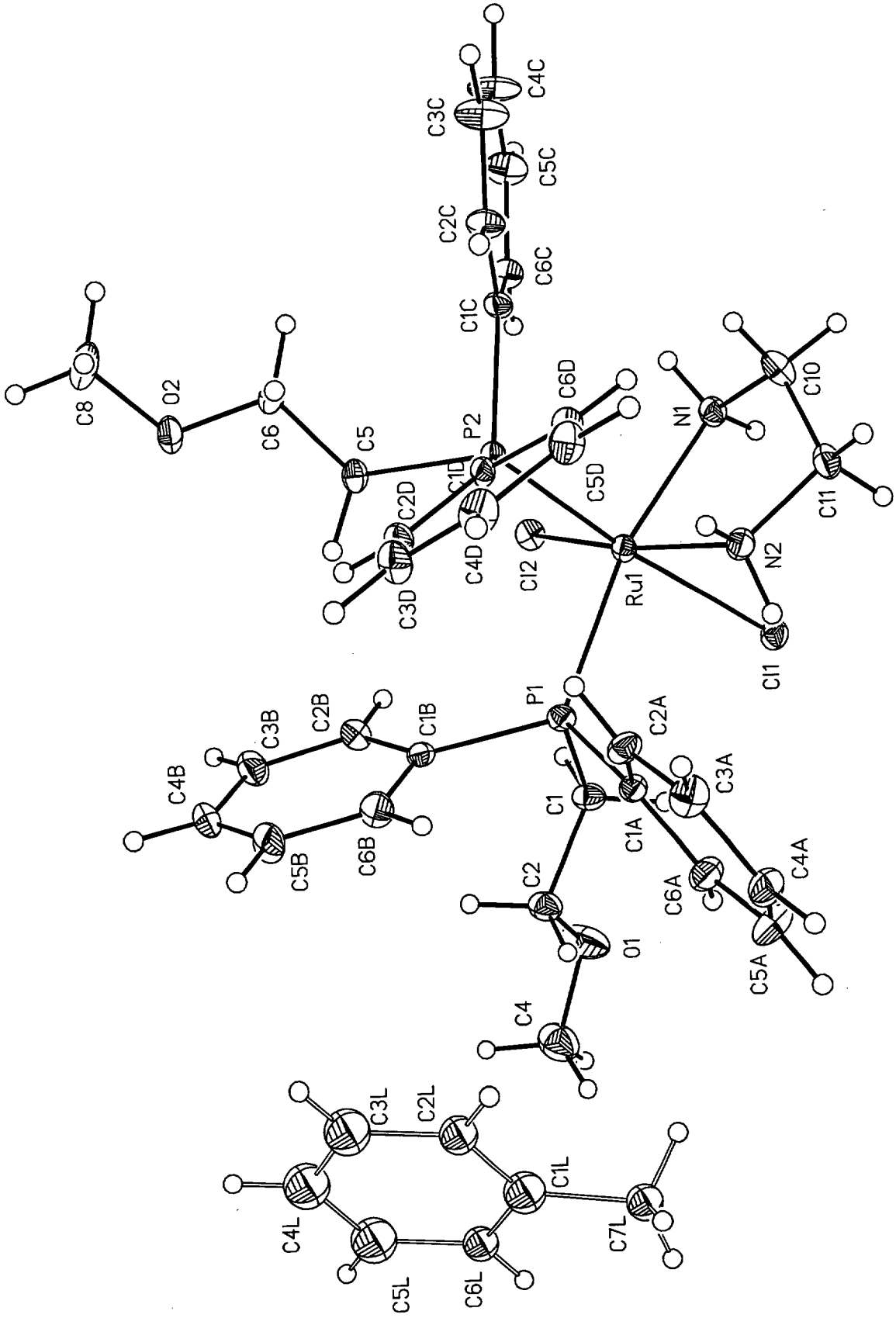

Figure S1: ORTEP plot of **3a**·0.5C_7H_8.

Table S1. Crystal data and structure refinement for **3a·0.5C_7H_8**.

Empirical formula	C35.50 H46 Cl2 N2 O2 P2 Ru
Formula weight	766.65
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 31.025(10) A alpha = 90 deg. b = 13.108(7) A beta = 100.44(2) deg. c = 18.054(4) A gamma = 90 deg.
Volume	7221(5) A^3
Z, Calculated density	8, 1.410 Mg/m^3
Absorption coefficient	0.704 mm^-1
F(000)	3176
Crystal size	0.1 x 0.3 x 0.2 mm
Theta range for data collection	2.11 to 24.98 deg.
Limiting indices	-1<=h<=36, -1<=k<=15, -21<=l<=21
Reflections collected / unique	7295 / 6285 [R(int) = 0.0489]
Completeness to theta = 24.98	98.9 %
Absorption correction	Empirical
Max. and min. transmission	0.3182 and 0.2226
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6285 / 10 / 385
Goodness-of-fit on F^2	1.771
Final R indices [I>2sigma(I)]	R1 = 0.0551, wR2 = 0.1380
R indices (all data)	R1 = 0.0830, wR2 = 0.1606
Extinction coefficient	0.00001(9)
Largest diff. peak and hole	1.204 and -1.450 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3a·0.5C$_7$H$_8$**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	3092(1)	7300(1)	8569(1)	25(1)
Cl(1)	2623(1)	5806(1)	8115(1)	37(1)
Cl(2)	3205(1)	6729(1)	9874(1)	34(1)
P(1)	3670(1)	6366(1)	8301(1)	29(1)
P(2)	3461(1)	8743(1)	8926(1)	24(1)
C(1)	3607(2)	5020(5)	8571(4)	36(1)
C(2)	3977(2)	4265(5)	8531(5)	42(2)
O(1)	3824(2)	3315(5)	8714(5)	78(2)
C(4)	4113(3)	2521(7)	8637(7)	70(3)
C(5)	3934(2)	8698(5)	9712(3)	32(1)
C(6)	4115(2)	9729(5)	9983(3)	36(1)
O(2)	4513(1)	9563(4)	10492(3)	42(1)
C(8)	4715(3)	10511(8)	10726(5)	61(2)
N(1)	2462(2)	7885(4)	8692(3)	34(1)
C(10)	2285(2)	8536(6)	8036(4)	44(2)
C(11)	2383(2)	8059(6)	7333(4)	40(2)
N(2)	2852(2)	7766(4)	7437(3)	33(1)
C(1C)	3146(2)	9763(5)	9299(3)	29(1)
C(2C)	3143(2)	10773(5)	9079(4)	38(1)
C(3C)	2929(3)	11480(7)	9436(5)	60(2)
C(4C)	2701(3)	11185(7)	10004(5)	63(2)
C(5C)	2703(3)	10185(6)	10221(4)	50(2)
C(6C)	2928(2)	9472(5)	9882(4)	35(1)
C(1D)	3688(2)	9385(5)	8186(3)	29(1)
C(2D)	4130(2)	9341(5)	8154(4)	33(1)
C(3D)	4287(2)	9776(6)	7548(4)	43(2)
C(4D)	4012(3)	10259(7)	6980(4)	50(2)
C(5D)	3572(2)	10301(6)	6999(4)	43(2)
C(6D)	3407(2)	9865(5)	7592(3)	33(1)
C(1A)	3678(2)	6343(5)	7290(3)	30(1)
C(2A)	3744(2)	7251(6)	6917(4)	38(1)
C(3A)	3720(2)	7291(7)	6143(4)	48(2)
C(4A)	3620(3)	6421(7)	5715(4)	52(2)
C(5A)	3552(3)	5522(7)	6063(5)	59(2)
C(6A)	3582(2)	5490(6)	6844(4)	46(2)
C(1B)	4249(2)	6549(4)	8737(3)	30(1)
C(2B)	4366(2)	6374(5)	9506(4)	38(1)
C(3B)	4803(2)	6404(7)	9862(4)	50(2)
C(4B)	5126(2)	6659(7)	9451(5)	52(2)
C(5B)	5012(2)	6836(7)	8693(5)	54(2)
C(6B)	4582(2)	6785(6)	8333(4)	44(2)
C(1L)	4741(3)	3218(8)	7197(6)	68(5)
C(2L)	4905(4)	4203(7)	7319(7)	53(4)
C(3L)	5268(4)	4386(7)	7876(8)	79(6)
C(4L)	5469(4)	3585(10)	8312(7)	84(6)
C(5L)	5305(4)	2600(8)	8191(6)	85(6)
C(6L)	4942(4)	2416(6)	7633(6)	50
C(7L)	4362(5)	2985(12)	6576(9)	50

Table S3. Bond lengths [A] and angles [deg] for **3a·0.5C$_7$H$_8$**.

Ru(1)-N(2)	2.134(5)	C(3C)-C(4C)	1.401(11)
Ru(1)-N(1)	2.147(5)	C(4C)-C(5C)	1.367(12)
Ru(1)-P(2)	2.2439(18)	C(5C)-C(6C)	1.375(10)
Ru(1)-P(1)	2.2961(17)	C(1D)-C(2D)	1.386(8)
Ru(1)-Cl(2)	2.4364(15)	C(1D)-C(6D)	1.403(9)
Ru(1)-Cl(1)	2.4879(18)	C(2D)-C(3D)	1.396(9)
Ru(1)-O(1)	5.682(7)	C(3D)-C(4D)	1.367(11)
Ru(1)-O(2)	5.893(5)	C(4D)-C(5D)	1.373(11)
P(1)-C(1A)	1.829(6)	C(5D)-C(6D)	1.390(9)
P(1)-C(1B)	1.840(6)	C(1A)-C(6A)	1.378(9)
P(1)-C(1)	1.849(6)	C(1A)-C(2A)	1.401(10)
P(1)-P(2)	3.416(3)	C(2A)-C(3A)	1.387(9)
P(2)-C(1D)	1.824(6)	C(3A)-C(4A)	1.381(12)
P(2)-C(5)	1.848(6)	C(4A)-C(5A)	1.370(13)
P(2)-C(1C)	1.852(6)	C(5A)-C(6A)	1.398(11)
C(1)-C(2)	1.528(9)	C(1B)-C(2B)	1.389(9)
C(2)-O(1)	1.394(9)	C(1B)-C(6B)	1.402(9)
O(1)-C(4)	1.398(11)	C(2B)-C(3B)	1.389(10)
C(5)-C(6)	1.511(9)	C(3B)-C(4B)	1.391(12)
C(6)-O(2)	1.416(8)	C(4B)-C(5B)	1.371(12)
O(2)-C(8)	1.423(10)	C(5B)-C(6B)	1.377(10)
N(1)-C(10)	1.482(9)	C(1L)-C(2L)	1.3900
N(1)-N(2)	2.759(7)	C(1L)-C(6L)	1.3900
C(10)-C(11)	1.495(10)	C(1L)-C(7L)	1.503(17)
C(11)-N(2)	1.482(8)	C(2L)-C(3L)	1.3900
C(1C)-C(2C)	1.380(9)	C(3L)-C(4L)	1.3900
C(1C)-C(6C)	1.404(8)	C(4L)-C(5L)	1.3900
C(2C)-C(3C)	1.370(10)	C(5L)-C(6L)	1.3900
N(2)-Ru(1)-N(1)	80.2(2)	C(1A)-P(1)-C(1)	105.5(3)
N(2)-Ru(1)-P(2)	96.08(15)	C(1B)-P(1)-C(1)	98.9(3)
N(1)-Ru(1)-P(2)	95.51(15)	C(1A)-P(1)-Ru(1)	111.8(2)
N(2)-Ru(1)-P(1)	95.82(15)	C(1B)-P(1)-Ru(1)	125.39(19)
N(1)-Ru(1)-P(1)	166.64(15)	C(1)-P(1)-Ru(1)	109.2(2)
P(2)-Ru(1)-P(1)	97.61(6)	C(1A)-P(1)-P(2)	112.5(2)
N(2)-Ru(1)-Cl(2)	168.03(14)	C(1B)-P(1)-P(2)	88.20(19)
N(1)-Ru(1)-Cl(2)	89.08(15)	C(1)-P(1)-P(2)	138.4(2)
P(2)-Ru(1)-Cl(2)	90.28(6)	Ru(1)-P(1)-P(2)	40.62(4)
P(1)-Ru(1)-Cl(2)	93.37(6)	C(1D)-P(2)-C(5)	102.7(3)
N(2)-Ru(1)-Cl(1)	80.05(15)	C(1D)-P(2)-C(1C)	103.4(3)
N(1)-Ru(1)-Cl(1)	80.02(15)	C(5)-P(2)-C(1C)	98.1(3)
P(2)-Ru(1)-Cl(1)	174.49(6)	C(1D)-P(2)-Ru(1)	115.00(19)
P(1)-Ru(1)-Cl(1)	86.73(6)	C(5)-P(2)-Ru(1)	119.1(2)
Cl(2)-Ru(1)-Cl(1)	92.86(6)	C(1C)-P(2)-Ru(1)	116.0(2)
N(2)-Ru(1)-O(1)	111.98(17)	C(1D)-P(2)-P(1)	93.3(2)
N(1)-Ru(1)-O(1)	133.37(16)	C(5)-P(2)-P(1)	93.0(2)
P(2)-Ru(1)-O(1)	125.63(9)	C(1C)-P(2)-P(1)	157.3(2)
P(1)-Ru(1)-O(1)	36.70(7)	Ru(1)-P(2)-P(1)	41.77(4)
Cl(2)-Ru(1)-O(1)	71.72(10)	C(2)-C(1)-P(1)	119.3(5)
Cl(1)-Ru(1)-O(1)	59.77(9)	O(1)-C(2)-C(1)	105.9(6)
N(2)-Ru(1)-O(2)	120.97(15)	C(2)-O(1)-C(4)	112.8(7)
N(1)-Ru(1)-O(2)	110.91(15)	C(2)-O(1)-Ru(1)	47.1(3)
P(2)-Ru(1)-O(2)	28.17(6)	C(4)-O(1)-Ru(1)	159.8(5)
P(1)-Ru(1)-O(2)	82.11(7)	C(6)-C(5)-P(2)	114.6(4)
Cl(2)-Ru(1)-O(2)	67.91(7)	O(2)-C(6)-C(5)	107.5(5)
Cl(1)-Ru(1)-O(2)	156.98(7)	C(6)-O(2)-C(8)	110.1(6)
O(1)-Ru(1)-O(2)	100.68(10)	C(6)-O(2)-Ru(1)	39.1(3)
C(1A)-P(1)-C(1B)	103.9(3)	C(8)-O(2)-Ru(1)	149.1(5)

C(10)-N(1)-Ru(1)	109.6(4)	C(6A)-C(1A)-C(2A)	116.3(6)
C(10)-N(1)-N(2)	62.0(3)	C(6A)-C(1A)-P(1)	123.7(5)
Ru(1)-N(1)-N(2)	49.68(15)	C(2A)-C(1A)-P(1)	119.7(5)
N(1)-C(10)-C(11)	109.6(6)	C(3A)-C(2A)-C(1A)	122.1(7)
N(2)-C(11)-C(10)	110.3(5)	C(4A)-C(3A)-C(2A)	119.9(8)
C(11)-N(2)-Ru(1)	111.1(4)	C(5A)-C(4A)-C(3A)	119.4(7)
C(11)-N(2)-N(1)	61.6(3)	C(4A)-C(5A)-C(6A)	120.1(7)
Ru(1)-N(2)-N(1)	50.08(15)	C(1A)-C(6A)-C(5A)	122.2(7)
C(2C)-C(1C)-C(6C)	119.8(6)	C(2B)-C(1B)-C(6B)	118.1(6)
C(2C)-C(1C)-P(2)	124.3(5)	C(2B)-C(1B)-P(1)	117.7(5)
C(6C)-C(1C)-P(2)	115.7(5)	C(6B)-C(1B)-P(1)	124.0(5)
C(3C)-C(2C)-C(1C)	119.4(6)	C(1B)-C(2B)-C(3B)	121.0(6)
C(2C)-C(3C)-C(4C)	120.7(7)	C(2B)-C(3B)-C(4B)	119.7(7)
C(5C)-C(4C)-C(3C)	119.8(7)	C(5B)-C(4B)-C(3B)	119.5(6)
C(4C)-C(5C)-C(6C)	120.1(7)	C(4B)-C(5B)-C(6B)	121.0(7)
C(5C)-C(6C)-C(1C)	120.1(6)	C(5B)-C(6B)-C(1B)	120.6(7)
C(2D)-C(1D)-C(6D)	118.0(6)	C(2L)-C(1L)-C(6L)	120.0
C(2D)-C(1D)-P(2)	121.9(5)	C(2L)-C(1L)-C(7L)	121.4(8)
C(6D)-C(1D)-P(2)	119.9(4)	C(6L)-C(1L)-C(7L)	118.6(8)
C(1D)-C(2D)-C(3D)	120.4(6)	C(1L)-C(2L)-C(3L)	120.0
C(4D)-C(3D)-C(2D)	121.2(6)	C(4L)-C(3L)-C(2L)	120.0
C(3D)-C(4D)-C(5D)	119.2(7)	C(5L)-C(4L)-C(3L)	120.0
C(4D)-C(5D)-C(6D)	120.7(7)	C(4L)-C(5L)-C(6L)	120.0
C(5D)-C(6D)-C(1D)	120.6(6)	C(5L)-C(6L)-C(1L)	120.0

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **3a·0.5C_7H_8**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	21(1)	31(1)	23(1)	-1(1)	7(1)	-2(1)
Cl(1)	30(1)	39(1)	41(1)	-5(1)	7(1)	-9(1)
Cl(2)	36(1)	39(1)	27(1)	5(1)	10(1)	-1(1)
P(1)	28(1)	32(1)	29(1)	-2(1)	11(1)	-1(1)
P(2)	22(1)	29(1)	22(1)	0(1)	6(1)	-2(1)
C(1)	39(3)	28(3)	44(4)	0(3)	16(3)	0(3)
C(2)	40(3)	30(3)	58(4)	0(3)	13(3)	3(3)
O(1)	72(4)	37(3)	138(7)	13(4)	54(4)	4(3)
C(4)	60(5)	51(5)	101(8)	3(5)	15(5)	8(4)
C(5)	30(3)	40(3)	23(3)	5(2)	1(2)	-4(3)
C(6)	38(3)	43(4)	26(3)	-6(3)	0(2)	-7(3)
O(2)	26(2)	64(3)	34(2)	-9(2)	2(2)	-6(2)
C(8)	49(4)	86(6)	48(4)	-25(4)	9(3)	-31(4)
N(1)	27(2)	39(3)	35(3)	-2(2)	7(2)	-2(2)
C(10)	32(3)	55(4)	46(4)	11(3)	7(3)	11(3)
C(11)	32(3)	45(4)	39(3)	4(3)	-4(3)	2(3)
N(2)	33(2)	31(3)	32(2)	-1(2)	2(2)	-2(2)
C(1C)	25(3)	34(3)	28(3)	-4(2)	9(2)	5(2)
C(2C)	45(3)	36(3)	38(3)	4(3)	20(3)	6(3)
C(3C)	86(6)	44(4)	62(5)	10(4)	42(5)	22(4)
C(4C)	87(6)	48(4)	66(5)	-1(4)	49(5)	28(4)
C(5C)	57(4)	58(5)	44(4)	1(3)	32(3)	10(4)
C(6C)	37(3)	37(3)	34(3)	2(3)	12(3)	1(3)
C(1D)	19(2)	41(3)	26(3)	-8(2)	6(2)	-3(2)
C(2D)	27(3)	44(3)	30(3)	-2(3)	8(2)	-1(3)
C(3D)	30(3)	66(5)	36(3)	1(3)	15(3)	-8(3)
C(4D)	54(4)	64(5)	34(4)	1(3)	17(3)	-17(4)
C(5D)	47(4)	49(4)	32(3)	6(3)	4(3)	-6(3)
C(6D)	32(3)	38(3)	30(3)	1(3)	8(2)	-3(3)
C(1A)	25(3)	32(3)	33(3)	-7(2)	9(2)	-2(2)
C(2A)	42(3)	42(3)	33(3)	-11(3)	15(3)	-6(3)
C(3A)	51(4)	60(4)	34(3)	1(3)	17(3)	-8(4)
C(4A)	50(4)	74(5)	32(3)	-15(4)	6(3)	1(4)
C(5A)	82(6)	50(5)	44(4)	-18(4)	6(4)	-11(4)
C(6A)	51(4)	42(4)	44(4)	-11(3)	6(3)	-5(3)
C(1B)	28(3)	28(3)	34(3)	-7(2)	9(2)	-1(2)
C(2B)	34(3)	41(3)	41(3)	2(3)	8(3)	3(3)
C(3B)	37(3)	63(5)	46(4)	-1(4)	-1(3)	10(3)
C(4B)	27(3)	69(5)	59(5)	-12(4)	0(3)	3(3)
C(5B)	29(3)	84(6)	55(4)	-15(4)	20(3)	-15(4)
C(6B)	38(3)	60(4)	39(3)	-6(3)	17(3)	-8(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3a·0.5C_7H_8**.

	x	y	z	U(eq)
H(1A)	3553	5016	9094	43
H(1B)	3339	4752	8247	43
H(2A)	4049	4252	8018	51
H(2B)	4244	4456	8893	51
H(4A)	3993	1876	8786	105
H(4B)	4397	2653	8961	105
H(4C)	4151	2477	8111	105
H(5A)	3844	8335	10141	38
H(5B)	4170	8296	9551	38
H(6A)	4168	10146	9551	43
H(6B)	3904	10096	10237	43
H(8A)	4993	10387	11069	91
H(8B)	4521	10911	10987	91
H(8C)	4771	10890	10285	91
H(1NA)	2273	7352	8723	40
H(1NB)	2489	8261	9128	40
H(10A)	2420	9222	8103	53
H(10B)	1964	8613	7997	53
H(11A)	2197	7447	7207	48
H(11B)	2314	8548	6910	48
H(2NA)	3013	8311	7319	39
H(2NB)	2884	7239	7114	39
H(2CA)	3289	10975	8683	46
H(3CA)	2934	12178	9298	72
H(4CA)	2544	11677	10237	75
H(5CA)	2550	9983	10607	60
H(6CA)	2936	8781	10043	43
H(2DA)	4328	9014	8545	40
H(3DA)	4591	9736	7532	51
H(4DA)	4123	10563	6575	60
H(5DA)	3378	10631	6604	52
H(6DA)	3101	9892	7595	40
H(2AA)	3808	7858	7203	45
H(3AA)	3772	7916	5908	57
H(4AA)	3599	6446	5184	63
H(5AA)	3485	4919	5773	71
H(6AA)	3534	4860	7076	55
H(2BA)	4145	6230	9792	46
H(3BA)	4880	6252	10383	60
H(4BA)	5423	6709	9695	63
H(5BA)	5234	6996	8411	65
H(6BA)	4510	6910	7807	53
H(2L)	4768	4751	7021	64
H(3L)	5380	5060	7959	95
H(4L)	5717	3710	8693	100
H(5L)	5442	2052	8488	102
H(6L)	4830	1743	7550	60
H(7L1)	4345	2247	6487	75
H(7L2)	4403	3335	6114	75
H(7L3)	4089	3220	6722	75

Table S6. Selected torsion angles [deg] for **3a·0.5C$_7$H$_8$**.

Ru(1)-P(1)-C(1)-C(2)	-173.1(5)
P(1)-C(1)-C(2)-O(1)	-176.0(6)
C(1)-C(2)-O(1)-C(4)	174.6(8)
Ru(1)-P(2)-C(5)-C(6)	-171.2(4)
P(2)-C(5)-C(6)-O(2)	-170.6(4)
C(5)-C(6)-O(2)-C(8)	176.0(5)
Ru(1)-N(1)-C(10)-C(11)	40.2(6)
N(1)-C(10)-C(11)-N(2)	-49.0(8)
C(10)-C(11)-N(2)-Ru(1)	33.6(7)
C(11)-N(2)-Ru(1)-N(1)	-9.0(4)
N(2)-Ru(1)-N(1)-C(10)	-17.0(4)

Table S7. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for **3a·0.5C$_7$H$_8$**.

```
11.5003 (0.0731) x + 11.8716 (0.0148) y + 2.4394 (0.0482) z = 14.3125
(0.0337)
 *     0.0000 (0.0001)  Ru1
 *     0.0000 (0.0001)  N1
 *     0.0000 (0.0000)  N2
       0.4093 (0.0108)  C10
      -0.2158 (0.0103)  C11
 Rms deviation of fitted atoms =   0.0000

14.8663 (0.0339) x + 11.0992 (0.0106) y + 2.5344 (0.0204) z = 14.7178
(0.0171)
Angle to previous plane (with approximate esd) =  7.23 ( 0.24 )
 *     0.1529 (0.0016)  Ru1
 *    -0.1030 (0.0024)  N1
 *     0.0253 (0.0024)  N2
 *    -0.0923 (0.0019)  P1
 *     0.0170 (0.0020)  C12
       0.1902 (0.0096)  C10
      -0.3717 (0.0088)  C11
 Rms deviation of fitted atoms =   0.0932

14.8908 (0.0337) x + 11.0965 (0.0106) y + 2.5162 (0.0204) z = 14.6695
(0.0174)
Angle to previous plane (with approximate esd) =  0.07 ( 0.16 )
 *    -0.0666 (0.0024)  N1
 *     0.0650 (0.0023)  N2
 *    -0.0518 (0.0018)  P1
 *     0.0534 (0.0019)  C12
       0.1912 (0.0020)  Ru1
       0.2272 (0.0098)  C10
      -0.3331 (0.0090)  C11
      -2.2788 (0.0030)  C11
       2.4315 (0.0027)  P2
 Rms deviation of fitted atoms =   0.0596
```

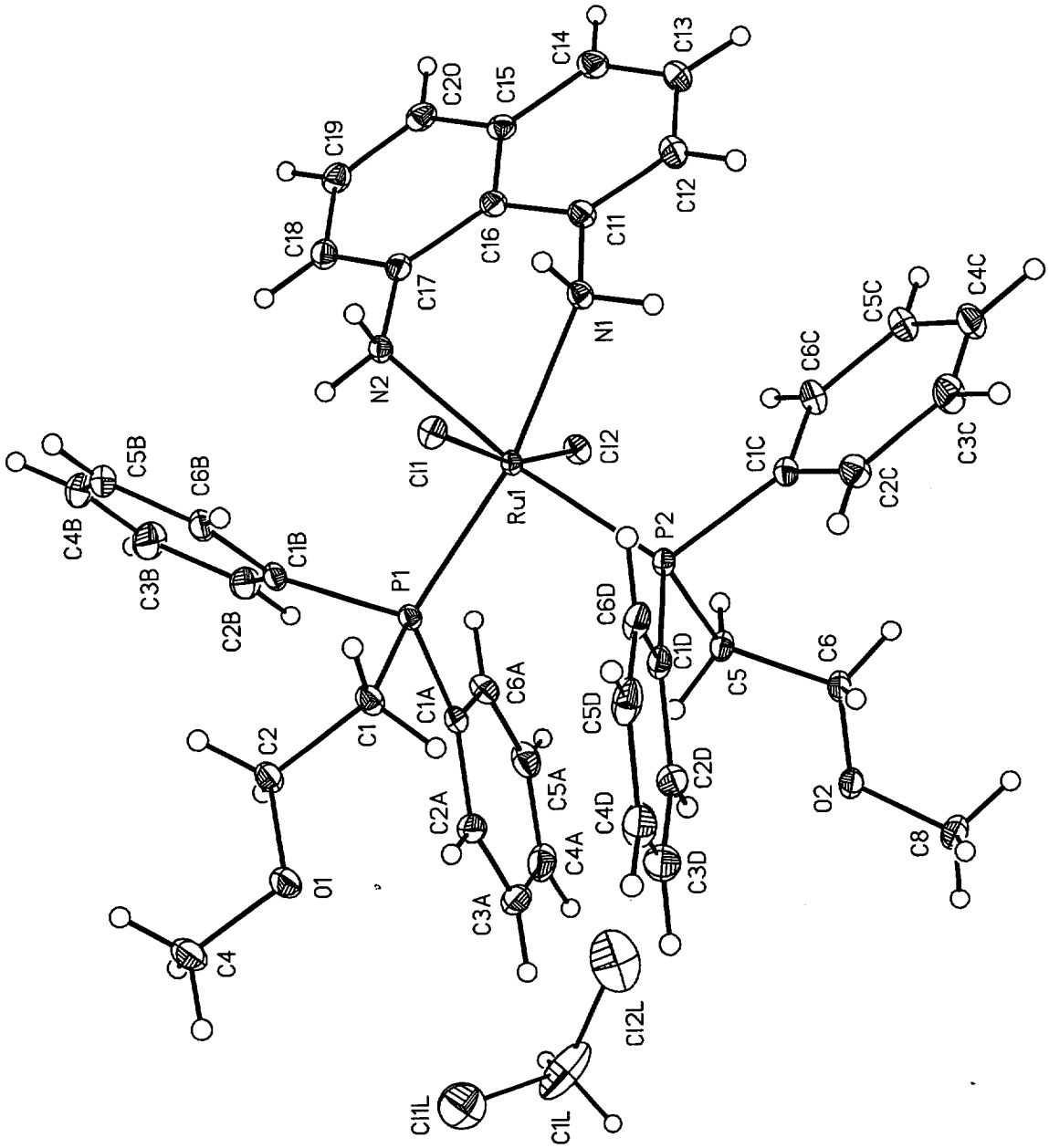

Figure S2. ORTEP plot of **3e·CH_2Cl_2**.

Table S8. Crystal data and structure refinement for **3e·CH_2Cl_2**.

Empirical formula	C41 H46 Cl4 N2 O2 P2 Ru
Formula weight	903.61
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.4917(18) A alpha = 90.025(19) deg.
	b = 13.070(3) A beta = 93.62(2) deg.
	c = 16.724(5) A gamma = 99.653(13) deg.
Volume	2041.1(9) A^3
Z, Calculated density	2, 1.470 Mg/m^3
Absorption coefficient	0.762 mm^-1
F(000)	928
Crystal size	0.2 x 0.3 x 0.2 mm
Theta range for data collection	2.01 to 27.50 deg.
Limiting indices	-1<=h<=12, -16<=k<=16, -21<=l<=21
Reflections collected / unique	11036 / 9345 [R(int) = 0.0665]
Completeness to theta = 27.50	99.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9345 / 0 / 470
Goodness-of-fit on F^2	1.845
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.1007
R indices (all data)	R1 = 0.0456, wR2 = 0.1064
Extinction coefficient	0.0081(9)
Largest diff. peak and hole	1.520 and -1.129 e.A^-3

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3e·CH_2Cl_2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	5746(1)	7867(1)	3124(1)	20(1)
Cl(1)	3434(1)	6979(1)	3491(1)	28(1)
Cl(2)	8001(1)	9006(1)	2993(1)	27(1)
P(1)	5013(1)	7705(1)	1802(1)	23(1)
P(2)	6844(1)	6453(1)	3085(1)	23(1)
C(1)	3637(3)	6581(2)	1511(2)	30(1)
C(2)	2787(3)	6682(2)	717(2)	33(1)
O(1)	2482(2)	5694(2)	336(1)	37(1)
C(4)	1596(4)	5722(3)	-372(2)	44(1)
C(5)	8426(3)	6568(2)	2487(2)	29(1)
C(6)	9369(3)	5742(2)	2655(2)	30(1)
O(2)	10046(2)	5583(2)	1947(1)	32(1)
C(8)	10813(3)	4743(3)	2036(2)	39(1)
N(1)	6054(2)	8146(2)	4433(1)	26(1)
N(2)	4771(2)	9257(2)	3329(1)	26(1)
C(11)	6752(3)	9134(2)	4776(2)	29(1)
C(12)	7712(3)	9139(2)	5429(2)	36(1)
C(13)	8427(3)	10079(3)	5784(2)	37(1)
C(14)	8162(3)	11005(2)	5488(2)	37(1)
C(15)	7203(3)	11034(2)	4801(2)	29(1)
C(16)	6478(3)	10085(2)	4431(2)	29(1)
C(17)	5556(3)	10171(2)	3732(2)	28(1)
C(18)	5408(3)	11119(2)	3424(2)	33(1)
C(19)	6127(3)	12055(2)	3801(2)	35(1)
C(20)	6985(3)	12004(2)	4479(2)	35(1)
C(1A)	6312(3)	7687(2)	1042(2)	29(1)
C(2A)	6218(4)	6849(2)	506(2)	37(1)
C(3A)	7306(4)	6803(3)	-15(2)	45(1)
C(4A)	8469(4)	7586(3)	-6(2)	49(1)
C(5A)	8573(4)	8429(3)	512(2)	45(1)
C(6A)	7501(3)	8478(3)	1034(2)	35(1)
C(1B)	4020(3)	8763(2)	1522(2)	28(1)
C(2B)	4577(4)	9644(2)	1100(2)	38(1)
C(3B)	3791(5)	10459(3)	993(2)	50(1)
C(4B)	2468(5)	10400(3)	1309(2)	50(1)
C(5B)	1897(4)	9531(3)	1725(2)	43(1)
C(6B)	2666(3)	8712(2)	1826(2)	33(1)
C(1C)	7661(3)	6167(2)	4071(2)	26(1)
C(2C)	7379(3)	5229(2)	4477(2)	34(1)
C(3C)	8059(4)	5108(3)	5227(2)	42(1)
C(4C)	9018(4)	5916(3)	5581(2)	41(1)
C(5C)	9318(3)	6853(3)	5190(2)	37(1)
C(6C)	8646(3)	6981(2)	4438(2)	32(1)
C(1D)	5790(3)	5193(2)	2760(2)	30(1)
C(2D)	6068(4)	4686(2)	2064(2)	40(1)
C(3D)	5194(4)	3759(3)	1810(3)	52(1)
C(4D)	4061(4)	3327(3)	2244(3)	54(1)
C(5D)	3788(3)	3819(2)	2936(3)	45(1)
C(6D)	4638(3)	4750(2)	3190(2)	36(1)
Cl(1L)	9682(2)	8163(1)	-2649(1)	95(1)
Cl(2L)	11717(3)	8557(2)	-1253(2)	122(1)
C(1L)	11534(8)	8426(4)	-2321(6)	106(3)

Table S10. Bond lengths [A] and angles [deg] for **3e·CH_2Cl_2**.

Ru(1)-N(2)	2.208(2)	C(16)-C(17)	1.433(4)
Ru(1)-N(1)	2.211(2)	C(17)-C(18)	1.366(4)
Ru(1)-P(2)	2.2717(8)	C(18)-C(19)	1.423(4)
Ru(1)-P(1)	2.2746(10)	C(19)-C(20)	1.361(4)
Ru(1)-Cl(2)	2.4160(7)	C(1A)-C(6A)	1.398(4)
Ru(1)-Cl(1)	2.4200(8)	C(1A)-C(2A)	1.403(4)
Ru(1)-O(2)	5.877(2)	C(2A)-C(3A)	1.401(5)
Ru(1)-O(1)	5.884(3)	C(3A)-C(4A)	1.373(6)
P(1)-C(1A)	1.829(3)	C(4A)-C(5A)	1.389(6)
P(1)-C(1)	1.837(3)	C(5A)-C(6A)	1.391(4)
P(1)-C(1B)	1.845(3)	C(1B)-C(2B)	1.396(4)
P(1)-P(2)	3.2841(12)	C(1B)-C(6B)	1.402(4)
P(2)-C(1D)	1.839(3)	C(2B)-C(3B)	1.405(4)
P(2)-C(5)	1.842(3)	C(3B)-C(4B)	1.383(6)
P(2)-C(1C)	1.843(3)	C(4B)-C(5B)	1.383(6)
C(1)-C(2)	1.527(4)	C(5B)-C(6B)	1.398(4)
C(2)-O(1)	1.416(3)	C(1C)-C(2C)	1.396(3)
O(1)-C(4)	1.413(4)	C(1C)-C(6C)	1.406(4)
C(5)-C(6)	1.529(3)	C(2C)-C(3C)	1.395(4)
C(6)-O(2)	1.414(3)	C(3C)-C(4C)	1.380(5)
O(2)-C(8)	1.419(3)	C(4C)-C(5C)	1.384(5)
N(1)-C(11)	1.449(3)	C(5C)-C(6C)	1.396(4)
N(2)-C(17)	1.441(3)	C(1D)-C(6D)	1.391(4)
C(11)-C(12)	1.377(4)	C(1D)-C(2D)	1.400(4)
C(11)-C(16)	1.426(4)	C(2D)-C(3D)	1.399(5)
C(12)-C(13)	1.411(4)	C(3D)-C(4D)	1.378(7)
C(13)-C(14)	1.364(5)	C(4D)-C(5D)	1.383(6)
C(14)-C(15)	1.424(4)	C(5D)-C(6D)	1.393(4)
C(15)-C(20)	1.420(4)	Cl(1L)-C(1L)	1.785(9)
C(15)-C(16)	1.433(3)	Cl(2L)-C(1L)	1.788(10)

N(2)-Ru(1)-N(1)	75.42(8)	C(1A)-P(1)-C(1B)	105.96(12)
N(2)-Ru(1)-P(2)	172.57(6)	C(1)-P(1)-C(1B)	99.64(12)
N(1)-Ru(1)-P(2)	97.19(6)	C(1A)-P(1)-Ru(1)	120.53(9)
N(2)-Ru(1)-P(1)	94.93(6)	C(1)-P(1)-Ru(1)	116.66(9)
N(1)-Ru(1)-P(1)	168.47(6)	C(1B)-P(1)-Ru(1)	109.14(9)
P(2)-Ru(1)-P(1)	92.50(3)	C(1A)-P(1)-P(2)	92.17(8)
N(2)-Ru(1)-Cl(2)	88.18(6)	C(1)-P(1)-P(2)	95.82(9)
N(1)-Ru(1)-Cl(2)	87.96(6)	C(1B)-P(1)-P(2)	152.85(8)
P(2)-Ru(1)-Cl(2)	90.86(3)	Ru(1)-P(1)-P(2)	43.71(2)
P(1)-Ru(1)-Cl(2)	98.15(3)	C(1D)-P(2)-C(5)	103.32(13)
N(2)-Ru(1)-Cl(1)	82.44(6)	C(1D)-P(2)-C(1C)	103.22(12)
N(1)-Ru(1)-Cl(1)	81.81(6)	C(5)-P(2)-C(1C)	99.71(11)
P(2)-Ru(1)-Cl(1)	97.39(3)	C(1D)-P(2)-Ru(1)	119.30(8)
P(1)-Ru(1)-Cl(1)	90.80(3)	C(5)-P(2)-Ru(1)	116.40(9)
Cl(2)-Ru(1)-Cl(1)	167.56(2)	C(1C)-P(2)-Ru(1)	112.34(8)
N(2)-Ru(1)-O(2)	155.19(6)	C(1D)-P(2)-P(1)	91.80(8)
N(1)-Ru(1)-O(2)	111.84(6)	C(5)-P(2)-P(1)	94.65(8)
P(2)-Ru(1)-O(2)	27.62(3)	C(1C)-P(2)-P(1)	156.11(8)
P(1)-Ru(1)-O(2)	79.56(3)	Ru(1)-P(2)-P(1)	43.78(2)
Cl(2)-Ru(1)-O(2)	68.95(3)	C(2)-C(1)-P(1)	115.38(19)
Cl(1)-Ru(1)-O(2)	121.52(3)	O(1)-C(2)-C(1)	108.5(2)
N(2)-Ru(1)-O(1)	106.02(6)	C(4)-O(1)-C(2)	111.0(2)
N(1)-Ru(1)-O(1)	150.28(6)	C(4)-O(1)-Ru(1)	149.54(18)
P(2)-Ru(1)-O(1)	80.73(3)	C(2)-O(1)-Ru(1)	38.62(13)
P(1)-Ru(1)-O(1)	26.40(3)	C(6)-C(5)-P(2)	114.74(18)
Cl(2)-Ru(1)-O(1)	121.61(3)	O(2)-C(6)-C(5)	108.0(2)
Cl(1)-Ru(1)-O(1)	69.20(4)	C(6)-O(2)-C(8)	110.8(2)
O(2)-Ru(1)-O(1)	79.65(4)	C(6)-O(2)-Ru(1)	39.38(12)
C(1A)-P(1)-C(1)	102.50(13)	C(8)-O(2)-Ru(1)	148.68(17)

C(11)-N(1)-Ru(1)	122.33(16)	C(5A)-C(6A)-C(1A)	120.7(3)
C(17)-N(2)-Ru(1)	122.21(16)	C(2B)-C(1B)-C(6B)	118.5(3)
C(12)-C(11)-C(16)	120.6(3)	C(2B)-C(1B)-P(1)	124.5(2)
C(12)-C(11)-N(1)	118.8(3)	C(6B)-C(1B)-P(1)	116.6(2)
C(16)-C(11)-N(1)	120.6(2)	C(1B)-C(2B)-C(3B)	120.1(3)
C(11)-C(12)-C(13)	121.1(3)	C(4B)-C(3B)-C(2B)	120.4(3)
C(14)-C(13)-C(12)	120.1(3)	C(5B)-C(4B)-C(3B)	120.3(3)
C(13)-C(14)-C(15)	120.4(3)	C(4B)-C(5B)-C(6B)	119.5(3)
C(20)-C(15)-C(14)	119.8(3)	C(5B)-C(6B)-C(1B)	121.1(3)
C(20)-C(15)-C(16)	120.2(3)	C(2C)-C(1C)-C(6C)	118.1(2)
C(14)-C(15)-C(16)	120.0(3)	C(2C)-C(1C)-P(2)	125.9(2)
C(11)-C(16)-C(17)	125.2(2)	C(6C)-C(1C)-P(2)	115.95(19)
C(11)-C(16)-C(15)	117.7(2)	C(3C)-C(2C)-C(1C)	120.7(3)
C(17)-C(16)-C(15)	117.0(2)	C(4C)-C(3C)-C(2C)	120.4(3)
C(18)-C(17)-C(16)	121.1(2)	C(3C)-C(4C)-C(5C)	120.0(3)
C(18)-C(17)-N(2)	118.3(2)	C(4C)-C(5C)-C(6C)	120.0(3)
C(16)-C(17)-N(2)	120.6(2)	C(5C)-C(6C)-C(1C)	120.7(3)
C(17)-C(18)-C(19)	121.3(3)	C(6D)-C(1D)-C(2D)	118.5(3)
C(20)-C(19)-C(18)	119.3(3)	C(6D)-C(1D)-P(2)	119.6(2)
C(19)-C(20)-C(15)	121.1(3)	C(2D)-C(1D)-P(2)	121.8(2)
C(6A)-C(1A)-C(2A)	118.5(3)	C(3D)-C(2D)-C(1D)	120.3(4)
C(6A)-C(1A)-P(1)	119.7(2)	C(4D)-C(3D)-C(2D)	120.5(4)
C(2A)-C(1A)-P(1)	121.6(2)	C(3D)-C(4D)-C(5D)	119.5(3)
C(3A)-C(2A)-C(1A)	120.5(3)	C(4D)-C(5D)-C(6D)	120.5(4)
C(4A)-C(3A)-C(2A)	119.9(3)	C(1D)-C(6D)-C(5D)	120.6(3)
C(3A)-C(4A)-C(5A)	120.5(3)	Cl(1L)-C(1L)-Cl(2L)	109.8(3)
C(4A)-C(5A)-C(6A)	119.9(3)		

Table S11. Anisotropic displacement parameters (A^2 x 10^3) for **3e·CH_2Cl_2**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	20(1)	19(1)	22(1)	1(1)	-2(1)	4(1)
Cl(1)	24(1)	25(1)	34(1)	2(1)	3(1)	2(1)
Cl(2)	26(1)	25(1)	28(1)	2(1)	-1(1)	-1(1)
P(1)	26(1)	21(1)	24(1)	1(1)	-4(1)	5(1)
P(2)	22(1)	21(1)	25(1)	2(1)	-1(1)	6(1)
C(1)	33(1)	26(1)	30(1)	-1(1)	-8(1)	3(1)
C(2)	37(1)	28(1)	33(1)	-2(1)	-12(1)	6(1)
O(1)	42(1)	32(1)	35(1)	-8(1)	-12(1)	7(1)
C(4)	50(2)	45(2)	34(1)	-7(1)	-13(1)	5(1)
C(5)	28(1)	32(1)	29(1)	7(1)	4(1)	13(1)
C(6)	27(1)	35(1)	30(1)	6(1)	0(1)	13(1)
O(2)	32(1)	38(1)	31(1)	4(1)	2(1)	16(1)
C(8)	38(1)	39(1)	45(2)	4(1)	5(1)	19(1)
N(1)	28(1)	24(1)	24(1)	3(1)	-1(1)	4(1)
N(2)	26(1)	22(1)	29(1)	-1(1)	-4(1)	6(1)
C(11)	28(1)	34(1)	26(1)	-3(1)	-1(1)	5(1)
C(12)	36(1)	38(1)	33(1)	-1(1)	-5(1)	9(1)
C(13)	33(1)	44(2)	33(1)	-7(1)	-9(1)	7(1)
C(14)	32(1)	41(1)	36(1)	-11(1)	-3(1)	2(1)
C(15)	26(1)	31(1)	30(1)	-7(1)	3(1)	2(1)
C(16)	26(1)	30(1)	30(1)	-4(1)	0(1)	4(1)
C(17)	25(1)	29(1)	31(1)	-2(1)	1(1)	7(1)
C(18)	32(1)	31(1)	37(1)	0(1)	-1(1)	8(1)
C(19)	38(1)	25(1)	43(2)	-1(1)	2(1)	8(1)
C(20)	33(1)	28(1)	44(2)	-9(1)	4(1)	4(1)
C(1A)	32(1)	34(1)	21(1)	2(1)	-3(1)	12(1)
C(2A)	48(2)	35(1)	30(1)	0(1)	-1(1)	16(1)
C(3A)	59(2)	47(2)	36(2)	1(1)	5(1)	28(2)
C(4A)	52(2)	66(2)	37(2)	12(2)	10(1)	31(2)
C(5A)	36(1)	63(2)	36(1)	12(1)	2(1)	10(1)
C(6A)	36(1)	43(2)	27(1)	3(1)	-3(1)	5(1)
C(1B)	31(1)	26(1)	27(1)	-1(1)	-8(1)	9(1)
C(2B)	52(2)	32(1)	34(1)	7(1)	2(1)	14(1)
C(3B)	70(2)	37(2)	48(2)	13(1)	4(2)	23(2)
C(4B)	65(2)	45(2)	48(2)	1(1)	-8(2)	34(2)
C(5B)	40(2)	49(2)	42(2)	-5(1)	-9(1)	22(1)
C(6B)	32(1)	33(1)	35(1)	-1(1)	-7(1)	10(1)
C(1C)	25(1)	27(1)	27(1)	6(1)	2(1)	7(1)
C(2C)	40(1)	30(1)	31(1)	9(1)	3(1)	5(1)
C(3C)	53(2)	40(2)	36(2)	17(1)	4(1)	12(1)
C(4C)	44(2)	55(2)	27(1)	10(1)	-1(1)	18(1)
C(5C)	34(1)	43(2)	33(1)	4(1)	-6(1)	7(1)
C(6C)	27(1)	35(1)	33(1)	7(1)	-5(1)	4(1)
C(1D)	27(1)	22(1)	40(1)	-1(1)	-8(1)	8(1)
C(2D)	45(2)	35(1)	42(2)	-7(1)	-9(1)	13(1)
C(3D)	56(2)	39(2)	59(2)	-18(2)	-18(2)	12(1)
C(4D)	47(2)	31(1)	81(3)	-13(2)	-27(2)	8(1)
C(5D)	29(1)	25(1)	79(2)	4(1)	-9(1)	4(1)
C(6D)	26(1)	26(1)	55(2)	1(1)	-3(1)	8(1)
Cl(1L)	115(1)	62(1)	104(1)	7(1)	2(1)	2(1)
Cl(2L)	107(1)	93(1)	151(2)	47(1)	-6(1)	-22(1)
C(1L)	103(4)	45(2)	184(8)	38(3)	96(5)	24(3)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3e·CH_2Cl_2**.

	x	y	z	U(eq)
H(1A)	4105	5962	1478	36
H(1B)	2956	6459	1940	36
H(2A)	1884	6932	814	40
H(2B)	3352	7187	371	40
H(4A)	1406	5033	-627	66
H(4B)	2078	6227	-741	66
H(4C)	689	5924	-240	66
H(5A)	8100	6530	1912	34
H(5B)	9015	7261	2591	34
H(6A)	10097	5977	3096	36
H(6B)	8778	5087	2816	36
H(8A)	11270	4644	1539	58
H(8B)	10151	4109	2153	58
H(8C)	11549	4895	2478	58
H(1NA)	5161	8008	4632	31
H(1NB)	6557	7652	4638	31
H(2NA)	4447	9463	2835	31
H(2NB)	3974	9043	3611	31
H(12A)	7897	8498	5644	43
H(13A)	9095	10067	6230	44
H(14A)	8619	11635	5741	44
H(18A)	4815	11154	2949	40
H(19A)	6010	12708	3583	42
H(20A)	7445	12628	4740	42
H(2AA)	5411	6309	495	44
H(3AA)	7239	6231	-375	54
H(4AA)	9209	7550	-357	59
H(5AA)	9375	8973	510	53
H(6AA)	7578	9055	1389	43
H(2BA)	5489	9693	885	46
H(3BA)	4171	11055	701	60
H(4BA)	1950	10960	1240	60
H(5BA)	987	9490	1941	51
H(6BA)	2265	8110	2104	40
H(2CA)	6718	4668	4241	40
H(3CA)	7860	4464	5496	51
H(4CA)	9472	5830	6093	49
H(5CA)	9981	7408	5432	44
H(6CA)	8858	7625	4172	39
H(2DA)	6854	4973	1764	48
H(3DA)	5384	3424	1333	62
H(4DA)	3471	2697	2069	65
H(5DA)	3015	3519	3241	54
H(6DA)	4429	5087	3661	43
H(1L1)	11999	9074	-2567	127
H(1L2)	12012	7852	-2491	127

Table S13. Selected torsion angles [deg] for **3e·CH_2Cl_2**.

Ru(1)-P(1)-C(1)-C(2)	158.97(18)
P(1)-C(1)-C(2)-O(1)	144.4(2)
C(1)-C(2)-O(1)-C(4)	175.2(3)
Ru(1)-P(2)-C(5)-C(6)	163.87(16)
P(2)-C(5)-C(6)-O(2)	151.09(19)
C(5)-C(6)-O(2)-C(8)	-173.5(2)

Table S14. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for **3e·CH_2Cl_2**.

```
7.4520 (0.0042) x + 5.9065 (0.0062) y - 3.9803 (0.0081) z = 7.6388 (0.0050)
 *    0.0463 (0.0006)  Ru1
 *   -0.0699 (0.0008)  P1
 *    0.0444 (0.0008)  P2
 *   -0.0802 (0.0009)  N1
 *    0.0593 (0.0009)  N2
 Rms deviation of fitted atoms =   0.0616

-7.6721 (0.0074) x + 1.9547 (0.0132) y + 10.6737 (0.0157) z = 1.6942
(0.0193)
Angle to previous plane (with approximate esd) = 42.82 ( 0.08 )
 *   -0.0151 (0.0015)  N1
 *    0.0075 (0.0012)  N2
 *    0.0087 (0.0013)  C11
 *   -0.0156 (0.0015)  C18
 *    0.0145 (0.0022)  C17
 Rms deviation of fitted atoms =   0.0127

7.4535 (0.0042) x + 5.9026 (0.0061) y - 3.9839 (0.0080) z = 7.6238 (0.0049)
Angle to previous plane (with approximate esd) = 42.80 ( 0.08 )
 *   -0.0578 (0.0008)  P1
 *    0.0567 (0.0008)  P2
 *   -0.0691 (0.0009)  N1
 *    0.0702 (0.0009)  N2
      0.0580 (0.0008)  Ru1
 Rms deviation of fitted atoms =   0.0638
```

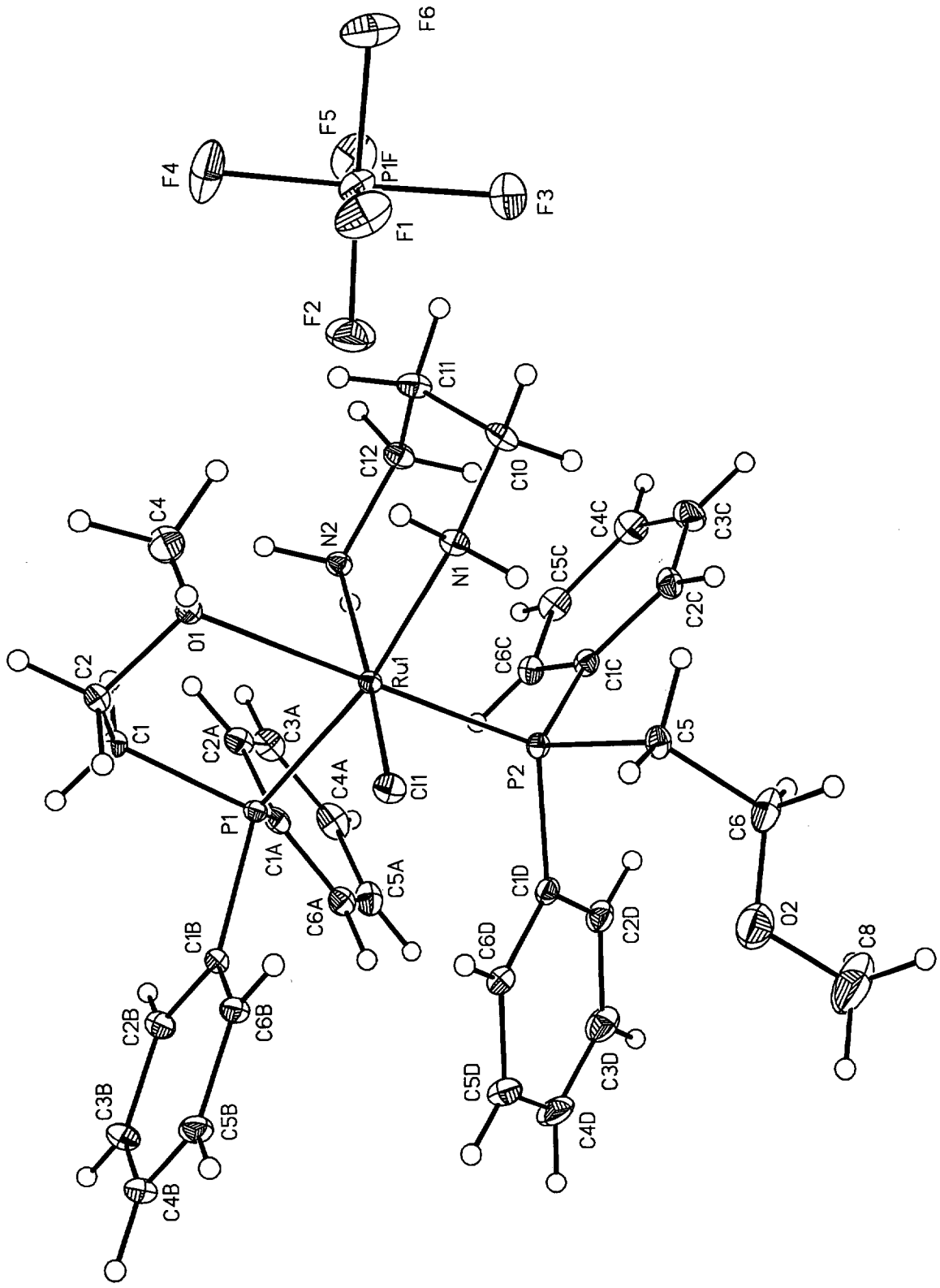

Figure S3. ORTEP plot of **4b·(PF$_6$)**.

Table S15. Crystal data and structure refinement for **4b·(PF$_6$)**.

Empirical formula	C33 H44 Cl F6 N2 O2 P3 Ru
Formula weight	844.13
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 13.730(3) A alpha = 90 deg. b = 11.869(4) A beta = 106.521(10) deg. c = 23.342(3) A gamma = 90 deg.
Volume	3647.1(15) A^3
Z, Calculated density	4, 1.537 Mg/m^3
Absorption coefficient	0.698 mm^-1
F(000)	1728
Crystal size	0.1 x 0.1 x 0.1 mm
Theta range for data collection	2.03 to 24.99 deg.
Limiting indices	-1<=h<=16, -1<=k<=14, -27<=l<=27
Reflections collected / unique	8022 / 6399 [R(int) = 0.0296]
Completeness to theta = 24.99	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6399 / 0 / 434
Goodness-of-fit on F^2	1.613
Final R indices [I>2sigma(I)]	R1 = 0.0406, wR2 = 0.0982
R indices (all data)	R1 = 0.0488, wR2 = 0.1060
Extinction coefficient	0.0014(3)
Largest diff. peak and hole	2.748 and -0.719 e.A^-3

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4b·(PF_6)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
P(1F)	-1927(1)	7613(1)	45(1)	31(1)
F(1)	-2938(2)	7237(3)	-433(1)	57(1)
F(2)	-1380(2)	7727(3)	-465(1)	56(1)
F(3)	-1561(3)	6322(2)	130(1)	56(1)
F(4)	-2271(3)	8887(3)	-14(2)	67(1)
F(5)	-901(2)	7969(3)	532(1)	55(1)
F(6)	-2463(3)	7447(3)	568(1)	64(1)
Ru(1)	1365(1)	8072(1)	-1351(1)	17(1)
P(1)	2107(1)	9360(1)	-1837(1)	18(1)
P(2)	2358(1)	6580(1)	-1381(1)	19(1)
Cl(1)	11(1)	7432(1)	-2193(1)	25(1)
C(1)	1561(3)	10684(3)	-1663(2)	25(1)
C(2)	444(3)	10491(3)	-1718(2)	26(1)
O(1)	390(2)	9628(2)	-1289(1)	24(1)
C(4)	-639(3)	9547(4)	-1253(2)	42(1)
C(5)	1643(3)	5244(3)	-1516(2)	27(1)
C(6)	2136(4)	4236(4)	-1702(2)	46(1)
O(2)	2209(3)	4297(3)	-2258(2)	61(1)
C(8)	2818(7)	3394(6)	-2380(5)	103(3)
N(2)	2262(2)	8743(2)	-512(1)	22(1)
C(12)	2315(3)	8216(3)	79(2)	28(1)
C(11)	1292(3)	7833(4)	132(2)	32(1)
C(10)	860(3)	6809(3)	-249(2)	29(1)
N(1)	472(2)	7103(3)	-888(1)	24(1)
C(1A)	3488(3)	9555(3)	-1555(2)	23(1)
C(2A)	3929(3)	10182(3)	-1037(2)	30(1)
C(3A)	4985(3)	10180(4)	-789(2)	36(1)
C(4A)	5602(3)	9568(4)	-1048(2)	39(1)
C(5A)	5176(3)	8971(3)	-1570(2)	36(1)
C(6A)	4125(3)	8974(3)	-1824(2)	28(1)
C(1B)	1875(3)	9554(3)	-2650(2)	22(1)
C(2B)	2491(3)	10290(3)	-2863(2)	31(1)
C(3B)	2285(4)	10503(4)	-3472(2)	38(1)
C(4B)	1463(3)	9992(4)	-3875(2)	37(1)
C(5B)	843(3)	9285(4)	-3672(2)	33(1)
C(6B)	1039(3)	9066(3)	-3057(2)	26(1)
C(1C)	3367(3)	6353(3)	-685(2)	24(1)
C(2C)	3296(3)	5529(3)	-270(2)	30(1)
C(3C)	3997(3)	5490(4)	294(2)	40(1)
C(4C)	4786(3)	6255(4)	449(2)	41(1)
C(5C)	4889(3)	7060(4)	34(2)	36(1)
C(6C)	4177(3)	7112(3)	-524(2)	26(1)
C(1D)	3024(3)	6528(3)	-1958(2)	24(1)
C(2D)	4032(3)	6174(3)	-1849(2)	33(1)
C(3D)	4479(3)	6162(4)	-2319(2)	43(1)
C(4D)	3933(4)	6487(4)	-2887(2)	49(1)
C(5D)	2930(4)	6806(4)	-2998(2)	41(1)
C(6D)	2470(3)	6820(3)	-2539(2)	30(1)

Table S17. Bond lengths [A] and angles [deg] for **4b·(PF_6)**.

P(1F)-F(1)	1.578(3)	C(11)-C(10)	1.523(5)
P(1F)-F(4)	1.578(3)	C(10)-N(1)	1.476(4)
P(1F)-F(2)	1.584(3)	C(1A)-C(6A)	1.396(5)
P(1F)-F(5)	1.594(3)	C(1A)-C(2A)	1.402(5)
P(1F)-F(3)	1.607(3)	C(2A)-C(3A)	1.399(6)
P(1F)-F(6)	1.608(3)	C(3A)-C(4A)	1.380(7)
Ru(1)-N(2)	2.148(3)	C(4A)-C(5A)	1.386(7)
Ru(1)-N(1)	2.178(3)	C(5A)-C(6A)	1.396(5)
Ru(1)-P(2)	2.2483(10)	C(1B)-C(6B)	1.392(5)
Ru(1)-P(1)	2.3070(9)	C(1B)-C(2B)	1.402(5)
Ru(1)-O(1)	2.309(2)	C(2B)-C(3B)	1.392(5)
Ru(1)-Cl(1)	2.4118(9)	C(3B)-C(4B)	1.387(7)
P(1)-C(1)	1.836(4)	C(4B)-C(5B)	1.371(6)
P(1)-C(1A)	1.836(3)	C(5B)-C(6B)	1.408(5)
P(1)-C(1B)	1.847(3)	C(1C)-C(6C)	1.397(5)
P(1)-P(2)	3.4544(16)	C(1C)-C(2C)	1.399(5)
P(2)-C(1C)	1.830(3)	C(2C)-C(3C)	1.392(6)
P(2)-C(1D)	1.833(4)	C(3C)-C(4C)	1.381(7)
P(2)-C(5)	1.845(4)	C(4C)-C(5C)	1.395(7)
C(1)-C(2)	1.520(5)	C(5C)-C(6C)	1.391(5)
C(2)-O(1)	1.447(4)	C(1D)-C(6D)	1.396(5)
O(1)-C(4)	1.443(5)	C(1D)-C(2D)	1.398(5)
C(5)-C(6)	1.499(5)	C(2D)-C(3D)	1.402(6)
C(6)-O(2)	1.330(7)	C(3D)-C(4D)	1.380(8)
O(2)-C(8)	1.438(8)	C(4D)-C(5D)	1.379(7)
N(2)-C(12)	1.499(4)	C(5D)-C(6D)	1.392(6)
C(12)-C(11)	1.513(5)		

F(1)-P(1F)-F(4)	91.65(18)	C(1)-P(1)-C(1B)	99.13(15)
F(1)-P(1F)-F(2)	90.16(18)	C(1A)-P(1)-C(1B)	102.17(16)
F(4)-P(1F)-F(2)	92.8(2)	C(1)-P(1)-Ru(1)	101.15(11)
F(1)-P(1F)-F(5)	178.9(2)	C(1A)-P(1)-Ru(1)	117.60(11)
F(4)-P(1F)-F(5)	89.44(18)	C(1B)-P(1)-Ru(1)	128.06(12)
F(2)-P(1F)-F(5)	90.09(18)	C(1)-P(1)-P(2)	139.55(11)
F(1)-P(1F)-F(3)	89.92(19)	C(1A)-P(1)-P(2)	90.46(11)
F(4)-P(1F)-F(3)	177.88(19)	C(1B)-P(1)-P(2)	114.10(11)
F(2)-P(1F)-F(3)	88.66(18)	Ru(1)-P(1)-P(2)	40.05(2)
F(5)-P(1F)-F(3)	88.98(18)	C(1C)-P(2)-C(1D)	103.75(16)
F(1)-P(1F)-F(6)	90.06(18)	C(1C)-P(2)-C(5)	104.89(16)
F(4)-P(1F)-F(6)	89.6(2)	C(1D)-P(2)-C(5)	101.43(16)
F(2)-P(1F)-F(6)	177.7(2)	C(1C)-P(2)-Ru(1)	113.64(11)
F(5)-P(1F)-F(6)	89.64(18)	C(1D)-P(2)-Ru(1)	118.92(12)
F(3)-P(1F)-F(6)	89.03(19)	C(5)-P(2)-Ru(1)	112.60(12)
N(2)-Ru(1)-N(1)	90.10(11)	C(1C)-P(2)-P(1)	113.45(12)
N(2)-Ru(1)-P(2)	97.18(8)	C(1D)-P(2)-P(1)	80.36(11)
N(1)-Ru(1)-P(2)	91.79(8)	C(5)-P(2)-P(1)	140.09(12)
N(2)-Ru(1)-P(1)	89.04(8)	Ru(1)-P(2)-P(1)	41.32(2)
N(1)-Ru(1)-P(1)	169.58(8)	C(2)-C(1)-P(1)	108.6(2)
P(2)-Ru(1)-P(1)	98.63(4)	O(1)-C(2)-C(1)	107.3(3)
N(2)-Ru(1)-O(1)	80.73(10)	C(4)-O(1)-C(2)	109.3(3)
N(1)-Ru(1)-O(1)	88.53(10)	C(4)-O(1)-Ru(1)	123.0(2)
P(2)-Ru(1)-O(1)	177.89(7)	C(2)-O(1)-Ru(1)	112.27(19)
P(1)-Ru(1)-O(1)	81.08(7)	C(6)-C(5)-P(2)	118.2(3)
N(2)-Ru(1)-Cl(1)	165.67(8)	O(2)-C(6)-C(5)	114.0(4)
N(1)-Ru(1)-Cl(1)	79.97(8)	C(6)-O(2)-C(8)	111.3(6)
P(2)-Ru(1)-Cl(1)	93.45(3)	C(12)-N(2)-Ru(1)	123.3(2)
P(1)-Ru(1)-Cl(1)	98.86(3)	N(2)-C(12)-C(11)	113.4(3)
O(1)-Ru(1)-Cl(1)	88.66(7)	C(12)-C(11)-C(10)	114.1(3)
C(1)-P(1)-C(1A)	104.94(16)	N(1)-C(10)-C(11)	111.7(3)

C(10)-N(1)-Ru(1)	122.3(2)	C(6C)-C(1C)-C(2C)	118.1(3)
C(6A)-C(1A)-C(2A)	118.5(3)	C(6C)-C(1C)-P(2)	119.2(3)
C(6A)-C(1A)-P(1)	119.5(3)	C(2C)-C(1C)-P(2)	122.2(3)
C(2A)-C(1A)-P(1)	121.7(3)	C(3C)-C(2C)-C(1C)	120.8(4)
C(3A)-C(2A)-C(1A)	119.9(4)	C(4C)-C(3C)-C(2C)	120.4(4)
C(4A)-C(3A)-C(2A)	120.8(4)	C(3C)-C(4C)-C(5C)	119.7(4)
C(3A)-C(4A)-C(5A)	119.7(4)	C(6C)-C(5C)-C(4C)	119.8(4)
C(4A)-C(5A)-C(6A)	119.9(4)	C(5C)-C(6C)-C(1C)	121.2(4)
C(1A)-C(6A)-C(5A)	121.0(4)	C(6D)-C(1D)-C(2D)	119.3(3)
C(6B)-C(1B)-C(2B)	118.7(3)	C(6D)-C(1D)-P(2)	117.2(3)
C(6B)-C(1B)-P(1)	121.2(3)	C(2D)-C(1D)-P(2)	123.4(3)
C(2B)-C(1B)-P(1)	119.8(3)	C(1D)-C(2D)-C(3D)	119.4(4)
C(3B)-C(2B)-C(1B)	120.5(4)	C(4D)-C(3D)-C(2D)	120.7(4)
C(4B)-C(3B)-C(2B)	120.2(4)	C(5D)-C(4D)-C(3D)	119.8(4)
C(5B)-C(4B)-C(3B)	119.9(3)	C(4D)-C(5D)-C(6D)	120.4(4)
C(4B)-C(5B)-C(6B)	120.5(4)	C(5D)-C(6D)-C(1D)	120.3(4)
C(1B)-C(6B)-C(5B)	120.1(3)		

Table S18. Anisotropic displacement parameters (A^2 x 10^3) for **4b·(PF_6)**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
P(1F)	29(1)	33(1)	33(1)	-10(1)	13(1)	-3(1)
F(1)	41(1)	74(2)	53(2)	-28(2)	10(1)	-11(1)
F(2)	64(2)	65(2)	53(2)	2(1)	38(2)	-11(2)
F(3)	74(2)	36(1)	62(2)	2(1)	27(2)	0(1)
F(4)	72(2)	37(2)	75(2)	-13(1)	-4(2)	18(1)
F(5)	39(1)	60(2)	57(2)	-15(1)	1(1)	-3(1)
F(6)	65(2)	87(2)	51(2)	-19(2)	36(2)	-13(2)
Ru(1)	17(1)	18(1)	15(1)	0(1)	4(1)	-1(1)
P(1)	21(1)	19(1)	16(1)	1(1)	5(1)	-1(1)
P(2)	18(1)	18(1)	21(1)	0(1)	4(1)	0(1)
Cl(1)	21(1)	31(1)	21(1)	-2(1)	1(1)	-4(1)
C(1)	31(2)	21(2)	24(2)	0(1)	9(1)	1(1)
C(2)	30(2)	24(2)	23(2)	5(1)	7(1)	4(1)
O(1)	24(1)	25(1)	25(1)	4(1)	11(1)	6(1)
C(4)	33(2)	45(2)	55(3)	10(2)	26(2)	9(2)
C(5)	26(2)	20(2)	31(2)	0(1)	3(1)	-4(1)
C(6)	43(2)	27(2)	71(3)	-10(2)	23(2)	0(2)
O(2)	71(2)	44(2)	70(2)	-9(2)	22(2)	-2(2)
C(8)	119(7)	53(4)	176(9)	-33(5)	103(7)	-10(4)
N(2)	24(1)	24(1)	18(1)	0(1)	5(1)	-3(1)
C(12)	30(2)	35(2)	17(2)	1(1)	2(1)	-2(1)
C(11)	36(2)	41(2)	19(2)	0(2)	10(1)	-5(2)
C(10)	30(2)	33(2)	24(2)	8(1)	10(1)	-5(1)
N(1)	22(1)	28(2)	22(1)	2(1)	7(1)	-2(1)
C(1A)	23(2)	23(2)	22(2)	4(1)	5(1)	-6(1)
C(2A)	31(2)	30(2)	26(2)	0(1)	6(1)	-8(1)
C(3A)	32(2)	37(2)	32(2)	0(2)	-1(2)	-11(2)
C(4A)	23(2)	43(2)	47(2)	10(2)	1(2)	-10(2)
C(5A)	29(2)	31(2)	51(2)	6(2)	17(2)	-1(2)
C(6A)	27(2)	26(2)	32(2)	2(1)	9(1)	-6(1)
C(1B)	28(2)	21(2)	20(2)	4(1)	9(1)	4(1)
C(2B)	36(2)	32(2)	24(2)	3(1)	9(1)	0(2)
C(3B)	50(2)	39(2)	30(2)	9(2)	21(2)	-1(2)
C(4B)	51(2)	40(2)	22(2)	4(2)	14(2)	9(2)
C(5B)	36(2)	40(2)	21(2)	-1(2)	4(1)	7(2)
C(6B)	30(2)	29(2)	20(2)	2(1)	7(1)	3(1)
C(1C)	22(2)	24(2)	25(2)	0(1)	4(1)	5(1)
C(2C)	31(2)	25(2)	33(2)	5(2)	8(2)	5(1)
C(3C)	42(2)	45(2)	31(2)	13(2)	8(2)	14(2)
C(4C)	33(2)	49(2)	33(2)	1(2)	-4(2)	8(2)
C(5C)	21(2)	41(2)	40(2)	-7(2)	1(2)	-1(2)
C(6C)	21(2)	26(2)	31(2)	0(1)	6(1)	1(1)
C(1D)	28(2)	19(2)	27(2)	-4(1)	10(1)	-2(1)
C(2D)	33(2)	29(2)	42(2)	-2(2)	15(2)	5(2)
C(3D)	40(2)	42(2)	56(3)	-10(2)	25(2)	2(2)
C(4D)	64(3)	48(3)	50(3)	-13(2)	40(2)	0(2)
C(5D)	59(3)	39(2)	30(2)	-8(2)	19(2)	-2(2)
C(6D)	36(2)	25(2)	28(2)	-5(1)	10(2)	1(1)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4b·(PF$_6$)**.

	x	y	z	U(eq)
H(1A)	1923	10929	-1252	30
H(1B)	1633	11281	-1944	30
H(2A)	128	11196	-1631	31
H(2B)	80	10243	-2127	31
H(4A)	-909	10305	-1230	62
H(4B)	-648	9119	-896	62
H(4C)	-1061	9163	-1609	62
H(5A)	1469	5044	-1144	32
H(5B)	995	5383	-1827	32
H(6A)	2825	4147	-1424	55
H(6B)	1740	3556	-1667	55
H(8A)	2808	3420	-2802	155
H(8B)	2543	2671	-2296	155
H(8C)	3519	3475	-2127	155
H(2NA)	2919	8784	-535	27
H(2NB)	2048	9474	-494	27
H(12A)	2608	8767	400	33
H(12B)	2777	7559	141	33
H(11A)	804	8464	14	38
H(11B)	1359	7653	556	38
H(10A)	1396	6229	-197	34
H(10B)	301	6485	-111	34
H(1NA)	-126	7489	-934	29
H(1NB)	305	6436	-1093	29
H(2AA)	3512	10607	-855	36
H(3AA)	5280	10605	-438	43
H(4AA)	6316	9555	-870	47
H(5AA)	5600	8560	-1754	43
H(6AA)	3839	8575	-2185	34
H(2BA)	3053	10647	-2590	37
H(3BA)	2709	11000	-3612	45
H(4BA)	1329	10131	-4291	44
H(5BA)	277	8940	-3949	40
H(6BA)	599	8585	-2920	31
H(2CA)	2764	4990	-374	36
H(3CA)	3931	4934	573	48
H(4CA)	5257	6233	836	49
H(5CA)	5445	7571	133	43
H(6CA)	4242	7674	-800	31
H(2DA)	4410	5944	-1459	40
H(3DA)	5165	5927	-2246	52
H(4DA)	4247	6492	-3201	59
H(5DA)	2551	7017	-3391	50
H(6DA)	1776	7029	-2620	36

Table S20. Selected torsion angles [deg] for **4b·(PF$_6$)**.

Ru(1)-P(1)-C(1)-C(2)	-41.5(2)
P(1)-C(1)-C(2)-O(1)	60.7(3)
C(1)-C(2)-O(1)-Ru(1)	-49.4(3)
C(2)-O(1)-Ru(1)-P(1)	18.6(2)
O(1)-Ru(1)-P(1)-C(1)	11.76(13)
Ru(1)-P(2)-C(5)-C(6)	164.5(3)
P(2)-C(5)-C(6)-O(2)	-71.4(5)
C(5)-C(6)-O(2)-C(8)	171.4(5)
Ru(1)-N(1)-C(10)-C(11)	49.4(4)
N(1)-C(10)-C(11)-C(12)	-74.4(4)
C(10)-C(11)-C(12)-N(2)	70.8(4)
C(11)-C(12)-N(2)-Ru(1)	-43.1(4)
C(12)-N(2)-Ru(1)-N(1)	18.7(3)
N(2)-Ru(1)-N(1)-C(10)	-22.2(3)

Table S21. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for **4b·(PF$_6$)**.

```
-9.5936 (0.0125) x + 8.1861 (0.0135) y + 8.8922 (0.0516) z = 4.5519
(0.0136)
 *    0.0198 (0.0016)  N1
 *   -0.0238 (0.0020)  C10
 *   -0.0195 (0.0016)  N2
 *    0.0235 (0.0019)  C12
     -0.4544 (0.0051)  Ru1
      0.7380 (0.0054)  C11
 Rms deviation of fitted atoms =   0.0217

5.7899 (0.0109) x + 2.9676 (0.0095) y + 16.7060 (0.0113) z = 0.9292
(0.0059)
Angle to previous plane (with approximate esd) = 87.51 ( 0.13 )
 *    0.0000 (0.0000)  Ru1
 *    0.0000 (0.0000)  P1
 *    0.0000 (0.0000)  O1
      0.3670 (0.0040)  C1
     -0.4280 (0.0046)  C2
 Rms deviation of fitted atoms =   0.0000

-9.1141 (0.0071) x + 8.8640 (0.0058) y + 5.3208 (0.0165) z = 5.3624
(0.0067)
 Angle to previous plane (with approximate esd) = 86.70 ( 0.06 )
 *   -0.1699 (0.0009)  Ru1
 *    0.0368 (0.0011)  P1
 *    0.0486 (0.0011)  C11
 *    0.0306 (0.0013)  N1
 *    0.0540 (0.0012)  N2
     -2.4136 (0.0015)  P2
      2.1305 (0.0026)  O1
 Rms deviation of fitted atoms =   0.0854

5.5595 (0.0084) x + 3.0933 (0.0065) y + 16.9257 (0.0123) z = 0.9814
(0.0066)
Angle to previous plane (with approximate esd) = 87.80 ( 0.05 )
 *   -0.0118 (0.0008)  Ru1
 *   -0.0234 (0.0010)  P1
 *    0.0281 (0.0009)  P2
```

```
*     0.0315 (0.0011)   O1
*    -0.0244 (0.0011)   N1
      2.1141 (0.0029)   N2
     -2.3874 (0.0015)   Cl1
 Rms deviation of fitted atoms =    0.0247

8.7996 (0.0066) x + 6.2444 (0.0061) y - 16.7638 (0.0116) z = 8.4309
(0.0041)
 Angle to previous plane (with approximate esd) = 84.64 ( 0.05 )
 *     0.0745 (0.0008)   Ru1
 *     0.0671 (0.0009)   P2
 *    -0.1053 (0.0010)   Cl1
 *     0.0863 (0.0011)   O1
 *    -0.1226 (0.0012)   N2
      2.3470 (0.0015)   P1
     -2.0916 (0.0030)   N1
 Rms deviation of fitted atoms =    0.0934
```

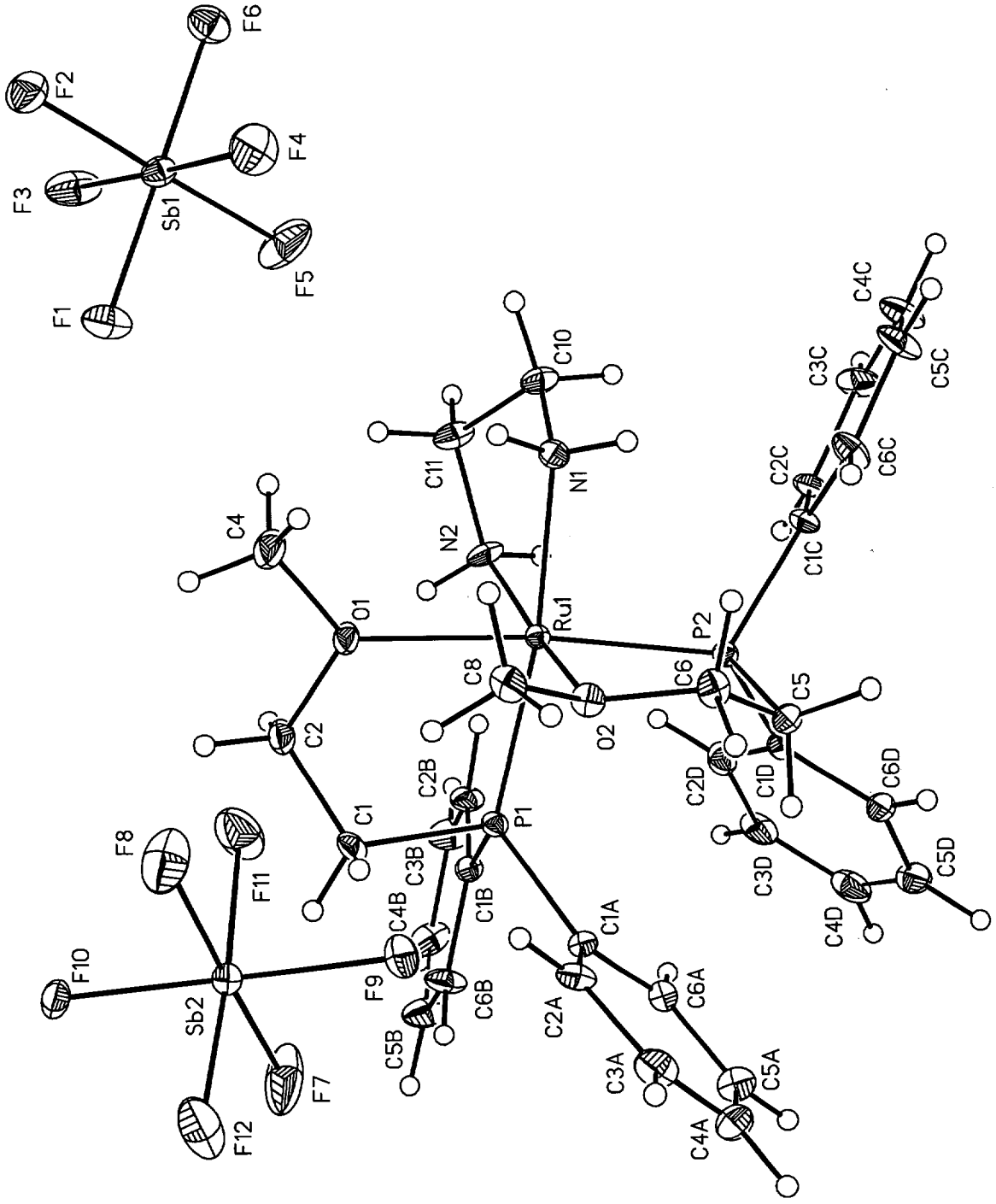

Figure S4. ORTEP plot of **5a**·$(SbF_6)_2$.

Table S22. Crystal data and structure refinement for **5a**·$(SbF_6)_2$.

Empirical formula	C32 H42 F12 N2 O2 P2 Ru Sb2
Formula weight	1121.19
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 15.348(5) A alpha = 90 deg. b = 15.163(6) A beta = 90 deg. c = 34.983(10) A gamma = 90 deg.
Volume	8141(5) A^3
Z, Calculated density	8, 1.830 Mg/m^3
Absorption coefficient	1.849 mm^-1
F(000)	4384
Crystal size	0.1 x 0.3 x 0.2 mm
Theta range for data collection	2.22 to 27.51 deg.
Limiting indices	-1<=h<=19, -1<=k<=19, -1<=l<=45
Reflections collected / unique	11052 / 9320 [R(int) = 0.0508]
Completeness to theta = 27.51	99.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9320 / 0 / 479
Goodness-of-fit on F^2	1.936
Final R indices [I>2sigma(I)]	R1 = 0.0602, wR2 = 0.1387
R indices (all data)	R1 = 0.1183, wR2 = 0.1764
Extinction coefficient	0.00017(6)
Largest diff. peak and hole	1.102 and -1.260 e.A^-3

Table S23. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5a·$(SbF_6)_2$**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sb(1)	5659(1)	7036(1)	367(1)	32(1)
Sb(2)	8428(1)	2759(1)	1919(1)	29(1)
F(1)	6058(5)	5913(5)	498(2)	57(2)
F(2)	4520(4)	6615(5)	330(2)	57(2)
F(3)	5839(5)	6804(6)	-153(2)	66(2)
F(4)	5476(6)	7310(6)	881(2)	67(2)
F(5)	6789(5)	7476(7)	400(3)	86(3)
F(6)	5268(5)	8166(4)	223(2)	49(2)
F(7)	9587(5)	2645(8)	1789(4)	104(4)
F(8)	7246(5)	2918(7)	2030(3)	73(3)
F(9)	8737(5)	3582(4)	2297(2)	49(2)
F(10)	8106(4)	1937(4)	1540(2)	39(1)
F(11)	8289(7)	3656(5)	1554(2)	75(3)
F(12)	8499(9)	1835(5)	2260(2)	108(5)
Ru(1)	9670(1)	6595(1)	1197(1)	20(1)
P(1)	10649(2)	5453(1)	1135(1)	23(1)
P(2)	10589(1)	7501(1)	1499(1)	22(1)
C(1)	9921(6)	4507(6)	1054(3)	36(2)
C(2)	9177(7)	4773(7)	800(3)	41(2)
O(1)	8748(4)	5538(5)	968(2)	35(2)
C(4)	7850(7)	5558(9)	882(4)	59(4)
C(5)	10497(6)	7147(6)	1999(2)	30(2)
C(6)	9636(7)	6731(6)	2083(2)	32(2)
O(2)	9399(4)	6154(4)	1779(2)	29(1)
C(8)	8614(6)	5668(6)	1873(3)	33(2)
N(1)	8596(5)	7536(5)	1234(2)	28(2)
C(10)	8580(7)	8103(7)	889(3)	36(2)
C(11)	8852(7)	7553(8)	546(3)	41(2)
N(2)	9698(5)	7106(6)	633(2)	32(2)
C(1A)	11274(6)	5133(6)	1561(3)	30(2)
C(2A)	10832(7)	4732(6)	1869(3)	36(2)
C(3A)	11311(11)	4559(8)	2202(3)	55(4)
C(4A)	12167(10)	4752(9)	2234(3)	56(3)
C(5A)	12601(9)	5159(8)	1928(4)	54(3)
C(6A)	12146(7)	5359(7)	1597(3)	38(2)
C(1B)	11438(6)	5312(6)	750(2)	28(2)
C(2B)	11504(7)	5870(7)	438(3)	36(2)
C(3B)	12107(8)	5752(9)	154(3)	52(3)
C(4B)	12652(7)	5031(9)	169(3)	50(3)
C(5B)	12593(8)	4434(10)	465(3)	54(3)
C(6B)	11993(8)	4575(8)	757(3)	45(3)
C(1C)	10318(6)	8676(5)	1496(3)	26(2)
C(2C)	10645(7)	9196(6)	1207(3)	35(2)
C(3C)	10392(8)	10098(7)	1168(4)	49(3)
C(4C)	9813(9)	10443(7)	1423(4)	54(3)
C(5C)	9482(9)	9937(7)	1708(3)	52(3)
C(6C)	9732(8)	9043(6)	1757(3)	39(2)
C(1D)	11751(6)	7516(6)	1421(3)	30(2)
C(2D)	12088(7)	7371(7)	1054(3)	37(2)
C(3D)	12989(7)	7329(7)	992(4)	46(3)
C(4D)	13545(8)	7427(7)	1294(5)	57(4)
C(5D)	13238(7)	7585(8)	1654(5)	51(3)
C(6D)	12339(6)	7632(7)	1722(4)	41(2)

Table S24. Bond lengths [A] and angles [deg] for **5a·$(SbF_6)_2$**.

Sb(1)-F(5)	1.862(8)	C(6)-O(2)	1.426(11)
Sb(1)-F(2)	1.864(7)	O(2)-C(8)	1.450(10)
Sb(1)-F(1)	1.867(7)	N(1)-C(10)	1.483(12)
Sb(1)-F(4)	1.867(7)	C(10)-C(11)	1.517(15)
Sb(1)-F(3)	1.874(7)	C(11)-N(2)	1.495(12)
Sb(1)-F(6)	1.884(7)	C(1A)-C(6A)	1.388(14)
Sb(2)-F(7)	1.843(8)	C(1A)-C(2A)	1.411(14)
Sb(2)-F(12)	1.845(7)	C(2A)-C(3A)	1.403(15)
Sb(2)-F(8)	1.871(7)	C(3A)-C(4A)	1.35(2)
Sb(2)-F(11)	1.876(8)	C(4A)-C(5A)	1.40(2)
Sb(2)-F(9)	1.880(6)	C(5A)-C(6A)	1.386(15)
Sb(2)-F(10)	1.885(6)	C(1B)-C(2B)	1.386(14)
Ru(1)-N(2)	2.122(7)	C(1B)-C(6B)	1.405(13)
Ru(1)-O(2)	2.182(6)	C(2B)-C(3B)	1.370(14)
Ru(1)-N(1)	2.184(7)	C(3B)-C(4B)	1.377(17)
Ru(1)-P(2)	2.234(2)	C(4B)-C(5B)	1.380(18)
Ru(1)-O(1)	2.283(7)	C(5B)-C(6B)	1.390(15)
Ru(1)-P(1)	2.304(2)	C(1C)-C(2C)	1.379(14)
P(1)-C(1B)	1.823(9)	C(1C)-C(6C)	1.396(13)
P(1)-C(1A)	1.836(9)	C(2C)-C(3C)	1.428(13)
P(1)-C(1)	1.840(10)	C(3C)-C(4C)	1.364(18)
P(1)-P(2)	3.358(3)	C(4C)-C(5C)	1.356(17)
P(2)-C(1D)	1.805(10)	C(5C)-C(6C)	1.419(14)
P(2)-C(1C)	1.829(8)	C(1D)-C(6D)	1.399(14)
P(2)-C(5)	1.836(8)	C(1D)-C(2D)	1.401(15)
C(1)-C(2)	1.502(14)	C(2D)-C(3D)	1.401(13)
C(2)-O(1)	1.457(12)	C(3D)-C(4D)	1.365(19)
O(1)-C(4)	1.411(12)	C(4D)-C(5D)	1.37(2)
C(5)-C(6)	1.493(13)	C(5D)-C(6D)	1.402(15)

F(5)-Sb(1)-F(2)	178.9(4)	F(9)-Sb(2)-F(10)	179.4(3)
F(5)-Sb(1)-F(1)	90.4(4)	N(2)-Ru(1)-O(2)	169.7(3)
F(2)-Sb(1)-F(1)	90.8(4)	N(2)-Ru(1)-N(1)	80.3(3)
F(5)-Sb(1)-F(4)	90.1(5)	O(2)-Ru(1)-N(1)	90.1(3)
F(2)-Sb(1)-F(4)	90.1(4)	N(2)-Ru(1)-P(2)	101.6(3)
F(1)-Sb(1)-F(4)	91.0(4)	O(2)-Ru(1)-P(2)	82.43(18)
F(5)-Sb(1)-F(3)	89.4(5)	N(1)-Ru(1)-P(2)	92.7(2)
F(2)-Sb(1)-F(3)	90.4(4)	N(2)-Ru(1)-O(1)	86.7(3)
F(1)-Sb(1)-F(3)	91.0(3)	O(2)-Ru(1)-O(1)	89.7(3)
F(4)-Sb(1)-F(3)	177.9(4)	N(1)-Ru(1)-O(1)	90.7(3)
F(5)-Sb(1)-F(6)	89.2(4)	P(2)-Ru(1)-O(1)	171.5(2)
F(2)-Sb(1)-F(6)	89.7(3)	N(2)-Ru(1)-P(1)	100.0(2)
F(1)-Sb(1)-F(6)	178.6(3)	O(2)-Ru(1)-P(1)	88.97(18)
F(4)-Sb(1)-F(6)	90.4(3)	N(1)-Ru(1)-P(1)	171.6(2)
F(3)-Sb(1)-F(6)	87.6(3)	P(2)-Ru(1)-P(1)	95.45(8)
F(7)-Sb(2)-F(12)	91.7(7)	O(1)-Ru(1)-P(1)	81.00(18)
F(7)-Sb(2)-F(8)	177.1(6)	C(1B)-P(1)-C(1A)	102.8(4)
F(12)-Sb(2)-F(8)	91.1(6)	C(1B)-P(1)-C(1)	101.5(4)
F(7)-Sb(2)-F(11)	90.6(6)	C(1A)-P(1)-C(1)	103.7(5)
F(12)-Sb(2)-F(11)	175.9(4)	C(1B)-P(1)-Ru(1)	126.3(3)
F(8)-Sb(2)-F(11)	86.5(5)	C(1A)-P(1)-Ru(1)	117.6(3)
F(7)-Sb(2)-F(9)	89.5(4)	C(1)-P(1)-Ru(1)	101.8(3)
F(12)-Sb(2)-F(9)	91.9(3)	C(1B)-P(1)-P(2)	114.0(3)
F(8)-Sb(2)-F(9)	90.7(3)	C(1A)-P(1)-P(2)	87.2(3)
F(11)-Sb(2)-F(9)	91.4(3)	C(1)-P(1)-P(2)	139.7(3)
F(7)-Sb(2)-F(10)	91.1(3)	Ru(1)-P(1)-P(2)	41.47(6)
F(12)-Sb(2)-F(10)	88.2(3)	C(1D)-P(2)-C(1C)	102.2(4)
F(8)-Sb(2)-F(10)	88.8(3)	C(1D)-P(2)-C(5)	102.9(5)
F(11)-Sb(2)-F(10)	88.4(3)	C(1C)-P(2)-C(5)	105.8(4)

C(1D)-P(2)-Ru(1)	124.1(3)	C(6A)-C(5A)-C(4A)	119.7(12)
C(1C)-P(2)-Ru(1)	116.9(3)	C(5A)-C(6A)-C(1A)	120.5(11)
C(5)-P(2)-Ru(1)	102.8(3)	C(2B)-C(1B)-C(6B)	117.0(9)
C(1D)-P(2)-P(1)	85.8(3)	C(2B)-C(1B)-P(1)	124.0(7)
C(1C)-P(2)-P(1)	154.8(3)	C(6B)-C(1B)-P(1)	119.0(7)
C(5)-P(2)-P(1)	95.3(3)	C(3B)-C(2B)-C(1B)	122.7(9)
Ru(1)-P(2)-P(1)	43.08(6)	C(2B)-C(3B)-C(4B)	119.2(11)
C(2)-C(1)-P(1)	110.1(7)	C(3B)-C(4B)-C(5B)	120.6(10)
O(1)-C(2)-C(1)	108.6(8)	C(4B)-C(5B)-C(6B)	119.6(10)
C(4)-O(1)-C(2)	111.9(8)	C(5B)-C(6B)-C(1B)	120.8(10)
C(4)-O(1)-Ru(1)	131.7(7)	C(2C)-C(1C)-C(6C)	119.1(8)
C(2)-O(1)-Ru(1)	114.9(5)	C(2C)-C(1C)-P(2)	118.6(7)
C(6)-C(5)-P(2)	112.2(6)	C(6C)-C(1C)-P(2)	122.1(7)
O(2)-C(6)-C(5)	109.7(7)	C(1C)-C(2C)-C(3C)	121.3(10)
C(6)-O(2)-C(8)	110.7(7)	C(4C)-C(3C)-C(2C)	118.8(11)
C(6)-O(2)-Ru(1)	117.3(5)	C(5C)-C(4C)-C(3C)	120.6(10)
C(8)-O(2)-Ru(1)	121.7(6)	C(4C)-C(5C)-C(6C)	121.8(10)
C(10)-N(1)-Ru(1)	110.1(6)	C(1C)-C(6C)-C(5C)	118.4(9)
N(1)-C(10)-C(11)	108.6(8)	C(6D)-C(1D)-C(2D)	118.2(9)
N(2)-C(11)-C(10)	109.2(8)	C(6D)-C(1D)-P(2)	121.7(8)
C(11)-N(2)-Ru(1)	109.6(6)	C(2D)-C(1D)-P(2)	120.1(7)
C(6A)-C(1A)-C(2A)	120.0(9)	C(3D)-C(2D)-C(1D)	120.9(10)
C(6A)-C(1A)-P(1)	120.8(8)	C(4D)-C(3D)-C(2D)	119.5(12)
C(2A)-C(1A)-P(1)	118.9(7)	C(3D)-C(4D)-C(5D)	121.1(11)
C(3A)-C(2A)-C(1A)	117.6(11)	C(4D)-C(5D)-C(6D)	120.4(12)
C(4A)-C(3A)-C(2A)	122.6(12)	C(1D)-C(6D)-C(5D)	120.0(12)
C(3A)-C(4A)-C(5A)	119.6(11)		

Table S25. Anisotropic displacement parameters (A^2 x 10^3) for **5a·$(SbF_6)_2$**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sb(1)	30(1)	41(1)	27(1)	2(1)	1(1)	6(1)
Sb(2)	28(1)	27(1)	34(1)	-3(1)	-5(1)	-1(1)
F(1)	65(5)	53(4)	55(4)	3(3)	4(4)	23(4)
F(2)	39(3)	57(4)	73(5)	4(4)	-4(3)	-4(3)
F(3)	67(5)	95(6)	37(3)	-1(4)	10(3)	41(5)
F(4)	92(6)	76(5)	34(3)	-1(4)	-9(4)	8(5)
F(5)	38(4)	108(7)	112(8)	38(6)	-16(4)	-22(4)
F(6)	62(4)	43(4)	43(3)	5(3)	2(3)	8(3)
F(7)	34(4)	131(9)	146(10)	-92(8)	-7(5)	1(5)
F(8)	40(4)	110(7)	71(5)	-37(5)	13(4)	-6(4)
F(9)	62(4)	38(3)	47(4)	-16(3)	-14(3)	5(3)
F(10)	31(3)	40(3)	45(3)	-15(3)	-11(3)	0(2)
F(11)	126(8)	43(4)	57(5)	9(4)	-10(5)	-4(5)
F(12)	230(14)	42(4)	51(4)	15(4)	-71(7)	-26(6)
Ru(1)	20(1)	21(1)	18(1)	-1(1)	1(1)	2(1)
P(1)	25(1)	22(1)	22(1)	-2(1)	1(1)	4(1)
P(2)	24(1)	21(1)	20(1)	0(1)	1(1)	1(1)
C(1)	34(5)	24(4)	49(6)	-15(4)	0(4)	8(4)
C(2)	32(5)	38(5)	53(6)	-22(5)	-6(5)	2(4)
O(1)	20(3)	36(4)	49(4)	-18(3)	-5(3)	1(3)
C(4)	30(5)	63(8)	83(9)	-37(7)	-16(6)	10(6)
C(5)	45(5)	30(4)	15(3)	3(3)	-8(3)	4(4)
C(6)	41(5)	36(5)	19(3)	0(3)	6(4)	-4(4)
O(2)	28(3)	31(3)	27(3)	5(3)	8(2)	-3(3)
C(8)	25(4)	28(4)	47(5)	4(4)	12(4)	-7(4)
N(1)	28(4)	27(3)	28(4)	0(3)	3(3)	1(3)
C(10)	36(5)	44(5)	30(4)	10(4)	-4(4)	11(4)
C(11)	29(5)	58(7)	36(5)	7(5)	1(4)	15(5)
N(2)	26(3)	51(5)	19(3)	5(3)	-2(3)	17(4)
C(1A)	32(4)	27(4)	31(4)	0(4)	-10(4)	7(4)
C(2A)	42(5)	29(5)	38(5)	8(4)	4(4)	10(4)
C(3A)	104(11)	42(6)	20(4)	6(4)	-7(6)	16(7)
C(4A)	82(9)	50(7)	35(6)	1(5)	-25(6)	10(7)
C(5A)	58(7)	48(7)	55(7)	0(6)	-17(6)	11(6)
C(6A)	42(5)	30(5)	42(5)	-6(4)	-11(5)	2(4)
C(1B)	30(4)	31(4)	22(4)	-5(3)	-2(3)	8(4)
C(2B)	35(5)	39(5)	33(5)	-7(4)	2(4)	20(4)
C(3B)	53(7)	70(8)	33(5)	7(5)	10(5)	24(6)
C(4B)	41(6)	81(9)	27(5)	-13(5)	6(4)	27(6)
C(5B)	52(7)	75(9)	36(5)	-2(6)	10(5)	39(7)
C(6B)	60(7)	40(6)	34(5)	1(4)	5(5)	29(6)
C(1C)	22(4)	16(3)	39(4)	1(3)	5(4)	2(3)
C(2C)	35(5)	22(4)	47(5)	-1(4)	0(5)	12(4)
C(3C)	46(6)	26(5)	74(8)	23(5)	3(6)	1(4)
C(4C)	71(8)	22(5)	69(8)	6(5)	13(7)	14(5)
C(5C)	74(8)	32(5)	49(6)	-8(5)	18(6)	24(6)
C(6C)	59(6)	23(4)	34(5)	1(4)	17(5)	0(5)
C(1D)	27(4)	21(4)	42(5)	-2(4)	-6(4)	-1(3)
C(2D)	33(5)	32(5)	44(5)	-5(4)	1(4)	-5(4)
C(3D)	26(5)	40(6)	72(8)	-13(6)	18(5)	9(4)
C(4D)	33(5)	28(5)	111(12)	-3(6)	2(7)	-1(4)
C(5D)	28(5)	34(6)	90(10)	1(6)	-16(6)	-4(4)
C(6D)	28(5)	30(5)	63(7)	-7(5)	-17(5)	1(4)

Table S26. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5a**·$(SbF_6)_2$.

	x	y	z	U(eq)
H(1A)	10250	4020	933	43
H(1B)	9691	4293	1302	43
H(2A)	9398	4922	542	49
H(2B)	8758	4281	775	49
H(4A)	7664	4975	793	88
H(4B)	7741	5996	682	88
H(4C)	7522	5717	1112	88
H(5A)	10967	6719	2056	36
H(5B)	10579	7664	2168	36
H(6A)	9671	6396	2326	38
H(6B)	9187	7195	2113	38
H(8A)	8591	5567	2150	50
H(8B)	8618	5099	1740	50
H(8C)	8102	6008	1794	50
H(1NA)	8076	7237	1254	33
H(1NB)	8661	7881	1448	33
H(10A)	8986	8605	921	44
H(10B)	7987	8341	848	44
H(11A)	8400	7107	490	49
H(11B)	8919	7936	319	49
H(2NA)	10149	7503	609	38
H(2NB)	9790	6656	462	38
H(2A)	10232	4585	1852	43
H(3A)	11022	4296	2413	66
H(4A)	12474	4614	2462	67
H(5A)	13203	5298	1948	64
H(6A)	12434	5652	1393	46
H(2B)	11114	6356	420	43
H(3B)	12148	6161	-51	63
H(4B)	13072	4944	-27	60
H(5B)	12961	3930	471	65
H(6B)	11958	4168	962	54
H(2C)	11047	8950	1030	42
H(3C)	10622	10451	967	58
H(4C)	9641	11043	1402	64
H(5C)	9070	10187	1879	62
H(6C)	9507	8702	1962	47
H(2D)	11701	7300	844	44
H(3D)	13211	7234	742	55
H(4D)	14155	7384	1252	69
H(5D)	13636	7663	1859	61
H(6D)	12130	7743	1973	49

Table S27. Selected torsion angles [deg] for **5a·(SbF$_6$)$_2$**.

Ru(1)-P(1)-C(1)-C(2)	39.3(8)
P(1)-C(1)-C(2)-O(1)	-54.5(10)
C(1)-C(2)-O(1)-Ru(1)	43.5(11)
C(2)-O(1)-Ru(1)-P(1)	-15.1(7)
O(1)-Ru(1)-P(1)-C(1)	-12.1(4)
Ru(1)-P(2)-C(5)-C(6)	-26.3(7)
P(2)-C(5)-C(6)-O(2)	42.7(9)
C(5)-C(6)-O(2)-Ru(1)	-40.4(9)
C(6)-O(2)-Ru(1)-P(2)	19.3(6)
O(2)-Ru(1)-P(2)-C(5)	4.2(4)
Ru(1)-N(1)-C(10)-C(11)	35.7(9)
N(1)-C(10)-C(11)-N(2)	-52.4(11)
C(10)-C(11)-N(2)-Ru(1)	43.1(11)
C(11)-N(2)-Ru(1)-N(1)	-18.0(7)
N(2)-Ru(1)-N(1)-C(10)	-10.0(6)

Table S28. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for **5a·(SbF$_6$)$_2$**.

```
3.0771 (0.0398) x + 4.4243 (0.0331) y - 32.7169 (0.0431) z = 1.9756
(0.0629)
 *     0.0000 (0.0000)  Ru1
 *     0.0000 (0.0000)  P1
 *     0.0000 (0.0000)  O1
      -0.3778 (0.0131)  C1
       0.3436 (0.0157)  C2
 Rms deviation of fitted atoms =   0.0000

3.2318 (0.0426) x + 2.7742 (0.0513) y - 33.5939 (0.0335) z = 1.0252
(0.0568)
 Angle to previous plane (with approximate esd) =  6.43 ( 0.27 )
 *    -0.0931 (0.0033)  Ru1
 *     0.1160 (0.0040)  P1
 *    -0.1099 (0.0037)  C1
 *     0.0871 (0.0030)  O1
       0.5782 (0.0152)  C2
 Rms deviation of fitted atoms =   0.1022

4.4548 (0.0477) x + 4.0376 (0.0464) y - 32.1544 (0.0449) z = 3.1461
(0.0567)
Angle to previous plane (with approximate esd) =  7.02 ( 0.28 )
 *    -0.0260 (0.0036)  Ru1
 *     0.1497 (0.0046)  P1
 *    -0.1250 (0.0059)  O1
 *    -0.2965 (0.0068)  C1
 *     0.2978 (0.0080)  C2
 Rms deviation of fitted atoms =   0.2075

11.1234 (0.0167) x - 10.3815 (0.0207) y - 2.7007 (0.0945) z = 3.5863
(0.0222)
 Angle to previous plane (with approximate esd) = 84.32 ( 0.23 )
 *     0.0000 (0.0000)  Ru1
 *     0.0000 (0.0000)  P2
 *     0.0000 (0.0000)  O2
       0.1310 (0.0113)  C5
      -0.4185 (0.0131)  C6
 Rms deviation of fitted atoms =   0.0000
```

```
10.9101 (0.0277) x - 10.5246 (0.0274) y - 3.9739 (0.1021) z = 3.1009
(0.0495)
Angle to previous plane (with approximate esd) =  2.30 ( 0.31 )
 *    0.0324 (0.0028)  Ru1
 *   -0.0386 (0.0033)  P2
 *    0.0358 (0.0031)  C5
 *   -0.0296 (0.0025)  O2
     -0.5002 (0.0127)  C6
 Rms deviation of fitted atoms =   0.0343

10.4863 (0.0317) x - 11.0695 (0.0293) y - 0.5105 (0.0903) z = 2.7997
(0.0532)
Angle to previous plane (with approximate esd) =  6.24 ( 0.37 )
 *   -0.0209 (0.0030)  Ru1
 *   -0.0757 (0.0039)  P2
 *    0.1541 (0.0049)  O2
 *    0.1951 (0.0056)  C5
 *   -0.2526 (0.0064)  C6
 Rms deviation of fitted atoms =   0.1623

-3.7995 (5.2399) x + 10.9009 (9.9990) y - 22.7215 (9.9990) z = 1.3651
(2.6421)
Angle to previous plane (with approximate esd) = 46.80 (62.95 )
 *    0.7809 (1.1288)  N1
 *    1.2584 (2.0978)  N2
 *   -0.5709 (0.8944)  Ru1
 *   -0.6173 (0.9663)  P2
 *   -0.8511 (1.3486)  O1
      2.1893 (3.3989)  C10
      2.2637 (3.6147)  C11
 Rms deviation of fitted atoms =   0.8514

9.8013 (0.0444) x + 10.7850 (0.0380) y + 10.2744 (0.1501) z = 17.8200
(0.0180)
Angle to previous plane (with approximate esd) = 80.65 (51.70 )
 *    0.0000 (0.0001)  Ru1
 *    0.0000 (0.0000)  N1
 *    0.0000 (0.0000)  N2
      0.2422 (0.0156)  C10
     -0.4357 (0.0171)  C11
 Rms deviation of fitted atoms =   0.0000

10.4136 (0.0443) x + 10.7412 (0.0378) y + 6.8024 (0.1493) z = 17.9925
(0.0131)
Angle to previous plane (with approximate esd) =  6.13 ( 0.55 )
 *   -0.0250 (0.0042)  Ru1
 *   -0.1075 (0.0057)  N1
 *    0.1704 (0.0064)  N2
 *    0.2511 (0.0073)  C10
 *   -0.2890 (0.0080)  C11
 Rms deviation of fitted atoms =   0.1938

10.5961 (0.0205) x + 9.8849 (0.0216) y + 10.9710 (0.0873) z = 17.9548
(0.0105)
Angle to previous plane (with approximate esd) =  7.59 ( 0.44 )
 *   -0.0440 (0.0039)  N1
 *    0.0405 (0.0036)  N2
 *   -0.0357 (0.0032)  P1
 *    0.0392 (0.0035)  O2
      0.1236 (0.0035)  Ru1
 Rms deviation of fitted atoms =   0.0399
```