

**From intercalation to groove binding: synthesis, photophysics and DNA binding
properties of tetracationic mononuclear Ruthenium(II)-based chromophore-quencher
complexes**
Supplementary Information

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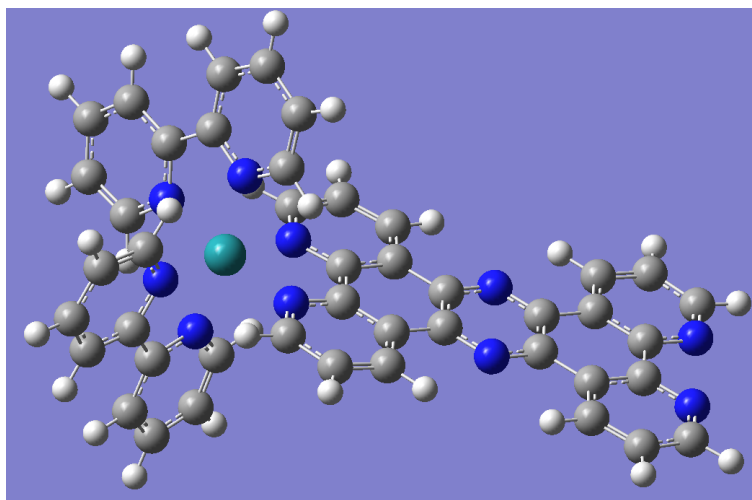
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CONTENTS

S1. Calculations on $\mathbf{1}^{2+}$ (^1A)	3
S1.1. Cartesian Co-ordinates (XYZ format)	3
S1.2. Frequencies	5
S2. Calculations on $\mathbf{2}^{2+}$ (^1A)	9
S2.1. Cartesian Co-ordinates (XYZ format)	9
S2.2. Frequencies	11
S3. Calculations on $\mathbf{3}^{4+}$ (^1A)	16
S3.1. Cartesian Co-ordinates (XYZ format)	16
S3.2. Frequencies	19
S4. Calculations on $\mathbf{4}^{4+}$ (^1A)	24
S4.1. Cartesian Co-ordinates (XYZ format)	24
S4.2. Frequencies	27
S5. Calculations on $\mathbf{1}^{2+}$ (^3A)	32
S5.1. Cartesian Co-ordinates (XYZ format)	32
S5.2. Frequencies	34
S6. Calculations on $\mathbf{2}^{2+}$ (^3A)	38
S6.1. Cartesian Co-ordinates (XYZ format)	38
S6.2. Frequencies	40
S7. Calculations on $\mathbf{3}^{4+}$ (^3A)	45
S7.1. Cartesian Co-ordinates (XYZ format)	45
S7.2. Frequencies	48
S8. Calculations on $\mathbf{4}^{4+}$ (^3A)	53
S8.1. Cartesian Co-ordinates (XYZ format)	53
S8.2. Frequencies	56

S1. CALCULATIONS ON 1²⁺ (¹A)



```

Route          : # opt freq b3lyp/genecp scrf=(solvent=acetonitrile) geom=connectivity
                : empiricdispersion=gd3bj int=ultrafine pop=regular
SMILES         : c1cc[n+]2c(c1)-c3cccc[n+]3[Ru]245([n+]6cccc6-c7[n+]4cccc7)
                : [n+]8cccc9c8c1[n+]5cccc1c1c9nc2c3ccnc3c3c(c2n1)cccn3
Formula        : C44H28N10Ru2+
Charge         : 2
Multiplicity   : 1
Energy         : -2336.71433335 a.u.
Gibbs Energy   : -2336.14894700 a.u.
Number of imaginary frequencies : 1

```

S1.1. Cartesian Co-ordinates (XYZ format)

83

```

Ru -2.58245111 -0.00005500 -0.00000600
N  -0.97099400 -1.19907904  0.57679302
N   3.85077095 -1.27071798  0.57447797
N   3.85077095  1.27049005 -0.57480502
N  -0.97099900  1.19881594 -0.57718801
C  -1.01818097 -2.41121411  1.13779402
H  -2.00172496 -2.81190991  1.33778596
C   0.13573501 -3.12839007  1.45919704
H   0.03997800 -4.10513020  1.91324103
C   1.37728405 -2.58054805  1.19582105
H   2.29178500 -3.10527897  1.43487704
C   1.44774997 -1.31069505  0.60461998
C   2.70648503 -0.64660197  0.29421201
C   4.99575090 -0.64975202  0.29163301
C   7.48183298 -0.67209101  0.29868799
C   7.48183393  0.67197102 -0.29875800
C   6.25618505  1.31289101 -0.58523202
C   4.99575186  0.64954698 -0.29190600
C   2.70648503  0.64635497 -0.29458201
C   1.44774699  1.31042099 -0.60504502
C   1.37727904  2.58024406 -1.19631004
H   2.29177904  3.10496807 -1.43538296

```

C	0.13573000	3.12806296	-1.45973206
H	0.03997000	4.10477304	-1.91383803
C	-1.01818705	2.41090703	-1.13827705
H	-2.00172997	2.81159401	-1.33829701
C	0.24621201	0.65282500	-0.30594701
C	0.24621300	-0.65308797	0.30554900
C	-3.59757304	-2.14627099	-1.72685599
C	-1.94908798	-0.93018401	-2.84336996
C	-3.74156904	-2.99300194	-2.82391596
C	-4.37460709	-2.27203608	-0.48368299
C	-2.05062604	-1.73782599	-3.96496511
H	-1.25678003	-0.10168900	-2.80725288
C	-2.96209502	-2.78874612	-3.95451403
H	-4.45262289	-3.80564690	-2.79700398
C	-5.36574984	-3.22954702	-0.27941900
H	-1.42321706	-1.54066598	-4.82333899
H	-3.06560993	-3.44055510	-4.81202412
C	-4.71629000	-1.41682601	1.66029096
C	-6.04007816	-3.27044201	0.93340802
H	-5.61116505	-3.93566990	-1.05899405
C	-5.70888090	-2.34821892	1.92092097
H	-4.42488813	-0.68318599	2.39760303
H	-6.81141615	-4.01028490	1.10235906
H	-6.20745277	-2.34268999	2.88047910
N	-4.05957222	-1.37462604	0.48894599
N	-2.70141506	-1.12323701	-1.74741495
C	-4.37386322	2.27241898	0.48409301
C	-4.71656513	1.41708803	-1.65966797
C	-5.36470604	3.23028302	0.28003401
C	-3.59651303	2.14649510	1.72705197
C	-5.70889616	2.34881997	-1.92008400
H	-4.42569399	0.68325198	-2.39699507
C	-6.03941107	3.27129602	-0.93257999
H	-5.60960388	3.93658900	1.05960298
C	-3.73996401	2.99333096	2.82410407
H	-6.20778704	2.34335804	-2.87947607
H	-6.81051207	4.01142120	-1.10137200
C	-1.94813704	0.92994797	2.84321809
C	-2.96026111	2.78889704	3.95451307
H	-4.45077896	3.80619001	2.79733992
C	-2.04912806	1.73768699	3.96479392
H	-1.25611603	0.10122000	2.80698705
H	-3.06335092	3.44078898	4.81201077
H	-1.42156506	1.54037297	4.82301903
N	-4.05946112	1.37479198	-0.48854601
N	-2.70066595	1.12318504	1.74743795
C	8.67364025	-2.46457601	1.09407699
C	8.67364407	2.46452308	-1.09399295
C	6.25618315	-1.31304598	0.58507401
C	6.29088020	-2.59560108	1.15491998
H	5.35951710	-3.09775209	1.37881899
C	6.29088497	2.59545588	-1.15505505
H	5.35952282	3.09757400	-1.37903094
C	7.51210117	-3.18130302	1.41371596
C	7.51210690	3.18120599	-1.41373503
H	7.58308506	-4.16833496	1.85189795
H	9.64997482	-2.89965606	1.28620303
H	7.58309412	4.16824722	-1.85189700
H	9.64997959	2.89964104	-1.28602898
N	8.66914368	-1.25215805	0.55529302
N	8.66914558	1.25209403	-0.55523300

S1.2. Frequencies

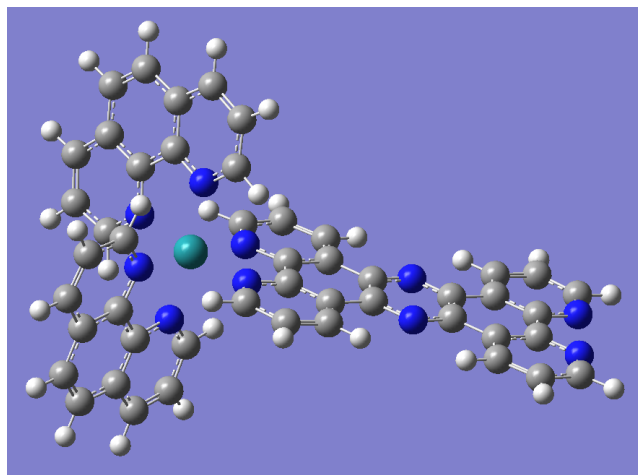
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4	29.31590000	0.05400000	0.00000000
5	34.42190000	0.31910000	0.00000000
6	37.26030000	0.22620000	0.00000000
7	44.30600000	0.56680000	0.00000000
8	47.25050000	0.71930000	0.00000000
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18	130.31760000	0.01290000	0.00000000
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21	175.63840000	1.98910000	0.00000000
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23	195.45850000	0.25600000	0.00000000
24	198.46650000	0.00400000	0.00000000
25	217.82790000	0.37440000	0.00000000
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27	222.71760000	0.21410000	0.00000000
28	233.57250000	0.60050000	0.00000000
29	246.77910000	0.51150000	0.00000000
30	250.12740000	0.45890000	0.00000000
31	269.74970000	11.17450000	0.00000000
32	272.62100000	0.73940000	0.00000000
33	277.07150000	6.96270000	0.00000000
34	286.56610000	0.42040000	0.00000000
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36	328.40560000	4.85010000	0.00000000
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38	342.83900000	1.85580000	0.00000000
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41	379.83250000	0.73890000	0.00000000
42	383.33250000	1.52150000	0.00000000
43	415.26390000	14.69010000	0.00000000
44	432.24590000	5.43950000	0.00000000
45	434.68050000	10.21480000	0.00000000
46	439.41760000	1.05320000	0.00000000
47	442.32790000	6.16930000	0.00000000
48	445.02640000	0.10930000	0.00000000
49	447.34160000	0.44970000	0.00000000
50	456.36350000	18.21390000	0.00000000
51	456.90820000	0.30830000	0.00000000
52	460.40170000	1.77370000	0.00000000
53	466.13500000	0.00710000	0.00000000
54	473.10950000	2.71260000	0.00000000
55	482.21910000	0.21280000	0.00000000
56	486.67480000	0.53370000	0.00000000
57	496.74060000	0.10810000	0.00000000
58	497.93990000	0.27010000	0.00000000
59	533.64420000	13.41010000	0.00000000
60	538.73560000	0.33640000	0.00000000

61	564.07940000	0.00830000	0.00000000
62	565.55650000	0.04300000	0.00000000
63	570.78950000	0.05390000	0.00000000
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89	776.30140000	139.19970000	0.00000000
90	777.34990000	127.13510000	0.00000000
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94	815.70050000	0.00040000	0.00000000
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96	821.64880000	0.02130000	0.00000000
97	823.12440000	0.28460000	0.00000000
98	833.06970000	102.79270000	0.00000000
99	833.63170000	0.00390000	0.00000000
100	837.64000000	0.74990000	0.00000000
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102	863.69370000	1.14660000	0.00000000
103	873.08880000	0.02430000	0.00000000
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105	908.80530000	0.00780000	0.00000000
106	908.97090000	0.01790000	0.00000000
107	909.28240000	0.08580000	0.00000000
108	933.09620000	0.51660000	0.00000000
109	975.48250000	0.00460000	0.00000000
110	975.91140000	0.02470000	0.00000000
111	984.51180000	0.14530000	0.00000000
112	985.81330000	0.00000000	0.00000000
113	989.05380000	0.27740000	0.00000000
114	989.31930000	1.16000000	0.00000000
115	991.07100000	1.31770000	0.00000000
116	991.10670000	1.40840000	0.00000000
117	1019.39230000	0.30420000	0.00000000
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121	1023.74580000	0.00620000	0.00000000
122	1023.76220000	0.00290000	0.00000000
123	1026.73590000	0.28150000	0.00000000
124	1026.76250000	0.15160000	0.00000000

125	1036.20700000	2.48990000	0.00000000
126	1039.24260000	1.56790000	0.00000000
127	1042.35380000	7.14990000	0.00000000
128	1044.55260000	27.72920000	0.00000000
129	1046.45310000	3.49810000	0.00000000
130	1055.09600000	0.19150000	0.00000000
131	1059.24570000	2.12630000	0.00000000
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133	1069.37390000	3.62810000	0.00000000
134	1070.27800000	0.80140000	0.00000000
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137	1090.10960000	2.33640000	0.00000000
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139	1094.95630000	8.61380000	0.00000000
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147	1146.60770000	25.09350000	0.00000000
148	1149.73140000	0.46490000	0.00000000
149	1150.50430000	2.75010000	0.00000000
150	1157.41460000	164.33290000	0.00000000
151	1158.32110000	8.10600000	0.00000000
152	1183.64390000	6.09670000	0.00000000
153	1183.99050000	10.17060000	0.00000000
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155	1195.94110000	1.39560000	0.00000000
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157	1218.97050000	20.27150000	0.00000000
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163	1292.14540000	1.88130000	0.00000000
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167	1312.37880000	4.30270000	0.00000000
168	1313.16720000	2.11500000	0.00000000
169	1316.77640000	39.75490000	0.00000000
170	1321.86470000	0.06280000	0.00000000
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173	1342.45410000	0.00450000	0.00000000
174	1342.83860000	0.20820000	0.00000000
175	1344.11680000	1.28370000	0.00000000
176	1345.10370000	10.51000000	0.00000000
177	1354.14530000	15.12380000	0.00000000
178	1360.51180000	27.20490000	0.00000000
179	1389.10990000	236.83320000	0.00000000
180	1392.76540000	135.79600000	0.00000000
181	1426.26100000	205.78180000	0.00000000
182	1438.13670000	9.79400000	0.00000000
183	1452.13560000	1.83640000	0.00000000
184	1461.97940000	20.53410000	0.00000000
185	1462.87780000	51.76220000	0.00000000
186	1469.29670000	53.01670000	0.00000000
187	1480.73430000	90.81290000	0.00000000
188	1480.83230000	35.59300000	0.00000000

189	1484.71450000	23.96530000	0.00000000
190	1496.55670000	75.83010000	0.00000000
191	1501.06370000	82.73790000	0.00000000
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193	1506.57460000	5.64070000	0.00000000
194	1511.92850000	162.94830000	0.00000000
195	1520.79770000	0.93440000	0.00000000
196	1521.57210000	2.55890000	0.00000000
197	1533.47230000	14.92790000	0.00000000
198	1541.96630000	45.31720000	0.00000000
199	1576.16500000	32.62820000	0.00000000
200	1592.82060000	1.81760000	0.00000000
201	1600.40820000	2.12280000	0.00000000
202	1600.67410000	0.59630000	0.00000000
203	1608.63140000	22.99970000	0.00000000
204	1609.45100000	5.46040000	0.00000000
205	1609.83380000	14.73210000	0.00000000
206	1612.14130000	0.22410000	0.00000000
207	1622.65750000	2.80950000	0.00000000
208	1624.34170000	99.49270000	0.00000000
209	1629.68930000	2.26170000	0.00000000
210	1637.46480000	22.82010000	0.00000000
211	1641.89340000	17.29950000	0.00000000
212	1642.71840000	10.67000000	0.00000000
213	1642.76320000	4.98060000	0.00000000
214	1648.74980000	6.63720000	0.00000000
215	1649.83280000	3.87000000	0.00000000
216	3153.02370000	32.71230000	0.00000000
217	3153.47570000	57.27670000	0.00000000
218	3199.43850000	17.07050000	0.00000000
219	3199.49440000	8.96690000	0.00000000
220	3202.45660000	2.92700000	0.00000000
221	3202.46000000	2.27420000	0.00000000
222	3203.40010000	3.80010000	0.00000000
223	3203.41770000	0.35730000	0.00000000
224	3209.45640000	0.86410000	0.00000000
225	3209.54020000	0.03330000	0.00000000
226	3215.09870000	18.47050000	0.00000000
227	3215.10650000	3.71870000	0.00000000
228	3215.11260000	1.94850000	0.00000000
229	3215.21130000	4.35670000	0.00000000
230	3216.08970000	0.52640000	0.00000000
231	3216.09410000	0.57120000	0.00000000
232	3221.42390000	1.59530000	0.00000000
233	3221.47310000	3.71950000	0.00000000
234	3223.19580000	0.21370000	0.00000000
235	3223.20940000	0.01370000	0.00000000
236	3227.08660000	10.29920000	0.00000000
237	3227.17470000	1.47850000	0.00000000
238	3230.38040000	3.57900000	0.00000000
239	3230.56550000	1.04330000	0.00000000
240	3231.64350000	3.61460000	0.00000000
241	3231.81990000	25.33430000	0.00000000
242	3232.95990000	6.13250000	0.00000000
243	3233.24000000	6.17280000	0.00000000

S2. CALCULATIONS ON 2^{2+} (1A)



```

Route      : # opt freq b3lyp/genecp scrf=(solvent=acetonitrile) geom=connectivity
            : empiricaldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1cc2c(c3c(cccn3)c4c2nc5c6ccc[n+]7c6c8c(c5n4)ccc[n+]8[Ru]792([n+]
            : 3ccc4c3c3[n+]9cccc3cc4)[n+]3cccc4c3c3[n+]2cccc3cc4)nc1
Formula    : C48H28N10Ru2+
Charge     : 2
Multiplicity : 1
Energy     : -2489.22648990 a.u.
Gibbs Energy : -2488.63655000 a.u.
Number of imaginary frequencies : 1

```

S2.1. Cartesian Co-ordinates (XYZ format)

87

```

Ru  2.27142096 -0.00000200  0.00000100
N   0.66395098 -1.03482997 -0.83458501
N  -4.15775204 -1.09343898 -0.86547101
N  -4.15775299  1.09342599  0.86547899
N   0.66395003  1.03481698  0.83459902
C   0.71242797 -2.08461905 -1.66017199
H   1.69675601 -2.43029690 -1.94246995
C  -0.44113800 -2.70446396 -2.14418888
H  -0.34452400 -3.54989290 -2.81148696
C  -1.68316102 -2.22931194 -1.76650798
H  -2.59716201 -2.68266010 -2.12401509
C  -1.75468695 -1.13147104 -0.89655900
C  -3.01344299 -0.55718899 -0.44079801
C  -5.30277300 -0.55831897 -0.44200799
C  -7.78902578 -0.57718199 -0.45589301
C  -7.78902721  0.57717198  0.45589599
C  -6.56323385  1.12712801  0.89193898
C  -5.30277395  0.55830699  0.44201499
C  -3.01344395  0.55717599  0.44080800
C  -1.75468802  1.13145697  0.89657098
C  -1.68316305  2.22929597  1.76652205
H  -2.59716392  2.68264389  2.12402892
C  -0.44114000  2.70444798  2.14420509

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H	-0.34452701	3.54987502	2.81150603
C	0.71242702	2.08460307	1.66018796
H	1.69675398	2.43028092	1.94248796
C	-0.55369800	0.56390297	0.44892901
C	-0.55369699	-0.56391603	-0.44891599
C	3.30480003	-2.43262291	1.22143304
C	1.67852497	-1.54540801	2.61551094
C	3.53737593	-3.52152205	2.08541393
C	4.04510117	-2.30859709	0.00816700
C	1.84567797	-2.59786797	3.52566004
H	0.96233702	-0.75689799	2.79940510
C	2.77213192	-3.58615398	3.26764607
C	5.01786804	-3.27077794	-0.32979199
H	1.24115801	-2.61594892	4.42212486
H	2.91841197	-4.40690994	3.95866799
C	4.44062710	-1.08550000	-1.92141497
C	5.71848106	-3.08745503	-1.53936994
C	5.42741585	-1.99395394	-2.32749391
H	4.19130516	-0.22460601	-2.52567005
H	6.47547913	-3.80251002	-1.83670902
H	5.94654608	-1.82082295	-3.26026702
N	3.76005197	-1.23507094	-0.78619200
N	2.38792706	-1.45747697	1.49161899
C	4.04507303	2.30861402	-0.00817700
C	4.44063520	1.08551705	1.92139804
C	5.01782990	3.27080798	0.32977501
C	3.30475998	2.43263197	-1.22143698
C	5.42741394	1.99398398	2.32747006
H	4.19133091	0.22461800	2.52565193
C	5.71845579	3.08749104	1.53934598
C	3.53731704	3.52153492	-2.08541894
H	5.94655514	1.82085896	3.26023793
H	6.47544622	3.80255795	1.83668101
C	1.67848897	1.54539597	-2.61550498
C	2.77206397	3.58615708	-3.26764607
C	1.84562194	2.59785891	-3.52565503
H	0.96231002	0.75687599	-2.79939604
H	2.91832805	4.40691519	-3.95866895
H	1.24109602	2.61593199	-4.42211723
N	3.76004696	1.23508203	0.78618097
N	2.38789892	1.45747399	-1.49161804
C	-8.98030376	-2.11678290	-1.67139804
C	-8.98030567	2.11677289	1.67139804
C	-6.56323385	-1.12713897	-0.89193499
C	-6.59765482	-2.22769189	-1.76287103
H	-5.66613197	-2.65805793	-2.10449505
C	-6.59765720	2.22768211	1.76287496
H	-5.66613293	2.65804696	2.10450006
C	-7.81861401	-2.73089790	-2.15950894
C	-7.81861496	2.73088789	2.15950990
H	-7.88940620	-3.57769608	-2.82974505
H	-9.95654297	-2.49093103	-1.96540797
H	-7.88940811	3.57768607	2.82974601
H	-9.95654488	2.49092197	1.96540594
N	-8.97610474	-1.07628798	-0.84832197
N	-8.97610569	1.07627797	0.84832299
C	4.52863979	4.49114180	-1.71935594
H	4.70236492	5.32580996	-2.38717198
C	5.23814297	4.37021494	-0.56445599
H	5.98557901	5.10714102	-0.29823199
C	5.23820305	-4.37018013	0.56443900
H	5.98564816	-5.10709715	0.29821101
C	4.52870989	-4.49111605	1.71934497
H	4.70245314	-5.32578087	2.38716102

S2.2. Frequencies

Mode	IR frequency	IR intensity	Raman intensity
1	-7.72530000	0.24140000	0.00000000
2	10.46060000	0.00000000	0.00000000
3	22.68840000	1.04800000	0.00000000
4	27.15430000	0.13890000	0.00000000
5	36.49830000	0.05630000	0.00000000
6	38.86470000	0.04500000	0.00000000
7	40.98930000	0.19500000	0.00000000
8	43.95530000	0.66930000	0.00000000
9	67.75300000	0.01290000	0.00000000
10	75.29420000	0.42510000	0.00000000
11	82.46440000	3.94500000	0.00000000
12	86.39020000	13.37290000	0.00000000
13	91.96120000	4.23640000	0.00000000
14	102.85650000	0.00580000	0.00000000
15	125.39490000	0.17020000	0.00000000
16	132.37520000	0.01600000	0.00000000
17	161.71220000	0.00000000	0.00000000
18	167.37790000	0.15270000	0.00000000
19	171.13360000	5.61280000	0.00000000
20	172.40050000	0.95020000	0.00000000
21	178.59890000	1.70860000	0.00000000
22	189.35590000	1.66840000	0.00000000
23	195.33190000	0.88990000	0.00000000
24	196.96610000	0.75450000	0.00000000
25	217.67350000	0.00030000	0.00000000
26	221.89600000	0.36140000	0.00000000
27	225.45070000	0.42040000	0.00000000
28	233.10180000	3.66850000	0.00000000
29	235.35070000	4.40720000	0.00000000
30	246.33420000	0.53710000	0.00000000
31	272.01520000	18.60070000	0.00000000
32	279.85070000	1.46970000	0.00000000
33	283.55540000	0.01230000	0.00000000
34	288.97570000	3.86520000	0.00000000
35	289.27230000	4.88450000	0.00000000
36	289.55280000	0.72890000	0.00000000
37	323.85190000	2.53700000	0.00000000
38	323.93820000	0.00230000	0.00000000
39	341.15080000	0.33020000	0.00000000
40	341.73080000	0.00860000	0.00000000
41	369.61570000	0.73720000	0.00000000
42	384.00190000	1.60250000	0.00000000
43	415.29620000	14.72110000	0.00000000
44	438.82690000	0.35750000	0.00000000
45	439.39450000	0.56090000	0.00000000
46	442.42270000	5.34700000	0.00000000
47	443.31470000	0.36000000	0.00000000
48	443.52760000	0.81450000	0.00000000
49	445.95020000	0.37020000	0.00000000
50	446.74060000	0.10260000	0.00000000
51	456.09180000	18.18770000	0.00000000
52	459.77580000	1.20260000	0.00000000
53	464.16540000	0.03290000	0.00000000
54	474.37870000	2.54500000	0.00000000
55	476.03320000	0.23630000	0.00000000
56	479.25550000	1.78640000	0.00000000
57	502.30130000	1.18900000	0.00000000
58	506.86030000	0.70850000	0.00000000
59	519.96720000	3.86030000	0.00000000
60	520.05670000	0.47200000	0.00000000

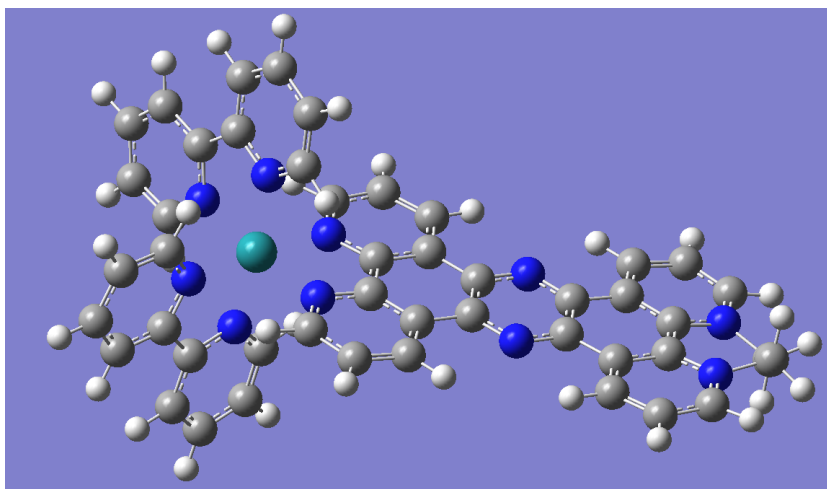
61	533.00600000	19.26920000	0.00000000
62	537.06730000	1.00680000	0.00000000
63	537.22950000	10.12640000	0.00000000
64	544.34480000	3.50090000	0.00000000
65	564.12520000	0.07720000	0.00000000
66	565.13440000	0.00680000	0.00000000
67	570.58180000	0.02540000	0.00000000
68	574.19050000	5.05230000	0.00000000
69	575.27830000	1.55510000	0.00000000
70	576.16240000	0.22160000	0.00000000
71	579.15720000	6.54700000	0.00000000
72	580.07830000	1.94160000	0.00000000
73	614.77290000	3.19570000	0.00000000
74	631.86230000	0.19180000	0.00000000
75	634.49380000	0.12830000	0.00000000
76	635.76850000	18.49130000	0.00000000
77	650.95320000	7.83590000	0.00000000
78	663.39940000	0.67910000	0.00000000
79	665.81410000	1.88940000	0.00000000
80	667.91200000	3.87350000	0.00000000
81	672.12830000	1.50920000	0.00000000
82	707.94720000	0.67450000	0.00000000
83	708.33130000	0.29330000	0.00000000
84	724.51490000	0.00050000	0.00000000
85	739.65780000	48.88490000	0.00000000
86	741.64770000	36.72180000	0.00000000
87	741.98070000	25.79060000	0.00000000
88	742.62770000	35.73930000	0.00000000
89	743.52940000	5.34020000	0.00000000
90	750.75620000	21.35980000	0.00000000
91	751.83260000	45.11200000	0.00000000
92	753.89310000	8.43090000	0.00000000
93	759.88050000	1.17640000	0.00000000
94	767.02210000	75.53420000	0.00000000
95	786.62030000	18.00160000	0.00000000
96	786.72540000	17.60960000	0.00000000
97	807.40420000	0.01770000	0.00000000
98	809.83790000	0.07590000	0.00000000
99	810.09360000	0.05510000	0.00000000
100	815.71440000	0.02180000	0.00000000
101	823.13420000	0.41220000	0.00000000
102	833.05270000	101.79780000	0.00000000
103	833.64660000	0.02310000	0.00000000
104	837.47960000	0.73920000	0.00000000
105	851.83920000	0.37980000	0.00000000
106	851.94510000	0.21530000	0.00000000
107	853.62520000	0.00030000	0.00000000
108	863.12170000	101.13670000	0.00000000
109	863.23580000	106.21790000	0.00000000
110	864.00020000	4.11010000	0.00000000
111	874.46790000	0.00280000	0.00000000
112	896.20120000	0.84530000	0.00000000
113	898.84670000	0.43230000	0.00000000
114	932.13400000	3.50220000	0.00000000
115	934.42000000	2.28860000	0.00000000
116	935.07470000	0.25370000	0.00000000
117	966.64640000	0.18230000	0.00000000
118	967.30670000	0.24150000	0.00000000
119	971.27970000	0.04920000	0.00000000
120	971.77110000	0.18430000	0.00000000
121	973.74520000	0.02270000	0.00000000
122	973.99770000	0.07820000	0.00000000
123	983.81270000	0.14510000	0.00000000
124	985.12960000	0.00030000	0.00000000

125	999.91280000	0.00060000	0.00000000
126	999.94160000	0.00000000	0.00000000
127	1014.75650000	1.04590000	0.00000000
128	1014.83130000	0.99500000	0.00000000
129	1017.30620000	0.05320000	0.00000000
130	1017.35270000	0.02600000	0.00000000
131	1018.31780000	0.12020000	0.00000000
132	1019.29010000	0.00020000	0.00000000
133	1021.37060000	0.81470000	0.00000000
134	1022.18800000	0.00010000	0.00000000
135	1043.48660000	4.78600000	0.00000000
136	1045.10890000	26.61880000	0.00000000
137	1059.23110000	1.93210000	0.00000000
138	1061.47820000	2.16720000	0.00000000
139	1063.17840000	0.09740000	0.00000000
140	1067.25470000	0.06800000	0.00000000
141	1074.55080000	3.27560000	0.00000000
142	1084.18770000	2.63470000	0.00000000
143	1085.04630000	1.94820000	0.00000000
144	1092.40110000	13.73270000	0.00000000
145	1105.17280000	4.71250000	0.00000000
146	1116.95670000	3.40670000	0.00000000
147	1117.02760000	3.47440000	0.00000000
148	1118.98070000	17.74330000	0.00000000
149	1119.20800000	13.34260000	0.00000000
150	1125.96290000	0.72300000	0.00000000
151	1130.01940000	0.48720000	0.00000000
152	1142.55940000	17.42590000	0.00000000
153	1146.10230000	24.40280000	0.00000000
154	1157.69850000	161.45000000	0.00000000
155	1159.17140000	7.50730000	0.00000000
156	1169.71240000	8.98100000	0.00000000
157	1170.01700000	6.73340000	0.00000000
158	1172.04080000	2.93520000	0.00000000
159	1172.21120000	0.04900000	0.00000000
160	1199.58650000	5.86680000	0.00000000
161	1217.29970000	20.24350000	0.00000000
162	1226.32590000	5.08070000	0.00000000
163	1231.15760000	10.26860000	0.00000000
164	1234.26450000	0.62350000	0.00000000
165	1234.40910000	0.52070000	0.00000000
166	1234.59500000	0.86610000	0.00000000
167	1250.13730000	1.60020000	0.00000000
168	1250.44460000	3.17340000	0.00000000
169	1263.99580000	0.51100000	0.00000000
170	1278.58730000	17.72650000	0.00000000
171	1286.58750000	1.63000000	0.00000000
172	1287.73860000	0.89100000	0.00000000
173	1292.86560000	24.45560000	0.00000000
174	1311.34510000	0.10790000	0.00000000
175	1316.51410000	39.45920000	0.00000000
176	1321.70390000	0.20600000	0.00000000
177	1330.72860000	9.87160000	0.00000000
178	1333.71820000	0.86890000	0.00000000
179	1333.86950000	1.25250000	0.00000000
180	1334.13580000	0.93170000	0.00000000
181	1347.78110000	5.92600000	0.00000000
182	1347.82670000	5.85310000	0.00000000
183	1352.96360000	12.14690000	0.00000000
184	1360.60790000	23.41940000	0.00000000
185	1373.81700000	8.93390000	0.00000000
186	1374.40490000	8.71500000	0.00000000
187	1388.35700000	214.69320000	0.00000000
188	1392.58580000	161.64800000	0.00000000

189	1425.90610000	207.65460000	0.00000000
190	1437.94180000	10.64950000	0.00000000
191	1442.02110000	32.17570000	0.00000000
192	1443.02570000	6.65880000	0.00000000
193	1450.88560000	1.43330000	0.00000000
194	1453.44160000	44.94580000	0.00000000
195	1453.55000000	12.72330000	0.00000000
196	1458.11780000	88.74220000	0.00000000
197	1458.50570000	24.90850000	0.00000000
198	1469.57650000	49.65580000	0.00000000
199	1482.57720000	1.22910000	0.00000000
200	1483.35150000	11.07940000	0.00000000
201	1484.32820000	21.84400000	0.00000000
202	1496.53690000	30.21930000	0.00000000
203	1506.16030000	1.01650000	0.00000000
204	1511.50870000	162.55790000	0.00000000
205	1529.00180000	17.23850000	0.00000000
206	1529.91300000	5.26110000	0.00000000
207	1533.48460000	15.00020000	0.00000000
208	1541.41390000	48.90330000	0.00000000
209	1550.15360000	5.56730000	0.00000000
210	1550.71150000	1.23610000	0.00000000
211	1576.06390000	31.75080000	0.00000000
212	1592.76130000	1.41870000	0.00000000
213	1608.62080000	24.05810000	0.00000000
214	1612.26460000	0.12160000	0.00000000
215	1617.48190000	1.36020000	0.00000000
216	1619.76330000	5.12720000	0.00000000
217	1619.96180000	9.56000000	0.00000000
218	1620.25630000	0.00010000	0.00000000
219	1622.80940000	2.57030000	0.00000000
220	1624.63770000	99.05330000	0.00000000
221	1629.66210000	2.34670000	0.00000000
222	1634.88900000	1.65480000	0.00000000
223	1635.19670000	5.49660000	0.00000000
224	1637.68180000	25.22770000	0.00000000
225	1642.39180000	3.83380000	0.00000000
226	1664.23730000	8.83910000	0.00000000
227	1664.54150000	2.19840000	0.00000000
228	3152.85030000	32.29710000	0.00000000
229	3153.29910000	56.69740000	0.00000000
230	3187.45570000	0.38190000	0.00000000
231	3187.45670000	0.19920000	0.00000000
232	3195.68570000	1.65790000	0.00000000
233	3195.69080000	1.22560000	0.00000000
234	3197.38960000	5.60280000	0.00000000
235	3197.39200000	0.10460000	0.00000000
236	3199.53520000	17.37850000	0.00000000
237	3199.59120000	9.03370000	0.00000000
238	3201.78560000	28.89410000	0.00000000
239	3201.81810000	11.50070000	0.00000000
240	3209.93880000	0.94430000	0.00000000
241	3210.02370000	0.05290000	0.00000000
242	3211.28850000	1.98590000	0.00000000
243	3211.31540000	0.65650000	0.00000000
244	3211.68370000	3.78140000	0.00000000
245	3211.72780000	0.10610000	0.00000000
246	3215.44590000	18.65370000	0.00000000
247	3215.55360000	4.32960000	0.00000000
248	3221.62200000	1.21960000	0.00000000
249	3221.65400000	4.57510000	0.00000000
250	3223.24090000	5.56330000	0.00000000
251	3223.25310000	3.26750000	0.00000000
252	3223.39930000	24.48870000	0.00000000

253	3223.66620000	0.04700000	0.00000000
254	3227.58680000	9.99570000	0.00000000
255	3227.67330000	1.49980000	0.00000000

S3. CALCULATIONS ON 3^{4+} (1A)



```

Route          : # opt freq b3lyp/genecp scrf=(solvent=acetonitrile) geom=connectivity
                : empiricaldispersion=gd3bj int=ultrafine pop=regular
SMILES         : c1cc[n+](c1)-c3cccc[n+](c3)[Ru]245([n+](c6cccc6-c7[n+](c4cccc7)[n+](c8cccc9c8c1[n+](c5cccc1c1c9nc2c3ccc[n+](c4c3c3c(c2n1)ccc[n+](c3CC4
Formula        : C46H32N10Ru4+
Charge         : 4
Multiplicity   : 1
Energy         : -2415.02198353
Gibbs Energy   : -2414.39640500
Number of imaginary frequencies : 0

```

a.u.

a.u.

S3.1. Cartesian Co-ordinates (XYZ format)

89

```

Ru  2.95185900  0.00000000  0.00000100
N   1.33976305 -1.23142505 -0.49943101
N  -3.47552109 -1.29758596 -0.51561201
N  -3.47552204  1.29758704  0.51561099
N   1.33976197  1.23142600  0.49943399
C   1.38710701 -2.47770500 -0.98375303
H   2.37127399 -2.88901997 -1.15698600
C   0.23552100 -3.21489811 -1.26202297
H   0.33305600 -4.21814919 -1.65297604
C  -1.00737906 -2.65252995 -1.03709900
H  -1.91980505 -3.19374704 -1.24452901
C  -1.07590997 -1.34849000 -0.52732301
C  -2.33407497 -0.66619700 -0.26126900
C  -4.61573505 -0.65539700 -0.26449299
C  -7.07956409 -0.64638400 -0.32341799
C  -7.07956409  0.64638400  0.32341799
C  -5.87333679  1.31302905  0.57692099
C  -4.61573601  0.65539700  0.26449201
C  -2.33407497  0.66619802  0.26126799
C  -1.07590997  1.34849095  0.52732301
C  -1.00737906  2.65253091  1.03709805
H  -1.91980600  3.19374895  1.24452698

```


C	0.23552001	3.21489906	1.26202297
H	0.33305600	4.21815109	1.65297496
C	1.38710701	2.47770596	0.98375499
H	2.37127399	2.88901997	1.15698898
C	0.12278600	0.67128599	0.26558501
C	0.12278600	-0.67128497	-0.26558301
C	3.97829294	-2.02662802	1.86100602
C	2.32511401	-0.75022399	2.90010095
C	4.13372707	-2.79510188	3.01269197
C	4.75134420	-2.23187304	0.62587702
C	2.43714499	-1.47902298	4.07341719
H	1.62639105	0.06881800	2.81250405
C	3.35751104	-2.52049208	4.13049221
H	4.85179281	-3.60152888	3.03855491
C	5.74431276	-3.19828391	0.48177800
H	1.81172001	-1.22878802	4.91926622
H	3.47078204	-3.11100101	5.03010511
C	5.08637619	-1.51662397	-1.56991398
C	6.41652822	-3.31581903	-0.72721201
H	5.99374008	-3.85156703	1.30484104
C	6.08123016	-2.46027589	-1.77143896
H	4.79285002	-0.83321601	-2.35317492
H	7.18972778	-4.06281424	-0.84961802
H	6.57857609	-2.51499510	-2.73002100
N	4.43146515	-1.40066195	-0.40251201
N	3.07514811	-1.01063895	1.81652403
C	4.75134277	2.23187208	-0.62587798
C	5.08637524	1.51662600	1.56991398
C	5.74431181	3.19828391	-0.48177999
C	3.97829294	2.02662611	-1.86100602
C	6.08123016	2.46027899	1.77143800
H	4.79284906	0.83321899	2.35317612
C	6.41652822	3.31581998	0.72720999
H	5.99373913	3.85156608	-1.30484402
C	4.13372898	2.79509807	-3.01269388
H	6.57857704	2.51499796	2.73001909
H	7.18972778	4.06281519	0.84961498
C	2.32511210	0.75022298	-2.90009999
C	3.35751295	2.52048707	-4.13049412
H	4.85179710	3.60152292	-3.03855896
C	2.43714499	1.47902000	-4.07341719
H	1.62638795	-0.06881700	-2.81250095
H	3.47078705	3.11099291	-5.03010798
H	1.81171894	1.22878504	-4.91926622
N	4.43146515	1.40066302	0.40251201
N	3.07514596	1.01063895	-1.81652296
C	-8.29333782	-2.43545794	-1.27892804
C	-8.29333782	2.43545794	1.27892804
C	-5.87333679	-1.31302798	-0.57692200
C	-5.91299391	-2.58908892	-1.16287804
H	-4.98027611	-3.10269809	-1.34961402
C	-5.91299391	2.58908892	1.16287804
H	-4.98027611	3.10269904	1.34961295
C	-7.12613583	-3.15614104	-1.49479401
C	-7.12613678	3.15614009	1.49479306
H	-7.19056416	-4.13768101	-1.94081795
H	-9.26862240	-2.80544591	-1.56002295
H	-7.19056416	4.13768101	1.94081795
H	-9.26862335	2.80544496	1.56002402
N	-8.25597763	-1.21970403	-0.71745402
N	-8.25597763	1.21970296	0.71745402
C	-9.49440289	0.40479201	0.63591897
H	-10.34802246	1.07575595	0.64679903
H	-9.52239227	-0.23197700	1.52059603

C	-9.49440289	-0.40479299	-0.63591897
H	-9.52239323	0.23197600	-1.52059603
H	-10.34802246	-1.07575703	-0.64679998

S3.2. Frequencies

Mode	IR frequency	IR intensity	Raman intensity
1	4.47750000	3.46750000	0.00000000
2	26.64340000	0.12370000	0.00000000
3	27.50690000	0.12450000	0.00000000
4	27.67960000	1.35030000	0.00000000
5	31.64210000	2.58910000	0.00000000
6	34.44070000	0.14580000	0.00000000
7	44.00680000	1.89620000	0.00000000
8	51.84300000	0.10630000	0.00000000
9	73.15020000	1.86990000	0.00000000
10	77.67260000	2.36190000	0.00000000
11	81.70840000	0.57390000	0.00000000
12	87.05090000	5.27300000	0.00000000
13	94.16390000	3.78570000	0.00000000
14	117.53030000	0.04610000	0.00000000
15	123.67900000	3.44260000	0.00000000
16	126.36250000	2.63190000	0.00000000
17	129.35820000	0.65720000	0.00000000
18	138.18230000	0.34590000	0.00000000
19	171.54840000	3.22710000	0.00000000
20	175.85880000	2.14930000	0.00000000
21	176.04890000	0.47550000	0.00000000
22	185.19300000	2.23370000	0.00000000
23	195.05250000	1.61300000	0.00000000
24	197.13070000	0.02510000	0.00000000
25	208.20550000	6.18060000	0.00000000
26	218.71910000	0.22360000	0.00000000
27	221.76790000	0.20800000	0.00000000
28	231.18620000	0.44680000	0.00000000
29	233.51750000	0.93330000	0.00000000
30	248.86880000	0.35670000	0.00000000
31	249.02630000	1.21290000	0.00000000
32	262.78200000	0.23530000	0.00000000
33	270.73650000	0.83460000	0.00000000
34	273.87770000	0.23550000	0.00000000
35	308.15550000	11.35670000	0.00000000
36	315.23560000	0.24460000	0.00000000
37	328.05090000	6.10540000	0.00000000
38	342.48680000	1.60490000	0.00000000
39	349.66810000	1.21710000	0.00000000
40	353.51710000	0.01960000	0.00000000
41	373.98920000	0.73830000	0.00000000
42	379.02550000	0.24890000	0.00000000
43	385.81870000	0.56780000	0.00000000
44	398.93690000	5.28270000	0.00000000
45	419.08890000	1.22440000	0.00000000
46	432.98420000	6.17890000	0.00000000
47	434.42460000	8.85210000	0.00000000
48	437.93090000	6.14830000	0.00000000
49	441.63360000	6.46230000	0.00000000
50	445.79500000	0.49060000	0.00000000
51	454.10090000	2.71200000	0.00000000
52	456.16300000	0.36860000	0.00000000
53	459.54320000	16.06620000	0.00000000
54	462.06010000	1.71330000	0.00000000
55	474.24700000	4.09740000	0.00000000
56	480.40590000	1.11510000	0.00000000
57	485.73660000	0.48950000	0.00000000
58	495.96700000	0.07010000	0.00000000
59	497.20930000	0.20260000	0.00000000
60	500.21620000	4.44250000	0.00000000

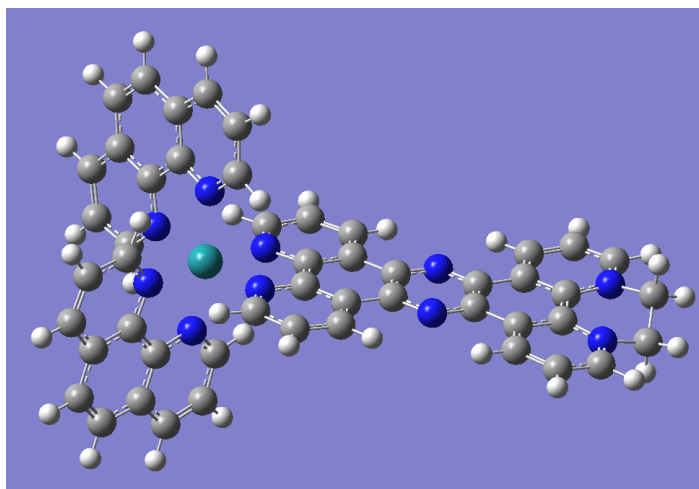
61	506.87300000	0.20460000	0.00000000
62	539.36860000	15.23590000	0.00000000
63	546.92600000	0.41840000	0.00000000
64	555.41990000	3.54960000	0.00000000
65	558.47610000	3.08430000	0.00000000
66	564.35130000	0.00720000	0.00000000
67	565.29810000	0.00320000	0.00000000
68	570.56000000	1.46320000	0.00000000
69	581.41970000	5.13630000	0.00000000
70	584.72130000	1.73700000	0.00000000
71	610.74800000	7.08730000	0.00000000
72	645.31220000	6.68860000	0.00000000
73	658.93530000	1.50350000	0.00000000
74	662.79790000	5.27140000	0.00000000
75	663.69820000	2.70010000	0.00000000
76	666.08230000	6.24930000	0.00000000
77	666.17640000	2.06930000	0.00000000
78	670.11660000	0.43650000	0.00000000
79	671.03300000	0.86470000	0.00000000
80	679.09310000	3.76900000	0.00000000
81	683.35730000	3.82460000	0.00000000
82	707.33500000	1.70740000	0.00000000
83	730.32570000	0.61250000	0.00000000
84	733.13990000	74.18300000	0.00000000
85	741.91070000	16.36370000	0.00000000
86	742.62160000	26.97550000	0.00000000
87	750.78560000	41.62360000	0.00000000
88	753.07310000	49.46420000	0.00000000
89	753.95710000	47.11220000	0.00000000
90	762.13710000	6.11650000	0.00000000
91	763.90390000	3.64590000	0.00000000
92	776.56580000	140.28700000	0.00000000
93	777.77760000	128.03060000	0.00000000
94	784.10900000	2.62230000	0.00000000
95	784.84960000	0.96350000	0.00000000
96	799.55260000	0.00000000	0.00000000
97	808.29190000	0.33250000	0.00000000
98	813.37020000	0.14250000	0.00000000
99	820.94570000	12.48700000	0.00000000
100	821.47130000	1.65100000	0.00000000
101	821.87000000	0.03160000	0.00000000
102	823.06670000	0.00010000	0.00000000
103	835.50700000	91.46830000	0.00000000
104	837.68440000	8.76910000	0.00000000
105	843.13020000	21.89140000	0.00000000
106	856.26610000	0.97640000	0.00000000
107	876.51160000	0.27820000	0.00000000
108	908.20180000	0.02980000	0.00000000
109	908.50480000	0.24520000	0.00000000
110	909.11520000	0.09290000	0.00000000
111	909.56900000	0.11820000	0.00000000
112	909.60740000	0.20370000	0.00000000
113	934.42440000	2.88950000	0.00000000
114	982.68270000	0.00290000	0.00000000
115	983.57130000	0.03220000	0.00000000
116	983.85930000	0.00540000	0.00000000
117	985.00080000	0.22700000	0.00000000
118	988.84130000	0.21400000	0.00000000
119	989.21010000	0.11140000	0.00000000
120	990.64090000	2.09510000	0.00000000
121	990.68420000	1.28840000	0.00000000
122	1014.65100000	14.92980000	0.00000000
123	1024.28880000	0.00380000	0.00000000
124	1024.30140000	0.02260000	0.00000000

125	1024.47130000	1.09080000	0.00000000
126	1025.36520000	0.33600000	0.00000000
127	1025.97140000	0.03030000	0.00000000
128	1027.64010000	0.26070000	0.00000000
129	1027.69320000	0.22150000	0.00000000
130	1036.52590000	0.91990000	0.00000000
131	1039.81840000	0.05680000	0.00000000
132	1044.79860000	0.20140000	0.00000000
133	1045.22800000	0.02020000	0.00000000
134	1046.15360000	3.79610000	0.00000000
135	1054.00590000	4.81310000	0.00000000
136	1060.12050000	3.68820000	0.00000000
137	1066.99240000	1.81350000	0.00000000
138	1069.44180000	3.91720000	0.00000000
139	1069.85860000	1.04200000	0.00000000
140	1077.72240000	2.79030000	0.00000000
141	1087.53210000	4.22500000	0.00000000
142	1088.62830000	0.76450000	0.00000000
143	1094.76880000	3.53050000	0.00000000
144	1095.24030000	7.70040000	0.00000000
145	1105.95470000	2.59940000	0.00000000
146	1108.29970000	0.53000000	0.00000000
147	1115.49030000	0.80800000	0.00000000
148	1118.99780000	25.69510000	0.00000000
149	1122.76540000	6.60150000	0.00000000
150	1133.97390000	5.84040000	0.00000000
151	1134.85570000	0.56850000	0.00000000
152	1146.25380000	0.75180000	0.00000000
153	1146.42050000	23.53190000	0.00000000
154	1150.17640000	0.34480000	0.00000000
155	1150.98050000	2.68290000	0.00000000
156	1160.13020000	225.23600000	0.00000000
157	1161.39030000	10.74590000	0.00000000
158	1184.74300000	6.71170000	0.00000000
159	1185.13520000	10.34850000	0.00000000
160	1195.19670000	4.65980000	0.00000000
161	1195.64700000	0.34060000	0.00000000
162	1196.53530000	26.21090000	0.00000000
163	1197.81780000	24.71300000	0.00000000
164	1219.67520000	1.03420000	0.00000000
165	1236.14340000	0.60920000	0.00000000
166	1246.76010000	55.41310000	0.00000000
167	1259.71500000	1.44340000	0.00000000
168	1275.10120000	14.16390000	0.00000000
169	1285.82460000	27.78790000	0.00000000
170	1286.13610000	48.24380000	0.00000000
171	1290.52440000	2.49410000	0.00000000
172	1290.69960000	24.46790000	0.00000000
173	1293.26220000	1.67470000	0.00000000
174	1297.55190000	6.41130000	0.00000000
175	1309.38670000	3.15780000	0.00000000
176	1309.96180000	1.47820000	0.00000000
177	1311.12380000	18.72290000	0.00000000
178	1318.40960000	2.31600000	0.00000000
179	1330.05570000	4.68310000	0.00000000
180	1339.15240000	8.26040000	0.00000000
181	1339.42580000	0.06420000	0.00000000
182	1340.54710000	3.72480000	0.00000000
183	1341.42650000	9.81050000	0.00000000
184	1342.05690000	0.04050000	0.00000000
185	1342.68500000	3.84240000	0.00000000
186	1349.61680000	51.28970000	0.00000000
187	1355.51500000	93.02480000	0.00000000
188	1386.32810000	25.16890000	0.00000000

189	1390.26470000	288.96490000	0.00000000
190	1396.22280000	32.80030000	0.00000000
191	1405.51170000	6.45520000	0.00000000
192	1430.25200000	106.50120000	0.00000000
193	1444.64080000	142.77280000	0.00000000
194	1461.16950000	21.01480000	0.00000000
195	1462.04230000	47.40540000	0.00000000
196	1470.18900000	27.61870000	0.00000000
197	1474.78490000	8.71860000	0.00000000
198	1474.83800000	83.09600000	0.00000000
199	1481.43430000	42.89480000	0.00000000
200	1481.44350000	102.39200000	0.00000000
201	1486.10530000	0.31140000	0.00000000
202	1488.95890000	3.25820000	0.00000000
203	1497.56970000	6.64720000	0.00000000
204	1499.31770000	136.11430000	0.00000000
205	1502.95870000	30.14380000	0.00000000
206	1512.10770000	37.17530000	0.00000000
207	1516.03570000	7.15810000	0.00000000
208	1520.24600000	0.02800000	0.00000000
209	1520.98680000	0.41620000	0.00000000
210	1524.64230000	61.01350000	0.00000000
211	1547.03250000	99.29510000	0.00000000
212	1569.95040000	49.03210000	0.00000000
213	1584.06480000	11.93000000	0.00000000
214	1600.81130000	2.34910000	0.00000000
215	1601.08060000	1.60740000	0.00000000
216	1608.09930000	43.34700000	0.00000000
217	1609.93940000	2.46940000	0.00000000
218	1610.29060000	14.06000000	0.00000000
219	1617.95960000	0.09630000	0.00000000
220	1622.95060000	0.17680000	0.00000000
221	1629.99680000	71.55750000	0.00000000
222	1635.29640000	15.07210000	0.00000000
223	1639.50700000	1.24350000	0.00000000
224	1641.29250000	12.05540000	0.00000000
225	1642.36050000	5.33920000	0.00000000
226	1642.58010000	15.17510000	0.00000000
227	1648.95390000	7.81680000	0.00000000
228	1650.10270000	4.12870000	0.00000000
229	1659.79710000	5.85100000	0.00000000
230	3098.72320000	1.21490000	0.00000000
231	3108.19170000	0.36380000	0.00000000
232	3176.36960000	0.15430000	0.00000000
233	3181.24530000	0.77320000	0.00000000
234	3202.70400000	1.29400000	0.00000000
235	3202.71060000	4.40840000	0.00000000
236	3203.46660000	2.69670000	0.00000000
237	3203.48950000	1.06500000	0.00000000
238	3213.79810000	0.18370000	0.00000000
239	3213.88190000	0.20450000	0.00000000
240	3215.29510000	1.23690000	0.00000000
241	3215.29790000	2.11040000	0.00000000
242	3216.06570000	0.79850000	0.00000000
243	3216.07930000	0.13100000	0.00000000
244	3223.28470000	0.03300000	0.00000000
245	3223.28500000	0.47960000	0.00000000
246	3225.10660000	1.14230000	0.00000000
247	3225.15820000	11.50770000	0.00000000
248	3228.85170000	1.74580000	0.00000000
249	3228.89100000	0.97610000	0.00000000
250	3229.85420000	1.40690000	0.00000000
251	3230.14710000	0.34810000	0.00000000
252	3230.78020000	5.91000000	0.00000000

253	3231.01300000	20.37500000	0.00000000
254	3231.44460000	10.10870000	0.00000000
255	3231.47000000	1.90240000	0.00000000
256	3232.76420000	6.68170000	0.00000000
257	3233.02280000	5.38700000	0.00000000
258	3235.67560000	30.78050000	0.00000000
259	3235.69220000	0.70970000	0.00000000
260	3243.40170000	2.95800000	0.00000000
261	3243.42230000	16.02550000	0.00000000

S4. CALCULATIONS ON 4^{4+} (1A)



```

Route          : # opt freq b3lyp/genecp scrf=(solvent=acetonitrile) geom=connectivity
                : empiricaldispersion=gd3bj int=ultrafine pop=regular
SMILES         : c1cc2ccc3ccc[n+](c1)[Ru]456([n+]7cccc8c7c9[n+]5cccc9cc8)[n+]
                : 1cccc2c1c1[n+]6cccc1c1c2nc2c3ccc[n+]4c3c3c(c2n1)ccc[n+]3CC4
Formula        : C50H32N10Ru4+
Charge         : 4
Multiplicity   : 1
Energy         : -2567.53405899                                     a.u.
Gibbs Energy   : -2566.88078300                                     a.u.
Number of imaginary frequencies : 1

```

S4.1. Cartesian Co-ordinates (XYZ format)

93

```

Ru  2.63054204  0.00000000  0.00000000
N   1.02203000  1.02690399  0.84144998
N  -3.79311395  1.08247995  0.88202202
N  -3.79311490 -1.08247900 -0.88202298
N   1.02203000 -1.02690399 -0.84145099
C   1.07033598  2.06942010  1.67834699
H   2.05526900  2.41346312  1.96032202
C  -0.08081400  2.68263602  2.17432690
H   0.01772000  3.52046895  2.85053492
C  -1.32416904  2.21010399  1.79688299
H  -2.23623991  2.65863609  2.16492009
C  -1.39353597  1.12311494  0.91424298
C  -2.65169692  0.55468202  0.45237300
C  -4.93339396  0.54841697  0.44562301
C  -7.39777184  0.59220600  0.41400900
C  -7.39777184 -0.59220499 -0.41400900
C  -6.19115591 -1.13543105 -0.87531000
C  -4.93339396 -0.54841602 -0.44562501
C  -2.65169692 -0.55467999 -0.45237401
C  -1.39353597 -1.12311399 -0.91424400
C  -1.32416904 -2.21010399 -1.79688394
H  -2.23623991 -2.65863490 -2.16492105

```


C	-0.08081400	-2.68263507	-2.17432690
H	0.01772000	-3.52046895	-2.85053396
C	1.07033598	-2.06942010	-1.67834699
H	2.05526900	-2.41346312	-1.96032202
C	-0.19544899	-0.55993497	-0.45526901
C	-0.19544899	0.55993599	0.45526901
C	3.67530298	2.43288302	-1.21257102
C	2.04958010	1.55575001	-2.61367989
C	3.91705704	3.52110100	-2.07496595
C	4.41271687	2.30232692	0.00168700
C	2.22583008	2.60779500	-3.52246809
H	1.33095300	0.77076602	-2.80243707
C	3.15642405	3.59087491	-3.25988197
C	5.39069891	3.25804090	0.34269500
H	1.62566996	2.62912512	-4.42176294
H	3.31018806	4.41102219	-3.94995689
C	4.79934311	1.07276595	1.92919695
C	6.08877420	3.06819391	1.55276203
C	5.79049921	1.97501504	2.33841991
H	4.54526281	0.21191300	2.53138304
H	6.84985685	3.77797604	1.85221398
H	6.30762100	1.79689205	3.27132297
N	4.12120819	1.22855604	0.79337001
N	2.75357008	1.46353495	-1.48681295
C	4.41271687	-2.30232692	-0.00168600
C	4.79934406	-1.07276702	-1.92919600
C	5.39069796	-3.25804210	-0.34269401
C	3.67530107	-2.43288398	1.21257102
C	5.79050016	-1.97501504	-2.33841801
H	4.54526520	-0.21191300	-2.53138089
C	6.08877420	-3.06819510	-1.55276000
C	3.91705394	-3.52110195	2.07496595
H	6.30762196	-1.79689205	-3.27132010
H	6.84985685	-3.77797699	-1.85221195
C	2.04957795	-1.55575097	2.61367893
C	3.15641999	-3.59087610	3.25988102
C	2.22582603	-2.60779595	3.52246594
H	1.33095098	-0.77076602	2.80243492
H	3.31018305	-4.41102314	3.94995594
H	1.62566602	-2.62912703	4.42176104
N	4.12120819	-1.22855604	-0.79336900
N	2.75356793	-1.46353495	1.48681295
C	-8.61031818	2.28576589	1.53077805
C	-8.61031723	-2.28576589	-1.53077698
C	-6.19115591	1.13543200	0.87530899
C	-6.23006296	2.25889301	1.71761501
H	-5.29687500	2.66842508	2.07827091
C	-6.23006296	-2.25889301	-1.71761596
H	-5.29687500	-2.66842389	-2.07827306
C	-7.44290781	2.82088709	2.05872703
C	-7.44290781	-2.82088590	-2.05872703
H	-7.50715113	3.68200493	2.70747495
H	-9.58525562	2.71011496	1.72060502
H	-7.50715113	-3.68200493	-2.70747495
H	-9.58525562	-2.71011591	-1.72060394
N	-8.57437611	1.21000600	0.73312998
N	-8.57437611	-1.21000600	-0.73312998
C	4.91340399	-4.48417997	1.70567799
H	5.09420919	-5.31820297	2.37238002
C	5.61954212	-4.35738516	0.54938400
H	6.37122822	-5.08907604	0.28082100
C	5.61954308	4.35738420	-0.54938298
H	6.37123013	5.08907509	-0.28082001
C	4.91340685	4.48417807	-1.70567703

H	5.09421206	5.31820107	-2.37238002
C	-9.81515217	-0.75160301	-0.05924800
H	-10.66563702	-1.07194901	-0.65417302
H	-9.85239887	-1.23545003	0.91730702
C	-9.81515312	0.75160199	0.05924900
H	-10.66563702	1.07194805	0.65417397
H	-9.85239983	1.23544896	-0.91730601

S4.2. Frequencies

Mode	IR frequency	IR intensity	Raman intensity
1	-5.41510000	3.06200000	0.00000000
2	12.65780000	0.00070000	0.00000000
3	23.66300000	0.00950000	0.00000000
4	27.51460000	2.61870000	0.00000000
5	35.65150000	1.09060000	0.00000000
6	39.99940000	0.00570000	0.00000000
7	41.56720000	0.80370000	0.00000000
8	44.74230000	0.03310000	0.00000000
9	67.37330000	2.16040000	0.00000000
10	74.13270000	2.42560000	0.00000000
11	82.82180000	1.19580000	0.00000000
12	87.27330000	7.46490000	0.00000000
13	90.99870000	1.73460000	0.00000000
14	122.86950000	7.63600000	0.00000000
15	133.63180000	0.01870000	0.00000000
16	133.99730000	0.59530000	0.00000000
17	167.32940000	0.09400000	0.00000000
18	167.56720000	0.77230000	0.00000000
19	171.74130000	6.21630000	0.00000000
20	173.64650000	2.24110000	0.00000000
21	179.40780000	2.57920000	0.00000000
22	189.72900000	1.64460000	0.00000000
23	195.59330000	0.50420000	0.00000000
24	195.62550000	0.67930000	0.00000000
25	209.14790000	6.10560000	0.00000000
26	214.16850000	0.59120000	0.00000000
27	223.97060000	1.15790000	0.00000000
28	229.18780000	0.40810000	0.00000000
29	235.20290000	2.63940000	0.00000000
30	236.24080000	4.14610000	0.00000000
31	246.62190000	0.61400000	0.00000000
32	259.13130000	0.07290000	0.00000000
33	279.73990000	1.31640000	0.00000000
34	284.77840000	7.05000000	0.00000000
35	288.70990000	3.19780000	0.00000000
36	289.15110000	4.88380000	0.00000000
37	312.29340000	1.94110000	0.00000000
38	323.84630000	2.90210000	0.00000000
39	324.57730000	0.25170000	0.00000000
40	341.36770000	0.04340000	0.00000000
41	347.93330000	2.85650000	0.00000000
42	353.91050000	0.52840000	0.00000000
43	386.33000000	0.54250000	0.00000000
44	396.91510000	4.17910000	0.00000000
45	420.03370000	1.74250000	0.00000000
46	437.19880000	5.58340000	0.00000000
47	438.93980000	0.26290000	0.00000000
48	441.75160000	6.02680000	0.00000000
49	443.21120000	0.00980000	0.00000000
50	443.38020000	1.25600000	0.00000000
51	446.64880000	0.35260000	0.00000000
52	452.27590000	4.71830000	0.00000000
53	457.84670000	12.36740000	0.00000000
54	463.03900000	2.76060000	0.00000000
55	473.44120000	2.09910000	0.00000000
56	475.18930000	0.48550000	0.00000000
57	480.17390000	2.78390000	0.00000000
58	495.60940000	3.07910000	0.00000000
59	505.37430000	8.19340000	0.00000000
60	506.82070000	0.75940000	0.00000000

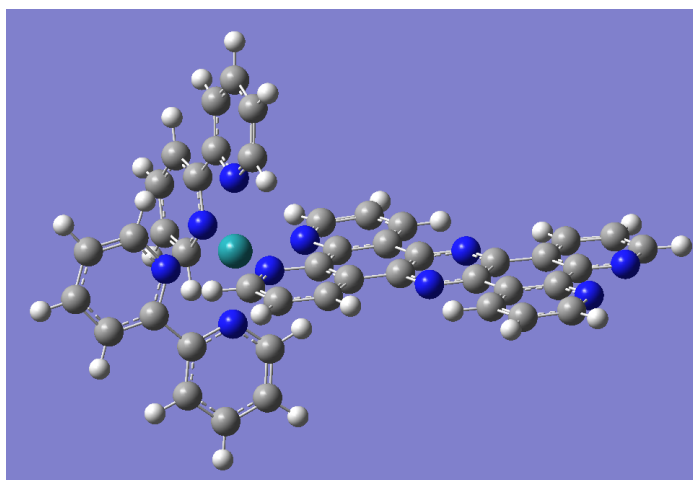
61	508.55420000	0.44460000	0.00000000
62	519.51050000	3.95670000	0.00000000
63	519.67980000	0.74060000	0.00000000
64	537.08450000	9.29930000	0.00000000
65	538.08750000	13.52570000	0.00000000
66	541.00480000	5.88160000	0.00000000
67	547.29220000	0.42010000	0.00000000
68	552.81180000	3.66910000	0.00000000
69	557.43690000	4.05050000	0.00000000
70	564.08640000	0.20580000	0.00000000
71	565.33120000	0.04650000	0.00000000
72	567.77910000	1.40290000	0.00000000
73	574.32490000	3.96120000	0.00000000
74	575.35730000	1.23570000	0.00000000
75	579.88080000	5.66920000	0.00000000
76	584.29420000	0.98160000	0.00000000
77	610.47130000	8.05330000	0.00000000
78	631.45720000	0.22350000	0.00000000
79	634.39250000	0.23070000	0.00000000
80	645.31870000	6.49340000	0.00000000
81	662.83150000	2.17660000	0.00000000
82	665.45240000	2.51960000	0.00000000
83	668.23750000	3.43780000	0.00000000
84	670.23130000	1.08130000	0.00000000
85	671.28970000	1.05080000	0.00000000
86	707.10570000	1.09070000	0.00000000
87	730.81770000	0.26010000	0.00000000
88	732.62960000	67.64150000	0.00000000
89	739.59820000	59.02100000	0.00000000
90	741.27090000	4.89630000	0.00000000
91	741.52960000	0.18740000	0.00000000
92	742.06840000	94.33370000	0.00000000
93	742.97070000	25.39670000	0.00000000
94	743.16220000	5.38060000	0.00000000
95	752.05450000	44.08630000	0.00000000
96	753.63060000	18.99050000	0.00000000
97	759.93230000	0.37200000	0.00000000
98	786.96360000	18.22560000	0.00000000
99	787.08510000	17.57100000	0.00000000
100	795.45650000	0.00130000	0.00000000
101	808.05080000	0.32660000	0.00000000
102	810.25550000	0.09920000	0.00000000
103	810.32570000	0.09510000	0.00000000
104	813.19900000	0.03800000	0.00000000
105	821.24360000	10.05140000	0.00000000
106	822.54190000	0.20900000	0.00000000
107	835.19140000	83.25300000	0.00000000
108	837.38010000	9.82840000	0.00000000
109	844.76520000	35.63650000	0.00000000
110	852.04490000	0.40890000	0.00000000
111	853.42900000	0.03160000	0.00000000
112	857.27700000	0.10690000	0.00000000
113	863.67120000	103.20560000	0.00000000
114	863.68960000	107.47860000	0.00000000
115	878.34000000	0.23790000	0.00000000
116	896.40690000	0.68840000	0.00000000
117	898.68080000	0.54280000	0.00000000
118	908.24460000	0.58480000	0.00000000
119	931.67220000	1.37100000	0.00000000
120	933.52240000	4.14120000	0.00000000
121	935.37730000	0.11250000	0.00000000
122	967.84760000	0.18510000	0.00000000
123	968.38750000	0.26390000	0.00000000
124	973.20360000	0.05010000	0.00000000

125	973.47430000	0.14540000	0.00000000
126	979.98320000	0.01420000	0.00000000
127	980.09190000	0.13720000	0.00000000
128	991.49760000	0.02300000	0.00000000
129	992.86220000	0.05480000	0.00000000
130	1000.56690000	0.00010000	0.00000000
131	1000.58650000	0.00000000	0.00000000
132	1014.57410000	16.62780000	0.00000000
133	1015.46690000	1.09120000	0.00000000
134	1015.50310000	0.59190000	0.00000000
135	1017.99820000	0.00560000	0.00000000
136	1018.00170000	0.00410000	0.00000000
137	1023.86870000	0.31060000	0.00000000
138	1024.43860000	0.00270000	0.00000000
139	1027.79210000	1.23940000	0.00000000
140	1042.85840000	0.21330000	0.00000000
141	1043.19460000	0.01030000	0.00000000
142	1059.01280000	3.07040000	0.00000000
143	1061.57890000	1.92290000	0.00000000
144	1063.30890000	0.00870000	0.00000000
145	1066.94750000	0.18690000	0.00000000
146	1076.47350000	0.44610000	0.00000000
147	1084.47210000	2.05380000	0.00000000
148	1085.37090000	2.65130000	0.00000000
149	1104.44160000	1.98170000	0.00000000
150	1108.02340000	0.17540000	0.00000000
151	1116.63160000	3.23720000	0.00000000
152	1117.02560000	1.12270000	0.00000000
153	1117.35790000	7.98310000	0.00000000
154	1120.45680000	25.96980000	0.00000000
155	1121.30660000	11.71580000	0.00000000
156	1126.08450000	0.86530000	0.00000000
157	1129.74360000	0.07610000	0.00000000
158	1146.05450000	0.77950000	0.00000000
159	1148.17390000	21.98370000	0.00000000
160	1160.05620000	218.95020000	0.00000000
161	1161.41370000	10.71080000	0.00000000
162	1169.79490000	8.39320000	0.00000000
163	1170.04340000	7.06500000	0.00000000
164	1172.46740000	4.20120000	0.00000000
165	1172.64680000	0.00000000	0.00000000
166	1195.57410000	23.77820000	0.00000000
167	1196.61340000	28.44050000	0.00000000
168	1217.22070000	1.27650000	0.00000000
169	1231.05990000	9.29850000	0.00000000
170	1234.19870000	2.24260000	0.00000000
171	1234.56470000	0.35210000	0.00000000
172	1234.71290000	0.17990000	0.00000000
173	1234.77410000	0.41320000	0.00000000
174	1248.33660000	52.24150000	0.00000000
175	1250.17880000	1.69060000	0.00000000
176	1250.50040000	3.58440000	0.00000000
177	1259.14650000	1.89460000	0.00000000
178	1276.56830000	14.04410000	0.00000000
179	1286.60330000	1.30430000	0.00000000
180	1287.74740000	0.69090000	0.00000000
181	1290.48840000	30.34860000	0.00000000
182	1297.91600000	5.25520000	0.00000000
183	1311.14260000	20.58400000	0.00000000
184	1317.99080000	2.41790000	0.00000000
185	1329.71140000	4.39070000	0.00000000
186	1334.39580000	1.30700000	0.00000000
187	1334.74590000	0.49480000	0.00000000
188	1339.06740000	0.00260000	0.00000000

189	1339.08990000	9.50940000	0.00000000
190	1347.82590000	6.06240000	0.00000000
191	1347.93670000	7.57050000	0.00000000
192	1350.29950000	49.37590000	0.00000000
193	1354.39980000	75.70200000	0.00000000
194	1373.81020000	9.51840000	0.00000000
195	1374.40320000	11.99050000	0.00000000
196	1385.94810000	54.17480000	0.00000000
197	1389.19480000	278.19510000	0.00000000
198	1396.75180000	35.90410000	0.00000000
199	1406.29270000	4.76660000	0.00000000
200	1428.19070000	106.27830000	0.00000000
201	1441.93720000	66.56460000	0.00000000
202	1443.00500000	6.25170000	0.00000000
203	1443.48020000	104.33540000	0.00000000
204	1453.40080000	45.83700000	0.00000000
205	1453.51380000	12.45710000	0.00000000
206	1457.98160000	88.22520000	0.00000000
207	1458.37160000	25.74290000	0.00000000
208	1470.33720000	32.16510000	0.00000000
209	1474.23340000	75.45040000	0.00000000
210	1474.49600000	10.77730000	0.00000000
211	1482.96880000	4.77870000	0.00000000
212	1483.65120000	7.44160000	0.00000000
213	1485.53400000	0.17930000	0.00000000
214	1487.62550000	12.79360000	0.00000000
215	1497.47050000	14.16600000	0.00000000
216	1511.74500000	38.41680000	0.00000000
217	1515.90070000	10.20200000	0.00000000
218	1523.95310000	57.56240000	0.00000000
219	1529.13850000	18.29640000	0.00000000
220	1530.12110000	4.12200000	0.00000000
221	1547.51870000	105.03280000	0.00000000
222	1550.72430000	6.14800000	0.00000000
223	1551.13770000	1.17250000	0.00000000
224	1571.09310000	49.20800000	0.00000000
225	1583.69440000	12.94880000	0.00000000
226	1608.38790000	42.11600000	0.00000000
227	1617.94820000	1.68350000	0.00000000
228	1618.01370000	0.19610000	0.00000000
229	1620.19850000	4.07250000	0.00000000
230	1620.39730000	8.93270000	0.00000000
231	1620.73860000	0.00550000	0.00000000
232	1623.12150000	0.23880000	0.00000000
233	1630.17920000	71.59310000	0.00000000
234	1635.05900000	1.53470000	0.00000000
235	1635.37960000	6.42320000	0.00000000
236	1636.00770000	14.67540000	0.00000000
237	1639.90560000	1.22250000	0.00000000
238	1641.67960000	1.35750000	0.00000000
239	1660.03110000	5.52840000	0.00000000
240	1664.33460000	9.67440000	0.00000000
241	1664.62360000	2.40390000	0.00000000
242	3094.73350000	0.61620000	0.00000000
243	3103.13120000	0.39790000	0.00000000
244	3169.92900000	0.05630000	0.00000000
245	3175.28100000	1.04720000	0.00000000
246	3187.94320000	0.26200000	0.00000000
247	3187.94440000	0.16140000	0.00000000
248	3196.17010000	1.67240000	0.00000000
249	3196.17420000	1.07650000	0.00000000
250	3197.89960000	5.24570000	0.00000000
251	3197.90250000	0.09630000	0.00000000
252	3202.28300000	26.74000000	0.00000000

253	3202.31430000	11.22150000	0.00000000
254	3211.87120000	1.15270000	0.00000000
255	3211.87670000	1.84520000	0.00000000
256	3211.98310000	3.36820000	0.00000000
257	3211.98630000	0.04560000	0.00000000
258	3213.38430000	0.11500000	0.00000000
259	3213.47350000	0.06990000	0.00000000
260	3223.68860000	11.85520000	0.00000000
261	3223.76450000	0.40510000	0.00000000
262	3223.91660000	28.01000000	0.00000000
263	3224.01970000	1.00770000	0.00000000
264	3224.10740000	1.86070000	0.00000000
265	3224.21650000	0.78540000	0.00000000
266	3228.59340000	1.90750000	0.00000000
267	3228.63650000	6.05320000	0.00000000
268	3230.76230000	3.48720000	0.00000000
269	3230.80400000	0.69200000	0.00000000
270	3237.24330000	25.20790000	0.00000000
271	3237.28570000	0.33890000	0.00000000
272	3245.52420000	6.11090000	0.00000000
273	3245.58540000	16.03120000	0.00000000

S5. CALCULATIONS ON 1^{2+} (3A)



```

Route          : # opt freq b3lyp/genecp scrf=(solvent=acetonitrile) geom=connectivity
                : empiricaldispersion=gd3bj int=ultrafine pop=regular
SMILES         : c1cc[n+](c1)-c3cccc[n+](c3)[Ru]245([n+](c6cccc6-c7[n+](c4cccc7)[n+](
                : 8cccc9c8c1[n+](c5cccc1c1c9nc2c3ccnc3c3c(c2n1)cccn3
Formula        : C44H28N10Ru2+,3
Charge         : 2
Multiplicity   : 3
Energy         : -2336.63745079 a.u.
Gibbs Energy   : -2336.07474800 a.u.
Number of imaginary frequencies : 2

```

S5.1. Cartesian Co-ordinates (XYZ format)

83

```

Ru -2.59259796 -0.00036000 -0.00011900
N  -1.01473296 -1.17948604  0.63172001
N   3.83782911 -1.24123001  0.63600498
N   3.83802891  1.23684299 -0.64159101
N  -1.01452899  1.17475402 -0.63922602
C  -1.05786300 -2.39499688  1.20381606
H  -2.04207802 -2.79414201  1.40959895
C   0.08496600 -3.09720302  1.53961694
H  -0.00528900 -4.06392813  2.01393604
C   1.34790802 -2.53407192  1.26546705
H   2.25781298 -3.05930495  1.52260697
C   1.43180895 -1.29725897  0.65408099
C   2.69239497 -0.63938802  0.32217401
C   4.98797512 -0.62977999  0.32482201
C   7.47552776 -0.64856702  0.34579399
C   7.47564220  0.64681703 -0.34521499
C   6.24698782  1.26662397 -0.66972297
C   4.98807001  0.62610602 -0.32867199
C   2.69248199  0.63439202 -0.32928300
C   1.43201900  1.29171801 -0.66257501
C   1.34830105  2.52776599 -1.27557099
H   2.25829196  3.05262089 -1.53318405

```


C	0.08550300	3.09054303	-1.55077100
H	-0.00464100	4.05644894	-2.02677488
C	-1.05746496	2.38921595	-1.21336496
H	-2.04166603	2.78834391	-1.41927898
C	0.22159000	0.61295801	-0.32875201
C	0.22150099	-0.61807400	0.32077399
C	-3.54384398	-2.29020095	-1.58798206
C	-1.81250799	-1.16932595	-2.69800210
C	-3.61610007	-3.23112893	-2.61018491
C	-4.38954115	-2.30756307	-0.38584301
C	-1.84551096	-2.07511306	-3.74576092
H	-1.12057197	-0.34021699	-2.68087411
C	-2.76051998	-3.12164807	-3.69916511
H	-4.32646990	-4.04272223	-2.55686212
C	-5.40246916	-3.23344588	-0.15640900
H	-1.16139102	-1.95692801	-4.57430887
H	-2.80751801	-3.84849811	-4.49932480
C	-4.85862589	-1.24214399	1.64297903
C	-6.15024424	-3.15060091	1.01119196
H	-5.60874224	-4.00782490	-0.88023102
C	-5.87581205	-2.13942790	1.92599201
H	-4.60685921	-0.44108400	2.32292199
H	-6.93956900	-3.86603904	1.20029998
H	-6.43600512	-2.03878999	2.84501600
N	-4.12923384	-1.32817900	0.51971900
N	-2.64592695	-1.27200902	-1.65031302
C	-4.37830877	2.31421995	0.39329901
C	-4.86360788	1.24807501	-1.63135099
C	-5.38877583	3.24393010	0.16853000
C	-3.52627110	2.29459310	1.59090400
C	-5.87881088	2.14909911	-1.90958500
H	-4.61898184	0.44518200	-2.31175089
C	-6.14371681	3.16261411	-0.99455303
H	-5.58776188	4.02003479	0.89254701
C	-3.58884501	3.23716903	2.61222911
H	-6.44482183	2.04956007	-2.82515597
H	-6.93119621	3.88104510	-1.17995095
C	-1.79546905	1.16632605	2.69410300
C	-2.72881389	3.12460589	3.69738197
H	-4.29520321	4.05238819	2.56120396
C	-1.81909800	2.07335591	3.74105191
H	-1.10774195	0.33380300	2.67471504
H	-2.76833510	3.85264993	4.49686098
H	-1.13183999	1.95250404	4.56660700
N	-4.12729979	1.33257902	-0.51247799
N	-2.63306403	1.27211106	1.65007806
C	8.66514397	-2.37817693	1.27529299
C	8.66556931	2.37738204	-1.27253902
C	6.24677277	-1.26936102	0.66804898
C	6.28148699	-2.50956702	1.32703805
H	5.34879589	-2.99540401	1.57980895
C	6.28190899	2.50687194	-1.32861495
H	5.34928799	2.99197412	-1.58304906
C	7.50129080	-3.07310200	1.63523805
C	7.50182009	3.07139111	-1.63458502
H	7.57043409	-4.02667284	2.14280295
H	9.64054489	-2.79656506	1.50634003
H	7.57112598	4.02503395	-2.14199090
H	9.64105511	2.79657197	-1.50176799
N	8.66270733	-1.20738196	0.65258002
N	8.66293240	1.20657802	-0.64984697

S5.2. Frequencies

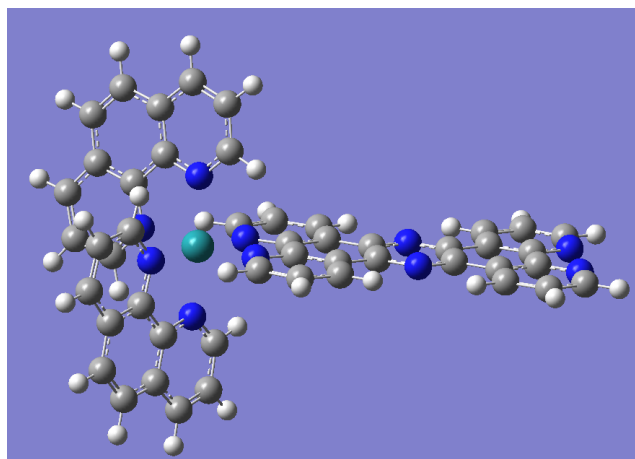
Mode	IR frequency	IR intensity	Raman intensity
1	-12.65020000	0.05070000	0.00000000
2	-10.41660000	0.01630000	0.00000000
3	24.22430000	0.04220000	0.00000000
4	27.30640000	0.49420000	0.00000000
5	33.08520000	3.39380000	0.00000000
6	34.24580000	1.19100000	0.00000000
7	43.67760000	0.37560000	0.00000000
8	44.79560000	0.56820000	0.00000000
9	69.55020000	0.03910000	0.00000000
10	77.02780000	1.27660000	0.00000000
11	82.22150000	6.39980000	0.00000000
12	87.31240000	10.12990000	0.00000000
13	89.46530000	4.62620000	0.00000000
14	98.02020000	0.08930000	0.00000000
15	109.83390000	0.16950000	0.00000000
16	116.70180000	0.22660000	0.00000000
17	127.43690000	8.96180000	0.00000000
18	131.82140000	2.44140000	0.00000000
19	154.94720000	7.49550000	0.00000000
20	163.30090000	4.73330000	0.00000000
21	170.66960000	2.84020000	0.00000000
22	180.69070000	0.34370000	0.00000000
23	193.03350000	3.27930000	0.00000000
24	193.46580000	6.27010000	0.00000000
25	216.23710000	14.62130000	0.00000000
26	221.75990000	2.69360000	0.00000000
27	222.26430000	0.08010000	0.00000000
28	230.07200000	4.16150000	0.00000000
29	240.82900000	1.53470000	0.00000000
30	242.19230000	10.86490000	0.00000000
31	261.56770000	1.67280000	0.00000000
32	266.21630000	22.46620000	0.00000000
33	273.27420000	29.83570000	0.00000000
34	277.90230000	2.85520000	0.00000000
35	288.87150000	3.73450000	0.00000000
36	312.08360000	132.79620000	0.00000000
37	318.29310000	23.10980000	0.00000000
38	326.12470000	22.40120000	0.00000000
39	365.36620000	2.45470000	0.00000000
40	372.08060000	3.98080000	0.00000000
41	378.26290000	1.87940000	0.00000000
42	379.33500000	0.60240000	0.00000000
43	411.86690000	12.67470000	0.00000000
44	414.48760000	107.06840000	0.00000000
45	430.55790000	6.99050000	0.00000000
46	430.56250000	11.13430000	0.00000000
47	437.39250000	16.96640000	0.00000000
48	440.00710000	9.95780000	0.00000000
49	441.23910000	8.76120000	0.00000000
50	442.00230000	13.47730000	0.00000000
51	447.96120000	1.42090000	0.00000000
52	449.47050000	20.82670000	0.00000000
53	451.06310000	7.38180000	0.00000000
54	458.44040000	29.94160000	0.00000000
55	470.26020000	4.57730000	0.00000000
56	473.41210000	8.75720000	0.00000000
57	483.46220000	0.68050000	0.00000000
58	495.30430000	0.89070000	0.00000000
59	509.09890000	38.58730000	0.00000000
60	528.54330000	0.17140000	0.00000000

61	537.80780000	43.01760000	0.00000000
62	561.05080000	0.39110000	0.00000000
63	561.37830000	0.07810000	0.00000000
64	569.47450000	7.98800000	0.00000000
65	575.61100000	9.25500000	0.00000000
66	578.06950000	0.50640000	0.00000000
67	594.44990000	4.54010000	0.00000000
68	634.72840000	16.80040000	0.00000000
69	647.05320000	131.35740000	0.00000000
70	648.98550000	1.88630000	0.00000000
71	663.99480000	6.10700000	0.00000000
72	664.14290000	1.67190000	0.00000000
73	665.77490000	13.65010000	0.00000000
74	670.26310000	15.27650000	0.00000000
75	672.81060000	0.45530000	0.00000000
76	683.68880000	10.59910000	0.00000000
77	685.27540000	2.85560000	0.00000000
78	698.17410000	67.85000000	0.00000000
79	706.24220000	141.08970000	0.00000000
80	706.78750000	0.22680000	0.00000000
81	712.38240000	12.26300000	0.00000000
82	739.66590000	78.31500000	0.00000000
83	747.58040000	35.76560000	0.00000000
84	750.54390000	43.22700000	0.00000000
85	755.62880000	10.95730000	0.00000000
86	758.89690000	0.09870000	0.00000000
87	759.44850000	2.48420000	0.00000000
88	761.83680000	10.99530000	0.00000000
89	767.35750000	57.11890000	0.00000000
90	777.57000000	140.70610000	0.00000000
91	779.22920000	99.65120000	0.00000000
92	779.71340000	114.96530000	0.00000000
93	780.61310000	0.35420000	0.00000000
94	784.04250000	3.89900000	0.00000000
95	784.50460000	4.48780000	0.00000000
96	816.54550000	276.13720000	0.00000000
97	819.82450000	0.27800000	0.00000000
98	821.98410000	0.19620000	0.00000000
99	822.81330000	0.12300000	0.00000000
100	835.21690000	36.08020000	0.00000000
101	836.44380000	0.85450000	0.00000000
102	860.75090000	4.17730000	0.00000000
103	861.22560000	173.68300000	0.00000000
104	909.48890000	0.34090000	0.00000000
105	910.01500000	0.27480000	0.00000000
106	913.69100000	1.29940000	0.00000000
107	914.35590000	0.64320000	0.00000000
108	923.17670000	81.18910000	0.00000000
109	958.91400000	3.84010000	0.00000000
110	960.20670000	21.62530000	0.00000000
111	970.61320000	6.89050000	0.00000000
112	971.64440000	26.34270000	0.00000000
113	980.52440000	0.16660000	0.00000000
114	981.83020000	0.01610000	0.00000000
115	996.22250000	0.09150000	0.00000000
116	996.57910000	0.09750000	0.00000000
117	997.96400000	0.77790000	0.00000000
118	998.59040000	0.21660000	0.00000000
119	1015.20180000	139.98770000	0.00000000
120	1018.08420000	0.83740000	0.00000000
121	1019.19590000	0.16380000	0.00000000
122	1032.40850000	3.74290000	0.00000000
123	1032.60970000	4.68650000	0.00000000
124	1034.83190000	1967.58050000	0.00000000

125	1035.96160000	0.17890000	0.00000000
126	1036.02990000	1.75510000	0.00000000
127	1041.72170000	18.69720000	0.00000000
128	1045.87960000	101.95770000	0.00000000
129	1049.78750000	20.17220000	0.00000000
130	1050.08390000	1932.67190000	0.00000000
131	1054.89810000	25.47170000	0.00000000
132	1057.51470000	49.78820000	0.00000000
133	1057.91950000	11.85020000	0.00000000
134	1068.87970000	10.76560000	0.00000000
135	1070.19220000	0.89280000	0.00000000
136	1078.58130000	18.96000000	0.00000000
137	1087.95340000	80.82300000	0.00000000
138	1088.86380000	49.82130000	0.00000000
139	1089.30820000	33.41100000	0.00000000
140	1094.98100000	17.49030000	0.00000000
141	1095.84390000	12.80220000	0.00000000
142	1103.26350000	1.63240000	0.00000000
143	1107.63640000	865.70830000	0.00000000
144	1132.82930000	607.03900000	0.00000000
145	1134.04240000	32.88590000	0.00000000
146	1135.89520000	127.74050000	0.00000000
147	1142.81890000	2655.16580000	0.00000000
148	1143.66840000	1.67900000	0.00000000
149	1148.88640000	95.73830000	0.00000000
150	1150.72300000	3.06400000	0.00000000
151	1151.25500000	12.16450000	0.00000000
152	1173.22860000	1587.51920000	0.00000000
153	1184.52790000	4.02050000	0.00000000
154	1184.78200000	6.40930000	0.00000000
155	1196.40400000	26.91210000	0.00000000
156	1196.50440000	28.24880000	0.00000000
157	1197.22640000	4.33510000	0.00000000
158	1197.56190000	119.35270000	0.00000000
159	1236.62890000	54.88360000	0.00000000
160	1239.68690000	2412.54090000	0.00000000
161	1251.04340000	0.64090000	0.00000000
162	1283.51780000	387.70750000	0.00000000
163	1289.65480000	51.82910000	0.00000000
164	1290.71180000	43.12070000	0.00000000
165	1296.92800000	10.05540000	0.00000000
166	1300.81400000	9.38350000	0.00000000
167	1307.14310000	362.49460000	0.00000000
168	1309.13650000	11.39930000	0.00000000
169	1316.67460000	2.13090000	0.00000000
170	1317.82260000	2.87860000	0.00000000
171	1321.06550000	1.20310000	0.00000000
172	1328.72470000	0.02910000	0.00000000
173	1344.38230000	24.66400000	0.00000000
174	1345.03980000	37.60470000	0.00000000
175	1347.40400000	5.83820000	0.00000000
176	1347.61960000	1.91590000	0.00000000
177	1352.49890000	202.65320000	0.00000000
178	1364.10120000	75.80420000	0.00000000
179	1384.98880000	18.28600000	0.00000000
180	1395.78100000	113.56750000	0.00000000
181	1417.31650000	237.44670000	0.00000000
182	1430.83440000	1560.84310000	0.00000000
183	1432.82370000	189.48050000	0.00000000
184	1434.60520000	359.99970000	0.00000000
185	1462.96300000	1.33590000	0.00000000
186	1463.42620000	8.70810000	0.00000000
187	1468.26950000	266.18190000	0.00000000
188	1481.38110000	146.22990000	0.00000000

189	1482.44470000	60.51350000	0.00000000
190	1485.74430000	37.65160000	0.00000000
191	1492.58560000	162.51530000	0.00000000
192	1500.33660000	69.00490000	0.00000000
193	1501.90260000	135.21310000	0.00000000
194	1504.93560000	13.75640000	0.00000000
195	1515.23160000	280.54810000	0.00000000
196	1526.04690000	44.81510000	0.00000000
197	1526.43470000	22.07560000	0.00000000
198	1529.11830000	2.63560000	0.00000000
199	1531.07790000	704.08600000	0.00000000
200	1557.27410000	3.90670000	0.00000000
201	1558.25780000	133.65920000	0.00000000
202	1596.68170000	27.85800000	0.00000000
203	1602.09760000	15.78770000	0.00000000
204	1602.60600000	6.84910000	0.00000000
205	1605.98960000	107.93770000	0.00000000
206	1607.77940000	52.47870000	0.00000000
207	1611.13180000	14.80290000	0.00000000
208	1611.30390000	6.99000000	0.00000000
209	1623.79360000	25.89770000	0.00000000
210	1632.36660000	81.35760000	0.00000000
211	1636.91930000	16.60170000	0.00000000
212	1641.76670000	31.10060000	0.00000000
213	1641.97690000	99.68980000	0.00000000
214	1650.38230000	40.26640000	0.00000000
215	1651.42730000	26.31880000	0.00000000
216	3149.49750000	31.57930000	0.00000000
217	3149.96220000	69.43520000	0.00000000
218	3196.46870000	24.43310000	0.00000000
219	3196.52100000	21.11090000	0.00000000
220	3203.32580000	4.30000000	0.00000000
221	3203.49580000	14.43970000	0.00000000
222	3207.32410000	3.60450000	0.00000000
223	3207.41330000	3.60080000	0.00000000
224	3208.71500000	2.80620000	0.00000000
225	3208.77410000	2.13110000	0.00000000
226	3209.64800000	23.93640000	0.00000000
227	3209.77880000	41.87770000	0.00000000
228	3213.35830000	23.66040000	0.00000000
229	3213.47790000	3.86460000	0.00000000
230	3219.66610000	0.21940000	0.00000000
231	3219.81500000	0.16700000	0.00000000
232	3222.17380000	0.42370000	0.00000000
233	3222.28970000	0.35440000	0.00000000
234	3223.03220000	14.79750000	0.00000000
235	3223.18630000	0.79700000	0.00000000
236	3225.31490000	0.42940000	0.00000000
237	3225.74730000	0.30530000	0.00000000
238	3232.19880000	7.47720000	0.00000000
239	3232.44500000	6.94670000	0.00000000
240	3235.92380000	3.65090000	0.00000000
241	3236.14560000	1.86730000	0.00000000
242	3237.39460000	9.49480000	0.00000000
243	3237.75300000	5.41910000	0.00000000

S6. CALCULATIONS ON 2²⁺ (³A)



```

Route      : # opt freq b3lyp/genecp scrf=(solvent=acetonitrile) geom=connectivity
            : empiricaldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1cc2c(c3c(cccn3)c4c2nc5c6ccc[n+]7c6c8c(c5n4)ccc[n+]8[Ru]792([n+]
            : 3cccc4c3c3[n+]9cccc3cc4)[n+]3cccc4c3c3[n+]2cccc3cc4)nc1
Formula    : C48H28N10Ru2+,3
Charge     : 2
Multiplicity : 3
Energy     : -2489.14885334 a.u.
Gibbs Energy : -2488.56454800 a.u.
Number of imaginary frequencies : 1

```

S6.1. Cartesian Co-ordinates (XYZ format)

87

```

Ru  2.27003503 -0.00000700  0.00001200
N   0.69912100  1.02026701  0.86175102
N  -4.15374184  1.09169400  0.86694402
N  -4.15373182 -1.09177005 -0.86690098
N   0.69913399 -1.02034700 -0.86165100
C   0.74440098  2.08826590  1.67664504
H   1.72944105  2.43542790  1.95869994
C  -0.39803901  2.70475197  2.15294290
H  -0.30676499  3.55077696  2.81897712
C  -1.66200900  2.21361494  1.76657403
H  -2.57101893  2.67558908  2.12734008
C  -1.74770999  1.13176596  0.91062802
C  -3.00823212  0.55910498  0.44642901
C  -5.30383492  0.55529398  0.43892500
C  -7.79168320  0.57800001  0.45269200
C  -7.79167795 -0.57807398 -0.45268601
C  -6.56276512 -1.12694895 -0.88595802
C  -5.30383110 -0.55536902 -0.43889600
C  -3.00822806 -0.55918300 -0.44637299
C  -1.74769795 -1.13185096 -0.91055101
C  -1.66198802 -2.21370697 -1.76648498
H  -2.57099199 -2.67568398 -2.12725997
C  -0.39800900 -2.70484996 -2.15283489

```

H	-0.30673000	-3.55088401	-2.81885695
C	0.74442297	-2.08835912	-1.67653596
H	1.72946703	-2.43552089	-1.95857704
C	-0.53815103	-0.53482002	-0.44466299
C	-0.53815699	0.53473800	0.44475099
C	3.27238798	2.48732591	-1.14282799
C	1.54315400	1.68124795	-2.47614193
C	3.46492505	3.61375403	-1.96528494
C	4.06865883	2.30409002	0.02334500
C	1.67102504	2.77493811	-3.34137106
H	0.80688697	0.90801299	-2.64383006
C	2.62783909	3.73748112	-3.09360790
C	5.07049704	3.23778009	0.35117599
H	1.01273298	2.84517908	-4.19592285
H	2.74091792	4.58777094	-3.75446296
C	4.54785490	0.98347998	1.87418401
C	5.82784414	2.98754501	1.51416194
C	5.56502295	1.86282802	2.26797009
H	4.31597185	0.09892000	2.45108199
H	6.60864019	3.67907906	1.80514002
H	6.12850904	1.64359605	3.16413593
N	3.81573606	1.20121396	0.78470302
N	2.32988000	1.53853297	-1.41134596
C	4.06877804	-2.30400991	-0.02343800
C	4.54775906	-0.98339999	-1.87433195
C	5.07062578	-3.23766208	-0.35134500
C	3.27262092	-2.48726201	1.14280796
C	5.56492281	-1.86271501	-2.26820111
H	4.31579399	-0.09885200	-2.45121193
C	5.82785511	-2.98741508	-1.51440406
C	3.46529007	-3.61365795	1.96527600
H	6.12832117	-1.64347303	-3.16442108
H	6.60864782	-3.67892408	-1.80544698
C	1.54348898	-1.68122005	2.47627807
C	2.62832999	-3.73738503	3.09369206
C	1.67150402	-2.77487302	3.34153104
H	0.80720401	-0.90801299	2.64401388
H	2.74151611	-4.58765078	3.75456095
H	1.01330900	-2.84511304	4.19615793
N	3.81574297	-1.20115304	-0.78478497
N	2.33009291	-1.53850603	1.41138995
C	-8.98078346	2.12565088	1.66215098
C	-8.98076820	-2.12572694	-1.66215301
C	-6.56277418	1.12687397	0.88597500
C	-6.59722519	2.23187995	1.75276005
H	-5.66436100	2.66140699	2.09189010
C	-6.59720898	-2.23195601	-1.75274098
H	-5.66434193	-2.66148400	-2.09186292
C	-7.81675720	2.73935795	2.14719796
C	-7.81673813	-2.73943496	-2.14718890
H	-7.88563681	3.58953309	2.81365609
H	-9.95611668	2.50361609	1.95494497
H	-7.88561106	-3.58961105	-2.81364608
H	-9.95609856	-2.50369501	-1.95495296
N	-8.97863102	1.08205104	0.84405202
N	-8.97862339	-1.08212698	-0.84405500
C	4.48717403	-4.55506182	1.61104095
H	4.63414097	-5.41835213	2.24756789
C	5.25744009	-4.37348223	0.50346398
H	6.02754879	-5.08933878	0.24585199
C	5.25718307	4.37362289	-0.50362903
H	6.02728415	5.08950901	-0.24607500
C	4.48680305	4.55519295	-1.61112797
H	4.63367081	5.41850424	-2.24764991

S6.2. Frequencies

Mode	IR frequency	IR intensity	Raman intensity
1	-9.02590000	0.18970000	0.00000000
2	9.78160000	0.00760000	0.00000000
3	18.90810000	1.29260000	0.00000000
4	23.71090000	0.01270000	0.00000000
5	30.37110000	0.84810000	0.00000000
6	36.33150000	1.01680000	0.00000000
7	41.53410000	0.60860000	0.00000000
8	41.66500000	0.06700000	0.00000000
9	65.90120000	0.04030000	0.00000000
10	71.87480000	2.18850000	0.00000000
11	76.81770000	8.06530000	0.00000000
12	86.06520000	13.31720000	0.00000000
13	90.11110000	3.20750000	0.00000000
14	102.21570000	0.00470000	0.00000000
15	124.66590000	5.78430000	0.00000000
16	129.08800000	2.66600000	0.00000000
17	157.17290000	7.59480000	0.00000000
18	160.39900000	3.34570000	0.00000000
19	163.52980000	0.94300000	0.00000000
20	170.23550000	1.12420000	0.00000000
21	178.09190000	0.46170000	0.00000000
22	184.90460000	1.34870000	0.00000000
23	191.72320000	4.00200000	0.00000000
24	192.95300000	1.18380000	0.00000000
25	217.25980000	12.74170000	0.00000000
26	218.91660000	0.00030000	0.00000000
27	224.33660000	4.38990000	0.00000000
28	228.84440000	12.49700000	0.00000000
29	230.66950000	5.46070000	0.00000000
30	239.07800000	4.27640000	0.00000000
31	268.24800000	14.45270000	0.00000000
32	268.78830000	54.44790000	0.00000000
33	273.00740000	33.36510000	0.00000000
34	278.79450000	3.34370000	0.00000000
35	282.04800000	0.06610000	0.00000000
36	288.04810000	58.40630000	0.00000000
37	289.39180000	0.81210000	0.00000000
38	317.50200000	8.88290000	0.00000000
39	325.83210000	53.51660000	0.00000000
40	327.59890000	12.04990000	0.00000000
41	366.83680000	2.23210000	0.00000000
42	377.53750000	2.45810000	0.00000000
43	410.15230000	8.16710000	0.00000000
44	414.63270000	105.69840000	0.00000000
45	431.52590000	3.86540000	0.00000000
46	433.86580000	26.38320000	0.00000000
47	437.83080000	5.95080000	0.00000000
48	439.41600000	7.31310000	0.00000000
49	442.75860000	5.26520000	0.00000000
50	443.86870000	16.67490000	0.00000000
51	444.99870000	16.87570000	0.00000000
52	449.30950000	18.58960000	0.00000000
53	451.63820000	7.27140000	0.00000000
54	456.85070000	26.86630000	0.00000000
55	468.46130000	2.22770000	0.00000000
56	469.69780000	1.85020000	0.00000000
57	501.87010000	1.71810000	0.00000000
58	503.58020000	0.05300000	0.00000000
59	509.59030000	31.89650000	0.00000000
60	518.39240000	4.37810000	0.00000000

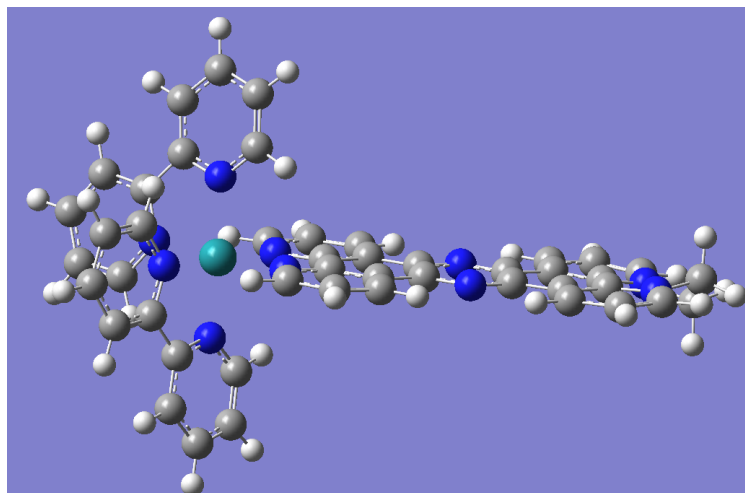
61	518.82160000	1.30130000	0.00000000
62	525.73400000	3.25890000	0.00000000
63	528.76510000	0.93240000	0.00000000
64	533.85280000	23.56760000	0.00000000
65	536.54220000	9.38970000	0.00000000
66	555.69740000	0.13090000	0.00000000
67	559.02880000	0.13700000	0.00000000
68	569.47650000	5.81530000	0.00000000
69	575.31670000	0.66240000	0.00000000
70	575.84740000	0.99440000	0.00000000
71	576.25060000	8.62750000	0.00000000
72	578.06370000	0.49240000	0.00000000
73	594.25280000	5.09550000	0.00000000
74	625.44630000	1.23270000	0.00000000
75	629.22930000	0.03080000	0.00000000
76	635.70050000	16.36820000	0.00000000
77	647.33850000	133.45490000	0.00000000
78	649.52790000	2.46900000	0.00000000
79	672.37930000	4.86370000	0.00000000
80	673.62750000	5.15460000	0.00000000
81	674.92410000	14.09920000	0.00000000
82	696.72630000	70.45630000	0.00000000
83	706.24810000	141.19330000	0.00000000
84	706.88830000	1.52820000	0.00000000
85	712.74720000	5.41650000	0.00000000
86	735.93260000	68.69030000	0.00000000
87	739.18290000	74.76890000	0.00000000
88	740.43630000	52.19640000	0.00000000
89	741.81400000	22.37510000	0.00000000
90	742.79280000	37.98820000	0.00000000
91	754.91070000	9.77980000	0.00000000
92	757.33920000	0.68790000	0.00000000
93	759.20560000	11.05880000	0.00000000
94	762.46130000	8.32390000	0.00000000
95	766.95360000	54.03440000	0.00000000
96	777.11220000	97.75320000	0.00000000
97	780.01940000	17.74670000	0.00000000
98	785.77100000	13.99670000	0.00000000
99	786.12440000	5.49340000	0.00000000
100	810.71630000	1.48740000	0.00000000
101	811.62810000	0.22320000	0.00000000
102	816.60780000	282.29570000	0.00000000
103	822.52430000	0.07340000	0.00000000
104	835.22660000	35.52380000	0.00000000
105	836.64580000	0.55450000	0.00000000
106	851.17960000	0.42850000	0.00000000
107	852.91430000	1.22320000	0.00000000
108	861.12800000	75.34130000	0.00000000
109	861.74000000	108.11550000	0.00000000
110	864.90830000	115.55060000	0.00000000
111	865.02810000	80.91200000	0.00000000
112	896.88200000	17.93360000	0.00000000
113	899.66930000	8.17930000	0.00000000
114	923.29750000	85.88660000	0.00000000
115	937.56380000	3.51460000	0.00000000
116	940.48750000	5.59450000	0.00000000
117	955.84490000	2.52960000	0.00000000
118	956.77190000	28.57380000	0.00000000
119	965.27320000	1.64120000	0.00000000
120	966.12880000	18.78480000	0.00000000
121	975.91980000	0.46850000	0.00000000
122	976.13660000	0.75320000	0.00000000
123	980.06070000	0.19860000	0.00000000
124	981.38150000	0.00090000	0.00000000

125	982.03300000	0.29640000	0.00000000
126	982.43380000	4.59180000	0.00000000
127	1000.15010000	0.00320000	0.00000000
128	1000.20220000	0.01910000	0.00000000
129	1014.10190000	151.94750000	0.00000000
130	1017.40240000	0.72920000	0.00000000
131	1018.54030000	0.07350000	0.00000000
132	1022.58700000	2.29140000	0.00000000
133	1022.76720000	0.08010000	0.00000000
134	1024.92250000	1.34790000	0.00000000
135	1025.13240000	0.08860000	0.00000000
136	1035.35860000	1855.00620000	0.00000000
137	1050.04980000	2118.72730000	0.00000000
138	1052.89440000	3.16970000	0.00000000
139	1058.01850000	9.18630000	0.00000000
140	1060.66050000	0.41630000	0.00000000
141	1062.56460000	0.70760000	0.00000000
142	1078.77280000	20.71410000	0.00000000
143	1086.34410000	0.84330000	0.00000000
144	1087.36800000	0.84210000	0.00000000
145	1089.12950000	106.35080000	0.00000000
146	1103.26740000	1.49560000	0.00000000
147	1107.65940000	926.30720000	0.00000000
148	1119.18950000	5.11090000	0.00000000
149	1119.86000000	12.08040000	0.00000000
150	1129.34130000	37.13190000	0.00000000
151	1131.35550000	610.84470000	0.00000000
152	1135.62450000	133.99960000	0.00000000
153	1142.91530000	2644.53000000	0.00000000
154	1143.60440000	1.22760000	0.00000000
155	1149.50470000	115.43510000	0.00000000
156	1173.57260000	1604.25370000	0.00000000
157	1174.66880000	14.08260000	0.00000000
158	1175.13010000	33.93430000	0.00000000
159	1175.44110000	14.82050000	0.00000000
160	1175.44610000	10.47210000	0.00000000
161	1195.46960000	139.82470000	0.00000000
162	1196.67010000	24.41140000	0.00000000
163	1232.38410000	15.32430000	0.00000000
164	1236.41390000	496.11320000	0.00000000
165	1237.15560000	36.64820000	0.00000000
166	1238.78700000	495.28810000	0.00000000
167	1238.98270000	1.59150000	0.00000000
168	1242.16980000	1376.26200000	0.00000000
169	1250.96250000	2.38240000	0.00000000
170	1252.00440000	35.31270000	0.00000000
171	1252.21800000	13.48110000	0.00000000
172	1283.68410000	408.64040000	0.00000000
173	1288.09000000	2.98810000	0.00000000
174	1288.29160000	3.48380000	0.00000000
175	1306.58710000	390.76430000	0.00000000
176	1309.08030000	8.20570000	0.00000000
177	1321.13830000	0.72700000	0.00000000
178	1328.82210000	0.00060000	0.00000000
179	1343.07580000	8.82420000	0.00000000
180	1343.10040000	0.26540000	0.00000000
181	1349.50330000	4.62320000	0.00000000
182	1350.72070000	32.48930000	0.00000000
183	1353.09810000	178.89250000	0.00000000
184	1364.26760000	77.75010000	0.00000000
185	1375.77960000	18.18720000	0.00000000
186	1377.70660000	11.76690000	0.00000000
187	1384.58060000	18.61330000	0.00000000
188	1395.84170000	119.74530000	0.00000000

189	1417.67300000	232.51820000	0.00000000
190	1431.01430000	1441.88120000	0.00000000
191	1432.35560000	220.24870000	0.00000000
192	1434.54200000	477.27510000	0.00000000
193	1443.46210000	13.63930000	0.00000000
194	1444.31800000	7.74230000	0.00000000
195	1455.83480000	57.47420000	0.00000000
196	1455.97080000	0.02490000	0.00000000
197	1459.72480000	118.19280000	0.00000000
198	1462.00620000	61.41880000	0.00000000
199	1467.99220000	203.90230000	0.00000000
200	1485.25870000	11.60360000	0.00000000
201	1485.54570000	6.92510000	0.00000000
202	1485.77530000	34.87240000	0.00000000
203	1492.14290000	173.37580000	0.00000000
204	1500.19890000	100.39360000	0.00000000
205	1514.68660000	281.71010000	0.00000000
206	1528.63180000	31.16550000	0.00000000
207	1529.10550000	2.94900000	0.00000000
208	1529.81200000	4.13450000	0.00000000
209	1531.02310000	682.68560000	0.00000000
210	1554.87540000	148.98560000	0.00000000
211	1555.22360000	53.62410000	0.00000000
212	1557.06920000	9.65670000	0.00000000
213	1558.68860000	113.72110000	0.00000000
214	1596.58390000	27.77120000	0.00000000
215	1606.05210000	110.26800000	0.00000000
216	1607.75620000	45.94350000	0.00000000
217	1620.45020000	11.11150000	0.00000000
218	1620.84190000	28.30530000	0.00000000
219	1621.45770000	46.87300000	0.00000000
220	1623.00160000	5.52220000	0.00000000
221	1624.10280000	26.39520000	0.00000000
222	1631.46130000	61.93030000	0.00000000
223	1635.90280000	0.85230000	0.00000000
224	1635.92280000	18.55260000	0.00000000
225	1637.09110000	16.74080000	0.00000000
226	1664.43350000	21.65430000	0.00000000
227	1664.58830000	1.73900000	0.00000000
228	3149.43040000	31.39050000	0.00000000
229	3149.89300000	69.13420000	0.00000000
230	3191.95650000	0.02650000	0.00000000
231	3191.95870000	0.02600000	0.00000000
232	3196.83190000	25.09970000	0.00000000
233	3196.88280000	22.64340000	0.00000000
234	3198.76620000	1.43980000	0.00000000
235	3198.77070000	1.53900000	0.00000000
236	3202.11840000	4.66280000	0.00000000
237	3202.12730000	0.78520000	0.00000000
238	3203.22110000	1.88950000	0.00000000
239	3203.34260000	16.06460000	0.00000000
240	3206.38510000	15.93550000	0.00000000
241	3206.40890000	8.98410000	0.00000000
242	3209.79860000	19.74800000	0.00000000
243	3209.87390000	45.51090000	0.00000000
244	3214.41250000	19.59110000	0.00000000
245	3214.52140000	5.33580000	0.00000000
246	3216.83010000	0.00970000	0.00000000
247	3216.86530000	0.05150000	0.00000000
248	3218.49510000	0.17070000	0.00000000
249	3218.57600000	1.01840000	0.00000000
250	3223.21110000	14.58700000	0.00000000
251	3223.36530000	0.14000000	0.00000000
252	3228.24170000	3.33340000	0.00000000

253	3228.25810000	6.99280000	0.00000000
254	3229.21030000	8.83020000	0.00000000
255	3229.43670000	1.55760000	0.00000000

S7. CALCULATIONS ON 3^{4+} (3A)



```

Route      : # opt freq b3lyp/genecp scrf=(solvent=acetonitrile) geom=connectivity
            : empiricaldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1cc[n+]2c(c1)-c3cccc[n+]3[Ru]245([n+]6cccc6-c7[n+]4cccc7)[n+]8cccc9c8c1[n+]
            : 5cccc1c1c9nc2c3ccc[n+]4c3c3c(c2n1)ccc[n+]3CC4
Formula    : C46H32N10Ru4+,3
Charge     : 4
Multiplicity : 3
Energy     : -2414.97348845
Gibbs Energy : -2414.34979500
Number of imaginary frequencies : 1

```

a.u.

a.u.

S7.1. Cartesian Co-ordinates (XYZ format)

89

```

Ru -2.96992993 -0.00003200 -0.00007200
N -1.34495401 1.19568503 -0.59103501
N 3.47022009 1.26329994 -0.59171999
N 3.47016907 -1.26433098 0.58996499
N -1.34496498 -1.19654596 0.58931100
C -1.40471399 2.40711498 -1.15058696
H -2.38742805 2.80683494 -1.35434496
C -0.24978800 3.12280989 -1.47069395
H -0.34571099 4.09808302 -1.92653501
C 0.99087900 2.57516694 -1.20388603
H 1.90378797 3.10361004 -1.44159698
C 1.06851995 1.30551696 -0.61058497
C 2.32523108 0.64275301 -0.29942399
C 4.61267900 0.64455801 -0.30585599
C 7.08868599 0.61442602 -0.33668599
C 7.08863306 -0.61479402 0.33670700
C 5.87210321 -1.29763103 0.63951099
C 4.61265087 -0.64541602 0.30458099
C 2.32520890 -0.64390802 0.29729500
C 1.06848097 -1.30669606 0.60831499
C 0.99080497 -2.57641912 1.20145297
H 1.90370202 -3.10497904 1.43895197

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C	-0.24987400	-3.12397099	1.46839404
H	-0.34582400	-4.09930086	1.92410696
C	-1.40477300	-2.40804291	1.14871204
H	-2.38749194	-2.80760288	1.35274804
C	-0.13125899	-0.64766800	0.31022200
C	-0.13124600	0.64664298	-0.31224599
C	-3.94590902	2.30086207	1.55345500
C	-2.22298694	1.20535004	2.70276308
C	-4.04244614	3.25058293	2.56449294
C	-4.77421093	2.29591489	0.34129199
C	-2.28128910	2.12055707	3.74065804
H	-1.52591205	0.38054201	2.71605706
C	-3.20338798	3.15920401	3.66790700
H	-4.76007223	4.05423021	2.49219298
C	-5.78790617	3.21085191	0.08079100
H	-1.61180103	2.01415396	4.58247185
H	-3.27002311	3.89317608	4.45994997
C	-5.21385098	1.18769896	-1.67668796
C	-6.52053213	3.10154891	-1.09458196
H	-6.00724602	3.99727511	0.78731102
C	-6.23062897	2.07504606	-1.98703802
H	-4.95237684	0.37578201	-2.33865809
H	-7.31136084	3.80874705	-1.30646706
H	-6.77927685	1.95347202	-2.91029096
N	-4.49843884	1.30083096	-0.54520899
N	-3.03918099	1.29076505	1.63947296
C	-4.77635384	-2.29463696	-0.33956400
C	-5.21306705	-1.18611395	1.67887294
C	-5.79046011	-3.20882106	-0.07802100
C	-3.94929790	-2.30020404	-1.55257297
C	-6.23019981	-2.07268810	1.99026203
H	-4.95032692	-0.37438101	2.34056807
C	-6.52179718	-3.09896803	1.09810400
H	-6.01111221	-3.99508691	-0.78430301
C	-4.04765415	-3.24981499	-2.56353903
H	-6.77781296	-1.95069301	2.91407299
H	-7.31294823	-3.80556202	1.31080496
C	-2.22665000	-1.20608497	-2.70361710
C	-3.20963693	-3.15911293	-3.66779804
H	-4.76589584	-4.05284977	-2.49054289
C	-2.28674293	-2.12123704	-3.74145794
H	-1.52889705	-0.38185701	-2.71759796
H	-3.27769208	-3.89301300	-4.45978689
H	-1.61801302	-2.01538110	-4.58394623
N	-4.49891806	-1.29977000	0.54665601
N	-3.04182506	-1.29084802	-1.63949299
C	8.30780792	2.42495704	-1.32132602
C	8.30759335	-2.42502999	1.32209003
C	5.87217808	1.29701602	-0.64013600
C	5.91747999	2.53975511	-1.24406803
H	4.98902702	3.04754090	-1.46422100
C	5.91733313	-2.54033303	1.24352598
H	4.98886585	-3.04829407	1.46321905
C	7.15456390	3.12513089	-1.56696200
C	7.15436220	-3.12543797	1.56711805
H	7.21343994	4.10173512	-2.02363300
H	9.28695393	2.79848909	-1.58588803
H	7.21319199	-4.10200787	2.02386808
H	9.28667164	-2.79833698	1.58722103
N	8.28332615	1.20157397	-0.74129701
N	8.28317165	-1.20167196	0.74200600
C	9.50543594	-0.38964000	0.65110600
H	10.36735916	-1.05090702	0.68936199
H	9.53718376	0.28816801	1.50680602

C	9.50571632	0.38981101	-0.64970601
H	9.53809071	-0.28799900	-1.50538003
H	10.36752033	1.05126095	-0.68748099

S7.2. Frequencies

Mode	IR frequency	IR intensity	Raman intensity
1	-17.38780000	0.88330000	0.00000000
2	9.24170000	0.01230000	0.00000000
3	28.34500000	0.09820000	0.00000000
4	29.14190000	1.19340000	0.00000000
5	33.57590000	3.98170000	0.00000000
6	34.62320000	1.63380000	0.00000000
7	44.30450000	1.44170000	0.00000000
8	45.46840000	0.42100000	0.00000000
9	62.03400000	0.53160000	0.00000000
10	73.59260000	2.35180000	0.00000000
11	84.23700000	3.50010000	0.00000000
12	85.08630000	3.04450000	0.00000000
13	87.15180000	4.04290000	0.00000000
14	113.36890000	0.71790000	0.00000000
15	114.21310000	0.80060000	0.00000000
16	123.02600000	0.09450000	0.00000000
17	131.27920000	0.60220000	0.00000000
18	137.92940000	0.62110000	0.00000000
19	155.40540000	5.93840000	0.00000000
20	163.02010000	0.01490000	0.00000000
21	172.56920000	0.09860000	0.00000000
22	180.26090000	8.69390000	0.00000000
23	184.21690000	0.84880000	0.00000000
24	196.01820000	2.44030000	0.00000000
25	196.87550000	0.67980000	0.00000000
26	210.90920000	0.51090000	0.00000000
27	220.93410000	1.23920000	0.00000000
28	229.34060000	4.21780000	0.00000000
29	233.04130000	2.38070000	0.00000000
30	241.17330000	3.06390000	0.00000000
31	244.34550000	0.92000000	0.00000000
32	253.94700000	2.14170000	0.00000000
33	266.17080000	1.46570000	0.00000000
34	268.39680000	1.30550000	0.00000000
35	288.34960000	3.14720000	0.00000000
36	307.54620000	1.45530000	0.00000000
37	313.38900000	0.41510000	0.00000000
38	336.87140000	21.98750000	0.00000000
39	343.81850000	24.54220000	0.00000000
40	349.38780000	16.82300000	0.00000000
41	373.49890000	9.95550000	0.00000000
42	376.06720000	0.74600000	0.00000000
43	380.01340000	2.78960000	0.00000000
44	393.07330000	41.84180000	0.00000000
45	413.63310000	0.05460000	0.00000000
46	417.86940000	3.11710000	0.00000000
47	429.28840000	12.46950000	0.00000000
48	431.19840000	15.19890000	0.00000000
49	431.56520000	17.21750000	0.00000000
50	439.07500000	1.78090000	0.00000000
51	440.53840000	118.20430000	0.00000000
52	446.10650000	20.68280000	0.00000000
53	452.36600000	25.37520000	0.00000000
54	455.69310000	1.13790000	0.00000000
55	460.09530000	9.38680000	0.00000000
56	470.80340000	9.45000000	0.00000000
57	471.14290000	2.49340000	0.00000000
58	481.50890000	4.16030000	0.00000000
59	485.76380000	0.81820000	0.00000000
60	496.12570000	0.55210000	0.00000000

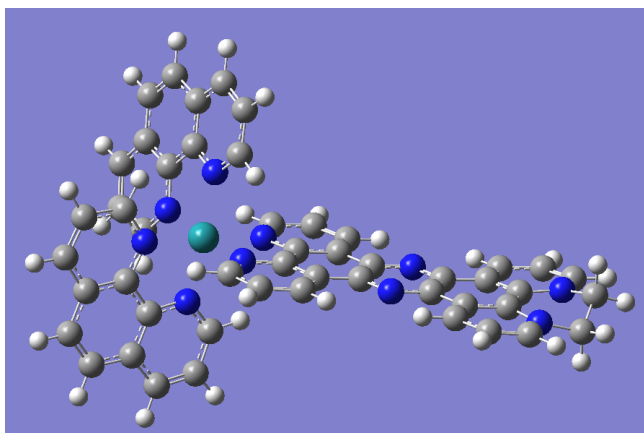
61	502.20910000	11.15500000	0.00000000
62	529.06130000	0.68480000	0.00000000
63	534.63390000	6.00240000	0.00000000
64	540.64490000	8.79460000	0.00000000
65	554.33170000	3.37120000	0.00000000
66	559.47320000	0.47970000	0.00000000
67	559.64800000	0.16880000	0.00000000
68	567.57560000	0.18120000	0.00000000
69	570.77380000	1.22860000	0.00000000
70	574.08250000	2.57460000	0.00000000
71	602.08120000	1.73280000	0.00000000
72	627.92370000	7.44640000	0.00000000
73	661.71310000	2.02360000	0.00000000
74	662.54260000	6.36790000	0.00000000
75	663.40410000	1.45280000	0.00000000
76	667.90950000	16.34080000	0.00000000
77	668.50470000	37.88160000	0.00000000
78	672.71170000	8.01690000	0.00000000
79	676.60350000	5.27110000	0.00000000
80	686.35210000	6.26220000	0.00000000
81	686.46730000	14.27630000	0.00000000
82	694.45960000	65.08740000	0.00000000
83	704.39230000	1.04610000	0.00000000
84	711.24130000	6.86230000	0.00000000
85	743.03950000	8.01440000	0.00000000
86	744.64970000	49.98010000	0.00000000
87	747.94990000	117.83300000	0.00000000
88	750.25750000	44.12970000	0.00000000
89	750.47000000	8.02350000	0.00000000
90	759.36900000	1.06250000	0.00000000
91	760.96120000	4.99620000	0.00000000
92	761.57970000	15.77510000	0.00000000
93	779.22720000	156.94360000	0.00000000
94	781.21160000	112.99170000	0.00000000
95	783.10240000	7.24380000	0.00000000
96	783.75020000	3.47720000	0.00000000
97	788.39370000	21.65850000	0.00000000
98	791.63520000	92.31820000	0.00000000
99	807.70010000	79.69290000	0.00000000
100	813.60950000	0.00050000	0.00000000
101	818.87450000	0.02670000	0.00000000
102	820.33790000	0.72400000	0.00000000
103	827.16450000	14.40980000	0.00000000
104	837.56790000	0.49410000	0.00000000
105	838.17160000	53.56850000	0.00000000
106	838.26390000	4.18570000	0.00000000
107	863.90940000	2.73710000	0.00000000
108	902.90730000	78.45600000	0.00000000
109	912.77460000	0.43870000	0.00000000
110	912.97510000	0.50060000	0.00000000
111	914.73410000	0.47570000	0.00000000
112	914.96440000	0.15980000	0.00000000
113	932.66940000	19.19080000	0.00000000
114	957.71850000	6.98490000	0.00000000
115	958.15720000	14.98000000	0.00000000
116	981.19520000	1.07910000	0.00000000
117	981.88030000	0.10660000	0.00000000
118	989.18180000	1.91370000	0.00000000
119	989.77030000	0.51260000	0.00000000
120	999.42740000	1.10800000	0.00000000
121	999.65830000	0.60100000	0.00000000
122	1000.77580000	1.09520000	0.00000000
123	1001.64400000	4.35380000	0.00000000
124	1003.72880000	85.89020000	0.00000000

125	1011.14780000	47.90210000	0.00000000
126	1031.55620000	134.93730000	0.00000000
127	1033.05890000	2.39260000	0.00000000
128	1033.55830000	0.21210000	0.00000000
129	1036.21660000	0.15010000	0.00000000
130	1036.24160000	0.25340000	0.00000000
131	1039.69420000	0.47560000	0.00000000
132	1039.79360000	0.00630000	0.00000000
133	1041.87080000	21.33800000	0.00000000
134	1045.26430000	73.32760000	0.00000000
135	1053.01530000	60.79450000	0.00000000
136	1057.21170000	58.98050000	0.00000000
137	1065.53490000	3.67100000	0.00000000
138	1070.25830000	7.66990000	0.00000000
139	1071.05130000	138.10850000	0.00000000
140	1074.08360000	878.50630000	0.00000000
141	1082.36210000	304.64240000	0.00000000
142	1091.01990000	9.38080000	0.00000000
143	1091.54620000	48.61510000	0.00000000
144	1092.01030000	59.26210000	0.00000000
145	1093.98900000	23.02610000	0.00000000
146	1095.15180000	15.56760000	0.00000000
147	1097.47890000	9.34270000	0.00000000
148	1108.68160000	27.97640000	0.00000000
149	1123.59570000	8.47710000	0.00000000
150	1135.05100000	37.42080000	0.00000000
151	1136.32690000	11.00840000	0.00000000
152	1140.16310000	5.96160000	0.00000000
153	1144.70500000	38.54720000	0.00000000
154	1151.76560000	0.03960000	0.00000000
155	1151.99570000	2.52420000	0.00000000
156	1162.85090000	217.29480000	0.00000000
157	1163.85750000	8.14880000	0.00000000
158	1185.29450000	11.39790000	0.00000000
159	1185.58280000	13.46680000	0.00000000
160	1191.35860000	33.26380000	0.00000000
161	1195.77240000	215.61690000	0.00000000
162	1197.87200000	16.16260000	0.00000000
163	1198.33180000	5.32410000	0.00000000
164	1211.80580000	1174.86480000	0.00000000
165	1216.71090000	154.62420000	0.00000000
166	1234.47480000	1517.18110000	0.00000000
167	1244.81520000	24.96200000	0.00000000
168	1245.90900000	23.86120000	0.00000000
169	1278.02370000	1.76810000	0.00000000
170	1288.05030000	203.09610000	0.00000000
171	1290.34540000	77.94720000	0.00000000
172	1290.61920000	8.11530000	0.00000000
173	1297.57370000	9.91160000	0.00000000
174	1303.03020000	6.52950000	0.00000000
175	1306.98640000	25.43960000	0.00000000
176	1319.10390000	2.90450000	0.00000000
177	1319.33620000	7.29430000	0.00000000
178	1322.01450000	11.40290000	0.00000000
179	1326.04430000	0.11970000	0.00000000
180	1335.10380000	60.45710000	0.00000000
181	1342.51730000	10.05360000	0.00000000
182	1344.45500000	22.39850000	0.00000000
183	1345.42660000	49.98430000	0.00000000
184	1349.67110000	12.66710000	0.00000000
185	1349.68280000	16.34310000	0.00000000
186	1354.99230000	667.94510000	0.00000000
187	1364.16790000	641.55850000	0.00000000
188	1372.09710000	37.85420000	0.00000000

189	1377.79570000	274.26680000	0.00000000
190	1392.51840000	763.53150000	0.00000000
191	1393.03450000	4.93530000	0.00000000
192	1406.47880000	325.67310000	0.00000000
193	1437.03620000	81.41080000	0.00000000
194	1453.33330000	703.09360000	0.00000000
195	1462.91930000	18.54600000	0.00000000
196	1463.48480000	2.83030000	0.00000000
197	1464.31580000	7.51130000	0.00000000
198	1469.26460000	126.62080000	0.00000000
199	1481.89760000	157.81400000	0.00000000
200	1482.53520000	77.37730000	0.00000000
201	1482.67480000	78.54100000	0.00000000
202	1491.19730000	72.45300000	0.00000000
203	1497.98930000	0.00590000	0.00000000
204	1499.94570000	91.95190000	0.00000000
205	1504.04700000	14.85130000	0.00000000
206	1504.19300000	18.40070000	0.00000000
207	1507.30750000	0.64210000	0.00000000
208	1527.82880000	69.13260000	0.00000000
209	1528.43030000	22.71040000	0.00000000
210	1529.72490000	3.89770000	0.00000000
211	1530.61600000	365.17390000	0.00000000
212	1548.51110000	457.54990000	0.00000000
213	1553.89610000	243.22760000	0.00000000
214	1585.23850000	299.76330000	0.00000000
215	1594.76300000	951.22470000	0.00000000
216	1601.57500000	17.18600000	0.00000000
217	1601.82880000	9.73670000	0.00000000
218	1609.99180000	7.33400000	0.00000000
219	1610.01350000	12.88090000	0.00000000
220	1610.54630000	51.73880000	0.00000000
221	1621.90070000	1.33580000	0.00000000
222	1623.22400000	22.96840000	0.00000000
223	1623.34290000	7.27570000	0.00000000
224	1636.47910000	2.18970000	0.00000000
225	1640.01920000	8.41790000	0.00000000
226	1640.50410000	42.79640000	0.00000000
227	1641.04380000	136.38100000	0.00000000
228	1649.05480000	47.51420000	0.00000000
229	1649.52430000	34.58340000	0.00000000
230	3064.90730000	48.69400000	0.00000000
231	3075.65750000	21.17910000	0.00000000
232	3154.41070000	22.71350000	0.00000000
233	3156.95090000	2.88130000	0.00000000
234	3210.70260000	2.52020000	0.00000000
235	3210.71580000	4.08360000	0.00000000
236	3211.80580000	1.92840000	0.00000000
237	3211.83590000	1.42370000	0.00000000
238	3217.19800000	0.05900000	0.00000000
239	3217.24860000	0.17690000	0.00000000
240	3218.89690000	38.91950000	0.00000000
241	3218.91420000	11.76480000	0.00000000
242	3223.55160000	0.60400000	0.00000000
243	3223.58180000	0.41730000	0.00000000
244	3224.34640000	3.35390000	0.00000000
245	3224.50170000	1.46530000	0.00000000
246	3225.04700000	0.41940000	0.00000000
247	3225.06740000	0.21950000	0.00000000
248	3225.67930000	3.53230000	0.00000000
249	3225.75110000	9.16360000	0.00000000
250	3227.51990000	0.99870000	0.00000000
251	3227.57520000	0.29670000	0.00000000
252	3233.91070000	1.69990000	0.00000000

253	3234.01750000	0.64640000	0.00000000
254	3236.98440000	4.16280000	0.00000000
255	3237.15920000	0.43300000	0.00000000
256	3237.39450000	0.00920000	0.00000000
257	3237.41300000	0.58540000	0.00000000
258	3238.71330000	0.61110000	0.00000000
259	3238.74850000	2.44200000	0.00000000
260	3240.31790000	3.66860000	0.00000000
261	3240.44880000	6.07430000	0.00000000

S8. CALCULATIONS ON 4^{4+} (3A)



```

Route      : # opt freq b3lyp/genecp scrf=(solvent=acetonitrile) geom=connectivity
            : empiricaldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1cc2ccc3ccc[n+]4c3c2[n+](c1)[Ru]456([n+]7cccc8c7c9[n+]5cccc9cc8)[n+]
            : 1cccc2c1c1[n+]6cccc1c1c2nc2c3ccc[n+]4c3c3c(c2n1)ccc[n+]3CC4
Formula    : C50H32N10Ru4+,3
Charge     : 4
Multiplicity : 3
Energy      : -2567.48505113 a.u.
Gibbs Energy : -2566.83527600 a.u.
Number of imaginary frequencies : 1

```

S8.1. Cartesian Co-ordinates (XYZ format)

93

```

Ru  2.63034105 -0.00335600 0.01970500
N   1.02234101 -1.08892798 -0.76593697
N   -3.79363394 -1.14269602 -0.82242799
N   -3.80081010 1.03488505 0.92211002
N   1.01348996 0.99609703 0.89156699
C   1.08857298 -2.15124989 -1.57349300
H   2.07413101 -2.49862695 -1.84843802
C   -0.06358800 -2.77782893 -2.05152607
H   0.03681800 -3.63113999 -2.70724106
C   -1.30710304 -2.29851794 -1.68418002
H   -2.21748304 -2.75990605 -2.04112101
C   -1.39126694 -1.19151604 -0.82518899
C   -2.65037894 -0.61418402 -0.38059899
C   -4.93781996 -0.60202301 -0.41158199
C   -7.41434479 -0.58899403 -0.41424900
C   -7.41623116 0.54612303 0.40767100
C   -6.20200920 1.10238802 0.91130102
C   -4.94141006 0.51068902 0.48183200
C   -2.65423393 0.49458301 0.50433201
C   -1.39994597 1.06911004 0.96456200
C   -1.32505202 2.16783595 1.83491695
H   -2.23906112 2.61729002 2.19777298
C   -0.08558400 2.65409303 2.20606089
H   0.00841600 3.49929309 2.87313795

```

C	1.07110906	2.04901195	1.71161795
H	2.05447412	2.40589809	1.98219800
C	-0.19916700	0.50700498	0.51395500
C	-0.19463100	-0.61573899	-0.38046801
C	3.77801108	-2.44337606	1.11560798
C	2.07754302	-1.71515095	2.53008604
C	4.05584002	-3.56242800	1.92295396
C	4.51432800	-2.22035003	-0.07960500
C	2.29325294	-2.80317712	3.38389802
H	1.31674898	-0.97739398	2.74112797
C	3.27641296	-3.72454691	3.08699107
C	5.54354191	-3.10379696	-0.45536399
H	1.68042898	-2.90173101	4.26876402
H	3.45444012	-4.57094383	3.73813891
C	4.86144114	-0.86028999	-1.93736398
C	6.24175882	-2.80842400	-1.64435601
C	5.90019512	-1.69005895	-2.37640190
H	4.56884003	0.01753300	-2.49562192
H	7.04155588	-3.46010804	-1.97257900
H	6.41937304	-1.43816102	-3.29036689
N	4.18196678	-1.12476897	-0.82273901
N	2.80551410	-1.53714597	1.42846406
C	4.38290501	2.32123804	-0.01137200
C	4.93126917	0.99596602	1.82256103
C	5.38898993	3.25931001	0.28753200
C	3.55379009	2.49799109	-1.15268099
C	5.95316410	1.88176405	2.18422103
H	4.72733307	0.10875800	2.40476108
C	6.18444395	3.01004505	1.42503703
C	3.71482897	3.62509203	-1.98038197
H	6.54657793	1.66297805	3.06076407
H	6.97156906	3.70403910	1.69202006
C	1.79573500	1.67621195	-2.43925095
C	2.84576106	3.74139404	-3.08494091
C	1.89095294	2.77054310	-3.30682206
H	1.06191099	0.89862001	-2.59662008
H	2.93303704	4.59214020	-3.74897289
H	1.21012795	2.83349299	-4.14393806
N	4.16201878	1.21440005	0.75720400
N	2.61149096	1.53994501	-1.39488697
C	-8.63094616	-2.23695898	-1.65396500
C	-8.63773155	2.22263789	1.60353196
C	-6.19593287	-1.16984105	-0.87919700
C	-6.23852777	-2.24416304	-1.74824500
H	-5.30878210	-2.66923904	-2.09930992
C	-6.25015593	2.18011189	1.77578700
H	-5.32344198	2.58777905	2.15429401
C	-7.47478819	-2.77045202	-2.16298294
C	-7.48791313	2.73317599	2.14909911
H	-7.53136396	-3.59780788	-2.85440803
H	-9.61064529	-2.62394595	-1.89593303
H	-7.54955578	3.56353498	2.83648610
H	-9.61629963	2.63094091	1.81233299
N	-8.60956860	-1.19192505	-0.79313201
N	-8.61019516	1.17533004	0.74557602
C	4.73993015	4.57317877	-1.65597904
H	4.86300993	5.43652105	-2.29713011
C	5.54318619	4.39659500	-0.57130998
H	6.31595993	5.11688995	-0.33624899
C	5.81597805	-4.23496723	0.38204700
H	6.60611391	-4.91385078	0.08786900
C	5.10170317	-4.45622921	1.51963103
H	5.31411886	-5.31463909	2.14388394
C	-9.82516193	0.75935102	0.02985300

H	-10.69339943	1.08641696	0.59666401
H	-9.83537102	1.24284196	-0.94944203
C	-9.83860302	-0.75018698	-0.11809300
H	-10.69414997	-1.05912006	-0.71353501
H	-9.89139843	-1.23299897	0.86016703

S8.2. Frequencies

Mode	IR frequency	IR intensity	Raman intensity
1	-7.41960000	0.35290000	0.00000000
2	10.47800000	0.46070000	0.00000000
3	22.85460000	0.14380000	0.00000000
4	25.46340000	1.23630000	0.00000000
5	34.57050000	2.66230000	0.00000000
6	39.72420000	0.33380000	0.00000000
7	46.90240000	0.63190000	0.00000000
8	49.23740000	0.17580000	0.00000000
9	61.60680000	0.14860000	0.00000000
10	74.33870000	3.47100000	0.00000000
11	84.02930000	8.39860000	0.00000000
12	85.91710000	4.75570000	0.00000000
13	94.28960000	2.02230000	0.00000000
14	122.73640000	1.83100000	0.00000000
15	131.53260000	0.48680000	0.00000000
16	137.50290000	0.01270000	0.00000000
17	161.56500000	1.60040000	0.00000000
18	167.14330000	0.65720000	0.00000000
19	171.03090000	8.16860000	0.00000000
20	175.98320000	4.00750000	0.00000000
21	180.69520000	1.23630000	0.00000000
22	182.41400000	5.62160000	0.00000000
23	195.03380000	0.47340000	0.00000000
24	195.84010000	0.86330000	0.00000000
25	197.84870000	0.70790000	0.00000000
26	208.96850000	0.25260000	0.00000000
27	223.06580000	1.65540000	0.00000000
28	228.23480000	0.37830000	0.00000000
29	234.08630000	8.92490000	0.00000000
30	235.94420000	11.56020000	0.00000000
31	243.19090000	0.47270000	0.00000000
32	253.04300000	0.02250000	0.00000000
33	274.46330000	7.89190000	0.00000000
34	282.73950000	2.09920000	0.00000000
35	285.15610000	5.98480000	0.00000000
36	288.04380000	10.02840000	0.00000000
37	288.89810000	6.96460000	0.00000000
38	309.44090000	6.38620000	0.00000000
39	329.97710000	0.17920000	0.00000000
40	338.68720000	1.63460000	0.00000000
41	339.84460000	12.86710000	0.00000000
42	346.64620000	31.22780000	0.00000000
43	377.15610000	0.15170000	0.00000000
44	390.72590000	39.51840000	0.00000000
45	413.81630000	0.29330000	0.00000000
46	418.88170000	5.37880000	0.00000000
47	429.56220000	17.43210000	0.00000000
48	432.18320000	2.59990000	0.00000000
49	439.42120000	5.59650000	0.00000000
50	442.80770000	138.43270000	0.00000000
51	445.09350000	29.31640000	0.00000000
52	447.20710000	2.98010000	0.00000000
53	452.09710000	21.49590000	0.00000000
54	457.65730000	2.45570000	0.00000000
55	459.55080000	3.29700000	0.00000000
56	469.22070000	5.59900000	0.00000000
57	472.12750000	7.37790000	0.00000000
58	480.22740000	0.15340000	0.00000000
59	501.98590000	10.64760000	0.00000000
60	503.52090000	2.66090000	0.00000000

61	506.09110000	1.58680000	0.00000000
62	521.29320000	2.00390000	0.00000000
63	521.45380000	3.10160000	0.00000000
64	526.39770000	2.67140000	0.00000000
65	531.40440000	0.04110000	0.00000000
66	533.03790000	1.31610000	0.00000000
67	535.58440000	3.93000000	0.00000000
68	539.19800000	11.08030000	0.00000000
69	553.89050000	2.19170000	0.00000000
70	554.88140000	1.81080000	0.00000000
71	556.12410000	0.10720000	0.00000000
72	566.96960000	1.28920000	0.00000000
73	570.59890000	0.97440000	0.00000000
74	573.15810000	0.50030000	0.00000000
75	575.73510000	0.53870000	0.00000000
76	577.19050000	0.29190000	0.00000000
77	603.87430000	2.89060000	0.00000000
78	624.59350000	4.97310000	0.00000000
79	626.88400000	1.81370000	0.00000000
80	629.39440000	0.54770000	0.00000000
81	661.68270000	2.35820000	0.00000000
82	668.90350000	37.81700000	0.00000000
83	675.42360000	11.76880000	0.00000000
84	676.94400000	9.73940000	0.00000000
85	678.24500000	4.76380000	0.00000000
86	696.00980000	62.83970000	0.00000000
87	704.80330000	3.71170000	0.00000000
88	712.72860000	14.41420000	0.00000000
89	734.69310000	84.45800000	0.00000000
90	736.71210000	74.94090000	0.00000000
91	742.36730000	25.37920000	0.00000000
92	743.02640000	10.91030000	0.00000000
93	745.20440000	8.41610000	0.00000000
94	748.57720000	65.33200000	0.00000000
95	751.76730000	86.52590000	0.00000000
96	759.97950000	0.32980000	0.00000000
97	761.57270000	28.57250000	0.00000000
98	764.33850000	4.14200000	0.00000000
99	787.78180000	10.18980000	0.00000000
100	788.90240000	22.78670000	0.00000000
101	792.13440000	14.10230000	0.00000000
102	792.95730000	93.24110000	0.00000000
103	807.77610000	78.55420000	0.00000000
104	809.67690000	0.07330000	0.00000000
105	811.34740000	0.47920000	0.00000000
106	813.59590000	0.06280000	0.00000000
107	825.77270000	14.75090000	0.00000000
108	837.78750000	47.07880000	0.00000000
109	838.50530000	3.46690000	0.00000000
110	839.88560000	9.88500000	0.00000000
111	850.48790000	0.47440000	0.00000000
112	851.81810000	0.64210000	0.00000000
113	866.52720000	104.37870000	0.00000000
114	866.68360000	20.86520000	0.00000000
115	866.93010000	73.54080000	0.00000000
116	900.49340000	22.39780000	0.00000000
117	901.59610000	0.44320000	0.00000000
118	903.35150000	84.85020000	0.00000000
119	930.54630000	16.28020000	0.00000000
120	940.21660000	4.00260000	0.00000000
121	942.14950000	10.12200000	0.00000000
122	962.12440000	10.55550000	0.00000000
123	962.88100000	19.10310000	0.00000000
124	979.03290000	0.77380000	0.00000000

125	980.41790000	1.29450000	0.00000000
126	982.32370000	0.72740000	0.00000000
127	983.54610000	1.54150000	0.00000000
128	984.00930000	0.28040000	0.00000000
129	984.54060000	1.06810000	0.00000000
130	986.45420000	0.24230000	0.00000000
131	988.22920000	0.45690000	0.00000000
132	1003.08170000	0.79940000	0.00000000
133	1003.55020000	88.15350000	0.00000000
134	1006.22910000	0.00160000	0.00000000
135	1011.91120000	54.77240000	0.00000000
136	1025.29550000	0.96620000	0.00000000
137	1025.60260000	0.86390000	0.00000000
138	1027.62730000	0.15160000	0.00000000
139	1028.76420000	0.22500000	0.00000000
140	1031.39550000	0.99430000	0.00000000
141	1031.63460000	132.23680000	0.00000000
142	1032.66910000	1.75110000	0.00000000
143	1062.08020000	4.29450000	0.00000000
144	1063.47490000	61.06760000	0.00000000
145	1065.33650000	2.10300000	0.00000000
146	1074.09020000	942.99340000	0.00000000
147	1083.48390000	347.44910000	0.00000000
148	1091.44120000	4.86260000	0.00000000
149	1092.42500000	97.80580000	0.00000000
150	1094.11190000	0.55170000	0.00000000
151	1096.47540000	9.28120000	0.00000000
152	1108.24940000	49.34010000	0.00000000
153	1123.01850000	7.41350000	0.00000000
154	1123.83900000	3.85820000	0.00000000
155	1125.28430000	9.56030000	0.00000000
156	1132.29520000	53.19110000	0.00000000
157	1135.76560000	27.81660000	0.00000000
158	1140.61280000	5.31110000	0.00000000
159	1146.45700000	46.50770000	0.00000000
160	1163.43420000	200.00000000	0.00000000
161	1165.96720000	8.30790000	0.00000000
162	1175.16540000	16.03670000	0.00000000
163	1178.18380000	13.18220000	0.00000000
164	1178.51410000	6.27230000	0.00000000
165	1179.24480000	10.32190000	0.00000000
166	1191.45110000	34.08360000	0.00000000
167	1195.97230000	194.78330000	0.00000000
168	1212.24890000	1025.81170000	0.00000000
169	1217.53550000	145.90840000	0.00000000
170	1234.54610000	1619.38550000	0.00000000
171	1239.04300000	22.12910000	0.00000000
172	1241.58930000	2.40580000	0.00000000
173	1241.73510000	2.93480000	0.00000000
174	1243.57630000	4.85020000	0.00000000
175	1244.31640000	24.67140000	0.00000000
176	1246.02690000	27.57450000	0.00000000
177	1253.00020000	12.35590000	0.00000000
178	1253.69630000	17.08640000	0.00000000
179	1277.44890000	2.63510000	0.00000000
180	1288.25980000	142.17780000	0.00000000
181	1289.69370000	4.16530000	0.00000000
182	1291.62720000	1.57550000	0.00000000
183	1307.97740000	23.91000000	0.00000000
184	1321.97360000	14.96880000	0.00000000
185	1325.74860000	0.45310000	0.00000000
186	1335.37150000	49.88050000	0.00000000
187	1343.12070000	18.30710000	0.00000000
188	1346.48490000	15.80380000	0.00000000

189	1346.64270000	18.94650000	0.00000000
190	1348.66340000	10.44450000	0.00000000
191	1349.63450000	2.14620000	0.00000000
192	1354.80820000	528.71670000	0.00000000
193	1365.62900000	785.86970000	0.00000000
194	1371.93830000	5.35430000	0.00000000
195	1379.10730000	283.80800000	0.00000000
196	1379.31690000	16.20930000	0.00000000
197	1381.76430000	20.47260000	0.00000000
198	1392.60500000	241.23330000	0.00000000
199	1392.85260000	493.02460000	0.00000000
200	1406.61890000	333.90320000	0.00000000
201	1436.85270000	81.68690000	0.00000000
202	1445.56990000	16.19140000	0.00000000
203	1447.13930000	3.81420000	0.00000000
204	1453.75030000	688.28130000	0.00000000
205	1458.05790000	52.82510000	0.00000000
206	1458.12320000	12.04450000	0.00000000
207	1461.92520000	35.98350000	0.00000000
208	1463.59770000	101.40670000	0.00000000
209	1465.61340000	44.24050000	0.00000000
210	1470.03870000	144.35500000	0.00000000
211	1479.59450000	56.47570000	0.00000000
212	1486.87270000	7.22200000	0.00000000
213	1488.33610000	6.17520000	0.00000000
214	1490.54440000	90.51110000	0.00000000
215	1493.92000000	2.24440000	0.00000000
216	1502.58210000	5.47050000	0.00000000
217	1505.72920000	0.87570000	0.00000000
218	1528.37970000	33.10040000	0.00000000
219	1529.44780000	14.43960000	0.00000000
220	1530.38380000	48.40190000	0.00000000
221	1530.58440000	335.90050000	0.00000000
222	1548.71140000	433.14270000	0.00000000
223	1553.54980000	252.31960000	0.00000000
224	1556.49570000	154.17000000	0.00000000
225	1558.12900000	129.69890000	0.00000000
226	1585.25480000	305.56760000	0.00000000
227	1595.15810000	930.50180000	0.00000000
228	1610.25600000	65.09030000	0.00000000
229	1619.66520000	48.31360000	0.00000000
230	1620.82190000	38.31730000	0.00000000
231	1621.03440000	21.78790000	0.00000000
232	1621.91720000	15.44730000	0.00000000
233	1622.17590000	1.49670000	0.00000000
234	1622.43440000	5.78360000	0.00000000
235	1623.40760000	10.47590000	0.00000000
236	1633.93620000	7.92360000	0.00000000
237	1634.16620000	20.52090000	0.00000000
238	1636.66510000	3.57590000	0.00000000
239	1640.70360000	26.78050000	0.00000000
240	1665.53190000	22.87210000	0.00000000
241	1665.69840000	7.31220000	0.00000000
242	3065.30300000	44.20720000	0.00000000
243	3076.07120000	21.19750000	0.00000000
244	3152.40350000	19.10180000	0.00000000
245	3155.31270000	2.51800000	0.00000000
246	3196.28710000	0.04940000	0.00000000
247	3197.81130000	0.00620000	0.00000000
248	3202.88380000	1.22810000	0.00000000
249	3203.90340000	1.69430000	0.00000000
250	3203.98080000	1.65210000	0.00000000
251	3205.14060000	1.53310000	0.00000000
252	3209.75960000	7.89210000	0.00000000

253	3210.71850000	8.41650000	0.00000000
254	3217.96510000	2.07920000	0.00000000
255	3218.02170000	0.21970000	0.00000000
256	3219.97880000	19.16440000	0.00000000
257	3220.04930000	0.30480000	0.00000000
258	3220.37680000	23.44670000	0.00000000
259	3220.55430000	0.29570000	0.00000000
260	3222.21130000	0.09090000	0.00000000
261	3223.60680000	0.03800000	0.00000000
262	3225.16570000	5.53270000	0.00000000
263	3226.12320000	8.38450000	0.00000000
264	3226.25430000	8.65750000	0.00000000
265	3226.79460000	2.03510000	0.00000000
266	3230.80990000	2.43560000	0.00000000
267	3231.54800000	2.14450000	0.00000000
268	3233.71080000	0.27060000	0.00000000
269	3234.28540000	1.96170000	0.00000000
270	3234.52810000	1.46860000	0.00000000
271	3237.61470000	0.18390000	0.00000000
272	3238.12100000	2.84660000	0.00000000
273	3238.26140000	0.15820000	0.00000000