SUPPORTING INFORMATION

to

Charge injection into nanostructured TiO_2 electrodes from the photogenerated reduced form of a new Ru(II) polypyridine compound: the "anti-biomimetic" mechanism at work

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Figure and Table Index

Additional Electrochemical and Spectroscopic Data

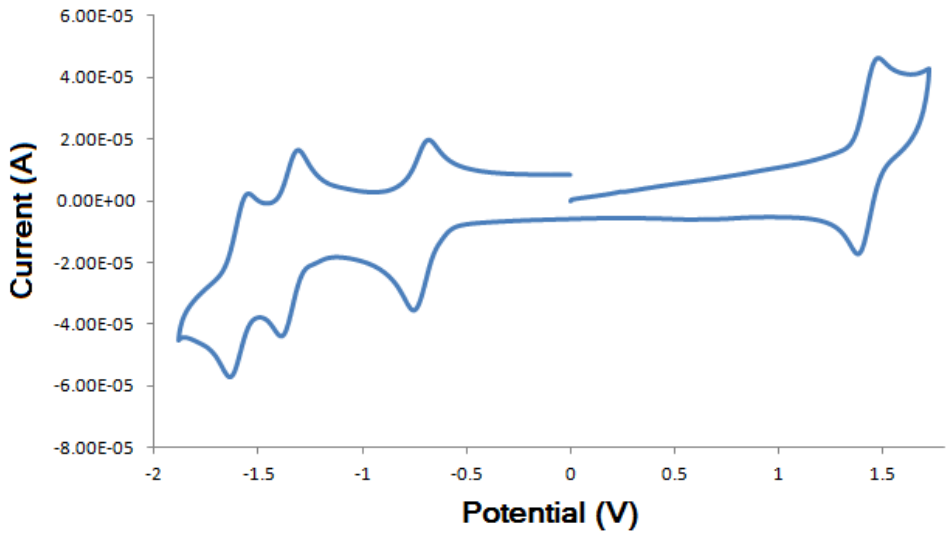


Figure S1. Cyclic voltammogram of **p1** in ACN/0.1 M $TBAPF_6$ (scan rate = 100 mV/s).

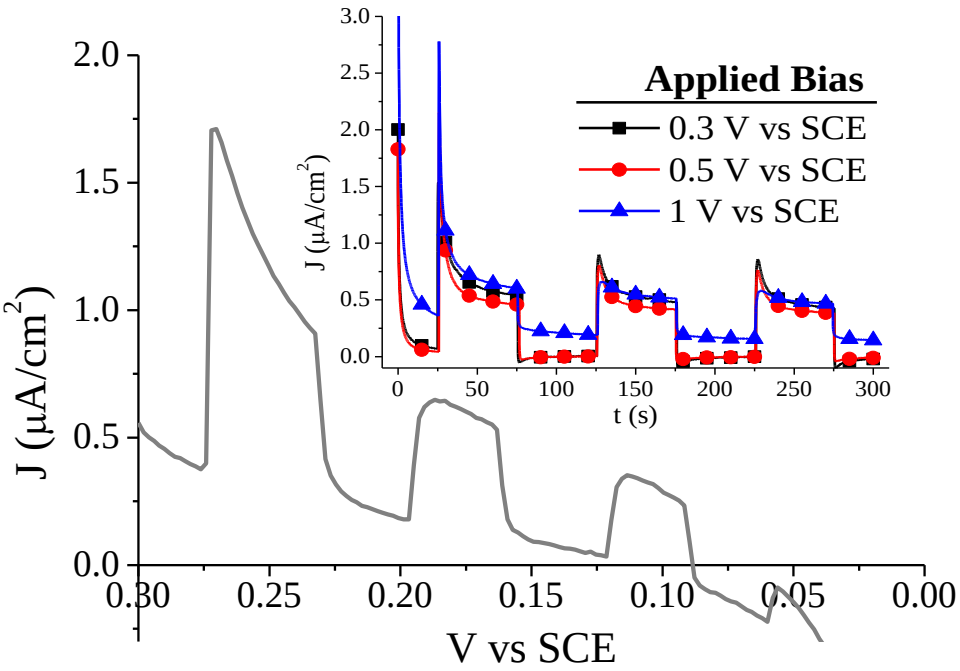


Figure S2. J-V curves of **1**/TiO_2 in 0.1 M $NaClO_4$ at pH 3. Inset: Constant potential chronoamperometry at 0.3 V (black), 0.5 V (red) and 1 V vs. SCE (blue) in the same electrolyte solution.

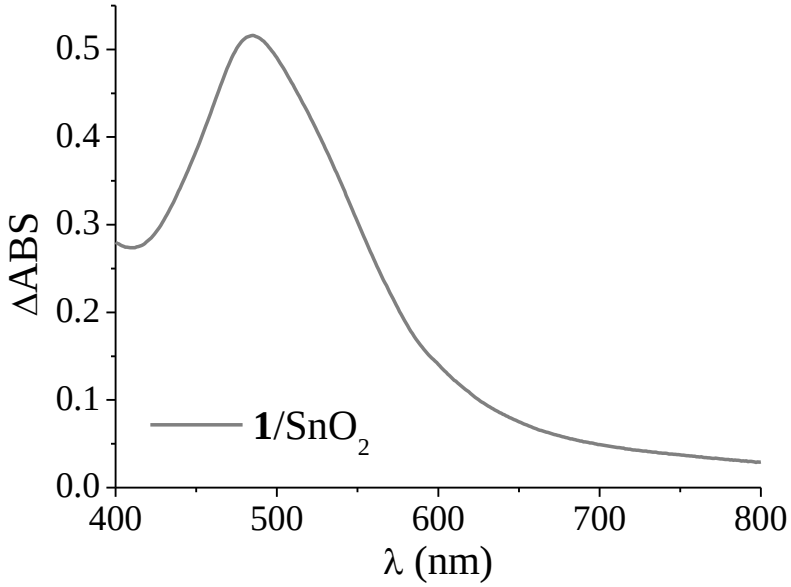


Figure S3. Absorption spectra of SnO_2 electrode dyad with **1**, corrected from scattering and intrinsic semiconductor absorption by subtracting the related identical bare semiconductor thin film.

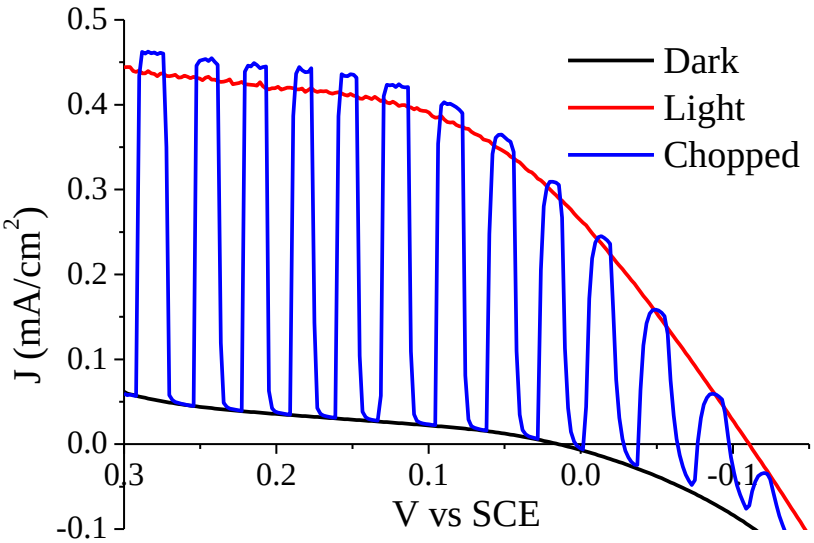


Figure S4. J-V curves of **1**/SnO_2 recorded under 490 nm, excitation (10 nm bandwidth, 5 mW/cm^2), in ACN/0.1M LiI.

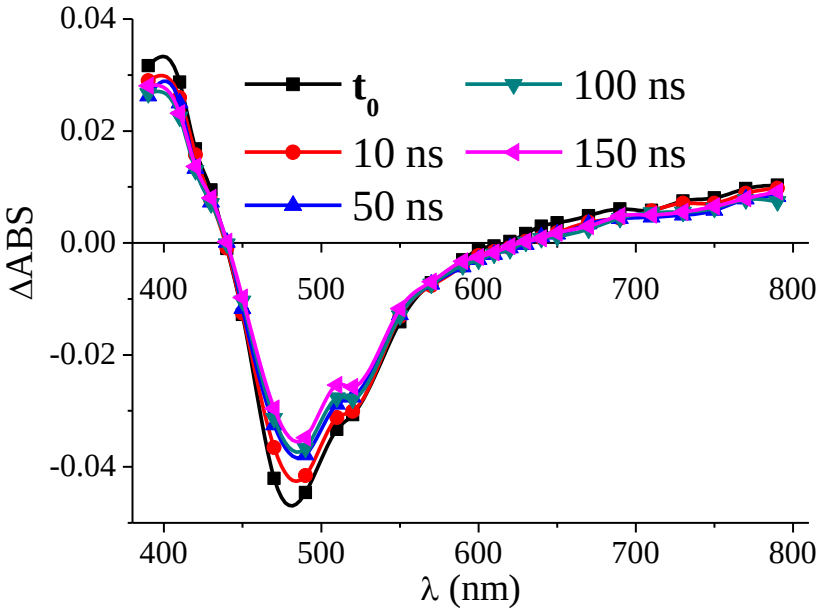


Figure S5. Transient spectrum of **1** loaded on SnO_2 recorded at delays 0-150 ns.

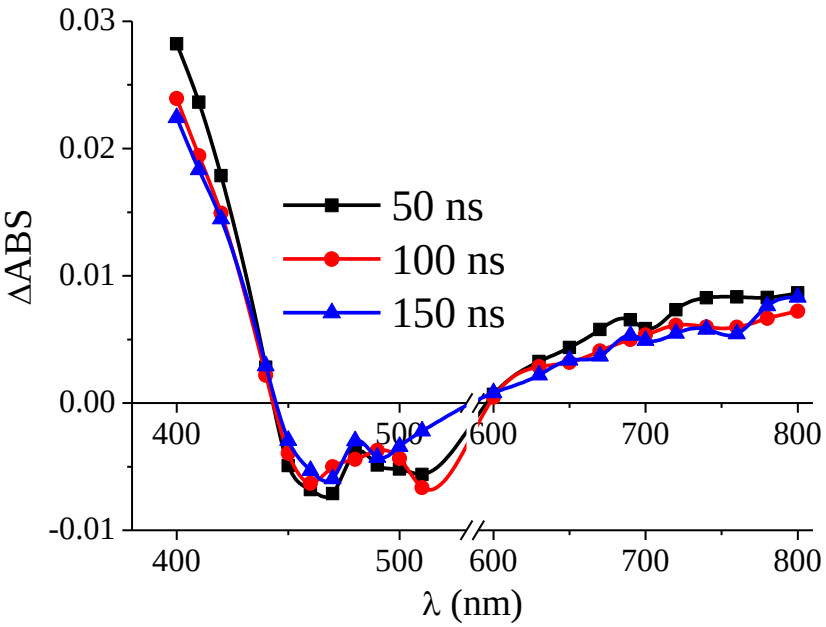


Figure S6. Transient spectrum of **1** loaded on TiO_2 recorded at delays > 50 ns.

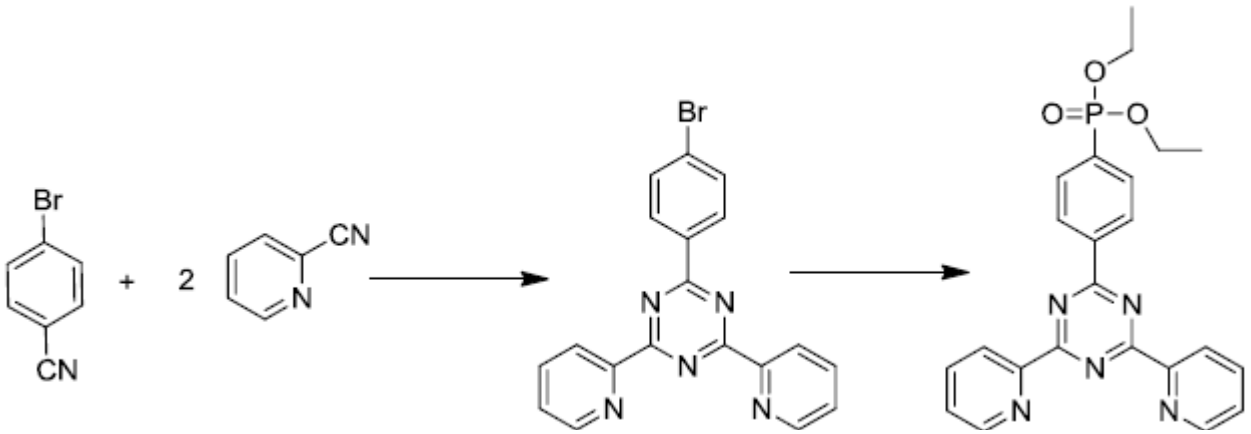


Figure S7. Simple synthesis pathway scheme of **L**.

NMR Spectra

Nuclear magnetic resonance spectra were recorded in deuterated solvents at room temperature on Bruker AV spectrometers at 300 MHz for ^{1}H NMR and at 75 MHz for ^{13}C NMR. Chemical shifts are reported in part per million (ppm) relative to residual solvent protons (for example, 1.94 ppm for acetonitrile-d_3) and the carbon resonance of the solvent.

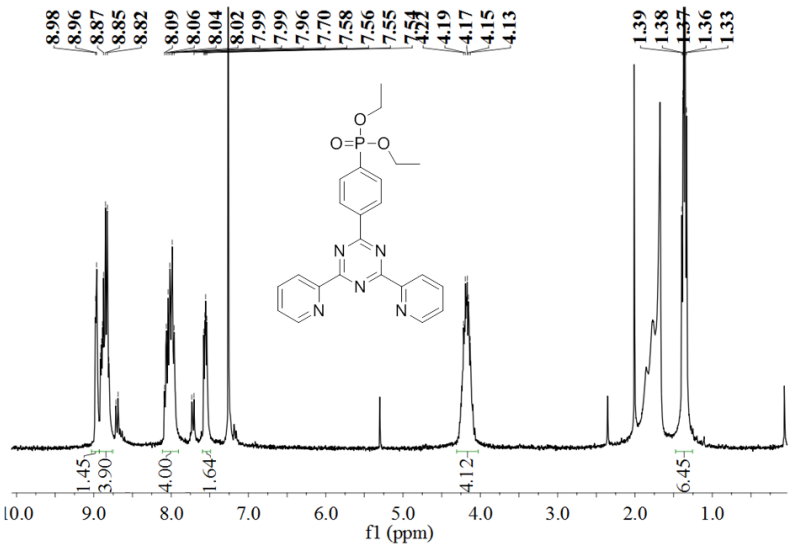


Figure S8. ^{1}H NMR spectrum of **L**.

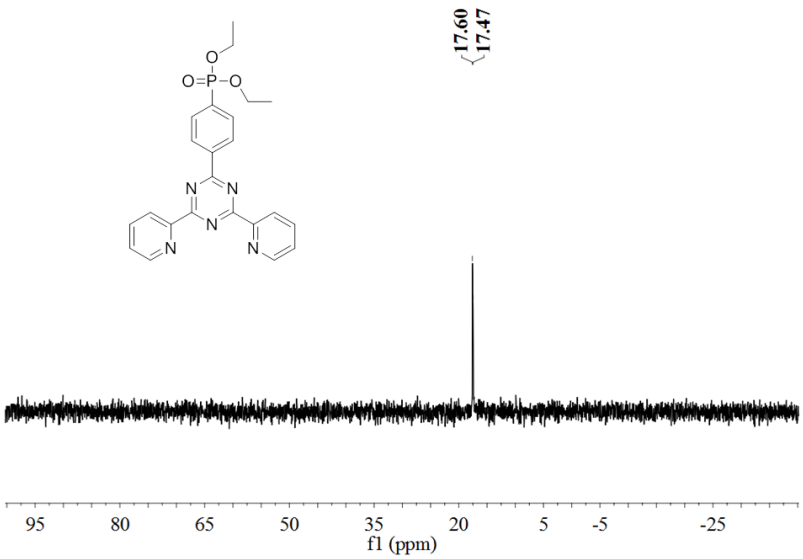


Figure S9. ^{31}P NMR spectrum of **L**.

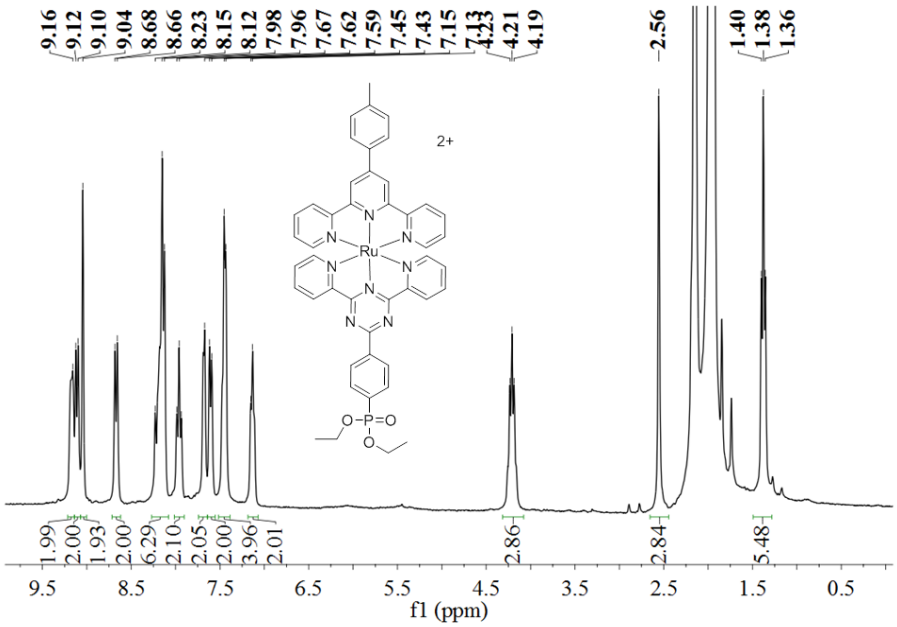


Figure S10. ^{1}H NMR spectrum of **p1**.

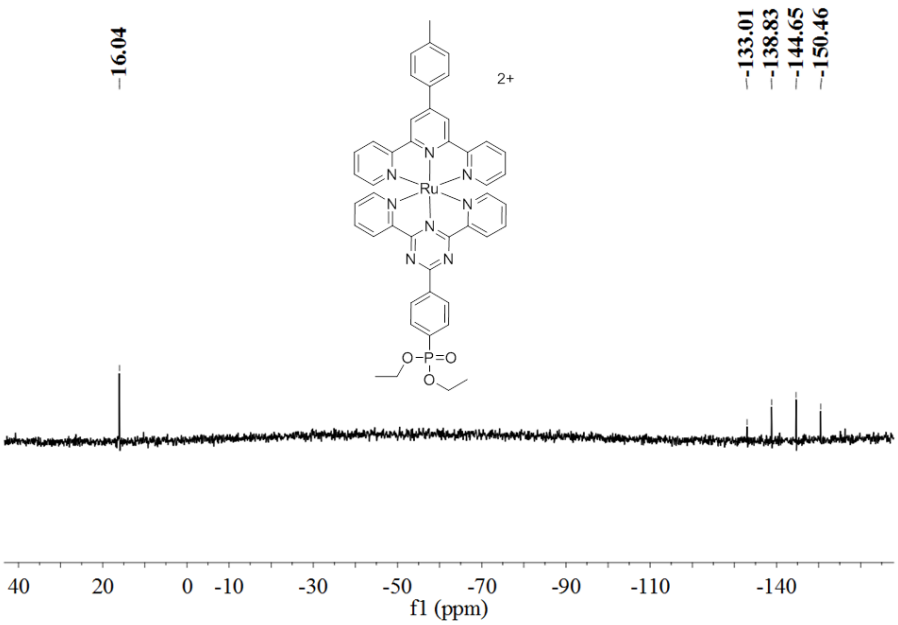


Figure S11. ^{31}P NMR spectrum of **p1**.

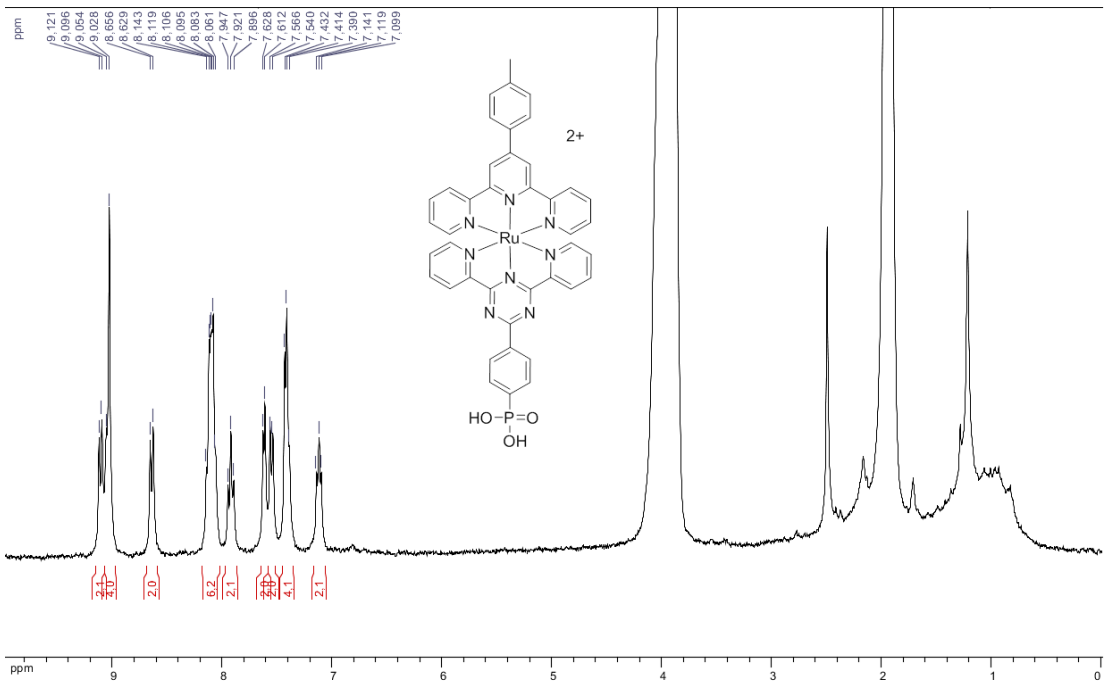


Figure S12. ^{1}H NMR spectrum of **1**.

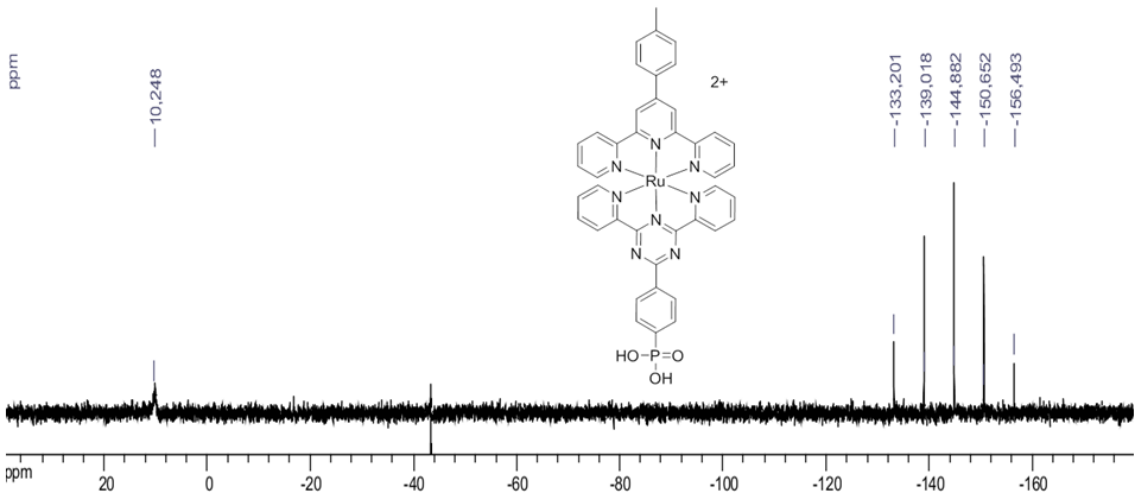


Figure S13. ^{31}P NMR spectrum of **1**.

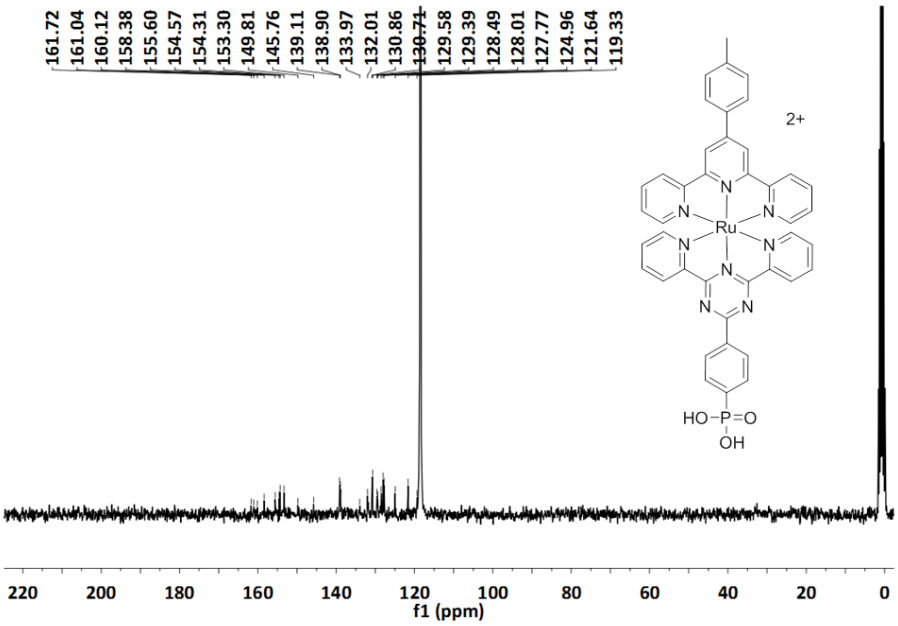


Figure S14. ^{31}C NMR spectrum of **1**.

Mass Spectra

High resolution mass spectra (HRMS) data were obtained using a QTOF LC/MS mass spectrometer with a dual-electrospray ionization (ESI) source. Samples were dissolved in 10 mM solution of formic acid (0.1%) in MeOH, and the compounds were detected in positive ion mode by HPLC-Chip Q/TOF-MS (nanospray) analysis using a quadrupole and a time-of-flight unit to produce spectra.

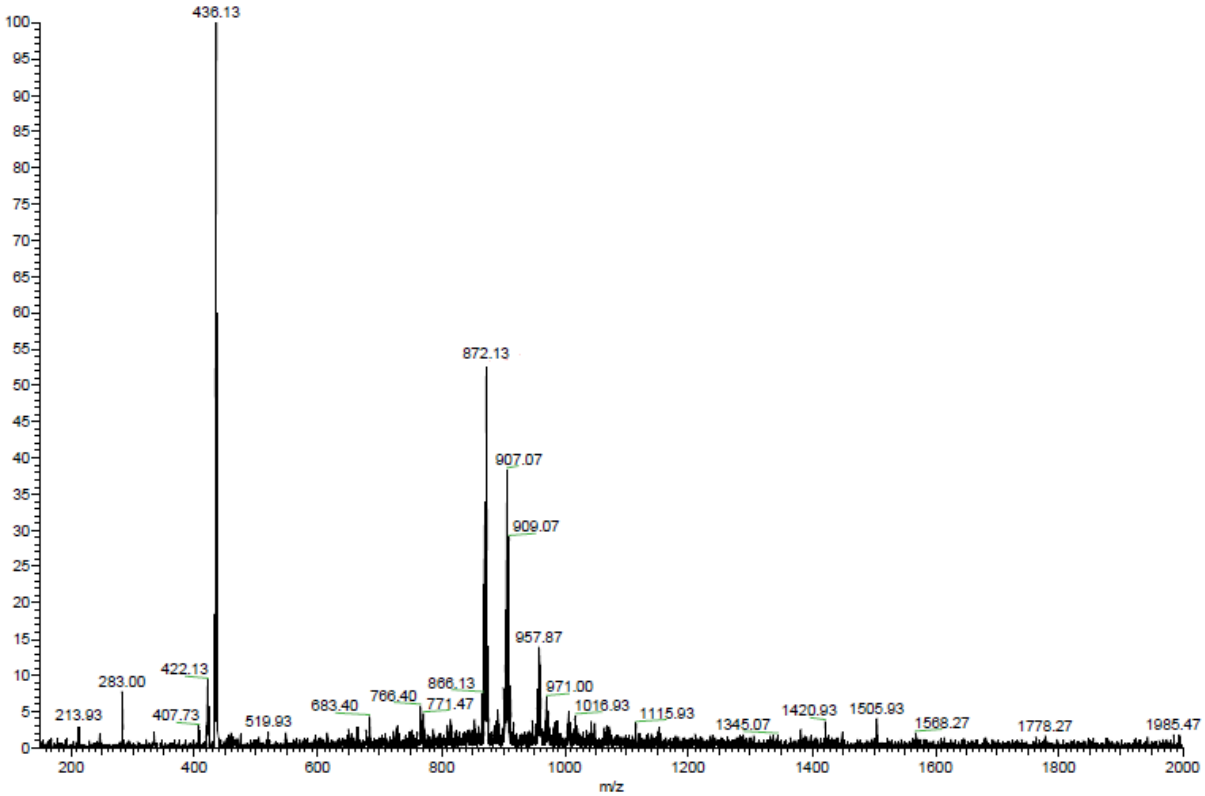
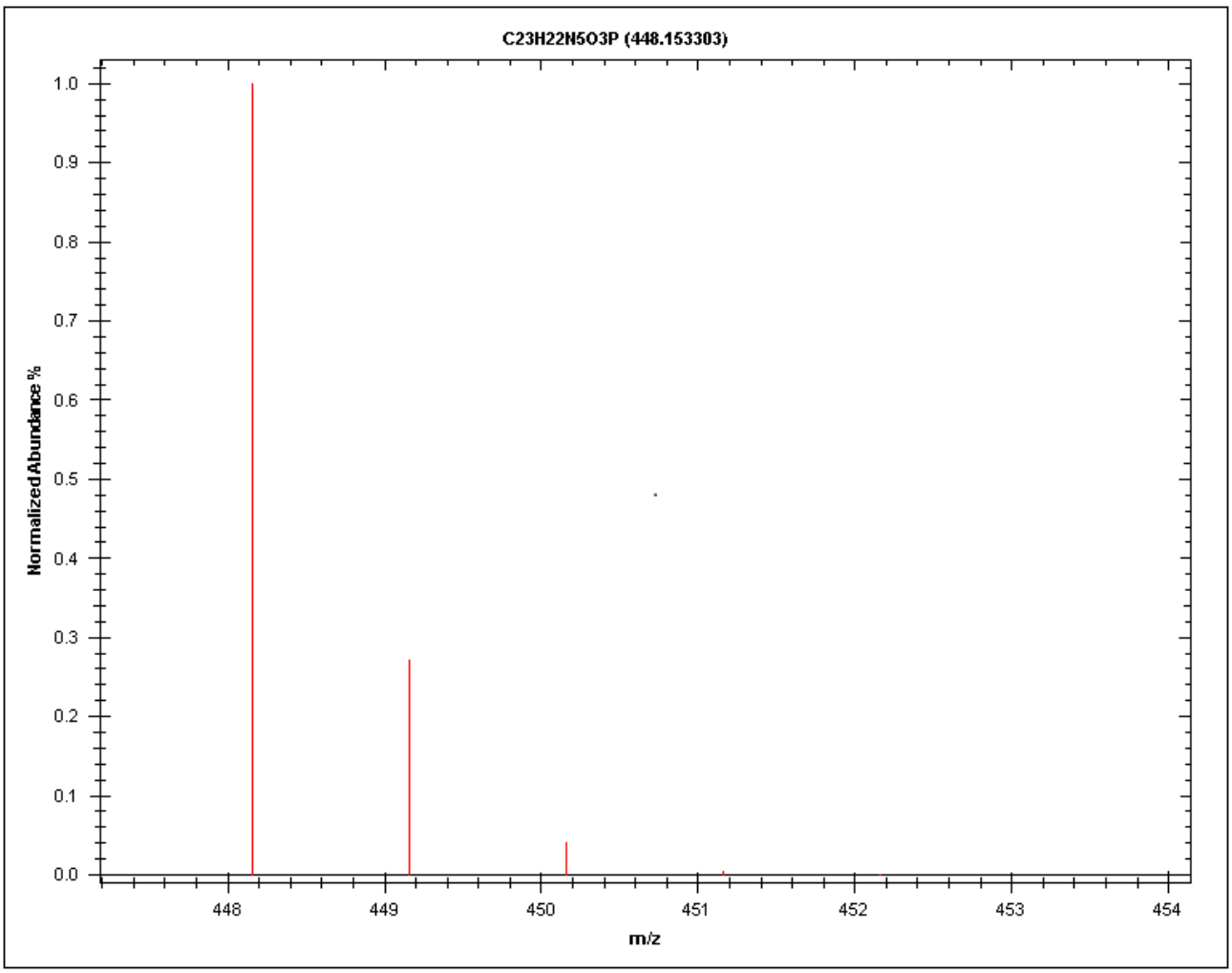


Figure S15. MS spectrum of **p1**.



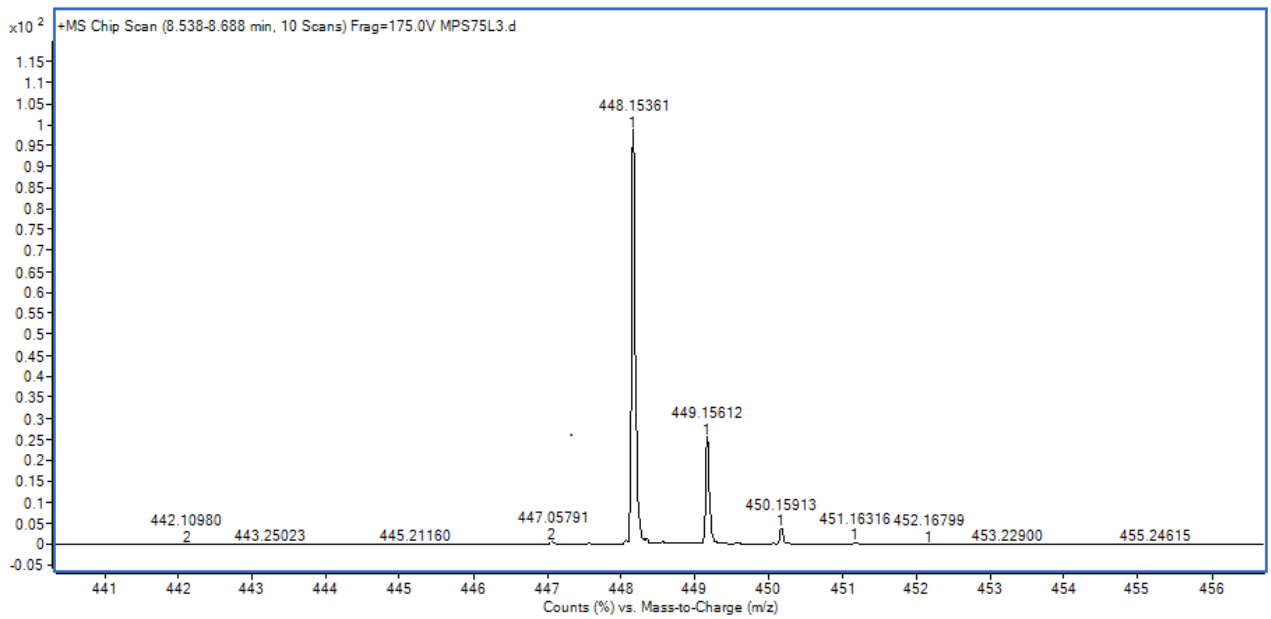
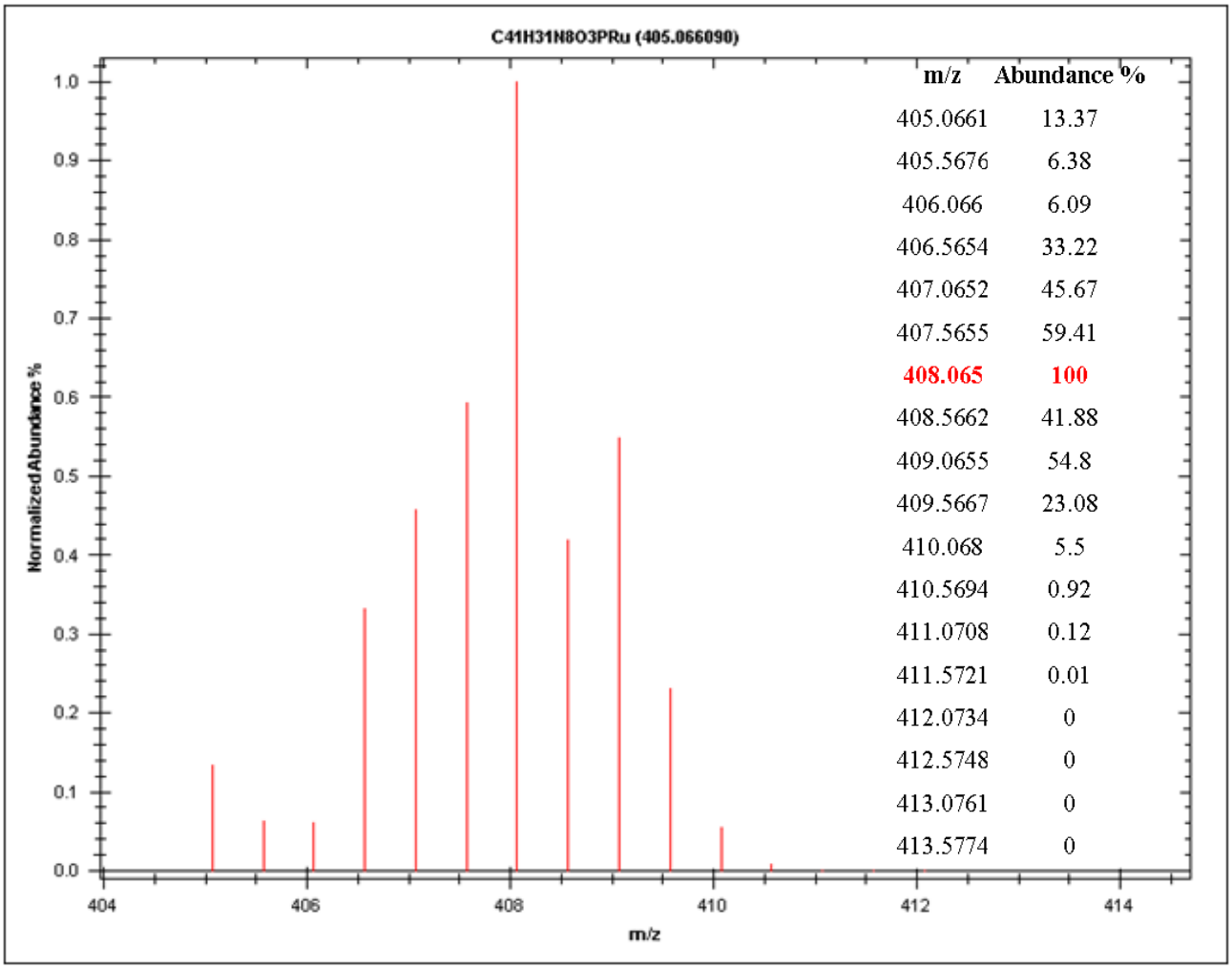


Figure S16. MS spectrum of **L** (above, calculated; below, experimental).



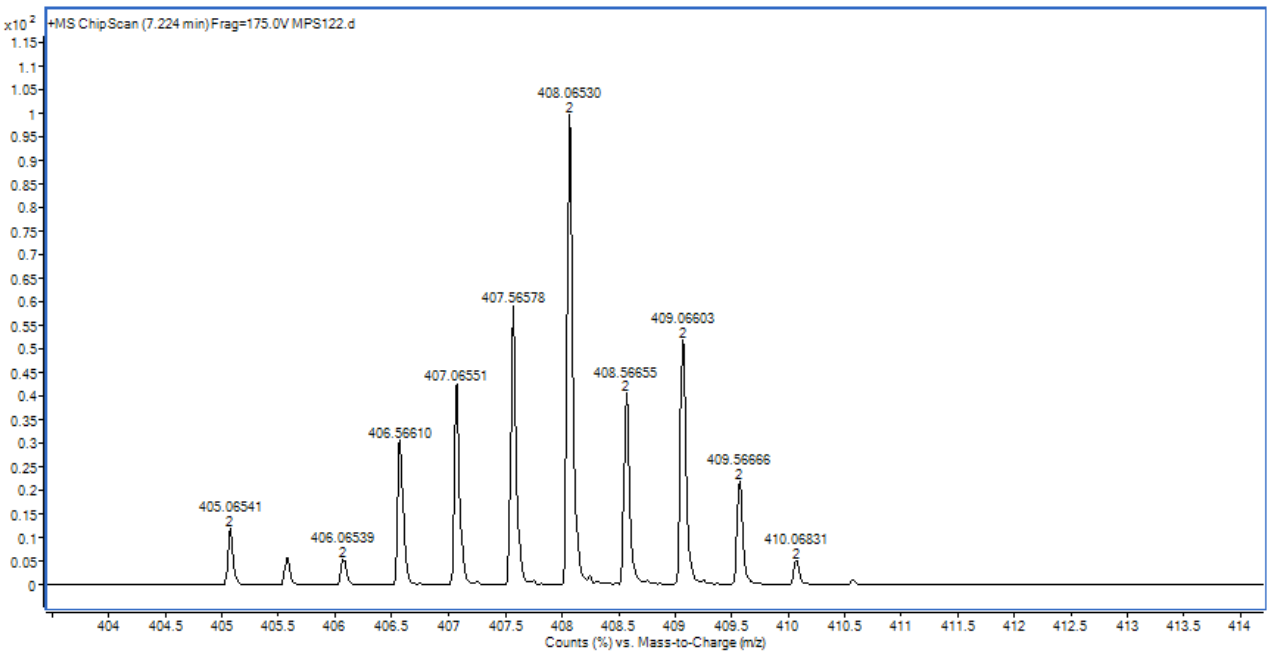


Figure S17. MS spectrum of **1** (above, calculated; below, experimental).

X-Ray Crystallography

Figure S18 shows a representation of the X-ray crystal of **p1**. Full details are deposited at Cambridge Crystallographic Data Center, deposition number CCDC 1474484.

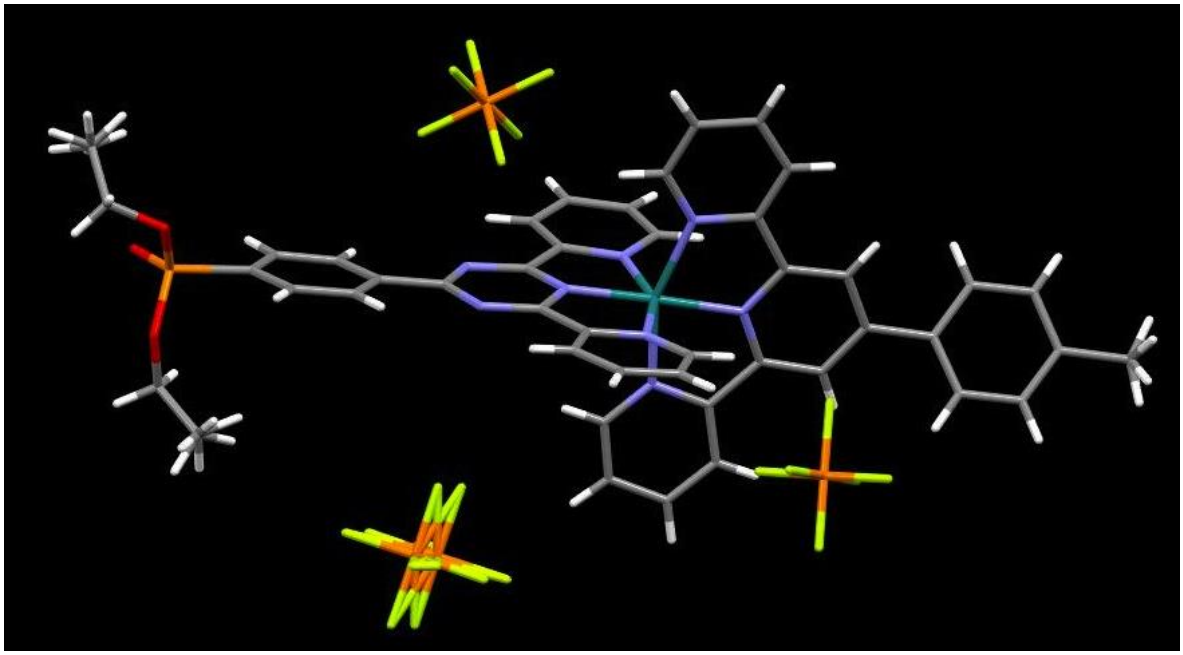


Figure S18. Ball-and-stick representation of **p1**.

Table S1. Crystallographic data for **p1**.

Formula	$RuC_{45}H_{39}P_3F_{12}N_8O_3$
Mw (g/mol); F(000)	1130.45; 1142
T (K); wavelength (Å)	293; 0.71073
Crystal System	Triclinic
Space Group	P(-1)
a (Å)	8.8081(7)
b (Å)	16.7037(18)
c (Å)	17.8490(17)
α (°)	77.72(1)
β (°)	86.79 (1)
γ(°)	79.71(1)
V ($Å^3$); Z; dcalc (g/cm^3)	2524.3(4); 2; 1.488
θ range (°); completeness	2.35 to 29.84; 0.918
collected reflections; R_{int}	75332; 0.1758
unique reflections; R_{int}	4275; 0.120
μ (mm^{-1}); exp abs coeff mu	4.654; 0.465
R1(F); wR(F^2) [$I > 2\sigma(I)$]	0.0975; 0.2964
R1a(F); wR(F2) (all data)	0.2105; 0.3027
GoF(F^2)	0.892
Residual electron density (e-/$Å^3$)	1.02; -1.10

Details of crystallographic data for p1

Table S2. Fractional atomic coordinates and isotropic temperature factors (Angstrom squared), with standard deviations in the least significant digits in parentheses. For anisotropic atoms, the equivalent isotropic temperature factors are shown.

	x/a	y/b	z/c	U
RU(1)	0.79874(7)	0.25374(5)	0.73968(4)	0.04586
P(3)	0.3426(3)	0.1676(2)	0.9629(2)	0.06515
P(2)	1.00000	0.50000	0.50000	0.07032
P(1)	0.6993(4)	0.4099(2)	0.1324(1)	0.07446
F(4)	0.4596(6)	0.2315(4)	0.9601(3)	0.08212
F(1)	0.9913(9)	0.4611(5)	0.4274(3)	0.10584
F(3)	1.0609(8)	0.4112(4)	0.5504(3)	0.09933
F(5)	0.4168(7)	0.1452(5)	0.8853(3)	0.09549
F(6)	0.2255(6)	0.2403(4)	0.9125(3)	0.08961
N(2)	0.8155(7)	0.2137(5)	0.8520(3)	0.03863
F(9)	0.4617(7)	0.0949(5)	1.0105(4)	0.10700
N(4)	1.0232(7)	0.2159(5)	0.7036(3)	0.04455
N(3)	0.8422(8)	0.3584(5)	0.7731(4)	0.04741
N(8)	0.8966(8)	0.2804(5)	0.5063(4)	0.05008
O(2)	0.6428(11)	0.5068(6)	0.1145(4)	0.09987
F(8)	0.2693(8)	0.1915(6)	1.0393(3)	0.11477
O(1)	0.8372(9)	0.3789(5)	0.0906(3)	0.08103
F(7)	0.2243(7)	0.1066(5)	0.9661(4)	0.10514
O(3)	0.5507(9)	0.3766(6)	0.1192(4)	0.08659
F(2)	0.8293(7)	0.4851(5)	0.5234(4)	0.11412
N(5)	0.7869(7)	0.2873(5)	0.6281(3)	0.04001
N(7)	0.6331(7)	0.3444(5)	0.5191(3)	0.04928
N(6)	0.5650(7)	0.3104(5)	0.7250(3)	0.04553
N(1)	0.7535(7)	0.1345(5)	0.7531(4)	0.05329
C(10)	0.8590(9)	0.2404(7)	0.9747(5)	0.05044
H(10)	0.87981	0.27675	1.00420	0.06053
C(12)	0.8561(9)	0.3498(6)	0.8514(4)	0.04605
C(37)	0.7496(10)	0.3430(6)	0.3936(5)	0.04892
C(9)	0.8435(9)	0.1594(7)	1.0086(5)	0.04995
C(39)	0.6002(12)	0.4126(8)	0.2814(5)	0.07650
H(39)	0.50974	0.44481	0.26000	0.09180
P(4)	0.50000	0.00000	0.50000	0.38792
C(28)	1.0460(9)	0.2271(6)	0.6261(4)	0.04348
C(38)	0.6126(11)	0.3903(7)	0.3598(5)	0.06857
H(38)	0.52953	0.40660	0.39084	0.08229
C(11)	0.8428(8)	0.2663(6)	0.8961(5)	0.04203
C(32)	0.5272(8)	0.3428(6)	0.6498(4)	0.04461
C(27)	1.1859(10)	0.2030(7)	0.5928(5)	0.06529
H(27)	1.19498	0.20829	0.53984	0.07835
C(16)	0.8526(9)	0.4348(7)	0.7288(5)	0.05407
H(16)	0.84149	0.44225	0.67615	0.06489
C(6)	0.7569(9)	0.0914(7)	0.8270(5)	0.04919
C(17)	0.8567(11)	0.1294(7)	1.0934(5)	0.05875
C(8)	0.8131(10)	0.1060(7)	0.9625(5)	0.05371
H(8)	0.80377	0.05116	0.98365	0.06446
C(4)	0.6787(13)	-0.0240(8)	0.7930(7)	0.08648

	x/a	y/b	z/c	U
H(4)	0.65123	-0.07652	0.80635	0.10378
C(42)	0.8688(11)	0.3187(7)	0.3456(5)	0.06218
H(42)	0.95941	0.28566	0.36626	0.07461
C(35)	0.3140(10)	0.3687(7)	0.7614(5)	0.06456
H(35)	0.24263	0.37733	0.80054	0.07747
C(33)	0.3836(10)	0.3857(7)	0.6296(5)	0.05731
H(33)	0.35899	0.40532	0.57817	0.06877
C(3)	0.6794(11)	0.0180(7)	0.7166(6)	0.06261
H(3)	0.65655	-0.00663	0.67751	0.07513
C(22)	0.9543(11)	0.1622(7)	1.1337(5)	0.07085
H(22)	1.01226	0.20094	1.10712	0.08501
C(40)	0.7213(11)	0.3874(7)	0.2341(5)	0.05925
C(29)	0.9048(9)	0.2658(6)	0.5826(4)	0.04331
C(41)	0.8544(11)	0.3432(7)	0.2664(5)	0.06628
H(41)	0.93819	0.32900	0.23494	0.07954
C(36)	0.4612(10)	0.3242(7)	0.7788(5)	0.05499
H(36)	0.48707	0.30353	0.82997	0.06598
C(31)	0.6507(9)	0.3247(6)	0.5947(4)	0.04417
C(2)	0.7144(10)	0.0961(7)	0.7007(5)	0.05904
H(2)	0.71070	0.12454	0.64991	0.07085
C(30)	0.7619(10)	0.3209(7)	0.4766(4)	0.05271
C(15)	0.8780(12)	0.4999(7)	0.7568(6)	0.06838
H(15)	0.88640	0.55015	0.72368	0.08206
C(14)	0.8912(13)	0.4917(7)	0.8344(6)	0.07549
H(14)	0.90719	0.53616	0.85503	0.09059
C(34)	0.2745(10)	0.3996(7)	0.6867(5)	0.07213
H(34)	0.17646	0.42946	0.67432	0.08656
C(5)	0.7189(11)	0.0135(7)	0.8470(6)	0.06406
H(5)	0.72094	-0.01378	0.89824	0.07687
C(21)	0.9657(14)	0.1375(9)	1.2128(7)	0.09586
H(21)	1.03132	0.15966	1.23875	0.11504
C(24)	1.1508(9)	0.1846(7)	0.7470(5)	0.05679
H(24)	1.14156	0.17925	0.79993	0.06815
C(13)	0.8802(12)	0.4158(7)	0.8808(6)	0.06770
H(13)	0.88929	0.40913	0.93354	0.08124
C(25)	1.2919(10)	0.1609(7)	0.7153(5)	0.06377
H(25)	1.37502	0.13745	0.74726	0.07653
C(18)	0.7698(14)	0.0747(8)	1.1340(6)	0.08501
H(18)	0.70245	0.05309	1.10856	0.10201
C(26)	1.3140(10)	0.1705(8)	0.6384(6)	0.07300
H(26)	1.41119	0.15597	0.61709	0.08760
C(7)	0.7972(8)	0.1377(6)	0.8834(5)	0.04019
C(43)	0.5510(15)	0.2894(10)	0.1346(7)	0.09667
H(43A)	0.64967	0.26025	0.15562	0.11601
H(43B)	0.53837	0.27226	0.08697	0.11601
C(46)	0.7819(16)	0.5841(10)	0.0128(7)	0.11496
H(46A)	0.77065	0.61668	-0.03844	0.17244
H(46B)	0.86225	0.53683	0.01329	0.17244
H(46C)	0.80829	0.61737	0.04621	0.17244
H(46D)	0.85681	0.56390	0.05248	0.17244
H(46E)	0.76521	0.64376	0.00075	0.17244
H(46F)	0.81917	0.56322	-0.03217	0.17244

	x/a	y/b	z/c	U
C(19)	0.7807(16)	0.0511(9)	1.2127(7)	0.10490
H(19)	0.71887	0.01437	1.23921	0.12588
C(20)	0.8797(17)	0.0800(9)	1.2532(6)	0.09431
C(45)	0.6393(15)	0.5562(10)	0.0387(7)	0.11140
H(45A)	0.55860	0.60441	0.03662	0.13368
H(45B)	0.61238	0.52404	0.00363	0.13368
C(23)	0.8878(19)	0.0532(11)	1.3427(5)	0.15598
H(23A)	0.81905	0.01432	1.36081	0.23397
H(23B)	0.85792	0.10126	1.36496	0.23397
H(23C)	0.99135	0.02749	1.35705	0.23397
H(23D)	0.95983	0.08106	1.36107	0.23397
H(23E)	0.92097	-0.00588	1.35692	0.23397
H(23F)	0.78753	0.06789	1.36483	0.23397
C(44)	0.428(2)	0.267(1)	0.188(1)	0.16580
H(44A)	0.43229	0.20760	0.19793	0.24870
H(44B)	0.33017	0.29416	0.16681	0.24870
H(44C)	0.44065	0.28342	0.23545	0.24870
H(44D)	0.36978	0.31585	0.20220	0.24870
H(44E)	0.47190	0.22929	0.23332	0.24870
H(44F)	0.36142	0.24003	0.16468	0.24870
F(10)	0.5329(19)	0.0287(18)	0.4148(10)	0.36716
F(11)	0.418(3)	-0.084(2)	0.485(1)	0.40762
F(12)	0.345(2)	0.058(3)	0.490(1)	0.52394

Table S3. Vibration parameters (Angstrom squared) in the expression: -2(pi squared)(U11((h.a*)squared) + U22((k.b*)squared) + U33((l.c*)squared) + 2.U12.h.k.a*.b* + 2.U13.h.l.a*.c* + 2.U23.k.l.b*.c*).

	U11	U22	U33	U12	U13	U23
RU(1)	0.0306(4)	0.0617(7)	0.0404(4)	-.0061(4)	-.0111(3)	0.0013(3)
P(3)	0.050(1)	0.078(2)	0.062(2)	-0.014(2)	-0.009(1)	0.002(1)
P(2)	0.066(2)	0.085(4)	0.056(2)	-0.035(3)	-0.030(2)	0.021(2)
P(1)	0.089(2)	0.088(3)	0.041(1)	-0.004(2)	-0.018(1)	-0.009(2)
F(4)	0.063(3)	0.105(6)	0.081(4)	-0.034(4)	-0.014(3)	-0.004(3)
F(1)	0.151(6)	0.110(7)	0.063(4)	-0.046(5)	-0.029(4)	-0.005(4)
F(3)	0.114(5)	0.074(5)	0.101(4)	-0.031(4)	-0.058(4)	0.030(4)
F(5)	0.088(4)	0.123(7)	0.077(4)	-0.011(4)	0.006(3)	-0.031(4)
F(6)	0.065(4)	0.088(6)	0.103(4)	-0.002(4)	-0.026(3)	0.006(4)
N(2)	0.032(4)	0.034(5)	0.050(4)	-0.009(4)	-0.006(3)	-0.003(4)
F(9)	0.068(4)	0.111(7)	0.118(5)	-0.012(4)	-0.033(4)	0.034(4)
N(4)	0.030(3)	0.055(6)	0.047(4)	-0.007(4)	-0.011(3)	-0.002(3)
N(3)	0.046(4)	0.040(6)	0.054(4)	-0.011(4)	-0.006(3)	-0.001(4)
N(8)	0.039(4)	0.063(6)	0.044(4)	-0.001(4)	-0.011(3)	-0.006(4)
O(2)	0.147(8)	0.083(7)	0.052(4)	0.011(6)	-0.003(4)	0.001(4)
F(8)	0.104(5)	0.172(9)	0.077(4)	-0.045(6)	0.021(4)	-0.034(4)
O(1)	0.107(6)	0.089(7)	0.047(4)	-0.017(5)	-0.007(4)	-0.015(4)
F(7)	0.065(4)	0.108(7)	0.139(6)	-0.034(4)	-0.016(4)	-0.001(5)
O(3)	0.091(6)	0.097(8)	0.071(5)	-0.006(5)	-0.041(4)	-0.014(4)
F(2)	0.071(4)	0.139(8)	0.125(5)	-0.044(5)	-0.018(4)	0.013(5)
N(5)	0.021(3)	0.047(5)	0.051(4)	-0.011(3)	0.003(3)	-0.005(3)
N(7)	0.038(4)	0.070(6)	0.038(4)	-0.014(4)	-0.007(3)	-0.002(4)
N(6)	0.040(4)	0.059(6)	0.037(4)	-0.011(4)	-0.004(3)	-0.005(4)
N(1)	0.034(4)	0.083(7)	0.034(4)	0.002(4)	-0.010(3)	-0.001(4)
C(10)	0.042(5)	0.065(8)	0.043(5)	-0.008(5)	-0.003(4)	-0.009(5)
C(12)	0.045(5)	0.057(8)	0.039(5)	-0.017(5)	0.002(4)	-0.011(5)
C(37)	0.048(5)	0.058(8)	0.042(5)	-0.015(5)	-0.013(4)	-0.004(4)
C(9)	0.039(5)	0.057(8)	0.050(5)	-0.007(5)	-0.002(4)	-0.004(5)
C(39)	0.070(7)	0.102(11)	0.047(6)	-0.001(7)	-0.025(5)	0.002(6)
P(4)	0.124(8)	0.865(47)	0.258(15)	0.025(17)	-0.016(8)	-0.391(22)
C(28)	0.032(4)	0.053(7)	0.044(5)	-0.009(5)	-0.003(4)	-0.006(4)
C(38)	0.057(6)	0.087(10)	0.049(6)	0.000(6)	-0.007(5)	0.004(5)
C(11)	0.029(4)	0.043(7)	0.049(5)	-0.009(4)	0.003(4)	0.005(4)
C(32)	0.022(4)	0.070(8)	0.040(5)	-0.009(4)	-0.010(3)	-0.006(4)
C(27)	0.046(5)	0.092(10)	0.050(5)	0.004(6)	0.003(4)	-0.012(5)
C(16)	0.035(5)	0.073(9)	0.051(5)	-0.007(5)	-0.009(4)	-0.007(5)
C(6)	0.033(4)	0.055(8)	0.059(6)	-0.002(5)	-0.001(4)	-0.013(5)
C(17)	0.053(5)	0.069(8)	0.043(5)	0.006(6)	-0.003(4)	0.002(5)
C(8)	0.047(5)	0.050(7)	0.058(6)	-0.005(5)	-0.009(4)	0.005(5)
C(4)	0.088(8)	0.081(10)	0.096(9)	-0.034(8)	-0.008(7)	-0.012(7)
C(42)	0.053(6)	0.086(9)	0.045(5)	-0.002(6)	-0.010(4)	-0.014(5)
C(35)	0.036(5)	0.092(10)	0.055(6)	0.007(6)	0.001(4)	-0.009(5)
C(33)	0.043(5)	0.075(9)	0.050(5)	-0.011(5)	-0.012(4)	0.001(5)
C(3)	0.076(7)	0.052(8)	0.061(6)	-0.010(6)	-0.013(5)	-0.012(5)
C(22)	0.063(6)	0.088(10)	0.049(6)	0.004(6)	-0.011(5)	0.002(6)
C(40)	0.061(6)	0.075(9)	0.042(5)	-0.007(6)	-0.007(5)	-0.013(5)

	U11	U22	U33	U12	U13	U23
C(29)	0.035(4)	0.049(7)	0.044(5)	-0.015(5)	-0.003(4)	0.000(4)
C(41)	0.056(6)	0.087(10)	0.056(6)	-0.012(6)	-0.005(5)	-0.014(6)
C(36)	0.047(5)	0.073(8)	0.040(5)	-0.007(5)	0.000(4)	-0.004(5)
C(31)	0.029(4)	0.050(7)	0.048(5)	-0.007(4)	-0.004(4)	0.004(4)
C(2)	0.047(5)	0.077(9)	0.047(5)	-0.002(6)	-0.010(4)	-0.004(5)
C(30)	0.051(5)	0.070(8)	0.038(5)	-0.017(6)	-0.008(4)	-0.004(5)
C(15)	0.077(7)	0.062(9)	0.068(7)	-0.028(7)	0.003(5)	-0.004(6)
C(14)	0.106(9)	0.058(9)	0.068(7)	-0.028(7)	0.001(6)	-0.015(6)
C(34)	0.042(5)	0.101(10)	0.060(6)	0.005(6)	-0.015(5)	0.003(6)
C(5)	0.067(6)	0.057(9)	0.064(6)	-0.009(6)	-0.009(5)	-0.001(6)
C(21)	0.081(8)	0.114(13)	0.082(9)	-0.002(8)	-0.025(7)	-0.002(8)
C(24)	0.033(5)	0.076(9)	0.054(5)	0.004(5)	-0.016(4)	-0.005(5)
C(13)	0.075(7)	0.071(9)	0.060(6)	-0.024(7)	-0.013(5)	-0.007(6)
C(25)	0.038(5)	0.086(9)	0.058(6)	0.003(5)	-0.018(4)	0.000(5)
C(18)	0.102(9)	0.092(11)	0.053(6)	-0.024(8)	-0.002(6)	0.012(6)
C(26)	0.030(5)	0.105(11)	0.074(7)	0.006(6)	-0.003(5)	-0.012(6)
C(7)	0.031(4)	0.036(7)	0.051(5)	-0.002(4)	-0.001(4)	-0.005(4)
C(43)	0.086(9)	0.110(14)	0.108(10)	-0.023(9)	-0.028(7)	-0.040(9)
C(46)	0.12(1)	0.14(2)	0.09(1)	-0.02(1)	0.00(1)	-0.02(1)
C(19)	0.13(1)	0.12(1)	0.06(1)	-0.03(1)	0.02(1)	0.00(1)
C(20)	0.12(1)	0.09(1)	0.06(1)	0.02(1)	-0.01(1)	-0.01(1)
C(45)	0.09(1)	0.12(1)	0.11(1)	-0.01(1)	-0.03(1)	0.00(1)
C(23)	0.20(2)	0.22(2)	0.02(1)	0.00(1)	0.00(1)	0.01(1)
C(44)	0.24(2)	0.14(2)	0.13(1)	-0.09(2)	0.00(1)	-0.02(1)
F(10)	0.22(2)	0.74(5)	0.22(1)	-0.07(2)	0.01(1)	-0.30(2)
F(11)	0.33(3)	0.69(5)	0.30(2)	-0.10(3)	0.02(2)	-0.32(3)
F(12)	0.18(2)	0.96(7)	0.41(3)	0.22(3)	-0.06(2)	-0.36(4)

Table S4. Complete listing of bond distances (Angstroms).

RU(1) - N(2)	1.979(7)	RU(1) - N(4)	2.076(7)
RU(1) - N(3)	2.065(8)	RU(1) - N(5)	1.955(7)
RU(1) - N(1)	2.062(9)	P(3) - F(4)	1.604(7)
P(3) - F(5)	1.587(7)	P(3) - F(6)	1.593(7)
P(3) - F(9)	1.583(8)	P(3) - F(8)	1.574(8)
P(3) - F(7)	1.573(8)	P(2) - F(1)	1.579(6)
P(2) - F(1)	1.579(6)	P(2) - F(3)	1.581(7)
P(2) - F(3)	1.581(7)	P(2) - F(2)	1.586(7)
P(2) - F(2)	1.586(7)	P(1) - O(2)	1.575(10)
P(1) - O(1)	1.463(9)	P(1) - O(3)	1.559(9)
P(1) - C(40)	1.788(9)	N(2) - C(11)	1.356(11)
N(2) - C(7)	1.309(12)	N(4) - C(28)	1.364(10)
N(4) - C(24)	1.360(11)	N(3) - C(12)	1.384(11)
N(3) - C(16)	1.366(14)	N(8) - C(29)	1.335(10)
N(8) - C(30)	1.334(12)	O(2) - C(45)	1.425(16)
O(3) - C(43)	1.424(19)	N(5) - C(29)	1.327(11)
N(5) - C(31)	1.356(10)	N(7) - C(31)	1.329(10)
N(7) - C(30)	1.374(11)	N(6) - C(32)	1.371(10)
N(6) - C(36)	1.316(11)	N(1) - C(6)	1.360(12)
N(1) - C(2)	1.333(12)	C(10) - H(10)	0.930(10)
C(10) - C(9)	1.388(15)	C(10) - C(11)	1.385(12)
C(12) - C(11)	1.474(14)	C(12) - C(13)	1.372(15)
C(37) - C(38)	1.408(14)	C(37) - C(42)	1.377(13)
C(37) - C(30)	1.453(11)	C(9) - C(17)	1.492(12)
C(9) - C(8)	1.404(14)	C(39) - H(39)	0.930(11)
C(39) - C(38)	1.374(13)	C(39) - C(40)	1.384(15)
P(4) - F(10)	1.523(18)	P(4) - F(10)	1.523(18)
P(4) - F(12)	1.52(3)	P(4) - F(12)	1.52(3)
C(28) - C(27)	1.370(12)	C(28) - C(29)	1.475(11)
C(38) - H(38)	0.930(10)	C(32) - C(33)	1.365(12)
C(32) - C(31)	1.460(11)	C(27) - H(27)	0.930(9)
C(27) - C(26)	1.389(13)	C(16) - H(16)	0.930(9)
C(16) - C(15)	1.346(16)	C(6) - C(5)	1.370(16)
C(6) - C(7)	1.485(13)	C(17) - C(22)	1.400(14)
C(17) - C(18)	1.362(16)	C(8) - H(8)	0.930(11)
C(8) - C(7)	1.403(12)	C(4) - H(4)	0.930(14)
C(4) - C(3)	1.395(16)	C(4) - C(5)	1.350(16)
C(42) - H(42)	0.930(10)	C(42) - C(41)	1.392(13)
C(35) - H(35)	0.930(10)	C(35) - C(36)	1.391(13)
C(35) - C(34)	1.363(13)	C(33) - H(33)	0.930(9)
C(33) - C(34)	1.389(13)	C(3) - H(3)	0.930(10)
C(3) - C(2)	1.361(16)	C(22) - H(22)	0.930(11)
C(22) - C(21)	1.388(15)	C(40) - C(41)	1.356(14)
C(41) - H(41)	0.930(10)	C(36) - H(36)	0.930(9)
C(2) - H(2)	0.930(10)	C(15) - H(15)	0.930(12)
C(15) - C(14)	1.373(15)	C(14) - H(14)	0.930(12)
C(14) - C(13)	1.375(17)	C(34) - H(34)	0.930(10)
C(5) - H(5)	0.930(11)	C(21) - H(21)	0.930(13)
C(21) - C(20)	1.39(2)	C(24) - H(24)	0.930(9)
C(24) - C(25)	1.365(13)	C(13) - H(13)	0.930(10)
C(25) - H(25)	0.930(9)	C(25) - C(26)	1.353(14)
C(18) - H(18)	0.930(12)	C(18) - C(19)	1.379(16)
C(26) - H(26)	0.930(10)	C(43) - H(43A)	0.970(13)

C(43) - H(43B)	0.970(14)	C(43) - C(44)	1.45(3)
C(46) - H(46A)	0.960(13)	C(46) - H(46B)	0.960(16)
C(46) - H(46C)	0.960(14)	C(46) - H(46D)	0.960(13)
C(46) - H(46E)	0.960(16)	C(46) - H(46F)	0.960(13)
C(46) - C(45)	1.44(2)	C(19) - H(19)	0.930(15)
C(19) - C(20)	1.373(19)	C(45) - H(45A)	0.970(15)
C(45) - H(45B)	0.970(14)	C(23) - H(23A)	0.960(17)
C(23) - H(23B)	0.960(17)	C(23) - H(23C)	0.960(17)
C(23) - H(23D)	0.960(16)	C(23) - H(23E)	0.960(18)
C(23) - H(23F)	0.960(16)	C(44) - H(44A)	0.960(19)
C(44) - H(44B)	0.96(2)	C(44) - H(44C)	0.960(16)
C(44) - H(44D)	0.960(19)	C(44) - H(44E)	0.960(17)
C(44) - H(44F)	0.960(19)		

Table S5. Complete listing of bond angles (degrees).

N(2)-RU(1)-N(4)	101.1(3)	N(2)-RU(1)-N(3)	78.8(3)
N(2)-RU(1)-N(5)	176.9(4)	N(2)-RU(1)-N(1)	78.3(3)
N(4)-RU(1)-N(3)	95.7(3)	N(4)-RU(1)-N(5)	77.1(3)
N(4)-RU(1)-N(1)	90.8(3)	N(3)-RU(1)-N(5)	103.7(3)
N(3)-RU(1)-N(1)	157.1(3)	N(5)-RU(1)-N(1)	99.1(3)
F(4)-P(3)-F(5)	89.8(4)	F(4)-P(3)-F(6)	89.1(4)
F(4)-P(3)-F(9)	90.7(4)	F(4)-P(3)-F(8)	89.3(4)
F(4)-P(3)-F(7)	178.6(4)	F(5)-P(3)-F(6)	88.0(4)
F(5)-P(3)-F(9)	90.2(4)	F(5)-P(3)-F(8)	178.9(5)
F(5)-P(3)-F(7)	91.2(4)	F(6)-P(3)-F(9)	178.2(4)
F(6)-P(3)-F(8)	91.3(4)	F(6)-P(3)-F(7)	89.9(4)
F(9)-P(3)-F(8)	90.4(4)	F(9)-P(3)-F(7)	90.4(4)
F(8)-P(3)-F(7)	89.7(5)	F(1)-P(2)-F(1)	180.0
F(1)-P(2)-F(3)	90.9(4)	F(1)-P(2)-F(3)	89.1(4)
F(1)-P(2)-F(2)	89.2(4)	F(1)-P(2)-F(2)	90.8(4)
F(1)-P(2)-F(3)	89.1(4)	F(1)-P(2)-F(3)	90.9(4)
F(1)-P(2)-F(2)	90.8(4)	F(1)-P(2)-F(2)	89.2(4)
F(3)-P(2)-F(3)	180.0	F(3)-P(2)-F(2)	88.4(4)
F(3)-P(2)-F(2)	91.6(4)	F(3)-P(2)-F(2)	91.6(4)
F(3)-P(2)-F(2)	88.4(4)	F(2)-P(2)-F(2)	180.0
O(2)-P(1)-O(1)	116.5(5)	O(2)-P(1)-O(3)	102.1(6)
O(2)-P(1)-C(40)	102.3(5)	O(1)-P(1)-O(3)	115.3(5)
O(1)-P(1)-C(40)	113.7(5)	O(3)-P(1)-C(40)	105.3(5)
P(2)-F(3)-P(2)	0.0	RU(1)-N(2)-C(11)	119.4(6)
RU(1)-N(2)-C(7)	120.1(6)	C(11)-N(2)-C(7)	120.5(7)
RU(1)-N(4)-C(28)	115.3(5)	RU(1)-N(4)-C(24)	128.4(6)
C(28)-N(4)-C(24)	116.2(7)	RU(1)-N(3)-C(12)	114.7(6)
RU(1)-N(3)-C(16)	128.7(6)	C(12)-N(3)-C(16)	116.6(8)
C(29)-N(8)-C(30)	116.0(7)	P(1)-O(2)-C(45)	122.9(9)
P(1)-O(3)-C(43)	119.8(8)	P(2)-F(2)-P(2)	0.0
RU(1)-N(5)-C(29)	121.7(6)	RU(1)-N(5)-C(31)	120.1(5)
C(29)-N(5)-C(31)	117.7(7)	C(31)-N(7)-C(30)	115.2(7)
C(32)-N(6)-C(36)	118.7(7)	RU(1)-N(1)-C(6)	114.3(7)
RU(1)-N(1)-C(2)	129.2(7)	C(6)-N(1)-C(2)	116.3(9)
H(10)-C(10)-C(9)	120.6(9)	H(10)-C(10)-C(11)	120.6(10)
C(9)-C(10)-C(11)	118.8(9)	N(3)-C(12)-C(11)	114.0(8)
N(3)-C(12)-C(13)	120.1(9)	C(11)-C(12)-C(13)	125.9(8)
C(38)-C(37)-C(42)	117.8(8)	C(38)-C(37)-C(30)	120.2(8)
C(42)-C(37)-C(30)	122.0(9)	C(10)-C(9)-C(17)	120.6(9)
C(10)-C(9)-C(8)	119.2(8)	C(17)-C(9)-C(8)	120.2(9)
H(39)-C(39)-C(38)	119.7(11)	H(39)-C(39)-C(40)	119.7(9)
C(38)-C(39)-C(40)	120.6(10)	F(10)-P(4)-F(10)	180.0
F(10)-P(4)-F(12)	88.5(13)	F(10)-P(4)-F(12)	91.5(13)
F(10)-P(4)-F(12)	91.5(13)	F(10)-P(4)-F(12)	88.5(13)
F(12)-P(4)-F(12)	180.0	N(4)-C(28)-C(27)	122.9(8)
N(4)-C(28)-C(29)	113.3(7)	C(27)-C(28)-C(29)	123.9(8)
C(37)-C(38)-C(39)	120.8(9)	C(37)-C(38)-H(38)	119.6(9)
C(39)-C(38)-H(38)	119.6(10)	N(2)-C(11)-C(10)	121.4(9)
N(2)-C(11)-C(12)	113.1(7)	C(10)-C(11)-C(12)	125.5(9)
N(6)-C(32)-C(33)	121.7(8)	N(6)-C(32)-C(31)	114.4(7)
C(33)-C(32)-C(31)	123.8(8)	C(28)-C(27)-H(27)	120.2(9)
C(28)-C(27)-C(26)	119.6(9)	H(27)-C(27)-C(26)	120.2(10)
N(3)-C(16)-H(16)	118.0(11)	N(3)-C(16)-C(15)	124.0(9)

H(16)-C(16)-C(15)	118.0(11)	N(1)-C(6)-C(5)	122.1(9)
N(1)-C(6)-C(7)	114.3(9)	C(5)-C(6)-C(7)	123.6(9)
C(9)-C(17)-C(22)	119.4(9)	C(9)-C(17)-C(18)	122.2(9)
C(22)-C(17)-C(18)	118.2(9)	C(9)-C(8)-H(8)	120.9(9)
C(9)-C(8)-C(7)	118.1(9)	H(8)-C(8)-C(7)	120.9(10)
H(4)-C(4)-C(3)	120.9(12)	H(4)-C(4)-C(5)	120.9(12)
C(3)-C(4)-C(5)	118.3(12)	C(37)-C(42)-H(42)	119.9(9)
C(37)-C(42)-C(41)	120.3(9)	H(42)-C(42)-C(41)	119.9(10)
H(35)-C(35)-C(36)	120.1(9)	H(35)-C(35)-C(34)	120.1(10)
C(36)-C(35)-C(34)	119.8(9)	C(32)-C(33)-H(33)	120.5(9)
C(32)-C(33)-C(34)	119.1(8)	H(33)-C(33)-C(34)	120.5(9)
C(4)-C(3)-H(3)	120.9(12)	C(4)-C(3)-C(2)	118.3(10)
H(3)-C(3)-C(2)	120.9(10)	C(17)-C(22)-H(22)	119.6(9)
C(17)-C(22)-C(21)	120.9(10)	H(22)-C(22)-C(21)	119.6(11)
P(1)-C(40)-C(39)	120.4(8)	P(1)-C(40)-C(41)	120.8(8)
C(39)-C(40)-C(41)	118.8(9)	N(8)-C(29)-N(5)	123.6(8)
N(8)-C(29)-C(28)	124.4(8)	N(5)-C(29)-C(28)	112.0(7)
C(42)-C(41)-C(40)	121.6(9)	C(42)-C(41)-H(41)	119.2(10)
C(40)-C(41)-H(41)	119.2(9)	N(6)-C(36)-C(35)	121.8(8)
N(6)-C(36)-H(36)	119.1(9)	C(35)-C(36)-H(36)	119.1(9)
N(5)-C(31)-N(7)	123.0(7)	N(5)-C(31)-C(32)	113.3(7)
N(7)-C(31)-C(32)	123.7(7)	N(1)-C(2)-C(3)	124.4(9)
N(1)-C(2)-H(2)	117.8(11)	C(3)-C(2)-H(2)	117.8(10)
N(8)-C(30)-N(7)	124.4(7)	N(8)-C(30)-C(37)	118.3(8)
N(7)-C(30)-C(37)	117.2(8)	C(16)-C(15)-H(15)	120.2(10)
C(16)-C(15)-C(14)	119.6(11)	H(15)-C(15)-C(14)	120.2(12)
C(15)-C(14)-H(14)	121.0(12)	C(15)-C(14)-C(13)	118.0(11)
H(14)-C(14)-C(13)	121.0(11)	C(35)-C(34)-C(33)	118.8(9)
C(35)-C(34)-H(34)	120.6(10)	C(33)-C(34)-H(34)	120.6(10)
C(6)-C(5)-C(4)	120.5(10)	C(6)-C(5)-H(5)	119.7(11)
C(4)-C(5)-H(5)	119.8(12)	C(22)-C(21)-H(21)	119.9(13)
C(22)-C(21)-C(20)	120.2(12)	H(21)-C(21)-C(20)	119.9(12)
N(4)-C(24)-H(24)	119.0(8)	N(4)-C(24)-C(25)	122.0(8)
H(24)-C(24)-C(25)	119.0(9)	C(12)-C(13)-C(14)	121.8(9)
C(12)-C(13)-H(13)	119.1(11)	C(14)-C(13)-H(13)	119.1(12)
C(24)-C(25)-H(25)	119.1(9)	C(24)-C(25)-C(26)	121.8(9)
H(25)-C(25)-C(26)	119.1(9)	C(17)-C(18)-H(18)	119.7(10)
C(17)-C(18)-C(19)	120.5(11)	H(18)-C(18)-C(19)	119.7(12)
C(27)-C(26)-C(25)	117.3(9)	C(27)-C(26)-H(26)	121.3(10)
C(25)-C(26)-H(26)	121.3(10)	N(2)-C(7)-C(6)	112.9(8)
N(2)-C(7)-C(8)	121.9(9)	C(6)-C(7)-C(8)	125.2(9)
O(3)-C(43)-H(43A)	109.3(12)	O(3)-C(43)-H(43B)	109.3(12)
O(3)-C(43)-C(44)	111.5(13)	H(43A)-C(43)-H(43B)	108.0(14)
H(43A)-C(43)-C(44)	109.3(13)	H(43B)-C(43)-C(44)	109.3(13)
H(46A)-C(46)-H(46B)	109.5(13)	H(46A)-C(46)-H(46C)	109.5(16)
H(46A)-C(46)-H(46D)	141.1(16)	H(46A)-C(46)-H(46E)	56.3(9)
H(46A)-C(46)-H(46F)	56.2(7)	H(46A)-C(46)-C(45)	109.5(13)
H(46B)-C(46)-H(46C)	109.5(14)	H(46B)-C(46)-H(46D)	56.2(9)
H(46B)-C(46)-H(46E)	141.1(16)	H(46B)-C(46)-H(46F)	56.3(9)
H(46B)-C(46)-C(45)	109.5(14)	H(46C)-C(46)-H(46D)	56.3(8)
H(46C)-C(46)-H(46E)	56.3(9)	H(46C)-C(46)-H(46F)	141.1(16)
H(46C)-C(46)-C(45)	109.5(13)	H(46D)-C(46)-H(46E)	109.5(15)
H(46D)-C(46)-H(46F)	109.5(15)	H(46D)-C(46)-C(45)	109.5(12)

H(46E)-C(46)-H(46F)	109.5(13)	H(46E)-C(46)-C(45)	109.5(14)
H(46F)-C(46)-C(45)	109.5(14)	C(18)-C(19)-H(19)	118.8(14)
C(18)-C(19)-C(20)	122.3(13)	H(19)-C(19)-C(20)	118.9(12)
C(21)-C(20)-C(19)	117.8(11)	O(2)-C(45)-C(46)	114.3(11)
O(2)-C(45)-H(45A)	108.7(12)	O(2)-C(45)-H(45B)	108.7(13)
C(46)-C(45)-H(45A)	108.7(14)	C(46)-C(45)-H(45B)	108.7(12)
H(45A)-C(45)-H(45B)	107.6(13)	H(23A)-C(23)-H(23B)	109.5(14)
H(23A)-C(23)-H(23C)	109.5(16)	H(23A)-C(23)-H(23D)	141.1(11)
H(23A)-C(23)-H(23E)	56.3(10)	H(23A)-C(23)-H(23F)	56.2(9)
H(23B)-C(23)-H(23C)	109.5(15)	H(23B)-C(23)-H(23D)	56.2(10)
H(23B)-C(23)-H(23E)	141.1(11)	H(23B)-C(23)-H(23F)	56.3(9)
H(23C)-C(23)-H(23D)	56.3(9)	H(23C)-C(23)-H(23E)	56.3(10)
H(23C)-C(23)-H(23F)	141.1(11)	H(23D)-C(23)-H(23E)	109.5(15)
H(23D)-C(23)-H(23F)	109.5(15)	H(23E)-C(23)-H(23F)	109.5(15)
C(43)-C(44)-H(44A)	109.5(17)	C(43)-C(44)-H(44B)	109.5(15)
C(43)-C(44)-H(44C)	109.5(17)	C(43)-C(44)-H(44D)	109.5(17)
C(43)-C(44)-H(44E)	109.5(18)	C(43)-C(44)-H(44F)	109.5(14)
H(44A)-C(44)-H(44B)	109.5(19)	H(44A)-C(44)-H(44C)	109.5(16)
H(44A)-C(44)-H(44D)	141.1(21)	H(44A)-C(44)-H(44E)	56.3(10)
H(44A)-C(44)-H(44F)	56.3(11)	H(44B)-C(44)-H(44C)	109.5(19)
H(44B)-C(44)-H(44D)	56.3(11)	H(44B)-C(44)-H(44E)	141.1(21)
H(44B)-C(44)-H(44F)	56.3(11)	H(44C)-C(44)-H(44D)	56.3(10)
H(44C)-C(44)-H(44E)	56.3(9)	H(44C)-C(44)-H(44F)	141.1(21)
H(44D)-C(44)-H(44E)	109.5(16)	H(44D)-C(44)-H(44F)	109.5(20)
H(44E)-C(44)-H(44F)	109.5(18)		

Computational Details

Table S6. Cartesian Coordinates of the atoms at the DFT optimized ground state geometry of **p1**.

Stoichiometry C45H39N8O3PRu(2+)
Framework group C1[X(C45H39N8O3PRu)]
Deg. of freedom 285
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.547493	0.014221	-0.053522
2	7	0	3.740289	0.002442	-0.014374
3	6	0	5.808678	-1.161798	-0.362440
4	6	0	5.807727	1.184013	0.276188
5	6	0	4.407340	1.158277	0.286436
6	6	0	4.408354	-1.147808	-0.333561
7	1	0	6.337750	-2.063227	-0.647223
8	1	0	6.337061	2.089611	0.546955
9	6	0	3.501155	-2.280677	-0.631555
10	6	0	1.635560	-4.285448	-1.152498
11	6	0	3.942753	-3.564702	-0.992992
12	7	0	2.145930	-2.001848	-0.532540
13	6	0	1.246642	-2.988663	-0.788723
14	6	0	3.007537	-4.579052	-1.256923
15	1	0	5.003824	-3.774200	-1.069528
16	1	0	0.198931	-2.726230	-0.698951
17	1	0	3.341117	-5.573150	-1.537130
18	1	0	0.880385	-5.039290	-1.347175
19	6	0	3.499314	2.283166	0.611019
20	6	0	1.632342	4.271421	1.187168
21	7	0	2.144292	1.992572	0.551095
22	6	0	3.940101	3.570759	0.960553
23	6	0	3.004159	4.576824	1.252308
24	6	0	1.244288	2.971522	0.833686
25	1	0	5.001122	3.789241	1.006717
26	1	0	3.337051	5.573566	1.523789
27	1	0	0.196663	2.700431	0.773656
28	1	0	0.876561	5.018508	1.404242
29	6	0	8.026003	0.020138	-0.073692
30	6	0	10.889192	0.030943	-0.114175
31	6	0	8.748399	1.202436	-0.370601
32	6	0	8.766187	-1.158556	0.202925
33	6	0	10.165641	-1.149433	0.186229
34	6	0	10.150532	1.203722	-0.393651
35	1	0	8.222847	2.119438	-0.627055
36	1	0	8.253790	-2.078913	0.473599
37	1	0	10.709003	-2.062743	0.417056
38	1	0	10.679566	2.120741	-0.639612
39	6	0	12.402672	0.027703	-0.131847
40	1	0	12.807604	-0.248557	0.850682
41	1	0	12.807986	1.008788	-0.397820
42	1	0	12.788091	-0.703468	-0.854433
43	6	0	-2.970710	-0.023199	0.092727
44	7	0	-0.268493	-0.015454	0.046753
45	7	0	-2.282920	-0.335193	1.251337
46	7	0	-2.325249	0.290352	-1.089369

47	6	0	-0.987160	0.285438	-1.076434
48	6	0	-0.946755	-0.321962	1.193530
49	6	0	-0.047432	-0.624857	2.322440
50	6	0	1.789542	-1.158458	4.321905
51	6	0	-0.513594	-0.965464	3.599045
52	7	0	1.308550	-0.546984	2.029780
53	6	0	2.196837	-0.811409	3.022330
54	6	0	0.416101	-1.237655	4.618403
55	1	0	-1.583997	-1.010143	3.769540
56	1	0	3.247682	-0.741900	2.765808
57	1	0	0.078998	-1.503373	5.615161
58	1	0	2.539260	-1.360135	5.079794
59	6	0	-0.127325	0.595093	-2.234075
60	6	0	1.640019	1.144226	-4.291583
61	7	0	1.238166	0.529386	-1.985156
62	6	0	-0.637004	0.931345	-3.495075
63	6	0	0.257098	1.211261	-4.543736
64	6	0	2.091773	0.801390	-3.005654
65	1	0	-1.712690	0.967090	-3.630917
66	1	0	-0.114084	1.473933	-5.529128
67	1	0	3.150805	0.741654	-2.782480
68	1	0	2.363225	1.352404	-5.073101
69	6	0	-4.432565	-0.022562	0.121973
70	6	0	-7.239489	-0.005024	0.185840
71	6	0	-5.171592	0.285447	-1.051355
72	6	0	-5.119438	-0.321524	1.326956
73	6	0	-6.518884	-0.310823	1.357508
74	6	0	-6.570679	0.293340	-1.018030
75	1	0	-4.642245	0.516779	-1.968832
76	1	0	-4.551573	-0.551892	2.221203
77	1	0	-7.059720	-0.525882	2.275242
78	1	0	-7.141013	0.538067	-1.908119
79	15	0	-9.088102	-0.007339	0.289782
80	8	0	-9.638457	-0.239671	1.761500
81	8	0	-9.411022	1.447774	-0.522751
82	8	0	-9.600134	-1.181925	-0.846491
83	6	0	-10.796091	1.923325	-0.800508
84	1	0	-10.650947	2.648641	-1.605316
85	1	0	-11.386679	1.081500	-1.183789
86	6	0	-11.434315	2.560468	0.434451
87	1	0	-12.424834	2.953995	0.169918
88	1	0	-10.821590	3.390863	0.801744
89	1	0	-11.554356	1.832396	1.244026
90	6	0	-10.477402	-2.324661	-0.457803
91	1	0	-10.357694	-2.520084	0.614831
92	1	0	-10.081395	-3.165255	-1.034724
93	6	0	-11.934012	-2.032535	-0.810967
94	1	0	-12.336809	-1.218126	-0.197189
95	1	0	-12.542884	-2.927029	-0.623426
96	1	0	-12.032205	-1.767682	-1.869653
97	44	0	1.726271	-0.006452	0.015247

Table S7. Computed vertical singlet excitation energies and oscillator strengths of **p1**.

```
Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      2.0821 eV  595.47 nm  f=0.0000
<S**2>=0.000
     201 ->205         0.15369
     204 ->205         0.68068
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-A      2.1872 eV  566.86 nm  f=0.0055
<S**2>=0.000
     202 ->206        -0.12269
     203 ->205         0.68581

 Excited State   3:      Singlet-A      2.1943 eV  565.02 nm  f=0.0000
<S**2>=0.000
     201 ->206         0.14012
     204 ->206         0.68872

 Excited State   4:      Singlet-A      2.3162 eV  535.29 nm  f=0.0162
<S**2>=0.000
     202 ->205        -0.32956
     203 ->206         0.62043

 Excited State   5:      Singlet-A      2.3953 eV  517.62 nm  f=0.0565
<S**2>=0.000
     202 ->206         0.68982
     203 ->205         0.12246

 Excited State   6:      Singlet-A      2.6110 eV  474.86 nm  f=0.7876
<S**2>=0.000
     202 ->205         0.47443
     203 ->206         0.26221
     204 ->207         0.44146

 Excited State   7:      Singlet-A      2.6543 eV  467.12 nm  f=0.0117
<S**2>=0.000
     203 ->207         0.70026

 Excited State   8:      Singlet-A      2.6996 eV  459.27 nm  f=0.0000
<S**2>=0.000
     202 ->207         0.69957

 Excited State   9:      Singlet-A      2.8709 eV  431.86 nm  f=0.0251
<S**2>=0.000
     202 ->205        -0.30662
     203 ->206        -0.17856
     203 ->208        -0.39499
     203 ->213         0.12173
     204 ->207         0.43932

 Excited State  10:      Singlet-A      2.9191 eV  424.73 nm  f=0.0352
<S**2>=0.000
     204 ->208         0.69031

 Excited State  11:      Singlet-A      3.0770 eV  402.93 nm  f=0.0001
<S**2>=0.000
```

```
     202 ->208         0.69737

 Excited State  12:      Singlet-A      3.2549 eV  380.92 nm  f=0.0326
<S**2>=0.000
     201 ->205         0.11707
     202 ->205        -0.19899
     203 ->208         0.56129
     203 ->213         0.14645
     204 ->207         0.28194

 Excited State  13:      Singlet-A      3.2600 eV  380.31 nm  f=0.0010
<S**2>=0.000
     201 ->205         0.66003
     204 ->205        -0.16725
     204 ->209         0.10792

 Excited State  14:      Singlet-A      3.2921 eV  376.61 nm  f=0.0000
<S**2>=0.000
     201 ->206         0.68701
     204 ->206        -0.14365

 Excited State  15:      Singlet-A      3.3625 eV  368.73 nm  f=0.0000
<S**2>=0.000
     203 ->216        -0.67781
     204 ->209         0.11334

 Excited State  16:      Singlet-A      3.3908 eV  365.65 nm  f=0.0000
<S**2>=0.000
     201 ->205        -0.11280
     201 ->209         0.11108
     203 ->216         0.12798
     204 ->209         0.65870

 Excited State  17:      Singlet-A      3.5436 eV  349.88 nm  f=0.0035
<S**2>=0.000
     199 ->205         0.63612
     200 ->205         0.26118
     204 ->216         0.10668

 Excited State  18:      Singlet-A      3.5686 eV  347.43 nm  f=0.1260
<S**2>=0.000
     199 ->206        -0.17360
     202 ->209         0.66437

 Excited State  19:      Singlet-A      3.5785 eV  346.47 nm  f=0.0834
<S**2>=0.000
     203 ->209         0.67738

 Excited State  20:      Singlet-A      3.5794 eV  346.38 nm  f=0.0137
<S**2>=0.000
     199 ->206         0.61776
     200 ->206         0.26892
     202 ->209         0.19045
```

Table S8. Cartesian Coordinates of the atoms in the $Ti_{64}O_{128}$ slab optimized at the Molecular Mechanics level.

Stoichiometry O128Ti64
Framework group C1[X(O128Ti64)]
Deg. of freedom 570
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	10081003	-8.273551	4.520786	-1.588236
2	8	10081003	-6.679554	1.177091	-2.156963
3	22	10221003	-8.006726	2.582240	-1.689196
4	8	10081003	-9.484468	2.303230	-2.922824
5	22	10221003	-10.692512	2.579400	-1.383052
6	8	10081003	-11.201792	0.902058	-0.544814
7	8	10081003	-9.177597	2.646574	-0.120908
8	22	10221006	-9.851762	1.098750	0.887428
9	8	10081003	-11.039037	2.355179	1.822907
10	8	10081003	-10.755577	-0.294711	1.895154
11	8	10081003	-8.626066	-0.152346	-0.075485
12	8	10081003	-4.588395	-1.635160	-2.669658
13	22	10221003	-6.266917	-0.761229	-1.898745
14	22	10221003	-8.596002	-2.545701	-2.333435
15	8	10081003	-9.710553	-2.601103	-0.694030
16	8	10081003	-7.206227	-2.210845	-1.064079
17	22	10221006	-8.219910	-2.048963	0.489365
18	8	10081003	-9.283102	-2.070829	2.119327
19	8	10081003	-7.735547	-3.989144	0.948191
20	8	10081003	-2.613466	-4.949876	-2.344856
21	22	10221003	-4.050820	-3.525465	-2.247546
22	8	10081003	-5.225668	-4.253218	-3.612593
23	22	10221003	-6.680151	-4.044572	-2.312999
24	8	10081003	-7.050323	-5.634540	-1.280290
25	8	10081003	-5.431894	-3.493413	-0.863004
26	22	10221006	-6.039569	-4.947734	0.272006
27	8	10081003	-4.452825	-5.787756	-0.468732
28	8	10081003	-0.459026	-7.704781	-2.305652
29	22	10221003	-2.112415	-6.800496	-1.696834
30	8	10081003	-3.480657	-7.709633	-2.827411
31	22	10221003	-3.754472	-9.205438	-1.575297
32	8	10081003	-5.247702	-8.857302	-0.335771
33	8	10081003	-2.625585	-8.160988	-0.389881
34	22	10221003	-4.162450	-7.431846	0.445000
35	22	10221003	0.540495	-6.899130	-0.834865
36	8	10081003	0.068826	-7.782249	0.880590
37	8	10081003	2.061423	-6.887814	0.458184
38	8	10081003	2.096002	-6.199293	-1.823254
39	22	10221003	2.762162	-5.240009	-0.278615
40	22	10221003	0.978504	-6.386644	1.961872
41	22	10221006	-1.407533	-3.916154	-1.264177
42	8	10081003	-2.358683	-3.887502	0.414938
43	8	10081003	-0.297356	-2.703834	-0.231941
44	8	10081003	-0.100038	-3.783495	-2.749074
45	22	10221003	1.042422	-2.608070	-1.650101
46	22	10221003	-0.729101	-3.438628	1.531162

47	8	10081003	-0.914193	-5.678448	-0.511514
48	8	10081003	2.488688	-3.966031	-1.663932
49	8	10081003	0.963398	-4.483212	1.367608
50	8	10081003	-0.418819	-6.700113	3.319890
51	22	10221003	-1.526241	-7.699773	2.066706
52	22	10221003	-3.226695	-4.990672	1.764717
53	8	10081003	-1.802448	-4.359434	2.943540
54	8	10081003	-3.357445	-6.931312	2.083940
55	8	10081003	-5.066525	-4.227605	1.853775
56	22	10221006	-3.377184	-0.891395	-1.321728
57	8	10081003	-3.546784	-1.919488	0.325159
58	8	10081003	-2.278274	0.077707	-0.120018
59	8	10081003	-2.401746	0.210225	-2.620377
60	22	10221003	-0.828427	0.495542	-1.356298
61	22	10221003	-2.472233	-0.769169	1.635822
62	8	10081003	-2.348193	-2.394311	-2.055574
63	8	10081003	0.525716	-0.730727	-2.170429
64	8	10081003	-0.826067	-1.663639	2.386538
65	22	10221003	-5.010519	-2.271754	1.507922
66	8	10081003	-3.935946	-1.360526	2.851222
67	8	10081003	-6.749214	-1.360846	1.559962
68	22	10221006	-5.228846	1.905229	-1.141102
69	8	10081003	-5.980769	2.053352	0.659355
70	8	10081003	-3.680415	2.464972	-0.178455
71	8	10081003	-4.093500	2.229004	-2.765552
72	22	10221003	-2.761186	3.322975	-1.708173
73	22	10221003	-4.224739	2.228214	1.735237
74	8	10081003	-4.901349	0.083186	-0.690153
75	8	10081003	-1.149738	2.208021	-2.175972
76	8	10081003	-2.617811	1.127045	2.369020
77	22	10221003	-6.750778	0.619448	1.681637
78	8	10081003	-5.320189	1.053166	2.930011
79	8	10081003	-8.471291	1.370069	2.293475
80	22	10221003	-6.783168	4.861946	-0.382484
81	8	10081003	-7.493879	4.914528	1.455612
82	8	10081003	-5.145593	4.441429	0.512150
83	8	10081003	-6.044793	6.583362	-0.930323
84	22	10221003	-4.324885	5.980201	-0.250733
85	22	10221003	-5.693531	4.893268	2.333660
86	8	10081003	-6.220438	3.513629	-1.645923
87	8	10081003	-3.277658	5.301010	-1.753235
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89	22	10221003	-8.162660	3.347469	2.490239
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92	8	10081003	-6.552824	-6.520607	1.333127
93	8	10081003	-7.763140	-0.975061	-3.209048
94	22	10221003	5.785569	-5.868597	-0.599914
95	8	10081003	6.157626	-6.428180	1.250823
96	8	10081003	7.618832	-5.386097	-0.077419
97	8	10081003	6.546282	-5.652038	-2.451828
98	22	10221003	7.977858	-4.486629	-1.793590
99	22	10221003	7.074069	-4.692782	1.680701
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101	22	10221006	3.867715	-2.845509	-1.002310
102	8	10081003	3.197597	-2.537151	0.745434
103	8	10081003	4.965593	-1.468162	-0.324653
104	8	10081003	5.031531	-2.912835	-2.550392
105	22	10221003	6.203904	-1.485798	-1.759007
106	22	10221003	4.995079	-2.000859	1.508730
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108	8	10081003	4.554895	-4.444542	-0.024300

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112	8	10081003	10.804801	-1.173081	-1.171782
113	22	10221003	10.866211	-2.253996	0.466745
114	8	10081003	10.080125	-1.544737	2.134588
115	8	10081003	9.096026	-2.849105	-0.038323
116	22	10221006	8.292580	-2.236380	1.667296
117	8	10081003	8.759197	-4.048318	2.340993
118	8	10081003	6.629491	-2.966628	0.986427
119	8	10081003	6.039879	-4.778681	3.361158
120	22	10221003	4.831210	-6.111161	2.679942
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124	8	10081003	7.520041	-1.850048	3.416394
125	8	10081003	7.819924	-0.466633	1.011806
126	8	10081003	1.445466	-2.289956	3.213983
127	22	10221006	2.096579	0.111508	-1.335173
128	8	10081003	2.087709	-0.618178	0.514176
129	8	10081003	3.729910	0.846095	-0.590102
130	8	10081003	2.663008	0.985887	-3.046148
131	22	10221003	4.407953	1.611180	-2.266464
132	22	10221003	3.319882	0.782954	1.346730
133	8	10081003	6.177951	2.688778	-2.651823
134	8	10081003	2.789882	-1.567115	-1.963568
135	8	10081003	5.745027	0.169296	-2.778551
136	22	10221006	7.234707	1.152672	-1.993140
137	8	10081003	8.124242	0.944342	-3.725894
138	8	10081003	8.761262	2.195751	-1.366662
139	22	10221003	7.725071	2.846803	0.081448
140	8	10081003	8.286968	2.085632	1.728566
141	8	10081003	6.332767	1.492350	-0.159430
142	22	10221006	6.692855	0.950075	1.795921
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144	22	10221003	0.892776	-0.730081	2.035896
145	8	10081003	1.999401	0.635972	2.865447
146	8	10081003	-0.257377	0.274993	0.932379
147	8	10081003	7.177808	0.525551	3.645167
148	8	10081003	5.628857	2.432999	2.602462
149	22	10221006	0.180962	3.198395	-1.249619
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152	8	10081003	1.318126	3.403117	-2.823310
153	22	10221003	2.544734	4.647398	-1.830802
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155	8	10081003	4.151056	5.744491	-1.270671
156	8	10081003	0.867569	1.504339	-0.659558
157	8	10081003	3.913294	3.500624	-2.602088
158	22	10221006	5.430548	4.416654	-1.925985
159	8	10081003	5.537486	5.251600	-3.697365
160	8	10081003	7.015242	5.436550	-1.298400
161	22	10221003	7.052592	4.648077	0.485038
162	8	10081003	6.078790	5.148144	2.104219
163	8	10081003	5.494649	3.605557	-0.062964
164	22	10221006	4.602014	3.896573	1.709043
165	8	10081003	3.070705	2.785407	1.241843
166	22	10221003	-0.915200	1.912382	1.735980
167	8	10081003	0.453037	2.679778	2.910189
168	8	10081003	3.635805	5.354176	0.926998
169	8	10081003	-1.651122	3.285671	0.562716
170	22	10221003	-1.603091	6.092907	-1.139768

171	8	10081003	-2.189060	6.424343	0.723289
172	8	10081003	0.156794	6.257820	-0.339973
173	8	10081003	-1.193514	7.600082	-2.362291
174	22	10221003	0.642519	7.559875	-1.711941
175	22	10221003	-0.367438	6.712634	1.505645
176	8	10081003	2.064351	8.911686	-2.123291
177	8	10081003	-1.090334	4.453594	-1.972877
178	8	10081003	1.897228	6.349135	-2.618242
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182	22	10221003	3.739895	9.072438	0.407395
183	8	10081003	4.559724	7.941993	1.726526
184	8	10081003	2.422335	7.664047	0.063766
185	22	10221006	2.926993	6.875302	1.888839
186	8	10081003	1.268298	5.774933	2.182721
187	22	10221003	-2.448215	4.714344	1.651794
188	8	10081003	-1.113496	5.444418	2.851738
189	8	10081003	3.535595	6.358119	3.667386
190	8	10081003	2.123603	8.420060	2.790962
191	8	10081003	-0.349866	8.614462	2.000276
192	8	10081003	3.758565	4.060253	3.459662