Supplementary Information for paper titled:

Molecular materials for switchable nonlinear optics in solid state, based on Ruthenium-nitrosyl complexes

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To be published in the *New Journal of Chemistry*.

1. Choice of the functional for the DFT computations

Selected bonds		DFT computed bond lengths (Å)		
	X-ray data*	PBE0	B3LYP	B3PW91
Ru-N(1,3) (lateral)	2.076(3)	2.081	2.107	2.087
Ru-N(2) (axial)	2.006(3)	2.014	2.031	2.019
Ru-NO	1.769(3)	1.750	1.767	1.756
Ru-Cl(1,2)	2.350(1)	2.384	2.420	2.394
N(4)-O(1)	1.121(4)	1.139	1.147	1.144

* Present work

The PBE0 method is selected as it provides a better description of the coordination sphere around the ruthenium atom.

2. Molecular geometries for 4a-b

2.1. cation $4a_{(NO)}$ – $[Ru^{II}(H_2N\text{-terpy})Cl_2(NO)]^+$

C	0.000000	3.023453	1.485711
H	0.000000	2.729431	2.528304
C	0.000000	4.362542	1.119183
H	0.000000	5.127368	1.887843
C	0.000000	4.685279	-0.231017
H	0.000000	5.721430	-0.554113
C	0.000000	3.659376	-1.168924
H	0.000000	3.888076	-2.228471
C	0.000000	2.337976	-0.740378
C	0.000000	1.176272	-1.647161
C	0.000000	1.213663	-3.026075
H	0.000000	2.157544	-3.559386
C	0.000000	0.000000	-3.750720
C	0.000000	-1.213663	-3.026075
H	0.000000	-2.157544	-3.559386
C	0.000000	-1.176272	-1.647161
C	0.000000	-2.337976	-0.740378
C	0.000000	-3.659376	-1.168924
H	0.000000	-3.888076	-2.228471
C	0.000000	-4.685279	-0.231017
H	0.000000	-5.721430	-0.554113
C	0.000000	-4.362542	1.119183
H	0.000000	-5.127368	1.887843
C	0.000000	-3.023453	1.485711
H	0.000000	-2.729431	2.528304
N	0.000000	2.038229	0.584032
N	0.000000	0.000000	-0.999037
N	0.000000	-2.038229	0.584032
N	0.000000	0.000000	2.754313
O	0.000000	0.000000	3.894417
Cl	2.381279	0.000000	0.823612
Cl	-2.381279	0.000000	0.823612
Ru	0.000000	0.000000	1.003262
N	0.000000	0.000000	-5.094758
H	0.000000	-0.859444	-5.620938
H	0.000000	0.859444	-5.620938

2.2. cation $4a_{(ON)}$ – $[Ru^{II}(H_2N\text{-terpy})Cl_2(ON)]^+$

C	0.000000	3.026914	1.482132
H	0.000000	2.733242	2.525598
C	0.000000	4.366986	1.117096

H	0.000000	5.132377	1.885231
C	0.000000	4.689833	-0.233240
H	0.000000	5.726099	-0.555938
C	0.000000	3.664145	-1.171734
H	0.000000	3.893787	-2.231115
C	0.000000	2.343333	-0.740945
C	0.000000	1.179011	-1.643486
C	0.000000	1.212988	-3.022209
H	0.000000	2.157338	-3.554643
C	0.000000	0.000000	-3.747165
C	0.000000	-1.212988	-3.022209
H	0.000000	-2.157338	-3.554643
C	0.000000	-1.179011	-1.643486
C	0.000000	-2.343333	-0.740945
C	0.000000	-3.664145	-1.171734
H	0.000000	-3.893787	-2.231115
C	0.000000	-4.689833	-0.233240
H	0.000000	-5.726099	-0.555938
C	0.000000	-4.366986	1.117096
H	0.000000	-5.132377	1.885231
C	0.000000	-3.026914	1.482132
H	0.000000	-2.733242	2.525598
N	0.000000	2.042281	0.582334
N	0.000000	0.000000	-0.993716
N	0.000000	-2.042281	0.582334
O	0.000000	0.000000	2.833608
N	0.000000	0.000000	3.966340
Cl	2.375727	0.000000	0.870631
Cl	-2.375727	0.000000	0.870631
Ru	0.000000	0.000000	0.966723
N	0.000000	0.000000	-5.091289
H	0.000000	-0.859458	-5.617402
H	0.000000	0.859458	-5.617402

2.3. cation $4b_{(NO)}$ – $[Ru^{II}(terpy)Cl_2(NO)]^+$

C	0.000000	3.025062	1.296826
H	0.000000	2.733139	2.340045
C	0.000000	4.364279	0.928150
H	0.000000	5.129759	1.696206
C	0.000000	4.686402	-0.422012
H	0.000000	5.722273	-0.745895
C	0.000000	3.659666	-1.359714
H	0.000000	3.887104	-2.419617
C	0.000000	2.339124	-0.928290
C	0.000000	1.181609	-1.836251
C	0.000000	1.209265	-3.227951

H	0.000000	2.147541	-3.769981
C	0.000000	0.000000	-3.916627
H	0.000000	0.000000	-5.002031
C	0.000000	-1.209265	-3.227951
H	0.000000	-2.147541	-3.769981
C	0.000000	-1.181609	-1.836251
C	0.000000	-2.339124	-0.928290
C	0.000000	-3.659666	-1.359714
H	0.000000	-3.887104	-2.419617
C	0.000000	-4.686402	-0.422012
H	0.000000	-5.722273	-0.745895
C	0.000000	-4.364279	0.928150
H	0.000000	-5.129759	1.696206
C	0.000000	-3.025062	1.296826
H	0.000000	-2.733139	2.340045
N	0.000000	2.039230	0.396441
N	0.000000	0.000000	-1.204398
N	0.000000	-2.039230	0.396441
N	0.000000	0.000000	2.559833
O	0.000000	0.000000	3.698946
Cl	2.375298	0.000000	0.607201
Cl	-2.375298	0.000000	0.607201
Ru	0.000000	0.000000	0.809467

2.4. cation $4b_{(ON)}$ – $[Ru^{II}(terpy)Cl_2(ON)]^+$

C	0.000000	3.027877	1.292780
H	0.000000	2.736021	2.336755
C	0.000000	4.368093	0.925931
H	0.000000	5.133943	1.693638
C	0.000000	4.690618	-0.424385
H	0.000000	5.726695	-0.747562
C	0.000000	3.664513	-1.362958
H	0.000000	3.892977	-2.422671
C	0.000000	2.344403	-0.929557
C	0.000000	1.183970	-1.832383
C	0.000000	1.208220	-3.223706
H	0.000000	2.147351	-3.764231
C	0.000000	0.000000	-3.913451
H	0.000000	0.000000	-4.998786
C	0.000000	-1.208220	-3.223706
H	0.000000	-2.147351	-3.764231
C	0.000000	-1.183970	-1.832383
C	0.000000	-2.344403	-0.929557
C	0.000000	-3.664513	-1.362958
H	0.000000	-3.892977	-2.422671
C	0.000000	-4.690618	-0.424385

H	0.000000	-5.726695	-0.747562
C	0.000000	-4.368093	0.925931
H	0.000000	-5.133943	1.693638
C	0.000000	-3.027877	1.292780
H	0.000000	-2.736021	2.336755
N	0.000000	2.042991	0.393796
N	0.000000	0.000000	-1.197498
N	0.000000	-2.042991	0.393796
O	0.000000	0.000000	2.639638
N	0.000000	0.000000	3.771053
Cl	2.371537	0.000000	0.656875
Cl	-2.371537	0.000000	0.656875
Ru	0.000000	0.000000	0.771820

2.5. cation $4c_{(NO)}$ – $[Ru^{II}(O_2N\text{-terpy})Cl_2(NO)]^+$

C	0.000000	3.028064	1.832731
H	0.000000	2.739106	2.876770
C	0.000000	4.367220	1.460656
H	0.000000	5.133856	2.227643
C	0.000000	4.688353	0.110500
H	0.000000	5.723717	-0.214860
C	0.000000	3.659879	-0.826067
H	0.000000	3.884866	-1.886697
C	0.000000	2.341332	-0.390136
C	0.000000	1.183892	-1.296359
C	0.000000	1.218022	-2.687788
H	0.000000	2.136203	-3.262173
C	0.000000	0.000000	-3.347328
C	0.000000	-1.218022	-2.687788
H	0.000000	-2.136203	-3.262173
C	0.000000	-1.183892	-1.296359
C	0.000000	-2.341332	-0.390136
C	0.000000	-3.659879	-0.826067
H	0.000000	-3.884866	-1.886697
C	0.000000	-4.688353	0.110500
H	0.000000	-5.723717	-0.214860
C	0.000000	-4.367220	1.460656
H	0.000000	-5.133856	2.227643
C	0.000000	-3.028064	1.832731
H	0.000000	-2.739106	2.876770
N	0.000000	2.040625	0.934682
N	0.000000	0.000000	-0.668257
N	0.000000	-2.040625	0.934682
N	0.000000	0.000000	3.098003
O	0.000000	0.000000	4.236346
Cl	2.372548	0.000000	1.134162
Cl	-2.372548	0.000000	1.134162

Ru	0.000000	0.000000	1.347462
N	0.000000	0.000000	-4.826957
O	0.000000	-1.086795	-5.367844
O	0.000000	1.086795	-5.367844

2.6. cation $4c_{(ON)}$ – $[Ru^{II}(O_2N\text{-terpy})Cl_2(ON)]^+$

C	0.000000	3.030748	1.827991
H	0.000000	2.741762	2.872716
C	0.000000	4.370873	1.457874
H	0.000000	5.137781	2.224587
C	0.000000	4.692572	0.107556
H	0.000000	5.728187	-0.216950
C	0.000000	3.664903	-0.829960
H	0.000000	3.890974	-1.890376
C	0.000000	2.346696	-0.392123
C	0.000000	1.186282	-1.292834
C	0.000000	1.216960	-2.683701
H	0.000000	2.136114	-3.256502
C	0.000000	0.000000	-3.344438
C	0.000000	-1.216960	-2.683701
H	0.000000	-2.136114	-3.256502
C	0.000000	-1.186282	-1.292834
C	0.000000	-2.346696	-0.392123
C	0.000000	-3.664903	-0.829960
H	0.000000	-3.890974	-1.890376
C	0.000000	-4.692572	0.107556
H	0.000000	-5.728187	-0.216950
C	0.000000	-4.370873	1.457874
H	0.000000	-5.137781	2.224587
C	0.000000	-3.030748	1.827991
H	0.000000	-2.741762	2.872716
N	0.000000	2.044330	0.931193
N	0.000000	0.000000	-0.661004
N	0.000000	-2.044330	0.931193
O	0.000000	0.000000	3.177436
N	0.000000	0.000000	4.308215
Cl	2.369844	0.000000	1.185357
Cl	-2.369844	0.000000	1.185357
Ru	0.000000	0.000000	1.308257
N	0.000000	0.000000	-4.823182
O	0.000000	-1.086842	-5.364238
O	0.000000	1.086842	-5.364238

3. R-ray data for [4b](PF)$_6$

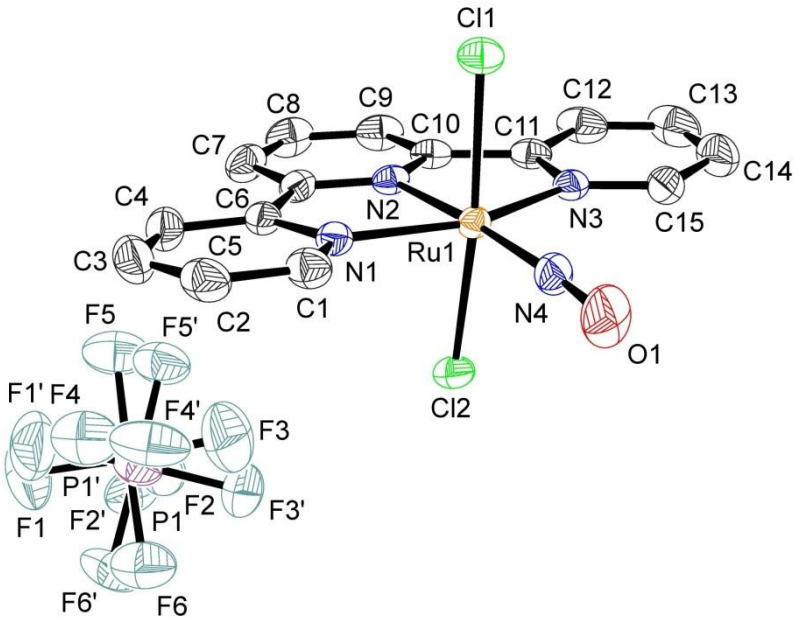

Table 1. Crystal data and structure refinement for rcb11-1m.

Identification code	RCB11-1
Empirical formula	C15 H11 Cl2 N4 O Ru, F6 P
Formula weight	580.22
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	orthorhombic, P b c a
Unit cell dimensions	a = 16.2048(5) A alpha = 90 deg. b = 12.3116(4) A beta = 90 deg. c = 19.4697(6) A gamma = 90 deg.
Volume	3884.3(2) A^3
Z, Calculated density	8, 1.984 Mg/m^3
Absorption coefficient	1.237 mm^-1
F(000)	2272
Crystal size	0.16 x 0.16 x 0.16 mm
Theta range for data collection	2.09 to 27.69 deg.
Limiting indices	-20<=h<=21, -16<=k<=16, -25<=l<=25
Reflections collected / unique	58235 / 4526 [R(int) = 0.0358]

Completeness to theta = 27.69	99.7 %
Max. and min. transmission	0.8267 and 0.8200
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4526 / 249 / 336
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0313, wR2 = 0.0727
R indices (all data)	R1 = 0.0438, wR2 = 0.0814
Largest diff. peak and hole	1.003 and -0.753 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for rcb11-1m.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3261(2)	2992(3)	3340(2)	33(1)
C(2)	3325(3)	2410(3)	2734(2)	41(1)
C(3)	2644(3)	1901(3)	2474(2)	44(1)
C(4)	1904(2)	1974(3)	2823(2)	38(1)
C(5)	1870(2)	2553(3)	3432(2)	28(1)
C(6)	1125(2)	2651(3)	3857(2)	27(1)
C(7)	353(2)	2204(3)	3731(2)	38(1)
C(8)	-271(2)	2384(3)	4200(2)	42(1)
C(9)	-142(2)	2996(3)	4783(2)	38(1)
C(10)	641(2)	3424(3)	4893(2)	28(1)
C(11)	909(2)	4099(3)	5475(2)	29(1)
C(12)	417(3)	4341(3)	6036(2)	43(1)
C(13)	742(3)	4967(4)	6560(2)	53(1)
C(14)	1538(3)	5326(3)	6517(2)	49(1)
C(15)	2008(3)	5073(3)	5950(2)	36(1)
N(1)	2548(2)	3076(2)	3680(1)	25(1)
N(2)	1240(2)	3236(2)	4433(1)	24(1)
N(3)	1697(2)	4475(2)	5435(1)	26(1)
N(4)	3279(2)	4667(2)	4667(1)	32(1)
O(1)	3844(2)	5191(3)	4691(2)	59(1)
Cl(1)	2703(1)	2421(1)	5236(1)	33(1)
Cl(2)	1779(1)	5349(1)	3904(1)	35(1)
Ru(1)	2340(1)	3947(1)	4579(1)	22(1)
P(1)	605(3)	4113(5)	1664(3)	38(1)
F(1)	145(4)	3638(6)	998(3)	82(2)
F(2)	-244(4)	4741(6)	1825(3)	50(1)
F(3)	996(4)	4540(6)	2339(3)	87(2)
F(4)	1391(3)	3414(4)	1495(3)	68(1)
F(5)	237(4)	3098(5)	2081(3)	66(2)
F(6)	988(6)	5136(6)	1269(4)	68(2)
P(1')	647(7)	4231(9)	1695(6)	48(1)
F(1')	470(8)	3325(9)	1157(6)	87(2)
F(2')	-260(6)	4696(10)	1548(6)	59(2)
F(3')	744(6)	5239(7)	2199(4)	66(2)
F(4')	1555(5)	3886(9)	1837(6)	73(2)
F(5')	329(7)	3517(8)	2307(5)	57(2)
F(6')	900(10)	4966(12)	1051(5)	63(2)

Table 3. Bond lengths [A] and angles [deg] for rcb11-1m.

C(1)-N(1)	1.336(4)
C(1)-C(2)	1.384(5)
C(1)-H(1)	0.9500
C(2)-C(3)	1.367(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.380(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(5)
C(4)-H(4)	0.9500
C(5)-N(1)	1.361(4)
C(5)-C(6)	1.470(5)
C(6)-N(2)	1.345(4)
C(6)-C(7)	1.389(5)
C(7)-C(8)	1.379(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.378(6)
C(8)-H(8)	0.9500
C(9)-C(10)	1.391(5)
C(9)-H(9)	0.9500
C(10)-N(2)	1.340(4)
C(10)-C(11)	1.472(5)
C(11)-N(3)	1.360(5)
C(11)-C(12)	1.384(5)
C(12)-C(13)	1.383(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.366(7)
C(13)-H(13)	0.9500
C(14)-C(15)	1.378(5)
C(14)-H(14)	0.9500
C(15)-N(3)	1.342(4)
C(15)-H(15)	0.9500
N(1)-Ru(1)	2.080(3)
N(2)-Ru(1)	2.006(3)
N(3)-Ru(1)	2.071(3)
N(4)-O(1)	1.121(4)
N(4)-Ru(1)	1.769(3)
Cl(1)-Ru(1)	2.3475(8)
Cl(2)-Ru(1)	2.3524(8)
P(1)-F(3)	1.551(7)
P(1)-F(4)	1.572(6)
P(1)-F(6)	1.601(7)
P(1)-F(5)	1.605(7)
P(1)-F(1)	1.605(6)
P(1)-F(2)	1.609(7)
P(1')-F(4')	1.556(12)
P(1')-F(1')	1.557(12)
P(1')-F(5')	1.566(12)
P(1')-F(3')	1.590(11)
P(1')-F(6')	1.600(12)
P(1')-F(2')	1.602(12)

N(1)-C(1)-C(2)	121.9(3)
N(1)-C(1)-H(1)	119.1
C(2)-C(1)-H(1)	119.1
C(3)-C(2)-C(1)	119.4(4)

C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
C(2)-C(3)-C(4)	119.3(4)
C(2)-C(3)-H(3)	120.3
C(4)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	119.3(4)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
N(1)-C(5)-C(4)	121.0(3)
N(1)-C(5)-C(6)	115.1(3)
C(4)-C(5)-C(6)	123.9(3)
N(2)-C(6)-C(7)	119.0(3)
N(2)-C(6)-C(5)	113.5(3)
C(7)-C(6)-C(5)	127.5(3)
C(8)-C(7)-C(6)	118.6(3)
C(8)-C(7)-H(7)	120.7
C(6)-C(7)-H(7)	120.7
C(9)-C(8)-C(7)	121.5(3)
C(9)-C(8)-H(8)	119.3
C(7)-C(8)-H(8)	119.3
C(8)-C(9)-C(10)	118.1(3)
C(8)-C(9)-H(9)	120.9
C(10)-C(9)-H(9)	120.9
N(2)-C(10)-C(9)	119.5(3)
N(2)-C(10)-C(11)	113.5(3)
C(9)-C(10)-C(11)	127.0(3)
N(3)-C(11)-C(12)	120.8(3)
N(3)-C(11)-C(10)	115.1(3)
C(12)-C(11)-C(10)	124.0(3)
C(13)-C(12)-C(11)	118.9(4)
C(13)-C(12)-H(12)	120.6
C(11)-C(12)-H(12)	120.6
C(14)-C(13)-C(12)	119.6(4)
C(14)-C(13)-H(13)	120.2
C(12)-C(13)-H(13)	120.2
C(13)-C(14)-C(15)	119.9(4)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
N(3)-C(15)-C(14)	121.0(4)
N(3)-C(15)-H(15)	119.5
C(14)-C(15)-H(15)	119.5
C(1)-N(1)-C(5)	119.0(3)
C(1)-N(1)-Ru(1)	126.7(2)
C(5)-N(1)-Ru(1)	114.3(2)
C(10)-N(2)-C(6)	123.2(3)
C(10)-N(2)-Ru(1)	118.3(2)
C(6)-N(2)-Ru(1)	118.3(2)
C(15)-N(3)-C(11)	119.8(3)
C(15)-N(3)-Ru(1)	125.7(3)
C(11)-N(3)-Ru(1)	114.3(2)
O(1)-N(4)-Ru(1)	174.1(3)
N(4)-Ru(1)-N(2)	175.18(12)
N(4)-Ru(1)-N(3)	101.38(12)
N(2)-Ru(1)-N(3)	78.67(11)
N(4)-Ru(1)-N(1)	101.57(12)
N(2)-Ru(1)-N(1)	78.47(11)
N(3)-Ru(1)-N(1)	157.04(11)
N(4)-Ru(1)-Cl(1)	97.62(10)

N(2)-Ru(1)-Cl(1)	87.20(7)
N(3)-Ru(1)-Cl(1)	86.47(7)
N(1)-Ru(1)-Cl(1)	90.36(8)
N(4)-Ru(1)-Cl(2)	91.08(10)
N(2)-Ru(1)-Cl(2)	84.10(7)
N(3)-Ru(1)-Cl(2)	91.41(7)
N(1)-Ru(1)-Cl(2)	88.31(8)
Cl(1)-Ru(1)-Cl(2)	171.29(3)
F(3)-P(1)-F(4)	91.9(4)
F(3)-P(1)-F(6)	88.9(4)
F(4)-P(1)-F(6)	91.0(5)
F(3)-P(1)-F(5)	89.3(4)
F(4)-P(1)-F(5)	88.9(4)
F(6)-P(1)-F(5)	178.2(5)
F(3)-P(1)-F(1)	175.8(5)
F(4)-P(1)-F(1)	90.5(4)
F(6)-P(1)-F(1)	94.5(5)
F(5)-P(1)-F(1)	87.3(4)
F(3)-P(1)-F(2)	91.2(4)
F(4)-P(1)-F(2)	175.3(5)
F(6)-P(1)-F(2)	92.6(5)
F(5)-P(1)-F(2)	87.6(4)
F(1)-P(1)-F(2)	86.2(4)
F(4')-P(1')-F(1')	95.6(8)
F(4')-P(1')-F(5')	91.3(8)
F(1')-P(1')-F(5')	92.9(8)
F(4')-P(1')-F(3')	90.6(8)
F(1')-P(1')-F(3')	173.1(10)
F(5')-P(1')-F(3')	90.1(7)
F(4')-P(1')-F(6')	92.9(9)
F(1')-P(1')-F(6')	85.7(9)
F(5')-P(1')-F(6')	175.6(11)
F(3')-P(1')-F(6')	90.9(8)
F(4')-P(1')-F(2')	174.9(10)
F(1')-P(1')-F(2')	88.1(8)
F(5')-P(1')-F(2')	92.0(8)
F(3')-P(1')-F(2')	85.6(7)
F(6')-P(1')-F(2')	83.8(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for rcb11-1m. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	33(2)	34(2)	33(2)	3(1)	6(1)	1(2)
C(2)	47(2)	40(2)	35(2)	5(2)	13(2)	7(2)
C(3)	59(3)	42(2)	30(2)	-5(2)	-1(2)	10(2)
C(4)	45(2)	33(2)	35(2)	-4(2)	-8(2)	2(2)
C(5)	32(2)	23(2)	27(2)	2(1)	-6(1)	2(1)
C(6)	26(2)	22(2)	33(2)	3(1)	-5(1)	-2(1)
C(7)	36(2)	30(2)	47(2)	2(2)	-11(2)	-6(2)
C(8)	25(2)	41(2)	61(2)	9(2)	-7(2)	-10(2)
C(9)	24(2)	40(2)	50(2)	12(2)	3(2)	-2(2)
C(10)	24(2)	28(2)	33(2)	10(1)	2(1)	2(1)
C(11)	29(2)	26(2)	31(2)	8(1)	4(1)	8(1)
C(12)	44(2)	44(2)	40(2)	12(2)	14(2)	13(2)
C(13)	76(3)	50(2)	34(2)	3(2)	17(2)	27(2)
C(14)	75(3)	39(2)	32(2)	-5(2)	-1(2)	12(2)
C(15)	50(2)	28(2)	30(2)	-2(1)	-4(2)	5(2)
N(1)	28(1)	24(1)	24(1)	2(1)	2(1)	0(1)
N(2)	20(1)	21(1)	30(1)	6(1)	-2(1)	0(1)
N(3)	32(2)	21(1)	25(1)	3(1)	-1(1)	4(1)
N(4)	33(2)	35(2)	29(1)	-1(1)	0(1)	-10(1)
O(1)	47(2)	78(2)	54(2)	-7(2)	3(1)	-35(2)
Cl(1)	30(1)	31(1)	37(1)	7(1)	-2(1)	5(1)
Cl(2)	43(1)	25(1)	36(1)	8(1)	-4(1)	-2(1)
Ru(1)	20(1)	22(1)	24(1)	1(1)	-1(1)	-3(1)
P(1)	35(1)	52(2)	29(1)	2(1)	5(1)	5(1)
F(1)	83(4)	107(4)	56(3)	-26(3)	-19(2)	17(3)
F(2)	50(2)	51(2)	49(3)	-3(2)	13(2)	12(2)
F(3)	81(3)	111(4)	68(3)	-16(3)	-23(2)	-10(3)
F(4)	56(3)	68(3)	79(3)	14(2)	30(2)	23(2)
F(5)	50(3)	70(4)	79(4)	30(3)	12(3)	5(3)
F(6)	66(3)	62(3)	76(4)	20(3)	14(3)	11(2)
P(1')	50(2)	52(2)	42(2)	9(2)	8(2)	12(2)
F(1')	114(5)	73(4)	74(4)	-31(4)	-3(4)	18(4)
F(2')	44(3)	53(4)	79(5)	10(4)	-15(4)	-11(3)
F(3')	83(5)	56(4)	59(4)	-10(3)	-16(4)	-18(4)
F(4')	48(3)	86(5)	87(5)	47(4)	16(3)	17(3)
F(5')	60(4)	59(4)	53(4)	16(3)	18(3)	9(4)
F(6')	75(5)	74(5)	39(4)	22(4)	19(4)	16(4)

3. R-ray data for $[Ru^{II}(DEAP\text{-}terpy)Cl_2(NO)](PF)_6$.

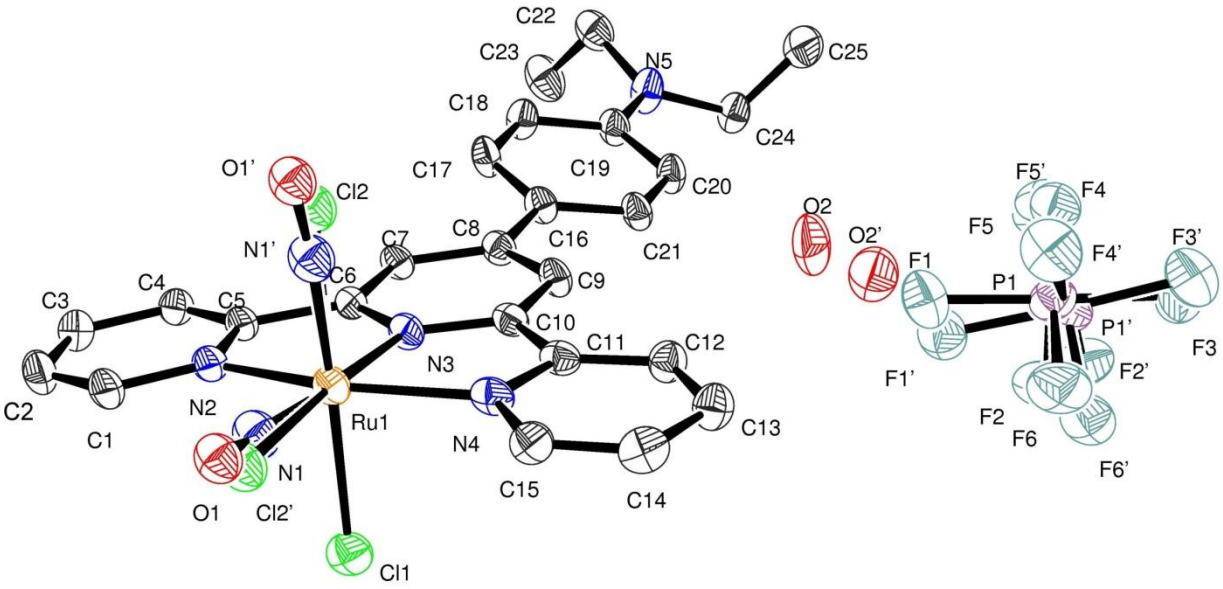

Table 1. Crystal data and structure refinement for rja83m.

Identification code	RJA83
Empirical formula	C25 H24 Cl2 N5 O Ru, F6 P, H2 O
Formula weight	745.43
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	orthorhombic, P b c n
Unit cell dimensions	a = 25.5380(16) A alpha = 90 deg. b = 15.5011(9) A beta = 90 deg. c = 14.6239(9) A gamma = 90 deg.
Volume	5789.1(6) A^3
Z, Calculated density	8, 1.706 Mg/m^3
Absorption coefficient	0.854 mm^-1
F(000)	2976
Crystal size	0.20 x 0.10 x 0.04 mm
Theta range for data collection	1.54 to 25.43 deg.
Limiting indices	-30<=h<=30, -18<=k<=18,

	-17<=l<=17
Reflections collected / unique	65294 / 5335 [R(int) = 0.0807]
Completeness to theta = 25.43	99.6 %
Max. and min. transmission	0.9666 and 0.9030
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5335 / 233 / 454
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0562, wR2 = 0.1420
R indices (all data)	R1 = 0.1029, wR2 = 0.1741
Largest diff. peak and hole	1.064 and -0.678 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for rja83m.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	4401(3)	324(4)	5941(5)	50(2)
C(2)	4798(3)	-227(4)	6172(5)	56(2)
C(3)	5277(3)	96(4)	6398(5)	52(2)
C(4)	5358(3)	978(4)	6415(4)	44(2)
C(5)	4950(2)	1512(4)	6189(4)	41(2)
C(6)	4981(2)	2466(4)	6197(4)	39(1)
C(7)	5418(2)	2955(4)	6384(4)	37(1)
C(8)	5390(2)	3861(4)	6371(4)	38(1)
C(9)	4906(2)	4240(4)	6181(4)	40(2)
C(10)	4473(2)	3738(4)	5998(4)	38(1)
C(11)	3937(2)	4019(4)	5778(4)	41(2)
C(12)	3777(2)	4864(4)	5788(5)	45(2)
C(13)	3259(2)	5063(4)	5619(5)	50(2)
C(14)	2916(3)	4395(5)	5455(5)	53(2)
C(15)	3092(2)	3562(4)	5440(4)	46(2)
C(16)	5864(2)	4367(4)	6552(4)	40(1)
C(17)	6360(2)	3997(4)	6492(5)	47(2)
C(18)	6806(2)	4452(4)	6647(5)	47(2)
C(19)	6790(2)	5325(4)	6898(5)	45(2)
C(20)	6291(2)	5708(4)	6958(5)	44(2)
C(21)	5847(2)	5240(4)	6785(4)	43(2)
C(22)	7764(3)	5441(5)	6808(5)	61(2)
C(23)	7987(3)	4954(5)	7569(6)	75(2)
C(24)	7229(2)	6642(4)	7479(5)	51(2)
C(25)	7225(3)	7359(5)	6786(6)	69(2)
N(2)	4470(2)	1196(3)	5942(4)	43(1)
N(3)	4522(2)	2859(3)	6007(4)	39(1)
N(4)	3593(2)	3374(3)	5590(3)	42(1)
N(5)	7240(2)	5788(3)	7048(5)	57(2)
Cl(1)	3651(1)	2078(1)	7159(1)	55(1)
Ru(1)	3914(1)	2136(1)	5642(1)	42(1)
Cl(2)	4251(1)	2206(2)	4182(2)	57(1)
N(1)	3390(4)	1470(6)	5300(7)	57(1)
O(1)	3075(4)	1156(6)	5035(7)	57(1)
Cl(2')	3138(3)	1331(5)	5250(5)	57(1)
N(1')	4001(10)	2122(14)	4385(13)	57(1)
O(1')	4072(7)	2062(10)	3661(11)	57(1)
P(1)	3590(4)	8025(7)	5534(6)	56(2)
F(1)	3738(6)	7016(7)	5513(8)	73(3)
F(2)	3682(5)	8032(8)	6609(7)	91(3)
F(3)	3451(8)	9027(8)	5523(12)	85(3)
F(4)	3517(4)	7983(7)	4451(6)	63(2)
F(5)	4203(4)	8243(14)	5406(10)	74(3)
F(6)	2996(4)	7780(9)	5655(9)	88(3)
P(1')	3548(6)	8120(10)	5602(9)	66(2)
F(1')	3680(9)	7135(10)	5843(12)	77(4)
F(2')	3773(6)	8426(10)	6562(9)	77(3)
F(3')	3431(11)	9105(10)	5322(16)	84(4)

F(4')	3320(6)	7852(12)	4637(10)	87(4)
F(5')	4124(6)	8217(19)	5173(13)	78(4)
F(6')	2989(5)	8023(11)	6042(11)	80(4)
O(2)	4774(3)	6467(6)	6098(7)	88(3)
O(2')	4759(9)	7011(18)	6540(20)	90(5)

Table 3. Bond lengths [A] and angles [deg] for rja83m.

C(1)-N(2)	1.362(8)
C(1)-C(2)	1.368(10)
C(1)-H(1)	0.9500
C(2)-C(3)	1.364(9)
C(2)-H(2)	0.9500
C(3)-C(4)	1.382(9)
C(3)-H(3)	0.9500
C(4)-C(5)	1.372(9)
C(4)-H(4)	0.9500
C(5)-N(2)	1.369(8)
C(5)-C(6)	1.482(8)
C(6)-N(3)	1.351(8)
C(6)-C(7)	1.376(8)
C(7)-C(8)	1.407(8)
C(7)-H(7)	0.9500
C(8)-C(9)	1.396(8)
C(8)-C(16)	1.466(8)
C(9)-C(10)	1.376(8)
C(9)-H(9)	0.9500
C(10)-N(3)	1.369(7)
C(10)-C(11)	1.472(8)
C(11)-N(4)	1.360(7)
C(11)-C(12)	1.372(9)
C(12)-C(13)	1.382(9)
C(12)-H(12)	0.9500
C(13)-C(14)	1.377(9)
C(13)-H(13)	0.9500
C(14)-C(15)	1.367(9)
C(14)-H(14)	0.9500
C(15)-N(4)	1.330(8)
C(15)-H(15)	0.9500
C(16)-C(17)	1.394(8)
C(16)-C(21)	1.397(8)
C(17)-C(18)	1.359(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.402(9)
C(18)-H(18)	0.9500
C(19)-N(5)	1.373(7)
C(19)-C(20)	1.408(8)
C(20)-C(21)	1.368(8)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.460(10)
C(22)-N(5)	1.484(9)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-N(5)	1.465(8)
C(24)-C(25)	1.505(10)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800

C(25)-H(25C)	0.9800
N(2)-Ru(1)	2.081(5)
N(3)-Ru(1)	1.988(5)
N(4)-Ru(1)	2.089(5)
Cl(1)-Ru(1)	2.3197(19)
Ru(1)-N(1)	1.762(10)
Ru(1)-N(1')	1.852(18)
Ru(1)-Cl(2)	2.305(3)
Ru(1)-Cl(2')	2.411(7)
N(1)-O(1)	1.017(12)
N(1')-O(1')	1.078(17)
P(1)-F(6)	1.573(9)
P(1)-F(2)	1.589(10)
P(1)-F(3)	1.592(10)
P(1)-F(4)	1.597(9)
P(1)-F(1)	1.610(9)
P(1)-F(5)	1.613(9)
P(1')-F(6')	1.573(12)
P(1')-F(4')	1.583(12)
P(1')-F(2')	1.588(12)
P(1')-F(1')	1.603(12)
P(1')-F(5')	1.605(12)
P(1')-F(3')	1.608(12)

N(2)-C(1)-C(2)	121.6(6)
N(2)-C(1)-H(1)	119.2
C(2)-C(1)-H(1)	119.2
C(3)-C(2)-C(1)	119.7(6)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
C(2)-C(3)-C(4)	120.1(7)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	118.6(6)
C(5)-C(4)-H(4)	120.7
C(3)-C(4)-H(4)	120.7
N(2)-C(5)-C(4)	121.9(5)
N(2)-C(5)-C(6)	114.1(6)
C(4)-C(5)-C(6)	124.0(6)
N(3)-C(6)-C(7)	119.9(5)
N(3)-C(6)-C(5)	113.6(5)
C(7)-C(6)-C(5)	126.5(6)
C(6)-C(7)-C(8)	120.3(6)
C(6)-C(7)-H(7)	119.8
C(8)-C(7)-H(7)	119.8
C(9)-C(8)-C(7)	117.9(5)
C(9)-C(8)-C(16)	122.8(5)
C(7)-C(8)-C(16)	119.3(5)
C(10)-C(9)-C(8)	120.8(5)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
N(3)-C(10)-C(9)	119.2(5)
N(3)-C(10)-C(11)	112.4(5)
C(9)-C(10)-C(11)	128.4(6)
N(4)-C(11)-C(12)	120.7(6)
N(4)-C(11)-C(10)	115.4(5)
C(12)-C(11)-C(10)	123.9(6)
C(11)-C(12)-C(13)	119.8(6)

C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(14)-C(13)-C(12)	118.2(6)
C(14)-C(13)-H(13)	120.9
C(12)-C(13)-H(13)	120.9
C(15)-C(14)-C(13)	120.3(6)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
N(4)-C(15)-C(14)	121.4(6)
N(4)-C(15)-H(15)	119.3
C(14)-C(15)-H(15)	119.3
C(17)-C(16)-C(21)	116.2(5)
C(17)-C(16)-C(8)	121.3(5)
C(21)-C(16)-C(8)	122.6(5)
C(18)-C(17)-C(16)	122.5(6)
C(18)-C(17)-H(17)	118.7
C(16)-C(17)-H(17)	118.7
C(17)-C(18)-C(19)	121.3(6)
C(17)-C(18)-H(18)	119.3
C(19)-C(18)-H(18)	119.3
N(5)-C(19)-C(18)	121.5(6)
N(5)-C(19)-C(20)	121.7(5)
C(18)-C(19)-C(20)	116.7(5)
C(21)-C(20)-C(19)	121.0(5)
C(21)-C(20)-H(20)	119.5
C(19)-C(20)-H(20)	119.5
C(20)-C(21)-C(16)	122.3(6)
C(20)-C(21)-H(21)	118.9
C(16)-C(21)-H(21)	118.9
C(23)-C(22)-N(5)	111.1(7)
C(23)-C(22)-H(22A)	109.4
N(5)-C(22)-H(22A)	109.4
C(23)-C(22)-H(22B)	109.4
N(5)-C(22)-H(22B)	109.4
H(22A)-C(22)-H(22B)	108.0
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(5)-C(24)-C(25)	112.2(6)
N(5)-C(24)-H(24A)	109.2
C(25)-C(24)-H(24A)	109.2
N(5)-C(24)-H(24B)	109.2
C(25)-C(24)-H(24B)	109.2
H(24A)-C(24)-H(24B)	107.9
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(1)-N(2)-C(5)	118.1(6)
C(1)-N(2)-Ru(1)	127.3(5)
C(5)-N(2)-Ru(1)	114.6(4)
C(6)-N(3)-C(10)	121.9(5)
C(6)-N(3)-Ru(1)	118.7(4)

C(10)-N(3)-Ru(1)	119.2(4)
C(15)-N(4)-C(11)	119.6(6)
C(15)-N(4)-Ru(1)	125.8(4)
C(11)-N(4)-Ru(1)	114.5(4)
C(19)-N(5)-C(24)	121.7(5)
C(19)-N(5)-C(22)	121.8(5)
C(24)-N(5)-C(22)	116.5(5)
N(1)-Ru(1)-N(1')	78.6(8)
N(1)-Ru(1)-N(3)	178.0(4)
N(1')-Ru(1)-N(3)	100.3(7)
N(1)-Ru(1)-N(2)	99.7(3)
N(1')-Ru(1)-N(2)	96.8(7)
N(3)-Ru(1)-N(2)	78.8(2)
N(1)-Ru(1)-N(4)	103.3(3)
N(1')-Ru(1)-N(4)	91.3(7)
N(3)-Ru(1)-N(4)	78.34(19)
N(2)-Ru(1)-N(4)	156.77(19)
N(1)-Ru(1)-Cl(2)	92.8(3)
N(1')-Ru(1)-Cl(2)	15.4(7)
N(3)-Ru(1)-Cl(2)	86.01(17)
N(2)-Ru(1)-Cl(2)	88.45(16)
N(4)-Ru(1)-Cl(2)	94.00(15)
N(1)-Ru(1)-Cl(1)	91.7(3)
N(1')-Ru(1)-Cl(1)	169.7(7)
N(3)-Ru(1)-Cl(1)	89.46(16)
N(2)-Ru(1)-Cl(1)	88.22(15)
N(4)-Ru(1)-Cl(1)	87.51(14)
Cl(2)-Ru(1)-Cl(1)	174.83(9)
N(1)-Ru(1)-Cl(2')	5.9(4)
N(1')-Ru(1)-Cl(2')	81.8(8)
N(3)-Ru(1)-Cl(2')	176.0(2)
N(2)-Ru(1)-Cl(2')	104.4(2)
N(4)-Ru(1)-Cl(2')	98.3(2)
Cl(2)-Ru(1)-Cl(2')	96.4(2)
Cl(1)-Ru(1)-Cl(2')	88.3(2)
O(1)-N(1)-Ru(1)	171.5(10)
O(1')-N(1')-Ru(1)	175(2)
F(6)-P(1)-F(2)	91.9(7)
F(6)-P(1)-F(3)	91.3(8)
F(2)-P(1)-F(3)	92.1(8)
F(6)-P(1)-F(4)	89.4(6)
F(2)-P(1)-F(4)	177.3(8)
F(3)-P(1)-F(4)	90.2(8)
F(6)-P(1)-F(1)	89.7(7)
F(2)-P(1)-F(1)	89.4(7)
F(3)-P(1)-F(1)	178.1(9)
F(4)-P(1)-F(1)	88.2(6)
F(6)-P(1)-F(5)	178.1(9)
F(2)-P(1)-F(5)	88.3(7)
F(3)-P(1)-F(5)	90.6(8)
F(4)-P(1)-F(5)	90.3(7)
F(1)-P(1)-F(5)	88.4(8)
F(6')-P(1')-F(4')	90.2(9)
F(6')-P(1')-F(2')	89.7(9)
F(4')-P(1')-F(2')	177.8(12)
F(6')-P(1')-F(1')	90.5(9)
F(4')-P(1')-F(1')	91.3(10)
F(2')-P(1')-F(1')	90.8(9)

F(6')-P(1')-F(5')	178.9(11)
F(4')-P(1')-F(5')	90.7(10)
F(2')-P(1')-F(5')	89.3(10)
F(1')-P(1')-F(5')	89.0(11)
F(6')-P(1')-F(3')	91.5(11)
F(4')-P(1')-F(3')	87.3(10)
F(2')-P(1')-F(3')	90.5(10)
F(1')-P(1')-F(3')	177.6(12)
F(5')-P(1')-F(3')	89.0(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for rja83m.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	56(4)	36(4)	57(4)	-7(3)	7(3)	-19(3)
C(2)	74(5)	33(4)	60(5)	-1(3)	3(4)	-11(3)
C(3)	59(4)	41(4)	56(4)	-4(3)	3(4)	-1(3)
C(4)	51(4)	39(4)	43(4)	-5(3)	3(3)	-6(3)
C(5)	44(4)	33(3)	44(4)	-5(3)	7(3)	-13(3)
C(6)	40(3)	31(3)	45(4)	-1(3)	10(3)	-4(3)
C(7)	31(3)	36(3)	44(4)	3(3)	-3(3)	-7(3)
C(8)	38(3)	36(3)	40(4)	0(3)	-1(3)	-7(3)
C(9)	38(3)	30(3)	53(4)	2(3)	-4(3)	-11(3)
C(10)	38(3)	37(3)	40(3)	5(3)	4(3)	-5(3)
C(11)	36(3)	45(4)	41(4)	1(3)	3(3)	-9(3)
C(12)	44(4)	41(4)	51(4)	-4(3)	-1(3)	-1(3)
C(13)	45(4)	47(4)	57(4)	-3(3)	-6(3)	4(3)
C(14)	40(4)	67(5)	52(4)	-6(4)	-8(3)	-3(3)
C(15)	38(4)	48(4)	53(4)	-7(3)	0(3)	-9(3)
C(16)	33(3)	36(3)	50(4)	3(3)	-6(3)	-6(3)
C(17)	45(4)	28(3)	67(5)	3(3)	-5(3)	-4(3)
C(18)	33(3)	38(4)	70(5)	-8(3)	-3(3)	-2(3)
C(19)	37(3)	34(3)	63(4)	-2(3)	1(3)	-8(3)
C(20)	37(3)	29(3)	66(5)	-4(3)	-3(3)	-3(3)
C(21)	32(3)	31(3)	64(4)	5(3)	-1(3)	-5(3)
C(22)	65(5)	53(4)	66(5)	3(4)	-8(4)	-20(4)
C(23)	88(6)	60(5)	79(6)	5(4)	-21(5)	-21(5)
C(24)	35(4)	41(4)	78(5)	-13(4)	-2(3)	-8(3)
C(25)	71(5)	54(5)	84(6)	-18(4)	11(4)	-20(4)
N(2)	48(3)	36(3)	44(3)	-4(2)	7(2)	-10(2)
N(3)	33(3)	35(3)	50(3)	-2(2)	2(2)	-10(2)
N(4)	33(3)	48(3)	45(3)	-2(2)	-1(2)	-16(2)
N(5)	31(3)	41(3)	99(5)	-18(3)	-4(3)	-8(2)
Cl(1)	44(1)	60(1)	62(1)	-5(1)	0(1)	-13(1)
Ru(1)	36(1)	39(1)	51(1)	-6(1)	2(1)	-13(1)
Cl(2)	59(2)	55(1)	56(2)	0(1)	-6(1)	-8(1)
N(1)	59(2)	55(1)	56(2)	0(1)	-6(1)	-8(1)
O(1)	59(2)	55(1)	56(2)	0(1)	-6(1)	-8(1)
Cl(2')	59(2)	55(1)	56(2)	0(1)	-6(1)	-8(1)
N(1')	59(2)	55(1)	56(2)	0(1)	-6(1)	-8(1)
O(1')	59(2)	55(1)	56(2)	0(1)	-6(1)	-8(1)
P(1)	44(3)	61(3)	64(3)	-7(2)	6(2)	-4(2)
F(1)	70(6)	57(4)	91(8)	9(5)	-17(6)	-6(4)
F(2)	95(6)	113(8)	65(4)	-2(5)	8(4)	-27(6)
F(3)	94(6)	63(5)	98(8)	-11(5)	11(7)	0(5)
F(4)	60(6)	63(5)	65(4)	0(4)	0(4)	-8(4)
F(5)	53(4)	89(6)	80(8)	-20(6)	6(4)	-30(4)
F(6)	50(4)	108(8)	105(8)	10(6)	9(5)	-15(4)
P(1')	58(4)	67(4)	73(4)	5(4)	2(3)	-18(4)
F(1')	64(7)	69(6)	99(10)	11(6)	7(7)	0(5)
F(2')	64(6)	97(9)	70(5)	-9(6)	4(5)	-3(7)

F(3')	92(8)	68(6)	93(10)	10(6)	-9(7)	-12(6)
F(4')	87(9)	87(7)	89(7)	-7(6)	-20(6)	-21(7)
F(5')	69(6)	91(7)	74(8)	-14(7)	19(6)	-23(6)
F(6')	49(5)	85(9)	106(10)	22(8)	5(6)	-4(5)
O(2)	82(5)	53(5)	129(8)	13(5)	-13(5)	22(4)
O(2')	74(9)	76(10)	120(12)	-6(9)	8(9)	-5(9)