094(4)	18(2)
C(22)	-8115(9)	4468(5)	1505(4)	22(2)
C(23)	-8754(10)	4180(6)	844(4)	38(3)
C(24)	-10292(11)	4341(6)	779(4)	41(3)
C(25)	-10995(9)	4018(6)	1352(4)	35(3)
C(26)	-10391(9)	4312(5)	2008(4)	26(2)
C(31)	-7985(10)	5408(5)	2917(4)	26(2)
C(32)	-6704(11)	5754(5)	2635(5)	29(3)
C(33)	-6870(11)	6593(5)	2551(5)	32(3)
C(34)	-7135(11)	6960(5)	3205(4)	39(3)
C(35)	-8377(12)	6628(5)	3513(5)	35(3)
C(36)	-8262(11)	5772(5)	3573(4)	28(3)
C(41)	-3565(10)	1233(6)	4318(4)	48(3)

Table S2. Bond lengths [Å] and angles [°] for **3a**.

Re(1)-C(2)	1.941(10)
Re(1)-C(4)	1.968(10)
Re(1)-C(3)	2.002(11)
Re(1)-C(1)	2.010(9)
Re(1)-P(1)	2.519(2)
Re(1)-S(1)	2.535(3)
Re(2)-C(5)	1.925(11)
Re(2)-C(7)	1.966(10)
Re(2)-C(6)	1.989(10)
Re(2)-C(8)	2.023(10)
Re(2)-P(1)	2.523(3)
Re(2)-S(1)	2.575(2)
Fe(1)-C(9)	1.758(11)
Fe(1)-C(11)	1.765(10)
Fe(1)-C(10)	1.822(11)
Fe(1)-S(2)	2.250(3)
Fe(1)-S(1)	2.320(3)
Fe(1)-Fe(2)	2.537(2)
Fe(2)-C(12)	1.771(10)
Fe(2)-C(14)	1.782(11)
Fe(2)-C(13)	1.803(11)
Fe(2)-S(2)	2.254(3)
Fe(2)-S(1)	2.290(3)
S(2)-C(41)	1.832(9)
P(1)-C(21)	1.870(8)
P(1)-C(31)	1.874(9)
O(1)-C(1)	1.130(10)
O(2)-C(2)	1.132(10)
O(3)-C(3)	1.117(11)
O(4)-C(4)	1.139(10)
C(5)-O(5)	1.140(11)
O(6)-C(6)	1.129(10)
O(7)-C(7)	1.135(10)
O(8)-C(8)	1.122(10)

O(9)-C(9)	1.152(12)
O(10)-C(10)	1.129(11)
O(11)-C(11)	1.158(11)
O(12)-C(12)	1.150(10)
O(13)-C(13)	1.142(11)
O(14)-C(14)	1.143(11)
C(21)-C(22)	1.545(10)
C(21)-C(26)	1.563(11)
C(22)-C(23)	1.534(10)
C(23)-C(24)	1.527(13)
C(24)-C(25)	1.504(12)
C(25)-C(26)	1.517(10)
C(31)-C(36)	1.523(11)
C(31)-C(32)	1.541(13)
C(32)-C(33)	1.522(11)
C(33)-C(34)	1.518(12)
C(34)-C(35)	1.522(13)
C(35)-C(36)	1.545(11)

C(2)-Re(1)-C(4)	87.2(4)
C(2)-Re(1)-C(3)	95.6(4)
C(4)-Re(1)-C(3)	88.9(4)
C(2)-Re(1)-C(1)	92.8(4)
C(4)-Re(1)-C(1)	89.6(4)
C(3)-Re(1)-C(1)	171.4(4)
C(2)-Re(1)-P(1)	92.7(3)
C(4)-Re(1)-P(1)	175.7(3)
C(3)-Re(1)-P(1)	86.8(3)
C(1)-Re(1)-P(1)	94.7(3)
C(2)-Re(1)-S(1)	171.9(3)
C(4)-Re(1)-S(1)	100.7(3)
C(3)-Re(1)-S(1)	83.3(3)
C(1)-Re(1)-S(1)	88.7(3)
P(1)-Re(1)-S(1)	79.26(8)
C(5)-Re(2)-C(7)	86.1(4)
C(5)-Re(2)-C(6)	89.3(4)

C(7)-Re(2)-C(6)	92.4(4)
C(5)-Re(2)-C(8)	90.7(4)
C(7)-Re(2)-C(8)	90.3(4)
C(6)-Re(2)-C(8)	177.4(4)
C(5)-Re(2)-P(1)	97.0(3)
C(7)-Re(2)-P(1)	176.0(3)
C(6)-Re(2)-P(1)	90.2(3)
C(8)-Re(2)-P(1)	87.2(3)
C(5)-Re(2)-S(1)	175.4(3)
C(7)-Re(2)-S(1)	98.5(3)
C(6)-Re(2)-S(1)	89.7(3)
C(8)-Re(2)-S(1)	90.1(3)
P(1)-Re(2)-S(1)	78.45(8)
C(9)-Fe(1)-C(11)	90.0(5)
C(9)-Fe(1)-C(10)	97.2(5)
C(11)-Fe(1)-C(10)	97.6(4)
C(9)-Fe(1)-S(2)	159.8(4)
C(11)-Fe(1)-S(2)	90.7(4)
C(10)-Fe(1)-S(2)	102.7(4)
C(9)-Fe(1)-S(1)	94.3(4)
C(11)-Fe(1)-S(1)	156.9(3)
C(10)-Fe(1)-S(1)	104.4(3)
S(2)-Fe(1)-S(1)	77.60(10)
C(9)-Fe(1)-Fe(2)	104.3(4)
C(11)-Fe(1)-Fe(2)	100.9(3)
C(10)-Fe(1)-Fe(2)	151.5(3)
S(2)-Fe(1)-Fe(2)	55.79(8)
S(1)-Fe(1)-Fe(2)	56.05(7)
C(12)-Fe(2)-C(14)	90.6(4)
C(12)-Fe(2)-C(13)	101.4(5)
C(14)-Fe(2)-C(13)	99.5(5)
C(12)-Fe(2)-S(2)	92.6(3)
C(14)-Fe(2)-S(2)	162.6(4)
C(13)-Fe(2)-S(2)	96.5(4)
C(12)-Fe(2)-S(1)	157.0(3)
C(14)-Fe(2)-S(1)	92.4(3)

C(13)-Fe(2)-S(1)	100.6(3)
S(2)-Fe(2)-S(1)	78.12(10)
C(12)-Fe(2)-Fe(1)	100.2(3)
C(14)-Fe(2)-Fe(1)	107.0(4)
C(13)-Fe(2)-Fe(1)	145.4(3)
S(2)-Fe(2)-Fe(1)	55.64(8)
S(1)-Fe(2)-Fe(1)	57.17(7)
Fe(2)-S(1)-Fe(1)	66.78(8)
Fe(2)-S(1)-Re(1)	124.83(10)
Fe(1)-S(1)-Re(1)	121.68(11)
Fe(2)-S(1)-Re(2)	119.66(11)
Fe(1)-S(1)-Re(2)	124.23(11)
Re(1)-S(1)-Re(2)	99.66(8)
C(41)-S(2)-Fe(1)	116.6(4)
C(41)-S(2)-Fe(2)	114.9(3)
Fe(1)-S(2)-Fe(2)	68.56(9)
C(21)-P(1)-C(31)	102.7(4)
C(21)-P(1)-Re(1)	110.0(3)
C(31)-P(1)-Re(1)	115.9(3)
C(21)-P(1)-Re(2)	111.4(3)
C(31)-P(1)-Re(2)	115.6(3)
Re(1)-P(1)-Re(2)	101.51(9)
O(1)-C(1)-Re(1)	176.3(9)
O(2)-C(2)-Re(1)	176.8(9)
O(3)-C(3)-Re(1)	176.3(9)
O(4)-C(4)-Re(1)	174.2(9)
O(5)-C(5)-Re(2)	177.0(9)
O(6)-C(6)-Re(2)	177.7(9)
O(7)-C(7)-Re(2)	171.2(9)
O(8)-C(8)-Re(2)	178.5(9)
O(9)-C(9)-Fe(1)	175.4(11)
O(10)-C(10)-Fe(1)	175.4(11)
O(11)-C(11)-Fe(1)	178.7(9)
O(12)-C(12)-Fe(2)	178.5(9)
O(13)-C(13)-Fe(2)	175.3(11)
O(14)-C(14)-Fe(2)	177.1(9)

C(22)-C(21)-C(26)	108.4(7)
C(22)-C(21)-P(1)	113.7(6)
C(26)-C(21)-P(1)	115.7(6)
C(23)-C(22)-C(21)	111.5(7)
C(24)-C(23)-C(22)	110.7(8)
C(25)-C(24)-C(23)	110.9(8)
C(24)-C(25)-C(26)	111.9(8)
C(25)-C(26)-C(21)	110.3(7)
C(36)-C(31)-C(32)	110.2(8)
C(36)-C(31)-P(1)	115.7(6)
C(32)-C(31)-P(1)	113.1(7)
C(33)-C(32)-C(31)	111.0(9)
C(34)-C(33)-C(32)	110.8(8)
C(33)-C(34)-C(35)	112.0(9)
C(34)-C(35)-C(36)	111.5(9)
C(31)-C(36)-C(35)	112.0(8)

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3a**. 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)	23(1)	20(1)	0(1)	3(1)	0(1)
Re(2)	14(1)	19(1)	24(1)	-1(1)	3(1)	-1(1)
Fe(1)	31(1)	20(1)	28(1)	3(1)	2(1)	-1(1)
Fe(2)	27(1)	28(1)	22(1)	1(1)	1(1)	4(1)
S(1)	18(1)	21(1)	20(1)	0(1)	3(1)	2(1)
S(2)	27(2)	31(1)	27(1)	4(1)	3(1)	9(1)
P(1)	15(1)	18(1)	20(1)	-2(1)	2(1)	3(1)
O(1)	79(7)	55(5)	29(4)	-18(4)	-16(5)	-18(5)
C(1)	25(6)	22(5)	32(6)	8(5)	-7(5)	-8(5)
O(2)	29(4)	42(5)	46(5)	-2(4)	2(4)	18(4)
C(2)	17(5)	32(6)	28(6)	-5(5)	5(5)	-3(5)
O(3)	43(5)	47(5)	45(5)	-23(4)	-5(4)	-5(4)
C(3)	15(6)	36(6)	35(6)	18(5)	4(5)	12(5)
O(4)	51(6)	68(6)	48(5)	17(5)	29(4)	-3(5)
C(4)	16(6)	39(6)	27(6)	8(5)	4(5)	7(5)
C(5)	18(6)	30(6)	44(7)	-18(5)	9(5)	7(5)
O(5)	50(5)	32(4)	47(5)	11(4)	21(4)	-9(4)
O(6)	54(5)	36(4)	35(4)	-14(4)	5(4)	-13(4)
C(6)	22(6)	26(6)	34(6)	-6(5)	7(5)	-8(5)
O(7)	7(4)	27(4)	103(7)	0(4)	0(4)	-1(3)
C(7)	25(6)	20(5)	36(6)	-3(5)	3(5)	-11(5)
O(8)	48(5)	35(5)	60(5)	-19(4)	-7(5)	2(4)
C(8)	20(6)	26(6)	35(6)	0(5)	-1(5)	1(5)
O(9)	36(5)	40(5)	91(7)	15(5)	19(5)	-2(4)
C(9)	30(7)	33(7)	58(8)	15(6)	1(6)	-3(6)
O(10)	132(9)	57(5)	35(4)	-9(5)	-12(5)	-9(7)
C(10)	50(8)	28(7)	42(6)	8(5)	4(6)	4(6)
O(11)	61(6)	32(4)	63(5)	19(4)	-7(5)	2(5)
C(11)	30(6)	32(6)	37(6)	-16(5)	-4(5)	0(6)
O(12)	74(6)	57(6)	37(4)	22(4)	-1(4)	22(5)
C(12)	38(7)	35(6)	28(6)	8(5)	7(5)	11(6)

O(13)	49(5)	54(5)	60(5)	-13(5)	-15(4)	-3(6)
C(13)	39(7)	42(7)	25(6)	8(5)	-11(6)	-6(6)
O(14)	57(6)	94(7)	38(5)	4(5)	13(5)	31(6)
C(14)	43(7)	47(7)	20(5)	17(5)	8(5)	18(6)
C(21)	18(5)	25(5)	10(4)	5(4)	2(4)	5(4)
C(22)	21(5)	31(5)	14(4)	4(4)	-1(4)	-10(5)
C(23)	32(7)	64(8)	18(5)	-10(5)	3(5)	0(6)
C(24)	44(8)	57(8)	19(5)	-9(5)	-11(5)	2(7)
C(25)	22(6)	54(7)	27(6)	-3(5)	-6(5)	0(6)
C(26)	31(6)	30(6)	16(5)	0(4)	0(5)	6(5)
C(31)	37(6)	14(5)	26(5)	-3(4)	0(5)	1(5)
C(32)	42(7)	20(5)	25(6)	2(5)	2(5)	-5(5)
C(33)	39(7)	23(6)	34(6)	10(5)	2(6)	2(5)
C(34)	57(8)	25(6)	34(6)	6(5)	-6(6)	1(6)
C(35)	60(9)	24(6)	24(6)	-2(5)	17(6)	18(6)
C(36)	30(6)	23(5)	30(6)	0(5)	-4(5)	5(5)
C(41)	56(8)	43(6)	46(6)	19(6)	8(6)	34(7)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3a**.

	x	y	z	U(eq)
H(21A)	-8749	3582	2047	21
H(22A)	-8196	5012	1518	27
H(22B)	-7137	4341	1544	27
H(23A)	-8309	4421	481	46
H(23B)	-8601	3642	812	46
H(24A)	-10442	4880	763	49
H(24B)	-10691	4126	366	49
H(25A)	-10908	3474	1345	42
H(25B)	-11975	4141	1304	42
H(26A)	-10865	4085	2368	31
H(26B)	-10524	4852	2027	31
H(31A)	-8766	5551	2608	31
H(32A)	-5898	5650	2933	35
H(32B)	-6556	5528	2206	35
H(33A)	-6036	6802	2382	38
H(33B)	-7638	6697	2230	38
H(34A)	-7284	7495	3134	47
H(34B)	-6324	6900	3511	47
H(35A)	-9209	6756	3241	42
H(35B)	-8455	6844	3952	42
H(36A)	-7517	5647	3901	33
H(36B)	-9117	5573	3729	33
H(41A)	-3110	1025	3949	72
H(41B)	-4091	846	4520	72
H(41C)	-2883	1429	4641	72

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	4260(1)	3788(1)	1194(1)	34(1)
Re(2)	648(1)	3825(1)	1985(1)	33(1)
Se(1)	1983(1)	3036(1)	1138(1)	34(1)
Se(2)	-401(1)	1997(1)	975(1)	57(1)
Fe(1)	1939(1)	1715(1)	1068(1)	44(1)
Fe(2)	868(1)	2550(1)	164(1)	44(1)
P(1)	2995(2)	4407(1)	2083(1)	33(1)
O(1)	6767(7)	4785(4)	1435(3)	69(2)
C(1)	5819(9)	4400(5)	1337(4)	43(2)
O(2)	3021(9)	4764(4)	51(3)	88(3)
C(2)	3465(10)	4430(5)	473(5)	52(3)
O(3)	5087(8)	2581(4)	2223(3)	74(2)
C(3)	4842(9)	3034(6)	1866(5)	49(2)
O(4)	5944(8)	2992(4)	198(4)	87(3)
C(4)	5270(10)	3265(6)	559(5)	54(3)
O(5)	-150(8)	4955(4)	866(3)	82(3)
C(5)	156(8)	4538(5)	1260(5)	45(2)
O(6)	-2243(7)	3167(4)	1816(4)	74(2)
C(6)	-1151(9)	3373(5)	1846(5)	45(2)
O(7)	-688(7)	4769(4)	3015(3)	76(2)
C(7)	-157(9)	4428(5)	2632(5)	47(2)
O(8)	1500(8)	2679(4)	3066(3)	74(2)
C(8)	1207(9)	3094(5)	2676(4)	40(2)
O(9)	4753(8)	1606(4)	757(5)	99(3)
C(9)	3647(11)	1665(6)	868(6)	64(3)
O(10)	1429(8)	284(4)	466(4)	83(2)
C(10)	1631(11)	836(6)	703(5)	62(3)
O(11)	2323(11)	1218(5)	2425(4)	115(4)
C(11)	2155(12)	1424(5)	1907(5)	65(3)
O(12)	3099(9)	3001(6)	-611(3)	105(3)
C(12)	2246(12)	2821(6)	-304(5)	65(3)

O(13)	-1071(9)	3723(5)	-137(4)	96(3)
C(13)	-303(12)	3263(6)	-40(5)	63(3)
O(14)	-1(9)	1467(5)	-812(4)	98(3)
C(14)	336(11)	1885(6)	-431(5)	64(3)
C(21)	3849(8)	4187(5)	2901(4)	40(2)
C(22)	5362(8)	4378(6)	2971(4)	51(2)
C(23)	6014(10)	4099(6)	3632(4)	68(3)
C(24)	5257(11)	4408(7)	4196(4)	75(3)
C(25)	3769(10)	4244(6)	4139(4)	68(3)
C(26)	3146(9)	4510(6)	3486(4)	53(2)
C(31)	3007(10)	5438(4)	2064(4)	50(2)
C(32)	1779(10)	5799(5)	2349(5)	51(2)
C(33)	1926(13)	6623(5)	2410(5)	79(3)
C(34)	2219(13)	6983(6)	1781(5)	80(3)
C(35)	3470(12)	6623(5)	1485(5)	70(3)
C(36)	3324(12)	5787(5)	1450(5)	64(3)
C(41)	-1538(10)	1192(6)	633(5)	81(4)

Table S6. Bond lengths [Å] and angles [°] for **3b**.

Re(1)-C(1)	1.909(10)
Re(1)-C(4)	1.932(9)
Re(1)-C(3)	2.006(10)
Re(1)-C(2)	2.007(10)
Re(1)-P(1)	2.529(2)
Re(1)-Se(1)	2.6270(11)
Re(2)-C(7)	1.926(9)
Re(2)-C(6)	1.962(9)
Re(2)-C(8)	1.999(9)
Re(2)-C(5)	2.012(10)
Re(2)-P(1)	2.543(2)
Re(2)-Se(1)	2.6585(10)
Se(1)-Fe(2)	2.3924(15)
Se(1)-Fe(1)	2.4139(15)
Se(2)-C(41)	1.952(9)
Se(2)-Fe(1)	2.3599(19)
Se(2)-Fe(2)	2.3620(17)
Fe(1)-C(9)	1.757(11)
Fe(1)-C(10)	1.786(11)
Fe(1)-C(11)	1.800(11)
Fe(1)-Fe(2)	2.5762(18)
Fe(2)-C(13)	1.773(12)
Fe(2)-C(12)	1.775(11)
Fe(2)-C(14)	1.776(10)
P(1)-C(21)	1.875(8)
P(1)-C(31)	1.880(8)
O(1)-C(1)	1.177(10)
O(2)-C(2)	1.124(10)
O(3)-C(3)	1.119(10)
O(4)-C(4)	1.137(10)
O(5)-C(5)	1.137(10)
O(6)-C(6)	1.138(10)
O(7)-C(7)	1.150(10)
O(8)-C(8)	1.125(9)

O(9)-C(9)	1.132(11)
O(10)-C(10)	1.129(11)
O(11)-C(11)	1.127(11)
O(12)-C(12)	1.127(11)
O(13)-C(13)	1.139(12)
O(14)-C(14)	1.128(10)
C(21)-C(22)	1.531(11)
C(21)-C(26)	1.535(10)
C(22)-C(23)	1.551(11)
C(23)-C(24)	1.519(13)
C(24)-C(25)	1.494(13)
C(25)-C(26)	1.520(11)
C(31)-C(36)	1.459(11)
C(31)-C(32)	1.524(11)
C(32)-C(33)	1.514(12)
C(33)-C(34)	1.489(13)
C(34)-C(35)	1.549(14)
C(35)-C(36)	1.534(12)

C(1)-Re(1)-C(4)	87.2(4)
C(1)-Re(1)-C(3)	95.6(4)
C(4)-Re(1)-C(3)	89.2(4)
C(1)-Re(1)-C(2)	92.8(4)
C(4)-Re(1)-C(2)	89.3(4)
C(3)-Re(1)-C(2)	171.3(4)
C(1)-Re(1)-P(1)	93.1(3)
C(4)-Re(1)-P(1)	176.0(3)
C(3)-Re(1)-P(1)	86.9(3)
C(2)-Re(1)-P(1)	94.6(3)
C(1)-Re(1)-Se(1)	172.0(2)
C(4)-Re(1)-Se(1)	100.7(3)
C(3)-Re(1)-Se(1)	83.3(3)
C(2)-Re(1)-Se(1)	88.6(3)
P(1)-Re(1)-Se(1)	78.99(6)
C(7)-Re(2)-C(6)	86.3(4)
C(7)-Re(2)-C(8)	90.1(4)

C(6)-Re(2)-C(8)	91.9(4)
C(7)-Re(2)-C(5)	92.8(4)
C(6)-Re(2)-C(5)	89.2(3)
C(8)-Re(2)-C(5)	177.0(3)
C(7)-Re(2)-P(1)	96.7(3)
C(6)-Re(2)-P(1)	176.2(3)
C(8)-Re(2)-P(1)	90.5(3)
C(5)-Re(2)-P(1)	88.2(2)
C(7)-Re(2)-Se(1)	174.6(3)
C(6)-Re(2)-Se(1)	98.9(3)
C(8)-Re(2)-Se(1)	88.5(2)
C(5)-Re(2)-Se(1)	88.6(3)
P(1)-Re(2)-Se(1)	78.18(5)
Fe(2)-Se(1)-Fe(1)	64.82(5)
Fe(2)-Se(1)-Re(1)	125.46(5)
Fe(1)-Se(1)-Re(1)	122.41(5)
Fe(2)-Se(1)-Re(2)	121.57(5)
Fe(1)-Se(1)-Re(2)	124.83(5)
Re(1)-Se(1)-Re(2)	98.20(3)
C(41)-Se(2)-Fe(1)	113.8(3)
C(41)-Se(2)-Fe(2)	112.7(3)
Fe(1)-Se(2)-Fe(2)	66.13(6)
C(9)-Fe(1)-C(10)	89.9(5)
C(9)-Fe(1)-C(11)	98.3(5)
C(10)-Fe(1)-C(11)	98.2(4)
C(9)-Fe(1)-Se(2)	159.6(4)
C(10)-Fe(1)-Se(2)	91.1(4)
C(11)-Fe(1)-Se(2)	101.7(4)
C(9)-Fe(1)-Se(1)	93.0(3)
C(10)-Fe(1)-Se(1)	157.2(3)
C(11)-Fe(1)-Se(1)	103.7(3)
Se(2)-Fe(1)-Se(1)	78.56(5)
C(9)-Fe(1)-Fe(2)	102.8(4)
C(10)-Fe(1)-Fe(2)	100.2(3)
C(11)-Fe(1)-Fe(2)	151.9(3)
Se(2)-Fe(1)-Fe(2)	56.97(5)

Se(1)-Fe(1)-Fe(2)	57.19(4)
C(13)-Fe(2)-C(12)	100.2(5)
C(13)-Fe(2)-C(14)	100.2(5)
C(12)-Fe(2)-C(14)	91.5(5)
C(13)-Fe(2)-Se(2)	96.6(4)
C(12)-Fe(2)-Se(2)	161.8(4)
C(14)-Fe(2)-Se(2)	92.4(3)
C(13)-Fe(2)-Se(1)	100.7(3)
C(12)-Fe(2)-Se(1)	91.0(3)
C(14)-Fe(2)-Se(1)	158.2(4)
Se(2)-Fe(2)-Se(1)	78.95(5)
C(13)-Fe(2)-Fe(1)	146.8(4)
C(12)-Fe(2)-Fe(1)	104.9(4)
C(14)-Fe(2)-Fe(1)	100.5(4)
Se(2)-Fe(2)-Fe(1)	56.90(5)
Se(1)-Fe(2)-Fe(1)	57.99(5)
C(21)-P(1)-C(31)	103.3(4)
C(21)-P(1)-Re(1)	109.4(3)
C(31)-P(1)-Re(1)	115.3(3)
C(21)-P(1)-Re(2)	110.0(3)
C(31)-P(1)-Re(2)	115.0(3)
Re(1)-P(1)-Re(2)	103.94(8)
O(1)-C(1)-Re(1)	178.6(8)
O(2)-C(2)-Re(1)	176.9(9)
O(3)-C(3)-Re(1)	174.6(9)
O(4)-C(4)-Re(1)	174.8(9)
O(5)-C(5)-Re(2)	177.3(9)
O(6)-C(6)-Re(2)	172.1(9)
O(7)-C(7)-Re(2)	177.0(8)
O(8)-C(8)-Re(2)	178.9(9)
O(9)-C(9)-Fe(1)	176.9(12)
O(10)-C(10)-Fe(1)	179.2(11)
O(11)-C(11)-Fe(1)	177.1(11)
O(12)-C(12)-Fe(2)	178.3(12)
O(13)-C(13)-Fe(2)	176.4(11)
O(14)-C(14)-Fe(2)	179.5(10)

C(22)-C(21)-C(26)	108.6(7)
C(22)-C(21)-P(1)	114.9(6)
C(26)-C(21)-P(1)	114.5(6)
C(21)-C(22)-C(23)	111.1(7)
C(24)-C(23)-C(22)	110.1(8)
C(25)-C(24)-C(23)	112.9(9)
C(24)-C(25)-C(26)	110.5(8)
C(25)-C(26)-C(21)	112.7(8)
C(36)-C(31)-C(32)	110.8(8)
C(36)-C(31)-P(1)	117.1(6)
C(32)-C(31)-P(1)	114.7(6)
C(33)-C(32)-C(31)	112.7(8)
C(34)-C(33)-C(32)	112.8(9)
C(33)-C(34)-C(35)	110.5(9)
C(36)-C(35)-C(34)	111.4(9)
C(31)-C(36)-C(35)	114.6(8)

Table S7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3b**. 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)	42(1)	31(1)	0(1)	5(1)	-1(1)
Re(2)	27(1)	33(1)	38(1)	2(1)	4(1)	1(1)
Se(1)	33(1)	37(1)	32(1)	-2(1)	1(1)	-2(1)
Se(2)	55(1)	59(1)	57(1)	-8(1)	8(1)	-12(1)
Fe(1)	51(1)	37(1)	44(1)	-5(1)	2(1)	0(1)
Fe(2)	49(1)	51(1)	33(1)	-4(1)	-2(1)	-9(1)
P(1)	31(1)	36(1)	32(1)	0(1)	3(1)	-2(1)
O(1)	51(4)	79(5)	77(5)	6(4)	-3(4)	-20(4)
C(1)	41(5)	52(6)	37(5)	-1(4)	9(4)	8(5)
O(2)	128(7)	81(6)	53(4)	24(4)	-16(5)	18(6)
C(2)	53(6)	58(6)	46(6)	-1(5)	12(5)	2(5)
O(3)	68(5)	71(5)	81(5)	29(4)	-11(4)	17(4)
C(3)	29(5)	61(7)	57(6)	-10(5)	2(5)	0(5)
O(4)	86(6)	99(6)	81(5)	-16(5)	42(5)	7(5)
C(4)	43(6)	67(7)	53(6)	-8(5)	18(5)	0(5)
O(5)	87(6)	75(5)	78(5)	39(4)	-35(5)	-8(5)
C(5)	24(5)	49(6)	61(6)	-3(5)	-3(4)	-1(4)
O(6)	36(4)	47(4)	140(7)	11(4)	9(4)	2(4)
C(6)	30(5)	29(5)	77(7)	6(4)	5(5)	6(4)
O(7)	85(6)	59(5)	88(5)	-3(4)	47(5)	16(4)
C(7)	30(5)	43(5)	70(6)	-4(5)	14(5)	1(4)
O(8)	98(6)	67(5)	58(4)	22(4)	0(4)	10(5)
C(8)	35(5)	51(6)	36(5)	0(4)	7(4)	10(5)
O(9)	55(5)	79(6)	168(9)	-33(6)	34(6)	6(5)
C(9)	52(7)	56(7)	84(8)	-22(6)	3(6)	7(6)
O(10)	99(6)	52(5)	100(6)	-33(4)	16(5)	-20(5)
C(10)	77(8)	49(6)	61(7)	-2(5)	11(6)	2(6)
O(11)	201(11)	79(6)	63(5)	8(5)	-25(6)	9(7)
C(11)	91(9)	45(6)	59(6)	-15(5)	-9(6)	5(6)
O(12)	104(7)	163(9)	52(5)	-12(5)	25(5)	-49(7)
C(12)	80(8)	79(8)	36(5)	-5(5)	5(5)	-25(7)

O(13)	101(7)	85(6)	98(6)	13(5)	-33(6)	11(6)
C(13)	72(8)	63(7)	52(6)	6(5)	-25(6)	-2(6)
O(14)	126(8)	104(7)	63(5)	-33(5)	3(5)	-56(6)
C(14)	66(7)	83(8)	44(6)	-13(6)	5(5)	-20(7)
C(21)	38(4)	51(5)	30(4)	-3(4)	-2(4)	0(4)
C(22)	38(5)	79(7)	34(4)	-8(5)	-6(4)	-8(5)
C(23)	46(5)	108(9)	47(5)	0(6)	-12(4)	-3(6)
C(24)	80(6)	111(9)	32(5)	-3(6)	-14(5)	-3(7)
C(25)	76(6)	96(8)	31(4)	8(5)	8(5)	-2(7)
C(26)	46(5)	79(7)	35(4)	-4(5)	7(4)	2(5)
C(31)	60(6)	35(5)	56(5)	4(4)	22(5)	3(5)
C(32)	51(6)	40(5)	62(6)	-3(4)	13(5)	5(5)
C(33)	113(10)	41(5)	87(7)	-8(5)	31(7)	9(6)
C(34)	127(10)	53(6)	58(6)	10(5)	1(6)	23(7)
C(35)	106(9)	41(5)	63(6)	6(5)	14(6)	-20(6)
C(36)	92(8)	42(5)	61(6)	10(5)	23(6)	3(6)
C(41)	64(7)	83(8)	95(9)	-35(7)	10(6)	-42(7)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3b**.

	x	y	z	U(eq)
H(21)	3794	3653	2947	48
H(22A)	5472	4906	2944	61
H(22B)	5825	4158	2614	61
H(23A)	5983	3567	3643	81
H(23B)	6959	4249	3676	81
H(24A)	5643	4205	4603	90
H(24B)	5384	4936	4212	90
H(25A)	3325	4484	4492	81
H(25B)	3629	3720	4178	81
H(26A)	3206	5041	3469	64
H(26B)	2192	4378	3451	64
H(31)	3769	5573	2368	59
H(32A)	974	5688	2072	61
H(32B)	1652	5593	2779	61
H(33A)	1093	6826	2566	95
H(33B)	2655	6734	2733	95
H(34A)	2393	7500	1854	96
H(34B)	1436	6937	1475	96
H(35A)	3572	6816	1049	84
H(35B)	4282	6747	1752	84
H(36A)	2611	5667	1120	77
H(36B)	4165	5581	1307	77
H(41A)	-1502	1171	166	121
H(41B)	-2459	1271	745	121
H(41C)	-1212	738	820	121

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Te(1)	-2341(1)	7359(1)	1764(1)	16(1)
Te(2)	-3776(1)	7595(1)	-177(1)	27(1)
Re(1)	-4348(1)	8740(1)	2149(1)	15(1)
Re(2)	-907(1)	6843(1)	3361(1)	15(1)
Fe(1)	-1166(1)	7433(1)	277(1)	24(1)
Fe(2)	-3098(1)	5898(1)	1154(1)	21(1)
P(1)	-2631(1)	8341(1)	3432(1)	14(1)
O(1)	-2586(4)	10862(3)	1037(2)	35(1)
C(1)	-3187(5)	10081(4)	1441(3)	24(1)
O(2)	-6284(4)	10109(3)	2936(3)	37(1)
C(2)	-5569(5)	9596(3)	2640(3)	23(1)
O(3)	-6140(4)	6590(3)	3147(2)	36(1)
C(3)	-5474(5)	7366(4)	2804(3)	23(1)
O(4)	-6434(4)	9278(3)	588(2)	35(1)
C(4)	-5620(5)	9042(3)	1150(3)	22(1)
O(5)	645(4)	6482(3)	5101(2)	36(1)
C(5)	23(5)	6620(3)	4466(3)	22(1)
O(6)	1149(4)	5045(3)	3158(3)	37(1)
C(6)	370(5)	5702(3)	3204(3)	24(1)
O(7)	1475(4)	8588(3)	2372(2)	34(1)
C(7)	590(5)	7973(3)	2714(3)	22(1)
O(8)	-3329(4)	5124(3)	4333(3)	40(1)
C(8)	-2456(5)	5742(3)	3984(3)	22(1)
O(9)	-443(4)	9728(3)	-808(3)	55(1)
C(9)	-724(5)	8847(4)	-374(4)	35(1)
O(10)	-343(5)	6342(4)	-975(3)	64(1)
C(10)	-686(6)	6777(4)	-491(3)	38(1)
O(11)	1586(4)	6902(3)	1158(3)	52(1)
C(11)	502(6)	7075(4)	825(3)	35(1)
O(12)	-1508(4)	4291(3)	2580(3)	46(1)
C(12)	-2113(5)	4932(3)	2009(3)	28(1)

O(13)	-6049(4)	5274(3)	1899(2)	38(1)
C(13)	-4891(5)	5530(3)	1620(3)	25(1)
O(14)	-2928(5)	4498(3)	89(3)	54(1)
C(14)	-2983(6)	5062(4)	489(3)	32(1)
C(21)	-3568(4)	8086(3)	4555(3)	18(1)
C(22)	-2669(5)	7446(4)	5360(3)	23(1)
C(23)	-3396(5)	7380(4)	6251(3)	29(1)
C(24)	-4907(5)	6882(4)	6369(3)	31(1)
C(25)	-5808(5)	7503(4)	5570(3)	25(1)
C(26)	-5064(4)	7549(3)	4681(3)	21(1)
C(31)	-1599(4)	9638(3)	3240(3)	16(1)
C(32)	-390(5)	9562(3)	3889(3)	22(1)
C(33)	505(5)	10615(3)	3552(3)	28(1)
C(34)	-416(5)	11623(4)	3468(4)	37(1)
C(35)	-1657(5)	11693(3)	2859(4)	30(1)
C(36)	-2535(5)	10634(3)	3187(3)	22(1)
C(41)	-3872(7)	7146(5)	-1339(3)	52(2)

Table S10. Bond lengths [Å] and angles [°] for **3c**.

Te(1)-Fe(1)	2.5432(7)
Te(1)-Fe(2)	2.5552(6)
Te(1)-Re(1)	2.7811(3)
Te(1)-Re(2)	2.7864(3)
Te(2)-C(41)	2.147(5)
Te(2)-Fe(2)	2.5422(7)
Te(2)-Fe(1)	2.5448(7)
Re(1)-C(2)	1.919(4)
Re(1)-C(4)	1.948(5)
Re(1)-C(3)	1.995(5)
Re(1)-C(1)	1.999(5)
Re(1)-P(1)	2.5516(10)
Re(2)-C(5)	1.925(5)
Re(2)-C(6)	1.973(4)
Re(2)-C(7)	1.997(4)
Re(2)-C(8)	2.001(4)
Re(2)-P(1)	2.5432(10)
Fe(1)-C(10)	1.774(5)
Fe(1)-C(11)	1.786(6)
Fe(1)-C(9)	1.798(5)
Fe(1)-Fe(2)	2.6476(9)
Fe(2)-C(12)	1.766(5)
Fe(2)-C(14)	1.778(5)
Fe(2)-C(13)	1.792(5)
P(1)-C(31)	1.872(4)
P(1)-C(21)	1.879(4)
O(1)-C(1)	1.126(5)
O(2)-C(2)	1.143(5)
O(3)-C(3)	1.135(5)
O(4)-C(4)	1.151(5)
O(5)-C(5)	1.145(5)
O(6)-C(6)	1.136(5)
O(7)-C(7)	1.129(5)
O(8)-C(8)	1.125(5)

O(9)-C(9)	1.131(6)
O(10)-C(10)	1.148(6)
O(11)-C(11)	1.140(6)
O(12)-C(12)	1.150(5)
O(13)-C(13)	1.152(6)
O(14)-C(14)	1.137(5)
C(21)-C(22)	1.531(6)
C(21)-C(26)	1.536(6)
C(22)-C(23)	1.524(6)
C(23)-C(24)	1.529(7)
C(24)-C(25)	1.520(6)
C(25)-C(26)	1.534(6)
C(31)-C(36)	1.532(5)
C(31)-C(32)	1.539(6)
C(32)-C(33)	1.521(6)
C(33)-C(34)	1.527(6)
C(34)-C(35)	1.522(6)
C(35)-C(36)	1.519(6)

Fe(1)-Te(1)-Fe(2)	62.57(2)
Fe(1)-Te(1)-Re(1)	130.889(17)
Fe(2)-Te(1)-Re(1)	121.434(18)
Fe(1)-Te(1)-Re(2)	124.692(18)
Fe(2)-Te(1)-Re(2)	122.664(17)
Re(1)-Te(1)-Re(2)	95.339(9)
C(41)-Te(2)-Fe(2)	108.45(15)
C(41)-Te(2)-Fe(1)	107.74(18)
Fe(2)-Te(2)-Fe(1)	62.73(2)
C(2)-Re(1)-C(4)	89.99(18)
C(2)-Re(1)-C(3)	92.32(18)
C(4)-Re(1)-C(3)	88.65(18)
C(2)-Re(1)-C(1)	90.58(18)
C(4)-Re(1)-C(1)	89.94(18)
C(3)-Re(1)-C(1)	176.78(17)
C(2)-Re(1)-P(1)	91.27(13)
C(4)-Re(1)-P(1)	178.56(13)

C(3)-Re(1)-P(1)	91.99(12)
C(1)-Re(1)-P(1)	89.35(12)
C(2)-Re(1)-Te(1)	168.78(13)
C(4)-Re(1)-Te(1)	100.93(12)
C(3)-Re(1)-Te(1)	85.44(12)
C(1)-Re(1)-Te(1)	91.99(13)
P(1)-Re(1)-Te(1)	77.85(2)
C(5)-Re(2)-C(6)	87.86(18)
C(5)-Re(2)-C(7)	88.75(18)
C(6)-Re(2)-C(7)	88.95(17)
C(5)-Re(2)-C(8)	92.67(18)
C(6)-Re(2)-C(8)	92.29(17)
C(7)-Re(2)-C(8)	178.15(16)
C(5)-Re(2)-P(1)	96.95(12)
C(6)-Re(2)-P(1)	175.17(13)
C(7)-Re(2)-P(1)	90.69(12)
C(8)-Re(2)-P(1)	87.96(11)
C(5)-Re(2)-Te(1)	174.54(12)
C(6)-Re(2)-Te(1)	97.29(13)
C(7)-Re(2)-Te(1)	89.54(12)
C(8)-Re(2)-Te(1)	88.94(12)
P(1)-Re(2)-Te(1)	77.89(2)
C(10)-Fe(1)-C(11)	92.4(2)
C(10)-Fe(1)-C(9)	101.8(2)
C(11)-Fe(1)-C(9)	97.0(2)
C(10)-Fe(1)-Te(1)	150.06(17)
C(11)-Fe(1)-Te(1)	88.42(15)
C(9)-Fe(1)-Te(1)	107.77(17)
C(10)-Fe(1)-Te(2)	91.28(19)
C(11)-Fe(1)-Te(2)	166.74(16)
C(9)-Fe(1)-Te(2)	94.71(16)
Te(1)-Fe(1)-Te(2)	82.04(2)
C(10)-Fe(1)-Fe(2)	92.69(17)
C(11)-Fe(1)-Fe(2)	108.50(17)
C(9)-Fe(1)-Fe(2)	150.09(16)
Te(1)-Fe(1)-Fe(2)	58.94(2)

Te(2)-Fe(1)-Fe(2)	58.59(2)
C(12)-Fe(2)-C(14)	91.6(2)
C(12)-Fe(2)-C(13)	99.7(2)
C(14)-Fe(2)-C(13)	98.3(2)
C(12)-Fe(2)-Te(2)	162.32(15)
C(14)-Fe(2)-Te(2)	92.53(16)
C(13)-Fe(2)-Te(2)	96.67(14)
C(12)-Fe(2)-Te(1)	87.78(13)
C(14)-Fe(2)-Te(1)	157.62(17)
C(13)-Fe(2)-Te(1)	103.87(13)
Te(2)-Fe(2)-Te(1)	81.860(19)
C(12)-Fe(2)-Fe(1)	103.66(15)
C(14)-Fe(2)-Fe(1)	100.11(17)
C(13)-Fe(2)-Fe(1)	149.65(14)
Te(2)-Fe(2)-Fe(1)	58.69(2)
Te(1)-Fe(2)-Fe(1)	58.491(19)
C(31)-P(1)-C(21)	102.10(18)
C(31)-P(1)-Re(2)	109.66(13)
C(21)-P(1)-Re(2)	115.75(13)
C(31)-P(1)-Re(1)	107.47(13)
C(21)-P(1)-Re(1)	113.66(13)
Re(2)-P(1)-Re(1)	107.78(4)
O(1)-C(1)-Re(1)	177.0(4)
O(2)-C(2)-Re(1)	179.3(4)
O(3)-C(3)-Re(1)	177.4(4)
O(4)-C(4)-Re(1)	174.2(4)
O(5)-C(5)-Re(2)	176.3(4)
O(6)-C(6)-Re(2)	175.8(4)
O(7)-C(7)-Re(2)	177.3(4)
O(8)-C(8)-Re(2)	179.9(5)
O(9)-C(9)-Fe(1)	177.8(5)
O(10)-C(10)-Fe(1)	178.2(5)
O(11)-C(11)-Fe(1)	176.6(5)
O(12)-C(12)-Fe(2)	178.0(5)
O(13)-C(13)-Fe(2)	177.5(4)
O(14)-C(14)-Fe(2)	177.6(5)

C(22)-C(21)-C(26)	109.1(3)
C(22)-C(21)-P(1)	114.2(3)
C(26)-C(21)-P(1)	115.0(3)
C(23)-C(22)-C(21)	112.4(4)
C(22)-C(23)-C(24)	111.2(4)
C(25)-C(24)-C(23)	110.9(4)
C(24)-C(25)-C(26)	111.5(4)
C(25)-C(26)-C(21)	110.8(3)
C(36)-C(31)-C(32)	107.9(3)
C(36)-C(31)-P(1)	114.6(3)
C(32)-C(31)-P(1)	116.6(3)
C(33)-C(32)-C(31)	110.2(3)
C(32)-C(33)-C(34)	111.6(4)
C(35)-C(34)-C(33)	109.8(4)
C(36)-C(35)-C(34)	111.2(4)
C(35)-C(36)-C(31)	111.5(4)

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3c**. 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}
Te(1)	17(1)	18(1)	15(1)	-8(1)	-1(1)	2(1)
Te(2)	36(1)	26(1)	19(1)	-9(1)	-7(1)	2(1)
Re(1)	13(1)	18(1)	14(1)	-6(1)	-2(1)	1(1)
Re(2)	14(1)	15(1)	16(1)	-5(1)	-2(1)	2(1)
Fe(1)	28(1)	23(1)	19(1)	-7(1)	5(1)	2(1)
Fe(2)	28(1)	19(1)	19(1)	-9(1)	-1(1)	-1(1)
P(1)	15(1)	14(1)	13(1)	-5(1)	-1(1)	0(1)
O(1)	36(2)	36(2)	25(2)	-1(2)	-2(2)	-13(2)
C(1)	23(2)	28(2)	19(2)	-7(2)	-6(2)	1(2)
O(2)	26(2)	37(2)	54(2)	-26(2)	5(2)	6(2)
C(2)	20(2)	22(2)	24(2)	-6(2)	-2(2)	-1(2)
O(3)	36(2)	35(2)	36(2)	-13(2)	4(2)	-12(2)
C(3)	19(2)	31(2)	23(2)	-16(2)	-5(2)	1(2)
O(4)	27(2)	54(2)	25(2)	-15(2)	-11(2)	4(2)
C(4)	19(2)	27(2)	22(2)	-12(2)	3(2)	-2(2)
O(5)	32(2)	50(2)	24(2)	-9(2)	-11(2)	6(2)
C(5)	23(2)	22(2)	21(2)	-8(2)	3(2)	-1(2)
O(6)	25(2)	32(2)	55(2)	-18(2)	3(2)	8(1)
C(6)	22(2)	21(2)	28(2)	-7(2)	0(2)	-4(2)
O(7)	23(2)	37(2)	36(2)	-8(2)	6(2)	-6(2)
C(7)	18(2)	22(2)	24(2)	-9(2)	-2(2)	3(2)
O(8)	38(2)	25(2)	51(2)	-7(2)	7(2)	-11(2)
C(8)	20(2)	19(2)	26(2)	-8(2)	-3(2)	5(2)
O(9)	47(3)	33(2)	63(3)	8(2)	7(2)	-2(2)
C(9)	24(3)	39(3)	37(3)	-8(2)	3(2)	1(2)
O(10)	74(3)	75(3)	59(3)	-48(3)	27(2)	-8(2)
C(10)	42(3)	40(3)	31(3)	-14(2)	15(2)	-7(2)
O(11)	30(2)	75(3)	44(2)	-15(2)	-7(2)	21(2)
C(11)	44(3)	37(3)	22(3)	-11(2)	9(2)	7(2)
O(12)	62(3)	21(2)	52(3)	-9(2)	-30(2)	7(2)
C(12)	35(3)	18(2)	35(3)	-15(2)	-3(2)	-5(2)

O(13)	37(2)	39(2)	35(2)	-11(2)	1(2)	-3(2)
C(13)	34(3)	23(2)	20(2)	-9(2)	-4(2)	-1(2)
O(14)	78(3)	49(2)	51(3)	-38(2)	-5(2)	2(2)
C(14)	43(3)	27(2)	27(3)	-12(2)	0(2)	-1(2)
C(21)	19(2)	20(2)	13(2)	-5(2)	4(2)	-4(2)
C(22)	22(2)	31(2)	16(2)	-9(2)	-1(2)	-1(2)
C(23)	32(3)	43(3)	14(2)	-13(2)	-1(2)	-5(2)
C(24)	37(3)	40(3)	16(2)	-9(2)	6(2)	-6(2)
C(25)	16(2)	37(3)	21(2)	-8(2)	4(2)	-3(2)
C(26)	19(2)	27(2)	16(2)	-7(2)	0(2)	1(2)
C(31)	17(2)	10(2)	19(2)	-4(2)	3(2)	-3(1)
C(32)	23(2)	25(2)	20(2)	-12(2)	-5(2)	2(2)
C(33)	21(2)	29(2)	39(3)	-18(2)	-7(2)	-2(2)
C(34)	28(3)	30(3)	61(4)	-26(3)	-6(3)	-3(2)
C(35)	27(3)	18(2)	46(3)	-11(2)	-4(2)	-1(2)
C(36)	21(2)	19(2)	28(2)	-11(2)	0(2)	0(2)
C(41)	93(5)	46(3)	21(3)	-16(3)	-10(3)	-2(3)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3c**.

	x	y	z	U(eq)
H(21)	-3730	8829	4590	21
H(22A)	-2505	6691	5369	27
H(22B)	-1718	7810	5290	27
H(23A)	-3460	8128	6274	34
H(23B)	-2805	6922	6752	34
H(24A)	-4835	6099	6431	37
H(24B)	-5385	6910	6925	37
H(25A)	-5973	8263	5551	30
H(25B)	-6757	7137	5644	30
H(26A)	-5664	7976	4174	25
H(26B)	-4965	6792	4680	25
H(31)	-1109	9834	2633	19
H(32A)	-815	9446	4495	26
H(32B)	236	8926	3934	26
H(33A)	964	10710	2958	33
H(33B)	1279	10554	3974	33
H(34A)	-800	11568	4070	44
H(34B)	183	12298	3215	44
H(35A)	-2289	12316	2842	36
H(35B)	-1270	11835	2240	36
H(36A)	-3322	10700	2773	27
H(36B)	-2977	10519	3789	27
H(41A)	-3319	6471	-1241	77
H(41B)	-3463	7742	-1866	77
H(41C)	-4878	7021	-1438	77

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	5168(1)	11402(1)	3025(1)	28(1)
Re(2)	6148(1)	12757(1)	4052(1)	32(1)
Re(3)	9036(1)	13039(1)	1321(1)	29(1)
Re(4)	9691(1)	10819(1)	886(1)	30(1)
Fe(1)	7055(1)	13190(1)	2846(1)	30(1)
Fe(2)	8076(1)	12127(1)	3313(1)	30(1)
Fe(3)	7505(1)	10975(1)	1623(1)	35(1)
Fe(4)	9056(1)	10774(1)	2100(1)	32(1)
S(1)	6542(2)	12356(2)	3339(1)	28(1)
S(2)	7343(2)	11835(2)	2644(1)	30(1)
S(3)	8127(2)	11889(2)	2159(1)	31(1)
S(4)	8835(2)	11419(2)	1434(1)	31(1)
P(1)	5102(2)	11491(3)	3805(1)	30(1)
P(2)	10266(2)	12342(3)	993(1)	28(1)
O(1)	3439(7)	10312(7)	2718(4)	55(3)
C(1)	4095(10)	10701(10)	2850(5)	37(3)
O(2)	5248(7)	11397(8)	2066(4)	50(3)
C(2)	5273(10)	11408(11)	2429(5)	39(3)
O(3)	6488(7)	9821(7)	3187(4)	54(3)
C(3)	5985(10)	10388(10)	3143(6)	37(3)
O(41) #	3826(16)	12972(15)	2910(20)	52(10)
O(42) #	4160(20)	13155(13)	2871(19)	61(13)
C(4)	4407(11)	12445(10)	2951(5)	43(4)
O(5)	4640(8)	14124(8)	3671(4)	58(3)
C(5)	5160(10)	13603(10)	3794(5)	36(3)
O(6)	7760(7)	11583(8)	4490(4)	55(3)
C(6)	7168(10)	11990(11)	4322(5)	41(3)
O(7)	5629(9)	12892(9)	4930(4)	67(4)
C(7)	5791(10)	12854(11)	4590(6)	45(4)
O(8)	7390(8)	14343(8)	4284(4)	65(4)

C(8)	6950(11)	13752(12)	4190(6)	47(4)
O(9)	6674(8)	14682(7)	3321(4)	60(4)
C(9)	6877(11)	14098(10)	3142(6)	39(4)
O(10)	8557(7)	14033(7)	2537(4)	47(3)
C(10)	7988(9)	13688(9)	2653(5)	29(3)
O(11)	5497(8)	13535(8)	2122(5)	73(4)
C(11)	6093(10)	13400(10)	2419(6)	44(4)
O(12)	8805(7)	13398(8)	3964(4)	60(4)
C(12)	8465(9)	12915(10)	3720(5)	31(3)
O(13)	9896(7)	12163(8)	3096(4)	60(4)
C(13)	9168(10)	12154(11)	3177(5)	40(4)
O(14)	8341(8)	10510(7)	3794(4)	55(3)
C(14)	8247(10)	11103(10)	3591(5)	36(3)
O(15)	7661(8)	13147(9)	448(4)	66(4)
C(15)	8182(10)	13055(11)	749(6)	41(3)
O(16)	7339(7)	13743(8)	1629(3)	48(3)
C(16)	7988(9)	13465(9)	1541(5)	31(3)
O(17)	10240(8)	13114(8)	2250(4)	54(3)
C(17)	9830(10)	13064(10)	1926(5)	33(3)
O(18)	9618(8)	14903(7)	1218(5)	59(4)
C(18)	9399(11)	14201(10)	1237(5)	38(3)
O(19)	10896(7)	10461(8)	235(4)	57(3)
C(19)	10448(10)	10590(11)	507(5)	37(3)
O(20)	9026(8)	8938(7)	749(4)	60(4)
C(20)	9239(10)	9655(10)	814(5)	35(3)
O(21)	7985(8)	11289(9)	187(5)	73(4)
C(21)	8638(11)	11177(10)	449(6)	40(3)
O(22)	11253(8)	10144(8)	1621(4)	55(3)
C(22)	10698(10)	10406(9)	1353(5)	34(3)
O(23)	7216(8)	9643(9)	969(5)	79(5)
C(23)	7349(10)	10165(12)	1230(6)	50(4)
O(24)	6051(9)	12110(10)	1172(5)	89(5)
C(24)	6625(11)	11656(13)	1342(6)	58(5)
O(25)	6567(8)	9930(8)	2156(4)	58(3)
C(25)	6914(11)	10342(11)	1960(6)	47(4)
O(26)	9343(9)	9088(7)	1761(4)	57(3)

C(26)	9227(12)	9748(11)	1882(6)	45(4)
O(27)	8700(9)	9940(8)	2868(4)	62(4)
C(27)	8851(10)	10278(11)	2577(6)	41(4)
O(28)	10997(7)	11223(8)	2458(4)	58(4)
C(28)	10254(11)	11081(11)	2334(5)	39(4)
C(31)	5605(11)	10511(10)	4087(5)	39(3)
C(32)	5737(10)	10521(10)	4565(5)	38(3)
C(33)	6294(11)	9766(10)	4773(6)	48(4)
C(34)	5885(13)	8918(11)	4605(6)	59(5)
C(35)	5704(12)	8889(10)	4131(6)	54(4)
C(36)	5117(10)	9647(9)	3927(5)	40(3)
C(41)	3925(10)	11525(11)	3936(7)	54(4)
C(42)	3203(12)	11114(16)	3623(9)	113(8)
C(43)	2245(13)	11035(18)	3778(10)	133(9)
C(44)	1952(12)	11948(17)	3877(9)	105(7)
C(45)	2650(13)	12212(18)	4216(9)	114(8)
C(46)	3601(13)	12272(16)	4076(9)	116(8)
C(51)	11395(9)	12329(9)	1395(5)	25(3)
C(52)	11751(9)	13208(8)	1588(5)	28(3)
C(53)	12502(9)	13034(10)	1971(5)	37(4)
C(54)	13300(10)	12605(10)	1836(5)	42(4)
C(55)	13013(10)	11776(10)	1613(5)	41(4)
C(56)	12197(9)	11904(10)	1230(5)	40(4)
C(61)	10542(9)	12840(9)	501(4)	29(3)
C(62)	10731(11)	13786(10)	529(5)	43(4)
C(63)	11124(13)	14105(12)	159(6)	64(5)
C(64)	10491(13)	13893(12)	-268(6)	59(5)
C(65)	10265(13)	12956(12)	-286(6)	58(5)
C(66)	9886(12)	12644(12)	95(5)	52(4)
Cl(1) #	6610(20)	16200(20)	4786(11)	295(14)
Cl(2) #	5550(20)	15280(20)	4629(11)	283(13)
C(100) #	5820(40)	16060(30)	4370(20)	149(19)

site occupation factor 0.5

Table S14. Bond lengths [Å] and angles [°] for **4a**.

Re(1)-C(1)	1.913(15)
Re(1)-C(2)	1.945(17)
Re(1)-C(4)	1.965(15)
Re(1)-C(3)	1.979(15)
Re(1)-P(1)	2.526(4)
Re(1)-S(1)	2.551(4)
Re(2)-C(7)	1.908(17)
Re(2)-C(8)	1.949(17)
Re(2)-C(6)	1.978(17)
Re(2)-C(5)	2.016(16)
Re(2)-P(1)	2.532(4)
Re(2)-S(1)	2.552(4)
Re(3)-C(18)	1.926(17)
Re(3)-C(16)	1.949(14)
Re(3)-C(15)	1.997(17)
Re(3)-C(17)	2.047(17)
Re(3)-P(2)	2.528(4)
Re(3)-S(4)	2.580(4)
Re(4)-C(19)	1.848(16)
Re(4)-C(20)	1.933(16)
Re(4)-C(21)	1.946(17)
Re(4)-C(22)	1.987(16)
Re(4)-P(2)	2.524(4)
Re(4)-S(4)	2.547(4)
Fe(1)-C(9)	1.755(17)
Fe(1)-C(11)	1.785(16)
Fe(1)-C(10)	1.803(15)
Fe(1)-S(2)	2.276(4)
Fe(1)-S(1)	2.293(4)
Fe(1)-Fe(2)	2.517(3)
Fe(2)-C(13)	1.759(15)
Fe(2)-C(12)	1.797(16)
Fe(2)-C(14)	1.820(16)
Fe(2)-S(2)	2.237(5)

Fe(2)-S(1)	2.315(4)
Fe(3)-C(23)	1.766(18)
Fe(3)-C(24)	1.774(18)
Fe(3)-C(25)	1.814(17)
Fe(3)-S(3)	2.273(5)
Fe(3)-S(4)	2.284(4)
Fe(3)-Fe(4)	2.497(3)
Fe(4)-C(26)	1.785(17)
Fe(4)-C(27)	1.794(17)
Fe(4)-C(28)	1.839(16)
Fe(4)-S(3)	2.250(4)
Fe(4)-S(4)	2.320(5)
S(2)-S(3)	2.127(5)
P(1)-C(31)	1.851(16)
P(1)-C(41)	1.875(14)
P(2)-C(61)	1.877(14)
P(2)-C(51)	1.886(14)
O(1)-C(1)	1.148(16)
O(2)-C(2)	1.158(18)
O(3)-C(3)	1.146(16)
O(41)-C(4)	1.18(2)
O(42)-C(4)	1.18(2)
O(5)-C(5)	1.132(17)
O(6)-C(6)	1.124(17)
O(7)-C(7)	1.165(19)
O(8)-C(8)	1.133(18)
O(9)-C(9)	1.150(17)
O(10)-C(10)	1.124(15)
O(11)-C(11)	1.174(18)
O(12)-C(12)	1.127(17)
O(13)-C(13)	1.158(16)
O(14)-C(14)	1.124(17)
O(15)-C(15)	1.110(18)
O(16)-C(16)	1.141(15)
O(17)-C(17)	1.091(18)
O(18)-C(18)	1.146(17)

O(19)-C(19)	1.216(17)
O(20)-C(20)	1.169(17)
O(21)-C(21)	1.153(18)
O(22)-C(22)	1.134(17)
O(23)-C(23)	1.155(19)
O(24)-C(24)	1.152(19)
O(25)-C(25)	1.099(18)
O(26)-C(26)	1.126(18)
O(27)-C(27)	1.131(18)
O(28)-C(28)	1.111(16)
C(31)-C(32)	1.50(2)
C(31)-C(36)	1.56(2)
C(32)-C(33)	1.51(2)
C(33)-C(34)	1.51(2)
C(34)-C(35)	1.49(2)
C(35)-C(36)	1.53(2)
C(41)-C(46)	1.37(2)
C(41)-C(42)	1.45(2)
C(42)-C(43)	1.60(3)
C(43)-C(44)	1.54(3)
C(44)-C(45)	1.39(3)
C(45)-C(46)	1.57(2)
C(51)-C(56)	1.545(18)
C(51)-C(52)	1.551(17)
C(52)-C(53)	1.497(18)
C(53)-C(54)	1.497(19)
C(54)-C(55)	1.50(2)
C(55)-C(56)	1.55(2)
C(61)-C(66)	1.48(2)
C(61)-C(62)	1.500(19)
C(62)-C(63)	1.51(2)
C(63)-C(64)	1.52(2)
C(64)-C(65)	1.50(2)
C(65)-C(66)	1.52(2)
Cl(1)-C(100)	1.60(5)
Cl(2)-C(100)	1.57(5)

C(1)-Re(1)-C(2)	87.0(7)
C(1)-Re(1)-C(4)	91.1(7)
C(2)-Re(1)-C(4)	92.3(7)
C(1)-Re(1)-C(3)	92.0(6)
C(2)-Re(1)-C(3)	91.2(7)
C(4)-Re(1)-C(3)	175.5(7)
C(1)-Re(1)-P(1)	96.9(5)
C(2)-Re(1)-P(1)	175.9(5)
C(4)-Re(1)-P(1)	86.2(5)
C(3)-Re(1)-P(1)	90.1(5)
C(1)-Re(1)-S(1)	173.5(5)
C(2)-Re(1)-S(1)	99.4(5)
C(4)-Re(1)-S(1)	87.4(5)
C(3)-Re(1)-S(1)	89.2(5)
P(1)-Re(1)-S(1)	76.70(12)
C(7)-Re(2)-C(8)	90.1(7)
C(7)-Re(2)-C(6)	89.1(7)
C(8)-Re(2)-C(6)	90.5(7)
C(7)-Re(2)-C(5)	90.3(7)
C(8)-Re(2)-C(5)	85.8(7)
C(6)-Re(2)-C(5)	176.3(7)
C(7)-Re(2)-P(1)	94.5(5)
C(8)-Re(2)-P(1)	175.0(5)
C(6)-Re(2)-P(1)	91.5(5)
C(5)-Re(2)-P(1)	92.3(4)
C(7)-Re(2)-S(1)	170.1(5)
C(8)-Re(2)-S(1)	99.0(5)
C(6)-Re(2)-S(1)	86.9(5)
C(5)-Re(2)-S(1)	94.3(5)
P(1)-Re(2)-S(1)	76.57(12)
C(18)-Re(3)-C(16)	89.7(6)
C(18)-Re(3)-C(15)	90.2(7)
C(16)-Re(3)-C(15)	85.9(6)
C(18)-Re(3)-C(17)	89.5(7)
C(16)-Re(3)-C(17)	89.6(6)

C(15)-Re(3)-C(17)	175.5(6)
C(18)-Re(3)-P(2)	95.9(5)
C(16)-Re(3)-P(2)	173.0(4)
C(15)-Re(3)-P(2)	89.8(5)
C(17)-Re(3)-P(2)	94.6(4)
C(18)-Re(3)-S(4)	170.4(5)
C(16)-Re(3)-S(4)	99.2(4)
C(15)-Re(3)-S(4)	94.1(5)
C(17)-Re(3)-S(4)	86.9(4)
P(2)-Re(3)-S(4)	75.57(12)
C(19)-Re(4)-C(20)	89.0(7)
C(19)-Re(4)-C(21)	95.0(7)
C(20)-Re(4)-C(21)	88.8(7)
C(19)-Re(4)-C(22)	88.2(6)
C(20)-Re(4)-C(22)	88.4(6)
C(21)-Re(4)-C(22)	175.6(6)
C(19)-Re(4)-P(2)	92.2(5)
C(20)-Re(4)-P(2)	178.8(5)
C(21)-Re(4)-P(2)	91.4(5)
C(22)-Re(4)-P(2)	91.4(4)
C(19)-Re(4)-S(4)	168.2(5)
C(20)-Re(4)-S(4)	102.6(5)
C(21)-Re(4)-S(4)	87.3(5)
C(22)-Re(4)-S(4)	90.1(5)
P(2)-Re(4)-S(4)	76.23(12)
C(9)-Fe(1)-C(11)	94.6(8)
C(9)-Fe(1)-C(10)	92.8(7)
C(11)-Fe(1)-C(10)	101.8(7)
C(9)-Fe(1)-S(2)	163.9(5)
C(11)-Fe(1)-S(2)	96.9(6)
C(10)-Fe(1)-S(2)	95.8(5)
C(9)-Fe(1)-S(1)	88.7(5)
C(11)-Fe(1)-S(1)	107.8(5)
C(10)-Fe(1)-S(1)	150.2(5)
S(2)-Fe(1)-S(1)	77.08(15)
C(9)-Fe(1)-Fe(2)	110.4(6)

C(11)-Fe(1)-Fe(2)	149.3(5)
C(10)-Fe(1)-Fe(2)	94.6(5)
S(2)-Fe(1)-Fe(2)	55.37(12)
S(1)-Fe(1)-Fe(2)	57.31(11)
C(13)-Fe(2)-C(12)	89.5(7)
C(13)-Fe(2)-C(14)	95.8(7)
C(12)-Fe(2)-C(14)	104.8(7)
C(13)-Fe(2)-S(2)	93.1(5)
C(12)-Fe(2)-S(2)	148.4(5)
C(14)-Fe(2)-S(2)	106.2(5)
C(13)-Fe(2)-S(1)	164.2(6)
C(12)-Fe(2)-S(1)	92.1(4)
C(14)-Fe(2)-S(1)	98.9(5)
S(2)-Fe(2)-S(1)	77.39(15)
C(13)-Fe(2)-Fe(1)	107.7(5)
C(12)-Fe(2)-Fe(1)	92.4(5)
C(14)-Fe(2)-Fe(1)	150.9(5)
S(2)-Fe(2)-Fe(1)	56.82(12)
S(1)-Fe(2)-Fe(1)	56.47(12)
C(23)-Fe(3)-C(24)	95.4(9)
C(23)-Fe(3)-C(25)	91.5(8)
C(24)-Fe(3)-C(25)	103.5(8)
C(23)-Fe(3)-S(3)	163.7(5)
C(24)-Fe(3)-S(3)	98.3(7)
C(25)-Fe(3)-S(3)	93.6(6)
C(23)-Fe(3)-S(4)	91.1(5)
C(24)-Fe(3)-S(4)	105.4(6)
C(25)-Fe(3)-S(4)	150.6(6)
S(3)-Fe(3)-S(4)	76.94(15)
C(23)-Fe(3)-Fe(4)	108.3(6)
C(24)-Fe(3)-Fe(4)	150.4(6)
C(25)-Fe(3)-Fe(4)	93.6(6)
S(3)-Fe(3)-Fe(4)	56.03(12)
S(4)-Fe(3)-Fe(4)	57.87(12)
C(26)-Fe(4)-C(27)	90.5(8)
C(26)-Fe(4)-C(28)	101.0(8)