Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **11•C_6H_6**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

	x	y	z	U(eq)
Re(1)	3321(1)	2212(1)	3127(1)	35(1)
P(1)	2943(2)	3876(2)	3251(2)	37(1)
P(2)	1649(2)	2589(2)	3585(2)	38(1)
P(3)	2660(2)	2229(2)	1140(2)	39(1)
C(1)	1985(7)	4402(7)	2276(9)	39(2)
C(2)	912(7)	3669(7)	3080(9)	41(2)
C(3)	1536(7)	3168(7)	1018(9)	40(2)
C(4)	1232(7)	3947(6)	2015(8)	35(2)
C(5)	360(8)	4667(7)	1564(10)	50(3)
C(6)	3581(8)	964(8)	3240(10)	51(3)
C(7)	3891(8)	2250(8)	4591(10)	50(3)
C(8)	4640(7)	1949(7)	2440(9)	39(2)
C(9)	5466(9)	1132(8)	2468(11)	60(3)
C(10)	5698(10)	645(10)	3311(13)	72(4)
C(11)	6527(12)	203(11)	-3369(15)	104(5)
C(12)	5598(9)	2497(9)	1338(12)	68(4)
O(1)	3797(6)	203(6)	3419(8)	73(3)
O(2)	4293(7)	2225(7)	5475(8)	79(3)
O(3)	4723(5)	2528(5)	1818(6)	52(2)
C(2,1)	2415(5)	4188(4)	5599(6)	51(3)
C(3,1)	2101(6)	4737(5)	6625(5)	66(3)
C(4,1)	1906(6)	5666(5)	6697(5)	71(4)
C(5,1)	2027(6)	6046(4)	5744(7)	67(3)
C(6,1)	2341(6)	5497(5)	4718(5)	56(3)
C(1,1)	2536(5)	4568(4)	4646(5)	45(3)
C(2,2)	3881(5)	4823(6)	2127(6)	65(3)
C(3,2)	4635(7)	5117(6)	2008(7)	103(5)
C(4,2)	5397(6)	4894(7)	2758(9)	92(5)
C(5,2)	5406(5)	4378(7)	3628(7)	78(4)
C(6,2)	4653(6)	4084(6)	3746(6)	64(3)
C(1,2)	3891(5)	4306(5)	2996(7)	47(3)
C(2,3)	331(4)	3166(5)	5358(5)	50(3)
C(3,3)	33(4)	3222(5)	6472(6)	56(3)
C(4,3)	673(5)	2821(6)	7299(5)	61(3)
C(5,3)	1610(5)	2364(5)	7012(5)	70(4)
C(6,3)	1908(4)	2308(5)	5898(6)	54(3)
C(1,3)	1268(5)	2709(5)	5071(5)	39(2)
C(2,4)	1499(6)	894(6)	3327(7)	68(4)
C(3,4)	1184(7)	194(4)	2852(9)	96(5)
C(4,4)	480(7)	347(5)	2018(9)	100(5)
C(5,4)	92(6)	1199(6)	1658(7)	82(4)
C(6,4)	407(5)	1899(5)	2132(7)	56(3)
C(1,4)	1110(5)	1746(5)	2967(6)	46(3)
C(2,5)	1716(5)	1343(4)	-461(7)	58(3)

C(3,5)	1529(6)	592(6)	-1028(6)	72(4)
C(4,5)	1991(7)	-261(5)	-698(8)	79(4)
C(5,5)	2640(6)	-363(4)	200(8)	85(4)
C(6,5)	2827(5)	387(5)	767(6)	67(3)
C(1,5)	2365(5)	1240(5)	437(6)	48(3)
C(2,6)	3298(6)	3154(5)	-379(8)	70(4)
C(3,6)	3884(7)	3188(6)	-1230(8)	94(5)
C(4,6)	4565(7)	2398(7)	-1708(8)	94(5)
C(5,6)	4660(6)	1575(6)	-1334(8)	108(6)
C(6,6)	4075(6)	1542(4)	-482(8)	69(4)
C(1,6)	3394(5)	2332(5)	-5(6)	46(3)
C(1,7)	8544(13)	1292(10)	4280(13)	161(9)
C(2,7)	8921(8)	1558(11)	5314(16)	138(8)
C(3,7)	8328(12)	2083(10)	6198(11)	119(6)
C(4,7)	7358(11)	2342(10)	6048(14)	154(9)
C(5,7)	6981(9)	2076(13)	5014(18)	177(11)
C(6,7)	7574(15)	1552(12)	4130(12)	161(9)
S(1)	8406(3)	3601(3)	9670(3)	69(1)
O(4)	8378(7)	3599(7)	8481(8)	79(3)
O(5)	7907(9)	4495(9)	10240(11)	121(4)
O(6)	9250(9)	3164(8)	10195(11)	111(4)
F(1)	7643(9)	2840(8)	10985(11)	141(4)
F(2)	8059(10)	2126(10)	9411(12)	166(5)
F(3)	6869(11)	3220(10)	9496(13)	173(5)
C(13)	7678(14)	2966(14)	9937(17)	103(5)

Table S2. Bond lengths [Å] and angles [deg] for **11•C_6H_6.**

Re(1)-C(7)	1.887(12)
Re(1)-C(6)	1.901(12)
Re(1)-C(8)	2.078(10)
Re(1)-P(2)	2.464(3)
Re(1)-P(1)	2.483(3)
Re(1)-P(3)	2.492(3)
P(1)-C(1)	1.834(10)
P(1)-C(1,2)	1.838(7)
P(1)-C(1,1)	1.853(6)
P(2)-C(1,3)	1.835(6)
P(2)-C(1,4)	1.841(7)
P(2)-C(2)	1.850(10)
P(3)-C(1,6)	1.848(7)
P(3)-C(1,5)	1.850(7)
P(3)-C(3)	1.851(10)
C(1)-C(4)	1.541(13)
C(2)-C(4)	1.535(14)
C(3)-C(4)	1.545(14)
C(4)-C(5)	1.544(13)
C(6)-O(1)	1.182(13)
C(7)-O(2)	1.176(13)
C(8)-O(3)	1.289(12)
C(8)-C(9)	1.462(15)
C(9)-C(10)	1.299(17)
C(10)-C(11)	1.50(2)
C(12)-O(3)	1.449(14)
C(2,1)-C(3,1)	1.3900
C(2,1)-C(1,1)	1.3900
C(3,1)-C(4,1)	1.3900
C(4,1)-C(5,1)	1.3900
C(5,1)-C(6,1)	1.3900
C(6,1)-C(1,1)	1.3900
C(2,2)-C(3,2)	1.3900
C(2,2)-C(1,2)	1.3900
C(3,2)-C(4,2)	1.3900
C(4,2)-C(5,2)	1.3900
C(5,2)-C(6,2)	1.3900
C(6,2)-C(1,2)	1.3900
C(2,3)-C(3,3)	1.3900
C(2,3)-C(1,3)	1.3900
C(3,3)-C(4,3)	1.3900
C(4,3)-C(5,3)	1.3900
C(5,3)-C(6,3)	1.3900
C(6,3)-C(1,3)	1.3900
C(2,4)-C(3,4)	1.3900
C(2,4)-C(1,4)	1.3900
C(3,4)-C(4,4)	1.3900

C(4,4)-C(5,4)	1.3900
C(5,4)-C(6,4)	1.3900
C(6,4)-C(1,4)	1.3900
C(2,5)-C(3,5)	1.3900
C(2,5)-C(1,5)	1.3900
C(3,5)-C(4,5)	1.3900
C(4,5)-C(5,5)	1.3900
C(5,5)-C(6,5)	1.3900
C(6,5)-C(1,5)	1.3900
C(2,6)-C(3,6)	1.3900
C(2,6)-C(1,6)	1.3900
C(3,6)-C(4,6)	1.3900
C(4,6)-C(5,6)	1.3900
C(5,6)-C(6,6)	1.3900
C(6,6)-C(1,6)	1.3900
C(1,7)-C(2,7)	1.3900
C(1,7)-C(6,7)	1.3900
C(2,7)-C(3,7)	1.3900
C(3,7)-C(4,7)	1.3900
C(4,7)-C(5,7)	1.3900
C(5,7)-C(6,7)	1.3900
S(1)-O(6)	1.385(12)
S(1)-O(4)	1.396(10)
S(1)-O(5)	1.445(13)
S(1)-C(13)	1.79(2)
F(1)-C(13)	1.28(2)
F(2)-C(13)	1.33(2)
F(3)-C(13)	1.26(2)
C(7)-Re(1)-C(6)	85.3(5)
C(7)-Re(1)-C(8)	87.4(4)
C(6)-Re(1)-C(8)	91.6(4)
C(7)-Re(1)-P(2)	102.8(3)
C(6)-Re(1)-P(2)	92.1(3)
C(8)-Re(1)-P(2)	169.4(3)
C(7)-Re(1)-P(1)	88.7(4)
C(6)-Re(1)-P(1)	172.6(3)
C(8)-Re(1)-P(1)	92.5(3)
P(2)-Re(1)-P(1)	84.97(9)
C(7)-Re(1)-P(3)	175.0(4)
C(6)-Re(1)-P(3)	97.9(4)
C(8)-Re(1)-P(3)	88.7(3)
P(2)-Re(1)-P(3)	81.03(9)
P(1)-Re(1)-P(3)	88.46(9)
C(1)-P(1)-C(1,2)	105.4(4)
C(1)-P(1)-C(1,1)	102.2(4)
C(1,2)-P(1)-C(1,1)	98.1(4)
C(1)-P(1)-Re(1)	112.7(3)
C(1,2)-P(1)-Re(1)	118.3(3)
C(1,1)-P(1)-Re(1)	117.9(2)

C(1,3)-P(2)-C(1,4)	97.8(4)
C(1,3)-P(2)-C(2)	103.4(4)
C(1,4)-P(2)-C(2)	105.6(4)
C(1,3)-P(2)-Re(1)	121.0(2)
C(1,4)-P(2)-Re(1)	115.3(3)
C(2)-P(2)-Re(1)	111.8(3)
C(1,6)-P(3)-C(1,5)	98.5(4)
C(1,6)-P(3)-C(3)	103.9(4)
C(1,5)-P(3)-C(3)	101.9(4)
C(1,6)-P(3)-Re(1)	117.4(3)
C(1,5)-P(3)-Re(1)	119.6(3)
C(3)-P(3)-Re(1)	113.0(3)
C(4)-C(1)-P(1)	116.6(7)
C(4)-C(2)-P(2)	118.1(7)
C(4)-C(3)-P(3)	119.1(7)
C(2)-C(4)-C(1)	113.6(8)
C(2)-C(4)-C(5)	106.4(8)
C(1)-C(4)-C(5)	106.3(8)
C(2)-C(4)-C(3)	113.2(8)
C(1)-C(4)-C(3)	111.2(8)
C(5)-C(4)-C(3)	105.4(8)
O(1)-C(6)-Re(1)	172.7(10)
O(2)-C(7)-Re(1)	175.7(10)
O(3)-C(8)-C(9)	115.1(9)
O(3)-C(8)-Re(1)	116.9(7)
C(9)-C(8)-Re(1)	127.7(8)
C(10)-C(9)-C(8)	125.2(13)
C(9)-C(10)-C(11)	127.0(15)
C(8)-O(3)-C(12)	124.9(9)
C(3,1)-C(2,1)-C(1,1)	120.0
C(4,1)-C(3,1)-C(2,1)	120.0
C(3,1)-C(4,1)-C(5,1)	120.0
C(6,1)-C(5,1)-C(4,1)	120.0
C(1,1)-C(6,1)-C(5,1)	120.0
C(6,1)-C(1,1)-C(2,1)	120.0
C(6,1)-C(1,1)-P(1)	117.8(4)
C(2,1)-C(1,1)-P(1)	122.2(4)
C(3,2)-C(2,2)-C(1,2)	120.0
C(4,2)-C(3,2)-C(2,2)	120.0
C(3,2)-C(4,2)-C(5,2)	120.0
C(6,2)-C(5,2)-C(4,2)	120.0
C(5,2)-C(6,2)-C(1,2)	120.0
C(6,2)-C(1,2)-C(2,2)	120.0
C(6,2)-C(1,2)-P(1)	115.5(5)
C(2,2)-C(1,2)-P(1)	124.5(5)
C(3,3)-C(2,3)-C(1,3)	120.0
C(2,3)-C(3,3)-C(4,3)	120.0
C(5,3)-C(4,3)-C(3,3)	120.0
C(4,3)-C(5,3)-C(6,3)	120.0

C(1,3)-C(6,3)-C(5,3)	120.0
C(6,3)-C(1,3)-C(2,3)	120.0
C(6,3)-C(1,3)-P(2)	120.0(4)
C(2,3)-C(1,3)-P(2)	119.9(4)
C(3,4)-C(2,4)-C(1,4)	120.0
C(2,4)-C(3,4)-C(4,4)	120.0
C(5,4)-C(4,4)-C(3,4)	120.0
C(4,4)-C(5,4)-C(6,4)	120.0
C(1,4)-C(6,4)-C(5,4)	120.0
C(6,4)-C(1,4)-C(2,4)	120.0
C(6,4)-C(1,4)-P(2)	124.2(5)
C(2,4)-C(1,4)-P(2)	115.6(5)
C(3,5)-C(2,5)-C(1,5)	120.0
C(2,5)-C(3,5)-C(4,5)	120.0
C(5,5)-C(4,5)-C(3,5)	120.0
C(6,5)-C(5,5)-C(4,5)	120.0
C(5,5)-C(6,5)-C(1,5)	120.0
C(6,5)-C(1,5)-C(2,5)	120.0
C(6,5)-C(1,5)-P(3)	120.0(4)
C(2,5)-C(1,5)-P(3)	119.9(4)
C(3,6)-C(2,6)-C(1,6)	120.0
C(4,6)-C(3,6)-C(2,6)	120.0
C(3,6)-C(4,6)-C(5,6)	120.0
C(6,6)-C(5,6)-C(4,6)	120.0
C(5,6)-C(6,6)-C(1,6)	120.0
C(6,6)-C(1,6)-C(2,6)	120.0
C(6,6)-C(1,6)-P(3)	117.1(5)
C(2,6)-C(1,6)-P(3)	122.9(5)
C(2,7)-C(1,7)-C(6,7)	120.0
C(3,7)-C(2,7)-C(1,7)	120.0
C(4,7)-C(3,7)-C(2,7)	120.0
C(3,7)-C(4,7)-C(5,7)	120.0
C(6,7)-C(5,7)-C(4,7)	120.0
C(5,7)-C(6,7)-C(1,7)	120.0
O(6)-S(1)-O(4)	119.2(7)
O(6)-S(1)-O(5)	113.9(8)
O(4)-S(1)-O(5)	110.8(7)
O(6)-S(1)-C(13)	103.2(9)
O(4)-S(1)-C(13)	104.9(8)
O(5)-S(1)-C(13)	102.7(9)
F(3)-C(13)-F(1)	111.2(18)
F(3)-C(13)-F(2)	102.7(18)
F(1)-C(13)-F(2)	102.8(17)
F(3)-C(13)-S(1)	115.0(15)
F(1)-C(13)-S(1)	115.5(15)
F(2)-C(13)-S(1)	107.9(14)

Symmetry transformations used to generate equivalent atoms:

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **11•C_6H_6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11 + ... + 2hka^*b^*U12]$

	U11	U22	U33	U23	U13	U12
Re(1)	35(1)	35(1)	35(1)	4(1)	1(1)	-11(1)
P(1)	37(1)	37(2)	40(2)	2(1)	-6(1)	-18(1)
P(2)	36(1)	37(2)	42(2)	8(1)	4(1)	-11(1)
P(3)	44(2)	40(2)	37(2)	2(1)	0(1)	-21(1)
C(1)	47(6)	33(6)	43(6)	7(5)	-8(5)	-21(5)
C(2)	33(5)	33(6)	53(6)	4(5)	0(5)	-8(4)
C(3)	40(6)	43(6)	45(6)	18(5)	-11(5)	-21(5)
C(4)	35(5)	28(5)	44(6)	8(4)	-13(4)	-14(4)
C(5)	53(7)	46(7)	58(7)	19(6)	-25(6)	-24(5)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **11•C_6H_6.**

	x	y	z	U(eq)
H(1A)	1673	5025	2601	57(12)
H(1B)	2259	4415	1555	57(12)
H(2A)	286	3640	2924	57(12)
H(2B)	857	4149	3706	57(12)
H(3A)	1565	3433	331	57(12)
H(3B)	1040	2906	897	57(12)
H(5A)	68	5120	2186	64(12)
H(5B)	-80	4383	1238	64(12)
H(5C)	548	4944	987	64(12)
H(9)	5855	947	1831	57(12)
H(10)	5308	845	3948	57(12)
H(11A)	6968	-87	3932	64(12)
H(11B)	6824	-396	2633	64(12)
H(11C)	6319	-669	3580	64(12)
H(12A)	5507	3056	1038	64(12)
H(12B)	5791	2003	732	64(12)
H(12C)	6074	2413	1926	64(12)
H(2,1)	2545	3566	5551	62
H(3,1)	2020	4483	7262	79
H(4,1)	1696	6034	7383	85
H(5,1)	1897	6668	5792	80
H(6,1)	2422	5751	4081	67
H(2,2)	3371	4972	1625	78
H(3,2)	4628	5463	1427	124
H(4,2)	5901	5091	2679	111
H(5,2)	5917	4229	4130	94
H(6,2)	4659	3738	4328	77
H(2,3)	-97	3434	4805	60
H(3,3)	-594	3528	6665	67
H(4,3)	474	2859	8045	73
H(5,3)	2038	2096	7565	84
H(6,3)	2535	2002	5706	65
H(2,4)	1970	792	3885	81
H(3,4)	1444	-376	3093	115
H(4,4)	269	-121	1700	119
H(5,4)	-379	1301	1099	99
H(6,4)	147	2469	1892	67
H(2,5)	1407	1913	-682	70
H(3,5)	1095	661	-1629	87
H(4,5)	1866	-763	-1077	95
H(5,5)	2949	-934	421	102
H(6,5)	3261	318	1368	80
H(2,6)	2843	3683	-59	84
H(3,6)	3820	3738	-1480	113

H(4,6)	4957	2420	-2277	113
H(5,6)	5116	1047	-1653	129
H(6,6)	4138	991	-232	83