Supplementary Information

for

Ruthenium nitrosyl complexes with NO release capability: the use of fluorene as an antenna

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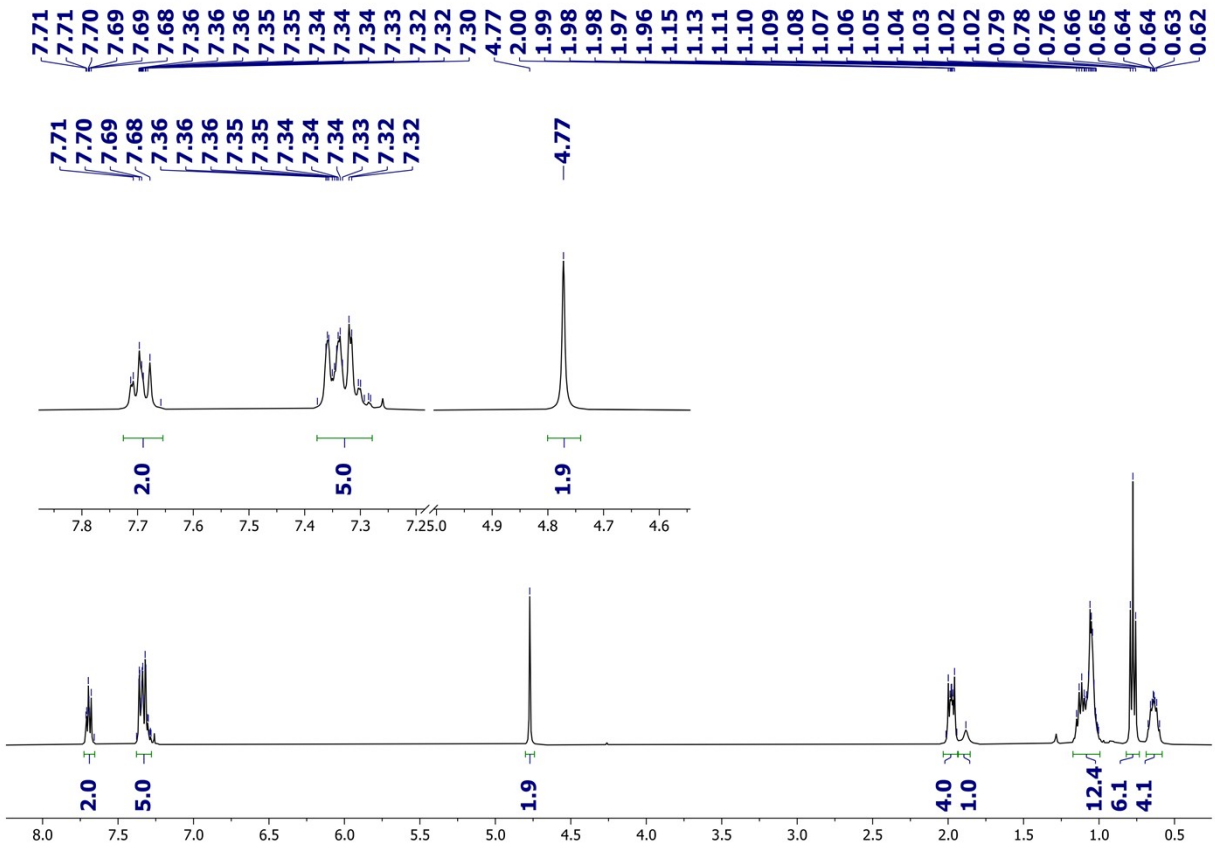
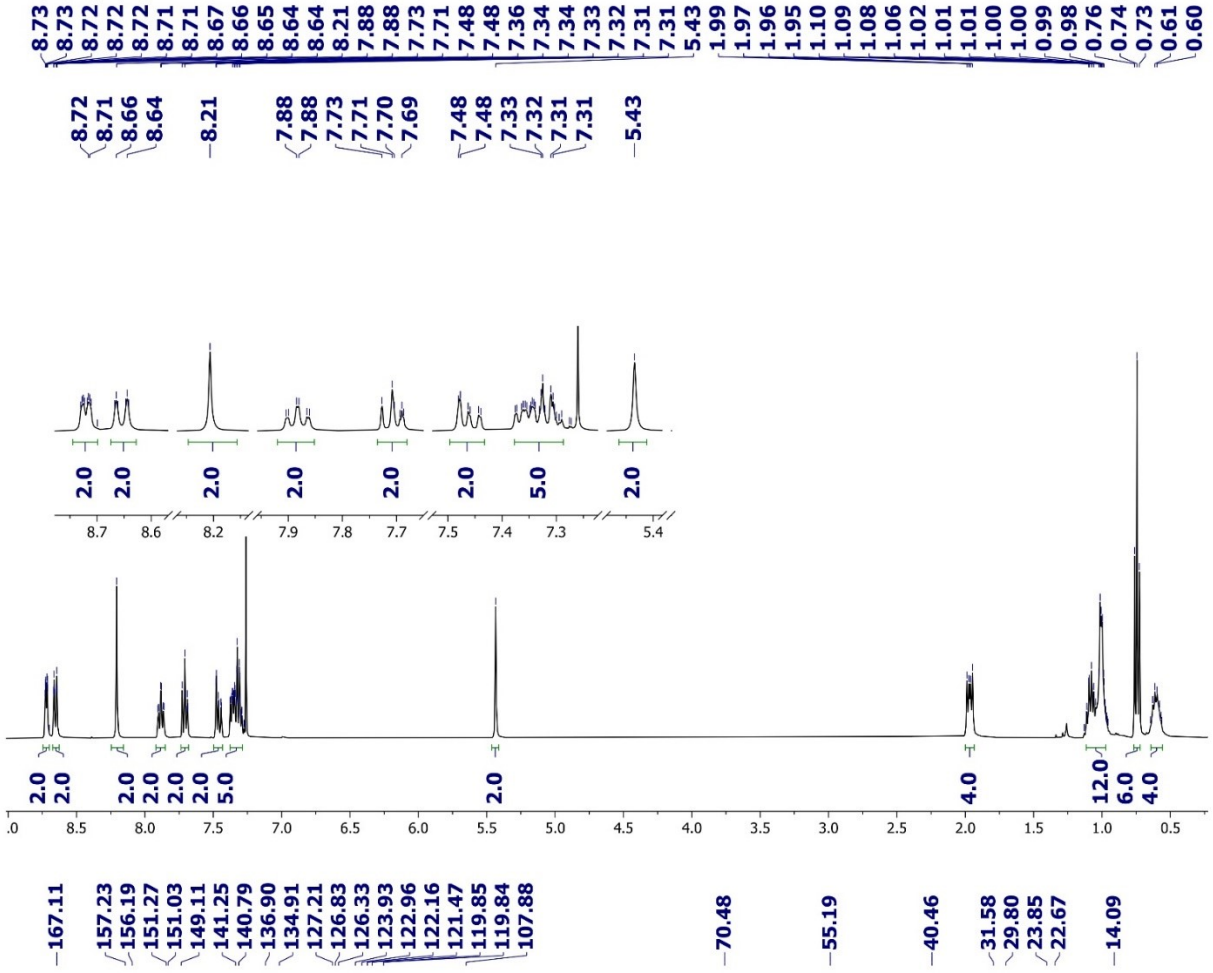
Summary

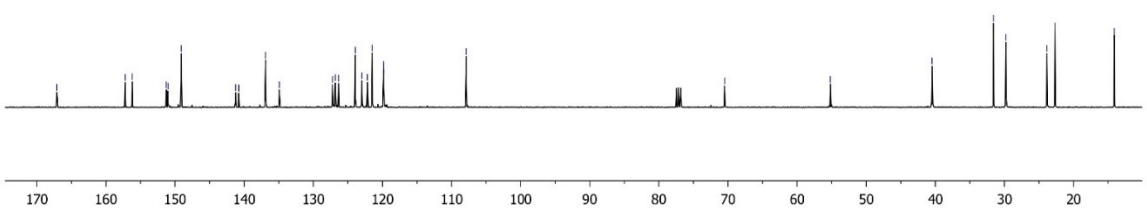
1. NMR Spectra

(9,9-dihexyl-9H-fluoren-2-yl)methanol

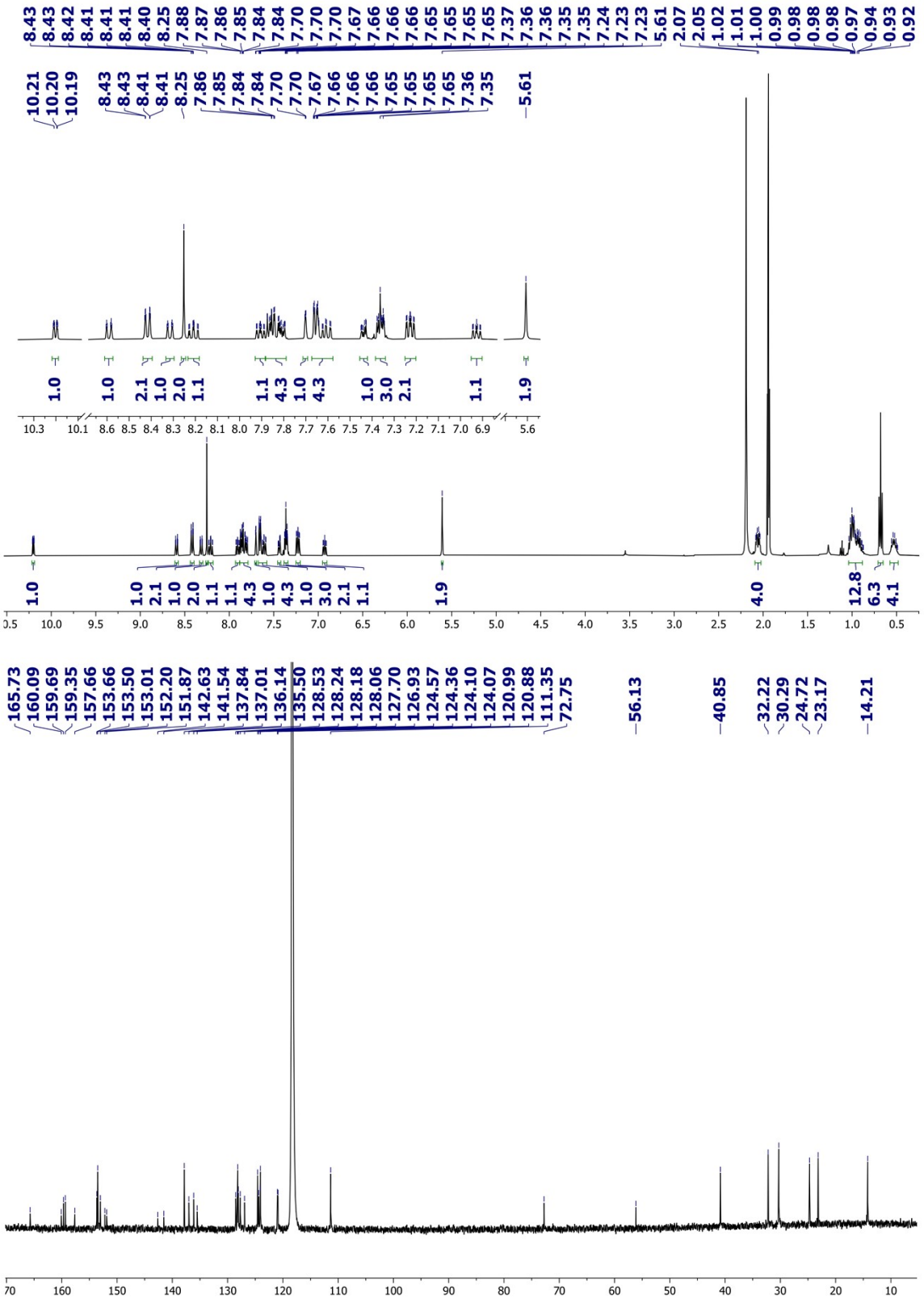


4'-((9,9-dihexyl-9H-fluoren-2-yl)methoxy)-2,2':6',2''-terpyridine (2Hex-flu-CH2O-tpy)

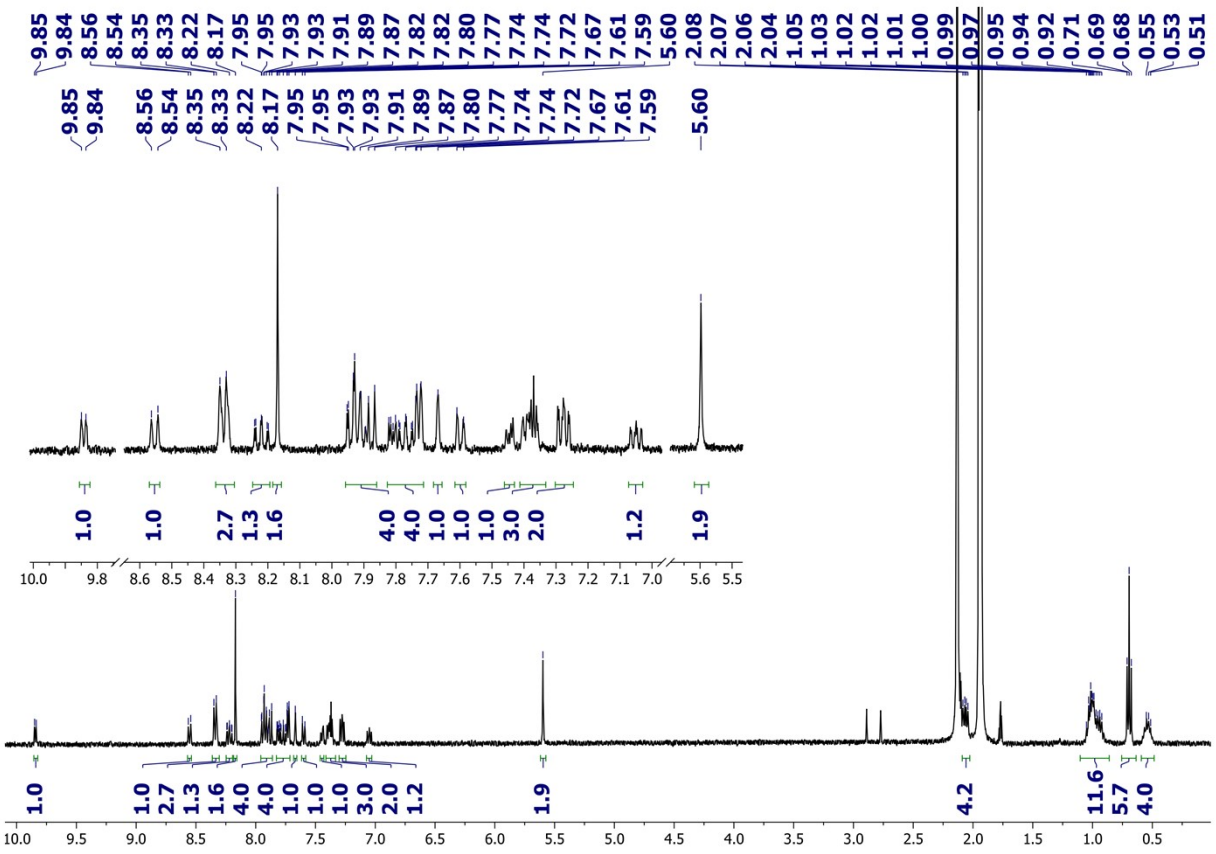




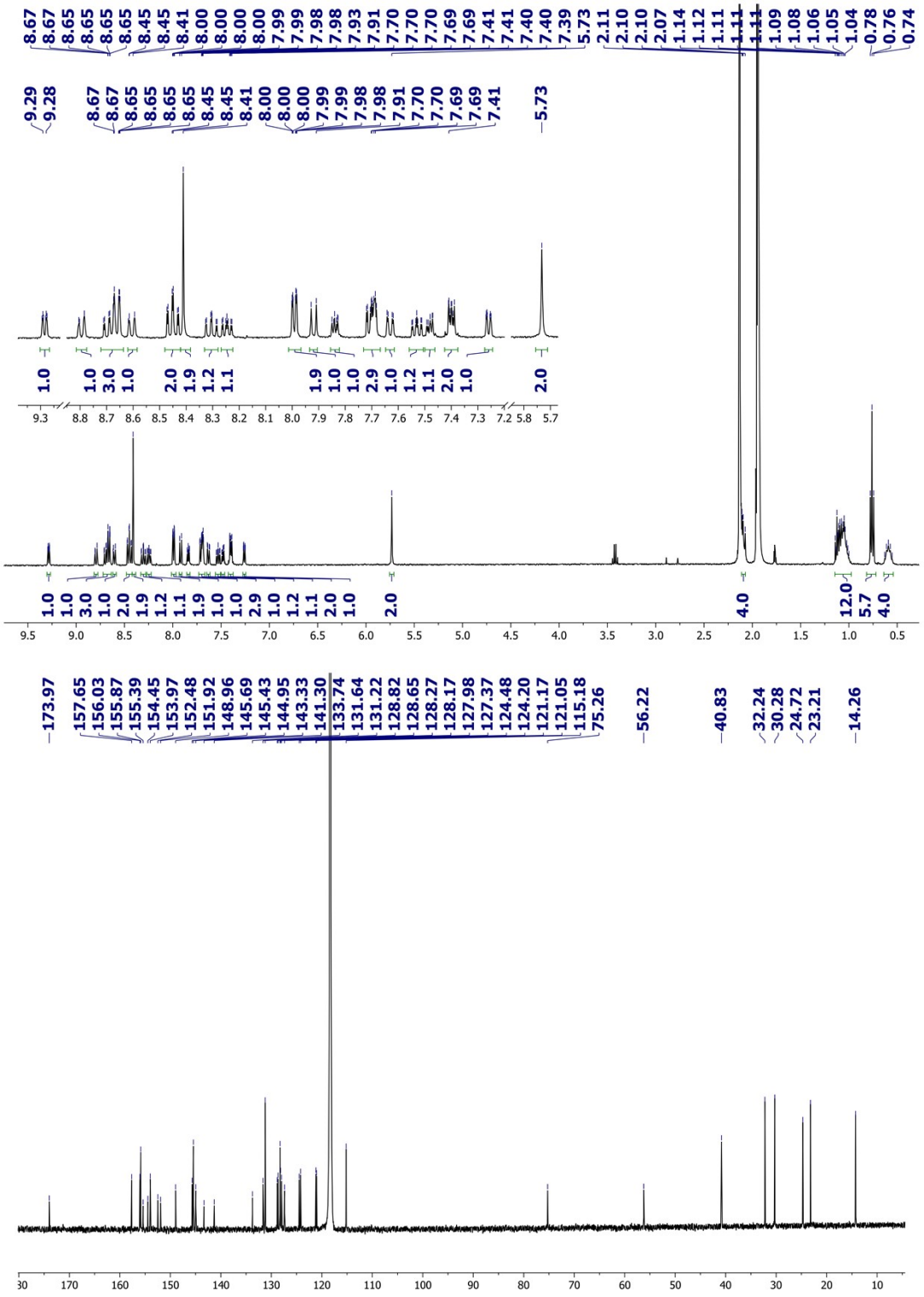
[Ru^{II}(2Hex-flu-CH2O-tpy)(bpy)Cl](PF_6)



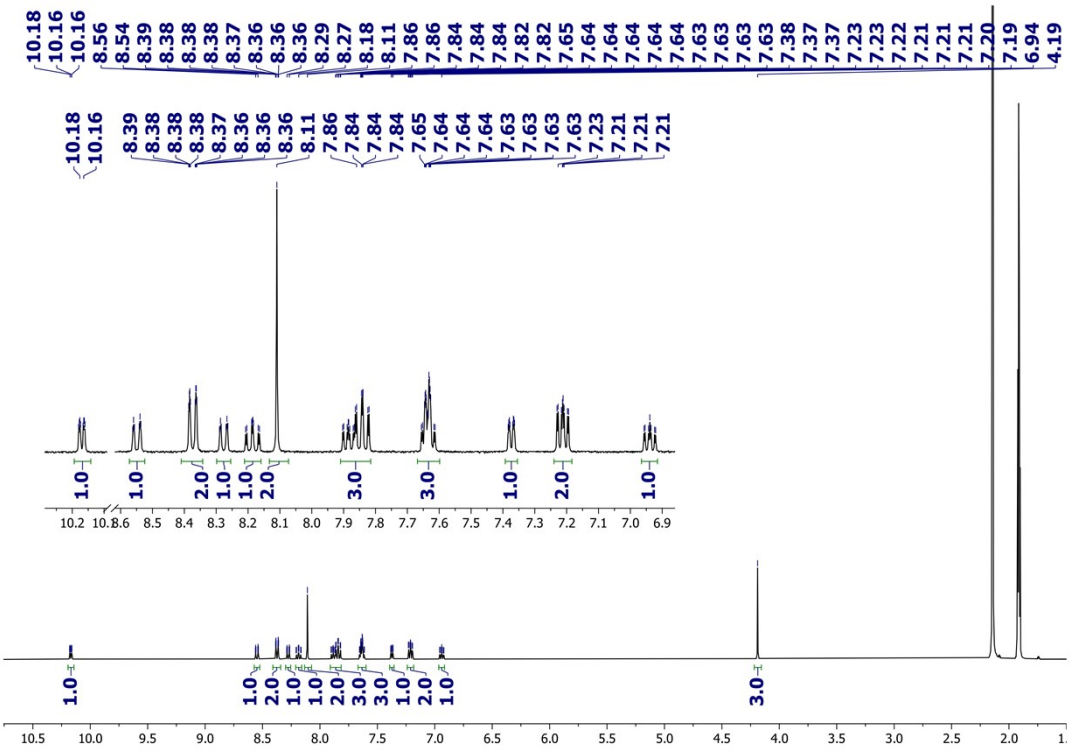
[Ru^{II}(2Hex-flu-CH2O-tpy)(bpy)(NO_2)](PF_6)



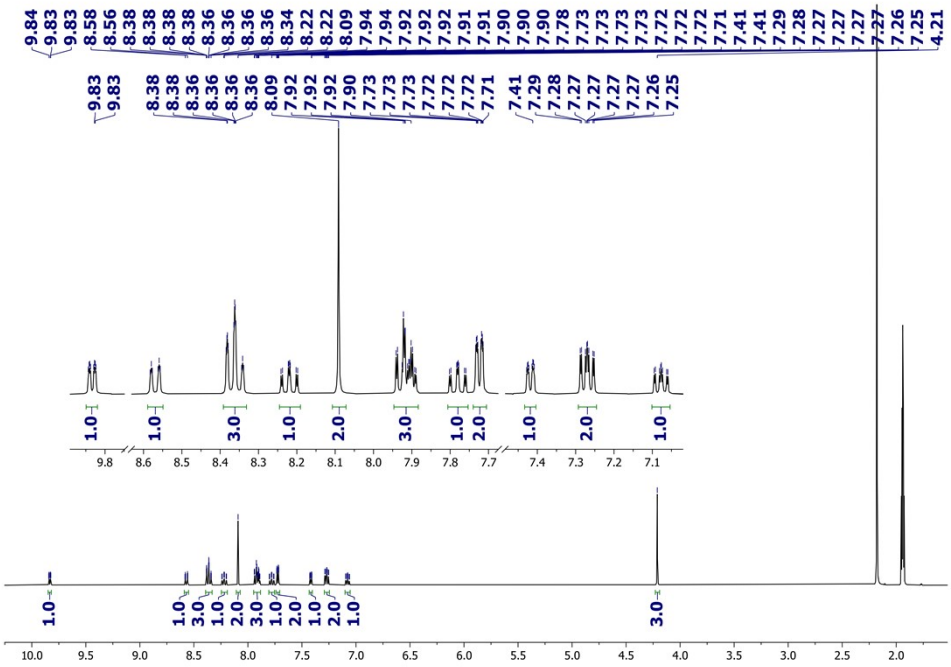
$[Ru^{II}(2Hex\text{-}flu\text{-}CH2O\text{-}tpy)(bpy)(NO)](PF_6)_3$

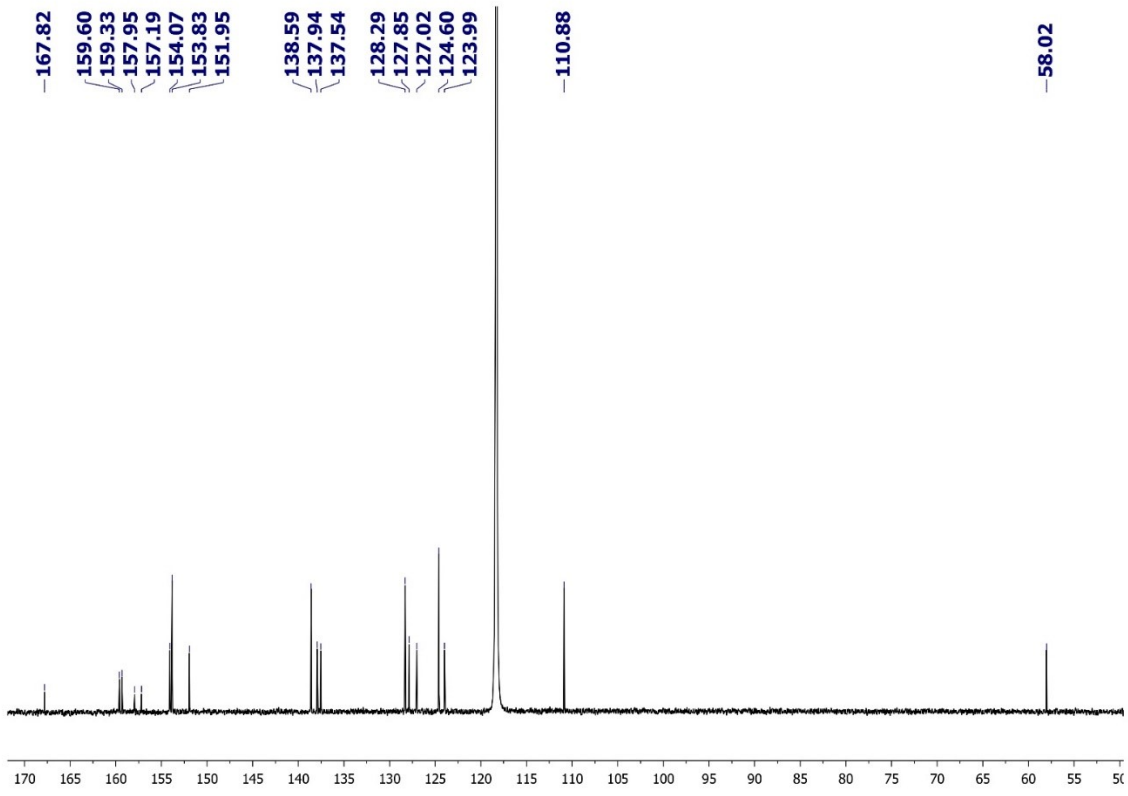


[Ru^{II}(MeO-tpy)(bpy)Cl](PF_6)

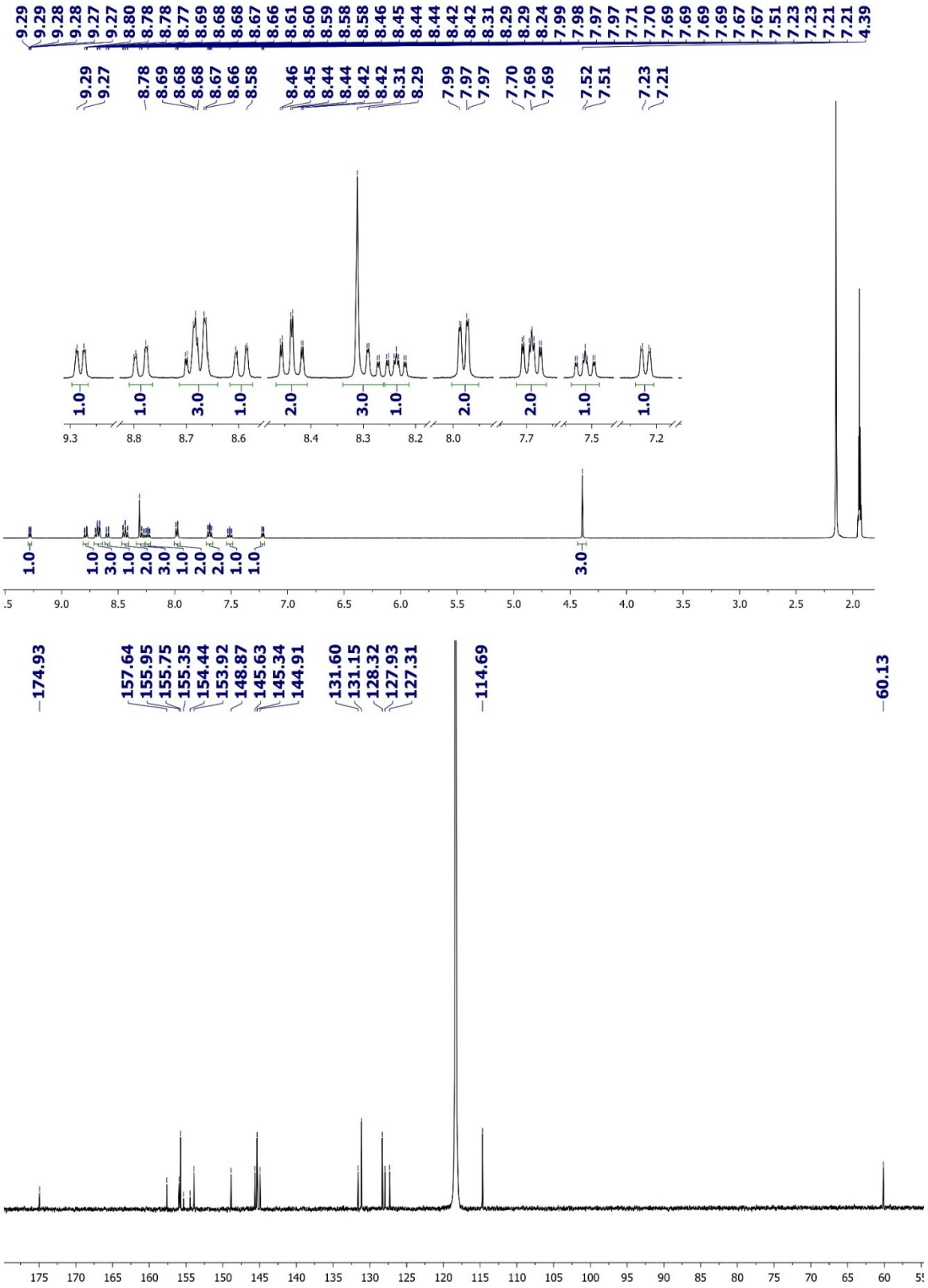


$[Ru^{II}(MeO\text{-}tpy)(bpy)(NO_2)](PF_6)$





$[Ru^{II}(MeO\text{-}tpy)(bpy)(NO)](PF_6)_3$



2. X-ray Data for $[C_{51}H_{53}N6O_3Ru]$ (PF_6) (*5b*)

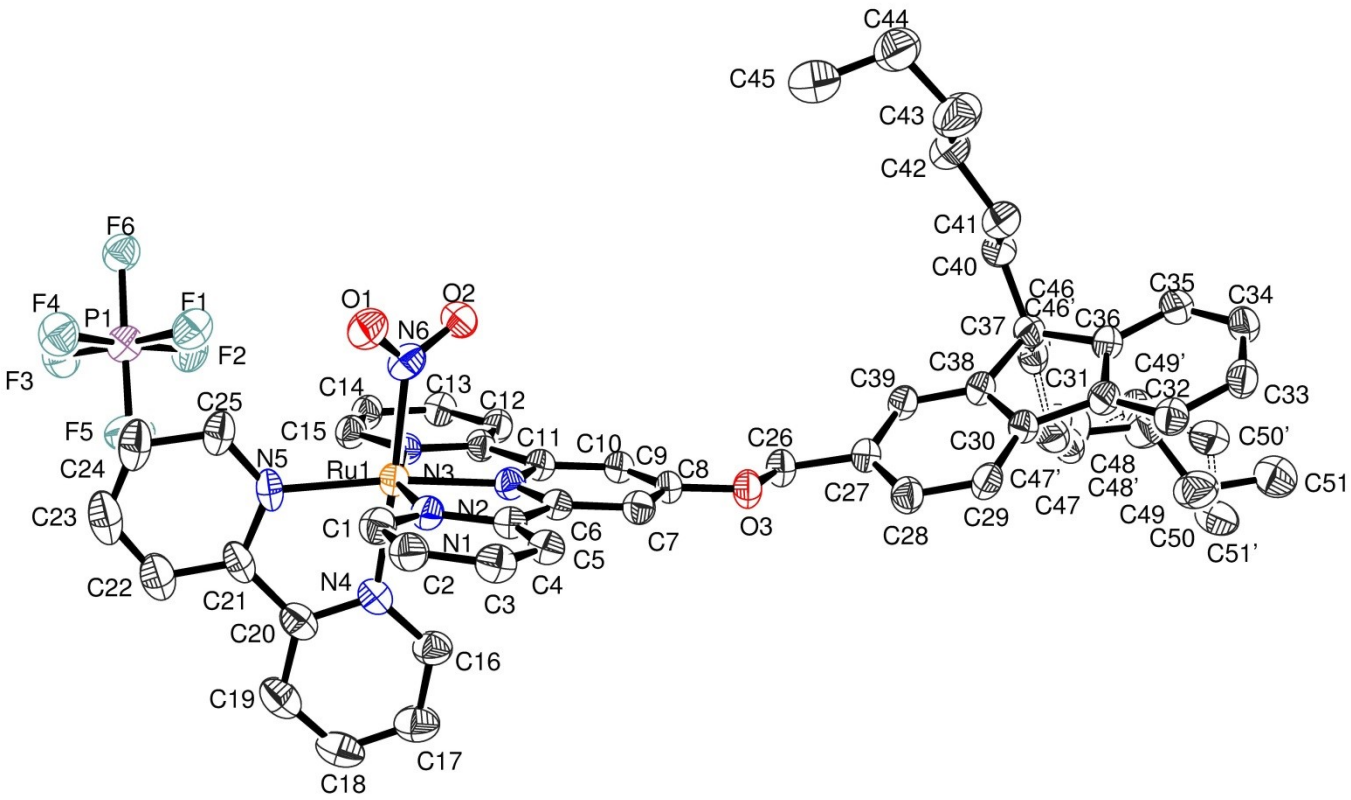


Figure 1 : Asymmetric Unit

Table 1. Crystal data and structure refinement

Empirical formula	C51 H53 N6 O3 Ru, P F6
Formula weight	1044.03
Temperature	100(2) K
Wavelength	1.54184 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 13.2505(2) A alpha = 90 deg. b = 11.0878(2) A beta = 92.6550(10) deg. c = 32.1285(4) A gamma = 90 deg.
Volume	4715.22(13) A^3
Z, Calculated density	4, 1.471 Mg/m^3
Absorption coefficient	3.642 mm^-1
F(000)	2152
Theta range for data collection	2.754 to 80.213 deg.

Limiting indices	-16<=h<=16, -10<=k<=13, -40<=l<=40
Reflections collected / unique	76605 / 10112 [R(int) = 0.0659]
Completeness to theta = 67.684	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10112 / 201 / 670
Goodness-of-fit on F^2	1.093
Final R indices [I>2sigma(I)]	R1 = 0.0520, wR2 = 0.1325
R indices (all data)	R1 = 0.0702, wR2 = 0.1428
Largest diff. peak and hole	0.858 and -1.827 e.A^-3

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

	x	y	z	U(eq)
C(1)	4786(3)	2966(4)	6063(1)	36(1)
C(2)	5833(3)	2922(4)	6114(1)	39(1)
C(3)	6408(3)	3030(4)	5768(1)	39(1)
C(4)	5928(3)	3201(4)	5382(1)	36(1)
C(5)	4882(3)	3230(3)	5347(1)	32(1)
C(6)	4300(3)	3420(3)	4947(1)	31(1)
C(7)	4690(3)	3603(4)	4562(1)	34(1)
C(8)	4006(3)	3793(3)	4219(1)	32(1)
C(9)	2972(3)	3769(3)	4268(1)	32(1)
C(10)	2629(3)	3587(4)	4664(1)	32(1)
C(11)	1560(3)	3535(4)	4780(1)	31(1)
C(12)	750(3)	3687(4)	4499(1)	36(1)
C(13)	-223(3)	3632(4)	4638(1)	37(1)
C(14)	-360(3)	3409(4)	5054(1)	37(1)
C(15)	480(3)	3266(4)	5322(1)	34(1)
C(16)	2982(3)	637(4)	5168(1)	41(1)
C(17)	2925(4)	-602(4)	5154(2)	51(1)
C(18)	2558(4)	-1220(4)	5488(2)	55(1)
C(19)	2254(4)	-565(4)	5828(2)	51(1)
C(20)	2336(3)	689(4)	5831(1)	40(1)
C(21)	2077(3)	1461(4)	6181(1)	41(1)
C(22)	1718(3)	1020(5)	6548(1)	52(1)
C(23)	1549(4)	1809(5)	6867(2)	58(1)
C(24)	1744(3)	3015(5)	6821(1)	51(1)
C(25)	2096(3)	3419(5)	6443(1)	42(1)
C(26)	3816(3)	4239(4)	3490(1)	36(1)
C(27)	4482(3)	4745(4)	3166(1)	35(1)
C(28)	5502(3)	4433(4)	3163(1)	39(1)
C(29)	6121(3)	4934(4)	2873(1)	37(1)
C(30)	5716(3)	5761(4)	2586(1)	33(1)
C(31)	6179(3)	6459(4)	2259(1)	35(1)
C(32)	7168(3)	6497(4)	2131(1)	39(1)
C(33)	7396(3)	7262(4)	1806(1)	41(1)
C(34)	6657(3)	7975(4)	1611(1)	42(1)
C(35)	5670(4)	7948(4)	1739(1)	43(1)
C(36)	5436(3)	7191(4)	2066(1)	36(1)
C(37)	4422(3)	7025(4)	2263(1)	37(1)
C(46)	3570(20)	6660(30)	1940(13)	41(5)
C(47)	3760(30)	5430(20)	1741(8)	50(5)
C(48)	3044(16)	5180(20)	1365(5)	70(5)
C(49)	3437(15)	5550(20)	955(6)	71(4)
C(50)	4253(10)	4750(13)	790(3)	63(3)
C(51)	4675(8)	5220(10)	390(3)	67(3)
C(46')	3630(30)	6520(40)	1941(14)	43(5)
C(47')	3810(30)	5290(20)	1749(8)	46(5)
C(48')	3105(16)	4999(18)	1373(5)	44(4)

C(49')	3240(17)	5770(20)	991(7)	62(4)
C(50')	4230(9)	5641(11)	774(4)	61(3)
C(51')	4444(12)	4364(11)	658(5)	59(4)
C(38)	4688(3)	6067(4)	2587(1)	34(1)
C(39)	4071(3)	5561(4)	2876(1)	34(1)
C(40)	4086(3)	8192(4)	2479(1)	45(1)
C(41)	4895(4)	8769(5)	2768(2)	52(1)
C(42)	4504(4)	9668(5)	3077(2)	57(1)
C(43)	5346(4)	10294(6)	3340(2)	73(2)
C(44)	4998(4)	11075(5)	3695(2)	66(2)
C(45)	4699(4)	10360(5)	4066(2)	62(1)
N(1)	4312(2)	3103(3)	5688(1)	32(1)
N(2)	3289(2)	3411(3)	4989(1)	31(1)
N(3)	1424(2)	3319(3)	5194(1)	30(1)
N(4)	2698(2)	1288(3)	5499(1)	35(1)
N(5)	2252(2)	2667(3)	6128(1)	36(1)
N(6)	2811(2)	4987(3)	5622(1)	39(1)
O(1)	3115(2)	5474(3)	5952(1)	48(1)
O(2)	2587(2)	5682(3)	5315(1)	41(1)
O(3)	4447(2)	4003(3)	3857(1)	37(1)
F(1)	91(2)	4520(2)	6288(1)	46(1)
F(2)	-1363(2)	3859(2)	5977(1)	47(1)
F(3)	-1966(2)	3390(2)	6605(1)	51(1)
F(4)	-499(2)	4060(3)	6920(1)	52(1)
F(5)	-462(2)	2632(3)	6417(1)	57(1)
F(6)	-1403(2)	5277(2)	6479(1)	43(1)
P(1)	-927(1)	3938(1)	6454(1)	40(1)
Ru(1)	2771(1)	3153(1)	5546(1)	30(1)

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

C(1)-N(1)	1.342(5)
C(1)-C(2)	1.389(6)
C(1)-H(1)	0.9500
C(2)-C(3)	1.380(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.382(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.386(5)
C(4)-H(4)	0.9500
C(5)-N(1)	1.367(5)
C(5)-C(6)	1.482(5)
C(6)-N(2)	1.353(5)
C(6)-C(7)	1.378(5)
C(7)-C(8)	1.407(5)
C(7)-H(7)	0.9500
C(8)-O(3)	1.348(4)
C(8)-C(9)	1.387(5)
C(9)-C(10)	1.385(5)
C(9)-H(9)	0.9500
C(10)-N(2)	1.345(5)
C(10)-C(11)	1.481(5)
C(11)-N(3)	1.372(5)
C(11)-C(12)	1.380(5)
C(12)-C(13)	1.384(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.381(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.383(5)
C(14)-H(14)	0.9500
C(15)-N(3)	1.336(5)
C(15)-H(15)	0.9500
C(16)-N(4)	1.352(5)
C(16)-C(17)	1.377(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.381(7)
C(17)-H(17)	0.9500
C(18)-C(19)	1.386(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.396(7)
C(19)-H(19)	0.9500
C(20)-N(4)	1.360(5)
C(20)-C(21)	1.467(6)
C(21)-N(5)	1.369(6)
C(21)-C(22)	1.381(6)
C(22)-C(23)	1.375(8)
C(22)-H(22)	0.9500
C(23)-C(24)	1.371(7)
C(23)-H(23)	0.9500
C(24)-C(25)	1.395(6)
C(24)-H(24)	0.9500
C(25)-N(5)	1.336(5)
C(25)-H(25)	0.9500
C(26)-O(3)	1.438(4)
C(26)-C(27)	1.505(5)

C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(39)	1.390(5)
C(27)-C(28)	1.395(5)
C(28)-C(29)	1.387(5)
C(28)-H(28)	0.9500
C(29)-C(30)	1.391(5)
C(29)-H(29)	0.9500
C(30)-C(38)	1.403(5)
C(30)-C(31)	1.463(5)
C(31)-C(32)	1.391(5)
C(31)-C(36)	1.399(6)
C(32)-C(33)	1.389(6)
C(32)-H(32)	0.9500
C(33)-C(34)	1.386(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.389(6)
C(34)-H(34)	0.9500
C(35)-C(36)	1.390(6)
C(35)-H(35)	0.9500
C(36)-C(37)	1.523(5)
C(37)-C(38)	1.516(5)
C(37)-C(40)	1.544(6)
C(37)-C(46')	1.549(13)
C(37)-C(46)	1.553(11)
C(46)-C(47)	1.529(12)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(48)	1.527(11)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.500(13)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(50)	1.516(14)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-C(51)	1.517(12)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(46')-C(47')	1.519(13)
C(46')-H(46C)	0.9900
C(46')-H(46D)	0.9900
C(47')-C(48')	1.531(13)
C(47')-H(47C)	0.9900
C(47')-H(47D)	0.9900
C(48')-C(49')	1.513(13)
C(48')-H(48C)	0.9900
C(48')-H(48D)	0.9900
C(49')-C(50')	1.521(14)
C(49')-H(49C)	0.9900
C(49')-H(49D)	0.9900
C(50')-C(51')	1.495(12)
C(50')-H(50C)	0.9900
C(50')-H(50D)	0.9900

C(51')-H(51D)	0.9800
C(51')-H(51E)	0.9800
C(51')-H(51F)	0.9800
C(38)-C(39)	1.386(5)
C(39)-H(39)	0.9500
C(40)-C(41)	1.526(7)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(42)	1.514(6)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-C(43)	1.534(8)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(44)	1.522(7)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(45)	1.499(8)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
N(1)-Ru(1)	2.073(3)
N(2)-Ru(1)	1.969(3)
N(3)-Ru(1)	2.077(3)
N(4)-Ru(1)	2.075(3)
N(5)-Ru(1)	2.091(3)
N(6)-O(1)	1.241(4)
N(6)-O(2)	1.275(4)
N(6)-Ru(1)	2.049(4)
F(1)-P(1)	1.608(3)
F(2)-P(1)	1.614(3)
F(3)-P(1)	1.600(3)
F(4)-P(1)	1.583(3)
F(5)-P(1)	1.580(3)
F(6)-P(1)	1.617(3)

N(1)-C(1)-C(2)	122.1(4)
N(1)-C(1)-H(1)	118.9
C(2)-C(1)-H(1)	118.9
C(3)-C(2)-C(1)	119.2(4)
C(3)-C(2)-H(2)	120.4
C(1)-C(2)-H(2)	120.4
C(2)-C(3)-C(4)	119.1(4)
C(2)-C(3)-H(3)	120.4
C(4)-C(3)-H(3)	120.4
C(3)-C(4)-C(5)	119.5(4)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
N(1)-C(5)-C(4)	121.4(3)
N(1)-C(5)-C(6)	115.1(3)
C(4)-C(5)-C(6)	123.5(3)
N(2)-C(6)-C(7)	120.3(3)
N(2)-C(6)-C(5)	113.0(3)
C(7)-C(6)-C(5)	126.7(3)
C(6)-C(7)-C(8)	118.0(3)
C(6)-C(7)-H(7)	121.0

C(8)-C(7)-H(7)	121.0
O(3)-C(8)-C(9)	124.8(3)
O(3)-C(8)-C(7)	114.4(3)
C(9)-C(8)-C(7)	120.9(3)
C(10)-C(9)-C(8)	118.3(3)
C(10)-C(9)-H(9)	120.9
C(8)-C(9)-H(9)	120.9
N(2)-C(10)-C(9)	120.3(3)
N(2)-C(10)-C(11)	113.2(3)
C(9)-C(10)-C(11)	126.5(3)
N(3)-C(11)-C(12)	121.4(3)
N(3)-C(11)-C(10)	114.9(3)
C(12)-C(11)-C(10)	123.7(3)
C(11)-C(12)-C(13)	119.5(4)
C(11)-C(12)-H(12)	120.2
C(13)-C(12)-H(12)	120.2
C(14)-C(13)-C(12)	119.0(4)
C(14)-C(13)-H(13)	120.5
C(12)-C(13)-H(13)	120.5
C(13)-C(14)-C(15)	119.0(4)
C(13)-C(14)-H(14)	120.5
C(15)-C(14)-H(14)	120.5
N(3)-C(15)-C(14)	122.7(4)
N(3)-C(15)-H(15)	118.6
C(14)-C(15)-H(15)	118.6
N(4)-C(16)-C(17)	122.8(4)
N(4)-C(16)-H(16)	118.6
C(17)-C(16)-H(16)	118.6
C(16)-C(17)-C(18)	119.3(5)
C(16)-C(17)-H(17)	120.3
C(18)-C(17)-H(17)	120.3
C(17)-C(18)-C(19)	118.6(5)
C(17)-C(18)-H(18)	120.7
C(19)-C(18)-H(18)	120.7
C(18)-C(19)-C(20)	120.1(4)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
N(4)-C(20)-C(19)	120.8(4)
N(4)-C(20)-C(21)	114.8(4)
C(19)-C(20)-C(21)	124.4(4)
N(5)-C(21)-C(22)	121.3(4)
N(5)-C(21)-C(20)	115.3(3)
C(22)-C(21)-C(20)	123.4(4)
C(23)-C(22)-C(21)	119.0(5)
C(23)-C(22)-H(22)	120.5
C(21)-C(22)-H(22)	120.5
C(24)-C(23)-C(22)	120.2(4)
C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
C(23)-C(24)-C(25)	118.6(5)
C(23)-C(24)-H(24)	120.7
C(25)-C(24)-H(24)	120.7
N(5)-C(25)-C(24)	122.0(5)
N(5)-C(25)-H(25)	119.0
C(24)-C(25)-H(25)	119.0
O(3)-C(26)-C(27)	107.2(3)
O(3)-C(26)-H(26A)	110.3
C(27)-C(26)-H(26A)	110.3

O(3)-C(26)-H(26B)	110.3
C(27)-C(26)-H(26B)	110.3
H(26A)-C(26)-H(26B)	108.5
C(39)-C(27)-C(28)	120.4(4)
C(39)-C(27)-C(26)	118.7(3)
C(28)-C(27)-C(26)	120.8(3)
C(29)-C(28)-C(27)	120.6(4)
C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(28)-C(29)-C(30)	119.2(4)
C(28)-C(29)-H(29)	120.4
C(30)-C(29)-H(29)	120.4
C(29)-C(30)-C(38)	120.2(3)
C(29)-C(30)-C(31)	131.5(4)
C(38)-C(30)-C(31)	108.3(3)
C(32)-C(31)-C(36)	120.3(4)
C(32)-C(31)-C(30)	131.3(4)
C(36)-C(31)-C(30)	108.4(3)
C(33)-C(32)-C(31)	118.7(4)
C(33)-C(32)-H(32)	120.6
C(31)-C(32)-H(32)	120.6
C(34)-C(33)-C(32)	121.0(4)
C(34)-C(33)-H(33)	119.5
C(32)-C(33)-H(33)	119.5
C(33)-C(34)-C(35)	120.6(4)
C(33)-C(34)-H(34)	119.7
C(35)-C(34)-H(34)	119.7
C(34)-C(35)-C(36)	118.8(4)
C(34)-C(35)-H(35)	120.6
C(36)-C(35)-H(35)	120.6
C(35)-C(36)-C(31)	120.6(4)
C(35)-C(36)-C(37)	128.2(4)
C(31)-C(36)-C(37)	111.2(3)
C(38)-C(37)-C(36)	100.9(3)
C(38)-C(37)-C(40)	110.0(3)
C(36)-C(37)-C(40)	111.3(4)
C(38)-C(37)-C(46')	110(2)
C(36)-C(37)-C(46')	111(2)
C(40)-C(37)-C(46')	113.7(12)
C(38)-C(37)-C(46)	114.4(19)
C(36)-C(37)-C(46)	112(2)
C(40)-C(37)-C(46)	107.7(10)
C(47)-C(46)-C(37)	112.5(14)
C(47)-C(46)-H(46A)	109.1
C(37)-C(46)-H(46A)	109.1
C(47)-C(46)-H(46B)	109.1
C(37)-C(46)-H(46B)	109.1
H(46A)-C(46)-H(46B)	107.8
C(48)-C(47)-C(46)	112.5(13)
C(48)-C(47)-H(47A)	109.1
C(46)-C(47)-H(47A)	109.1
C(48)-C(47)-H(47B)	109.1
C(46)-C(47)-H(47B)	109.1
H(47A)-C(47)-H(47B)	107.8
C(49)-C(48)-C(47)	114.6(15)
C(49)-C(48)-H(48A)	108.6
C(47)-C(48)-H(48A)	108.6
C(49)-C(48)-H(48B)	108.6

C(47)-C(48)-H(48B)	108.6
H(48A)-C(48)-H(48B)	107.6
C(48)-C(49)-C(50)	115.3(14)
C(48)-C(49)-H(49A)	108.4
C(50)-C(49)-H(49A)	108.4
C(48)-C(49)-H(49B)	108.5
C(50)-C(49)-H(49B)	108.5
H(49A)-C(49)-H(49B)	107.5
C(49)-C(50)-C(51)	113.0(12)
C(49)-C(50)-H(50A)	109.0
C(51)-C(50)-H(50A)	109.0
C(49)-C(50)-H(50B)	109.0
C(51)-C(50)-H(50B)	109.0
H(50A)-C(50)-H(50B)	107.8
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(47')-C(46')-C(37)	118.4(17)
C(47')-C(46')-H(46C)	107.7
C(37)-C(46')-H(46C)	107.7
C(47')-C(46')-H(46D)	107.7
C(37)-C(46')-H(46D)	107.7
H(46C)-C(46')-H(46D)	107.1
C(46')-C(47')-C(48')	113.9(16)
C(46')-C(47')-H(47C)	108.8
C(48')-C(47')-H(47C)	108.8
C(46')-C(47')-H(47D)	108.8
C(48')-C(47')-H(47D)	108.8
H(47C)-C(47')-H(47D)	107.7
C(49')-C(48')-C(47')	115.4(15)
C(49')-C(48')-H(48C)	108.4
C(47')-C(48')-H(48C)	108.4
C(49')-C(48')-H(48D)	108.4
C(47')-C(48')-H(48D)	108.4
H(48C)-C(48')-H(48D)	107.5
C(48')-C(49')-C(50')	117.0(15)
C(48')-C(49')-H(49C)	108.1
C(50')-C(49')-H(49C)	108.1
C(48')-C(49')-H(49D)	108.0
C(50')-C(49')-H(49D)	108.0
H(49C)-C(49')-H(49D)	107.3
C(51')-C(50')-C(49')	112.5(13)
C(51')-C(50')-H(50C)	109.1
C(49')-C(50')-H(50C)	109.1
C(51')-C(50')-H(50D)	109.1
C(49')-C(50')-H(50D)	109.1
H(50C)-C(50')-H(50D)	107.8
C(50')-C(51')-H(51D)	109.5
C(50')-C(51')-H(51E)	109.5
H(51D)-C(51')-H(51E)	109.5
C(50')-C(51')-H(51F)	109.5
H(51D)-C(51')-H(51F)	109.5
H(51E)-C(51')-H(51F)	109.5
C(39)-C(38)-C(30)	120.4(4)
C(39)-C(38)-C(37)	128.2(4)

C(30)-C(38)-C(37)	111.3(3)
C(38)-C(39)-C(27)	119.2(3)
C(38)-C(39)-H(39)	120.4
C(27)-C(39)-H(39)	120.4
C(41)-C(40)-C(37)	114.6(4)
C(41)-C(40)-H(40A)	108.6
C(37)-C(40)-H(40A)	108.6
C(41)-C(40)-H(40B)	108.6
C(37)-C(40)-H(40B)	108.6
H(40A)-C(40)-H(40B)	107.6
C(42)-C(41)-C(40)	115.0(4)
C(42)-C(41)-H(41A)	108.5
C(40)-C(41)-H(41A)	108.5
C(42)-C(41)-H(41B)	108.5
C(40)-C(41)-H(41B)	108.5
H(41A)-C(41)-H(41B)	107.5
C(41)-C(42)-C(43)	113.4(4)
C(41)-C(42)-H(42A)	108.9
C(43)-C(42)-H(42A)	108.9
C(41)-C(42)-H(42B)	108.9
C(43)-C(42)-H(42B)	108.9
H(42A)-C(42)-H(42B)	107.7
C(44)-C(43)-C(42)	115.7(5)
C(44)-C(43)-H(43A)	108.4
C(42)-C(43)-H(43A)	108.4
C(44)-C(43)-H(43B)	108.4
C(42)-C(43)-H(43B)	108.4
H(43A)-C(43)-H(43B)	107.4
C(45)-C(44)-C(43)	113.3(5)
C(45)-C(44)-H(44A)	108.9
C(43)-C(44)-H(44A)	108.9
C(45)-C(44)-H(44B)	108.9
C(43)-C(44)-H(44B)	108.9
H(44A)-C(44)-H(44B)	107.7
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(1)-N(1)-C(5)	118.6(3)
C(1)-N(1)-Ru(1)	128.0(3)
C(5)-N(1)-Ru(1)	113.4(2)
C(10)-N(2)-C(6)	122.2(3)
C(10)-N(2)-Ru(1)	119.1(2)
C(6)-N(2)-Ru(1)	118.7(2)
C(15)-N(3)-C(11)	118.3(3)
C(15)-N(3)-Ru(1)	128.4(3)
C(11)-N(3)-Ru(1)	113.3(2)
C(16)-N(4)-C(20)	118.4(4)
C(16)-N(4)-Ru(1)	125.1(3)
C(20)-N(4)-Ru(1)	116.5(3)
C(25)-N(5)-C(21)	118.8(3)
C(25)-N(5)-Ru(1)	125.9(3)
C(21)-N(5)-Ru(1)	115.3(3)
O(1)-N(6)-O(2)	116.9(4)
O(1)-N(6)-Ru(1)	122.6(3)
O(2)-N(6)-Ru(1)	120.3(3)

C(8)-O(3)-C(26)	118.7(3)
F(5)-P(1)-F(4)	91.35(15)
F(5)-P(1)-F(3)	91.06(16)
F(4)-P(1)-F(3)	91.22(15)
F(5)-P(1)-F(1)	90.43(15)
F(4)-P(1)-F(1)	90.48(14)
F(3)-P(1)-F(1)	177.71(16)
F(5)-P(1)-F(2)	90.25(15)
F(4)-P(1)-F(2)	178.20(17)
F(3)-P(1)-F(2)	89.57(14)
F(1)-P(1)-F(2)	88.68(13)
F(5)-P(1)-F(6)	178.69(16)
F(4)-P(1)-F(6)	89.83(14)
F(3)-P(1)-F(6)	89.48(14)
F(1)-P(1)-F(6)	89.00(14)
F(2)-P(1)-F(6)	88.56(14)
N(2)-Ru(1)-N(6)	87.44(13)
N(2)-Ru(1)-N(1)	79.71(12)
N(6)-Ru(1)-N(1)	88.87(13)
N(2)-Ru(1)-N(4)	95.47(13)
N(6)-Ru(1)-N(4)	177.08(13)
N(1)-Ru(1)-N(4)	91.79(12)
N(2)-Ru(1)-N(3)	79.52(12)
N(6)-Ru(1)-N(3)	89.63(12)
N(1)-Ru(1)-N(3)	159.22(12)
N(4)-Ru(1)-N(3)	90.75(12)
N(2)-Ru(1)-N(5)	173.37(14)
N(6)-Ru(1)-N(5)	99.08(14)
N(1)-Ru(1)-N(5)	99.13(12)
N(4)-Ru(1)-N(5)	78.01(14)
N(3)-Ru(1)-N(5)	101.57(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for vlad150322_auto.
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)	38(2)	36(2)	33(2)	-2(2)	-1(2)	0(2)
C(2)	41(2)	38(2)	37(2)	0(2)	-1(2)	1(2)
C(3)	33(2)	39(2)	45(2)	0(2)	-1(2)	0(2)
C(4)	39(2)	31(2)	39(2)	1(2)	5(2)	0(2)
C(5)	35(2)	28(2)	33(2)	0(2)	4(1)	1(2)
C(6)	35(2)	26(2)	32(2)	0(1)	6(1)	-1(1)
C(7)	32(2)	33(2)	36(2)	2(2)	5(2)	1(2)
C(8)	37(2)	30(2)	28(2)	2(1)	10(1)	-1(2)
C(9)	37(2)	30(2)	30(2)	0(2)	5(1)	0(2)
C(10)	36(2)	30(2)	29(2)	0(1)	4(1)	0(2)
C(11)	33(2)	32(2)	26(2)	0(1)	2(1)	-1(2)
C(12)	38(2)	38(2)	31(2)	-1(2)	5(2)	-2(2)
C(13)	36(2)	39(2)	36(2)	-1(2)	1(2)	-1(2)
C(14)	33(2)	41(2)	38(2)	-1(2)	8(2)	-1(2)
C(15)	32(2)	35(2)	35(2)	-1(2)	7(1)	-2(2)
C(16)	48(2)	34(2)	41(2)	-4(2)	-2(2)	0(2)
C(17)	58(3)	40(3)	56(3)	-6(2)	-4(2)	0(2)
C(18)	62(3)	32(3)	69(3)	4(2)	-7(2)	-4(2)
C(19)	49(3)	45(3)	60(3)	16(2)	2(2)	-6(2)
C(20)	37(2)	39(2)	45(2)	11(2)	-2(2)	-1(2)
C(21)	36(2)	48(3)	38(2)	19(2)	4(2)	-2(2)
C(22)	47(2)	65(3)	45(2)	18(2)	7(2)	2(2)
C(23)	48(3)	84(4)	42(2)	24(3)	7(2)	2(3)
C(24)	44(2)	80(4)	28(2)	4(2)	4(2)	4(2)
C(25)	39(2)	60(3)	27(2)	1(2)	5(2)	3(2)
C(26)	35(2)	44(2)	29(2)	3(2)	4(1)	-1(2)
C(27)	39(2)	36(2)	30(2)	1(2)	7(2)	1(2)
C(28)	40(2)	43(2)	33(2)	5(2)	5(2)	3(2)
C(29)	34(2)	45(2)	33(2)	-1(2)	9(2)	6(2)
C(30)	39(2)	33(2)	28(2)	0(2)	6(1)	-1(2)
C(31)	41(2)	37(2)	28(2)	-3(2)	5(2)	-1(2)
C(32)	37(2)	42(2)	38(2)	-2(2)	4(2)	-3(2)
C(33)	45(2)	44(2)	35(2)	-4(2)	12(2)	-8(2)
C(34)	56(3)	38(2)	34(2)	2(2)	13(2)	-5(2)
C(35)	54(2)	38(3)	38(2)	4(2)	8(2)	2(2)
C(36)	43(2)	37(2)	30(2)	1(2)	7(2)	1(2)
C(37)	40(2)	37(2)	33(2)	5(2)	5(2)	4(2)
C(46)	39(8)	45(9)	39(9)	3(7)	-2(6)	5(6)
C(47)	39(7)	67(10)	43(7)	-13(8)	-3(6)	4(8)
C(48)	51(8)	109(13)	48(7)	-24(7)	-5(5)	-7(9)
C(49)	83(9)	82(10)	46(6)	-16(6)	-2(5)	13(7)
C(50)	85(8)	56(9)	49(6)	-3(6)	1(5)	15(6)
C(51)	71(7)	63(7)	67(6)	9(5)	4(5)	5(5)
C(46')	40(10)	52(11)	37(9)	15(7)	7(8)	6(8)
C(47')	53(11)	44(8)	40(7)	9(7)	-1(7)	2(7)
C(48')	42(8)	48(7)	43(7)	15(5)	5(5)	4(6)
C(49')	93(10)	56(9)	39(6)	6(6)	16(6)	7(7)
C(50')	79(7)	43(7)	61(7)	7(5)	16(5)	9(6)
C(51')	72(8)	40(7)	64(9)	6(6)	0(6)	1(6)
C(38)	39(2)	36(2)	29(2)	-2(2)	7(2)	1(2)
C(39)	33(2)	39(2)	29(2)	0(2)	5(1)	2(2)

C(40)	52(2)	39(2)	44(2)	7(2)	12(2)	10(2)
C(41)	57(3)	44(3)	55(3)	-6(2)	15(2)	0(2)
C(42)	59(3)	48(3)	65(3)	-9(2)	20(2)	1(2)
C(43)	65(3)	62(4)	93(4)	-30(3)	25(3)	-16(3)
C(44)	66(3)	56(3)	77(4)	-15(3)	18(3)	-5(3)
C(45)	64(3)	54(3)	68(3)	-8(3)	-5(3)	4(3)
N(1)	32(2)	32(2)	32(2)	0(1)	4(1)	0(1)
N(2)	30(2)	30(2)	32(2)	-1(1)	5(1)	-2(1)
N(3)	29(1)	31(2)	30(2)	2(1)	1(1)	2(1)
N(4)	33(2)	35(2)	36(2)	6(1)	-1(1)	-3(1)
N(5)	32(2)	50(2)	26(2)	10(1)	6(1)	-3(1)
N(6)	35(2)	44(2)	38(2)	-6(2)	1(1)	6(2)
O(1)	57(2)	48(2)	40(2)	-9(1)	3(1)	-2(2)
O(2)	44(2)	37(2)	42(2)	5(1)	4(1)	0(1)
O(3)	36(1)	47(2)	30(1)	7(1)	8(1)	3(1)
F(1)	35(1)	53(2)	52(1)	-9(1)	4(1)	-2(1)
F(2)	44(1)	59(2)	40(1)	-6(1)	1(1)	-7(1)
F(3)	44(1)	57(2)	51(1)	6(1)	7(1)	-4(1)
F(4)	55(2)	60(2)	41(1)	1(1)	-6(1)	5(1)
F(5)	47(1)	46(2)	77(2)	-8(1)	-4(1)	5(1)
F(6)	41(1)	47(2)	42(1)	-2(1)	2(1)	4(1)
P(1)	37(1)	43(1)	40(1)	-2(1)	1(1)	0(1)
Ru(1)	31(1)	33(1)	27(1)	1(1)	4(1)	0(1)

3. Atomic coordinates (B3PW91/6-31G*)

A

O	-2.618534	-0.509918	0.222921
C	-3.299266	-1.283733	-0.754479
H	-2.857897	-1.142445	-1.753232
H	-3.215619	-2.357415	-0.519260
C	-4.756166	-0.894892	-0.787998
C	-8.875970	0.096253	-0.610501
C	-9.023426	0.338556	0.768648
C	-11.351755	0.827988	0.419594
C	-9.964353	0.219907	-1.475674
H	-9.855073	0.033699	-2.541456
C	-11.203457	0.587755	-0.949654
H	-12.060835	0.688096	-1.610472
C	-10.260567	0.703778	1.286062
H	-10.387808	0.892936	2.349886
C	-5.429445	-0.561843	0.396135
H	-4.876487	-0.544185	1.331661
C	-6.819219	-0.600256	-2.051057
H	-7.344319	-0.612546	-3.003139
C	-6.781060	-0.249386	0.353093
C	-5.459212	-0.904479	-1.999833
H	-4.932339	-1.152201	-2.919178
C	-7.480507	-0.270260	-0.868114
C	-7.702402	0.142455	1.501628
C	-7.235451	1.447056	2.173667
H	-7.940611	1.750768	2.955800
H	-6.253268	1.309579	2.640091
H	-7.158695	2.261160	1.445232
C	-7.803440	-0.980552	2.550125
H	-8.517642	-0.709907	3.336224
H	-8.134718	-1.919187	2.093429
H	-6.830482	-1.153439	3.024016
H	-12.323462	1.113569	0.814637
H	-1.753953	-0.921390	0.363608

C

Ru	0.448318	0.014662	-0.607328
N	-1.503769	0.158118	-0.251240
C	-2.226322	-0.977066	-0.174922
C	-1.414322	-2.207005	-0.283889
N	0.246464	2.100091	-0.418519
N	-0.072103	-2.019672	-0.465457
C	0.275177	-4.379020	-0.474299
H	0.973449	-5.204035	-0.555277
C	-2.042135	1.394756	-0.134389
C	-3.402017	1.524887	0.058266
H	-3.883914	2.489315	0.160062
C	0.950940	4.377991	-0.370827
H	1.765577	5.089235	-0.443217
C	-1.048888	2.485369	-0.210628

C	-4.197752	0.360078	0.125929
C	-1.939147	-3.490068	-0.195047
H	-3.002529	-3.638438	-0.050879
C	-3.597658	-0.909605	0.015547
H	-4.188867	-1.812548	0.080063
C	0.747175	-3.073175	-0.558459
H	1.799069	-2.861016	-0.705983
C	1.216063	3.019289	-0.501720
H	2.219663	2.652934	-0.679599
C	-1.369084	3.830079	-0.071470
H	-2.395284	4.132677	0.098480
C	-0.358968	4.786706	-0.151320
H	-0.600283	5.838896	-0.043498
C	-1.086031	-4.588086	-0.291911
H	-1.488457	-5.593240	-0.225082
N	0.274269	0.038115	-2.366722
O	0.201438	0.037340	-3.497616
C	2.194547	-0.178749	1.765006
C	2.596088	-0.253348	3.096420
H	3.643776	-0.357907	3.347639
C	1.645121	-0.192112	4.108543
H	1.952261	-0.249643	5.147429
C	0.304000	-0.056757	3.767825
H	-0.475057	-0.003246	4.519262
C	-0.039791	0.008471	2.426163
H	-1.074576	0.110952	2.130854
N	0.877447	-0.051811	1.444934
C	3.341140	-0.178658	-1.691284
H	2.852608	-0.110068	-2.654310
C	4.721925	-0.288862	-1.612064
H	5.306848	-0.307816	-2.524336
C	5.316036	-0.370613	-0.357540
H	6.392583	-0.457216	-0.256310
C	4.509728	-0.338493	0.774426
H	4.958471	-0.399138	1.757539
C	3.127910	-0.226168	0.633694
N	2.559001	-0.148443	-0.597306
O	-5.491315	0.563183	0.303596
C	-6.384866	-0.556576	0.391824
H	-7.373878	-0.121138	0.522760
H	-6.355842	-1.143778	-0.530438
H	-6.134996	-1.178501	1.256347

***AC* (fluorene ⊥ terpyridine)**

O	2.536916	0.131224	-0.730470
C	3.317492	1.358806	-0.629743
H	3.031847	2.011879	-1.460723
H	3.068057	1.842742	0.320039
C	4.767028	0.988646	-0.691435
C	8.847467	-0.129382	-0.605022
C	9.031832	-0.335112	0.775316
C	11.330147	-0.907914	0.365479
C	9.901016	-0.312187	-1.502730

H	9.761105	-0.154810	-2.569407
C	11.144598	-0.703333	-1.005817
H	11.976410	-0.850395	-1.689830
C	10.273871	-0.724952	1.263748
H	10.431568	-0.887431	2.327639
C	5.458518	0.663675	0.485247
H	4.939379	0.700331	1.441051
C	6.775101	0.593125	-2.004732
H	7.277992	0.573637	-2.967969
C	6.797001	0.305758	0.414421
C	5.430602	0.950754	-1.925091
H	4.887918	1.209101	-2.831488
C	7.456027	0.269923	-0.829876
C	7.743322	-0.075285	1.544874
C	7.262492	-1.341860	2.277638
H	7.988821	-1.641432	3.041581
H	6.304795	-1.158131	2.777967
H	7.132624	-2.176966	1.581134
C	7.911487	1.081355	2.548126
H	8.644494	0.816691	3.318457
H	8.253474	1.993159	2.047200
H	6.960863	1.298773	3.048487
H	12.305354	-1.212238	0.736931
Ru	-3.495835	-0.004541	-0.583901
N	-1.508494	0.074130	-0.585718
C	-0.912895	1.279113	-0.484382
C	-1.863052	2.396523	-0.305684
N	-3.032929	-2.052654	-0.687227
N	-3.186761	2.053318	-0.280395
C	-3.791955	4.335927	0.050907
H	-4.581265	5.066041	0.187315
C	-0.824259	-1.086344	-0.718390
C	0.553779	-1.058064	-0.766811
H	1.147723	-1.958056	-0.865674
C	-3.460373	-4.395533	-0.802126
H	-4.190634	-5.196399	-0.814696
C	-1.687697	-2.283634	-0.764802
C	1.218044	0.185765	-0.676166
C	-1.478324	3.722261	-0.152865
H	-0.429947	3.994655	-0.171478
C	0.469679	1.371110	-0.526430
H	0.958842	2.331391	-0.440578
C	-4.121923	2.993932	-0.108676
H	-5.152884	2.661030	-0.103962
C	-3.893369	-3.077529	-0.706531
H	-4.946274	-2.829903	-0.651913
C	-1.200984	-3.580853	-0.865112
H	-0.134254	-3.760126	-0.926985
C	-2.096254	-4.648558	-0.883822
H	-1.725166	-5.664963	-0.961834
C	-2.452466	4.702944	0.026754
H	-2.159831	5.740793	0.145725
N	-3.656187	0.175844	-2.335073
O	-3.809774	0.297471	-3.451485
C	-4.794854	-0.302054	2.049171

C	-4.954231	-0.437117	3.425992
H	-5.944257	-0.502410	3.858250
C	-3.835197	-0.489806	4.249054
H	-3.953785	-0.594893	5.322218
C	-2.571217	-0.408216	3.675667
H	-1.667836	-0.447170	4.272957
C	-2.471061	-0.272724	2.299366
H	-1.501481	-0.207874	1.826297
N	-3.551584	-0.217955	1.501274
C	-6.540120	-0.080786	-1.138977
H	-6.228590	0.012739	-2.171025
C	-7.887728	-0.152945	-0.816900
H	-8.626468	-0.112801	-1.609023
C	-8.250967	-0.275515	0.519689
H	-9.294815	-0.333466	0.809254
C	-7.255166	-0.326208	1.488341
H	-7.524056	-0.425068	2.532313
C	-5.917397	-0.248837	1.105577
N	-5.575219	-0.123741	-0.202924

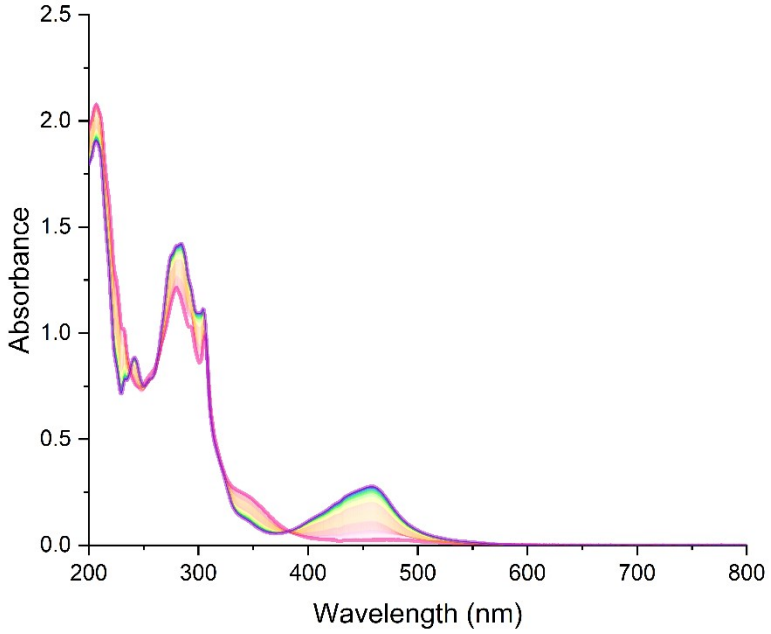
***AC* (fluorene // terpyridine)**

O	2.580965	0.387170	-0.346319
C	3.287136	1.637725	-0.309247
H	3.063944	2.192024	-1.229498
H	2.926410	2.223135	0.545630
C	4.766122	1.375958	-0.180914
C	8.907215	0.568921	0.184513
C	8.896142	-0.838876	0.170345
C	11.290308	-0.845243	0.388583
C	10.107525	1.272193	0.300347
H	10.120320	2.359408	0.311318
C	11.299370	0.553171	0.402019
H	12.243103	1.084936	0.492776
C	10.086799	-1.548925	0.272849
H	10.091929	-2.636667	0.263897
C	5.302486	0.084067	-0.151804
H	4.644894	-0.777044	-0.220796
C	6.993044	2.331421	0.028717
H	7.634902	3.205930	0.097047
C	6.677891	-0.076924	-0.027297
C	5.615077	2.488849	-0.092120
H	5.192132	3.491006	-0.117156
C	7.525162	1.040797	0.062571
C	7.475832	-1.372766	0.035991
C	7.305125	-2.200892	-1.251076
H	7.934181	-3.097729	-1.217758
H	6.264129	-2.524434	-1.365542
H	7.583716	-1.618531	-2.135735
C	7.076442	-2.215849	1.261527
H	7.705429	-3.110477	1.332973
H	7.187531	-1.642916	2.188252
H	6.033216	-2.542410	1.181446
H	12.227194	-1.390604	0.469142

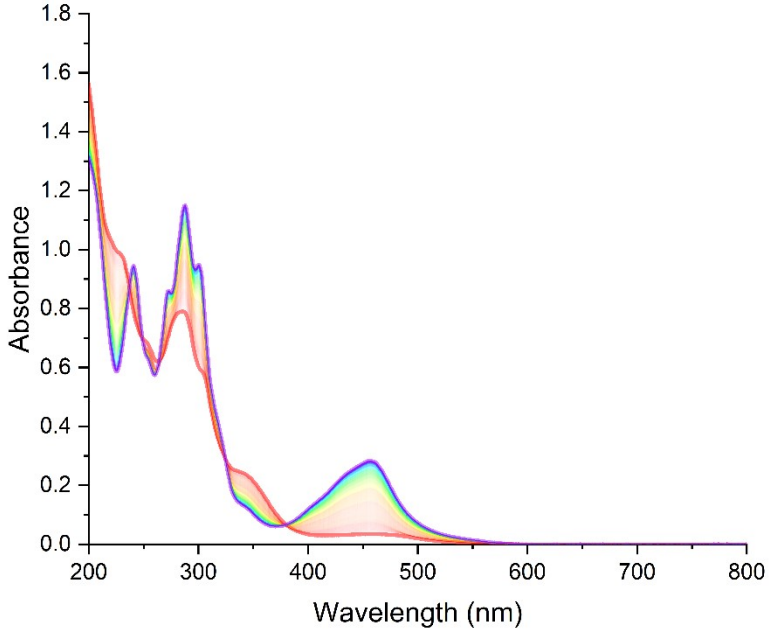
Ru	-3.435641	-0.045393	-0.591611
N	-1.456921	0.132416	-0.472747
C	-0.926596	1.370178	-0.421927
C	-1.936397	2.447999	-0.374711
N	-2.871400	-2.070850	-0.522837
N	-3.241852	2.041951	-0.406597
C	-3.969792	4.307475	-0.241548
H	-4.798445	5.004312	-0.191772
C	-0.712799	-0.998168	-0.473307
C	0.663114	-0.903363	-0.429748
H	1.303310	-1.776455	-0.421119
C	-3.179518	-4.435875	-0.505110
H	-3.868818	-5.272273	-0.511635
C	-1.514715	-2.237848	-0.493369
C	1.258969	0.375589	-0.390205
C	-1.622590	3.797850	-0.279304
H	-0.588883	4.120805	-0.253776
C	0.450567	1.528852	-0.384561
H	0.887723	2.516598	-0.346696
C	-4.227802	2.944272	-0.342366
H	-5.240421	2.561783	-0.379275
C	-3.678907	-3.138195	-0.530204
H	-4.743863	-2.943188	-0.558806
C	-0.962206	-3.512182	-0.469085
H	0.113227	-3.640939	-0.444118
C	-1.803005	-4.623458	-0.475177
H	-1.380025	-5.622215	-0.456661
C	-2.649506	4.737904	-0.212131
H	-2.412327	5.793846	-0.137534
N	-3.483247	-0.003096	-2.358539
O	-3.564737	0.020319	-3.488662
C	-4.893013	-0.222132	1.968251
C	-5.136696	-0.252873	3.339050
H	-6.148817	-0.333331	3.713785
C	-4.072972	-0.177280	4.230996
H	-4.257598	-0.201222	5.299724
C	-2.779100	-0.070996	3.733048
H	-1.916754	-0.010559	4.386568
C	-2.594998	-0.039848	2.359222
H	-1.602458	0.044537	1.939461
N	-3.621751	-0.112299	1.494678
C	-6.428611	-0.309283	-1.332817
H	-6.051235	-0.260134	-2.345850
C	-7.788708	-0.441803	-1.093743
H	-8.473665	-0.492252	-1.932214
C	-8.233274	-0.507524	0.222224
H	-9.289192	-0.611907	0.447857
C	-7.304314	-0.437604	1.254042
H	-7.637762	-0.489338	2.282681
C	-5.950046	-0.303443	0.953569
N	-5.527859	-0.242059	-0.335735

4. Photorelease experiments at $\lambda = 300$ nm

AC



C



5. Rotation barrier