Electronic Supplementary Information for Dalton Transactions

Supplementary Material

Synthesis and Lanthanide Coordination Chemistry of Trifluoromethyl Derivatives of Phosphinoylmethyl-pyridine N-oxides

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Contents

Electronic Supplementary Information for Dalton Transactions

X-ray Crystallographic data for **3c**.

Crystal Structure Report

Prepared for:

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Compound:

Rps21/slp-11-38

C20 H14 F6 N O P

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277-6649

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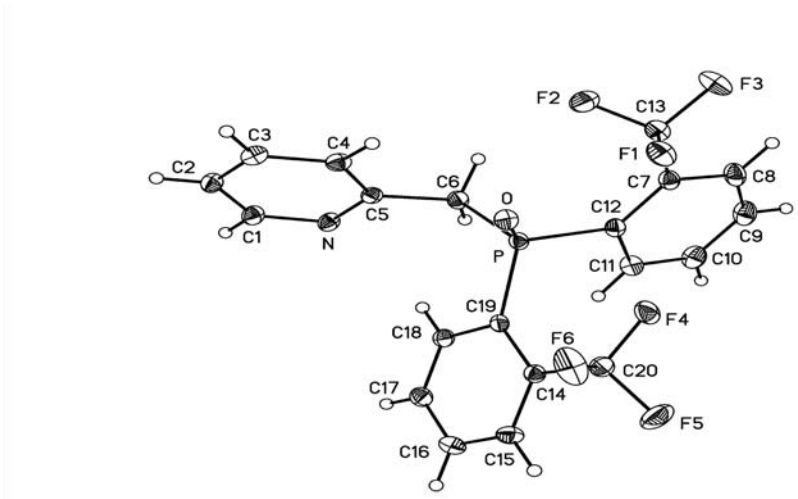

Rpsl21l1b.jpg $225

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Table 1. Crystal data and structure refinement for rpsl21.

Identification code	rpsl21	
Empirical formula	C20 H14 F6 N O P	
Formula weight	429.29	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.9554(4) Å	α= 88.599(2)°.
	b = 9.6902(4) Å	β= 74.127(2)°.
	c = 11.0339(4) Å	γ = 88.578(2)°.
Volume	920.57(7) $Å^3$	
Z	2	
Density (calculated)	1.549 Mg/m^3	
Absorption coefficient	0.219 mm^{-1}	
F(000)	436	
Crystal size	0.48 x 0.28 x 0.12 mm^3	
Theta range for data collection	2.61 to 32.13°.	
Index ranges	-10<=h<=13, -14<=k<=14, -16<=l<=16	
Reflections collected	19527	
Independent reflections	6424 [R(int) = 0.0162]	
Completeness to theta = 32.13°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.97 and 0.90	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6424 / 0 / 262	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1459	
R indices (all data)	R1 = 0.0628, wR2 = 0.1615	
Largest diff. peak and hole	0.785 and -0.294 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rpsl21. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P	7616(1)	2455(1)	3893(1)	30(1)
O	6641(1)	3652(1)	3723(1)	38(1)
N	6873(2)	1901(2)	7434(1)	39(1)
C(1)	6315(2)	2507(2)	8550(2)	42(1)
C(2)	5088(2)	3443(2)	8813(2)	42(1)
C(3)	4418(2)	3813(2)	7862(2)	43(1)
C(4)	4970(2)	3196(2)	6701(2)	39(1)
C(5)	6174(2)	2223(2)	6531(1)	33(1)
C(6)	6745(2)	1445(2)	5320(2)	37(1)
C(7)	6960(2)	731(2)	2005(2)	36(1)
C(8)	7329(3)	-384(2)	1194(2)	49(1)
C(9)	8651(3)	-1172(2)	1102(2)	56(1)
C(10)	9647(3)	-859(2)	1806(2)	52(1)
C(11)	9317(2)	264(2)	2595(2)	43(1)
C(12)	7962(2)	1082(2)	2720(1)	34(1)
C(13)	5466(2)	1505(2)	2087(2)	43(1)
F(1)	5666(2)	2808(1)	1665(1)	51(1)
F(2)	4557(1)	1542(1)	3281(1)	56(1)
F(3)	4623(2)	929(2)	1405(2)	66(1)
C(14)	10522(2)	3814(2)	3038(1)	33(1)
C(15)	11899(2)	4266(2)	3227(2)	43(1)
C(16)	12329(2)	3907(2)	4306(2)	46(1)
C(17)	11391(2)	3059(2)	5203(2)	44(1)
C(18)	10006(2)	2594(2)	5029(2)	39(1)
C(19)	9534(2)	2962(2)	3955(1)	32(1)
C(20)	10183(2)	4318(2)	1840(2)	40(1)
F(4)	9238(2)	3535(1)	1433(1)	53(1)
F(5)	11470(2)	4413(2)	893(1)	87(1)
F(6)	9527(2)	5571(1)	1958(2)	78(1)

Table 3. Bond lengths [Å] and angles [°] for rpsl21.

P-O	1.4734(12)
P-C(19)	1.8175(15)
P-C(6)	1.8262(15)
P-C(12)	1.8396(15)
N-C(1)	1.339(2)
N-C(5)	1.342(2)
C(1)-C(2)	1.380(3)
C(1)-H(1)	0.9400
C(2)-C(3)	1.380(3)
C(2)-H(2)	0.9400
C(3)-C(4)	1.385(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.390(2)
C(4)-H(4)	0.9400
C(5)-C(6)	1.507(2)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(7)-C(8)	1.394(2)
C(7)-C(12)	1.401(2)
C(7)-C(13)	1.499(3)
C(8)-C(9)	1.374(3)
C(8)-H(8)	0.9400
C(9)-C(10)	1.377(3)
C(9)-H(9)	0.9400
C(10)-C(11)	1.385(3)
C(10)-H(10)	0.9400
C(11)-C(12)	1.409(2)
C(11)-H(11)	0.9400
C(13)-F(1)	1.334(2)
C(13)-F(3)	1.341(2)
C(13)-F(2)	1.347(2)
C(14)-C(15)	1.389(2)
C(14)-C(19)	1.411(2)
C(14)-C(20)	1.504(2)

C(15)-C(16)	1.383(3)
C(15)-H(15)	0.9400
C(16)-C(17)	1.378(3)
C(16)-H(16)	0.9400
C(17)-C(18)	1.393(2)
C(17)-H(17)	0.9400
C(18)-C(19)	1.399(2)
C(18)-H(18)	0.9400
C(20)-F(4)	1.323(2)
C(20)-F(6)	1.329(2)
C(20)-F(5)	1.331(2)

O-P-C(19)	112.11(7)
O-P-C(6)	112.66(8)
C(19)-P-C(6)	107.93(7)
O-P-C(12)	117.96(7)
C(19)-P-C(12)	105.31(7)
C(6)-P-C(12)	99.77(7)
C(1)-N-C(5)	117.25(15)
N-C(1)-C(2)	124.04(16)
N-C(1)-H(1)	118.0
C(2)-C(1)-H(1)	118.0
C(1)-C(2)-C(3)	118.30(16)
C(1)-C(2)-H(2)	120.8
C(3)-C(2)-H(2)	120.8
C(2)-C(3)-C(4)	118.73(16)
C(2)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(3)-C(4)-C(5)	119.18(15)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
N-C(5)-C(4)	122.39(15)
N-C(5)-C(6)	116.08(14)
C(4)-C(5)-C(6)	121.52(14)
C(5)-C(6)-P	117.13(11)
C(5)-C(6)-H(6A)	108.0

P-C(6)-H(6A)	108.0
C(5)-C(6)-H(6B)	108.0
P-C(6)-H(6B)	108.0
H(6A)-C(6)-H(6B)	107.3
C(8)-C(7)-C(12)	119.94(17)
C(8)-C(7)-C(13)	117.83(16)
C(12)-C(7)-C(13)	122.22(14)
C(9)-C(8)-C(7)	121.12(19)
C(9)-C(8)-H(8)	119.4
C(7)-C(8)-H(8)	119.4
C(8)-C(9)-C(10)	120.11(17)
C(8)-C(9)-H(9)	119.9
C(10)-C(9)-H(9)	119.9
C(9)-C(10)-C(11)	119.56(19)
C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2
C(10)-C(11)-C(12)	121.65(18)
C(10)-C(11)-H(11)	119.2
C(12)-C(11)-H(11)	119.2
C(7)-C(12)-C(11)	117.60(14)
C(7)-C(12)-P	125.90(12)
C(11)-C(12)-P	116.38(12)
F(1)-C(13)-F(3)	105.36(15)
F(1)-C(13)-F(2)	107.23(15)
F(3)-C(13)-F(2)	106.37(16)
F(1)-C(13)-C(7)	113.45(15)
F(3)-C(13)-C(7)	112.45(15)
F(2)-C(13)-C(7)	111.49(15)
C(15)-C(14)-C(19)	120.01(15)
C(15)-C(14)-C(20)	115.50(14)
C(19)-C(14)-C(20)	124.48(14)
C(16)-C(15)-C(14)	121.34(16)
C(16)-C(15)-H(15)	119.3
C(14)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	119.48(16)
C(17)-C(16)-H(16)	120.3

C(15)-C(16)-H(16)	120.3
C(16)-C(17)-C(18)	119.97(16)
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	121.59(16)
C(17)-C(18)-H(18)	119.2
C(19)-C(18)-H(18)	119.2
C(18)-C(19)-C(14)	117.60(14)
C(18)-C(19)-P	118.17(11)
C(14)-C(19)-P	123.96(11)
F(4)-C(20)-F(6)	105.56(16)
F(4)-C(20)-F(5)	105.89(16)
F(6)-C(20)-F(5)	106.10(17)
F(4)-C(20)-C(14)	114.87(13)
F(6)-C(20)-C(14)	111.98(15)
F(5)-C(20)-C(14)	111.81(16)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rpsl21. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P	35(1)	31(1)	25(1)	1(1)	-9(1)	-4(1)
O	41(1)	36(1)	37(1)	0(1)	-12(1)	2(1)
N	38(1)	48(1)	29(1)	5(1)	-8(1)	3(1)
C(1)	43(1)	55(1)	28(1)	4(1)	-10(1)	0(1)
C(2)	43(1)	46(1)	35(1)	-3(1)	-4(1)	-3(1)
C(3)	36(1)	43(1)	46(1)	3(1)	-6(1)	1(1)
C(4)	34(1)	48(1)	37(1)	7(1)	-12(1)	-3(1)
C(5)	33(1)	38(1)	27(1)	6(1)	-7(1)	-7(1)
C(6)	44(1)	37(1)	30(1)	3(1)	-8(1)	-10(1)
C(7)	46(1)	32(1)	32(1)	0(1)	-11(1)	-5(1)
C(8)	69(1)	38(1)	41(1)	-9(1)	-16(1)	-7(1)
C(9)	76(1)	39(1)	49(1)	-14(1)	-8(1)	4(1)
C(10)	60(1)	40(1)	52(1)	-6(1)	-7(1)	9(1)
C(11)	48(1)	38(1)	44(1)	-1(1)	-16(1)	3(1)
C(12)	41(1)	30(1)	30(1)	0(1)	-9(1)	-2(1)
C(13)	47(1)	41(1)	44(1)	0(1)	-18(1)	-5(1)
F(1)	65(1)	42(1)	53(1)	4(1)	-31(1)	0(1)
F(2)	44(1)	64(1)	55(1)	2(1)	-7(1)	1(1)
F(3)	69(1)	63(1)	81(1)	-10(1)	-46(1)	-8(1)
C(14)	37(1)	31(1)	32(1)	-1(1)	-9(1)	-3(1)
C(15)	40(1)	40(1)	50(1)	6(1)	-14(1)	-10(1)
C(16)	41(1)	47(1)	55(1)	-2(1)	-21(1)	-7(1)
C(17)	42(1)	56(1)	39(1)	-3(1)	-18(1)	0(1)
C(18)	38(1)	50(1)	30(1)	2(1)	-11(1)	-4(1)
C(19)	35(1)	34(1)	26(1)	-3(1)	-9(1)	-2(1)
C(20)	46(1)	40(1)	34(1)	7(1)	-10(1)	-9(1)
F(4)	71(1)	58(1)	36(1)	10(1)	-24(1)	-22(1)
F(5)	57(1)	155(2)	42(1)	28(1)	-2(1)	-24(1)
F(6)	140(2)	41(1)	71(1)	3(1)	-58(1)	13(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rpsl21.

	x	y	z	U(eq)
H(1)	6789	2280	9192	51
H(2)	4717	3819	9620	51
H(3)	3604	4472	7999	52
H(4)	4535	3431	6037	47
H(6A)	5868	948	5182	45
H(6B)	7514	752	5432	45
H(8)	6662	-601	703	59
H(9)	8875	-1926	558	67
H(10)	10545	-1404	1752	63
H(11)	10014	487	3057	51
H(15)	12552	4828	2608	52
H(16)	13254	4239	4428	55
H(17)	11686	2794	5931	53
H(18)	9374	2019	5648	47

Table 6. Torsion angles [°] for rpsl21.

C(5)-N-C(1)-C(2)	-0.7(3)
N-C(1)-C(2)-C(3)	-2.0(3)
C(1)-C(2)-C(3)-C(4)	2.2(3)
C(2)-C(3)-C(4)-C(5)	0.1(3)
C(1)-N-C(5)-C(4)	3.3(2)
C(1)-N-C(5)-C(6)	-175.47(15)
C(3)-C(4)-C(5)-N	-3.0(2)
C(3)-C(4)-C(5)-C(6)	175.65(15)
N-C(5)-C(6)-P	-117.58(14)
C(4)-C(5)-C(6)-P	63.67(19)
O-P-C(6)-C(5)	-50.03(15)
C(19)-P-C(6)-C(5)	74.29(14)
C(12)-P-C(6)-C(5)	-176.00(13)
C(12)-C(7)-C(8)-C(9)	1.4(3)
C(13)-C(7)-C(8)-C(9)	-177.71(18)
C(7)-C(8)-C(9)-C(10)	-0.7(3)
C(8)-C(9)-C(10)-C(11)	-0.8(3)
C(9)-C(10)-C(11)-C(12)	1.6(3)
C(8)-C(7)-C(12)-C(11)	-0.7(2)
C(13)-C(7)-C(12)-C(11)	178.41(16)
C(8)-C(7)-C(12)-P	-176.58(13)
C(13)-C(7)-C(12)-P	2.5(2)
C(10)-C(11)-C(12)-C(7)	-0.8(3)
C(10)-C(11)-C(12)-P	175.49(15)
O-P-C(12)-C(7)	-28.36(17)
C(19)-P-C(12)-C(7)	-154.31(14)
C(6)-P-C(12)-C(7)	93.91(15)
O-P-C(12)-C(11)	155.72(13)
C(19)-P-C(12)-C(11)	29.77(14)
C(6)-P-C(12)-C(11)	-82.02(14)
C(8)-C(7)-C(13)-F(1)	-115.04(18)
C(12)-C(7)-C(13)-F(1)	65.8(2)
C(8)-C(7)-C(13)-F(3)	4.4(2)
C(12)-C(7)-C(13)-F(3)	-174.73(15)

C(8)-C(7)-C(13)-F(2)	123.77(17)
C(12)-C(7)-C(13)-F(2)	-55.4(2)
C(19)-C(14)-C(15)-C(16)	-0.4(3)
C(20)-C(14)-C(15)-C(16)	178.29(17)
C(14)-C(15)-C(16)-C(17)	1.4(3)
C(15)-C(16)-C(17)-C(18)	-1.3(3)
C(16)-C(17)-C(18)-C(19)	0.3(3)
C(17)-C(18)-C(19)-C(14)	0.7(2)
C(17)-C(18)-C(19)-P	-173.59(14)
C(15)-C(14)-C(19)-C(18)	-0.6(2)
C(20)-C(14)-C(19)-C(18)	-179.21(15)
C(15)-C(14)-C(19)-P	173.29(13)
C(20)-C(14)-C(19)-P	-5.3(2)
O-P-C(19)-C(18)	121.83(13)
C(6)-P-C(19)-C(18)	-2.81(15)
C(12)-P-C(19)-C(18)	-108.69(13)
O-P-C(19)-C(14)	-52.06(15)
C(6)-P-C(19)-C(14)	-176.71(13)
C(12)-P-C(19)-C(14)	77.42(14)
C(15)-C(14)-C(20)-F(4)	156.35(16)
C(19)-C(14)-C(20)-F(4)	-25.0(2)
C(15)-C(14)-C(20)-F(6)	-83.3(2)
C(19)-C(14)-C(20)-F(6)	95.4(2)
C(15)-C(14)-C(20)-F(5)	35.7(2)
C(19)-C(14)-C(20)-F(5)	-145.71(18)

Table 7. Possible Hydrogen bonds for rpsl21 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...F(3)	0.94	2.30	2.664(3)	102.5
C(18)-H(18)...N	0.94	2.55	3.362(2)	144.8

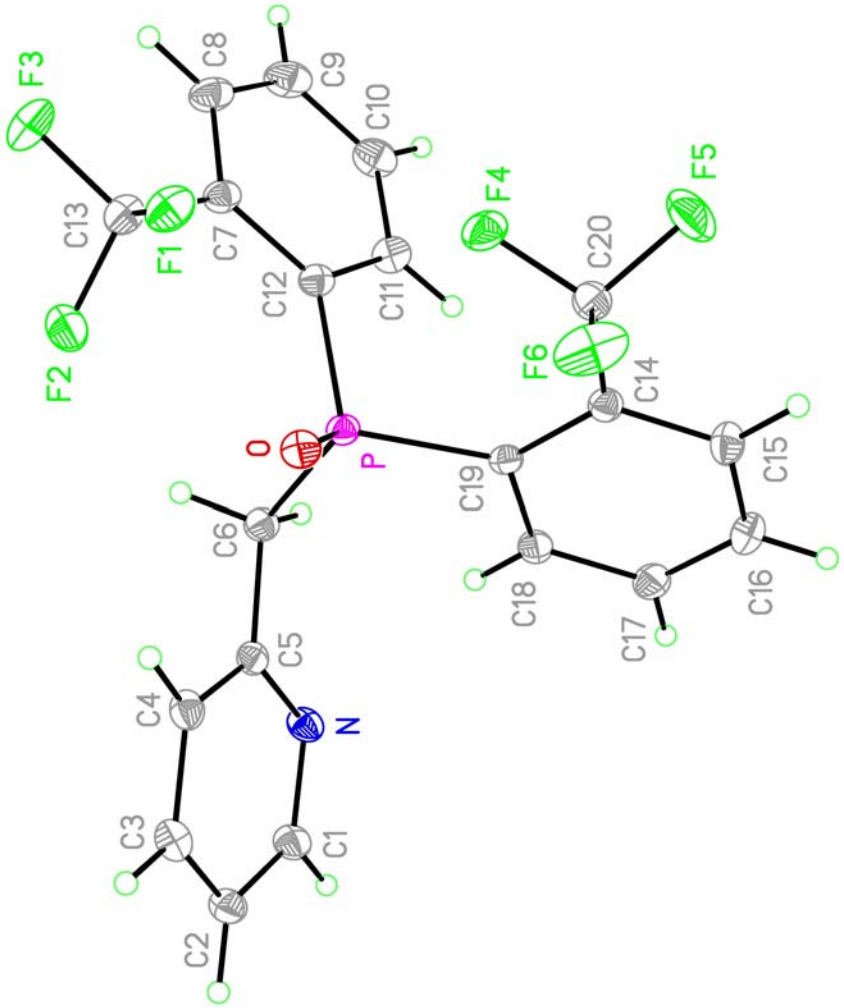

Figure 1. rpsl21l1.jpg, Single molecule view, 20% thermal displacement ellipsoids 20%, rpsl21l1b.jpg=b/w

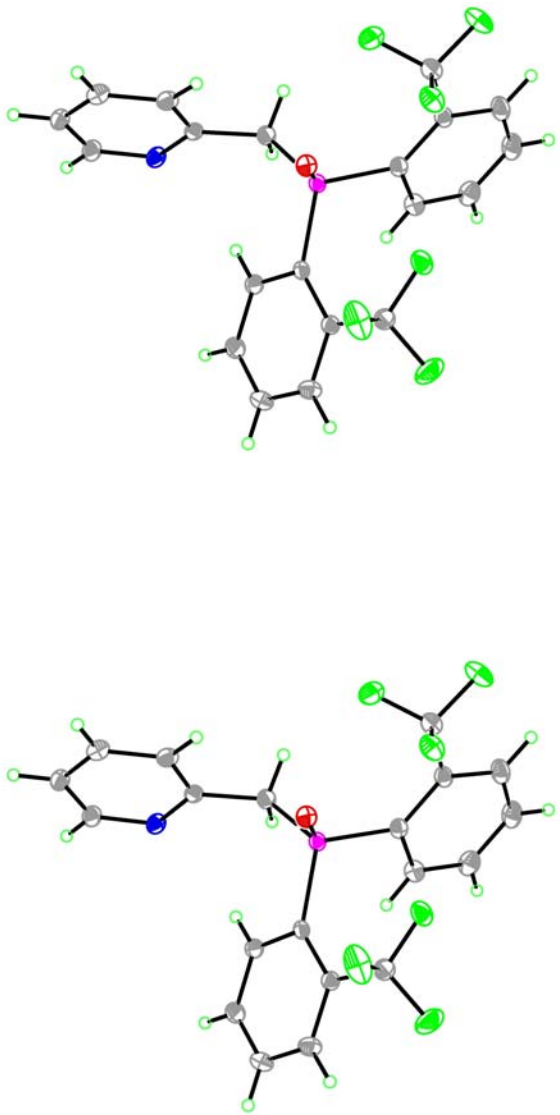

Figure 1.rpsl21s1.jpg also rpsl21s1b.jpg[b/w], stereoview of single molecule.

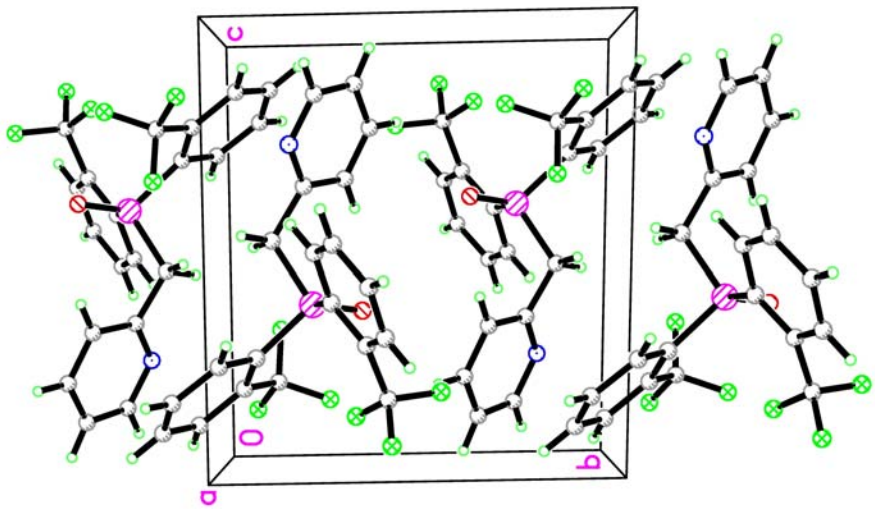

Figure 3.rpsl21al1.jpg packing view down a-axis,color,also rpsl21al1b.jpg b/w

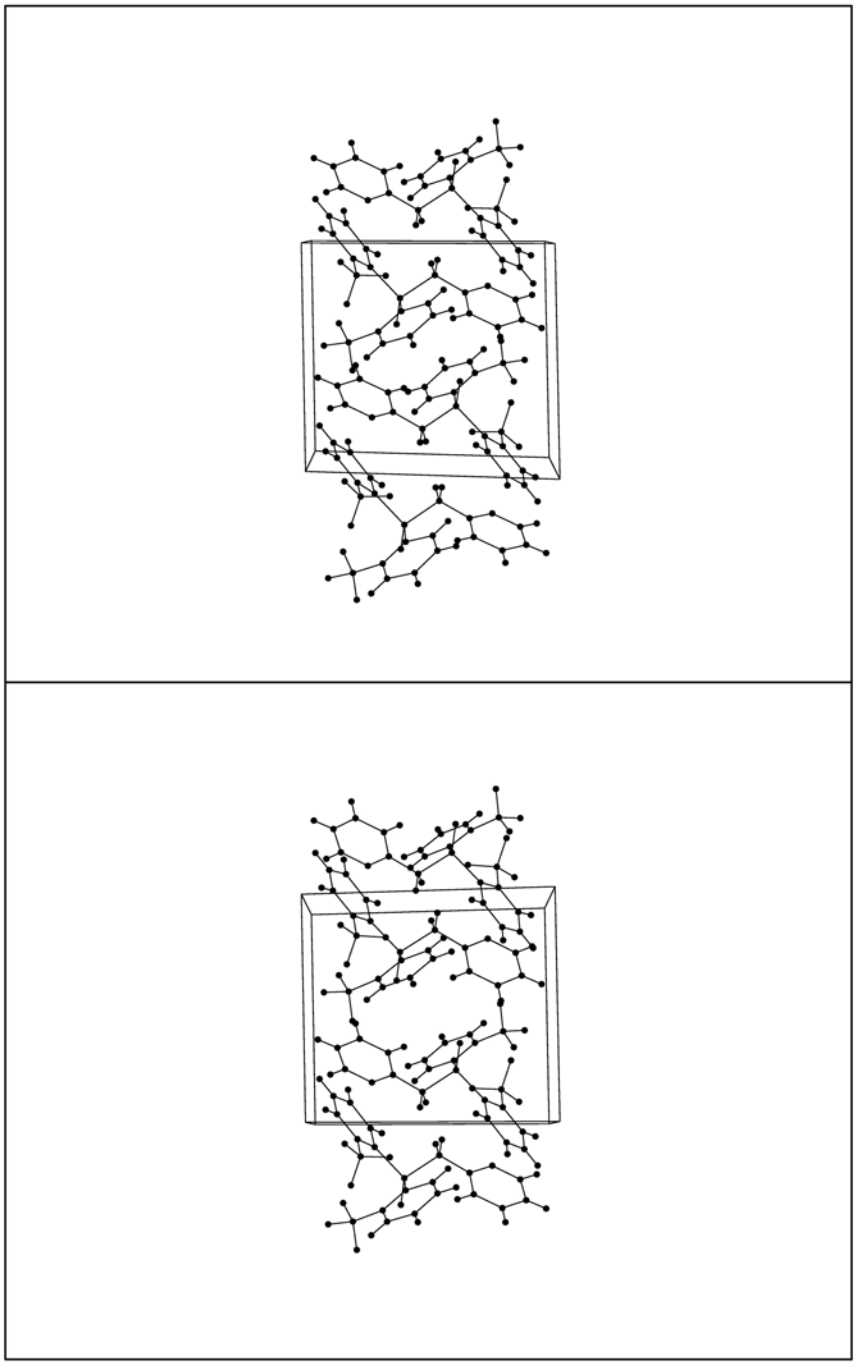

Figure 4.rpsl21as.jpg stereoview packing, down a-axis

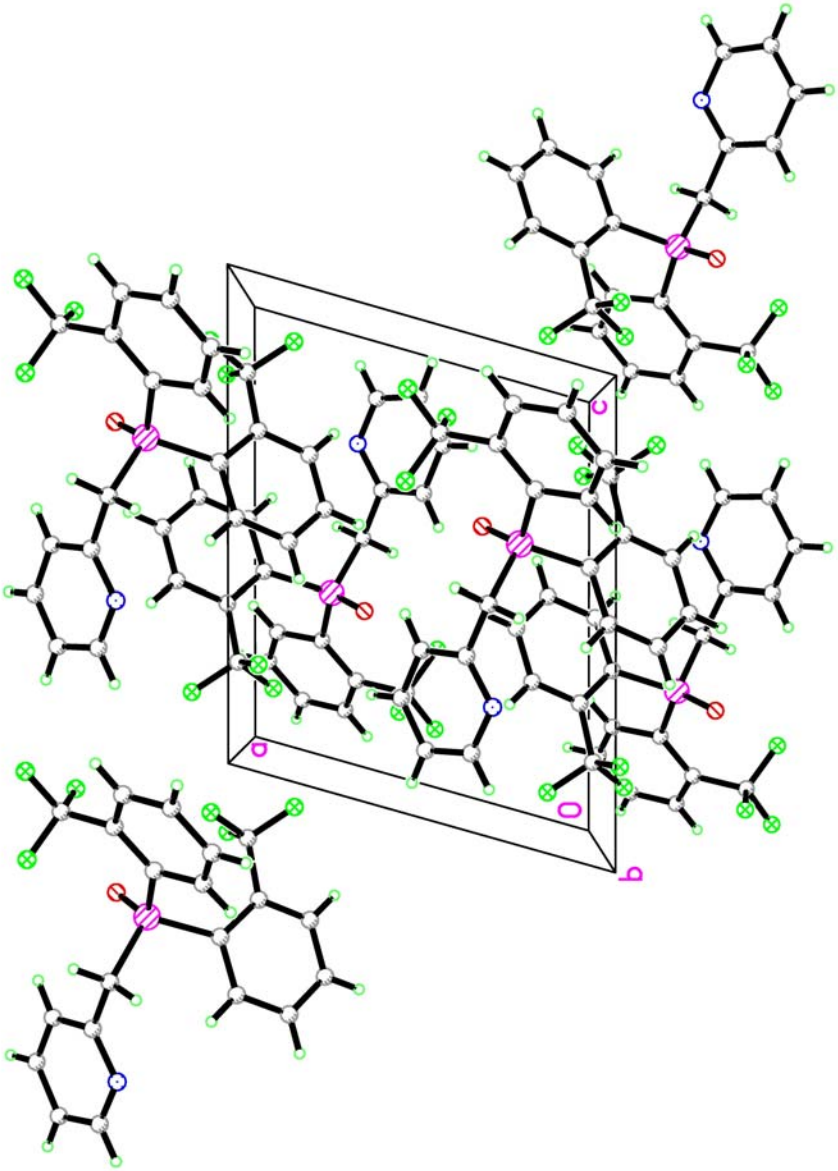

Figure 5.rpsl21bl.jpg packing view down b-axis,color,also rpsl21blb.jpg b/w, also see rpsl21bs.jpg

Electronic Supplementary Information for Dalton Transactions

X-ray Crystallographic data for **1c**.

Crystal Structure Report

Prepared for:

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Compound:

Rpsl32/slp-13.05

C20 H14 F6 N O2 P

Prepared by:

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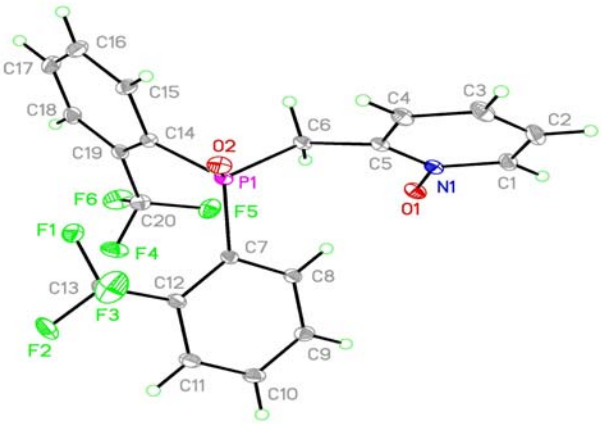
277-6649

Issue date:

November 9, 2007



Rpsl32l1.jpg $225

Table 1. Crystal data and structure refinement for rpsl32.

Identification code	rpsl32	
Empirical formula	C20 H14 F6 N O2 P	
Formula weight	445.29	
Temperature	225(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.8219(6) Å	α= 84.198(4)°.
	b = 8.8196(7) Å	β= 81.657(4)°.
	c = 14.4992(12) Å	γ = 72.516(4)°.
Volume	942.18(13) $Å^3$	
Z	2	
Density (calculated)	1.570 Mg/m^3	
Absorption coefficient	0.221 mm^{-1}	
F(000)	452	
Crystal size	0.51 x 0.28 x 0.14 mm^3	
Theta range for data collection	2.74 to 33.07°.	
Index ranges	-11<=h<=11, -13<=k<=13, -22<=l<=21	
Reflections collected	25744	
Independent reflections	7013 [R(int) = 0.0237]	
Completeness to theta = 33.07°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.970 and 0.900	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7013 / 0 / 271	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0426, wR2 = 0.1187	
R indices (all data)	R1 = 0.0515, wR2 = 0.1254	
Largest diff. peak and hole	0.693 and -0.518 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rpsl32. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	1770(1)	6569(1)	2068(1)	22(1)
O(1)	6751(1)	6216(1)	531(1)	34(1)
O(2)	132(1)	7898(1)	1909(1)	32(1)
N(1)	5493(2)	7250(1)	104(1)	26(1)
C(1)	5987(2)	8227(2)	-602(1)	34(1)
C(2)	4718(2)	9332(2)	-1072(1)	40(1)
C(3)	2905(2)	9479(2)	-828(1)	40(1)
C(4)	2423(2)	8453(2)	-123(1)	33(1)
C(5)	3715(2)	7316(1)	340(1)	25(1)
C(6)	3290(2)	6037(1)	1001(1)	26(1)
C(7)	3001(2)	7063(1)	2910(1)	23(1)
C(8)	4764(2)	7112(2)	2607(1)	27(1)
C(9)	5757(2)	7611(2)	3172(1)	32(1)
C(10)	5011(2)	8052(2)	4060(1)	35(1)
C(11)	3267(2)	8017(2)	4379(1)	34(1)
C(12)	2250(2)	7541(2)	3815(1)	28(1)
C(13)	350(2)	7613(2)	4214(1)	41(1)
C(14)	1211(2)	4687(2)	2339(1)	25(1)
C(15)	-289(2)	4704(2)	1913(1)	32(1)
C(16)	-864(2)	3353(2)	1941(1)	40(1)
C(17)	20(2)	1968(2)	2405(1)	43(1)
C(18)	1505(2)	1923(2)	2839(1)	36(1)
C(19)	2115(2)	3260(2)	2802(1)	27(1)
C(20)	3754(2)	3107(2)	3267(1)	35(1)
F(1)	-252(1)	6516(1)	3914(1)	44(1)
F(2)	161(2)	7440(3)	5133(1)	92(1)
F(3)	-830(2)	9017(2)	3988(1)	77(1)
F(4)	3382(2)	3934(1)	4030(1)	50(1)
F(5)	4999(1)	3628(1)	2695(1)	46(1)
F(6)	4583(2)	1604(1)	3537(1)	59(1)

Table 3. Bond lengths [Å] and angles [°] for rpsl32.

P(1)-O(2)	1.4822(9)
P(1)-C(7)	1.8177(12)
P(1)-C(6)	1.8180(13)
P(1)-C(14)	1.8325(13)
O(1)-N(1)	1.3064(14)
N(1)-C(1)	1.3591(17)
N(1)-C(5)	1.3682(17)
C(1)-C(2)	1.371(2)
C(1)-H(1A)	0.9400
C(2)-C(3)	1.381(3)
C(2)-H(2)	0.9400
C(3)-C(4)	1.383(2)
C(3)-H(3)	0.9400
C(4)-C(5)	1.3883(17)
C(4)-H(4)	0.9400
C(5)-C(6)	1.4885(17)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(7)-C(8)	1.3970(17)
C(7)-C(12)	1.4089(17)
C(8)-C(9)	1.3905(18)
C(8)-H(8)	0.9400
C(9)-C(10)	1.377(2)
C(9)-H(9)	0.9400
C(10)-C(11)	1.384(2)
C(10)-H(10)	0.9400
C(11)-C(12)	1.3911(19)
C(11)-H(11)	0.9400
C(12)-C(13)	1.499(2)
C(13)-F(2)	1.319(2)
C(13)-F(1)	1.3284(19)
C(13)-F(3)	1.346(2)
C(14)-C(15)	1.3976(18)
C(14)-C(19)	1.4028(17)

C(15)-C(16)	1.389(2)
C(15)-H(15)	0.9400
C(16)-C(17)	1.373(3)
C(16)-H(16)	0.9400
C(17)-C(18)	1.388(2)
C(17)-H(17)	0.9400
C(18)-C(19)	1.3923(19)
C(18)-H(18)	0.9400
C(19)-C(20)	1.498(2)
C(20)-F(4)	1.3345(18)
C(20)-F(6)	1.3354(16)
C(20)-F(5)	1.3438(19)

O(2)-P(1)-C(7)	110.83(6)
O(2)-P(1)-C(6)	112.74(6)
C(7)-P(1)-C(6)	108.69(6)
O(2)-P(1)-C(14)	110.77(6)
C(7)-P(1)-C(14)	115.13(5)
C(6)-P(1)-C(14)	98.13(6)
O(1)-N(1)-C(1)	118.71(12)
O(1)-N(1)-C(5)	120.83(11)
C(1)-N(1)-C(5)	120.43(11)
N(1)-C(1)-C(2)	120.94(14)
N(1)-C(1)-H(1A)	119.5
C(2)-C(1)-H(1A)	119.5
C(1)-C(2)-C(3)	120.29(13)
C(1)-C(2)-H(2)	119.9
C(3)-C(2)-H(2)	119.9
C(2)-C(3)-C(4)	118.13(13)
C(2)-C(3)-H(3)	120.9
C(4)-C(3)-H(3)	120.9
C(3)-C(4)-C(5)	121.38(14)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
N(1)-C(5)-C(4)	118.73(12)
N(1)-C(5)-C(6)	117.68(10)

C(4)-C(5)-C(6)	123.17(12)
C(5)-C(6)-P(1)	119.53(8)
C(5)-C(6)-H(6A)	107.4
P(1)-C(6)-H(6A)	107.4
C(5)-C(6)-H(6B)	107.4
P(1)-C(6)-H(6B)	107.4
H(6A)-C(6)-H(6B)	107.0
C(8)-C(7)-C(12)	117.69(11)
C(8)-C(7)-P(1)	117.46(9)
C(12)-C(7)-P(1)	124.58(10)
C(9)-C(8)-C(7)	121.70(12)
C(9)-C(8)-H(8)	119.2
C(7)-C(8)-H(8)	119.2
C(10)-C(9)-C(8)	119.81(13)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(11)	119.74(13)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-H(10)	120.1
C(10)-C(11)-C(12)	120.99(12)
C(10)-C(11)-H(11)	119.5
C(12)-C(11)-H(11)	119.5
C(11)-C(12)-C(7)	120.06(12)
C(11)-C(12)-C(13)	116.64(12)
C(7)-C(12)-C(13)	123.28(12)
F(2)-C(13)-F(1)	106.70(15)
F(2)-C(13)-F(3)	106.38(16)
F(1)-C(13)-F(3)	105.25(14)
F(2)-C(13)-C(12)	112.15(14)
F(1)-C(13)-C(12)	113.83(12)
F(3)-C(13)-C(12)	111.97(14)
C(15)-C(14)-C(19)	117.82(12)
C(15)-C(14)-P(1)	110.74(9)
C(19)-C(14)-P(1)	131.11(10)
C(16)-C(15)-C(14)	121.37(14)
C(16)-C(15)-H(15)	119.3

C(14)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	120.30(14)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	119.46(14)
C(16)-C(17)-H(17)	120.3
C(18)-C(17)-H(17)	120.3
C(17)-C(18)-C(19)	120.81(14)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(18)-C(19)-C(14)	120.23(13)
C(18)-C(19)-C(20)	117.68(12)
C(14)-C(19)-C(20)	122.10(11)
F(4)-C(20)-F(6)	106.21(12)
F(4)-C(20)-F(5)	106.52(13)
F(6)-C(20)-F(5)	105.97(13)
F(4)-C(20)-C(19)	112.93(13)
F(6)-C(20)-C(19)	112.89(12)
F(5)-C(20)-C(19)	111.80(11)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rpsl32. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	24(1)	21(1)	21(1)	0(1)	-5(1)	-4(1)
O(1)	30(1)	40(1)	27(1)	-1(1)	-8(1)	-1(1)
O(2)	30(1)	27(1)	35(1)	0(1)	-10(1)	0(1)
N(1)	30(1)	26(1)	20(1)	-3(1)	-3(1)	-5(1)
C(1)	41(1)	33(1)	26(1)	-3(1)	4(1)	-12(1)
C(2)	59(1)	29(1)	26(1)	3(1)	1(1)	-11(1)
C(3)	53(1)	30(1)	28(1)	5(1)	-9(1)	0(1)
C(4)	35(1)	32(1)	28(1)	2(1)	-8(1)	-1(1)
C(5)	30(1)	24(1)	19(1)	-2(1)	-4(1)	-4(1)
C(6)	32(1)	23(1)	21(1)	-1(1)	-4(1)	-6(1)
C(7)	27(1)	22(1)	20(1)	-1(1)	-4(1)	-6(1)
C(8)	27(1)	29(1)	23(1)	-1(1)	-4(1)	-8(1)
C(9)	30(1)	35(1)	33(1)	0(1)	-10(1)	-11(1)
C(10)	41(1)	36(1)	31(1)	-2(1)	-13(1)	-13(1)
C(11)	43(1)	38(1)	24(1)	-6(1)	-5(1)	-13(1)
C(12)	32(1)	29(1)	23(1)	-3(1)	-2(1)	-9(1)
C(13)	41(1)	53(1)	32(1)	-14(1)	7(1)	-18(1)
C(14)	25(1)	26(1)	24(1)	-2(1)	-3(1)	-8(1)
C(15)	27(1)	35(1)	36(1)	-5(1)	-6(1)	-9(1)
C(16)	32(1)	48(1)	46(1)	-10(1)	-2(1)	-20(1)
C(17)	48(1)	44(1)	44(1)	-6(1)	4(1)	-28(1)
C(18)	47(1)	30(1)	31(1)	2(1)	1(1)	-17(1)
C(19)	32(1)	26(1)	23(1)	1(1)	-2(1)	-9(1)
C(20)	43(1)	26(1)	36(1)	7(1)	-15(1)	-8(1)
F(1)	38(1)	54(1)	44(1)	-11(1)	4(1)	-22(1)
F(2)	85(1)	189(2)	28(1)	-27(1)	19(1)	-85(1)
F(3)	40(1)	52(1)	125(1)	-24(1)	19(1)	-2(1)
F(4)	69(1)	48(1)	38(1)	0(1)	-24(1)	-15(1)
F(5)	32(1)	47(1)	60(1)	9(1)	-13(1)	-12(1)
F(6)	71(1)	28(1)	79(1)	15(1)	-40(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rpsl32.

	x	y	z	U(eq)
H(1A)	7217	8145	-770	40
H(2)	5084	9992	-1562	48
H(3)	2022	10255	-1133	48
H(4)	1196	8526	47	40
H(6A)	4436	5330	1182	31
H(6B)	2782	5411	656	31
H(8)	5292	6798	2005	32
H(9)	6935	7648	2949	38
H(10)	5683	8376	4448	42
H(11)	2762	8318	4985	41
H(15)	-921	5648	1602	38
H(16)	-1863	3388	1640	48
H(17)	-376	1057	2429	51
H(18)	2106	979	3162	43

Table 6. Torsion angles [°] for rpsl32.

O(1)-N(1)-C(1)-C(2)	179.93(12)
C(5)-N(1)-C(1)-C(2)	2.11(19)
N(1)-C(1)-C(2)-C(3)	0.6(2)
C(1)-C(2)-C(3)-C(4)	-2.0(2)
C(2)-C(3)-C(4)-C(5)	0.9(2)
O(1)-N(1)-C(5)-C(4)	179.00(11)
C(1)-N(1)-C(5)-C(4)	-3.21(18)
O(1)-N(1)-C(5)-C(6)	-8.14(16)
C(1)-N(1)-C(5)-C(6)	169.65(11)
C(3)-C(4)-C(5)-N(1)	1.7(2)
C(3)-C(4)-C(5)-C(6)	-170.72(13)
N(1)-C(5)-C(6)-P(1)	124.22(10)
C(4)-C(5)-C(6)-P(1)	-63.27(15)
O(2)-P(1)-C(6)-C(5)	45.19(12)
C(7)-P(1)-C(6)-C(5)	-78.10(11)
C(14)-P(1)-C(6)-C(5)	161.82(10)
O(2)-P(1)-C(7)-C(8)	-118.67(10)
C(6)-P(1)-C(7)-C(8)	5.75(11)
C(14)-P(1)-C(7)-C(8)	114.64(10)
O(2)-P(1)-C(7)-C(12)	55.17(12)
C(6)-P(1)-C(7)-C(12)	179.60(10)
C(14)-P(1)-C(7)-C(12)	-71.52(12)
C(12)-C(7)-C(8)-C(9)	0.03(18)
P(1)-C(7)-C(8)-C(9)	174.31(10)
C(7)-C(8)-C(9)-C(10)	0.9(2)
C(8)-C(9)-C(10)-C(11)	-0.9(2)
C(9)-C(10)-C(11)-C(12)	0.0(2)
C(10)-C(11)-C(12)-C(7)	1.0(2)
C(10)-C(11)-C(12)-C(13)	-177.45(14)
C(8)-C(7)-C(12)-C(11)	-0.97(18)
P(1)-C(7)-C(12)-C(11)	-174.80(10)
C(8)-C(7)-C(12)-C(13)	177.35(13)
P(1)-C(7)-C(12)-C(13)	3.52(19)
C(11)-C(12)-C(13)-F(2)	-27.7(2)

C(7)-C(12)-C(13)-F(2)	153.88(16)
C(11)-C(12)-C(13)-F(1)	-149.02(14)
C(7)-C(12)-C(13)-F(1)	32.6(2)
C(11)-C(12)-C(13)-F(3)	91.75(17)
C(7)-C(12)-C(13)-F(3)	-86.62(17)
O(2)-P(1)-C(14)-C(15)	29.00(11)
C(7)-P(1)-C(14)-C(15)	155.72(9)
C(6)-P(1)-C(14)-C(15)	-89.15(10)
O(2)-P(1)-C(14)-C(19)	-157.91(12)
C(7)-P(1)-C(14)-C(19)	-31.19(14)
C(6)-P(1)-C(14)-C(19)	83.94(13)
C(19)-C(14)-C(15)-C(16)	-0.4(2)
P(1)-C(14)-C(15)-C(16)	173.68(12)
C(14)-C(15)-C(16)-C(17)	1.1(2)
C(15)-C(16)-C(17)-C(18)	-0.6(2)
C(16)-C(17)-C(18)-C(19)	-0.6(2)
C(17)-C(18)-C(19)-C(14)	1.2(2)
C(17)-C(18)-C(19)-C(20)	-178.48(14)
C(15)-C(14)-C(19)-C(18)	-0.72(19)
P(1)-C(14)-C(19)-C(18)	-173.41(11)
C(15)-C(14)-C(19)-C(20)	178.97(13)
P(1)-C(14)-C(19)-C(20)	6.3(2)
C(18)-C(19)-C(20)-F(4)	-110.65(14)
C(14)-C(19)-C(20)-F(4)	69.64(17)
C(18)-C(19)-C(20)-F(6)	9.85(19)
C(14)-C(19)-C(20)-F(6)	-169.86(13)
C(18)-C(19)-C(20)-F(5)	129.23(13)
C(14)-C(19)-C(20)-F(5)	-50.48(18)

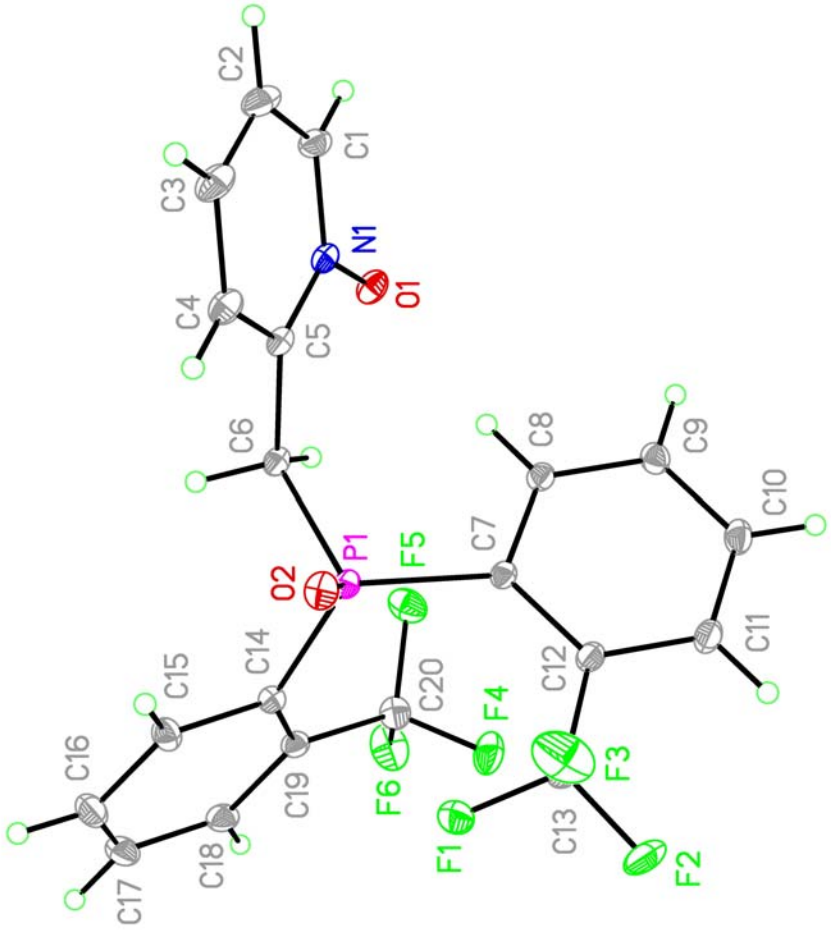


Figure 1. rpsl32l1.jpg, Single molecule view, 20% thermal displacement ellipsoids 20%, rpsl32l1b.jpg=b/w

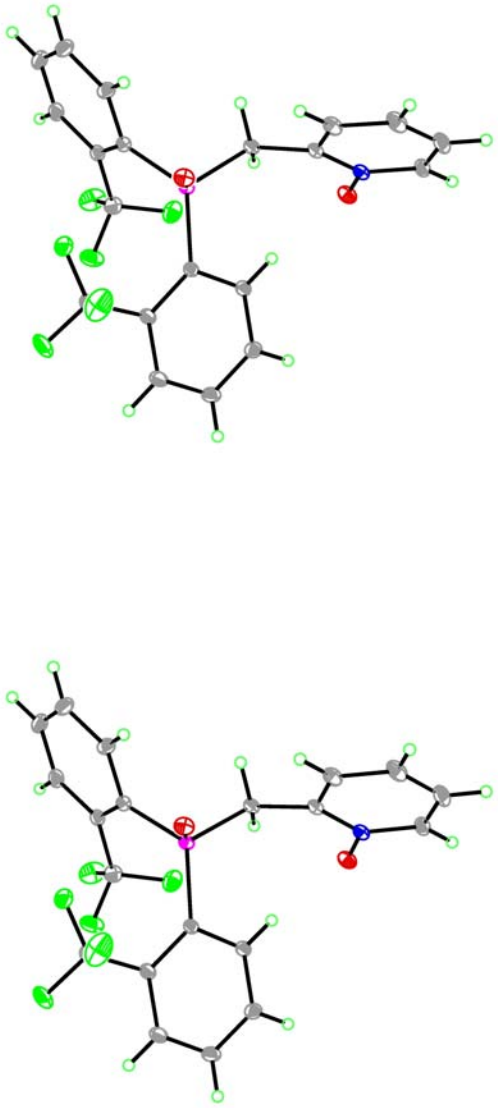


Figure 2.rpsl32s1.jpg also rpsl32s1b.jpg[b/w], stereoview of single molecule.

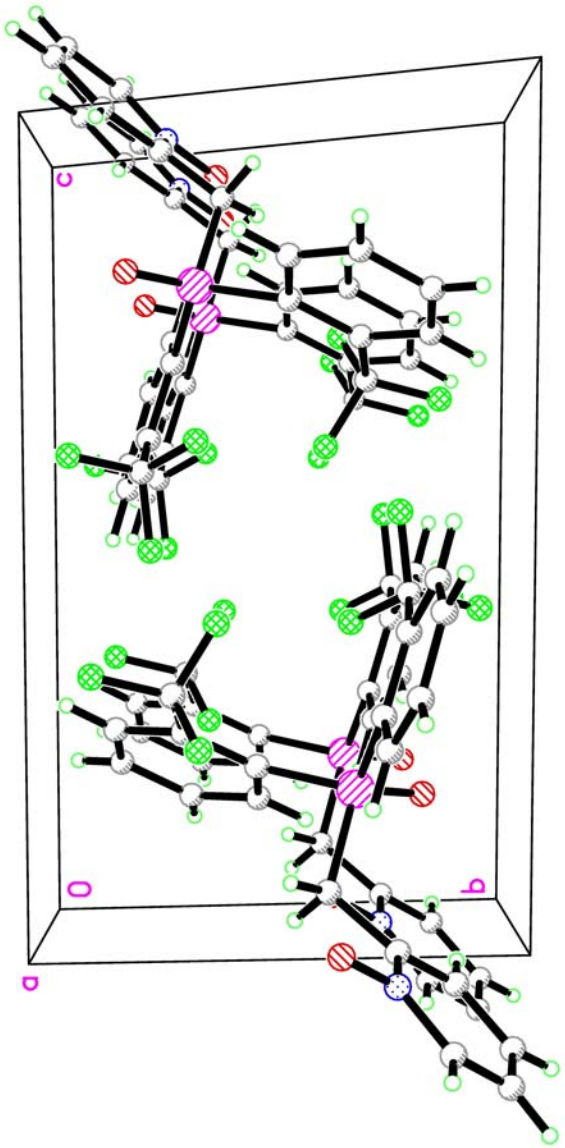


Figure 3.rpsl32al.jpg packing view down a-axis,color,also rpsl32alb.jpg b/w

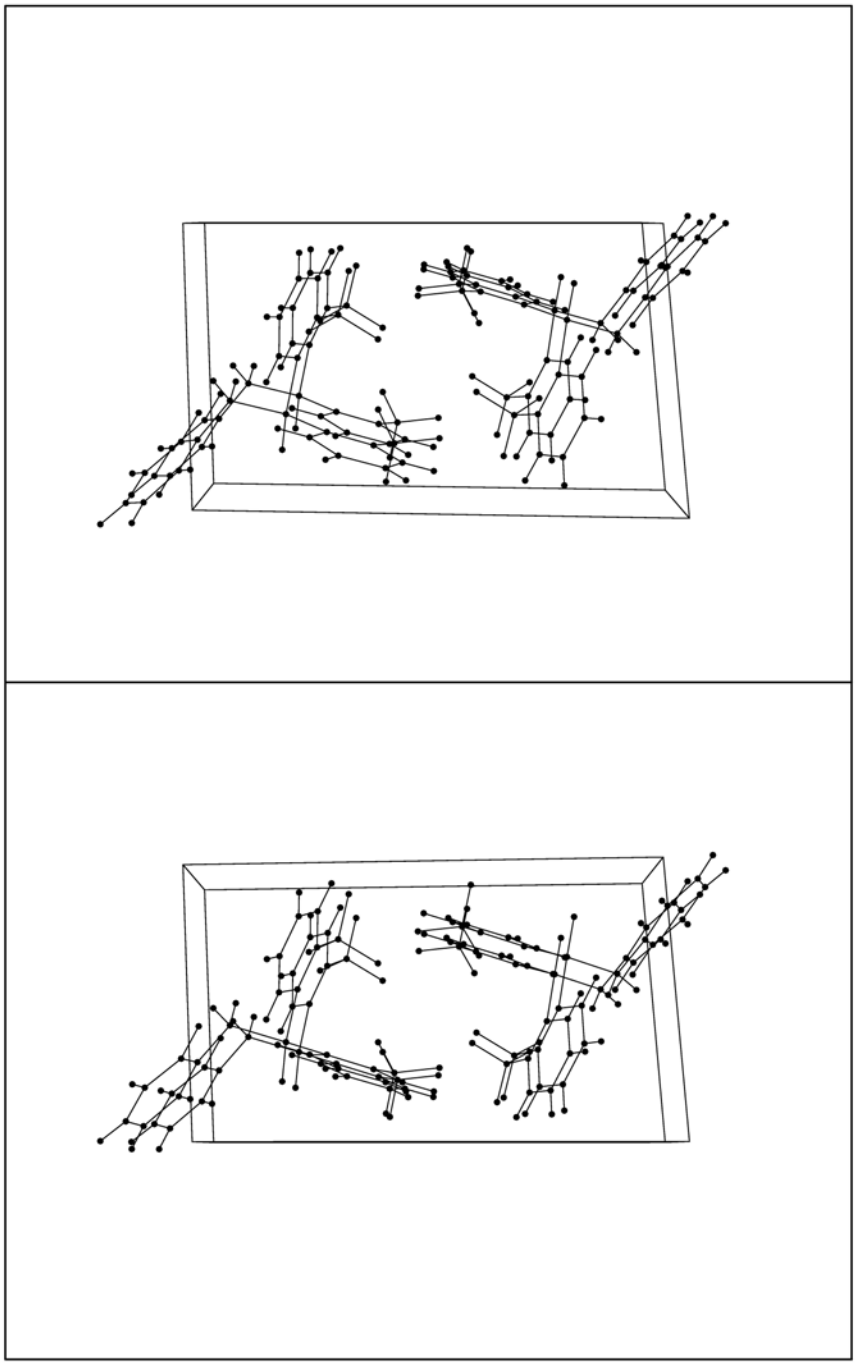


Figure 4.rpsl32asb.jpg stereoview packing, down a-axis

Electronic Supplementary Information for Dalton Transactions

X-ray Crystallographic data for **3d**.

Crystal Structure Report

Prepared for:

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Compound:

Rps20/slp-11-39-L1

C22 H12 F12 N O P

Prepared by:

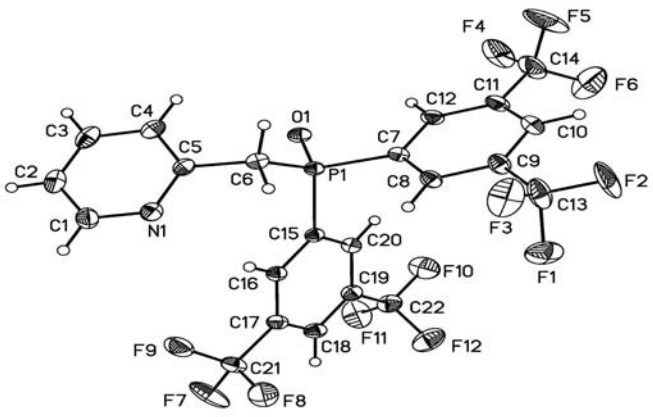
Eileen Duesler

Duesler@unm.edu

277-6649

Issue date:

January 18, 2007



Rpsl20l1b.jpg $257 = $225+ 2[46*-30] *includes disordered F's

Table 1. Crystal data and structure refinement for rpsl20a.

Identification code	rpsl20a	
Empirical formula	C22 H12 F12 N O P	
Formula weight	565.30	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.6362(12) Å	α= 90°.
	b = 19.362(3) Å	β= 104.192(6)°.
	c = 10.6850(13) Å	γ = 90°.
Volume	2333.9(5) $Å^3$	
Z	4	
Density (calculated)	1.609 Mg/m^3	
Absorption coefficient	0.230 mm^{-1}	
F(000)	1128	
Crystal size	0.46 x 0.44 x 0.28 mm^3	
Theta range for data collection	2.09 to 29.13°.	
Index ranges	-15<=h<=15, -26<=k<=26, -14<=l<=14	
Reflections collected	32662	
Independent reflections	6258 [R(int) = 0.0172]	
Completeness to theta = 29.13°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.93 and 0.90	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6258 / 0 / 415	
Goodness-of-fit on F^2	0.987	
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1970	
R indices (all data)	R1 = 0.0687, wR2 = 0.2327	
Largest diff. peak and hole	0.634 and -0.272 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rpsl20a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	4117(1)	2536(1)	4257(1)	33(1)
O(1)	4205(1)	2467(1)	2898(1)	44(1)
N(1)	5760(2)	1112(1)	6114(2)	52(1)
C(1)	6651(2)	674(1)	6096(3)	61(1)
C(2)	6765(2)	331(1)	5001(3)	64(1)
C(3)	5942(2)	439(1)	3889(3)	64(1)
C(4)	5019(2)	900(1)	3862(2)	53(1)
C(5)	4962(2)	1224(1)	5003(2)	41(1)
C(6)	3985(1)	1729(1)	5059(2)	40(1)
C(7)	2803(1)	3036(1)	4292(2)	38(1)
C(8)	2442(1)	3176(1)	5406(2)	42(1)
C(9)	1408(2)	3551(1)	5321(2)	49(1)
C(10)	745(2)	3794(1)	4156(2)	53(1)
C(11)	1133(2)	3669(1)	3052(2)	54(1)
C(12)	2150(2)	3290(1)	3115(2)	47(1)
C(13)	1033(2)	3705(2)	6545(3)	80(1)
F(1)	1938(3)	4112(3)	7398(4)	100(1)
F(2)	109(5)	4080(5)	6437(7)	128(3)
F(3)	1025(7)	3191(3)	7279(6)	115(2)
F(1A)	1659(8)	3527(8)	7501(6)	130(4)
F(2A)	85(12)	3224(7)	6477(13)	191(5)
F(3A)	504(13)	4253(8)	6480(12)	168(7)
C(14)	484(3)	3978(3)	1782(3)	103(1)
F(4)	934(7)	3855(6)	843(6)	115(3)
F(5)	-585(6)	3662(8)	1395(7)	160(4)
F(6)	209(18)	4613(5)	1868(8)	215(7)
F(4A)	-528(6)	4182(7)	1742(9)	139(4)
F(5A)	1097(7)	4559(7)	1548(10)	163(5)
F(6A)	437(15)	3537(11)	864(10)	244(8)
C(15)	5359(1)	3006(1)	5235(2)	34(1)
C(16)	6068(1)	2749(1)	6372(2)	37(1)

C(17)	7050(1)	3128(1)	7025(2)	42(1)
C(18)	7305(2)	3758(1)	6572(2)	46(1)
C(19)	6580(2)	4018(1)	5448(2)	45(1)
C(20)	5613(1)	3639(1)	4751(2)	41(1)
C(21)	7829(2)	2833(1)	8240(2)	57(1)
F(7)	8924(4)	2950(5)	8465(7)	109(3)
F(8)	7468(8)	3004(5)	9290(7)	106(3)
F(9)	7726(5)	2120(2)	8343(6)	96(2)
F(7A)	7328(6)	2765(6)	9114(7)	123(4)
F(8A)	8360(7)	2306(4)	7976(6)	132(3)
F(9A)	8715(6)	3288(4)	8689(7)	121(3)
C(22)	6854(2)	4707(1)	4985(3)	62(1)
F(10)	6049(2)	4931(1)	3958(2)	100(1)
F(11)	7876(2)	4723(1)	4666(2)	105(1)
F(12)	6886(2)	5196(1)	5873(2)	107(1)

Table 3. Bond lengths [Å] and angles [°] for rpsl20a.

P(1)-O(1)	1.4874(14)
P(1)-C(15)	1.8070(15)
P(1)-C(6)	1.8077(18)
P(1)-C(7)	1.8178(17)
N(1)-C(5)	1.334(3)
N(1)-C(1)	1.344(3)
C(1)-C(2)	1.379(4)
C(1)-H(1)	0.9400
C(2)-C(3)	1.347(4)
C(2)-H(2)	0.9400
C(3)-C(4)	1.392(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.387(3)
C(4)-H(4)	0.9400
C(5)-C(6)	1.510(2)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(7)-C(8)	1.383(2)
C(7)-C(12)	1.389(2)
C(8)-C(9)	1.389(2)
C(8)-H(8)	0.9400
C(9)-C(10)	1.376(3)
C(9)-C(13)	1.506(3)
C(10)-C(11)	1.384(3)
C(10)-H(10)	0.9400
C(11)-C(12)	1.380(3)
C(11)-C(14)	1.507(4)
C(12)-H(12)	0.9400
C(13)-F(1A)	1.152(7)
C(13)-F(3A)	1.221(12)
C(13)-F(3)	1.269(5)
C(13)-F(2)	1.279(5)
C(13)-F(2A)	1.432(10)
C(13)-F(1)	1.446(6)

C(14)-F(4A)	1.233(7)
C(14)-F(4)	1.263(8)
C(14)-F(6)	1.279(8)
C(14)-F(6A)	1.292(12)
C(14)-F(5)	1.356(9)
C(14)-F(5A)	1.387(10)
C(15)-C(16)	1.383(2)
C(15)-C(20)	1.390(2)
C(16)-C(17)	1.393(2)
C(16)-H(16)	0.9400
C(17)-C(18)	1.372(3)
C(17)-C(21)	1.501(3)
C(18)-C(19)	1.382(3)
C(18)-H(18)	0.9400
C(19)-C(20)	1.396(2)
C(19)-C(22)	1.484(3)
C(20)-H(20)	0.9400
C(21)-F(7A)	1.224(6)
C(21)-F(7)	1.259(5)
C(21)-F(8A)	1.260(6)
C(21)-F(8)	1.333(7)
C(21)-F(9A)	1.352(7)
C(21)-F(9)	1.394(5)
C(22)-F(11)	1.315(3)
C(22)-F(10)	1.328(3)
C(22)-F(12)	1.334(3)

O(1)-P(1)-C(15)	111.91(7)
O(1)-P(1)-C(6)	114.72(8)
C(15)-P(1)-C(6)	108.08(8)
O(1)-P(1)-C(7)	109.15(8)
C(15)-P(1)-C(7)	106.12(7)
C(6)-P(1)-C(7)	106.37(8)
C(5)-N(1)-C(1)	117.5(2)
N(1)-C(1)-C(2)	123.4(2)
N(1)-C(1)-H(1)	118.3

C(2)-C(1)-H(1)	118.3
C(3)-C(2)-C(1)	118.6(2)
C(3)-C(2)-H(2)	120.7
C(1)-C(2)-H(2)	120.7
C(2)-C(3)-C(4)	119.7(2)
C(2)-C(3)-H(3)	120.2
C(4)-C(3)-H(3)	120.2
C(5)-C(4)-C(3)	118.4(2)
C(5)-C(4)-H(4)	120.8
C(3)-C(4)-H(4)	120.8
N(1)-C(5)-C(4)	122.38(18)
N(1)-C(5)-C(6)	115.93(16)
C(4)-C(5)-C(6)	121.69(18)
C(5)-C(6)-P(1)	112.88(11)
C(5)-C(6)-H(6A)	109.0
P(1)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6B)	109.0
P(1)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(8)-C(7)-C(12)	119.77(16)
C(8)-C(7)-P(1)	123.78(13)
C(12)-C(7)-P(1)	116.45(14)
C(7)-C(8)-C(9)	119.10(17)
C(7)-C(8)-H(8)	120.4
C(9)-C(8)-H(8)	120.4
C(10)-C(9)-C(8)	121.49(19)
C(10)-C(9)-C(13)	119.99(18)
C(8)-C(9)-C(13)	118.50(19)
C(9)-C(10)-C(11)	118.92(17)
C(9)-C(10)-H(10)	120.5
C(11)-C(10)-H(10)	120.5
C(12)-C(11)-C(10)	120.42(18)
C(12)-C(11)-C(14)	119.3(2)
C(10)-C(11)-C(14)	120.2(2)
C(11)-C(12)-C(7)	120.25(18)
C(11)-C(12)-H(12)	119.9

C(7)-C(12)-H(12)	119.9
F(1A)-C(13)-F(3A)	120.7(9)
F(3)-C(13)-F(2)	111.6(5)
F(1A)-C(13)-F(2A)	99.4(8)
F(3A)-C(13)-F(2A)	101.0(9)
F(3)-C(13)-F(1)	98.7(4)
F(2)-C(13)-F(1)	102.3(5)
F(1A)-C(13)-C(9)	117.1(3)
F(3A)-C(13)-C(9)	111.8(6)
F(3)-C(13)-C(9)	115.4(3)
F(2)-C(13)-C(9)	116.8(4)
F(2A)-C(13)-C(9)	102.2(5)
F(1)-C(13)-C(9)	109.5(2)
F(4)-C(14)-F(6)	113.5(9)
F(4A)-C(14)-F(6A)	108.9(7)
F(4)-C(14)-F(5)	101.5(6)
F(6A)-C(14)-F(5A)	109.1(10)
F(4A)-C(14)-C(11)	115.0(5)
F(4)-C(14)-C(11)	115.2(4)
F(6)-C(14)-C(11)	113.3(4)
F(6A)-C(14)-C(11)	109.9(7)
F(5)-C(14)-C(11)	108.4(6)
F(5A)-C(14)-C(11)	108.5(4)
C(16)-C(15)-C(20)	120.52(15)
C(16)-C(15)-P(1)	123.16(13)
C(20)-C(15)-P(1)	116.24(13)
C(15)-C(16)-C(17)	119.37(17)
C(15)-C(16)-H(16)	120.3
C(17)-C(16)-H(16)	120.3
C(18)-C(17)-C(16)	120.87(16)
C(18)-C(17)-C(21)	120.41(16)
C(16)-C(17)-C(21)	118.72(18)
C(17)-C(18)-C(19)	119.49(15)
C(17)-C(18)-H(18)	120.3
C(19)-C(18)-H(18)	120.3
C(18)-C(19)-C(20)	120.78(17)

C(18)-C(19)-C(22)	118.81(17)
C(20)-C(19)-C(22)	120.40(19)
C(15)-C(20)-C(19)	118.90(17)
C(15)-C(20)-H(20)	120.6
C(19)-C(20)-H(20)	120.6
F(7A)-C(21)-F(8A)	115.7(7)
F(7)-C(21)-F(8)	107.9(6)
F(7A)-C(21)-F(9A)	105.3(6)
F(8A)-C(21)-F(9A)	103.5(5)
F(7)-C(21)-F(9)	105.4(5)
F(7A)-C(21)-C(17)	113.7(4)
F(7)-C(21)-C(17)	117.7(4)
F(8A)-C(21)-C(17)	109.9(3)
F(8)-C(21)-C(17)	112.7(4)
F(9A)-C(21)-C(17)	107.8(4)
F(9)-C(21)-C(17)	113.6(2)
F(11)-C(22)-F(10)	106.2(2)
F(11)-C(22)-F(12)	107.4(2)
F(10)-C(22)-F(12)	104.3(2)
F(11)-C(22)-C(19)	112.9(2)
F(10)-C(22)-C(19)	113.71(17)
F(12)-C(22)-C(19)	111.8(2)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rpsl20a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	34(1)	40(1)	27(1)	-3(1)	8(1)	-4(1)
O(1)	48(1)	57(1)	28(1)	-5(1)	11(1)	-7(1)
N(1)	56(1)	46(1)	51(1)	-2(1)	11(1)	1(1)
C(1)	58(1)	51(1)	72(2)	5(1)	11(1)	5(1)
C(2)	66(1)	45(1)	90(2)	2(1)	33(1)	5(1)
C(3)	80(1)	50(1)	76(2)	-15(1)	43(1)	-6(1)
C(4)	67(1)	48(1)	49(1)	-9(1)	23(1)	-8(1)
C(5)	48(1)	35(1)	45(1)	-2(1)	17(1)	-8(1)
C(6)	43(1)	43(1)	37(1)	-2(1)	14(1)	-8(1)
C(7)	33(1)	45(1)	33(1)	-1(1)	4(1)	-3(1)
C(8)	37(1)	52(1)	37(1)	6(1)	9(1)	3(1)
C(9)	40(1)	61(1)	50(1)	8(1)	17(1)	6(1)
C(10)	37(1)	61(1)	57(1)	7(1)	4(1)	5(1)
C(11)	40(1)	69(1)	44(1)	3(1)	-6(1)	3(1)
C(12)	45(1)	60(1)	31(1)	-5(1)	1(1)	0(1)
C(13)	71(1)	113(2)	68(2)	28(2)	40(1)	46(2)
F(1)	98(2)	151(4)	57(2)	-32(2)	29(2)	-13(3)
F(2)	78(2)	227(9)	86(3)	28(3)	35(2)	101(4)
F(3)	172(6)	98(3)	107(4)	32(3)	96(5)	13(4)
F(1A)	104(6)	239(13)	56(3)	13(7)	34(4)	87(7)
F(2A)	212(10)	222(11)	204(11)	-32(9)	175(10)	-69(9)
F(3A)	269(16)	155(8)	125(8)	23(6)	134(10)	113(11)
C(14)	87(2)	151(4)	55(2)	0(2)	-16(2)	47(2)
F(4)	108(4)	188(9)	42(3)	45(5)	8(3)	54(4)
F(5)	78(4)	294(12)	77(4)	-4(6)	-40(3)	7(6)
F(6)	368(16)	114(6)	92(5)	-8(5)	-78(10)	131(9)
F(4A)	69(3)	234(12)	100(7)	58(7)	-6(3)	66(5)
F(5A)	137(5)	210(10)	122(6)	117(8)	-9(4)	-23(5)
F(6A)	229(14)	358(19)	81(6)	-84(8)	-84(7)	148(12)
C(15)	33(1)	39(1)	32(1)	-6(1)	11(1)	-4(1)
C(16)	37(1)	43(1)	32(1)	-4(1)	11(1)	-3(1)

C(17)	34(1)	56(1)	34(1)	-8(1)	8(1)	-2(1)
C(18)	38(1)	57(1)	46(1)	-11(1)	11(1)	-12(1)
C(19)	45(1)	42(1)	51(1)	-3(1)	14(1)	-10(1)
C(20)	40(1)	43(1)	39(1)	1(1)	8(1)	-2(1)
C(21)	44(1)	72(2)	47(1)	-2(1)	-3(1)	-3(1)
F(7)	32(1)	197(9)	90(4)	65(5)	0(2)	-10(3)
F(8)	146(6)	135(5)	38(2)	-3(2)	23(3)	54(4)
F(9)	108(3)	64(2)	85(4)	20(2)	-36(3)	-4(3)
F(7A)	61(2)	237(11)	71(4)	89(6)	15(2)	-7(4)
F(8A)	133(5)	142(6)	89(4)	-13(4)	-36(4)	88(5)
F(9A)	89(4)	162(7)	75(3)	17(4)	-49(3)	-54(4)
C(22)	71(1)	47(1)	66(2)	1(1)	14(1)	-18(1)
F(10)	110(1)	67(1)	108(1)	34(1)	-3(1)	-24(1)
F(11)	82(1)	91(1)	154(2)	38(1)	50(1)	-20(1)
F(12)	156(2)	55(1)	112(2)	-14(1)	39(1)	-35(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rpsl20a.

	x	y	z	U(eq)
H(1)	7226	596	6871	73
H(2)	7403	29	5031	77
H(3)	5992	204	3134	77
H(4)	4448	990	3090	64
H(6A)	4000	1821	5964	48
H(6B)	3218	1517	4654	48
H(8)	2890	3019	6211	50
H(10)	40	4040	4111	64
H(12)	2402	3202	2359	57
H(16)	5890	2322	6700	44
H(18)	7968	4011	7021	56
H(20)	5142	3809	3968	49

Table 6. Torsion angles [°] for rpsl20a.

C(5)-N(1)-C(1)-C(2)	-1.0(3)
N(1)-C(1)-C(2)-C(3)	-0.1(4)
C(1)-C(2)-C(3)-C(4)	1.3(4)
C(2)-C(3)-C(4)-C(5)	-1.5(3)
C(1)-N(1)-C(5)-C(4)	0.8(3)
C(1)-N(1)-C(5)-C(6)	-179.13(17)
C(3)-C(4)-C(5)-N(1)	0.4(3)
C(3)-C(4)-C(5)-C(6)	-179.66(17)
N(1)-C(5)-C(6)-P(1)	109.07(16)
C(4)-C(5)-C(6)-P(1)	-70.86(19)
O(1)-P(1)-C(6)-C(5)	53.98(15)
C(15)-P(1)-C(6)-C(5)	-71.65(14)
C(7)-P(1)-C(6)-C(5)	174.76(12)
O(1)-P(1)-C(7)-C(8)	177.77(15)
C(15)-P(1)-C(7)-C(8)	-61.46(17)
C(6)-P(1)-C(7)-C(8)	53.48(17)
O(1)-P(1)-C(7)-C(12)	-2.75(16)
C(15)-P(1)-C(7)-C(12)	118.02(14)
C(6)-P(1)-C(7)-C(12)	-127.04(15)
C(12)-C(7)-C(8)-C(9)	1.9(3)
P(1)-C(7)-C(8)-C(9)	-178.65(14)
C(7)-C(8)-C(9)-C(10)	-0.8(3)
C(7)-C(8)-C(9)-C(13)	-179.4(2)
C(8)-C(9)-C(10)-C(11)	-1.1(3)
C(13)-C(9)-C(10)-C(11)	177.5(2)
C(9)-C(10)-C(11)-C(12)	1.9(3)
C(9)-C(10)-C(11)-C(14)	-174.9(3)
C(10)-C(11)-C(12)-C(7)	-0.8(3)
C(14)-C(11)-C(12)-C(7)	176.0(3)
C(8)-C(7)-C(12)-C(11)	-1.1(3)
P(1)-C(7)-C(12)-C(11)	179.38(16)
C(10)-C(9)-C(13)-F(1A)	-175.2(10)
C(8)-C(9)-C(13)-F(1A)	3.5(11)
C(10)-C(9)-C(13)-F(3A)	-29.9(10)

C(8)-C(9)-C(13)-F(3A)	148.8(9)
C(10)-C(9)-C(13)-F(3)	132.2(5)
C(8)-C(9)-C(13)-F(3)	-49.2(6)
C(10)-C(9)-C(13)-F(2)	-2.0(7)
C(8)-C(9)-C(13)-F(2)	176.7(6)
C(10)-C(9)-C(13)-F(2A)	77.5(8)
C(8)-C(9)-C(13)-F(2A)	-103.9(7)
C(10)-C(9)-C(13)-F(1)	-117.6(3)
C(8)-C(9)-C(13)-F(1)	61.1(4)
C(12)-C(11)-C(14)-F(4A)	165.6(9)
C(10)-C(11)-C(14)-F(4A)	-17.6(10)
C(12)-C(11)-C(14)-F(4)	0.7(8)
C(10)-C(11)-C(14)-F(4)	177.5(7)
C(12)-C(11)-C(14)-F(6)	-132.5(12)
C(10)-C(11)-C(14)-F(6)	44.3(13)
C(12)-C(11)-C(14)-F(6A)	42.4(12)
C(10)-C(11)-C(14)-F(6A)	-140.8(11)
C(12)-C(11)-C(14)-F(5)	113.6(7)
C(10)-C(11)-C(14)-F(5)	-69.6(7)
C(12)-C(11)-C(14)-F(5A)	-76.8(8)
C(10)-C(11)-C(14)-F(5A)	100.0(8)
O(1)-P(1)-C(15)-C(16)	-125.55(14)
C(6)-P(1)-C(15)-C(16)	1.71(15)
C(7)-P(1)-C(15)-C(16)	115.48(14)
O(1)-P(1)-C(15)-C(20)	51.33(15)
C(6)-P(1)-C(15)-C(20)	178.60(12)
C(7)-P(1)-C(15)-C(20)	-67.64(14)
C(20)-C(15)-C(16)-C(17)	-0.5(2)
P(1)-C(15)-C(16)-C(17)	176.21(12)
C(15)-C(16)-C(17)-C(18)	1.5(3)
C(15)-C(16)-C(17)-C(21)	-178.47(16)
C(16)-C(17)-C(18)-C(19)	-0.2(3)
C(21)-C(17)-C(18)-C(19)	179.69(18)
C(17)-C(18)-C(19)-C(20)	-1.9(3)
C(17)-C(18)-C(19)-C(22)	178.79(19)
C(16)-C(15)-C(20)-C(19)	-1.5(3)

P(1)-C(15)-C(20)-C(19)	-178.51(13)
C(18)-C(19)-C(20)-C(15)	2.8(3)
C(22)-C(19)-C(20)-C(15)	-177.92(18)
C(18)-C(17)-C(21)-F(7A)	116.1(6)
C(16)-C(17)-C(21)-F(7A)	-63.9(6)
C(18)-C(17)-C(21)-F(7)	-35.1(6)
C(16)-C(17)-C(21)-F(7)	144.9(5)
C(18)-C(17)-C(21)-F(8A)	-112.4(6)
C(16)-C(17)-C(21)-F(8A)	67.5(6)
C(18)-C(17)-C(21)-F(8)	91.6(5)
C(16)-C(17)-C(21)-F(8)	-88.5(5)
C(18)-C(17)-C(21)-F(9A)	-0.2(5)
C(16)-C(17)-C(21)-F(9A)	179.7(4)
C(18)-C(17)-C(21)-F(9)	-158.9(4)
C(16)-C(17)-C(21)-F(9)	21.0(4)
C(18)-C(19)-C(22)-F(11)	64.1(3)
C(20)-C(19)-C(22)-F(11)	-115.2(2)
C(18)-C(19)-C(22)-F(10)	-174.9(2)
C(20)-C(19)-C(22)-F(10)	5.8(3)
C(18)-C(19)-C(22)-F(12)	-57.1(3)
C(20)-C(19)-C(22)-F(12)	123.6(2)

Table 7. Possible Hydrogen bonds for rpsl20a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(6)-H(6A)...O(1)#1	0.98	2.45	3.364(2)	155.7
C(8)-H(8)...O(1)#1	0.94	2.26	3.188(2)	168.0
C(12)-H(12)...O(1)	0.94	2.48	2.930(2)	109.1
C(16)-H(16)...F(9)	0.94	2.44	2.766(5)	100.1
C(16)-H(16)...N(1)	0.94	2.42	3.193(3)	139.4
C(18)-H(18)...F(9A)	0.94	2.27	2.611(7)	100.9

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z+1/2

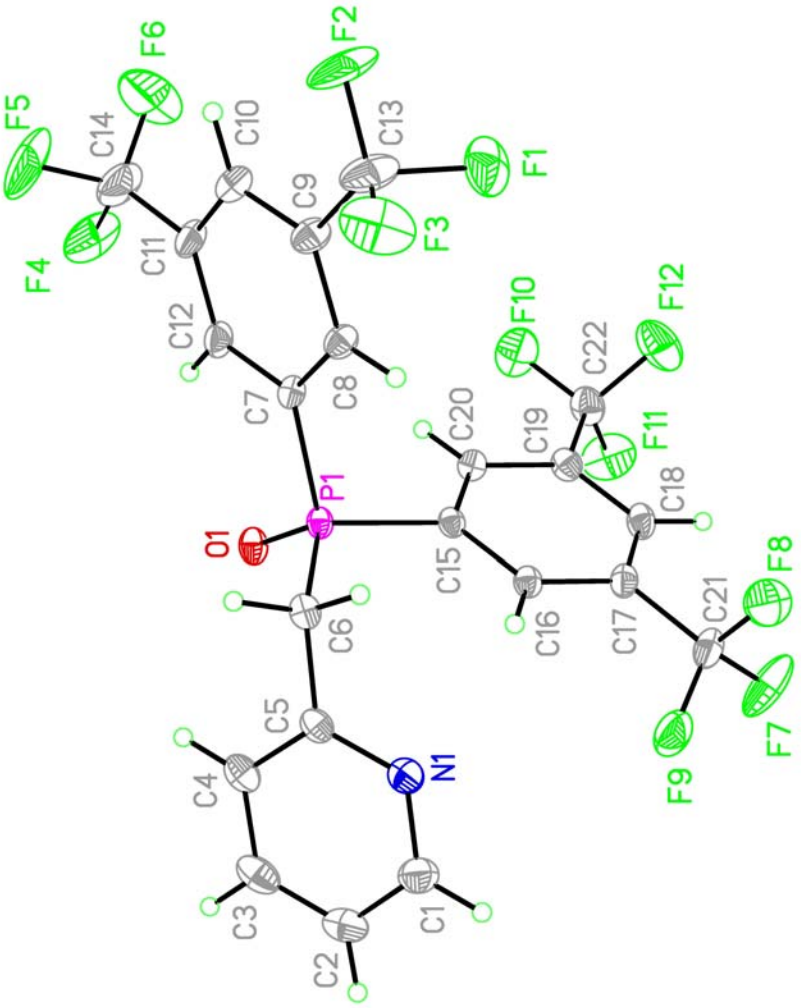


Figure 1. rpsl20l1.jpg, Single molecule view, only part one of all disordered F's included, thermal displacement ellipsoids at 20%, rpsl20l1b.jpg=b/w; only F1,F2,F3,F4,F5,F6,F7,F8 F9 of disorder shown.

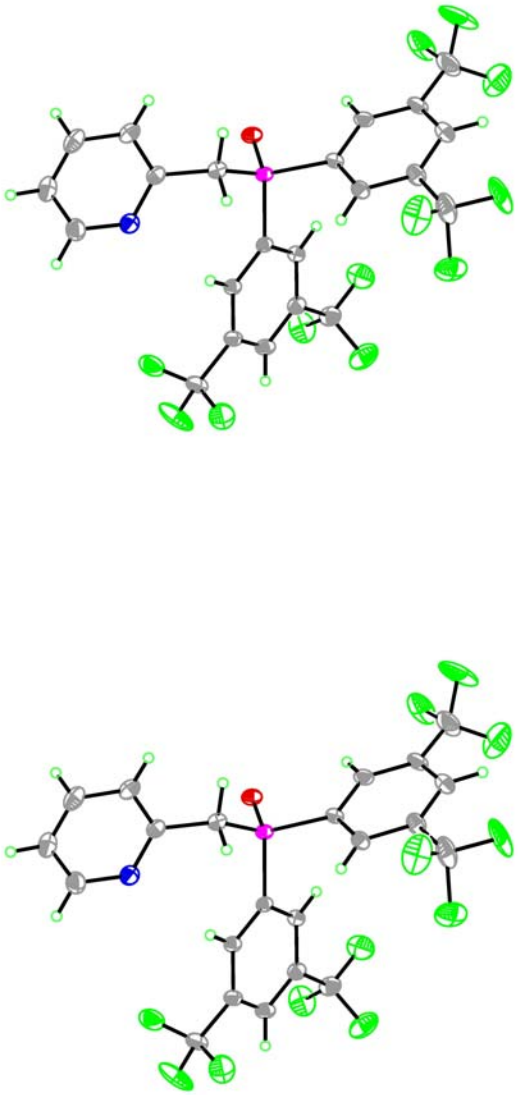


Figure 3.rpsl20s1.jpg also rpsl20s1b.jpg[b/w], stereoview of single molecule. Disorder not shown.

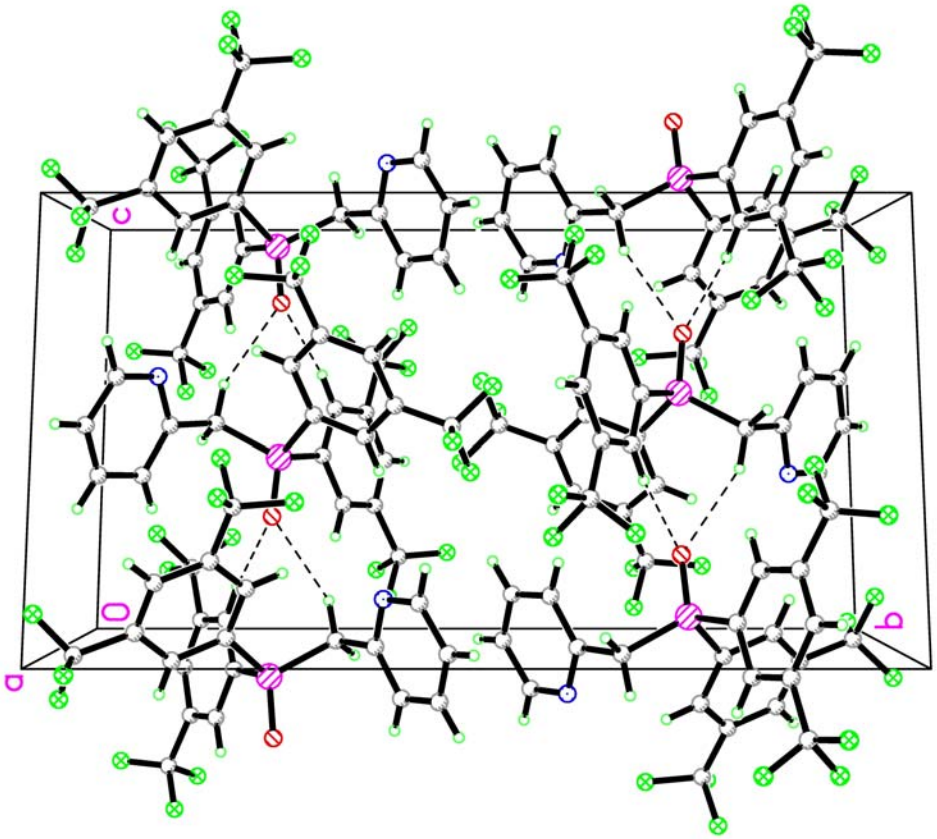


Figure 3.rpsl20al1.jpg packing view down a-axis,color,also rpsl20al1b.jpg b/w, O1—H6, and O1—H8 distances shown [dotted lines]. Disorder not shown.

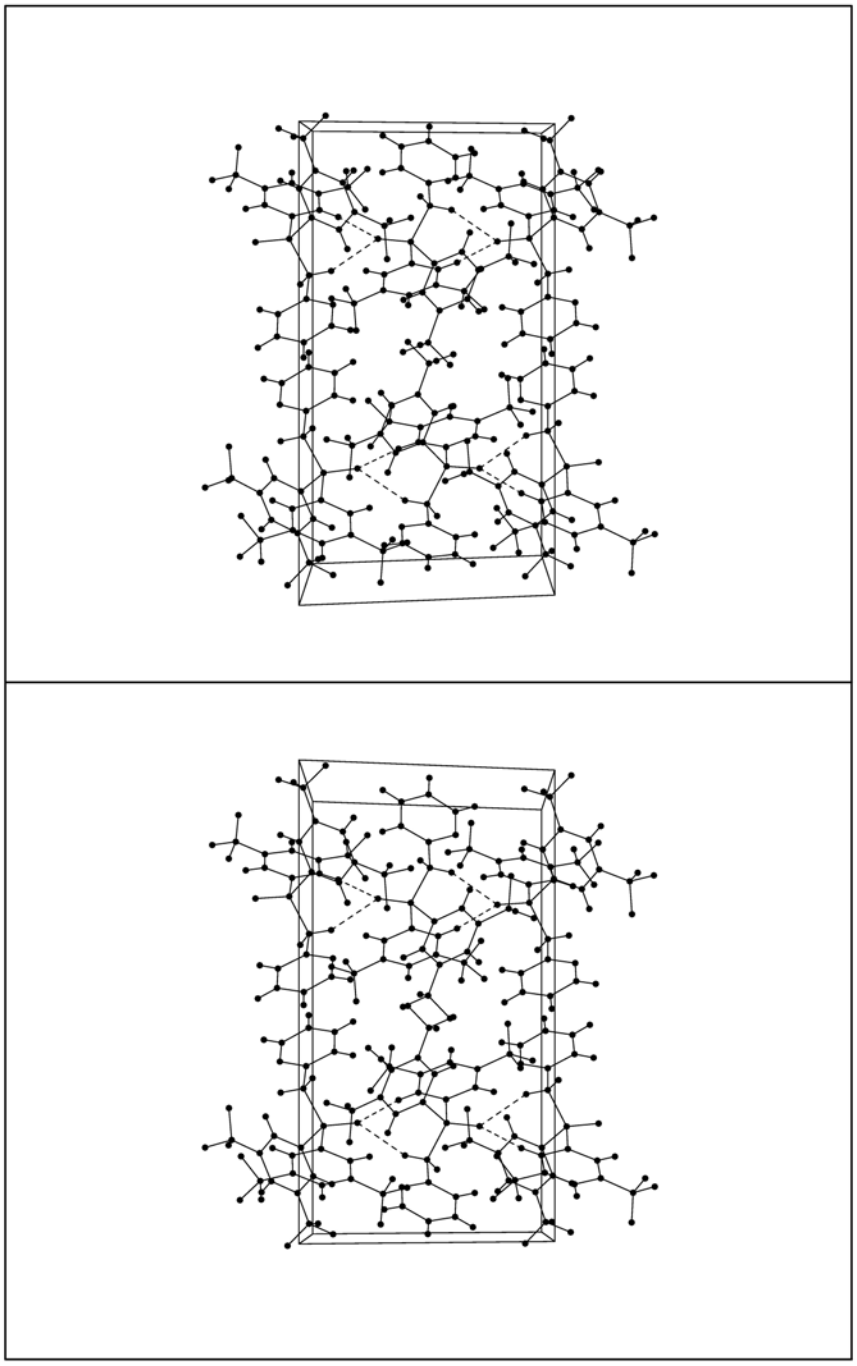


Figure 4.rpsl20.jpg, stereoview of packing, view down a-axis,b/w only.Disorder not shown.

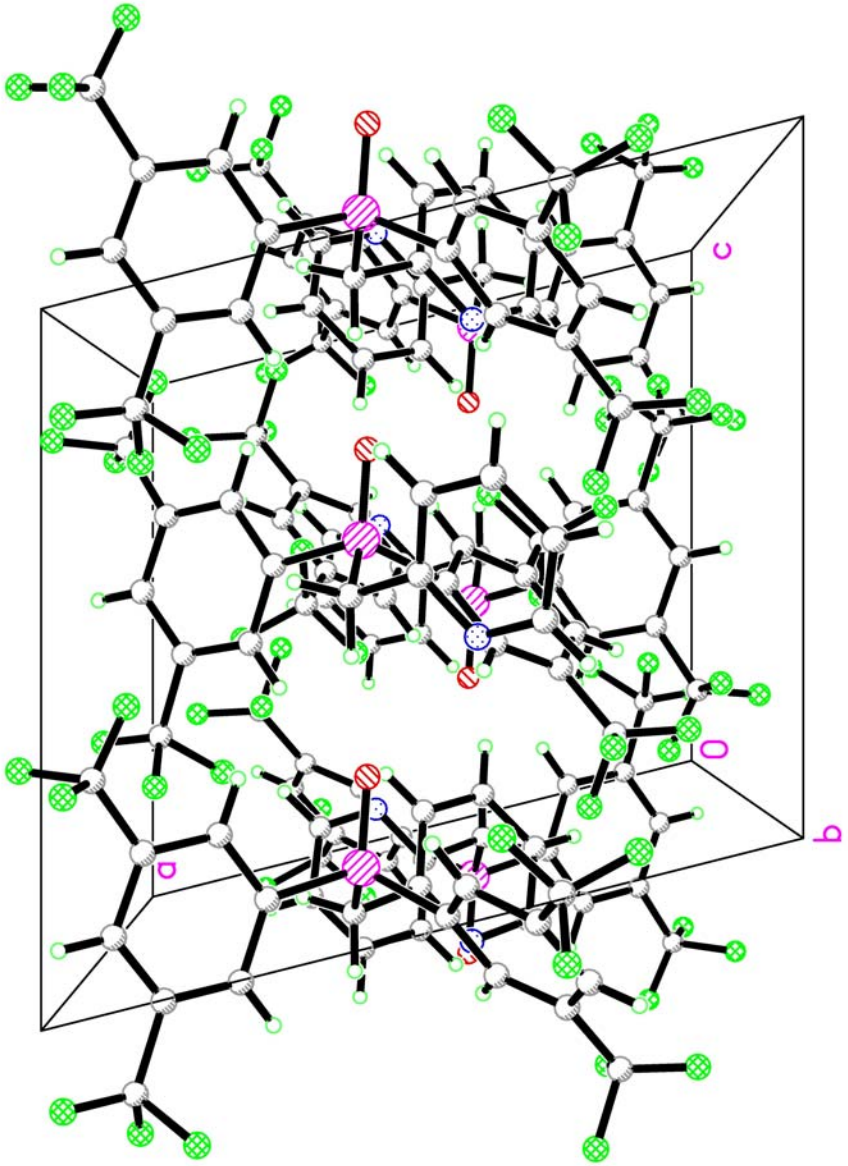


Figure 5. rpsl20bl.jpg packing view down b-axis,color,also rpsl20blb.jpg b/w, also see rpsl20bs.jpg, stereo view of same. Disorder not shown.

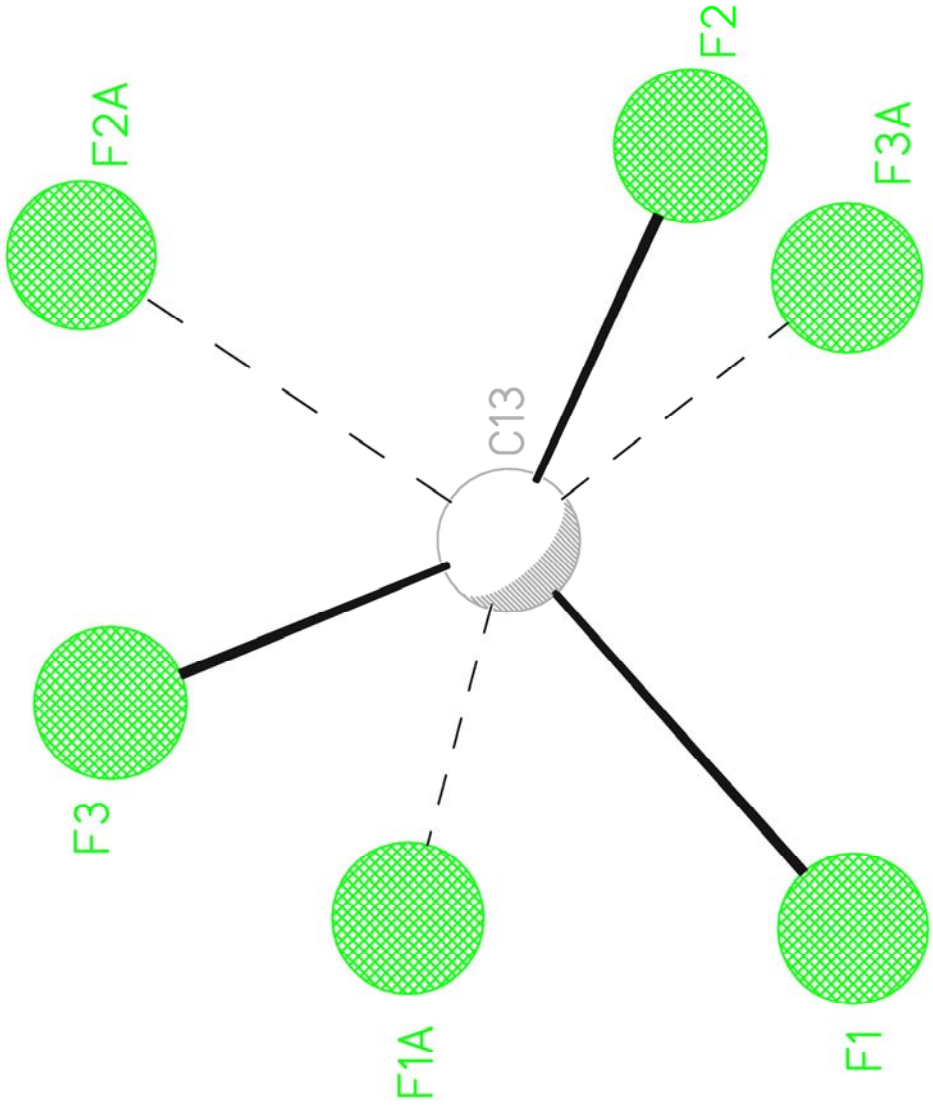


Figure 6. rpsl20c13.jpg CF3 of C13, showing two sets of F's; F1-3 at 60% occupancy, F1A-3A at 40% occupancy. rpsl20c13b.jpg=b/w version

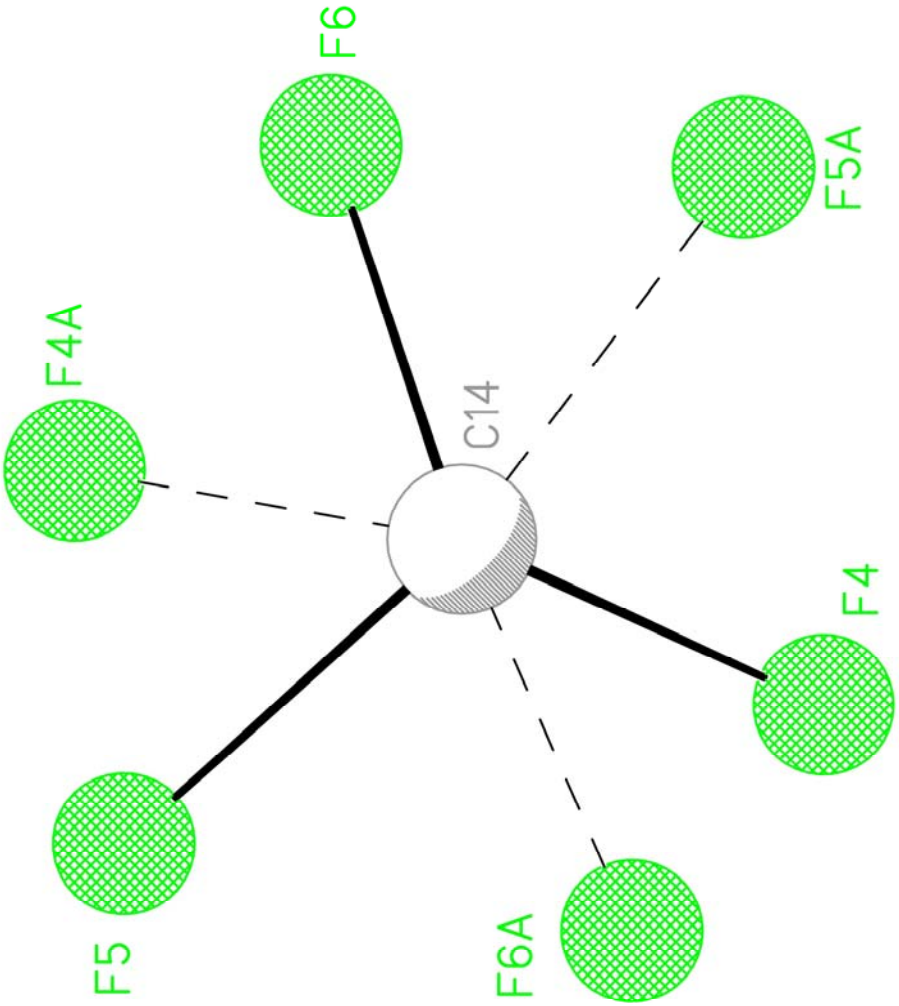


Figure 7 . rpsl20c14.jpg and rpsl20c14b.jpg, CF3 plan of C14, two sets of F's, each at 50% occupancy

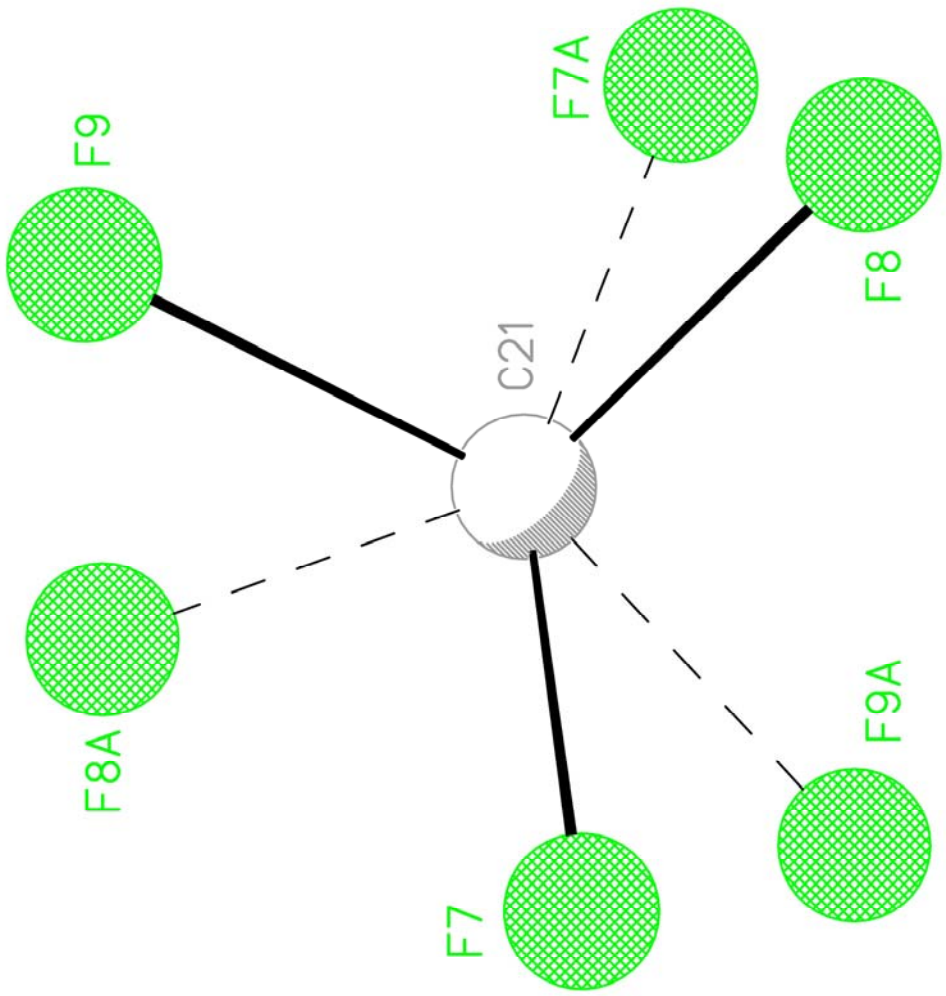


Figure 8. rps20c21p.jpg and rpsl20c21b.jpg, CF3 plan of C21, two sets of F's each at 50% occupancy

Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information for Dalton Transactions

X-ray Crystallographic data for **1d**.

Crystal Structure Report

Prepared for:

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Compound:

Rps22/slp-11-41

C22 H12 F12 N O2 P

Prepared by:

Eileen Duesler

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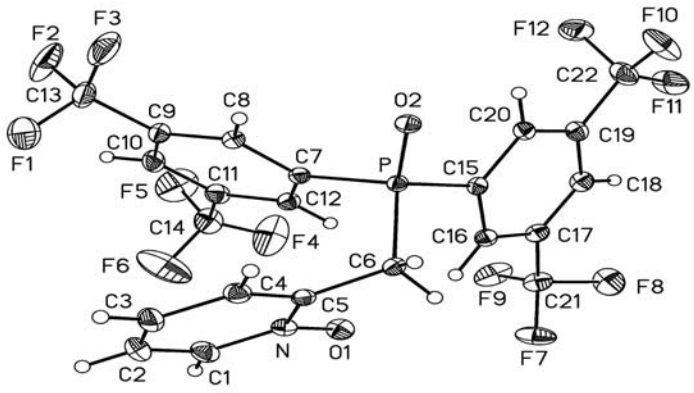
277-6649

Issue date:

January 26, 2007



Rpsl22l1b.jpg $253=$[225+2[44-30]]

Table 1. Crystal data and structure refinement for rpsl22.

Identification code	rpsl22	
Empirical formula	C22 H12 F12 N O2 P	
Formula weight	581.30	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.7789(6) Å	α= 90°.
	b = 24.0769(8) Å	β= 117.727(2)°.
	c = 11.4618(4) Å	γ = 90°.
Volume	4587.2(3) $Å^3$	
Z	8	
Density (calculated)	1.683 Mg/m^3	
Absorption coefficient	0.239 mm^{-1}	
F(000)	2320	
Crystal size	0.32 x 0.23 x 0.16 mm^3	
Theta range for data collection	2.63 to 28.32°.	
Index ranges	-24<=h<=25, -32<=k<=32, -15<=l<=15	
Reflections collected	38656	
Independent reflections	5720 [R(int) = 0.0219]	
Completeness to theta = 28.32°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.960 and 0.926	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5720 / 0 / 397	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0473, wR2 = 0.1265	
R indices (all data)	R1 = 0.0567, wR2 = 0.1354	
Largest diff. peak and hole	0.578 and -0.444 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rpsl22. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P	1528(1)	130(1)	1061(1)	26(1)
N	1457(1)	1285(1)	-681(2)	35(1)
O(1)	2099(1)	1039(1)	-588(2)	44(1)
O(2)	1014(1)	-168(1)	1520(1)	35(1)
C(1)	1420(1)	1849(1)	-679(2)	48(1)
C(2)	763(2)	2115(1)	-738(2)	55(1)
C(3)	119(2)	1812(1)	-814(2)	50(1)
C(4)	157(1)	1239(1)	-822(2)	39(1)
C(5)	831(1)	976(1)	-743(2)	30(1)
C(6)	952(1)	364(1)	-650(2)	30(1)
C(7)	1956(1)	744(1)	2067(2)	29(1)
C(8)	1520(1)	971(1)	2650(2)	33(1)
C(9)	1791(1)	1447(1)	3412(2)	40(1)
C(10)	2498(1)	1699(1)	3605(2)	46(1)
C(11)	2935(1)	1469(1)	3034(2)	43(1)
C(12)	2671(1)	993(1)	2270(2)	35(1)
C(13)	1303(2)	1698(1)	4007(2)	56(1)
F(1)	856(1)	2104(1)	3312(2)	104(1)
F(2)	1757(1)	1906(1)	5192(2)	111(1)
F(3)	830(2)	1342(1)	4151(3)	117(1)
C(14)	3690(2)	1751(1)	3219(3)	66(1)
F(4)	4148(1)	1442(1)	2925(3)	129(1)
F(5)	4149(1)	1910(1)	4450(2)	115(1)
F(6)	3544(2)	2207(1)	2554(3)	151(1)
C(15)	2371(1)	-283(1)	1220(2)	30(1)
C(16)	2854(1)	-125(1)	654(2)	33(1)
C(17)	3535(1)	-431(1)	909(2)	37(1)
C(18)	3726(1)	-902(1)	1689(2)	41(1)
C(19)	3239(1)	-1061(1)	2233(2)	41(1)
C(20)	2566(1)	-752(1)	2022(2)	35(1)
C(21)	4093(1)	-225(1)	405(2)	49(1)

F(7)	3731(6)	-34(5)	-780(10)	71(3)
F(8)	4497(4)	-687(3)	236(7)	83(2)
F(9)	4614(4)	89(3)	1154(6)	81(2)
F(7A)	4743(3)	-489(3)	769(6)	84(2)
F(8A)	4368(5)	319(3)	920(9)	87(2)
F(9A)	3731(7)	-116(6)	-851(10)	72(3)
C(22)	3467(2)	-1563(1)	3123(3)	60(1)
F(10)	2877(3)	-1890(3)	2918(6)	95(2)
F(11)	4080(3)	-1839(2)	3177(5)	93(2)
F(12)	3732(4)	-1412(3)	4392(5)	81(2)
F(10A)	3990(8)	-1499(5)	4216(13)	178(8)
F(11A)	2816(7)	-1811(5)	3062(12)	82(3)
F(12A)	3610(7)	-1992(3)	2401(10)	121(3)

Table 3. Bond lengths [Å] and angles [°] for rpsl22.

P-O(2)	1.4825(12)
P-C(15)	1.8052(17)
P-C(7)	1.8165(17)
P-C(6)	1.8325(17)
N-O(1)	1.303(2)
N-C(1)	1.359(3)
N-C(5)	1.364(2)
C(1)-C(2)	1.364(3)
C(1)-H(1A)	0.9400
C(2)-C(3)	1.381(3)
C(2)-H(2)	0.9400
C(3)-C(4)	1.380(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.381(3)
C(4)-H(4)	0.9400
C(5)-C(6)	1.488(2)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(7)-C(12)	1.387(2)
C(7)-C(8)	1.388(2)
C(8)-C(9)	1.386(3)
C(8)-H(8)	0.9400
C(9)-C(10)	1.381(3)
C(9)-C(13)	1.501(3)
C(10)-C(11)	1.382(3)
C(10)-H(10)	0.9400
C(11)-C(12)	1.387(3)
C(11)-C(14)	1.494(3)
C(12)-H(12)	0.9400
C(13)-F(1)	1.294(3)
C(13)-F(3)	1.299(3)
C(13)-F(2)	1.321(3)
C(14)-F(6)	1.291(4)
C(14)-F(4)	1.295(3)

C(14)-F(5)	1.323(3)
C(15)-C(16)	1.392(2)
C(15)-C(20)	1.394(2)
C(16)-C(17)	1.385(3)
C(16)-H(16)	0.9400
C(17)-C(18)	1.383(3)
C(17)-C(21)	1.496(3)
C(18)-C(19)	1.380(3)
C(18)-H(18)	0.9400
C(19)-C(20)	1.388(3)
C(19)-C(22)	1.508(3)
C(20)-H(20)	0.9400
C(21)-F(9)	1.219(6)
C(21)-F(7A)	1.264(6)
C(21)-F(7)	1.287(10)
C(21)-F(9A)	1.300(11)
C(21)-F(8)	1.410(7)
C(21)-F(8A)	1.430(8)
C(22)-F(10A)	1.189(12)
C(22)-F(10)	1.288(6)
C(22)-F(11)	1.305(5)
C(22)-F(11A)	1.332(11)
C(22)-F(12)	1.350(6)
C(22)-F(12A)	1.424(8)

O(2)-P-C(15)	112.48(8)
O(2)-P-C(7)	109.71(7)
C(15)-P-C(7)	106.07(8)
O(2)-P-C(6)	111.74(8)
C(15)-P-C(6)	109.35(8)
C(7)-P-C(6)	107.21(8)
O(1)-N-C(1)	120.08(17)
O(1)-N-C(5)	119.86(15)
C(1)-N-C(5)	120.04(17)
N-C(1)-C(2)	121.0(2)
N-C(1)-H(1A)	119.5

C(2)-C(1)-H(1A)	119.5
C(1)-C(2)-C(3)	120.0(2)
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-H(2)	120.0
C(4)-C(3)-C(2)	118.8(2)
C(4)-C(3)-H(3)	120.6
C(2)-C(3)-H(3)	120.6
C(3)-C(4)-C(5)	120.46(19)
C(3)-C(4)-H(4)	119.8
C(5)-C(4)-H(4)	119.8
N-C(5)-C(4)	119.68(16)
N-C(5)-C(6)	115.96(15)
C(4)-C(5)-C(6)	124.29(16)
C(5)-C(6)-P	112.07(11)
C(5)-C(6)-H(6A)	109.2
P-C(6)-H(6A)	109.2
C(5)-C(6)-H(6B)	109.2
P-C(6)-H(6B)	109.2
H(6A)-C(6)-H(6B)	107.9
C(12)-C(7)-C(8)	119.46(16)
C(12)-C(7)-P	124.44(13)
C(8)-C(7)-P	116.10(13)
C(9)-C(8)-C(7)	120.13(17)
C(9)-C(8)-H(8)	119.9
C(7)-C(8)-H(8)	119.9
C(10)-C(9)-C(8)	120.61(18)
C(10)-C(9)-C(13)	119.63(19)
C(8)-C(9)-C(13)	119.74(19)
C(9)-C(10)-C(11)	119.11(18)
C(9)-C(10)-H(10)	120.4
C(11)-C(10)-H(10)	120.4
C(10)-C(11)-C(12)	120.87(19)
C(10)-C(11)-C(14)	118.96(19)
C(12)-C(11)-C(14)	120.1(2)
C(7)-C(12)-C(11)	119.80(18)
C(7)-C(12)-H(12)	120.1

C(11)-C(12)-H(12)	120.1
F(1)-C(13)-F(3)	107.0(3)
F(1)-C(13)-F(2)	105.6(2)
F(3)-C(13)-F(2)	105.8(2)
F(1)-C(13)-C(9)	112.6(2)
F(3)-C(13)-C(9)	112.94(19)
F(2)-C(13)-C(9)	112.4(2)
F(6)-C(14)-F(4)	108.6(3)
F(6)-C(14)-F(5)	103.8(3)
F(4)-C(14)-F(5)	105.1(3)
F(6)-C(14)-C(11)	112.1(3)
F(4)-C(14)-C(11)	113.8(2)
F(5)-C(14)-C(11)	112.7(2)
C(16)-C(15)-C(20)	120.10(16)
C(16)-C(15)-P	122.17(13)
C(20)-C(15)-P	117.55(13)
C(17)-C(16)-C(15)	119.59(17)
C(17)-C(16)-H(16)	120.2
C(15)-C(16)-H(16)	120.2
C(18)-C(17)-C(16)	120.59(17)
C(18)-C(17)-C(21)	120.29(18)
C(16)-C(17)-C(21)	118.98(18)
C(19)-C(18)-C(17)	119.57(18)
C(19)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(18)-C(19)-C(20)	120.90(18)
C(18)-C(19)-C(22)	119.30(19)
C(20)-C(19)-C(22)	119.73(19)
C(19)-C(20)-C(15)	119.21(17)
C(19)-C(20)-H(20)	120.4
C(15)-C(20)-H(20)	120.4
F(9)-C(21)-F(7)	112.3(7)
F(7A)-C(21)-F(7)	118.9(6)
F(9)-C(21)-F(9A)	119.3(7)
F(7A)-C(21)-F(9A)	113.2(7)
F(9)-C(21)-F(8)	106.1(4)

F(7)-C(21)-F(8)	101.0(6)
F(7A)-C(21)-F(8A)	102.5(4)
F(9A)-C(21)-F(8A)	100.0(7)
F(9)-C(21)-C(17)	114.3(4)
F(7A)-C(21)-C(17)	116.6(3)
F(7)-C(21)-C(17)	113.9(5)
F(9A)-C(21)-C(17)	113.3(6)
F(8)-C(21)-C(17)	108.0(3)
F(8A)-C(21)-C(17)	109.1(4)
F(10)-C(22)-F(11)	111.3(5)
F(10A)-C(22)-F(11A)	113.7(9)
F(10)-C(22)-F(12)	102.5(5)
F(11)-C(22)-F(12)	102.2(4)
F(10A)-C(22)-F(12A)	114.9(9)
F(11A)-C(22)-F(12A)	93.5(6)
F(10A)-C(22)-C(19)	116.3(6)
F(10)-C(22)-C(19)	114.6(4)
F(11)-C(22)-C(19)	113.9(3)
F(11A)-C(22)-C(19)	111.0(5)
F(12)-C(22)-C(19)	111.0(3)
F(12A)-C(22)-C(19)	105.0(4)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rpsl22. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P	28(1)	27(1)	28(1)	-2(1)	16(1)	-3(1)
N	37(1)	38(1)	33(1)	4(1)	19(1)	-2(1)
O(1)	37(1)	50(1)	52(1)	4(1)	26(1)	-1(1)
O(2)	35(1)	36(1)	39(1)	2(1)	22(1)	-5(1)
C(1)	55(1)	38(1)	53(1)	6(1)	27(1)	-8(1)
C(2)	74(2)	31(1)	63(1)	6(1)	35(1)	4(1)
C(3)	58(1)	42(1)	59(1)	9(1)	34(1)	15(1)
C(4)	38(1)	42(1)	39(1)	6(1)	22(1)	4(1)
C(5)	34(1)	33(1)	25(1)	2(1)	15(1)	-1(1)
C(6)	32(1)	32(1)	27(1)	-3(1)	14(1)	-3(1)
C(7)	33(1)	28(1)	26(1)	0(1)	13(1)	-2(1)
C(8)	37(1)	33(1)	31(1)	0(1)	16(1)	1(1)
C(9)	52(1)	35(1)	35(1)	-3(1)	20(1)	5(1)
C(10)	57(1)	33(1)	44(1)	-10(1)	18(1)	-5(1)
C(11)	46(1)	36(1)	42(1)	-3(1)	17(1)	-11(1)
C(12)	37(1)	35(1)	34(1)	-2(1)	17(1)	-6(1)
C(13)	67(2)	50(1)	54(1)	-12(1)	31(1)	10(1)
F(1)	114(2)	103(2)	116(2)	30(1)	70(1)	64(1)
F(2)	108(2)	145(2)	73(1)	-55(1)	35(1)	28(1)
F(3)	178(2)	82(1)	180(2)	-36(1)	159(2)	-21(1)
C(14)	63(2)	55(1)	81(2)	-17(1)	36(1)	-27(1)
F(4)	93(1)	123(2)	212(3)	-80(2)	106(2)	-67(1)
F(5)	78(1)	142(2)	105(2)	-45(1)	25(1)	-61(1)
F(6)	104(2)	123(2)	201(3)	78(2)	50(2)	-43(2)
C(15)	29(1)	30(1)	31(1)	-4(1)	14(1)	-2(1)
C(16)	32(1)	36(1)	32(1)	-1(1)	16(1)	-1(1)
C(17)	31(1)	46(1)	35(1)	-2(1)	16(1)	1(1)
C(18)	35(1)	46(1)	43(1)	0(1)	18(1)	7(1)
C(19)	42(1)	36(1)	43(1)	3(1)	19(1)	5(1)
C(20)	38(1)	31(1)	38(1)	-1(1)	20(1)	-2(1)
C(21)	34(1)	71(2)	45(1)	4(1)	21(1)	5(1)

F(7)	46(4)	110(5)	66(5)	44(4)	34(4)	21(4)
F(8)	82(4)	81(3)	128(5)	10(3)	83(4)	21(3)
F(9)	61(3)	126(6)	58(2)	-28(3)	31(2)	-56(4)
F(7A)	47(3)	118(6)	104(4)	55(4)	51(3)	36(3)
F(8A)	89(5)	81(4)	120(5)	-27(3)	74(4)	-42(3)
F(9A)	61(5)	120(6)	35(3)	-5(3)	21(3)	-36(4)
C(22)	62(2)	45(1)	78(2)	20(1)	36(1)	17(1)
F(10)	89(3)	54(3)	99(3)	26(2)	7(3)	-19(2)
F(11)	112(3)	80(3)	116(4)	53(3)	78(3)	66(3)
F(12)	102(4)	84(2)	50(2)	27(2)	30(3)	26(2)
F(10A)	115(10)	115(10)	149(12)	89(9)	-68(7)	-40(7)
F(11A)	125(7)	55(4)	123(6)	41(4)	105(6)	33(4)
F(12A)	202(10)	50(3)	176(9)	39(5)	143(8)	63(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rpsl22.

	x	y	z	U(eq)
H(1A)	1854	2058	-636	57
H(2)	749	2505	-727	65
H(3)	-338	1992	-858	60
H(4)	-279	1027	-882	46
H(6A)	1236	255	-1146	36
H(6B)	426	180	-1053	36
H(8)	1039	801	2528	40
H(10)	2679	2023	4118	56
H(12)	2975	839	1891	42
H(16)	2719	188	102	39
H(18)	4185	-1111	1848	50
H(20)	2245	-858	2416	42

Table 6. Torsion angles [°] for rpsl22.

O(1)-N-C(1)-C(2)	-178.15(19)
C(5)-N-C(1)-C(2)	0.1(3)
N-C(1)-C(2)-C(3)	-0.6(4)
C(1)-C(2)-C(3)-C(4)	0.3(4)
C(2)-C(3)-C(4)-C(5)	0.6(3)
O(1)-N-C(5)-C(4)	179.05(15)
C(1)-N-C(5)-C(4)	0.8(3)
O(1)-N-C(5)-C(6)	2.1(2)
C(1)-N-C(5)-C(6)	-176.09(17)
C(3)-C(4)-C(5)-N	-1.2(3)
C(3)-C(4)-C(5)-C(6)	175.48(18)
N-C(5)-C(6)-P	81.79(16)
C(4)-C(5)-C(6)-P	-94.98(18)
O(2)-P-C(6)-C(5)	107.82(13)
C(15)-P-C(6)-C(5)	-126.99(12)
C(7)-P-C(6)-C(5)	-12.42(14)
O(2)-P-C(7)-C(12)	154.06(15)
C(15)-P-C(7)-C(12)	32.34(17)
C(6)-P-C(7)-C(12)	-84.42(16)
O(2)-P-C(7)-C(8)	-26.37(15)
C(15)-P-C(7)-C(8)	-148.09(13)
C(6)-P-C(7)-C(8)	95.15(14)
C(12)-C(7)-C(8)-C(9)	1.0(3)
P-C(7)-C(8)-C(9)	-178.64(14)
C(7)-C(8)-C(9)-C(10)	-0.2(3)
C(7)-C(8)-C(9)-C(13)	178.24(18)
C(8)-C(9)-C(10)-C(11)	-0.4(3)
C(13)-C(9)-C(10)-C(11)	-178.9(2)
C(9)-C(10)-C(11)-C(12)	0.3(3)
C(9)-C(10)-C(11)-C(14)	178.6(2)
C(8)-C(7)-C(12)-C(11)	-1.0(3)
P-C(7)-C(12)-C(11)	178.52(14)
C(10)-C(11)-C(12)-C(7)	0.4(3)
C(14)-C(11)-C(12)-C(7)	-177.9(2)

C(10)-C(9)-C(13)-F(1)	81.0(3)
C(8)-C(9)-C(13)-F(1)	-97.5(3)
C(10)-C(9)-C(13)-F(3)	-157.7(2)
C(8)-C(9)-C(13)-F(3)	23.8(3)
C(10)-C(9)-C(13)-F(2)	-38.1(3)
C(8)-C(9)-C(13)-F(2)	143.4(2)
C(10)-C(11)-C(14)-F(6)	-71.9(3)
C(12)-C(11)-C(14)-F(6)	106.4(3)
C(10)-C(11)-C(14)-F(4)	164.4(3)
C(12)-C(11)-C(14)-F(4)	-17.3(4)
C(10)-C(11)-C(14)-F(5)	44.8(3)
C(12)-C(11)-C(14)-F(5)	-136.9(2)
O(2)-P-C(15)-C(16)	169.17(13)
C(7)-P-C(15)-C(16)	-70.89(15)
C(6)-P-C(15)-C(16)	44.42(16)
O(2)-P-C(15)-C(20)	-15.69(16)
C(7)-P-C(15)-C(20)	104.25(14)
C(6)-P-C(15)-C(20)	-140.45(13)
C(20)-C(15)-C(16)-C(17)	-0.9(3)
P-C(15)-C(16)-C(17)	174.09(14)
C(15)-C(16)-C(17)-C(18)	1.9(3)
C(15)-C(16)-C(17)-C(21)	-174.02(17)
C(16)-C(17)-C(18)-C(19)	-1.0(3)
C(21)-C(17)-C(18)-C(19)	174.84(19)
C(17)-C(18)-C(19)-C(20)	-0.9(3)
C(17)-C(18)-C(19)-C(22)	-177.8(2)
C(18)-C(19)-C(20)-C(15)	1.8(3)
C(22)-C(19)-C(20)-C(15)	178.7(2)
C(16)-C(15)-C(20)-C(19)	-0.9(3)
P-C(15)-C(20)-C(19)	-176.10(14)
C(18)-C(17)-C(21)-F(9)	-87.3(4)
C(16)-C(17)-C(21)-F(9)	88.6(4)
C(18)-C(17)-C(21)-F(7A)	-2.5(5)
C(16)-C(17)-C(21)-F(7A)	173.4(4)
C(18)-C(17)-C(21)-F(7)	141.8(6)
C(16)-C(17)-C(21)-F(7)	-42.3(7)

C(18)-C(17)-C(21)-F(9A)	131.6(7)
C(16)-C(17)-C(21)-F(9A)	-52.5(7)
C(18)-C(17)-C(21)-F(8)	30.5(4)
C(16)-C(17)-C(21)-F(8)	-153.6(3)
C(18)-C(17)-C(21)-F(8A)	-117.9(4)
C(16)-C(17)-C(21)-F(8A)	58.0(4)
C(18)-C(19)-C(22)-F(10A)	77.2(11)
C(20)-C(19)-C(22)-F(10A)	-99.8(11)
C(18)-C(19)-C(22)-F(10)	-136.9(4)
C(20)-C(19)-C(22)-F(10)	46.1(5)
C(18)-C(19)-C(22)-F(11)	-7.1(5)
C(20)-C(19)-C(22)-F(11)	175.9(4)
C(18)-C(19)-C(22)-F(11A)	-150.7(5)
C(20)-C(19)-C(22)-F(11A)	32.2(6)
C(18)-C(19)-C(22)-F(12)	107.6(4)
C(20)-C(19)-C(22)-F(12)	-69.4(4)
C(18)-C(19)-C(22)-F(12A)	-50.9(6)
C(20)-C(19)-C(22)-F(12A)	132.0(5)

Table 7. Possible Hydrogen bonds for rpsl22 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(4)-H(4)...O(2)#1	0.94	2.40	3.240(2)	147.9
C(6)-H(6A)...O(2)#2	0.98	2.52	3.334(2)	140.7
C(6)-H(6B)...O(2)#1	0.98	2.50	3.380(2)	149.1
C(8)-H(8)...O(2)	0.94	2.59	2.992(2)	105.9
C(12)-H(12)...O(1)	0.94	2.58	2.936(2)	102.8
C(16)-H(16)...O(1)	0.94	2.31	3.163(2)	151.4
C(20)-H(20)...O(1)#3	0.94	2.47	3.314(2)	149.9

Symmetry transformations used to generate equivalent atoms:

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

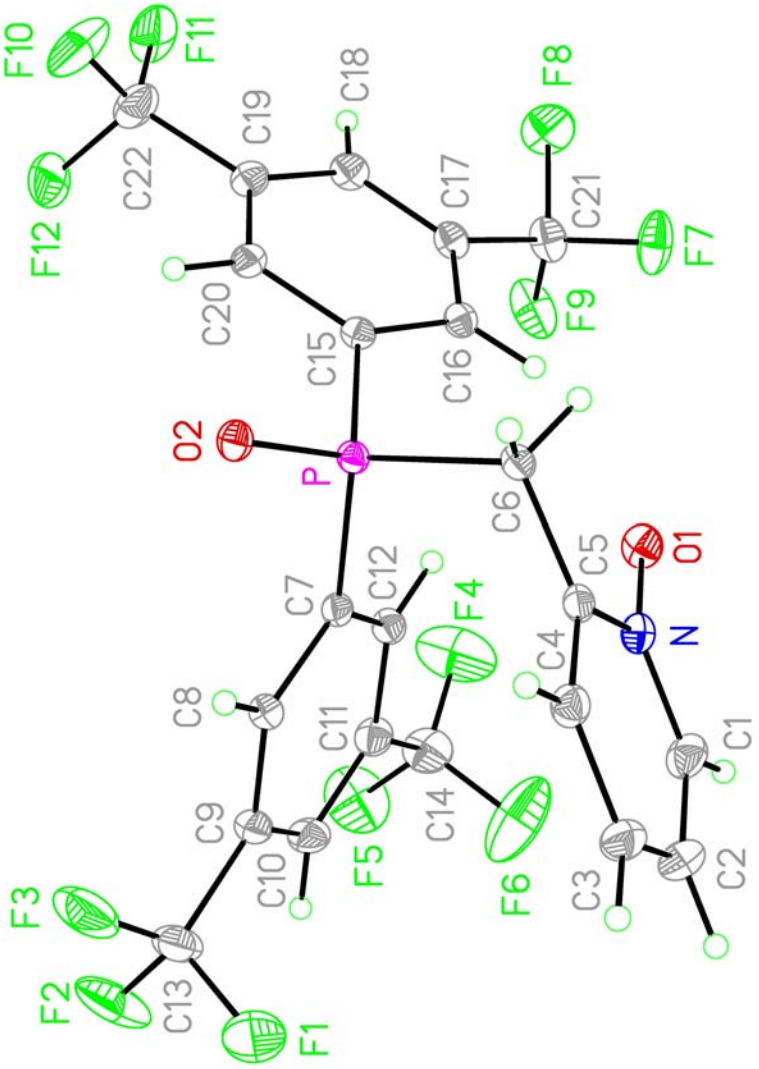


Figure 1. rpsl22l1.jpg, Single molecule view, 20% thermal displacement ellipsoids 20%, rpsl22l1b.jpg=b/w only major disorder part is shown. F7-F9 [51% occupancy] and F10-F12[63% occupancy].

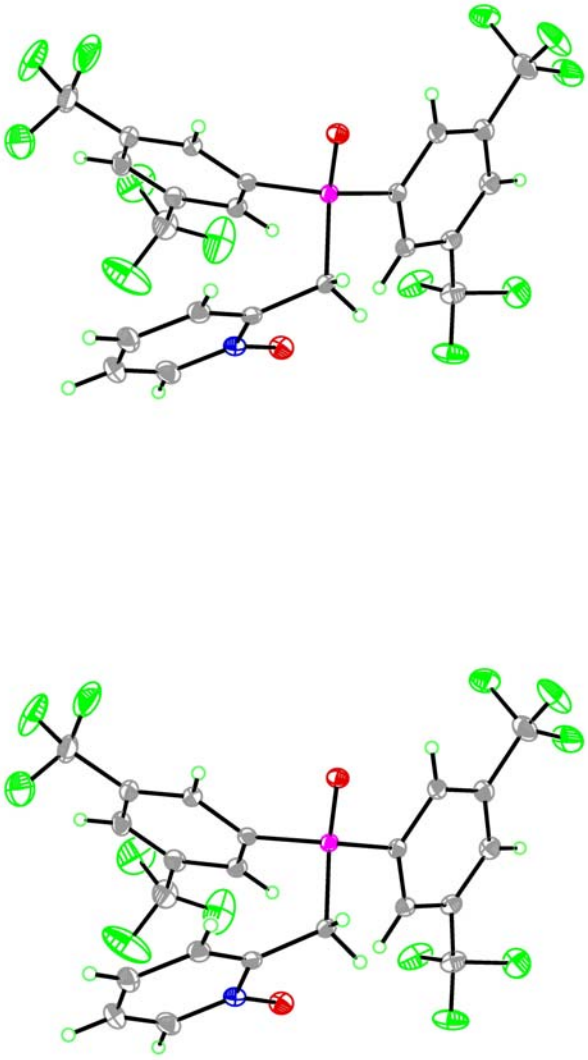


Figure 4.rpsl22s1.jpg also rpsl22s1b.jpg[b/w], stereoview of rpsl22l1.

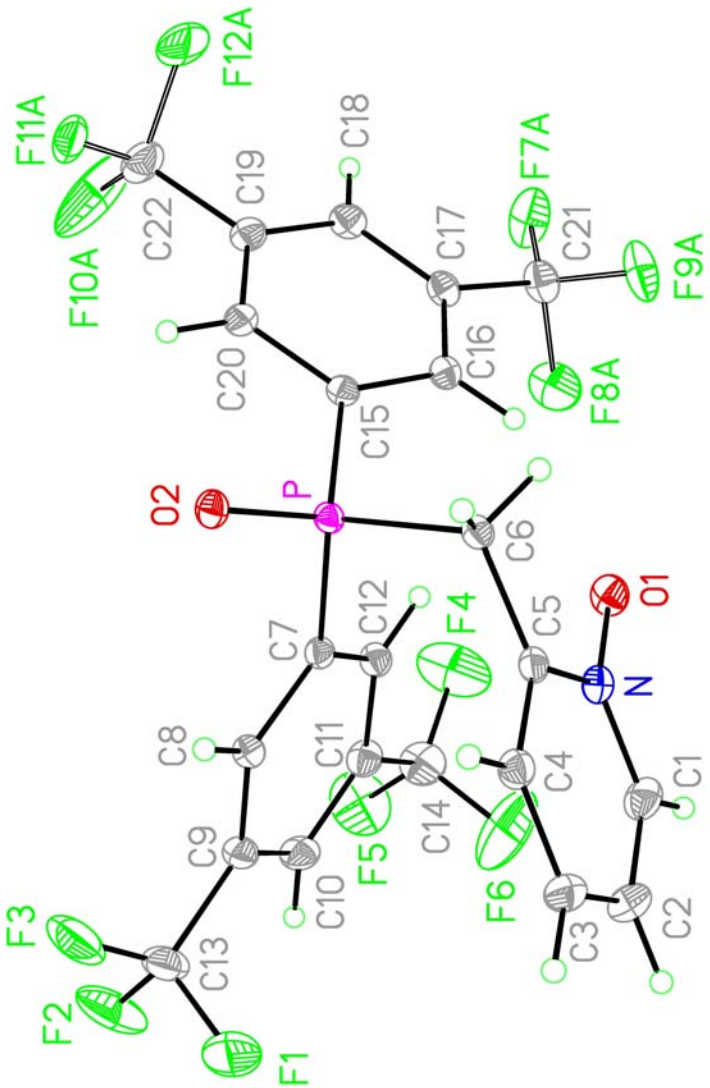


Figure 3 rpsl22l2.jpg molecule showing minor disorder postions: F7a-F9a [49% occupancy], F10a-F12a [37% occupancy].

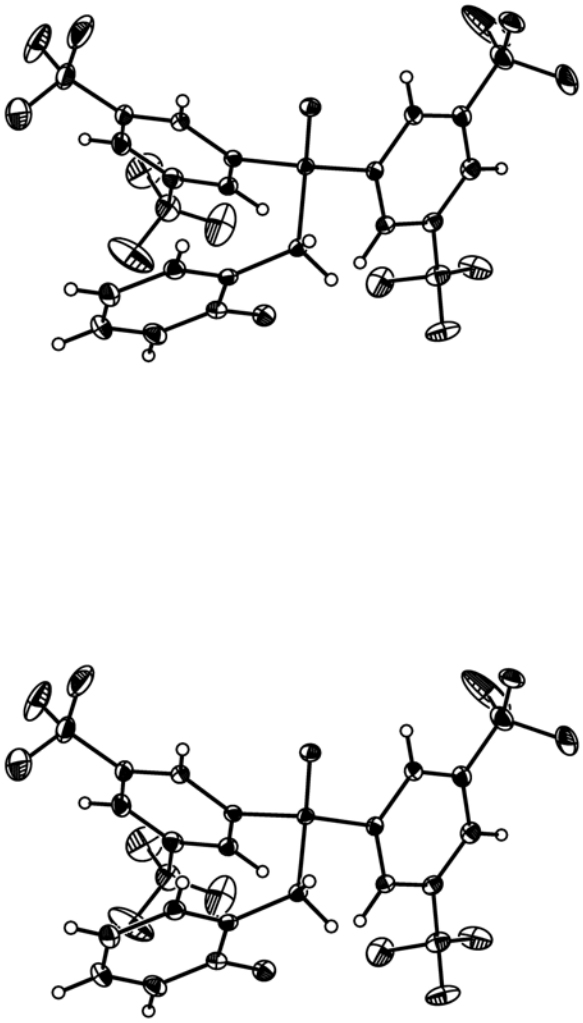


Figure 4. rpsl22s2b.jpg stereoview molecule showing minor disorder positions, b/w only

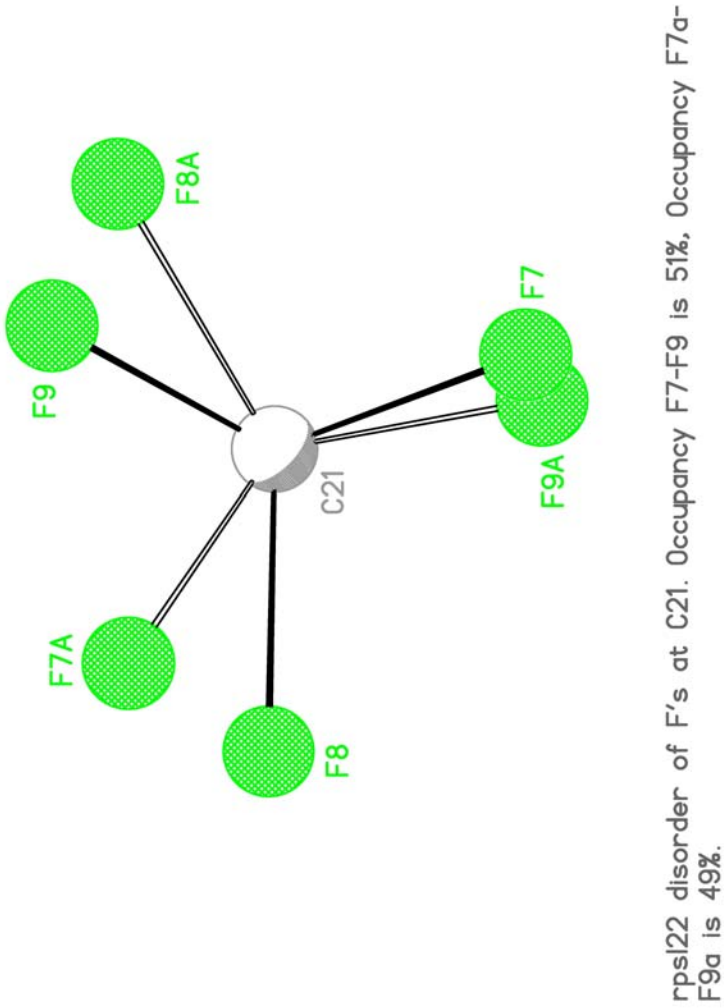


Figure 5. rpsl22c21p.jpg [rpsl22c21.jpg no notes] superposition of F's about C21

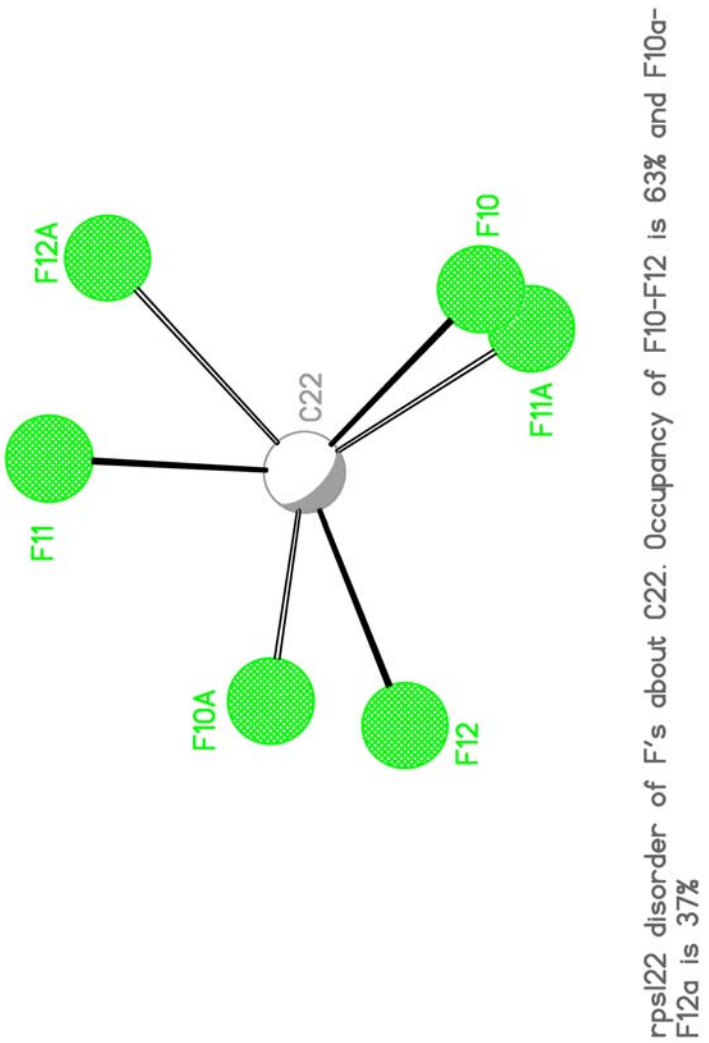


Figure 6. rpsl22c22p.jpg [rpsl22c22.jpg no notes] superposition of F's about C22

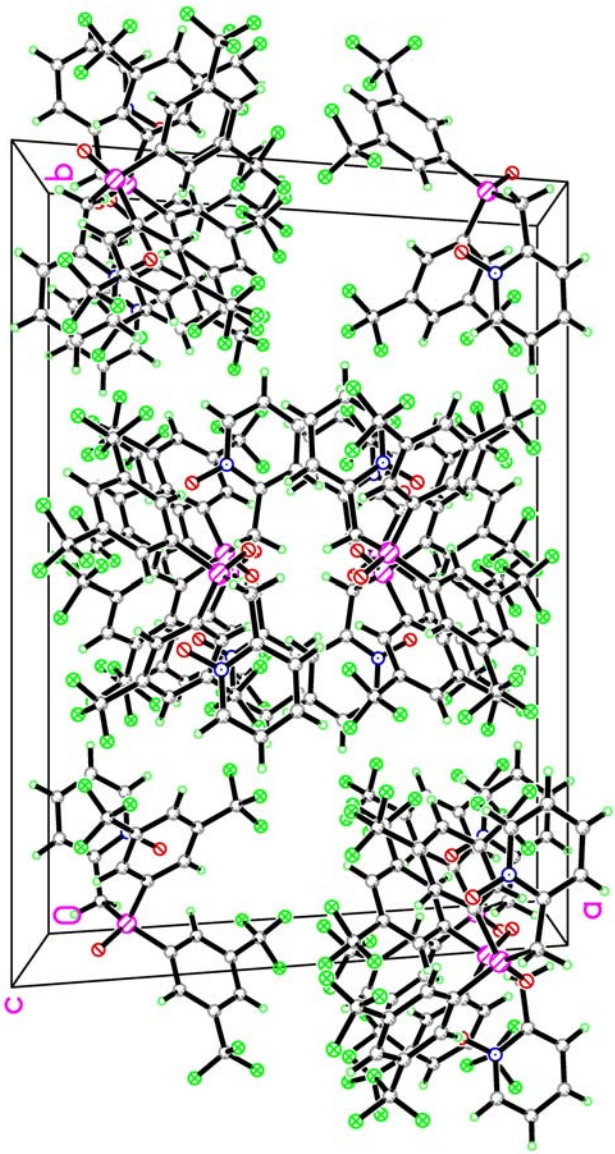


Figure 7.rpsl22cl.jpg packing view down c-axis, color, also rpsl22clb.jpg b/w, only major disorder positions shown

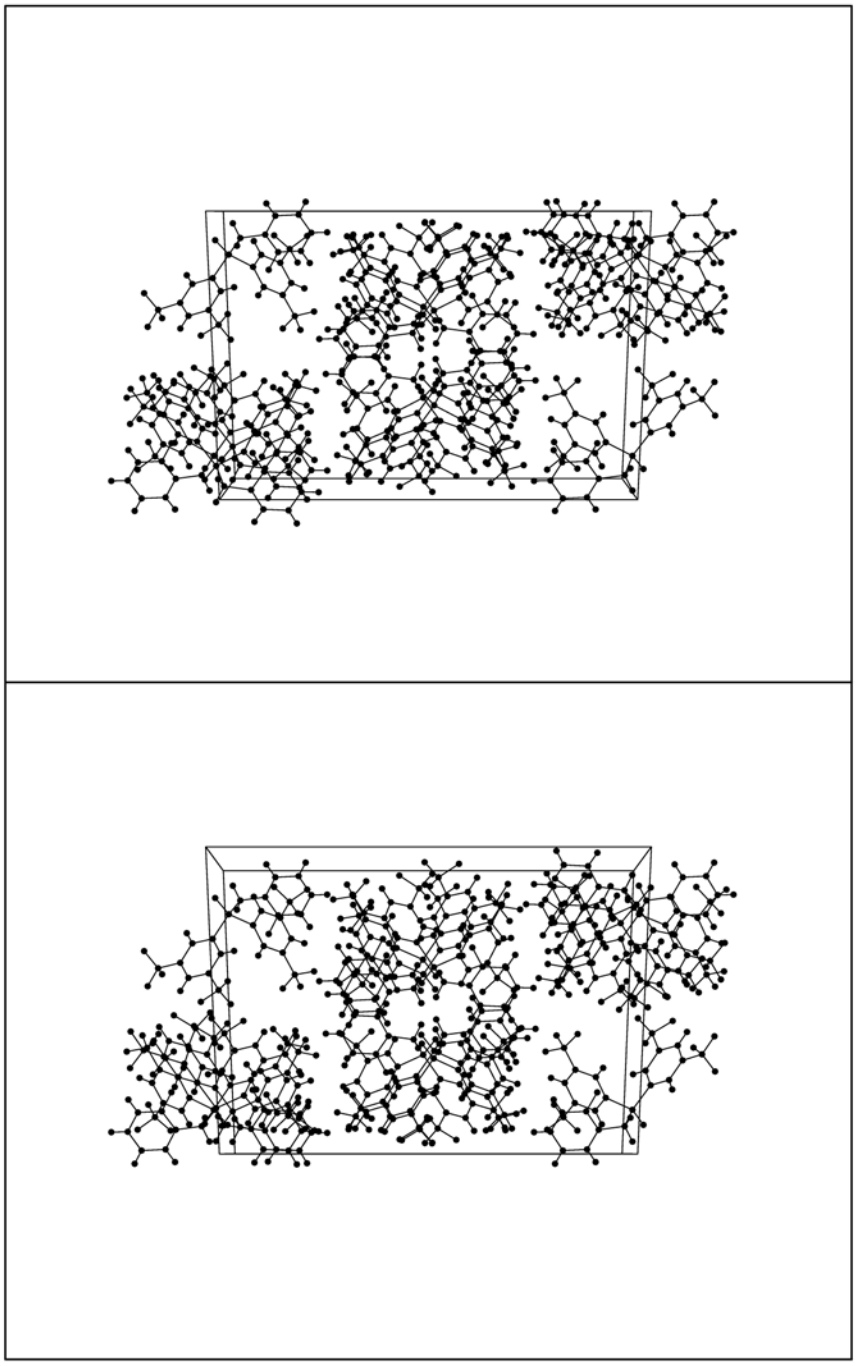


Figure 8. rpsl22cs.jpg stereoview packing, down c-axis, only major disorder positions shown

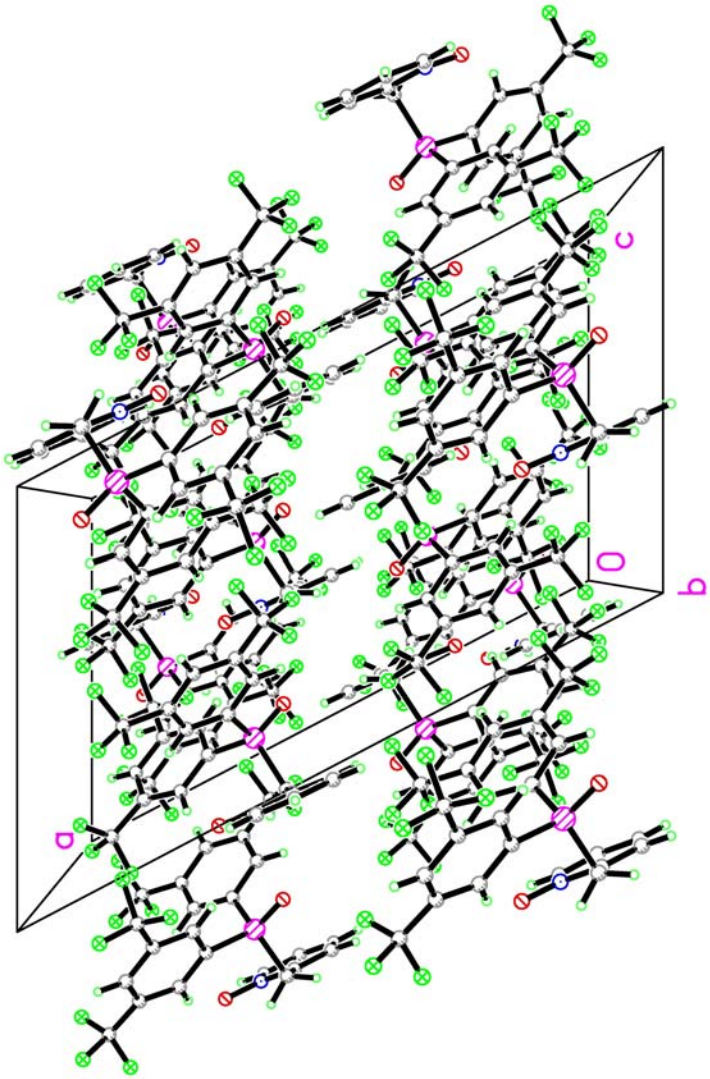


Figure 9.rpsl22bl.jpg packing view down b-axis, color, also rpsl22blb.jpg b/w, also see rpsl22bs.jpg only major disorder position shown

Electronic Supplementary Information for Dalton Transactions

X-ray Crystallographic data for [Yb(**1c**)$(NO_3)_3$(DMF)](DMF)$(H_2O)_{½}$.

Crystal Structure Report

Prepared for:

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Compound: **rpec17/SLP.12.10.Yb1.1**

[C22 H14 F6 N O2 P]Yb[NO3]3[C3H7NO]2,0.5H2O

Prepared by:

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277-6649

Issue date:

June 27 2007

Rpec17l1.jpg,$287=225+2[61-30]

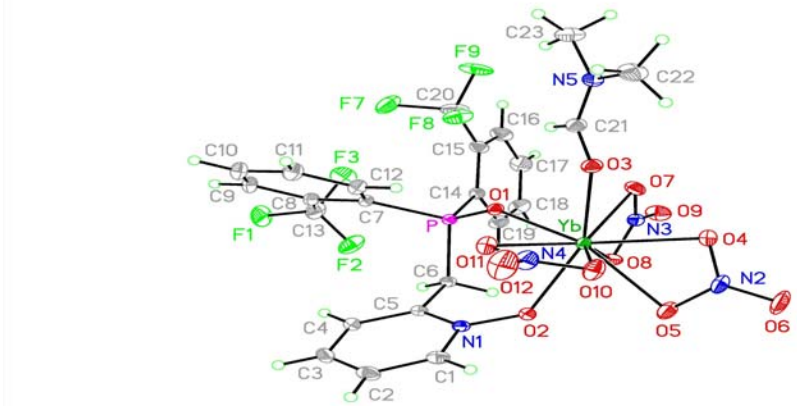


Table 1. Crystal data and structure refinement for rpec17.

Identification code	rpec17	
Empirical formula	C26 H29 F6 N6 O13.50 P Yb	
Formula weight	959.56	
Temperature	225(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.2303(17) Å	α= 90°.
	b = 13.5964(8) Å	β= 124.507(2)°.
	c = 21.6915(12) Å	γ = 90°.
Volume	7104.0(7) $Å^3$	
Z	8	
Density (calculated)	1.794 Mg/m^3	
Absorption coefficient	2.781 mm^{-1}	
F(000)	3792	
Crystal size	0.13 x 0.12 x 0.09 mm^3	
Theta range for data collection	2.59 to 32.70°.	
Index ranges	-44<=h<=41, -20<=k<=18, -32<=l<=32	
Reflections collected	100265	
Independent reflections	13060 [R(int) = 0.0336]	
Completeness to theta = 32.70°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.780 and 0.720	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13060 / 0 / 554	
Goodness-of-fit on F^2	1.010	
Final R indices [I>2sigma(I)]	R1 = 0.0204, wR2 = 0.0463	
R indices (all data)	R1 = 0.0293, wR2 = 0.0500	
Largest diff. peak and hole	0.882 and -0.340 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rpec17. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Yb	7449(1)	9874(1)	9302(1)	24(1)
P	6649(1)	9358(1)	10027(1)	24(1)
O(1)	6851(1)	9947(1)	9640(1)	28(1)
O(2)	7944(1)	8928(1)	10342(1)	31(1)
O(3)	7040(1)	11297(1)	8707(1)	37(1)
O(4)	7570(1)	9881(1)	8292(1)	53(1)
O(5)	8068(1)	8868(1)	9178(1)	50(1)
O(6)	8145(1)	8946(2)	8244(1)	83(1)
O(7)	6534(1)	9421(1)	8150(1)	41(1)
O(8)	7028(1)	8273(1)	8921(1)	39(1)
O(9)	6251(1)	7914(1)	7876(1)	52(1)
O(10)	8247(1)	10862(1)	9713(1)	48(1)
O(11)	7870(1)	11080(1)	10310(1)	43(1)
O(12)	8554(1)	12014(1)	10544(1)	79(1)
N(1)	8068(1)	9063(1)	11029(1)	27(1)
N(2)	7933(1)	9223(1)	8559(1)	44(1)
N(3)	6590(1)	8517(1)	8300(1)	31(1)
N(4)	8234(1)	11340(1)	10205(1)	46(1)
N(5)	6321(1)	12318(1)	7986(1)	38(1)
C(1)	8581(1)	9393(1)	11564(1)	37(1)
C(2)	8740(1)	9510(1)	12289(1)	45(1)
C(3)	8368(1)	9301(1)	12466(1)	45(1)
C(4)	7846(1)	8962(1)	11914(1)	38(1)
C(5)	7697(1)	8825(1)	11189(1)	27(1)
C(6)	7153(1)	8406(1)	10581(1)	27(1)
C(7)	6611(1)	10179(1)	10661(1)	30(1)
C(8)	6395(1)	9988(1)	11086(1)	39(1)
C(9)	6420(1)	10722(2)	11554(1)	54(1)
C(10)	6650(1)	11620(2)	11606(1)	59(1)
C(11)	6864(1)	11817(2)	11196(1)	52(1)
C(12)	6843(1)	11097(1)	10727(1)	39(1)

C(13)	6119(1)	9044(2)	11052(2)	58(1)
F(1)	6049(2)	8929(6)	11596(3)	77(1)
F(2)	6351(1)	8248(2)	11008(2)	68(1)
F(3)	5585(1)	8985(2)	10402(2)	70(1)
F(4)	6639(5)	8430(9)	11611(11)	154(6)
F(5)	5972(11)	8553(11)	10597(8)	170(9)
F(6)	5954(7)	9030(20)	11472(13)	83(6)
C(14)	5999(1)	8736(1)	9372(1)	30(1)
C(15)	5480(1)	9198(1)	8880(1)	38(1)
C(16)	5018(1)	8637(2)	8389(1)	53(1)
C(17)	5051(1)	7632(2)	8366(1)	57(1)
C(18)	5548(1)	7169(2)	8838(1)	53(1)
C(19)	6018(1)	7718(1)	9331(1)	41(1)
C(20)	5389(1)	10285(2)	8877(2)	58(1)
F(7)	5305(1)	10538(2)	9436(2)	73(1)
F(8)	5817(2)	10841(4)	9067(3)	60(1)
F(9)	4949(1)	10623(2)	8273(2)	84(1)
F(10)	5296(6)	10507(6)	8096(4)	132(4)
F(11)	4964(5)	10479(7)	8723(12)	149(7)
F(12)	5791(6)	10809(10)	9200(9)	69(4)
C(21)	6554(1)	11556(1)	8426(1)	38(1)
C(22)	6635(1)	12935(2)	7816(2)	61(1)
C(23)	5757(1)	12610(2)	7702(2)	62(1)
O(13)	5052(1)	4489(2)	6343(1)	110(1)
N(6)	4896(1)	3658(2)	5349(1)	79(1)
C(24)	4757(1)	4015(3)	5782(2)	86(1)
C(25)	5441(2)	3826(3)	5522(2)	110(1)
C(26)	4515(2)	3075(4)	4690(3)	160(2)
O(14)	5000	5257(19)	7500	72(15)
O(15)	4836(17)	5123(14)	7270(20)	87(7)

Table 3. Bond lengths [Å] and angles [°] for rpec17.

Yb-O(1)	2.2499(11)
Yb-O(3)	2.2575(11)
Yb-O(2)	2.2660(11)
Yb-O(10)	2.3831(13)
Yb-O(5)	2.3997(13)
Yb-O(8)	2.4055(12)
Yb-O(4)	2.4079(14)
Yb-O(11)	2.4362(13)
Yb-O(7)	2.4908(13)
P-O(1)	1.5016(11)
P-C(6)	1.8123(14)
P-C(14)	1.8127(17)
P-C(7)	1.8236(16)
O(2)-N(1)	1.3318(16)
O(3)-C(21)	1.238(2)
O(4)-N(2)	1.252(2)
O(5)-N(2)	1.262(2)
O(6)-N(2)	1.2145(19)
O(7)-N(3)	1.2591(18)
O(8)-N(3)	1.2682(17)
O(9)-N(3)	1.2118(19)
O(10)-N(4)	1.267(2)
O(11)-N(4)	1.261(2)
O(12)-N(4)	1.215(2)
N(1)-C(1)	1.351(2)
N(1)-C(5)	1.353(2)
N(5)-C(21)	1.308(2)
N(5)-C(22)	1.439(3)
N(5)-C(23)	1.450(3)
C(1)-C(2)	1.374(3)
C(1)-H(1)	0.9400
C(2)-C(3)	1.373(3)
C(2)-H(2)	0.9400
C(3)-C(4)	1.381(3)

C(3)-H(3)	0.9400
C(4)-C(5)	1.386(2)
C(4)-H(4)	0.9400
C(5)-C(6)	1.489(2)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(7)-C(12)	1.388(2)
C(7)-C(8)	1.407(2)
C(8)-C(9)	1.395(3)
C(8)-C(13)	1.495(3)
C(9)-C(10)	1.368(4)
C(9)-H(9)	0.9400
C(10)-C(11)	1.372(3)
C(10)-H(10)	0.9400
C(11)-C(12)	1.388(3)
C(11)-H(11)	0.9400
C(12)-H(12)	0.9400
C(13)-F(5)	1.060(10)
C(13)-F(6)	1.249(16)
C(13)-F(2)	1.310(3)
C(13)-F(1)	1.316(5)
C(13)-F(3)	1.391(4)
C(13)-F(4)	1.547(11)
C(14)-C(19)	1.390(2)
C(14)-C(15)	1.414(2)
C(15)-C(16)	1.383(3)
C(15)-C(20)	1.501(3)
C(16)-C(17)	1.372(3)
C(16)-H(16)	0.9400
C(17)-C(18)	1.368(3)
C(17)-H(17)	0.9400
C(18)-C(19)	1.386(3)
C(18)-H(18)	0.9400
C(19)-H(19)	0.9400
C(20)-F(11)	1.119(7)
C(20)-F(12)	1.203(14)

C(20)-F(9)	1.293(3)
C(20)-F(8)	1.312(5)
C(20)-F(7)	1.408(4)
C(20)-F(10)	1.585(8)
C(21)-H(21)	0.9400
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(22)-H(22C)	0.9700
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(23)-H(23C)	0.9700
O(13)-C(24)	1.206(4)
N(6)-C(24)	1.309(4)
N(6)-C(25)	1.433(4)
N(6)-C(26)	1.452(4)
C(24)-H(24)	0.9400
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(25)-H(25C)	0.9700
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(26)-H(26C)	0.9700
O(14)-H(1W)	0.94(5)
O(15)-H(1W)	0.72(6)

O(1)-Yb-O(3)	83.72(4)
O(1)-Yb-O(2)	82.88(4)
O(3)-Yb-O(2)	152.69(4)
O(1)-Yb-O(10)	129.01(4)
O(3)-Yb-O(10)	79.63(5)
O(2)-Yb-O(10)	90.59(5)
O(1)-Yb-O(5)	146.67(4)
O(3)-Yb-O(5)	127.84(4)
O(2)-Yb-O(5)	72.04(4)
O(10)-Yb-O(5)	73.99(5)
O(1)-Yb-O(8)	79.11(4)

O(3)-Yb-O(8)	125.22(4)
O(2)-Yb-O(8)	75.08(4)
O(10)-Yb-O(8)	147.21(5)
O(5)-Yb-O(8)	73.56(5)
O(1)-Yb-O(4)	146.92(5)
O(3)-Yb-O(4)	77.23(5)
O(2)-Yb-O(4)	124.63(4)
O(10)-Yb-O(4)	73.86(5)
O(5)-Yb-O(4)	52.63(5)
O(8)-Yb-O(4)	90.05(5)
O(1)-Yb-O(11)	76.54(4)
O(3)-Yb-O(11)	76.76(5)
O(2)-Yb-O(11)	77.03(5)
O(10)-Yb-O(11)	52.83(4)
O(5)-Yb-O(11)	117.09(5)
O(8)-Yb-O(11)	144.82(4)
O(4)-Yb-O(11)	123.69(5)
O(1)-Yb-O(7)	75.32(4)
O(3)-Yb-O(7)	73.60(4)
O(2)-Yb-O(7)	125.12(4)
O(10)-Yb-O(7)	141.40(5)
O(5)-Yb-O(7)	101.29(5)
O(8)-Yb-O(7)	51.80(4)
O(4)-Yb-O(7)	73.47(5)
O(11)-Yb-O(7)	140.85(4)
O(1)-P-C(6)	108.82(7)
O(1)-P-C(14)	112.37(7)
C(6)-P-C(14)	106.51(7)
O(1)-P-C(7)	107.80(7)
C(6)-P-C(7)	108.10(7)
C(14)-P-C(7)	113.10(7)
P-O(1)-Yb	141.54(6)
N(1)-O(2)-Yb	130.63(9)
C(21)-O(3)-Yb	127.86(11)
N(2)-O(4)-Yb	95.65(11)
N(2)-O(5)-Yb	95.76(10)

N(3)-O(7)-Yb	94.26(9)
N(3)-O(8)-Yb	98.10(9)
N(4)-O(10)-Yb	96.62(10)
N(4)-O(11)-Yb	94.27(10)
O(2)-N(1)-C(1)	118.26(14)
O(2)-N(1)-C(5)	120.32(12)
C(1)-N(1)-C(5)	121.33(14)
O(6)-N(2)-O(4)	122.06(18)
O(6)-N(2)-O(5)	121.99(18)
O(4)-N(2)-O(5)	115.95(14)
O(9)-N(3)-O(7)	122.30(14)
O(9)-N(3)-O(8)	121.95(15)
O(7)-N(3)-O(8)	115.74(14)
O(12)-N(4)-O(11)	122.76(18)
O(12)-N(4)-O(10)	121.19(18)
O(11)-N(4)-O(10)	116.05(15)
C(21)-N(5)-C(22)	120.33(17)
C(21)-N(5)-C(23)	121.59(17)
C(22)-N(5)-C(23)	117.91(17)
N(1)-C(1)-C(2)	120.86(17)
N(1)-C(1)-H(1)	119.6
C(2)-C(1)-H(1)	119.6
C(3)-C(2)-C(1)	119.29(17)
C(3)-C(2)-H(2)	120.4
C(1)-C(2)-H(2)	120.4
C(2)-C(3)-C(4)	119.22(17)
C(2)-C(3)-H(3)	120.4
C(4)-C(3)-H(3)	120.4
C(3)-C(4)-C(5)	120.71(17)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
N(1)-C(5)-C(4)	118.55(15)
N(1)-C(5)-C(6)	118.29(13)
C(4)-C(5)-C(6)	123.14(15)
C(5)-C(6)-P	111.89(10)
C(5)-C(6)-H(6A)	109.2

P-C(6)-H(6A)	109.2
C(5)-C(6)-H(6B)	109.2
P-C(6)-H(6B)	109.2
H(6A)-C(6)-H(6B)	107.9
C(12)-C(7)-C(8)	118.27(16)
C(12)-C(7)-P	113.14(12)
C(8)-C(7)-P	128.57(14)
C(9)-C(8)-C(7)	119.15(19)
C(9)-C(8)-C(13)	117.05(18)
C(7)-C(8)-C(13)	123.77(17)
C(10)-C(9)-C(8)	121.2(2)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(9)-C(10)-C(11)	120.32(19)
C(9)-C(10)-H(10)	119.8
C(11)-C(10)-H(10)	119.8
C(10)-C(11)-C(12)	119.4(2)
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.3
C(7)-C(12)-C(11)	121.66(18)
C(7)-C(12)-H(12)	119.2
C(11)-C(12)-H(12)	119.2
F(5)-C(13)-F(6)	123.5(15)
F(5)-C(13)-F(2)	50.5(14)
F(6)-C(13)-F(2)	118.2(12)
F(5)-C(13)-F(1)	125.0(7)
F(6)-C(13)-F(1)	12.7(12)
F(2)-C(13)-F(1)	108.5(4)
F(5)-C(13)-F(3)	52.5(15)
F(6)-C(13)-F(3)	93.7(10)
F(2)-C(13)-F(3)	102.0(3)
F(1)-C(13)-F(3)	104.4(3)
F(5)-C(13)-C(8)	120.7(5)
F(6)-C(13)-C(8)	113.2(13)
F(2)-C(13)-C(8)	115.2(2)
F(1)-C(13)-C(8)	114.2(4)

F(3)-C(13)-C(8)	111.4(2)
F(5)-C(13)-F(4)	95.1(14)
F(6)-C(13)-F(4)	92.0(12)
F(2)-C(13)-F(4)	44.8(7)
F(1)-C(13)-F(4)	79.4(7)
F(3)-C(13)-F(4)	143.5(7)
C(8)-C(13)-F(4)	99.2(5)
C(19)-C(14)-C(15)	117.34(16)
C(19)-C(14)-P	116.89(12)
C(15)-C(14)-P	125.72(14)
C(16)-C(15)-C(14)	119.88(18)
C(16)-C(15)-C(20)	116.48(18)
C(14)-C(15)-C(20)	123.58(17)
C(17)-C(16)-C(15)	121.23(19)
C(17)-C(16)-H(16)	119.4
C(15)-C(16)-H(16)	119.4
C(18)-C(17)-C(16)	119.9(2)
C(18)-C(17)-H(17)	120.0
C(16)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	119.8(2)
C(17)-C(18)-H(18)	120.1
C(19)-C(18)-H(18)	120.1
C(18)-C(19)-C(14)	121.80(18)
C(18)-C(19)-H(19)	119.1
C(14)-C(19)-H(19)	119.1
F(11)-C(20)-F(12)	126.0(10)
F(11)-C(20)-F(9)	46.9(10)
F(12)-C(20)-F(9)	117.5(8)
F(11)-C(20)-F(8)	131.1(6)
F(12)-C(20)-F(8)	14.7(10)
F(9)-C(20)-F(8)	109.7(4)
F(11)-C(20)-F(7)	59.7(11)
F(12)-C(20)-F(7)	86.7(8)
F(9)-C(20)-F(7)	103.2(2)
F(8)-C(20)-F(7)	100.8(3)
F(11)-C(20)-C(15)	113.4(6)

F(12)-C(20)-C(15)	117.8(7)
F(9)-C(20)-C(15)	115.3(3)
F(8)-C(20)-C(15)	115.5(3)
F(7)-C(20)-C(15)	110.7(2)
F(11)-C(20)-F(10)	98.4(11)
F(12)-C(20)-F(10)	91.7(9)
F(9)-C(20)-F(10)	51.6(5)
F(8)-C(20)-F(10)	77.4(5)
F(7)-C(20)-F(10)	149.9(5)
C(15)-C(20)-F(10)	96.6(4)
O(3)-C(21)-N(5)	124.18(17)
O(3)-C(21)-H(21)	117.9
N(5)-C(21)-H(21)	117.9
N(5)-C(22)-H(22A)	109.5
N(5)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(5)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(5)-C(23)-H(23A)	109.5
N(5)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
N(5)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(24)-N(6)-C(25)	120.2(3)
C(24)-N(6)-C(26)	122.1(3)
C(25)-N(6)-C(26)	117.7(3)
O(13)-C(24)-N(6)	126.0(3)
O(13)-C(24)-H(24)	117.0
N(6)-C(24)-H(24)	117.0
N(6)-C(25)-H(25A)	109.5
N(6)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
N(6)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5

H(25B)-C(25)-H(25C)	109.5
N(6)-C(26)-H(26A)	109.5
N(6)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
N(6)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rpec17. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Yb	26(1)	25(1)	27(1)	3(1)	18(1)	3(1)
P	22(1)	28(1)	25(1)	4(1)	15(1)	5(1)
O(1)	30(1)	31(1)	32(1)	7(1)	22(1)	7(1)
O(2)	30(1)	37(1)	27(1)	5(1)	17(1)	7(1)
O(3)	43(1)	30(1)	46(1)	9(1)	29(1)	8(1)
O(4)	58(1)	72(1)	41(1)	11(1)	35(1)	22(1)
O(5)	71(1)	40(1)	70(1)	15(1)	58(1)	18(1)
O(6)	118(2)	88(1)	104(2)	13(1)	100(1)	30(1)
O(7)	49(1)	34(1)	31(1)	7(1)	18(1)	5(1)
O(8)	31(1)	32(1)	34(1)	1(1)	7(1)	6(1)
O(9)	39(1)	44(1)	47(1)	-9(1)	8(1)	-8(1)
O(10)	46(1)	51(1)	59(1)	-19(1)	38(1)	-15(1)
O(11)	50(1)	42(1)	46(1)	-5(1)	32(1)	-3(1)
O(12)	81(1)	72(1)	93(1)	-47(1)	54(1)	-43(1)
N(1)	24(1)	27(1)	27(1)	3(1)	12(1)	4(1)
N(2)	55(1)	43(1)	58(1)	-3(1)	46(1)	1(1)
N(3)	28(1)	34(1)	29(1)	0(1)	15(1)	3(1)
N(4)	46(1)	41(1)	49(1)	-12(1)	27(1)	-9(1)
N(5)	45(1)	30(1)	39(1)	8(1)	24(1)	7(1)
C(1)	26(1)	35(1)	41(1)	2(1)	14(1)	1(1)
C(2)	36(1)	37(1)	36(1)	-6(1)	6(1)	1(1)
C(3)	51(1)	44(1)	26(1)	-3(1)	14(1)	10(1)
C(4)	40(1)	43(1)	29(1)	6(1)	20(1)	12(1)
C(5)	26(1)	28(1)	26(1)	5(1)	13(1)	7(1)
C(6)	24(1)	28(1)	28(1)	5(1)	14(1)	4(1)
C(7)	28(1)	36(1)	27(1)	4(1)	17(1)	9(1)
C(8)	43(1)	49(1)	33(1)	9(1)	27(1)	15(1)
C(9)	69(1)	70(2)	38(1)	4(1)	39(1)	19(1)
C(10)	75(2)	59(1)	41(1)	-10(1)	32(1)	14(1)
C(11)	61(1)	45(1)	49(1)	-10(1)	29(1)	1(1)
C(12)	42(1)	38(1)	40(1)	-2(1)	25(1)	3(1)

C(13)	76(2)	62(1)	69(2)	14(1)	61(1)	11(1)
F(1)	117(3)	87(2)	70(2)	20(2)	78(2)	8(2)
F(2)	86(2)	48(1)	115(3)	12(2)	85(2)	8(1)
F(3)	52(1)	87(2)	72(1)	6(1)	37(1)	-12(1)
F(4)	100(8)	97(8)	279(17)	115(11)	115(10)	40(6)
F(5)	360(30)	110(12)	108(11)	-59(9)	175(17)	-148(15)
F(6)	65(6)	116(12)	121(13)	5(9)	85(8)	-5(6)
C(14)	24(1)	38(1)	28(1)	2(1)	15(1)	3(1)
C(15)	26(1)	50(1)	34(1)	10(1)	15(1)	5(1)
C(16)	27(1)	71(2)	44(1)	7(1)	11(1)	1(1)
C(17)	34(1)	72(2)	50(1)	-15(1)	14(1)	-13(1)
C(18)	39(1)	49(1)	63(1)	-17(1)	24(1)	-7(1)
C(19)	28(1)	41(1)	47(1)	-6(1)	18(1)	3(1)
C(20)	31(1)	56(1)	71(2)	24(1)	19(1)	14(1)
F(7)	89(2)	63(1)	104(2)	8(1)	76(2)	22(1)
F(8)	46(2)	49(2)	93(3)	19(2)	43(2)	11(1)
F(9)	52(2)	77(2)	66(2)	28(1)	-1(1)	28(1)
F(10)	256(13)	60(4)	55(4)	15(3)	72(6)	-20(6)
F(11)	77(7)	65(5)	340(20)	28(11)	140(12)	35(5)
F(12)	63(8)	37(5)	46(4)	-9(3)	-5(4)	25(5)
C(21)	46(1)	30(1)	47(1)	11(1)	31(1)	8(1)
C(22)	71(2)	45(1)	77(2)	27(1)	47(1)	8(1)
C(23)	51(1)	53(1)	74(2)	21(1)	30(1)	19(1)
O(13)	106(2)	136(2)	56(1)	-23(1)	28(1)	-28(2)
N(6)	60(1)	86(2)	67(1)	-10(1)	21(1)	-4(1)
C(24)	64(2)	110(3)	65(2)	-4(2)	26(2)	-15(2)
C(25)	78(2)	115(3)	127(3)	15(3)	52(2)	19(2)
C(26)	119(4)	192(6)	118(4)	-87(4)	37(3)	-31(4)
O(14)	100(50)	48(6)	100(40)	0	70(40)	0
O(15)	74(13)	110(11)	90(17)	34(13)	54(13)	36(12)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rpec17.

	x	y	z	U(eq)
H(1)	8833	9543	11439	44
H(2)	9099	9731	12660	53
H(3)	8468	9388	12958	54
H(4)	7588	8822	12031	45
H(6A)	7009	7985	10802	32
H(6B)	7206	7996	10256	32
H(9)	6276	10597	11839	65
H(10)	6662	12104	11924	71
H(11)	7023	12433	11232	63
H(12)	6990	11234	10447	47
H(16)	4674	8949	8065	63
H(17)	4733	7263	8026	68
H(18)	5571	6480	8828	64
H(19)	6359	7392	9646	49
H(21)	6339	11181	8536	45
H(22A)	6821	13445	8193	92
H(22B)	6387	13236	7329	92
H(22C)	6910	12541	7811	92
H(23A)	5596	12141	7865	93
H(23B)	5538	12628	7160	93
H(23C)	5760	13258	7892	93
H(24)	4394	3889	5642	103
H(25A)	5660	4188	5988	164
H(25B)	5414	4203	5123	164
H(25C)	5618	3200	5572	164
H(26A)	4689	2455	4715	239
H(26B)	4420	3431	4245	239
H(26C)	4180	2948	4670	239
H(1W)	4970(20)	4890(30)	7110(30)	105(18)

Table 6. Torsion angles [°] for rpec17.

C(6)-P-O(1)-Yb	18.78(14)
C(14)-P-O(1)-Yb	-98.92(12)
C(7)-P-O(1)-Yb	135.79(11)
O(3)-Yb-O(1)-P	173.06(12)
O(2)-Yb-O(1)-P	-30.78(12)
O(10)-Yb-O(1)-P	-115.74(12)
O(5)-Yb-O(1)-P	10.13(18)
O(8)-Yb-O(1)-P	45.32(12)
O(4)-Yb-O(1)-P	118.25(12)
O(11)-Yb-O(1)-P	-109.09(12)
O(7)-Yb-O(1)-P	98.41(12)
O(1)-Yb-O(2)-N(1)	-46.24(12)
O(3)-Yb-O(2)-N(1)	14.92(18)
O(10)-Yb-O(2)-N(1)	83.04(12)
O(5)-Yb-O(2)-N(1)	155.99(13)
O(8)-Yb-O(2)-N(1)	-126.81(13)
O(4)-Yb-O(2)-N(1)	153.72(11)
O(11)-Yb-O(2)-N(1)	31.52(12)
O(7)-Yb-O(2)-N(1)	-112.66(12)
O(1)-Yb-O(3)-C(21)	-30.99(15)
O(2)-Yb-O(3)-C(21)	-91.97(18)
O(10)-Yb-O(3)-C(21)	-162.58(16)
O(5)-Yb-O(3)-C(21)	137.23(15)
O(8)-Yb-O(3)-C(21)	40.93(17)
O(4)-Yb-O(3)-C(21)	121.79(16)
O(11)-Yb-O(3)-C(21)	-108.59(16)
O(7)-Yb-O(3)-C(21)	45.52(15)
O(1)-Yb-O(4)-N(2)	-139.01(10)
O(3)-Yb-O(4)-N(2)	164.58(13)
O(2)-Yb-O(4)-N(2)	2.63(14)
O(10)-Yb-O(4)-N(2)	81.86(12)
O(5)-Yb-O(4)-N(2)	-0.08(11)
O(8)-Yb-O(4)-N(2)	-69.18(12)
O(11)-Yb-O(4)-N(2)	100.25(12)

O(7)-Yb-O(4)-N(2)	-118.99(12)
O(1)-Yb-O(5)-N(2)	139.33(11)
O(3)-Yb-O(5)-N(2)	-18.98(14)
O(2)-Yb-O(5)-N(2)	-177.57(13)
O(10)-Yb-O(5)-N(2)	-81.59(12)
O(8)-Yb-O(5)-N(2)	103.18(12)
O(4)-Yb-O(5)-N(2)	0.08(11)
O(11)-Yb-O(5)-N(2)	-113.09(12)
O(7)-Yb-O(5)-N(2)	58.93(12)
O(1)-Yb-O(7)-N(3)	-89.31(9)
O(3)-Yb-O(7)-N(3)	-176.98(10)
O(2)-Yb-O(7)-N(3)	-19.25(11)
O(10)-Yb-O(7)-N(3)	135.05(9)
O(5)-Yb-O(7)-N(3)	56.63(10)
O(8)-Yb-O(7)-N(3)	-1.75(9)
O(4)-Yb-O(7)-N(3)	101.82(10)
O(11)-Yb-O(7)-N(3)	-134.67(9)
O(1)-Yb-O(8)-N(3)	81.56(10)
O(3)-Yb-O(8)-N(3)	7.36(12)
O(2)-Yb-O(8)-N(3)	167.00(10)
O(10)-Yb-O(8)-N(3)	-126.20(10)
O(5)-Yb-O(8)-N(3)	-117.71(10)
O(4)-Yb-O(8)-N(3)	-66.99(10)
O(11)-Yb-O(8)-N(3)	128.37(10)
O(7)-Yb-O(8)-N(3)	1.75(9)
O(1)-Yb-O(10)-N(4)	5.33(14)
O(3)-Yb-O(10)-N(4)	78.40(12)
O(2)-Yb-O(10)-N(4)	-75.96(12)
O(5)-Yb-O(10)-N(4)	-147.08(13)
O(8)-Yb-O(10)-N(4)	-138.61(11)
O(4)-Yb-O(10)-N(4)	157.97(13)
O(11)-Yb-O(10)-N(4)	-2.79(11)
O(7)-Yb-O(10)-N(4)	124.82(12)
O(1)-Yb-O(11)-N(4)	-170.73(12)
O(3)-Yb-O(11)-N(4)	-84.13(11)
O(2)-Yb-O(11)-N(4)	103.61(11)

O(10)-Yb-O(11)-N(4)	2.79(11)
O(5)-Yb-O(11)-N(4)	41.85(12)
O(8)-Yb-O(11)-N(4)	141.87(11)
O(4)-Yb-O(11)-N(4)	-19.58(13)
O(7)-Yb-O(11)-N(4)	-125.69(11)
Yb-O(2)-N(1)-C(1)	-101.26(14)
Yb-O(2)-N(1)-C(5)	82.15(16)
Yb-O(4)-N(2)-O(6)	-179.38(19)
Yb-O(4)-N(2)-O(5)	0.14(18)
Yb-O(5)-N(2)-O(6)	179.38(19)
Yb-O(5)-N(2)-O(4)	-0.14(18)
Yb-O(7)-N(3)-O(9)	-176.33(15)
Yb-O(7)-N(3)-O(8)	2.90(14)
Yb-O(8)-N(3)-O(9)	176.21(14)
Yb-O(8)-N(3)-O(7)	-3.02(15)
Yb-O(11)-N(4)-O(12)	174.7(2)
Yb-O(11)-N(4)-O(10)	-4.65(18)
Yb-O(10)-N(4)-O(12)	-174.59(19)
Yb-O(10)-N(4)-O(11)	4.78(18)
O(2)-N(1)-C(1)-C(2)	-177.51(15)
C(5)-N(1)-C(1)-C(2)	-1.0(2)
N(1)-C(1)-C(2)-C(3)	-0.8(3)
C(1)-C(2)-C(3)-C(4)	1.0(3)
C(2)-C(3)-C(4)-C(5)	0.5(3)
O(2)-N(1)-C(5)-C(4)	178.94(13)
C(1)-N(1)-C(5)-C(4)	2.5(2)
O(2)-N(1)-C(5)-C(6)	0.42(19)
C(1)-N(1)-C(5)-C(6)	-176.07(14)
C(3)-C(4)-C(5)-N(1)	-2.2(2)
C(3)-C(4)-C(5)-C(6)	176.23(16)
N(1)-C(5)-C(6)-P	-86.52(14)
C(4)-C(5)-C(6)-P	95.03(16)
O(1)-P-C(6)-C(5)	63.54(12)
C(14)-P-C(6)-C(5)	-175.10(11)
C(7)-P-C(6)-C(5)	-53.27(13)
O(1)-P-C(7)-C(12)	-8.45(14)

C(6)-P-C(7)-C(12)	109.03(13)
C(14)-P-C(7)-C(12)	-133.30(13)
O(1)-P-C(7)-C(8)	173.23(15)
C(6)-P-C(7)-C(8)	-69.29(17)
C(14)-P-C(7)-C(8)	48.38(18)
C(12)-C(7)-C(8)-C(9)	0.2(3)
P-C(7)-C(8)-C(9)	178.41(15)
C(12)-C(7)-C(8)-C(13)	178.14(19)
P-C(7)-C(8)-C(13)	-3.6(3)
C(7)-C(8)-C(9)-C(10)	0.0(3)
C(13)-C(8)-C(9)-C(10)	-178.1(2)
C(8)-C(9)-C(10)-C(11)	-0.1(4)
C(9)-C(10)-C(11)-C(12)	0.1(4)
C(8)-C(7)-C(12)-C(11)	-0.2(3)
P-C(7)-C(12)-C(11)	-178.69(16)
C(10)-C(11)-C(12)-C(7)	0.0(3)
C(9)-C(8)-C(13)-F(5)	160.6(18)
C(7)-C(8)-C(13)-F(5)	-17.4(18)
C(9)-C(8)-C(13)-F(6)	-1.6(11)
C(7)-C(8)-C(13)-F(6)	-179.6(11)
C(9)-C(8)-C(13)-F(2)	-142.0(3)
C(7)-C(8)-C(13)-F(2)	40.0(4)
C(9)-C(8)-C(13)-F(1)	-15.4(4)
C(7)-C(8)-C(13)-F(1)	166.6(3)
C(9)-C(8)-C(13)-F(3)	102.5(2)
C(7)-C(8)-C(13)-F(3)	-75.5(3)
C(9)-C(8)-C(13)-F(4)	-97.8(8)
C(7)-C(8)-C(13)-F(4)	84.2(8)
O(1)-P-C(14)-C(19)	109.91(14)
C(6)-P-C(14)-C(19)	-9.16(15)
C(7)-P-C(14)-C(19)	-127.76(14)
O(1)-P-C(14)-C(15)	-67.45(16)
C(6)-P-C(14)-C(15)	173.48(14)
C(7)-P-C(14)-C(15)	54.88(16)
C(19)-C(14)-C(15)-C(16)	0.5(3)
P-C(14)-C(15)-C(16)	177.83(15)

C(19)-C(14)-C(15)-C(20)	177.65(19)
P-C(14)-C(15)-C(20)	-5.0(3)
C(14)-C(15)-C(16)-C(17)	-0.2(3)
C(20)-C(15)-C(16)-C(17)	-177.6(2)
C(15)-C(16)-C(17)-C(18)	0.4(4)
C(16)-C(17)-C(18)-C(19)	-0.9(4)
C(17)-C(18)-C(19)-C(14)	1.2(3)
C(15)-C(14)-C(19)-C(18)	-1.0(3)
P-C(14)-C(19)-C(18)	-178.54(17)
C(16)-C(15)-C(20)-F(11)	29.9(13)
C(14)-C(15)-C(20)-F(11)	-147.4(13)
C(16)-C(15)-C(20)-F(12)	-167.7(9)
C(14)-C(15)-C(20)-F(12)	15.0(10)
C(16)-C(15)-C(20)-F(9)	-21.9(4)
C(14)-C(15)-C(20)-F(9)	160.8(3)
C(16)-C(15)-C(20)-F(8)	-151.5(3)
C(14)-C(15)-C(20)-F(8)	31.3(4)
C(16)-C(15)-C(20)-F(7)	94.8(3)
C(14)-C(15)-C(20)-F(7)	-82.5(3)
C(16)-C(15)-C(20)-F(10)	-72.3(6)
C(14)-C(15)-C(20)-F(10)	110.4(6)
Yb-O(3)-C(21)-N(5)	-168.37(14)
C(22)-N(5)-C(21)-O(3)	-1.9(3)
C(23)-N(5)-C(21)-O(3)	-177.1(2)
C(25)-N(6)-C(24)-O(13)	-0.5(6)
C(26)-N(6)-C(24)-O(13)	178.6(4)

Table 7. Hydrogen bonds for rpec17 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...O(13)#2	0.94	2.42	3.354(3)	170.4
C(6)-H(6A)...F(2)	0.98	2.24	2.975(3)	131.2
C(6)-H(6A)...O(5)#2	0.98	2.53	3.259(2)	131.0
C(6)-H(6B)...O(8)#2	0.98	2.58	3.0293(18)	108.1
C(9)-H(9)...F(1)	0.94	2.34	2.689(8)	101.7
C(9)-H(9)...O(7)#3	0.94	2.49	3.289(2)	142.4
C(12)-H(12)...O(1)	0.94	2.34	2.839(2)	112.6
C(16)-H(16)...F(9)	0.94	2.37	2.710(4)	100.8
C(17)-H(17)...O(9)#1	0.94	2.55	3.204(2)	126.9
C(21)-H(21)...F(8)	0.94	2.42	3.304(5)	156.7
C(21)-H(21)...O(1)	0.94	2.59	3.145(2)	117.8
C(22)-H(22B)...O(6)#4	0.97	2.50	3.042(3)	114.9
C(25)-H(25A)...O(13)	0.97	2.34	2.751(5)	104.9

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2 #2 -x+3/2,-y+3/2,-z+2 #3 x,-y+2,z+1/2
#4 -x+3/2,y+1/2,-z+3/2

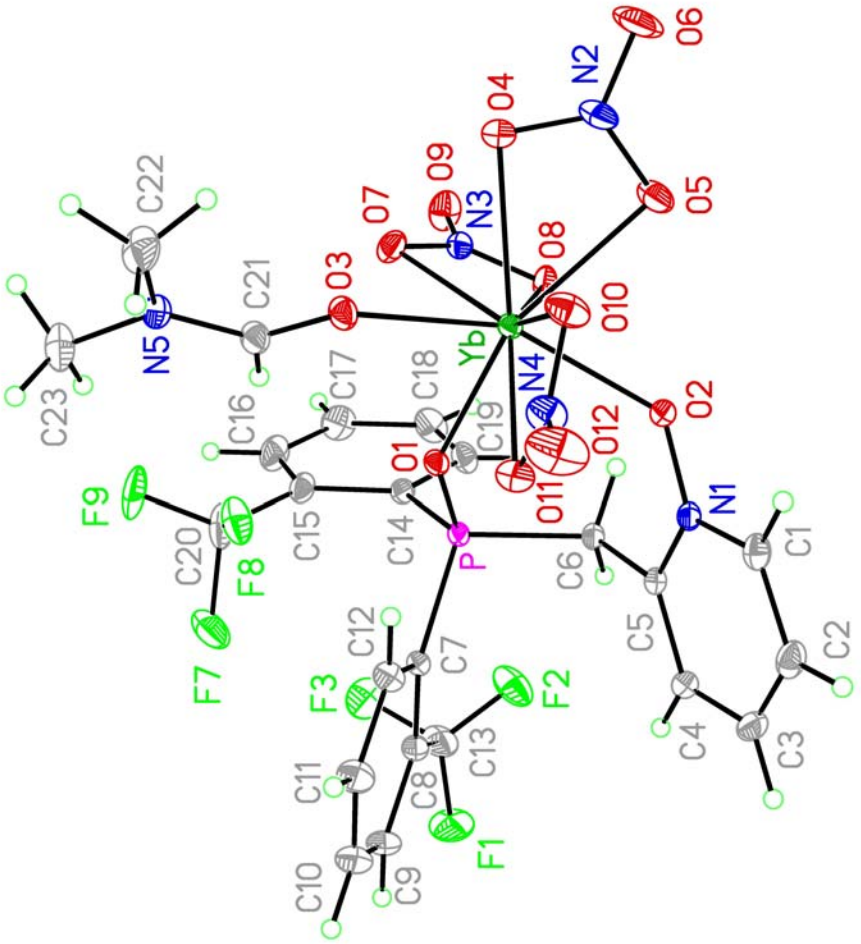


Figure 1. rpec17l1.jpg single molecule with 20% displacement ellipsoids, also see rpec17l1b.jpg b/w, note that only major disorder parts shown [F1,F2,F3 and F7,F8,F9]

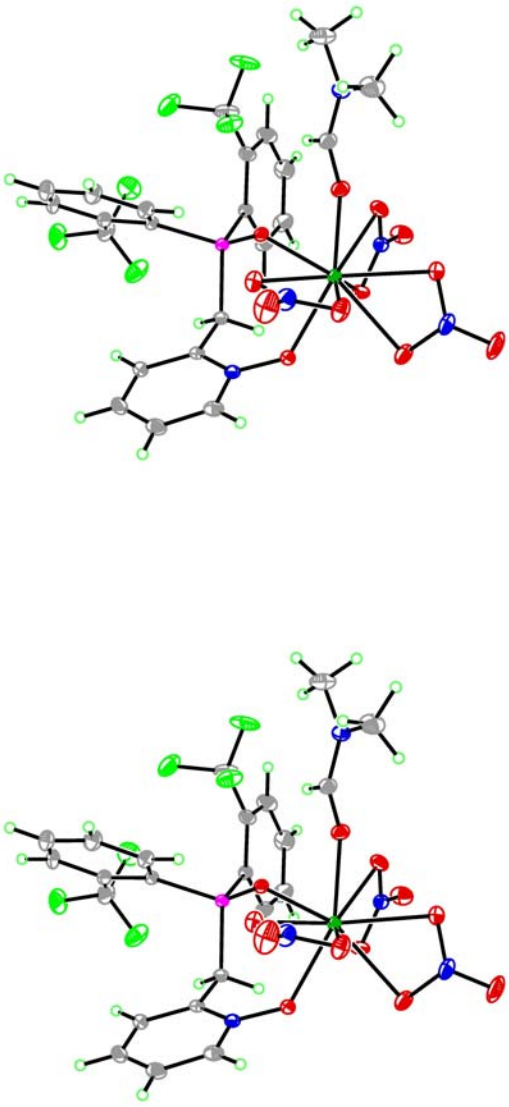


Figure 2. rpec17s1.jpg stereoview of molecule at 20% displacement ellipsoids, also rpec17s1b.jpg, note that only major disorder parts shown [F1,F2,F3 and F7,F8,F9]

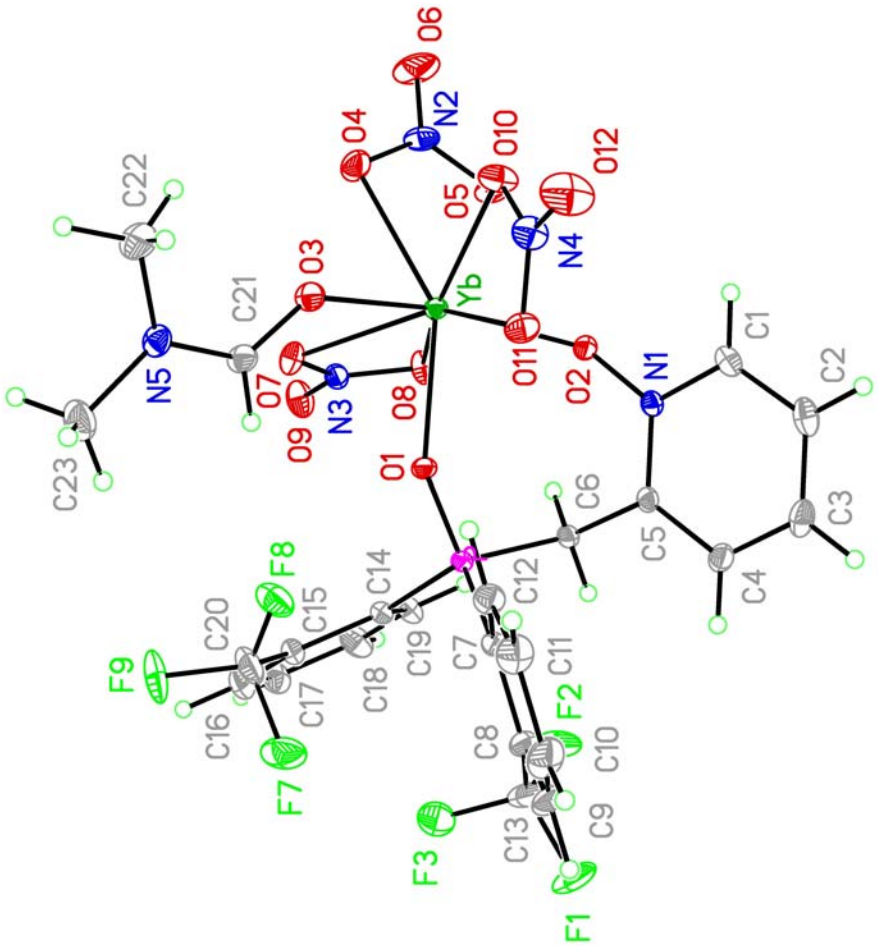


Figure 3. rpec17l2.jpg, another view of molecule 20% displacement ellipsoids, also rpec17l2b.jpg b/w and rpec17s2.jpg, rpec17s2b.jpg stereo views

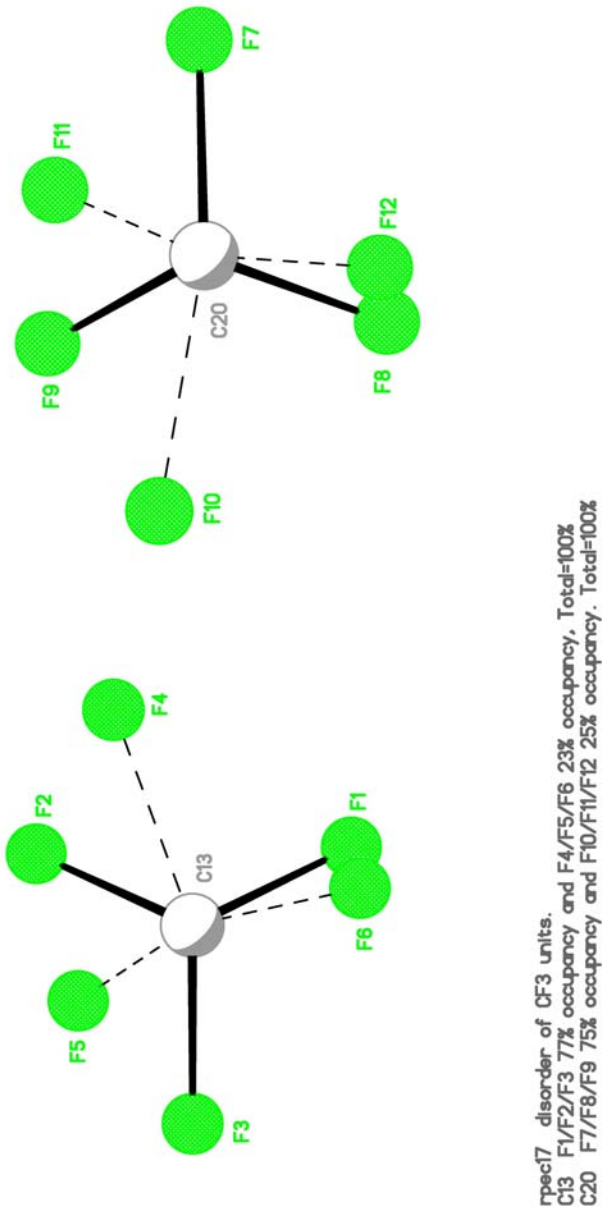


Figure 4. rpec17cf.jpg disorder of CF3 units, also rpec17c13.jpg and rpec17c20.jpg, note that only major disorder parts shown [F1,F2,F3 and F7,F8,F9]

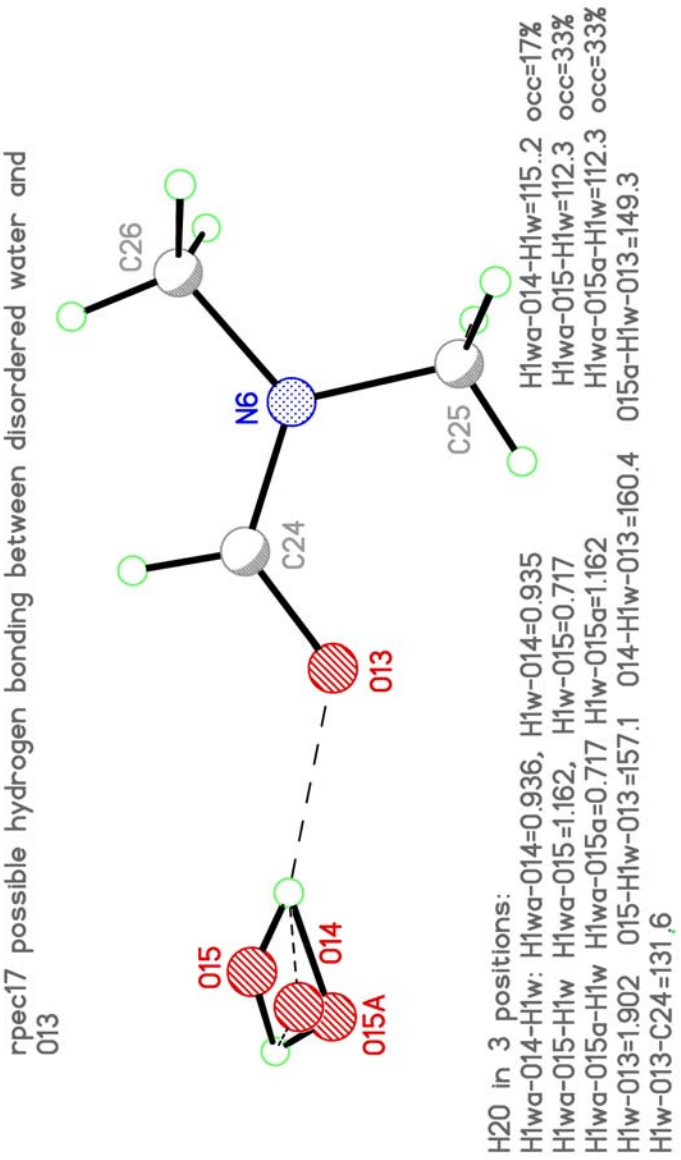


Figure 5. rpec17w1q.jpg disorder of water molecule over 3 positions..H14a-O14-H14,H15a-O15-H15,H15a-O15a-H15, also rpec17w1b.jpg b/w, rpec17w1.jpg [no notation],rpec17w1b.jpg b/w

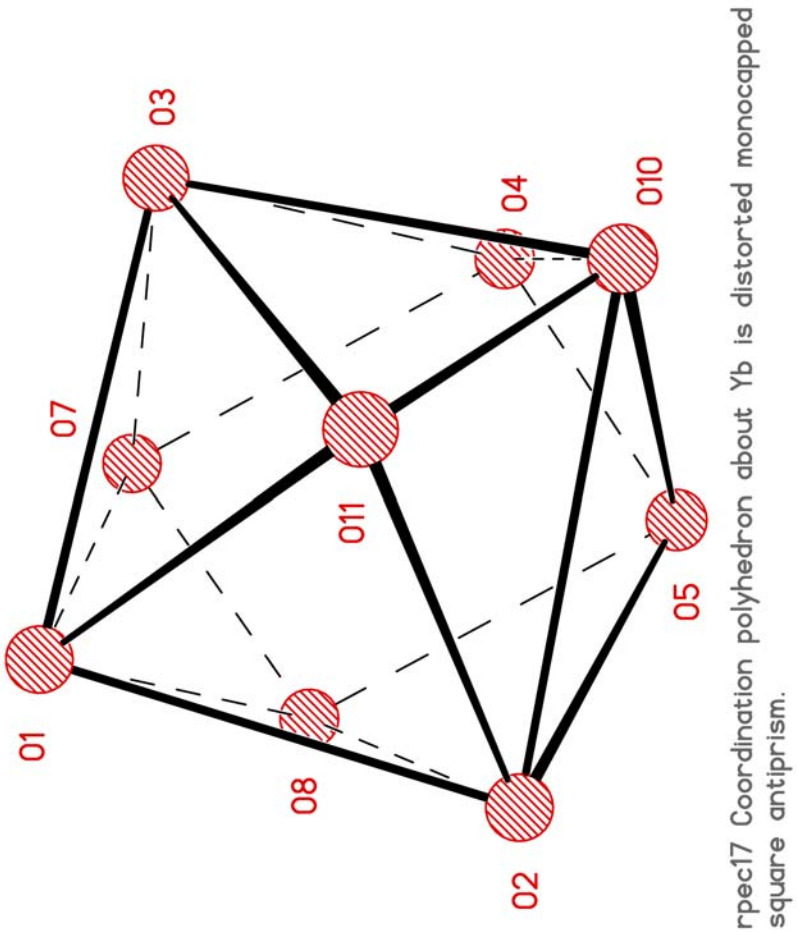


Figure 6. rpec17ybp.jpg coordination polyhedron of Yb, also rpec17yb.jpg no notation, rpec17ybb.jpg b/w

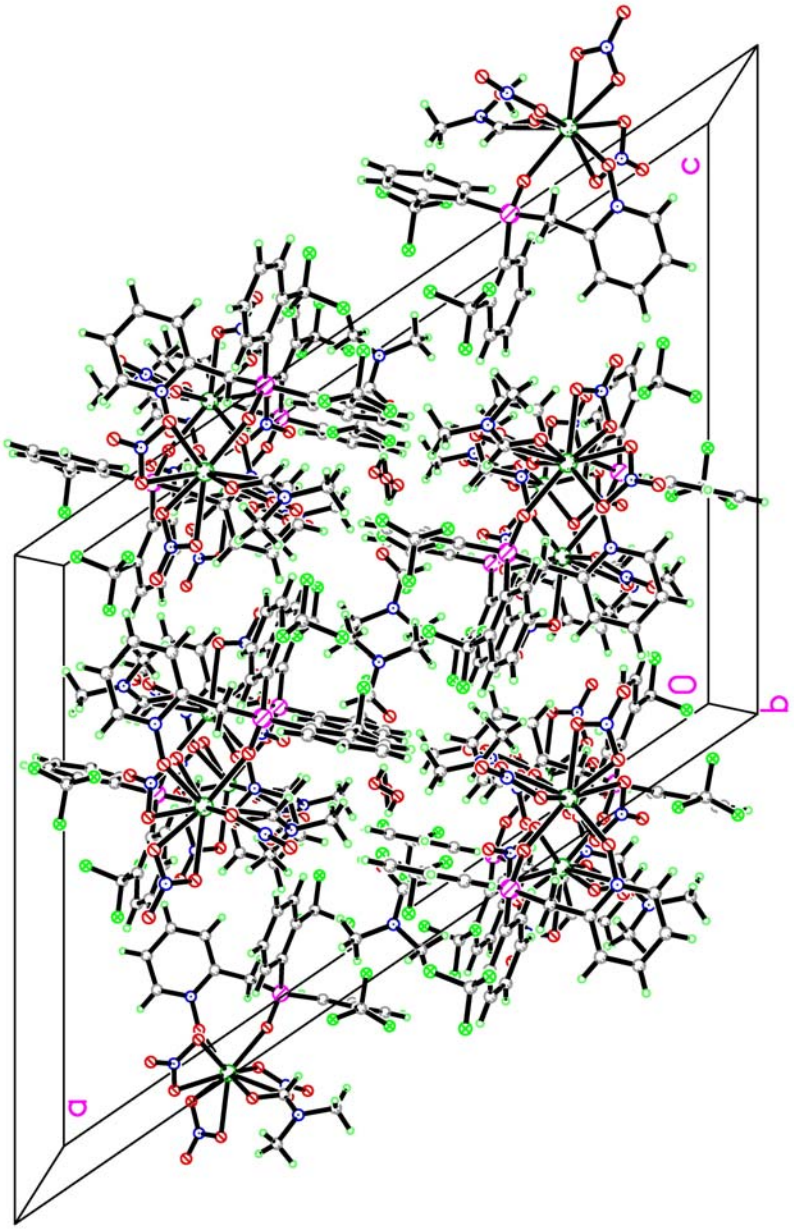


Figure 7. rpec17bl.jpg packing of cell, view down b-axis; also rpec16blb.jpg b/w, note that only major disorder parts shown [F1,F2,F3 and F7,F8,F9]

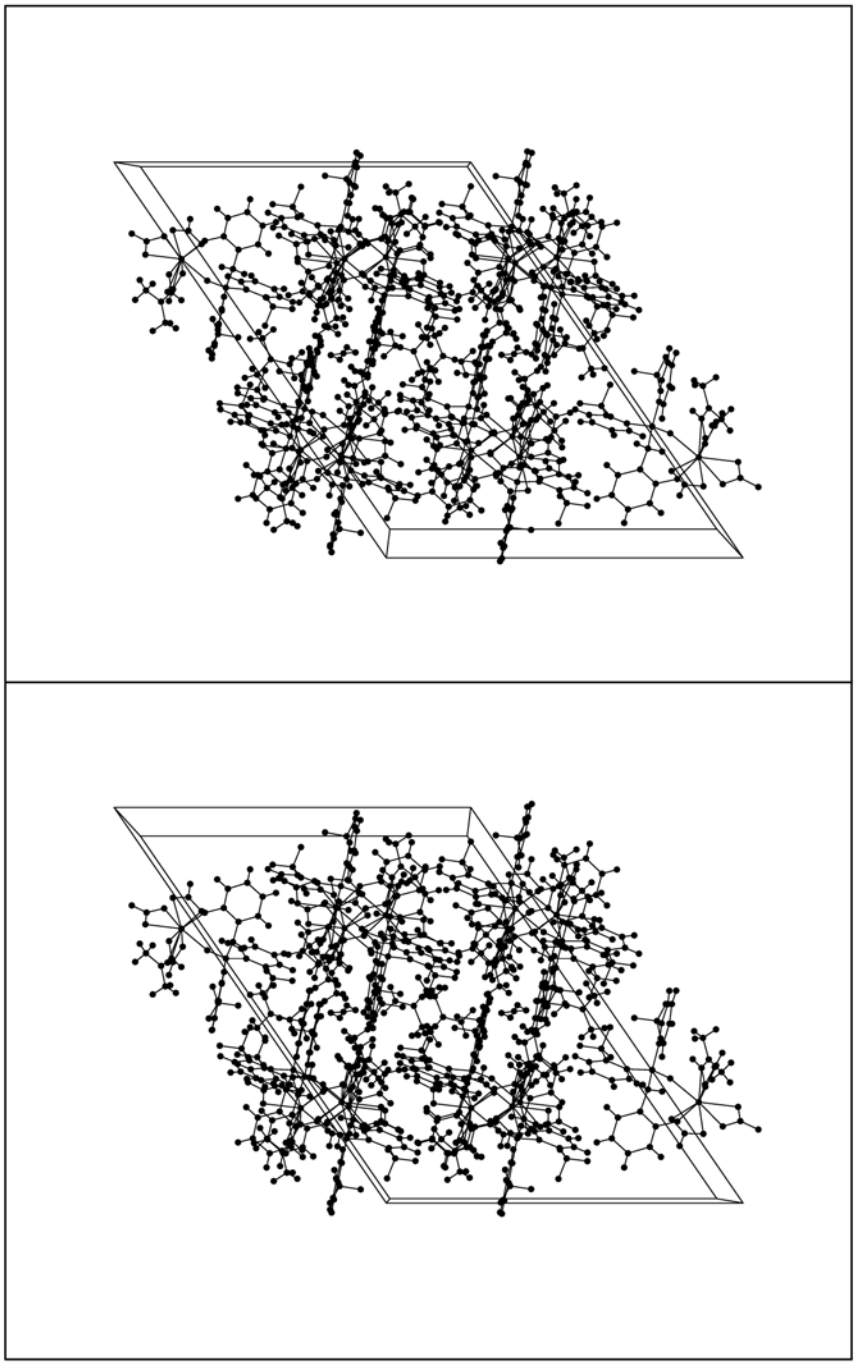
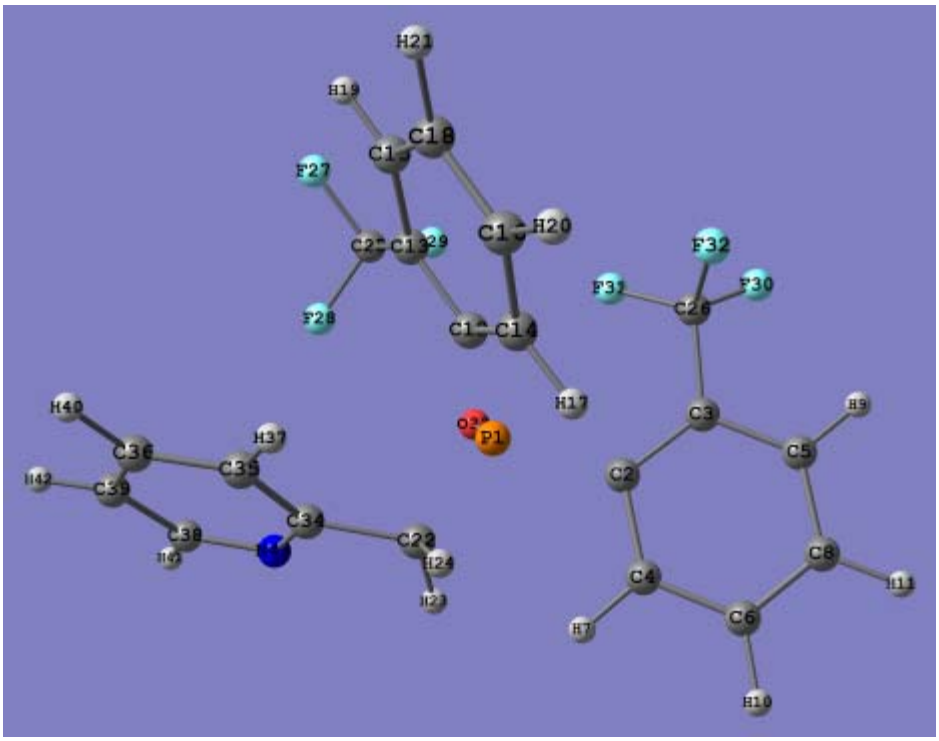


Figure 8. rpec17bsb.jpg stereoview of packing, view down b-axis, note that only major disorder parts shown [F1,F2,F3 and F7,F8,F9]

Computational material for **3c**, **1c**, **3d**, **1d**.

$\{[2\text{-}(CF_3)C_6H_4]_2P(O)CH_2]\}C_5H_4N$, 3c



Atom Coordinates
(Angstroms)

1	P	-0.180440000	0.829101000	-0.417800000
2	C	-1.949627000	1.289094000	-0.021354000
3	C	-3.073737000	0.450446000	-0.200306000
4	C	-2.195780000	2.625190000	0.325562000
5	C	-4.362636000	0.950998000	-0.007430000
6	C	-3.483907000	3.118511000	0.513301000
7	H	-1.370611000	3.311696000	0.448653000
8	C	-4.574980000	2.277573000	0.348261000
9	H	-5.207496000	0.290597000	-0.150603000
10	H	-3.625304000	4.159247000	0.780827000
11	H	-5.584477000	2.645842000	0.486557000
12	C	0.173104000	-0.642928000	0.661008000
13	C	0.968226000	-1.756321000	0.319973000
14	C	-0.371070000	-0.589442000	1.949586000
15	C	1.172634000	-2.770049000	1.257974000
16	C	-0.156581000	-1.599658000	2.881411000
17	H	-0.995874000	0.251025000	2.229784000
18	C	0.616091000	-2.698387000	2.530711000

Atom Coordinates

(continued)

19	H	1.779087000	-3.621837000	0.984833000
20	H	-0.601352000	-1.529232000	3.867183000
21	H	0.788204000	-3.500354000	3.238872000
22	C	0.834173000	2.156497000	0.409191000
23	H	0.619787000	3.081877000	-0.127037000
24	H	0.516366000	2.252770000	1.450024000
25	C	1.634813000	-1.924821000	-1.036596000
26	C	-2.996762000	-1.026994000	-0.527586000
27	F	2.455814000	-3.008537000	-1.041481000
28	F	2.406759000	-0.870048000	-1.353226000
39	F	0.749444000	-2.117295000	-2.022876000
30	F	-4.088392000	-1.437865000	-1.210116000
31	F	-1.927075000	-1.362364000	-1.260032000
32	F	-2.957052000	-1.772830000	0.607295000
33	O	0.063863000	0.711903000	-1.880418000
34	C	2.322880000	1.921139000	0.313834000
35	C	3.008276000	1.146091000	1.255494000
36	C	4.378653000	0.967808000	1.107762000
37	H	2.477080000	0.693348000	2.083869000
38	C	4.255334000	2.327501000	-0.849907000
39	C	5.020786000	1.564924000	0.028068000
40	H	4.934497000	0.372102000	1.823122000
41	H	4.718044000	2.819787000	-1.700670000
42	H	6.086232000	1.449685000	-0.130249000
43	N	2.940958000	2.512732000	-0.714947000

Bond Angles and Lengths

R(1-33)	1.488
R(2-3)	1.414
R(2-4)	1.402
R(3-5)	1.396
R(3-26)	1.515
R(4-6)	1.392
R(4-7)	1.080
R(5-8)	1.390
R(5-9)	1.082
R(6-8)	1.387
R(6-10)	1.084
R(8-11)	1.083
R(12-13)	1.410
R(12-14)	1.400
R(13-15)	1.396
R(13-25)	1.521
R(14-16)	1.391
R(14-17)	1.084
R(15-18)	1.391
R(15-19)	1.081
R(16-18)	1.388
R(16-20)	1.084
R(18-21)	1.084
R(22-23)	1.091
R(22-24)	1.093
R(22-34)	1.510
R(25-27)	1.360
R(25-28)	1.345
R(25-29)	1.339
R(26-30)	1.351
R(26-31)	1.339
R(26-32)	1.359
R(34-35)	1.399
R(34-43)	1.338
R(35-36)	1.390
R(35-37)	1.083
R(36-39)	1.391
R(36-40)	1.084
R(38-39)	1.392
R(38-41)	1.086
R(38-43)	1.334
R(39-42)	1.083

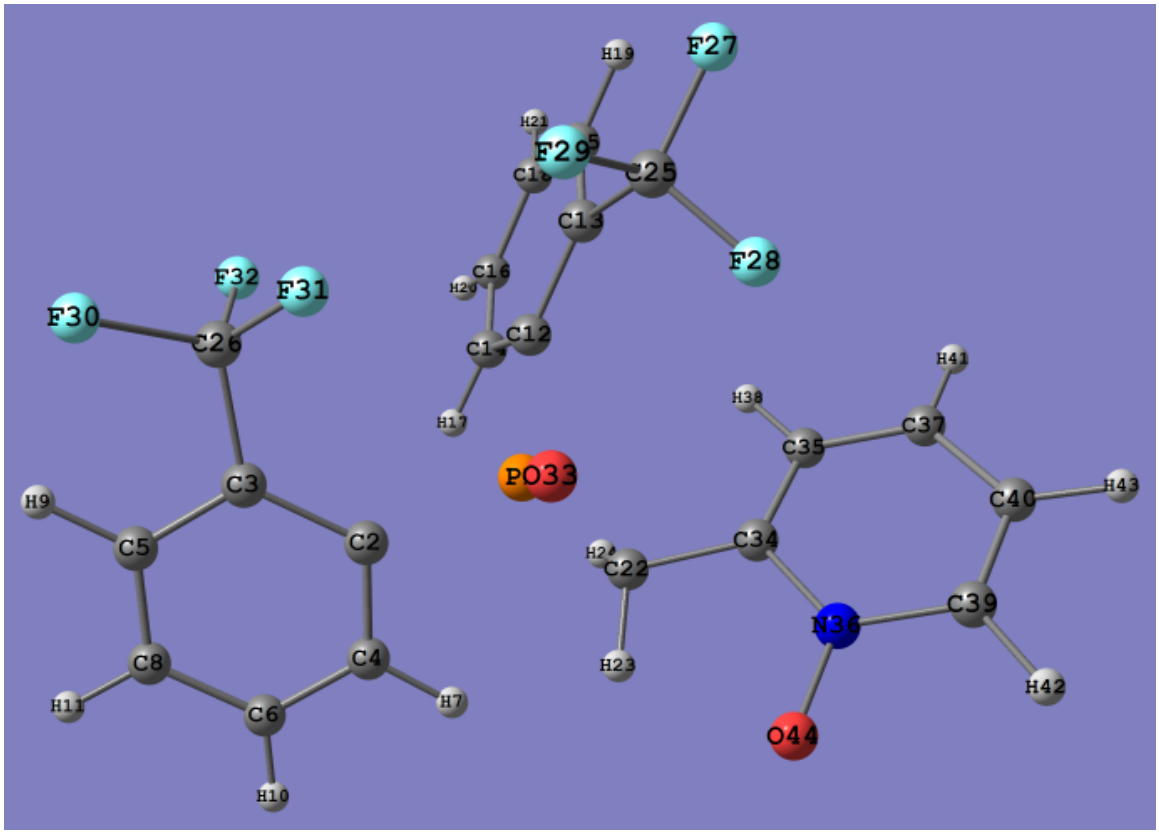
Bond Angles

A(3-2-4)	117.2
A(2-3-5)	120.3
A(2-3-26)	124.4
A(2-4-6)	122.2
A(2-4-7)	120.0
A(5-3-26)	115.2
A(3-5-8)	121.2
A(3-5-9)	118.9
A(3-26-30)	111.4
A(3-26-31)	113.8
A(3-26-32)	110.9
A(6-4-7)	117.8
A(4-6-8)	119.8
A(4-6-10)	119.6
A(8-5-9)	119.8
A(5-8-6)	119.3
A(5-8-11)	120.0
A(8-6-10)	120.6
A(6-8-11)	120.8
A(13-12-14)	118.2
A(12-13-15)	119.6
A(12-13-25)	123.4
A(12-14-16)	121.9
A(12-14-17)	119.4
A(15-13-25)	117.0
A(13-15-18)	121.2
A(13-15-19)	119.0
A(13-25-27)	110.9
A(13-25-28)	112.0
A(13-25-29)	112.5
A(16-14-17)	118.6
A(14-16-18)	119.4
A(14-16-20)	119.9
A(18-15-19)	119.8
A(15-18-16)	119.6
A(15-18-21)	119.8
A(18-16-20)	120.6
A(16-18-21)	120.6
A(23-22-24)	109.7
A(23-22-34)	107.2
A(24-22-34)	111.1
A(22-34-35)	121.8
A(22-34-43)	115.8
A(27-25-28)	106.1

Bond Angles
(continued)

A(27-25-29)	106.4
A(28-25-29)	108.6
A(30-26-31)	107.0
A(30-26-32)	106.2
A(31-26-32)	107.2
A(35-34-43)	122.4
A(34-35-36)	118.9
A(34-35-37)	120.4
A(34-43-38)	118.1
A(36-35-37)	120.7
A(35-36-39)	118.9
A(35-36-40)	120.4
A(39-36-40)	120.8
A(36-39-38)	118.1
A(36-39-42)	121.5
A(39-38-41)	120.5
A(39-38-43)	123.6
A(38-39-42)	120.5
A(41-38-43)	115.8

{[2-(CF_3)C_6H_4]$_2$P9O)CH_2}C_5H_4NO, 1c



Coordinates
(Angstroms)

1	P	0.121308000	-0.719198000	-0.250565000
2	C	1.828189000	-1.402277000	0.089043000
3	C	3.046328000	-0.752490000	-0.218569000
4	C	1.907283000	-2.725238000	0.546649000
5	C	4.262087000	-1.414218000	-0.039407000
6	C	3.123681000	-3.379420000	0.721865000
7	H	1.005365000	-3.276120000	0.768337000
8	C	4.309281000	-2.721344000	0.430073000
9	H	5.179992000	-0.896864000	-0.284462000
10	H	3.133590000	-4.403103000	1.077484000
11	H	5.264329000	-3.217212000	0.555785000
12	C	0.058240000	0.880006000	0.701622000
13	C	-0.551583000	2.081670000	0.284001000
14	C	0.647461000	0.845178000	1.971089000
15	C	-0.537569000	3.191065000	1.132645000
16	C	0.651748000	1.952335000	2.812632000
17	H	1.137801000	-0.061886000	2.306030000
18	C	0.058340000	3.133345000	2.388024000

19	H	-1.002421000	4.108931000	0.802247000
20	H	1.125760000	1.890648000	3.785230000
21	H	0.057695000	4.010406000	3.024398000
22	C	-1.010426000	-1.800510000	0.768814000
23	H	-0.879014000	-2.825215000	0.418859000
24	H	-0.736400000	-1.718980000	1.822205000
25	C	-1.241292000	2.254019000	-1.061782000
26	C	3.156236000	0.685293000	-0.681758000
27	F	-1.852702000	3.466302000	-1.138654000
28	F	-2.208492000	1.338338000	-1.254075000
29	F	-0.387878000	2.196027000	-2.090572000
30	F	4.254431000	0.875934000	-1.445525000
31	F	2.103238000	1.099406000	-1.398115000
32	F	3.280230000	1.528376000	0.376309000
33	O	-0.226459000	-0.678731000	-1.695352000
34	C	-2.455353000	-1.475006000	0.570029000
35	C	-3.138509000	-0.452143000	1.212337000
36	N	-3.136835000	-2.305413000	-0.306362000
37	C	-4.487139000	-0.216763000	0.977563000
38	H	-2.584058000	0.170930000	1.902838000
39	C	-4.465029000	-2.068696000	-0.549211000
40	C	-5.145592000	-1.044063000	0.071153000
41	H	-5.005206000	0.589706000	1.479258000
42	H	-4.898687000	-2.761588000	-1.254479000
43	H	-6.193881000	-0.905030000	-0.161977000
44	O	-2.556586000	-3.289103000	-0.872639000

Bond Lengths
(Angstroms)

R(1-33)	1.487
R(2-3)	1.414
R(2-4)	1.402
R(3-5)	1.396
R(3-26)	1.515
R(4-6)	1.392
R(4-7)	1.080
R(5-8)	1.390
R(5-9)	1.082
R(6-8)	1.387
R(6-10)	1.084
R(8-11)	1.083
R(12-13)	1.411
R(12-14)	1.400
R(13-15)	1.397
R(13-25)	1.522
R(14-16)	1.391

Bond Lengths
Continued

R(14-17)	1.084
R(15-18)	1.391
R(15-19)	1.081
R(16-18)	1.388
R(16-20)	1.084
R(18-21)	1.084
R(22-23)	1.091
R(22-24)	1.091
R(22-34)	1.494
R(25-27)	1.360
R(25-28)	1.346
R(25-29)	1.338
R(26-30)	1.351
R(26-31)	1.339
R(26-32)	1.359
R(34-35)	1.388
R(34-36)	1.386
R(35-37)	1.389
R(35-38)	1.083
R(36-39)	1.371
R(36-44)	1.275
R(37-40)	1.393
R(37-41)	1.082
R(39-40)	1.378
R(39-42)	1.080
R(40-43)	1.083

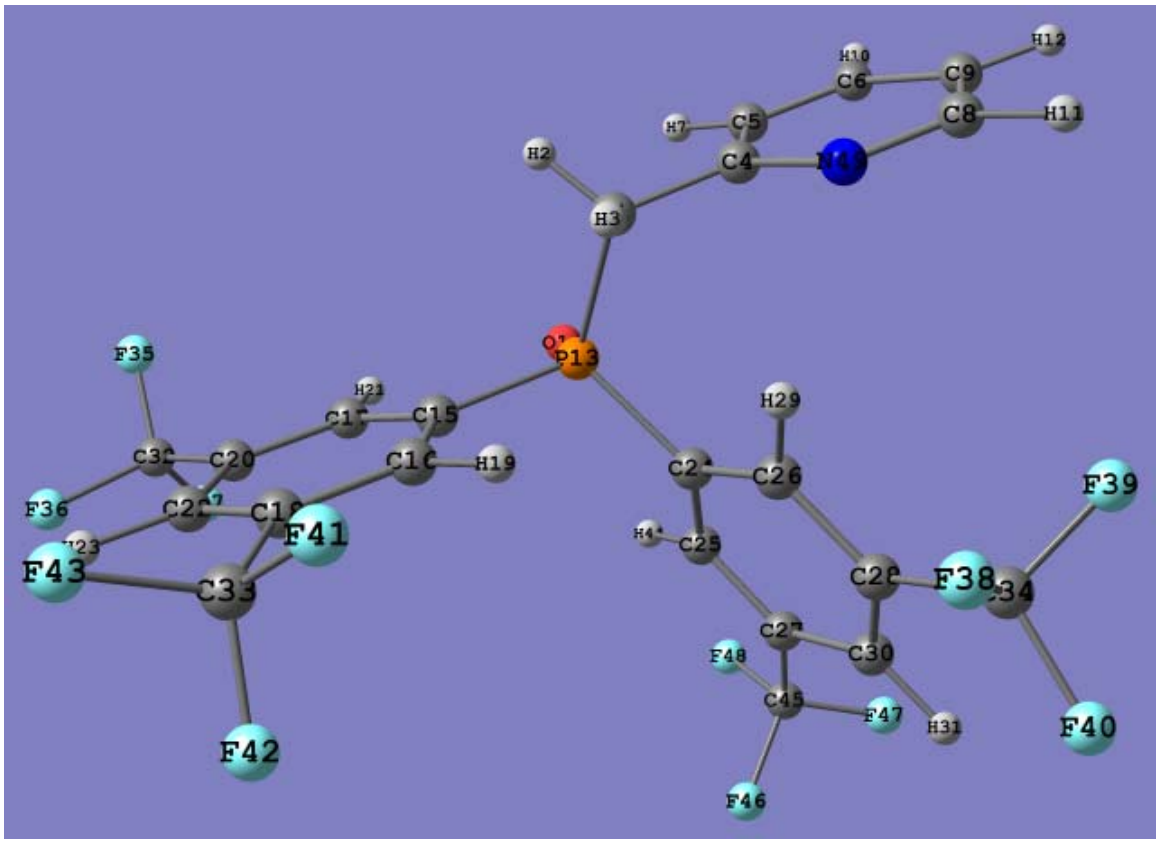
Bond Angles

A(3-2-4)	117.1
A(2-3-5)	120.3
A(2-3-26)	124.4
A(2-4-6)	122.3
A(2-4-7)	120.1
A(5-3-26)	115.2
A(3-5-8)	121.3
A(3-5-9)	118.9
A(3-26-30)	111.5
A(3-26-31)	113.6
A(3-26-32)	111.0
A(6-4-7)	117.7
A(4-6-8)	119.8
A(4-6-10)	119.5
A(8-5-9)	119.8
A(5-8-6)	119.2
A(5-8-11)	120.0
A(8-6-10)	120.6
A(6-8-11)	120.8
A(13-12-14)	118.1
A(12-13-15)	119.5
A(12-13-25)	123.6
A(12-14-16)	122.0
A(12-14-17)	119.4
A(15-13-25)	116.9
A(13-15-18)	121.3
A(13-15-19)	119.0
A(13-25-27)	110.8
A(13-25-28)	112.0
A(13-25-29)	112.7
A(16-14-17)	118.5
A(14-16-18)	119.4
A(14-16-20)	119.9
A(18-15-19)	119.7
A(15-18-16)	119.6
A(15-18-21)	119.8
A(18-16-20)	120.7
A(16-18-21)	120.6
A(23-22-24)	110.5
A(23-22-34)	106.2
A(24-22-34)	110.8
A(22-34-35)	125.1
A(22-34-36)	115.4
A(27-25-28)	106.0

Bond Angles
(continued)

A(27-25-29)	106.4
A(28-25-29)	108.6
A(30-26-31)	107.0
A(30-26-32)	106.2
A(31-26-32)	107.2
A(35-34-36)	119.5
A(34-35-37)	121.6
A(34-35-38)	117.9
A(34-36-39)	119.0
A(34-36-44)	121.3
A(37-35-38)	120.5
A(35-37-40)	117.9
A(35-37-41)	120.9
A(39-36-44)	119.7
A(36-39-40)	121.8
A(36-39-42)	113.2
A(40-37-41)	121.2
A(37-40-39)	120.1
A(37-40-43)	121.4
A(40-39-42)	125.0
A(39-40-43)	118.5

{[3,5-(CF$_3$)2C$_6$H$_3$]$_2$P(O)CH$_2$}C$_5$H$_4$N, 3d



Atom Coordinates

1	C	0.250551000	2.715490000	0.266424000
2	H	-0.524985000	3.448507000	0.024455000
3	H	0.119478000	2.420338000	1.308876000
4	C	1.632853000	3.294017000	0.083922000
5	C	1.961362000	4.066731000	-1.033565000
6	C	3.253204000	4.569693000	-1.137799000
7	H	1.222656000	4.252943000	-1.803417000
8	C	3.754359000	3.497668000	0.937531000
9	C	4.171528000	4.285245000	-0.131307000
10	H	3.537853000	5.172413000	-1.992652000
11	H	4.440371000	3.240571000	1.739073000
12	H	5.187647000	4.657942000	-0.172821000
13	P	-0.130012000	1.292432000	-0.845654000
14	O	-0.244185000	1.643382000	-2.296333000
15	C	-1.717239000	0.626908000	-0.195081000
16	C	-1.859287000	0.099189000	1.092122000
17	C	-2.817783000	0.670655000	-1.049606000
18	C	-3.097239000	-0.370735000	1.517233000

19	H	-1.016044000	0.046913000	1.770221000
20	C	-4.056956000	0.197986000	-0.613251000
21	H	-2.693790000	1.069653000	-2.050032000
22	C	-4.202368000	-0.322076000	0.666725000
23	H	-5.164676000	-0.682742000	1.003195000
24	C	1.115838000	-0.015819000	-0.530551000
25	C	1.337918000	-0.929543000	-1.568577000
26	C	1.836319000	-0.130178000	0.657711000
27	C	2.256466000	-1.958630000	-1.401269000
28	C	2.764878000	-1.162140000	0.809732000
29	H	1.724129000	0.595913000	1.452342000
30	C	2.974203000	-2.080633000	-0.210512000
31	H	3.695892000	-2.877119000	-0.086748000
32	C	-5.236522000	0.283279000	-1.549151000
33	C	-3.240903000	-0.988760000	2.884549000
34	C	3.577234000	-1.225873000	2.077416000
35	F	-5.562726000	1.567874000	-1.809309000
36	F	-6.333367000	-0.313929000	-1.042667000
37	F	-4.967774000	-0.300415000	-2.734891000
38	F	2.811284000	-1.010597000	3.167918000
39	F	4.547413000	-0.284184000	2.089352000
40	F	4.181481000	-2.419869000	2.234902000
41	F	-2.328435000	-0.504518000	3.752518000
42	F	-3.072744000	-2.328154000	2.840798000
43	F	-4.462136000	-0.762115000	3.409714000
44	H	0.805639000	-0.817476000	-2.504812000
45	C	2.475059000	-2.980041000	-2.488329000
46	F	1.890872000	-4.158832000	-2.177457000
47	F	3.788962000	-3.233628000	-2.671130000
48	F	1.969357000	-2.582982000	-3.670259000
49	N	2.515564000	3.009448000	1.050886000

Bond Lengths
(Angstroms)

R(1-2)	1.094
R(1-3)	1.091
R(1-4)	1.510
R(1-13)	1.846
R(4-5)	1.398
R(4-49)	1.340
R(5-6)	1.390
R(5-7)	1.083
R(6-9)	1.392
R(6-10)	1.084
R(8-9)	1.392

Bond Lenghts

(continued)

R(8-11)	1.086
R(8-49)	1.336
R(9-12)	1.083
R(13-14)	1.497
R(13-15)	1.840
R(13-24)	1.834
R(15-16)	1.398
R(15-17)	1.394
R(16-18)	1.391
R(16-19)	1.083
R(17-20)	1.396
R(17-21)	1.084
R(18-22)	1.395
R(18-33)	1.507
R(20-22)	1.389
R(20-32)	1.508
R(22-23)	1.081
R(24-25)	1.401
R(24-26)	1.394
R(25-27)	1.390
R(25-44)	1.083
R(26-28)	1.397
R(26-29)	1.082
R(27-30)	1.396
R(27-45)	1.508
R(28-30)	1.389
R(28-34)	1.507
R(30-31)	1.082
R(32-35)	1.351
R(32-36)	1.348
R(32-37)	1.349
R(33-41)	1.349
R(33-42)	1.351
R(33-43)	1.349
R(34-38)	1.350
R(34-39)	1.352
R(34-40)	1.347
R(45-46)	1.352
R(45-47)	1.351
R(45-48)	1.345

Bond Angles

A(2-1-3)	107.9
A(2-1-4)	111.4
A(2-1-13)	103.7
A(3-1-4)	109.2
A(3-1-13)	110.0
A(4-1-13)	114.3
A(1-4-5)	121.6
A(1-4-49)	115.8
A(1-13-14)	114.8
A(1-13-15)	104.1
A(1-13-24)	107.8
A(5-4-49)	122.7
A(4-5-6)	118.6
A(4-5-7)	120.2
A(4-49-8)	118.2
A(6-5-7)	121.2
A(5-6-9)	119.0
A(5-6-10)	120.3
A(9-6-10)	120.7
A(6-9-8)	118.2
A(6-9-12)	121.4
A(9-8-11)	120.8
A(9-8-49)	123.4
A(8-9-12)	120.4
A(11-8-49)	115.9
A(14-13-15)	111.2
A(14-13-24)	112.7
A(15-13-24)	105.5
A(13-15-16)	123.3
A(13-15-17)	116.9
A(13-24-25)	116.5
A(13-24-26)	123.8
A(16-15-17)	119.7
A(15-16-18)	120.0
A(15-16-19)	121.0
A(15-17-20)	119.9
A(15-17-21)	119.1
A(18-16-19)	119.0
A(16-18-22)	120.5
A(16-18-33)	120.0
A(20-17-21)	121.0
A(17-20-22)	120.5
A(17-20-32)	118.8
A(22-18-33)	119.5

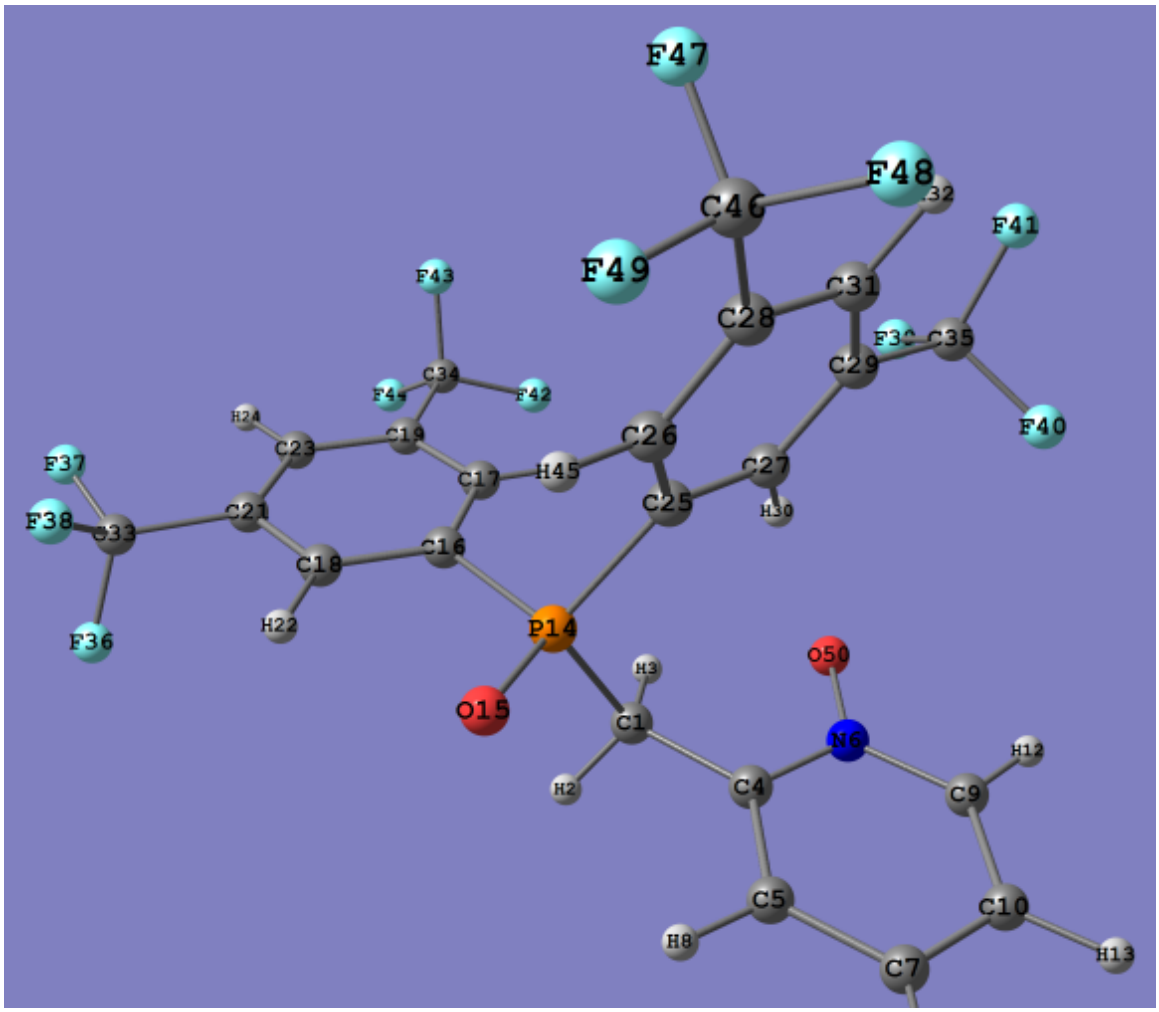
Bond Angles
(continued)

A(18-22-20)	119.5
A(18-22-23)	120.2
A(18-33-41)	111.8
A(18-33-42)	111.4
A(18-33-43)	111.8
A(22-20-32)	120.7
A(20-22-23)	120.3
A(20-32-35)	111.2
A(20-32-36)	112.2
A(20-32-37)	111.4
A(25-24-26)	119.7
A(24-25-27)	119.9
A(24-25-44)	119.7
A(24-26-28)	119.8
A(24-26-29)	121.1
A(27-25-44)	120.4
A(25-27-30)	120.5
A(25-27-45)	120.7
A(28-26-29)	119.0
A(26-28-30)	120.6
A(26-28-34)	118.8
A(30-27-45)	118.8
A(27-30-28)	119.4
A(27-30-31)	120.3
A(27-45-46)	111.2
A(27-45-47)	111.5
A(27-45-48)	112.3
A(30-28-34)	120.6
A(28-30-31)	120.2
A(28-34-38)	111.5
A(28-34-39)	111.4
A(28-34-40)	112.2
A(35-32-36)	107.3
A(35-32-37)	106.9
A(36-32-37)	107.5
A(41-33-42)	107.0
A(41-33-43)	107.6
A(42-33-43)	107.0
A(38-34-39)	106.8
A(38-34-40)	107.5
A(39-34-40)	107.1
A(46-45-47)	106.7

Bond Angles (continued)

A(46-45-48)	107.3
A(47-45-48)	107.6

{[3,5-(CF$_3$)2C$_6$H$_3$]$_2$P(O)CH$_2$}C$_5$H$_4$NO, 1d



Atom Coordinates
(Angstroms)

1	C	-0.226259000	-2.525755000	-0.841027000
2	H	0.498692000	-3.114232000	-1.411005000
3	H	-0.057188000	-2.694386000	0.222780000
4	C	-1.621438000	-2.942216000	-1.179369000
5	C	-2.102620000	-3.092359000	-2.474539000
6	N	-2.458023000	-3.187320000	-0.107419000
7	C	-3.411268000	-3.491525000	-2.712563000
8	H	-1.427139000	-2.871098000	-3.291756000
9	C	-3.747169000	-3.582827000	-0.337151000
10	C	-4.235129000	-3.740322000	-1.616159000
11	H	-3.779316000	-3.602551000	-3.723991000

12	H	-4.313895000	-3.744040000	0.567638000
13	H	-5.263933000	-4.052948000	-1.742283000
14	P	0.183615000	-0.783087000	-1.300456000
15	O	0.301571000	-0.557652000	-2.776337000
16	C	1.777779000	-0.463774000	-0.444250000
17	C	1.922033000	-0.505110000	0.946635000
18	C	2.878119000	-0.170956000	-1.248174000
19	C	3.164125000	-0.257761000	1.520323000
20	H	1.078583000	-0.725630000	1.589663000
21	C	4.121723000	0.071882000	-0.662040000
22	H	2.751151000	-0.128978000	-2.323875000
23	C	4.269688000	0.029812000	0.718441000
24	H	5.235088000	0.217116000	1.168768000
25	C	-1.047774000	0.331661000	-0.524032000
26	C	-1.258034000	1.554950000	-1.174974000
27	C	-1.762955000	0.026702000	0.633409000
28	C	-2.163370000	2.469527000	-0.653169000
29	C	-2.679701000	0.952660000	1.139677000
30	H	-1.656866000	-0.935520000	1.128207000
31	C	-2.879028000	2.172827000	0.508285000
32	H	-3.591844000	2.882169000	0.907513000
33	C	5.308919000	0.341686000	-1.551962000
34	C	3.323555000	-0.246714000	3.019587000
35	C	-3.489766000	0.578295000	2.355527000
36	F	5.713349000	-0.782894000	-2.182387000
37	F	6.365468000	0.812870000	-0.860341000
38	F	5.014359000	1.243677000	-2.509716000
39	F	-2.717040000	0.052745000	3.325674000
40	F	-4.429208000	-0.345897000	2.053143000
41	F	-4.134400000	1.640430000	2.881011000
42	F	2.341439000	-0.932014000	3.636951000
43	F	3.298713000	1.012808000	3.507082000
44	F	4.499380000	-0.790098000	3.397466000
45	H	-0.727700000	1.772111000	-2.093514000
46	C	-2.383727000	3.804845000	-1.317006000
47	F	-1.879573000	4.813173000	-0.571419000
48	F	-3.699968000	4.062956000	-1.479539000
49	F	-1.804443000	3.874604000	-2.529396000
50	O	-2.045644000	-3.042208000	1.102720000

Bond Lengths

R(1-2)	1.094
R(1-3)	1.090
R(1-4)	1.495
R(1-14)	1.848
R(4-5)	1.390
R(4-6)	1.382
R(5-7)	1.389
R(5-8)	1.083
R(6-9)	1.368
R(6-50)	1.287
R(7-10)	1.394
R(7-11)	1.082
R(9-10)	1.378
R(9-12)	1.080
R(10-13)	1.083
R(14-15)	1.498
R(14-16)	1.838
R(14-25)	1.834
R(16-17)	1.399
R(16-18)	1.394
R(17-19)	1.390
R(17-20)	1.083
R(18-21)	1.396
R(18-22)	1.084
R(19-23)	1.396
R(19-34)	1.508
R(21-23)	1.389
R(21-33)	1.508
R(23-24)	1.082
R(25-26)	1.402
R(25-27)	1.394
R(26-28)	1.389
R(26-45)	1.083
R(27-29)	1.398
R(27-30)	1.087
R(28-31)	1.396
R(28-46)	1.507
R(29-31)	1.388
R(29-35)	1.508
R(31-32)	1.082
R(33-36)	1.351
R(33-37)	1.348
R(33-38)	1.348

Bond Lengths (continued)

R(34-42)	1.347
R(34-43)	1.351
R(34-44)	1.349
R(35-39)	1.347
R(35-40)	1.352
R(35-41)	1.349
R(46-47)	1.352
R(46-48)	1.351
R(46-49)	1.345

Bond Angles

A(2-1-3)	108.8
A(2-1-4)	110.5
A(2-1-14)	103.3
A(3-1-4)	108.8
A(3-1-14)	110.7
A(4-1-14)	114.4
A(1-4-5)	124.3
A(1-4-6)	116.0
A(1-14-15)	113.9
A(1-14-16)	103.9
A(1-14-25)	108.6
A(5-4-6)	119.6
A(4-5-7)	121.1
A(4-5-8)	117.7
A(4-6-9)	119.4
A(4-6-50)	121.0
A(7-5-8)	121.1
A(5-7-10)	118.3
A(5-7-11)	120.7
A(9-6-50)	119.5
A(6-9-10)	121.5
A(6-9-12)	113.4
A(10-7-11)	121.1
A(7-10-9)	120.0
A(7-10-13)	121.4
A(10-9-12)	125.1
A(9-10-13)	118.5
A(15-14-16)	111.4
A(15-14-25)	112.3
A(16-14-25)	106.2
A(14-16-17)	123.2
A(14-16-18)	116.9
A(14-25-26)	115.8
A(14-25-27)	124.3

Bond Angles (continued)

A(17-16-18)	119.9
A(16-17-19)	119.8
A(16-17-20)	121.1
A(16-18-21)	119.8
A(16-18-22)	119.2
A(19-17-20)	119.1
A(17-19-23)	120.5
A(17-19-34)	120.4
A(21-18-22)	120.9
A(18-21-23)	120.5
A(18-21-33)	119.0
A(23-19-34)	119.1
A(19-23-21)	119.5
A(19-23-24)	120.2
A(19-34-42)	112.0
A(19-34-43)	111.3
A(19-34-44)	111.6
A(23-21-33)	120.5
A(21-23-24)	120.2
A(21-33-36)	111.2
A(21-33-37)	112.1
A(21-33-38)	111.5
A(26-25-27)	120.0
A(25-26-28)	119.9
A(25-26-45)	119.7
A(25-27-29)	119.5
A(25-27-30)	121.4
A(28-26-45)	120.4
A(26-28-31)	120.5
A(26-28-46)	120.9
A(29-27-30)	119.0
A(27-29-31)	120.8
A(27-29-35)	118.7
A(31-28-46)	118.7
A(28-31-29)	119.4
A(28-31-32)	120.4
A(28-46-47)	111.3
A(28-46-48)	111.4
A(28-46-49)	112.3
A(31-29-35)	120.5
A(29-31-32)	120.2
A(29-35-39)	111.7
A(29-35-40)	111.3

Bond Angles (continued)

A(29-35-41)	112.0
A(36-33-37)	107.2
A(36-33-38)	106.9
A(37-33-38)	107.6
A(42-34-43)	107.2
A(42-34-44)	107.6
A(43-34-44)	106.9
A(39-35-40)	107.0
A(39-35-41)	107.5
A(40-35-41)	107.1
A(47-46-48)	106.7
A(47-46-49)	107.3
A(48-46-49)	107.5