Supporting Information

for

Zinc Oxide Nanocrystal Quenching of Emission from Electron-Rich Ruthenium-Bipyridine Complexes

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Synthesis of 4,4'-bis(diethylamino)-2,2'-bipyridine, $(Et_2N)_2$bpy. 4,4'-Dichloro-2,2'-bipyridine-N,N'-dioxide (0.60 g, 0.0023 mol) was added to 27 mL of 2:1 diethylamine/water and heated in a sealed autoclave with stirring for 22 hours at 135°C. The reaction was then cooled to room temperature and the solvent was evaporated. The crude brown oil was dissolved in dry, deoxygenated chloroform (~30 mL) to which 5 mL (0.047 mol, 20 eq) of phosphorus trichloride (PCl_3) was added at 0°C. The reaction was then refluxed for 3 h, cooled to room temperature, and poured onto ice (~200 g). The organic layer was separated from the aqueous layer and further extracted with water (3 x 20 mL). The aqueous layers were combined and the volume was reduced to ~100 mL under vacuum. The reaction mixture was then basified with concentrated NaOH(aq) causing the desired compound to precipitate. The precipitate was filtered and washed thoroughly with water and dried under vacuum. $(Et_2N)_2$bpy was isolated as a grey solid by filtration to yield 0.57 g (82%). ^{1}H-NMR (300 MHz; CD_2Cl_2): δ 8.21 (d, J = 5.9 Hz, 2H), 7.67 (d, J = 2.7 Hz, 2H), 6.49 (dd, J = 5.9, 2.8 Hz, 2H), 3.46 (q, J = 7.1 Hz, 8H), 1.22 (t, J = 7.1 Hz, 12H).

Synthesis of 4,4'-dipyrrolidino-2,2'-bipyridine, **(pyrrol)$_2$bpy**. 4,4'-Dichloro-2,2'-bipyridine-N,N'-dioxide (0.50 g, 0.0022 mol) was added to 40 mL pyrrolidine and the reaction was refluxed neat for 23 h. Using the same procedure as above, (pyrrol)$_2$bpy was isolated after treatment with PCl_3 as a light brown solid by filtration to yield 0.27 g (47%). ^{1}H-NMR (300 MHz; $CDCl_3$): δ 8.29 (d, *J* = 5.7 Hz, 2H), 7.55 (d, *J* = 2.3 Hz, 2H), 6.40 (dd, *J* = 5.7, 2.4 Hz, 2H), 3.44 (t, *J* = 6.5 Hz, 8H), 2.05 (q, *J* = 6.5 Hz, 8H).

Synthesis of 4,4'-dipiperidino-2,2'-bipyridine, **(pip)$_2$bpy**. 4,4'-Dichloro-2,2'-bipyridine-N,N'-dioxide (0.50 g, 0.0022 mol) was added to 50 mL piperidine and the reaction was refluxed neat for 23 h. After treatment with PCl_3, (pip)$_2$bpy was isolated as a light brown solid by filtration to yield 0.50 g (80%). ^{1}H-NMR (300 MHz; $CDCl_3$): δ 8.31 (d, *J* = 5.9 Hz, 2H), 7.85 (d, *J* = 2.7 Hz, 2H), 6.66 (dd, *J* = 5.9, 2.7 Hz, 2H), 3.44 (d, *J* = 4.9 Hz, 8H), 1.67-1.63 (m, 12H).

Synthesis of 4,4'-dimorpholino-2,2'-bipyridine, **(morph)$_2$bpy**. 4,4'-Dichloro-2,2'-bipyridine-N,N'-dioxide (0.50 g, 0.0022 mol) was added to 50 mL morpholine, and the reaction was refluxed for 24 h. After treatment with PCl_3, (morph)$_2$bpy was isolated as a light brown solid by filtration to yield 0.47 g (74%). ^{1}H-NMR (300 MHz; $CDCl_3$): δ 8.36 (d, *J* = 5.9 Hz, 2H), 7.88 (d, *J* = 2.6 Hz, 2H), 6.69 (dd, *J* = 5.9, 2.7 Hz, 2H), 3.86 (t, *J* = 4.9 Hz, 8H), 3.42 (t, *J* = 5.0 Hz, 8H).

Synthesis of 4,4'-di(N-methylpiperazino)-2,2'-bipyridine, **(mepipz)$_2$bpy**. 4,4'-Dichloro-2,2'-bipyridine-1,1'-dioxide (0.50 g, 0.0022 mol) was added to 50 mL N-methylpiperazine and the reaction was refluxed for 22 h. After treatment with PCl_3, (mepipz)$_2$bpy was isolated as a light brown solid by filtration to yield 0.61 g (90%). ^{1}H-NMR (300 MHz; $CDCl_3$): δ 8.33 (d, *J* = 5.9 Hz, 2H), 7.87 (d, *J* = 2.5 Hz, 2H), 6.68 (dd, *J* = 5.9, 2.7 Hz, 2H), 3.47 (t, *J* = 5.1 Hz, 8H), 2.54 (t, *J* = 5.0 Hz, 8H), 2.35 (s, 6H).

Synthesis of 4,4'-dimethoxy-2,2'-bipyridine, **$(MeO)_2$bpy**. Solid 4,4'-dichloro-2,2'-bipyridine-N,N'-dioxide (1.50 g, 0.0058 mol) was added to freshly prepared sodium methoxide (0.025 mol) in dry methanol (75 mL). The yellow suspension was stirred at 60 ˚C for 5 h, resulting in a yellow solution. The reaction was cooled to 0°C and neutralized with concentrated sulfuric acid. The excess solvent was evaporated and the crude solid was dried under vacuum. The crude solid 4,4'-dimethoxy-2,2'-bipyridine-N,N'-dioxide was treated with PCl_3 as above to yield 1.0 g (80%) of $(MeO)_2$bpy as an off-white solid. ^{1}H-NMR (300 MHz; CD_2Cl_2): δ 8.46 (d, *J* = 5.6 Hz, 2H), 8.01 (d, *J* = 2.6 Hz, 2H), 6.86 (dd, *J* = 5.6, 2.6 Hz, 2H), 3.94 (s, 6H).

{Ru[$(Et_2N)_2$bpy]$_2Cl_2$}Cl. $RuCl_3$•$3H_2O$ (0.25 g, 1 mmol, 1 eq) was added to a solution of LiCl (1.7 g, 39 mmol) in ethylene glycol/water (25 mL, 4:1) at 110 ˚C. The LiCl was used to maintain a total Cl^- ion concentration of 1.7 M. After 15 min, $(Et_2N)_2$bpy (0.60 g, 2.0 mmol, 2 eq) was added. After 12 min glucose (0.36 g, 2.0 mmol, 2 eq) was added and allowed to react for 10 min, at which point ascorbic acid (0.089 g, 0.5 mmol, 0.5 eq) was added. The reaction solution was maintained at 110 ˚C for 30 min. The reaction was quenched with the addition of 10 mL of a saturated NaCl solution and cooled to 0°C for 60 min. The dark purple precipitate was filtered, washed with the NaCl solution, and chromatographed on a neutral alumina column using methylene chloride/methanol (99:1) as the eluent. First to elute was a dark purple band, which yielded 0.30 g (37%) of paramagnetic {Ru[$(Et_2N)_2$bpy]$_2Cl_2$}Cl. Further elution yielded a dark red band of {Ru[$(Et_2N)_2$bpy]$_3$}Cl_2 (0.17 g, 24%). HR ESI-MS of {Ru[$(Et_2N)_2$bpy]$_2Cl_2$}Cl m/z (obs) 768.2724 (M^+), m/z (calcd) 768.2736.

{Ru[$(pyrrol)_2$bpy]$_2Cl_2$}Cl. The same procedure was repeated with $RuCl_3$•$3H_2O$ (0.21 g, 0.8 mmol) and $(pyrrol)_2$bpy (0.50 g, 1.6 mmol). The dark dark purple precipitate was filtered and

chromatographed to yield 0.17 g (25%) of {Ru[(pyrrol)$_2$bpy]$_2$Cl$_2$}Cl. HR ESI-MS m/z (obs) 760.2119 (M^+), m/z (calcd) 760.2110.

{Ru[(pip)$_2$bpy]$_2$Cl$_2$}Cl. The same procedure was repeated with $RuCl_3$•3H_2O (0.17 g, 0.7 mmol) and (pip)$_2$bpy (0.45 g, 1.4 mmol). The dark purple precipitate was filtered and chromatographed to yield 0.14 g (25%) of {Ru[(pip)$_2$bpy]$_2$Cl$_2$}Cl. Further elution produced a dark red band of {Ru[(Et$_2$N)$_2$bpy]$_3$}Cl$_2$ (0.16 g, 22%). HR ESI-MS of {Ru[(pip)$_2$bpy]$_2$Cl$_2$}Cl m/z (obs) 816.2713 (M^+), m/z (calcd) 816.2736.

{Ru[(morph)$_2$bpy]$_2$Cl$_2$}Cl. The same procedure was repeated with $RuCl_3$•3H_2O (0.17 g, 0.7 mmol) and (morph)$_2$bpy (0.45 g, 1.4 mmol). The reaction was quenched, and the dark purple precipitate was filtered. Due to its limited solubility crude {Ru[(morph)$_2$bpy]$_2$Cl$_2$}Cl was used in the subsequent reaction. HR ESI-MS showed the presence of m/z 824.1890 (M^+), m/z (calcd) 824.1906.

Ru[(MeO)$_2$bpy]$_2$Cl$_2$. The same procedure was repeated with $RuCl_3$•3H_2O (0.30 g, 1.3 mmol) and (MeO)$_2$bpy (0.54 g, 2.5 mmol). The purple/brown precipitate was filtered, dissolved in a warm 1:1 mixture of methanol:methylene chloride, and filtered a second time. The red/orange filtrate was evaporated to yield 0.47 g of a mixture containing Ru[(MeO)$_2$bpy]$_2$Cl$_2$, which was used in the next step without further purification. HR ESI-MS m/z (obs) 302.0120 (M^{2+}), m/z (calcd) 302.0109.

S. I. Figure 1. Electronic absorption spectra for **1** - **6** in methanol.

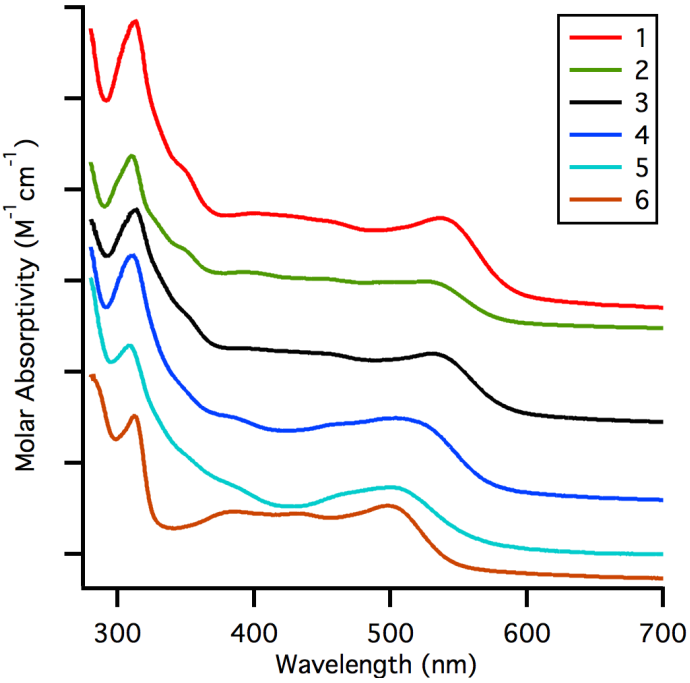
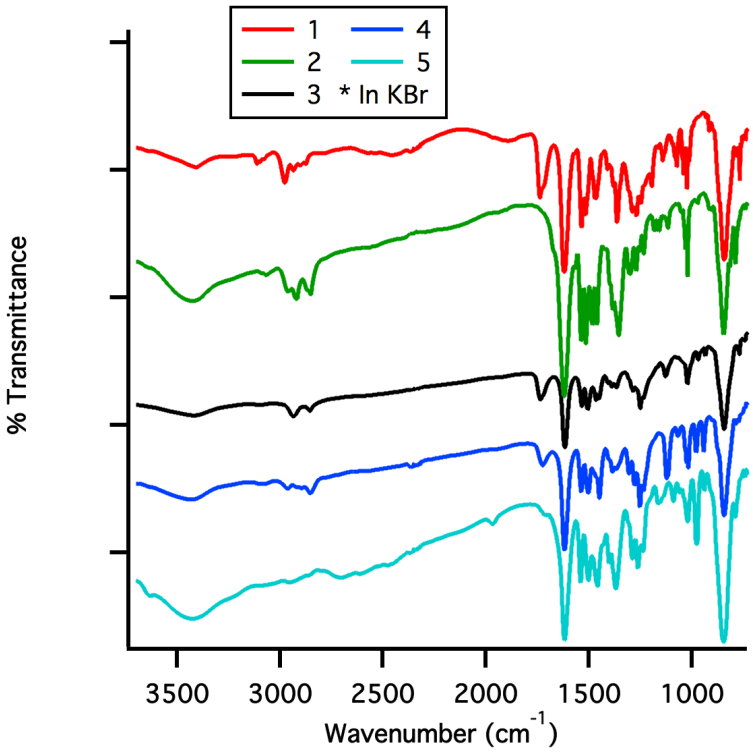


Figure 2. IR (KBr) of compounds **1** - **5**.



S. I. Table 1. Spectroscopic and electrochemical properties of complexes **1-6**, and their deprotonated analogues.

Dyes	λ_{abs} (nm)[a]	λ_{em} (nm)[a,b]	E° (V)[c] Ru^{III}/Ru^{II}	E° (V)[c] RuL_3^{2+}/RuL_3^{+}	E° (V)[c] RuL_3^{+}/RuL_3^{0}	E° (V)[c] RuL_3^{0}/RuL_3^{-}	E*[d] Ru^{III}/Ru^{II}
1	540	778	0.953	-0.993 (ir)	-1.29 (ir)	-	-0.99
1-COO$^-$	515	748	0.832	-1.40	-1.71	-1.92	-1.20
2	535	760	0.801	-1.43 (ir)	-	-	-1.17
2-COO$^-$	520	752	0.779	-	-	-	-1.23
3	542	786	0.980	-0.940 (ir)	-1.30 (ir)	-	-0.95
3-COO$^-$	502	742	0.865	-1.37	-1.64	-1.82	-1.21
4	527	777	1.04	-0.948 (ir)	-1.21 (ir)	-1.62 (ir)	-0.94
4-COO$^-$	499	723	0.942	-1.33	-1.55	-1.76	-1.15
5	505	775	1.21	-0.880 (ir)	-1.35 (ir)	-	-0.82
5-COO$^-$	498	725	0.940	-1.34	-1.58	-1.78	-1.16
6	500	740	1.37	-0.840 (ir)	-1.35 (ir)	-1.75 (ir)	-0.70
6-COO$^-$	475	680	1.22	-1.20	-1.36	-1.57	-0.99
1-Cl[e]	545	-	0.927	-0.946 (ir)	-1.57 (ir)	-1.70 (ir)	

[a] Measured in CH_3OH at 25 °C. [b] $\lambda_{Excit} = \lambda_{abs}$. [c] recorded under argon at 100 mV/s using $[^nBu_4N][PF_6]$ as the supporting electrolyte in dimethylformamide and referenced to a Ag/AgCl electrode. All potentials are listed vs. NHE. [d] Excited state reduction potential. e abbreviation for $\{Ru[(Et_2N)_2bpy]_2[(Cl)_2bpy]\}(PF_6)_2$

S. I. Table 2. The geometry in Cartesian coordinates for all optimized structures reported in angstroms.

{Ru[$(Et_2N)_2$bpy]$_2$dcbpy}$(PF_6)_2$, 1

C	2.40349400	-3.20931000	-2.41636600
C	2.93698500	-2.48757800	-1.31346400
C	2.21166000	-1.48576400	-0.68387000
C	0.43214600	-1.82265800	-2.12660900
C	1.08942300	-2.82671100	-2.80478800
H	3.93340700	-2.70948300	-0.96190000
H	-0.57135200	-1.53650100	-2.42022100
H	0.57053600	-3.31925500	-3.61604300
C	2.73078600	-0.70021500	0.46414700
C	4.00464800	-0.86670300	0.98948000
C	2.27544200	0.95719200	2.01508600
C	4.46030400	-0.09833000	2.09611800
H	4.66233800	-1.59114800	0.53378000
C	3.52217200	0.84958100	2.59244500
H	1.56425200	1.67938400	2.40037200
H	3.75916800	1.50814200	3.41656300
N	0.95321100	-1.13833400	-1.08523800
N	1.84996300	0.21241500	0.97134900
Ru	0.00144800	0.38251000	-0.00046700
N	-0.98632500	-1.10028500	1.10311300
C	-0.48296200	-1.78019600	2.15592300
C	-2.25048200	-1.42675400	0.70225400
C	-1.16373700	-2.75982700	2.84670600
H	0.52606700	-1.51157200	2.44738200
C	-2.99952300	-2.40256600	1.34491300
C	-2.48488800	-3.11902400	2.46006300
H	-0.65766500	-3.25261600	3.66587000
H	-3.99989500	-2.60743000	0.99420800
N	-1.84822900	0.24204700	-0.97327500
C	-2.74803600	-0.64854500	-0.46023000
C	-2.25330500	0.97939400	-2.03040100
C	-4.02016400	-0.80199400	-0.99383000
C	-3.49714600	0.88400400	-2.61609700
H	-1.52715600	1.68392200	-2.42040100
C	-4.45412600	-0.04229200	-2.11503600
H	-4.69268900	-1.51042700	-0.53462600
H	-3.71652300	1.53406300	-3.45172200
C	-0.38242300	3.23113100	0.58024300
C	-0.82333000	4.39981700	1.20071800
C	-1.63042000	4.32438000	2.33445400
C	-1.98158700	3.06166800	2.82320300

C	-1.51232600	1.93503500	2.16060600
N	-0.72597200	1.99734000	1.06369800
H	-0.55726100	5.38085800	0.82526900
H	-2.60809800	2.95713600	3.70110100
H	-1.75860000	0.93807000	2.50502500
C	0.47122300	3.21102900	-0.61759600
C	0.94885500	4.36233000	-1.25001200
N	0.77244400	1.96265100	-1.08637500
C	1.75109800	4.24387200	-2.38374700
H	0.70527700	5.34623700	-0.86974700
C	1.55373400	1.86052900	-2.18524900
C	2.05670700	2.96365000	-2.85727700
H	1.76517900	0.85213500	-2.51884900
H	2.67949800	2.84753500	-3.73728100
C	-6.66032700	-1.15153000	-2.12361300
H	-6.14182900	-2.08592400	-1.88069700
H	-7.35432600	-1.39821100	-2.93106800
C	-6.10759000	0.63183300	-3.81731500
H	-5.27866800	0.69865400	-4.52995700
H	-6.89975000	0.08191700	-4.33159900
C	-2.69537800	-4.73683800	4.32056700
H	-2.14397200	-4.00888000	4.92299300
H	-3.56884400	-5.01645000	4.91737100
C	-4.52414200	-4.51316800	2.63710100
H	-4.52789600	-4.53341000	1.54259900
H	-4.64431800	-5.55377100	2.95287900
C	-7.44278300	-0.63337800	-0.91067900
H	-8.04112100	0.24455500	-1.17124600
H	-8.12624100	-1.41016400	-0.55090900
H	-6.77825600	-0.35371900	-0.08608900
C	-6.60925700	2.02967400	-3.43682000
H	-7.49736100	1.97333400	-2.80034100
H	-5.84616000	2.60425100	-2.90146900
H	-6.87882400	2.58408000	-4.34203000
C	-5.68124200	-3.66735600	3.17941000
H	-6.63694300	-4.06256100	2.81890400
H	-5.70209000	-3.68634100	4.27396600
H	-5.60076300	-2.62133200	2.86427000
C	-1.84080900	-5.97515900	4.03236200
H	-0.94712500	-5.72290100	3.45176900
H	-1.51965200	-6.43553900	4.97261700
H	-2.40865100	-6.72302700	3.46880800
C	6.13826000	0.57232500	3.77518700
H	5.31602000	0.66138700	4.49316000
H	6.92563800	0.01662300	4.29061000
C	6.65860100	1.95721300	3.37295300

H	5.90077200	2.53592500	2.83458600
H	6.94229400	2.51945700	4.26898000
H	7.54167000	1.87921000	2.73182300
C	6.64998400	-1.23985200	2.09885800
H	7.34961200	-1.48407300	2.90218300
H	6.11607400	-2.17049600	1.87555800
C	7.42560300	-0.75015900	0.86986500
H	6.75589400	-0.47275700	0.04880400
H	8.03925100	0.12268500	1.11088800
H	8.09382600	-1.54171400	0.51372600
C	2.57162400	-4.86039300	-4.25161400
H	2.03444900	-4.13026600	-4.86417200
H	3.43641400	-5.16921600	-4.84661100
C	1.69077800	-6.07439900	-3.93998600
H	2.24404700	-6.82551900	-3.36632400
H	0.80541800	-5.79249200	-3.36029200
H	1.35552200	-6.54268900	-4.87137200
C	4.41299300	-4.64745800	-2.58045700
H	4.51082700	-5.69503700	-2.88052700
H	4.42231200	-4.65078800	-1.48579900
C	5.58323600	-3.83299500	-3.14209500
H	5.59760200	-3.86954200	-4.23629100
H	5.52468200	-2.78077400	-2.84322400
H	6.53308100	-4.24099100	-2.78037700
C	-2.07601900	5.60877900	2.96305700
C	2.30296400	5.42690900	-3.11831200
N	-3.20162000	-4.07426200	3.10744100
N	-5.68353700	-0.19865200	-2.67524400
N	3.09679500	-4.18983500	-3.05090200
N	5.69222600	-0.26582100	2.64732000
O	-2.84866400	5.40581200	4.04600100
H	-3.09595100	6.28390700	4.39610600
O	-1.76897600	6.69898500	2.53491400
O	3.00285800	5.33006000	-4.10066600
O	1.93090400	6.59454300	-2.55946500
H	2.32713300	7.31192200	-3.09145400

{Ru[(pyrrol)$_2$bpy]$_2$dcbpy}(PF$_6$)$_2$, 2

C	2.24400900	-3.11101700	-2.56507400
C	2.85752100	-2.38825000	-1.50818100
C	2.17084700	-1.38844000	-0.83387800
C	0.28917800	-1.74616200	-2.14392400
C	0.90361000	-2.74713000	-2.86514400
H	3.86836600	-2.63275900	-1.21499500

H	-0.73245800	-1.46232000	-2.36816200
H	0.35253400	-3.23542900	-3.65828200
C	2.76147000	-0.60193700	0.27711400
C	4.07044700	-0.75786100	0.70968400
C	2.39223600	1.03981100	1.87570400
C	4.58460900	0.01883400	1.78179200
H	4.71497200	-1.46809300	0.21225700
C	3.67529300	0.94072800	2.36798100
H	1.69512800	1.74282600	2.31718700
H	3.96758200	1.56836300	3.19976400
N	0.88332400	-1.05418200	-1.14603800
N	1.91015200	0.29955000	0.85187100
Ru	0.00119200	0.46315700	0.00197000
N	-0.90716300	-1.02532900	1.16665500
C	-0.32514700	-1.71499700	2.17318300
C	-2.19740300	-1.34689300	0.85245200
C	-0.95436400	-2.70182800	2.90115600
H	0.69939400	-1.44199500	2.39787200
C	-2.89886900	-2.33182000	1.53363600
C	-2.29777600	-3.05253400	2.59895000
H	-0.41200700	-3.18994100	3.70039800
H	-3.91146100	-2.56687900	1.23867600
N	-1.90836000	0.32044800	-0.84896800
C	-2.77314200	-0.56515500	-0.26972700
C	-2.37606900	1.05547600	-1.88326100
C	-4.08107100	-0.71159600	-0.70900400
C	-3.65718000	0.96529100	-2.38224700
H	-1.66838000	1.74548000	-2.32829400
C	-4.57975200	0.05874600	-1.79291900
H	-4.73623000	-1.41001900	-0.20867400
H	-3.93728700	1.58725800	-3.22244800
C	-0.35362900	3.30824400	0.61012100
C	-0.75249000	4.47494000	1.26181400
C	-1.47406500	4.39497300	2.45122300
C	-1.78293800	3.13080600	2.96393900
C	-1.35874500	2.00644400	2.26853600
N	-0.65516800	2.07286600	1.11661300
H	-0.51888500	5.45762600	0.87004700
H	-2.34333400	3.02453800	3.88491200
H	-1.57513900	1.00875300	2.62968000
C	0.41098900	3.29257000	-0.64629800
C	0.83252300	4.44662300	-1.31248200
N	0.68804000	2.04581300	-1.13381800
C	1.55427400	4.33201100	-2.49911400
H	0.60764100	5.42944800	-0.91890000
C	1.39238400	1.94773600	-2.28428600

C	1.83776200	3.05365500	-2.99090200
H	1.58954600	0.94103800	-2.63072200
H	2.39935200	2.94251300	-3.91150000
C	-1.87906100	5.67689900	3.11196600
C	2.04299100	5.51834900	-3.27246900
O	-2.56937000	5.46997400	4.24729000
H	-2.79514200	6.34189800	4.61524100
O	-1.60899900	6.76859700	2.66272900
O	2.67254700	5.42439900	-4.30177300
O	1.70150600	6.68327300	-2.69123500
H	2.05092100	7.40132200	-3.24690300
C	6.81253100	-1.09932100	1.68859300
C	6.45530300	0.73415500	3.26638400
C	7.98514300	-1.03409400	2.67735100
H	7.12480500	-0.82304000	0.67167100
H	6.35698100	-2.09473900	1.64662600
C	7.95485500	0.42076300	3.17111500
H	6.04595600	0.46585000	4.24995500
H	6.23700600	1.79123300	3.08350700
H	7.80873400	-1.72257000	3.51033800
H	8.93277200	-1.30995900	2.21017300
H	8.46562100	0.56063000	4.12596400
H	8.42785700	1.08195700	2.43763100
C	2.26820100	-4.91227100	-4.28769200
C	4.30785000	-4.43492700	-3.02676500
C	3.29252100	-6.03086100	-4.52271100
H	2.10170100	-4.31728600	-5.19618900
H	1.29984500	-5.29617200	-3.95035800
C	4.63690000	-5.35457800	-4.21161500
H	4.43205100	-4.95311400	-2.06540000
H	4.93192900	-3.53470400	-3.01152400
H	3.11103600	-6.85540700	-3.82543700
H	3.23813700	-6.43193700	-5.53681400
H	5.43054500	-6.06534400	-3.97227500
H	4.96906600	-4.75631000	-5.06636500
C	-6.81806300	-1.03946300	-1.70812700
C	-6.43175600	0.77607900	-3.29976600
C	-7.98067100	-0.97451200	-2.70870200
H	-7.13810400	-0.75186900	-0.69673400
H	-6.37034700	-2.03779000	-1.65283600
C	-7.93449900	0.47543700	-3.21546800
H	-6.01543400	0.49458200	-4.27669600
H	-6.20660800	1.83318200	-3.12556000
H	-7.80142300	-1.67185700	-3.53366300
H	-8.93484000	-1.23903200	-2.24830900
H	-8.43539900	0.61049900	-4.17620600

H	-8.40891300	1.14703800	-2.49239500
C	-2.34746900	-4.84100900	4.33418400
C	-4.37742500	-4.35110500	3.06263300
C	-3.38425400	-5.94735500	4.57286800
H	-2.17713600	-4.24246200	5.23965700
H	-1.38227600	-5.23727700	4.00211900
C	-4.72042700	-5.25936900	4.25232100
H	-4.50256400	-4.87476300	2.10435200
H	-4.99279700	-3.44510000	3.03838200
H	-3.20881800	-6.77836400	3.88177500
H	-3.33768600	-6.34227400	5.58978100
H	-5.52050400	-5.96350200	4.01479200
H	-5.04946800	-4.65199200	5.10186500
N	-2.96030200	-4.01192600	3.27989400
N	5.85579600	-0.11048300	2.21587600
N	2.89300200	-4.08351800	-3.24009800
N	-5.84901300	-0.06254300	-2.23505100

{Ru[(pip)$_2$bpy]$_2$dcbpy}(PF$_6$)$_2$, 3

C	-2.06380700	-2.77860700	2.80079400
C	-2.74658400	-2.05777100	1.78366200
C	-2.11093900	-1.08209800	1.02774700
C	-0.14133900	-1.42159100	2.19146000
C	-0.70359200	-2.40079800	2.98099300
H	-3.79414200	-2.24395500	1.60570700
H	0.89893600	-1.14890100	2.32611000
H	-0.06903700	-2.88512800	3.71005500
C	-2.79124200	-0.30651800	-0.04023000
C	-4.12364800	-0.48407500	-0.38148200
C	-2.56423900	1.32773400	-1.66074700
C	-4.74131800	0.27398200	-1.41532100
H	-4.68964200	-1.23832800	0.14255100
C	-3.87949900	1.21000000	-2.05434700
H	-1.91862500	2.04949400	-2.14793700
H	-4.22990700	1.86916400	-2.83565200
N	-0.80288300	-0.74766500	1.22501600
N	-1.99264000	0.60032200	-0.67721300
Ru	-0.01896700	0.76377100	0.00209500
N	0.78256800	-0.72251500	-1.24021600
C	0.12194600	-1.41200300	-2.19359800
C	2.09842600	-1.03832400	-1.05188700
C	0.69125100	-2.38901200	-2.98371800
H	-0.91878100	-1.14285800	-2.33261700
C	2.74016600	-2.00714100	-1.80926000

C	2.05927700	-2.74020000	-2.81906500
H	0.07151000	-2.84873100	-3.74041100
H	3.77446200	-2.22639800	-1.59308900
N	1.95668700	0.61527400	0.67893700
C	2.76960100	-0.26524800	0.02386900
C	2.51883100	1.33672400	1.67239000
C	4.10770600	-0.42026700	0.35396700
C	3.83702100	1.23575600	2.06013000
H	1.86209600	2.03824000	2.17403500
C	4.71448500	0.32773600	1.40180800
H	4.68798400	-1.14582500	-0.19420100
H	4.17629600	1.88614800	2.85351400
C	0.29337700	3.60864800	-0.63060800
C	0.64194600	4.77522800	-1.31076500
C	1.25908900	4.69513500	-2.55749500
C	1.51550100	3.43092300	-3.09820300
C	1.14581700	2.30676500	-2.37210400
N	0.54345700	2.37322100	-1.16413300
H	0.44884700	5.75790700	-0.89751500
H	1.99453500	3.32453600	-4.06396400
H	1.32521500	1.30929700	-2.75349100
C	-0.36236700	3.59382000	0.68560600
C	-0.72258600	4.74883800	1.38516000
N	-0.60206400	2.34758500	1.19387400
C	-1.34401500	4.63609900	2.62739900
H	-0.52791100	5.73113100	0.97454600
C	-1.21011400	2.25146000	2.39818500
C	-1.59131400	3.35839500	3.13989500
H	-1.38288500	1.24550900	2.75929600
H	-2.07584800	3.24852100	4.10341000
C	1.61417700	5.97669600	-3.24706400
C	-1.76224300	5.82361400	3.43938400
O	2.20231400	5.76902000	-4.43842100
H	2.40158600	6.64066500	-4.82202300
O	1.39096000	7.06857300	-2.77332300
O	-2.30387700	5.73097700	4.51764900
O	-1.46629700	6.98765900	2.83213000
H	-1.76597100	7.70667300	3.41495100
C	-7.03761200	-0.58447200	-0.93010100
C	-6.66027800	0.80093300	-2.91749500
C	-7.86020900	-1.59671500	-1.73495000
H	-7.70699800	0.18055400	-0.50828100
H	-6.54795100	-1.06856800	-0.08785700
C	-7.49453500	-0.16718300	-3.77012300
H	-7.29419300	1.61646800	-2.53915800
H	-5.88754200	1.24662700	-3.54025500

C	-8.53581300	-0.91496000	-2.93032200
H	-8.60467700	-2.05061500	-1.07206000
H	-7.20046100	-2.40149800	-2.08324700
H	-7.97558900	0.40496900	-4.57045800
H	-6.81752600	-0.88531500	-4.24957200
H	-9.06382900	-1.65064500	-3.54458500
H	-9.29294600	-0.20733000	-2.56642900
C	-2.14344900	-4.20339400	4.84411100
C	-4.02044800	-4.24789800	3.25709900
C	-2.17347800	-5.72803800	4.98853400
H	-2.77524300	-3.74821300	5.62253700
H	-1.13531700	-3.82432200	4.99608900
C	-4.10635500	-5.77636900	3.38771900
H	-4.72594500	-3.76661300	3.95182700
H	-4.30920100	-3.96896500	2.24444900
C	-3.58745300	-6.26696900	4.74302200
H	-1.82301200	-5.99094800	5.99220600
H	-1.47107100	-6.17215700	4.27223800
H	-5.14858300	-6.07663100	3.23510600
H	-3.51850200	-6.22989500	2.57999100
H	-3.59507700	-7.36055400	4.77999500
H	-4.25554000	-5.91990800	5.54281300
C	7.01954400	-0.50843200	0.91353900
C	6.63300500	0.87158600	2.90100600
C	7.84005100	-1.52145100	1.72016800
H	7.68922000	0.25887300	0.49657400
H	6.53555500	-0.99270300	0.06821400
C	7.46314600	-0.09699000	3.75704900
H	7.26986100	1.68509200	2.52347800
H	5.85967100	1.32082300	3.52002000
C	8.50899400	-0.84240200	2.92077200
H	8.58825500	-1.97280600	1.05972300
H	7.17948100	-2.32790500	2.06287200
H	7.94005400	0.47442500	4.56038500
H	6.78424900	-0.81608300	4.23235900
H	9.03424000	-1.57947200	3.53573700
H	9.26762000	-0.13340900	2.56265900
C	1.91708100	-4.54122000	-4.51906200
C	4.12684300	-3.76050900	-3.75984300
C	2.43172000	-5.98766400	-4.54477800
H	1.99605900	-4.09146700	-5.52122400
H	0.86372500	-4.55196900	-4.24196300
C	4.67113000	-5.19194500	-3.74948200
H	4.34529500	-3.29170100	-4.73239800
H	4.62857800	-3.16193900	-3.00217100
C	3.94284700	-6.05643700	-4.78367400

H	1.88608400	-6.53078000	-5.32362000
H	2.18651800	-6.46483400	-3.58783200
H	5.74642500	-5.15679400	-3.95466100
H	4.54477100	-5.61913300	-2.74681400
H	4.29028200	-7.09277100	-4.73328300
H	4.17534500	-5.69396800	-5.79404700
N	2.66641000	-3.71916600	-3.55204900
N	6.02092700	0.17746800	1.75336600
N	-6.04413100	0.10591900	-1.77286900
N	-2.65805200	-3.76345200	3.53277900

{Ru[(morph)$_2$bpy]$_2$dcbpy}(PF$_6$)$_2$, 4

C	2.17823000	-2.88893800	-2.67623700
C	2.81719700	-2.15688300	-1.64053700
C	2.14764900	-1.17353300	-0.92383200
C	0.23221000	-1.52567800	-2.17163700
C	0.83237700	-2.50879800	-2.92946300
H	3.84923100	-2.35588100	-1.39839700
H	-0.79730900	-1.24736500	-2.36455100
H	0.24330000	-2.97159600	-3.70814500
C	2.77599800	-0.38825100	0.16813700
C	4.10252300	-0.53510200	0.55064200
C	2.46406000	1.24742700	1.77430600
C	4.66040000	0.22399700	1.61396000
H	4.71584700	-1.24171800	0.01428400
C	3.76720400	1.15296800	2.21396700
H	1.78956400	1.95951100	2.23573000
H	4.07758500	1.81415700	3.00998100
N	0.84755200	-0.84694600	-1.17982600
N	1.94047900	0.50388500	0.77645300
Ru	0.00122000	0.66093100	0.00272800
N	-0.86177000	-0.82593500	1.19979600
C	-0.25409600	-1.50137700	2.19847600
C	-2.16247000	-1.14744000	0.94034200
C	-0.86228400	-2.47716200	2.95948900
H	0.77623300	-1.22738200	2.39350600
C	-2.83986800	-2.12334300	1.66000600
C	-2.20848000	-2.85299100	2.70193300
H	-0.27864500	-2.93850600	3.74311800
H	-3.87158300	-2.31935300	1.41401400
N	-1.93778900	0.51481300	-0.77223500
C	-2.78151700	-0.36705700	-0.16048500
C	-2.45172500	1.25265200	-1.77934300
C	-4.10694300	-0.50971700	-0.54867900

C	-3.75294200	1.16143000	-2.22526700
H	-1.77051200	1.95626000	-2.24379700
C	-4.65443600	0.24245900	-1.62232500
H	-4.72710300	-1.20819100	-0.00944900
H	-4.05486900	1.81677600	-3.02931300
C	-0.33999700	3.50719600	0.62624400
C	-0.71728500	4.67303300	1.29228000
C	-1.39367800	4.59144300	2.50784200
C	-1.67983300	3.32704800	3.03212000
C	-1.27850200	2.20356700	2.32126200
N	-0.61859200	2.27157500	1.14422900
H	-0.50153500	5.65650300	0.89228400
H	-2.20535500	3.21963000	3.97332500
H	-1.47925500	1.20588200	2.69127700
C	0.37679700	3.49484800	-0.65853100
C	0.76770300	4.65165100	-1.33865700
N	0.64009100	2.25033500	-1.15834900
C	1.44419000	4.54171300	-2.55210200
H	0.55394500	5.63319600	-0.93579600
C	1.30077600	2.15685500	-2.33447500
C	1.71441800	3.26563900	-3.05625000
H	1.48965300	1.15195700	-2.69049000
H	2.24115800	3.15830500	-3.99771100
C	-1.77725800	5.87369500	3.18297200
C	1.89799800	5.73168400	-3.34294700
O	-2.42327500	5.66479100	4.34280100
H	-2.63898700	6.53522700	4.72054600
O	-1.52577900	6.96449200	2.72173400
O	2.48632700	5.63919300	-4.39609700
O	1.57520900	6.89344800	-2.74648900
H	1.89925000	7.61530700	-3.31274800
C	6.92966400	-0.67629100	1.22013800
C	6.55390100	1.03224300	2.97475600
C	8.10490100	-1.16801400	2.06785900
H	7.30076800	-0.03136400	0.41049100
H	6.45378500	-1.55088100	0.77393100
C	7.75434200	0.42625600	3.70390700
H	6.86606200	1.93400900	2.42867500
H	5.81959000	1.32140200	3.72754300
H	8.87512500	-1.58205700	1.41237800
H	7.76358100	-1.96165500	2.75204400
H	8.26244100	1.20722800	4.27465200
H	7.41114700	-0.35201300	4.40419600
C	2.24015500	-4.39797200	-4.63192000
C	4.25301300	-4.11699800	-3.21873300
C	2.75634300	-5.80234900	-4.94805100

H	2.50142600	-3.71357400	-5.45180600
H	1.15348400	-4.44955400	-4.56055500
C	4.63765000	-5.54006800	-3.63035900
H	4.80919900	-3.38995100	-3.82848900
H	4.54195200	-3.98653100	-2.17435600
H	2.43680000	-6.08821900	-5.95307500
H	2.33810000	-6.52420700	-4.22836000
H	5.72664600	-5.62995000	-3.64762400
H	4.23854000	-6.25860400	-2.89642200
C	-6.92950000	-0.64543100	-1.23595500
C	-6.53549000	1.04883200	-3.00114600
C	-8.10290300	-1.13662400	-2.08650700
H	-7.30169800	0.00609100	-0.43204200
H	-6.46007400	-1.51963700	-0.78207100
C	-7.73580400	0.44425000	-3.73166600
H	-6.84487500	1.95710300	-2.46432200
H	-5.79557000	1.32721000	-3.75250500
H	-8.87851800	-1.54259400	-1.43232300
H	-7.76217400	-1.93637800	-2.76381100
H	-8.23674200	1.22392800	-4.31041500
H	-7.39381700	-0.34094900	-4.42470500
C	-2.28403100	-4.35396200	4.66324900
C	-4.29049900	-4.07029800	3.24126800
C	-2.80802600	-5.75444100	4.98392100
H	-2.54432800	-3.66479000	5.47950000
H	-1.19740900	-4.41133800	4.59549200
C	-4.68304600	-5.48966700	3.65802500
H	-4.84618400	-3.33801300	3.84526200
H	-4.57466600	-3.94353000	2.19512200
H	-2.49336900	-6.03733100	5.99132700
H	-2.39067800	-6.48146500	4.26896500
H	-5.77248600	-5.57474800	3.67138000
H	-4.28424300	-6.21343400	2.92911300
N	-2.84186100	-3.84862700	3.39355300
N	-5.94315400	0.08683200	-2.05116100
N	5.95102500	0.06585000	2.03600700
N	2.80464200	-3.88988800	-3.36615300
O	-8.68358500	-0.08063800	-2.82314900
O	-4.22133500	-5.79419300	4.95786100
O	4.16951000	-5.84873400	-4.92686100
O	8.69480600	-0.11038000	2.79481800

{Ru[(mepipz)$_2$bpy]$_2$dcbpy}(PF_6)$_2$, 5

C	2.14670400	-2.74477900	-2.63155000

C	2.78691600	-2.01333900	-1.59468600
C	2.13098900	-1.00592400	-0.89985800
C	0.22675300	-1.32746800	-2.17205500
C	0.81526500	-2.33016200	-2.91213000
H	3.81263300	-2.22872600	-1.34015300
H	-0.79427200	-1.02986500	-2.38092800
H	0.22394200	-2.79088800	-3.69041400
C	2.76550200	-0.21678000	0.18577800
C	4.08821500	-0.37741500	0.57459400
C	2.47503800	1.45084500	1.76212700
C	4.65652500	0.38877300	1.62876800
H	4.69266200	-1.09807900	0.04737400
C	3.77552400	1.34541500	2.20587800
H	1.81061800	2.18123400	2.20959400
H	4.09361200	2.01750700	2.98941100
N	0.84135100	-0.65490000	-1.17484200
N	1.94088000	0.69624200	0.77790000
Ru	0.00241100	0.86033600	0.00423000
N	-0.85821600	-0.62841900	1.20138200
C	-0.25409700	-1.29578800	2.20846200
C	-2.14880500	-0.97265300	0.92227800
C	-0.85385100	-2.28763400	2.95420100
H	0.76834500	-1.00427500	2.41931100
C	-2.81563500	-1.96937700	1.62229500
C	-2.18600700	-2.69628500	2.66865800
H	-0.26969000	-2.74681600	3.73885000
H	-3.84143500	-2.18012200	1.36401400
N	-1.93571200	0.71060900	-0.77130200
C	-2.77090400	-0.19006600	-0.17528800
C	-2.45733200	1.45838100	-1.76744600
C	-4.09182800	-0.34616700	-0.57235000
C	-3.75506700	1.35661200	-2.21992000
H	-1.78444800	2.17887900	-2.21817600
C	-4.64652000	0.41156300	-1.63985700
H	-4.70507000	-1.05719600	-0.04211000
H	-4.06228700	2.02183100	-3.01358700
C	-0.33504200	3.70598500	0.62406800
C	-0.71120000	4.87252400	1.28945200
C	-1.38744200	4.79216600	2.50516700
C	-1.67499500	3.52793200	3.02980000
C	-1.27496800	2.40375600	2.31980300
N	-0.61439800	2.47056400	1.14282000
H	-0.49440500	5.85536900	0.88850900
H	-2.20071200	3.42139300	3.97096600
H	-1.47683400	1.40610800	2.68935300
C	0.38153100	3.69113300	-0.66038800

C	0.77435900	4.84593400	-1.34267100
N	0.64299700	2.44490700	-1.15763800
C	1.45167800	4.73252600	-2.55531900
H	0.56147700	5.82844700	-0.94170300
C	1.30514600	2.34801300	-2.33288600
C	1.72095500	3.45470300	-3.05623600
H	1.49294200	1.34176700	-2.68571100
H	2.24870400	3.34451700	-3.99675400
C	-1.76939900	6.07411100	3.18003500
C	1.90744700	5.91983000	-3.34757700
O	-2.41517900	5.86657600	4.34093900
H	-2.62840100	6.73810200	4.71731800
O	-1.51811400	7.16564900	2.71985100
O	2.49893100	5.82630200	-4.39916200
O	1.58331400	7.08399200	-2.75535800
H	1.90929300	7.80303200	-3.32390300
C	6.89466100	-0.60285400	1.28351400
C	6.56001900	1.19006100	2.98090700
C	8.04253900	-1.13475800	2.16468600
H	7.28892100	-0.00928100	0.44546200
H	6.37636400	-1.46655500	0.86505100
C	7.72479100	0.56792800	3.77509200
H	6.90004000	2.06684200	2.41060600
H	5.81621700	1.53031800	3.70145700
H	8.76942300	-1.63725300	1.51847500
H	7.63383000	-1.88956900	2.84907900
H	8.21039000	1.36015200	4.35345300
H	7.31107200	-0.15444500	4.49063000
C	2.24944700	-4.25517200	-4.59382200
C	4.16333400	-4.12292500	-3.02258700
C	2.60567200	-5.73490800	-4.82658900
H	2.66313500	-3.62610300	-5.39552900
H	1.16520000	-4.15938500	-4.62742000
C	4.43910600	-5.60977200	-3.33021900
H	4.82905500	-3.47109600	-3.60802300
H	4.38022800	-3.96226400	-1.96552200
H	2.29021700	-6.01522200	-5.83646100
H	2.03096900	-6.34746300	-4.11971000
H	5.51027500	-5.79771700	-3.20557100
H	3.90899100	-6.21744200	-2.58526500
C	-6.89198900	-0.56610500	-1.30503500
C	-6.53359900	1.21009200	-3.01613200
C	-8.03683500	-1.09809400	-2.19012600
H	-7.28867300	0.03558200	-0.47389700
H	-6.38145900	-1.42973000	-0.87677600
C	-7.69650800	0.58806200	-3.81308700

H	-6.87191500	2.09502300	-2.45750600
H	-5.78198900	1.53781900	-3.73435800
H	-8.77153700	-1.59053900	-1.54499800
H	-7.62805100	-1.86126000	-2.86511700
H	-8.17271600	1.37798300	-4.40226700
H	-7.28243300	-0.14362900	-4.51882100
C	-2.31726700	-4.18619600	4.64586700
C	-4.20816500	-4.07025800	3.04689300
C	-2.67221000	-5.66528700	4.88468200
H	-2.74661900	-3.55252500	5.43569700
H	-1.23420100	-4.08515300	4.69651000
C	-4.48456800	-5.55572200	3.36083900
H	-4.88312400	-3.41599800	3.61897500
H	-4.41100200	-3.91699300	1.98593600
H	-2.37109900	-5.93719600	5.90121200
H	-2.08525800	-6.28132000	4.19102800
H	-5.55333200	-5.74764600	3.22244700
H	-3.94217700	-6.16684600	2.62766500
N	-2.80643700	-3.71586000	3.33330600
N	-5.92826400	0.23981900	-2.07982300
N	5.94106700	0.21441500	2.05930900
N	2.75721500	-3.77242200	-3.29271500
N	4.01669100	-6.04106400	-4.65124600
N	8.71097000	-0.11854800	2.95827100
N	-8.69303200	-0.08452300	-2.99713100
N	-4.07970900	-5.97675600	4.69069700
C	-4.96565800	-5.55540300	5.77269800
H	-4.62406100	-6.00459300	6.70970700
H	-5.03687600	-4.46450400	5.92932600
H	-5.97431100	-5.92954500	5.57412300
C	4.88540000	-5.62404900	-5.74889200
H	4.95008700	-4.53409400	-5.91429900
H	5.89822800	-5.99301900	-5.56230100
H	4.53199200	-6.08118400	-6.67764100
C	-9.60117700	0.79802000	-2.26878300
H	-9.12778200	1.43456600	-1.50050000
H	-10.10661400	1.45631700	-2.98120800
H	-10.36712400	0.19296200	-1.77483500
C	9.62020300	0.75142900	2.21617100
H	9.14599800	1.38487500	1.44588400
H	10.13530800	1.41200900	2.91951600
H	10.37831000	0.13678700	1.72200400

{Ru[$(Et_2N)_2$bpy]$_2$[$(Cl)_2$bpy]}$(PF_6)_2$

C	2.34390700	-3.00955900	-2.52230900
C	2.91352600	-2.28660800	-1.43889000
C	2.20232100	-1.29536200	-0.77695300
C	0.37124300	-1.64465800	-2.15146600
C	1.01188800	-2.63953000	-2.85802100
H	3.92494600	-2.49919500	-1.12728600
H	-0.64593400	-1.36897600	-2.40463300
H	0.46740700	-3.13493400	-3.65004900
C	2.75631700	-0.51107000	0.35542200
C	4.04923600	-0.67057600	0.83484900
C	2.34363000	1.13799300	1.92676900
C	4.53619200	0.09651300	1.92863000
H	4.69582300	-1.38833900	0.35396300
C	3.61057400	1.03795100	2.45929500
H	1.64142600	1.85368700	2.33896500
H	3.87235700	1.69536400	3.27630400
N	0.92581200	-0.95873200	-1.12801700
N	1.88667000	0.39207800	0.89715800
Ru	0.00006900	0.54146800	0.00002000
N	-0.92590200	-0.95857700	1.12806300
C	-0.37146600	-1.64448500	2.15159800
C	-2.20249200	-1.29495900	0.77706800
C	-1.01233500	-2.63909000	2.85832500
H	0.64578800	-1.36900900	2.40468600
C	-2.91394300	-2.28588500	1.43921900
C	-2.34447200	-3.00880300	2.52273600
H	-0.46795300	-3.13452500	3.65040200
H	-3.92545800	-2.49821200	1.12774800
N	-1.88653300	0.39231600	-0.89716200
C	-2.75629300	-0.51074900	-0.35546000
C	-2.34333500	1.13816400	-1.92689000
C	-4.04913900	-0.67027800	-0.83507500
C	-3.61021400	1.03812500	-2.45957600
H	-1.64106000	1.85380700	-2.33905200
C	-4.53592700	0.09674400	-1.92897700
H	-4.69579100	-1.38803400	-0.35426800
H	-3.87186400	1.69548900	-3.27666700
C	-0.40139700	3.39150400	0.61784700
C	-0.83058400	4.55590600	1.25933500
C	-1.58545300	4.45289700	2.42507000
C	-1.89716800	3.18665300	2.92640500
C	-1.43826200	2.07454800	2.23532600
N	-0.70227600	2.15166500	1.10594500
H	-0.58847000	5.53440900	0.86529900
H	-2.48292300	3.06893600	3.83031000
H	-1.65601500	1.07397800	2.58837800

C	0.40182000	3.39141200	-0.61794800
C	0.83109800	4.55576800	-1.25950900
N	0.70259300	2.15154600	-1.10594400
C	1.58596100	4.45261300	-2.42522000
H	0.58904700	5.53430600	-0.86552900
C	1.43860300	2.07427700	-2.23533500
C	1.89758500	3.18629300	-2.92646200
H	1.65626000	1.07365000	-2.58827700
H	2.48334200	3.06849200	-3.83035500
C	-6.72697600	-1.03966000	-1.86389600
H	-6.18650100	-1.96918200	-1.65401900
H	-7.44768800	-1.28638700	-2.64704000
C	-6.26377000	0.77274200	-3.55384700
H	-5.46656800	0.85403300	-4.30000700
H	-7.07174000	0.22183600	-4.04078700
C	-2.45415700	-4.65361000	4.36745000
H	-1.88261600	-3.92903300	4.95425300
H	-3.29547100	-4.95000200	5.00045200
C	-4.36008500	-4.42527200	2.77262900
H	-4.41576700	-4.42831400	1.67974500
H	-4.45606500	-5.47175300	3.07553800
C	-7.46942800	-0.55027000	-0.61486200
H	-8.09100800	0.32013600	-0.83923900
H	-8.12535600	-1.34169900	-0.23923000
H	-6.77832400	-0.27076300	0.18613400
C	-6.76004900	2.16244100	-3.13936300
H	-7.61998200	2.09374700	-2.46811500
H	-5.98059000	2.73741400	-2.63077000
H	-7.07061500	2.72321600	-4.02610800
C	-5.49790200	-3.59989200	3.38200700
H	-6.46528900	-3.99696400	3.05995600
H	-5.46809100	-3.63710800	4.47488000
H	-5.44070100	-2.54909000	3.08157500
C	-1.60170700	-5.87853500	4.02287600
H	-0.74045300	-5.60891700	3.40426200
H	-1.23124100	-6.34719400	4.93942000
H	-2.18716200	-6.62492000	3.47767300
C	6.26425900	0.77258000	3.55322900
H	5.46715500	0.85392900	4.29948800
H	7.07228100	0.22168800	4.04009900
C	6.76050900	2.16224600	3.13860100
H	5.98099600	2.73720100	2.63007100
H	7.07119300	2.72306800	4.02527600
H	7.62035900	2.09349900	2.46725300
C	6.72720700	-1.03994800	1.86334000
H	7.44800500	-1.28664500	2.64641400

H	6.18667600	-1.96946600	1.65359000
C	7.46952800	-0.55066700	0.61418600
H	6.77834200	-0.27120400	-0.18675400
H	8.09115400	0.31974100	0.83842800
H	8.12539600	-1.34214000	0.23853900
C	2.45321300	-4.65476000	-4.36669800
H	1.88190600	-3.93014500	-4.95368200
H	3.29447100	-4.95152400	-4.99959900
C	1.60039400	-5.87936500	-4.02189900
H	2.18561700	-6.62581300	-3.47653300
H	0.73921200	-5.60935800	-3.40335300
H	1.22980300	-6.34809900	-4.93835300
C	4.35916500	-4.42658300	-2.77188900
H	4.45489900	-5.47314500	-3.07459800
H	4.41484000	-4.42943500	-1.67900500
C	5.49717800	-3.60158500	-3.38141700
H	5.46737300	-3.63901500	-4.47428300
H	5.44020600	-2.55071100	-3.08119500
H	6.46447100	-3.99881200	-3.05927200
Cl	-2.12966400	5.88088800	3.23955600
Cl	2.13030600	5.88047400	-3.23983100
N	-3.02169300	-3.98031800	3.18800300
N	-5.78612400	-0.06525300	-2.43922700
N	3.02088400	-3.98139000	-3.18736000
N	5.78645500	-0.06547300	2.43872000