How to elucidate and control the redox sequence in vinylbenzoate and vinylpyridine bridged diruthenium complexes

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Supporting Information

Table S1 Cartesian coordinates and energy data of the stationary points for complexes studied.

1a

Ru,0,-0.4714009871,-1.174800791,0.0136268159
C,0,-1.3018564591,-2.7794269809,0.057580043
O,0,-1.8356429597,-3.815906708,0.0869095745
C,0,-2.2680996868,-0.2243603862,-0.001195002
C,0,-2.3793937076,1.1222344233,-0.0109532845
H,0,-1.4615852942,1.7168559059,-0.0026158277
H,0,-3.2012486767,-0.7984616662,0.0001874066
P,0,-0.4887447764,-1.0211968779,2.3561945243
P,0,-0.5134809734,-1.1261012353,-2.3315263425
C,0,0.813176477,-2.0715448642,-3.1748267367
C,0,-2.0424903535,-1.7558165461,-3.1190409346
C,0,-0.3540297673,0.5583992633,-3.0283752407
C,0,0.8127472883,-1.9825963273,3.2203453005
C,0,-0.253575713,0.682399711,2.9830967062
C,0,-2.0302462269,-1.5533813123,3.1899469999
H,0,-0.2598643632,0.7067705498,4.0783042178
H,0,0.6919094137,1.0827257667,2.6079997106
H,0,-1.0627073061,1.309184593,2.5962796408
H,0,0.7965633458,-1.8075982772,4.3019080103
H,0,0.6638245491,-3.0491735555,3.0245740754
H,0,1.7901752456,-1.70468516,2.8158560092
H,0,-1.9645049847,-1.4223983981,4.2754945352
H,0,-2.8624029952,-0.9574872851,2.8027597898
H,0,-2.2286518261,-2.6062554438,2.9658967084
H,0,-0.4050037841,0.5449689773,-4.1226396487
H,0,-1.1641728441,1.1748986778,-2.6275775489
H,0,0.5941298585,0.9974481576,-2.7065987797
H,0,0.7797482486,-1.9362247777,-4.2617145074
H,0,1.784297246,-1.7450423454,-2.7921162185
H,0,0.7044565091,-3.1349263165,-2.9393983782
H,0,-1.9926068825,-1.6777173325,-4.2104229901
H,0,-2.198065355,-2.8023756853,-2.8389197449
H,0,-2.8931677791,-1.1727048782,-2.7531331391
H,0,2.5211692886,2.4600327575,-0.0660352135
C,0,3.4133156297,1.8417033108,-0.0471843488
C,0,4.675772044,2.4152116257,-0.0500077109
C,0,3.2708631441,0.4513444818,-0.0193108308
C,0,5.8219441345,1.6035847055,-0.024634235
H,0,4.7915561047,3.4944083045,-0.0712518003
C,0,4.4085223356,-0.3609021021,0.0051937121
C,0,5.67313978,0.2069803414,0.0027223109
C,0,7.1216488618,2.1897108448,-0.0257596518
H,0,4.2811440533,-1.438813346,0.0262718596
H,0,6.5594473029,-0.4196454374,0.0221856512
C,0,8.2249930489,2.6856024115,-0.0259790996
H,0,9.1982699448,3.12312255,-0.0263223414
C,0,1.9183572511,-0.1652971818,-0.0131799385

O,0,1.7907272906,-1.4228957759,0.0131784337
O,0,0.8833746311,0.5774115708,-0.0316888091
C,0,-3.6125644342,1.9228529392,-0.0241767435
C,0,-3.5143889745,3.3213777821,0.0580979263
C,0,-4.9019572558,1.3710616057,-0.1177956906
C,0,-4.6440340874,4.1325959806,0.0537510193
H,0,-2.526730693,3.7737007844,0.1282636599
C,0,-6.0312288125,2.1791988602,-0.1218980065
H,0,-5.0213793215,0.2931812255,-0.1924080615
C,0,-5.9126018319,3.5663356354,-0.0354414118
H,0,-4.5317964468,5.2121492655,0.119914093
H,0,-7.0155376597,1.7228587056,-0.1962397713
H,0,-6.798421808,4.1957002797,-0.0403307452

Sum of electronic and zero-point Energies= -1933.842041
Sum of electronic and thermal Energies= -1933.806092
Sum of electronic and thermal Enthalpies= -1933.805148
Sum of electronic and thermal Free Energies= -1933.913173

1a^{+}
Charge = 1 Multiplicity = 2
Ru,0,0.6145673587,0.1610046532,0.2323489146
C,0,-2.1384568811,-0.5330714564,-0.2210609678
C,0,-1.1715115948,-0.2830172002,0.7495116629
H,0,-1.8334330338,-0.4646403892,-1.264392859
H,0,-1.4758485357,-0.3512479813,1.7961823341
C,0,1.0385528932,0.2811967454,2.0179649412
P,0,0.2752285112,2.5255989891,0.0258876959
P,0,1.4321841039,-2.0865373556,0.0616175615
O,0,1.3349998458,0.3641766199,3.1304983163
C,0,1.7526136304,3.320829745,-0.6959992893
C,0,-1.099076427,2.9788432838,-1.083712171
C,0,-0.0481905176,3.4459769528,1.5714759032
C,0,1.5759088159,-3.0279395453,1.6216324458
C,0,0.438491722,-3.15089123,-1.0361446301
C,0,3.1125752057,-2.1007714969,-0.6541041437
H,0,1.5808500169,4.3951417944,-0.8238970723
H,0,2.619589295,3.1773533102,-0.0435563929
H,0,1.9619853398,2.866621843,-1.6687739475
H,0,-1.1431383538,4.0660984027,-1.2078306077
H,0,-0.9432386897,2.5035475911,-2.0559836851
H,0,-2.0457837662,2.6265173295,-0.6634894322
H,0,-0.1621268471,4.5154788169,1.3652211719
H,0,-0.9656891611,3.0776082036,2.0406114794
H,0,0.7782515738,3.3083122124,2.2752405816
H,0,1.9810777316,-4.0274431857,1.4314012542
H,0,2.2369242512,-2.5062126008,2.320275849
H,0,0.5914800573,-3.1295102291,2.0887199079
H,0,0.9132475159,-4.1319040223,-1.1442698244
H,0,-0.5639245113,-3.2810112441,-0.6175681099
H,0,0.3550349653,-2.6725485116,-2.0158012402

H,0,3.4686904324,-3.1306998296,-0.7656229459
H,0,3.0862623102,-1.6158438189,-1.6341981022
H,0,3.8068238386,-1.5555122498,-0.0070915572
Cl,0,0.71214562,0.1669298857,-2.1615623387
C,0,-3.5131194169,-0.8760884178,0.010166639
C,0,-4.3390721914,-1.092000174,-1.1195675987
C,0,-4.0870208199,-1.0100720256,1.2985939856
C,0,-5.673659371,-1.4255990156,-0.9709069193
H,0,-3.9093389617,-0.991899084,-2.1131301167
C,0,-5.4207836344,-1.3435217807,1.4400151305
H,0,-3.4828892579,-0.851672469,2.1865963826
C,0,-6.2190106577,-1.5524857367,0.3090822795
H,0,-6.2947119851,-1.588147246,-1.8463771229
H,0,-5.8511709374,-1.4438039776,2.4317526386
H,0,-7.2662752722,-1.8142441246,0.4283779094

Sum of electronic and zero-point Energies= -1897.965310
Sum of electronic and thermal Energies= -1897.937462
Sum of electronic and thermal Enthalpies= -1897.936517
Sum of electronic and thermal Free Energies= -1898.025756

1b

Charge = 0 Multiplicity = 1
Ru,0,0.8720056283,0.1057402609,0.1407624978
C,0,-1.9944411838,-0.2664623983,-0.3951657246
C,0,-1.0597542719,-0.1670546037,0.5624202919
H,0,-1.7569767885,-0.2115392853,-1.4556190702
H,0,-1.4051724653,-0.2286935987,1.5964201138
C,0,1.2086479584,0.1353723352,1.9233697461
P,0,0.5130386814,2.4329123863,0.0235171607
P,0,1.1909971892,-2.2229274414,-0.0294555346
O,0,1.4636321331,0.16046682,3.0595257504
C,0,1.9886723672,3.3818423486,-0.5083066984
C,0,-0.7682950043,2.9304028968,-1.1818012437
C,0,-0.0102918553,3.2712101467,1.5672111398
C,0,0.9311607119,-3.2148019566,1.4897603137
C,0,0.1023676416,-3.0358003847,-1.2523741058
C,0,2.8757778696,-2.6988688108,-0.5733669097
H,0,1.7617438889,4.4491389936,-0.608263669
H,0,2.7967549033,3.2542698086,0.2190240101
H,0,2.3233481015,2.9872034584,-1.4725799832
H,0,-0.8699381632,4.0205269298,-1.2176838941
H,0,-0.4825858448,2.5501881622,-2.1667265354
H,0,-1.7260397653,2.4807203951,-0.9032644837
H,0,-0.1636815258,4.3441784946,1.408791314
H,0,-0.9468689249,2.8250191034,1.9165350165
H,0,0.745180321,3.1277453009,2.3459448906
H,0,1.0906127101,-4.2821199047,1.3020454089
H,0,1.6160375177,-2.8821959856,2.2758772145
H,0,-0.093153566,-3.0630385115,1.8444482224
H,0,0.3226172537,-4.1064898549,-1.3241375779

H,0,-0.9418489516,-2.894589965,-0.9586142571
H,0,0.2541102805,-2.5563994849,-2.2234643024
H,0,2.9637913349,-3.7844968096,-0.6933310702
H,0,3.0829424706,-2.2065831459,-1.5284774143
H,0,3.6140767498,-2.358994467,0.1598975683
Cl,0,1.1797033124,0.1774696103,-2.2591656336
C,0,-3.443490323,-0.4087982991,-0.1016680846
F,0,-3.7110556399,-0.5617457898,1.2066422934
F,0,-3.9805591315,-1.4686386888,-0.7425051211
F,0,-4.1422316195,0.6722859351,-0.5196086394

Sum of electronic and zero-point Energies= -2004.216661
Sum of electronic and thermal Energies= -2004.190308
Sum of electronic and thermal Enthalpies= -2004.189363
Sum of electronic and thermal Free Energies= -2004.274699

1b^{+}

Charge = 1 Multiplicity = 2
C,0,-1.1073994009,0.0070075268,-1.8496058385
C,0,-1.2587768543,-0.0082089993,-0.4951229338
H,0,-0.1353229026,0.022121009,-2.3351577178
Ru,0,0.3308324595,-0.0025506811,0.6043389064
H,0,-2.2720118986,-0.0229254997,-0.0930326679
C,0,-0.8063058186,-0.0286231672,2.063744484
P,0,0.7091552333,2.3606155823,0.8582028526
P,0,0.7578011759,-2.3619195805,0.8118540569
O,0,-1.4897147626,-0.0448008384,2.9896386107
C,0,2.3184226044,2.6499599914,1.6652504899
C,0,0.7804736464,3.2298420466,-0.7413964147
C,0,-0.5152084481,3.2735513932,1.8565549377
C,0,-0.4465805318,-3.3191956388,1.7928300582
C,0,0.8454490711,-3.1980555763,-0.8044861146
C,0,2.373391075,-2.6338818328,1.6122893088
H,0,2.4995169233,3.7268656484,1.7549197241
H,0,2.3302255901,2.2067058718,2.6657363984
H,0,3.1095900212,2.1951169361,1.0628184303
H,0,1.0382414504,4.2822787275,-0.5793773042
H,0,1.536401021,2.7585728519,-1.3749657524
H,0,-0.1913570882,3.1707812024,-1.2397873815
H,0,-0.2369605481,4.3314269343,1.9150345602
H,0,-1.5068331366,3.1956532217,1.4003860659
H,0,-0.5653484614,2.8660738538,2.8706500266
H,0,-0.1465425532,-4.3720528084,1.8304207613
H,0,-0.5040979823,-2.9327620697,2.8147409944
H,0,-1.4400516757,-3.252834899,1.3388580203
H,0,1.1250111118,-4.2479192582,-0.6632520973
H,0,-0.1278808165,-3.1493007775,-1.3010618179
H,0,1.5908743408,-2.698990178,-1.4291494242
H,0,2.576518136,-3.7083985965,1.6809707262
H,0,3.1545576308,-2.1513620896,1.0184056679
H,0,2.3770286019,-2.2099504333,2.6211777807

Cl,0,2.2208193126,0.0310542607,-0.8384872776
C,0,-2.2827023118,0.0040900157,-2.7893113187
F,0,-2.2226953579,-1.070509013,-3.5823936975
F,0,-2.2459097641,1.0958103369,-3.5601208191
F,0,-3.4514667432,-0.0150788951,-2.1427797881

Sum of electronic and zero-point Energies= -2003.960284
Sum of electronic and thermal Energies= -2003.933309
Sum of electronic and thermal Enthalpies= -2003.932364
Sum of electronic and thermal Free Energies= -2004.020676

2a

Charge = 0 Multiplicity = 1
Ru,0,-0.4714009871,-1.174800791,0.0136268159
C,0,-1.3018564591,-2.7794269809,0.057580043
O,0,-1.8356429597,-3.815906708,0.0869095745
C,0,-2.2680996868,-0.2243603862,-0.001195002
C,0,-2.3793937076,1.1222344233,-0.0109532845
H,0,-1.4615852942,1.7168559059,-0.0026158277
H,0,-3.2012486767,-0.7984616662,0.0001874066
P,0,-0.4887447764,-1.0211968779,2.3561945243
P,0,-0.5134809734,-1.1261012353,-2.3315263425
C,0,0.813176477,-2.0715448642,-3.1748267367
C,0,-2.0424903535,-1.7558165461,-3.1190409346
C,0,-0.3540297673,0.5583992633,-3.0283752407
C,0,0.8127472883,-1.9825963273,3.2203453005
C,0,-0.253575713,0.682399711,2.9830967062
C,0,-2.0302462269,-1.5533813123,3.1899469999
H,0,-0.2598643632,0.7067705498,4.0783042178
H,0,0.6919094137,1.0827257667,2.6079997106
H,0,-1.0627073061,1.309184593,2.5962796408
H,0,0.7965633458,-1.8075982772,4.3019080103
H,0,0.6638245491,-3.0491735555,3.0245740754
H,0,1.7901752456,-1.70468516,2.8158560092
H,0,-1.9645049847,-1.4223983981,4.2754945352
H,0,-2.8624029952,-0.9574872851,2.8027597898
H,0,-2.2286518261,-2.6062554438,2.9658967084
H,0,-0.4050037841,0.5449689773,-4.1226396487
H,0,-1.1641728441,1.1748986778,-2.6275775489
H,0,0.5941298585,0.9974481576,-2.7065987797
H,0,0.7797482486,-1.9362247777,-4.2617145074
H,0,1.784297246,-1.7450423454,-2.7921162185
H,0,0.7044565091,-3.1349263165,-2.9393983782
H,0,-1.9926068825,-1.6777173325,-4.2104229901
H,0,-2.198065355,-2.8023756853,-2.8389197449
H,0,-2.8931677791,-1.1727048782,-2.7531331391
H,0,2.5211692886,2.4600327575,-0.0660352135
C,0,3.4133156297,1.8417033108,-0.0471843488
C,0,4.675772044,2.4152116257,-0.0500077109
C,0,3.2708631441,0.4513444818,-0.0193108308

C,0,5.8219441345,1.6035847055,-0.024634235
H,0,4.7915561047,3.4944083045,-0.0712518003
C,0,4.4085223356,-0.3609021021,0.0051937121
C,0,5.67313978,0.2069803414,0.0027223109
C,0,7.1216488618,2.1897108448,-0.0257596518
H,0,4.2811440533,-1.438813346,0.0262718596
H,0,6.5594473029,-0.4196454374,0.0221856512
C,0,8.2249930489,2.6856024115,-0.0259790996
H,0,9.1982699448,3.12312255,-0.0263223414
C,0,1.9183572511,-0.1652971818,-0.0131799385
O,0,1.7907272906,-1.4228957759,0.0131784337
O,0,0.8833746311,0.5774115708,-0.0316888091
C,0,-3.6125644342,1.9228529392,-0.0241767435
C,0,-3.5143889745,3.3213777821,0.0580979263
C,0,-4.9019572558,1.3710616057,-0.1177956906
C,0,-4.6440340874,4.1325959806,0.0537510193
H,0,-2.526730693,3.7737007844,0.1282636599
C,0,-6.0312288125,2.1791988602,-0.1218980065
H,0,-5.0213793215,0.2931812255,-0.1924080615
C,0,-5.9126018319,3.5663356354,-0.0354414118
H,0,-4.5317964468,5.2121492655,0.119914093
H,0,-7.0155376597,1.7228587056,-0.1962397713
H,0,-6.798421808,4.1957002797,-0.0403307452

Sum of electronic and zero-point Energies= -1933.842041
Sum of electronic and thermal Energies= -1933.806092
Sum of electronic and thermal Enthalpies= -1933.805148
Sum of electronic and thermal Free Energies= -1933.913173

2a^{+}
Charge = 1 Multiplicity = 2
Ru,0,0.5972576546,-1.1248511203,0.0000786552
C,0,1.4900511042,-2.7243485399,0.0006601682
O,0,2.0646256519,-3.7270414506,0.0010665988
C,0,2.2962144193,-0.1889701594,0.0000953636
C,0,2.3129181274,1.2028118132,-0.0003146773
H,0,1.3482971261,1.7130287147,-0.0007416222
H,0,3.2693270954,-0.6887891782,0.0005078219
P,0,0.4104932772,-1.216651304,-2.3883164448
P,0,0.4098330635,-1.2156284116,2.3884706988
C,0,-0.8002720342,-2.4644457421,2.9441991283
C,0,1.9501297171,-1.6354669434,3.2775212122
C,0,-0.1391742893,0.3501156697,3.1502845055
C,0,-0.8024426152,-2.4628039193,-2.9438499782
C,0,-0.1345858175,0.350076312,-3.1509393255
C,0,1.9500387286,-1.6406145239,-3.2766985812
H,0,-0.2094144445,0.2376134114,-4.2377460964
H,0,-1.1071322283,0.646976384,-2.750361039
H,0,0.5855561298,1.1396519966,-2.9174568986
H,0,-0.9285049847,-2.4230448675,-4.0309881551
H,0,-0.4614337463,-3.4629723427,-2.659372546

H,0,-1.7607331099,-2.2763442778,-2.4519507136
H,0,1.7754683478,-1.6794912917,-4.3571291332
H,0,2.7159732141,-0.888355783,-3.0654881764
H,0,2.3194427924,-2.6152869018,-2.9431559363
H,0,-0.2133751221,0.2380197244,4.2371743531
H,0,0.5788130829,1.1414601979,2.9161639871
H,0,-1.1126477288,0.6442761499,2.7499349209
H,0,-0.9268901956,-2.4243883837,4.0312620663
H,0,-1.7588059268,-2.2805546401,2.4517988482
H,0,-0.4566872389,-3.4639354384,2.660442088
H,0,1.7752955819,-1.6744555372,4.3579061653
H,0,2.3220967846,-2.6093119093,2.9444038644
H,0,2.7142505489,-0.8813609295,3.0663253986
H,0,-2.3481833909,2.5168940619,-0.0006777413
C,0,-3.2386424684,1.8959722669,-0.0004709151
C,0,-4.4982074035,2.4719990035,-0.0004999856
C,0,-3.1026120375,0.5022931156,-0.0001643569
C,0,-5.6475105196,1.6623334791,-0.0002245232
H,0,-4.6113216836,3.5512362358,-0.0007306659
C,0,-4.2438882548,-0.3093435293,0.0001133034
C,0,-5.5045788733,0.2636858072,0.0000798002
C,0,-6.9428129823,2.252075734,-0.0002539102
H,0,-4.1280400563,-1.3887540539,0.0003484943
H,0,-6.3931286291,-0.3592318728,0.0002890694
C,0,-8.043847073,2.7519032042,-0.0001356829
H,0,-9.0168234333,3.1925650131,-0.000215857
C,0,-1.764759334,-0.111310704,-0.0001383355
O,0,-1.6201183342,-1.3775692898,0.0003081877
O,0,-0.7090711349,0.6104067481,-0.0005170928
C,0,3.4665525158,2.0619501287,-0.0002396726
C,0,3.2560257257,3.4607317336,-0.0009468346
C,0,4.7991153586,1.5852881222,0.0005234533
C,0,4.3232202324,4.3426247861,-0.0009310778
H,0,2.2364838315,3.838844749,-0.0015131355
C,0,5.8618599223,2.47040948,0.0005523103
H,0,4.9959400657,0.5175613141,0.0011183743
C,0,5.6300403093,3.850219647,-0.0001813576
H,0,4.1446113293,5.413591834,-0.0014908548
H,0,6.8800870247,2.0931754929,0.0011507069
H,0,6.4693643278,4.5395187143,-0.0001582209

Sum of electronic and zero-point Energies= -1933.624826
Sum of electronic and thermal Energies= -1933.588807
Sum of electronic and thermal Enthalpies= -1933.587863
Sum of electronic and thermal Free Energies= -1933.696683

2b

Charge = 0 Multiplicity = 1
Ru,0,-0.1852814735,-0.0025389085,1.222300103
C,0,-0.1950658308,0.0002129548,3.0321901397
O,0,-0.1915877474,0.0013015761,4.1975437981

C,0,-2.2051250407,0.0016890423,1.1763658165
C,0,-2.8988386902,0.0009433811,0.0253640129
H,0,-2.4104593636,-0.001703146,-0.9490681569
H,0,-2.8075086241,0.003973606,2.0896442352
P,0,-0.2467674622,2.345599444,1.1453736441
P,0,-0.2533941889,-2.3507261409,1.1535572068
C,0,1.3621411816,-3.1907568225,1.3686116703
C,0,-1.3204854299,-3.1598290699,2.4027187166
C,0,-0.8867961777,-3.0206280192,-0.426912006
C,0,1.3707277844,3.1814046013,1.3615370651
C,0,-0.8764081899,3.0162832985,-0.4368323606
C,0,-1.3127275397,3.1614110987,2.3911005535
H,0,-0.881077447,4.1117696418,-0.4308383795
H,0,-0.2545888915,2.6534933202,-1.2597861561
H,0,-1.8942147156,2.6465129816,-0.5947381856
H,0,1.2837679479,4.2683382538,1.2545042868
H,0,1.7673747688,2.9464582094,2.3542911991
H,0,2.0779519483,2.7938268619,0.6229753482
H,0,-1.3070637038,4.2502384867,2.2717064701
H,0,-2.3370212759,2.7924260425,2.2791928163
H,0,-0.9668375539,2.9085337346,3.3983041364
H,0,-0.9032025448,-4.1159562999,-0.4176550234
H,0,-1.9000043582,-2.6396283007,-0.5873113313
H,0,-0.2599299613,-2.6667464867,-1.2498463806
H,0,1.2742834072,-4.2766494808,1.2520440883
H,0,2.0717151671,-2.7976716806,0.635128044
H,0,1.7566400421,-2.9651586316,2.3644406643
H,0,-1.3188412882,-4.249033867,2.2866959694
H,0,-0.9725277668,-2.9051738313,3.4087522596
H,0,-2.3437052652,-2.7877925089,2.2912739042
C,0,-4.3815055902,0.0078529078,-0.0499960066
H,0,0.806712814,-0.0218134915,-3.3697578871
C,0,1.8831629363,-0.0129908105,-3.2291062082
C,0,2.7409734495,-0.0115546864,-4.3182259822
C,0,2.3960544568,-0.0028837298,-1.9285130365
C,0,4.132089116,0.0006247677,-4.1235578447
H,0,2.3477669313,-0.01949826,-5.3300388592
C,0,3.7797309088,0.0087494125,-1.7290827757
C,0,4.6419612398,0.010699071,-2.8145931228
C,0,5.0161053106,0.0031209134,-5.2419794472
H,0,4.1628311877,0.0160184435,-0.7132891298
H,0,5.7171454336,0.0200485736,-2.6651428983
C,0,5.7654809034,0.0053652443,-6.1914603482
H,0,6.4264442512,0.0074451183,-7.0292763669
C,0,1.4772183097,-0.0042783151,-0.7613575744
O,0,1.9359781454,0.0014145257,0.4174074086
O,0,0.2164370587,-0.0080355236,-0.9482147054
F,0,-4.8450667174,1.0937406755,-0.7113109783
F,0,-4.9783378631,0.0021551482,1.1547659083
F,0,-4.8543309573,-1.0640848155,-0.7266651014

Sum of electronic and zero-point Energies= -2039.868233
Sum of electronic and thermal Energies= -2039.833356
Sum of electronic and thermal Enthalpies= -2039.832412
Sum of electronic and thermal Free Energies= -2039.938204

2b^{+}

Charge = 1 Multiplicity = 2
Ru,0,-0.4185960803,0.0012131549,1.1670918658
C,0,-0.4597134859,0.0040289143,3.0094617412
O,0,-0.4958464637,0.0061976955,4.1613116909
C,0,-2.379659903,0.00426415,1.1702930051
C,0,-3.0093262624,0.0014098763,-0.0389045972
H,0,-2.4564002041,-0.0014654138,-0.9767862937
H,0,-3.0151843052,0.0075274887,2.0580152149
P,0,-0.0736262684,2.3866200362,1.207347565
P,0,-0.0771083433,-2.3847977478,1.2130941174
C,0,1.4727765427,-2.8162102037,2.0713777522
C,0,-1.391314732,-3.3126771566,2.074918727
C,0,0.0493476137,-3.1586324792,-0.4334482177
C,0,1.4822804894,2.8173251598,2.0549508259
C,0,0.0427915908,3.1572351267,-0.4414188559
C,0,-1.3812738523,3.3169767365,2.076425804
H,0,0.1763592376,4.2390525323,-0.3325669478
H,0,0.8938565509,2.7506576113,-0.9943119291
H,0,-0.8679374765,2.9611600806,-1.0136701528
H,0,1.6677936487,3.8947508659,1.9917964342
H,0,1.4288049968,2.5267396374,3.1084900953
H,0,2.3064317652,2.2745671476,1.584083217
H,0,-1.1485756115,4.3871546925,2.0847755228
H,0,-2.3409027232,3.1628074059,1.574600996
H,0,-1.4686017954,2.9647845827,3.1086726886
H,0,0.1804076984,-4.2404442051,-0.3215329346
H,0,-0.8571014484,-2.9623521616,-1.0123786306
H,0,0.9049723042,-2.7546109916,-0.9811387813
H,0,1.6579096407,-3.8938164287,2.010055883
H,0,2.3006267948,-2.2745451039,1.6057013576
H,0,1.4124558153,-2.5250548604,3.1243854801
H,0,-1.1593061751,-4.382985567,2.0863052692
H,0,-1.4851765617,-2.9589858184,3.1060853657
H,0,-2.3474732466,-3.1585274006,1.5665169541
C,0,-4.5014011798,-0.0014065931,-0.1990226597
H,0,0.3619324769,-0.0017571045,-3.4297044475
C,0,1.4422290079,-0.0022768267,-3.3235705967
C,0,2.2569264725,-0.0024475535,-4.4427598218
C,0,2.0092496515,-0.0027144491,-2.0418625852
C,0,3.6561970444,-0.0030410317,-4.3013379903
H,0,1.8254888593,-0.0020484568,-5.4383563873
C,0,3.4031549518,-0.0034238515,-1.8944864921
C,0,4.2192996916,-0.0036135677,-3.0126118421
C,0,4.4944217336,-0.0029374835,-5.4505227257
H,0,3.8345898048,-0.0038007251,-0.8982478812

H,0,5.2991582673,-0.0041260961,-2.9066785648
C,0,5.207773148,-0.0027265729,-6.4268322084
H,0,5.8377811068,-0.0025318039,-7.2896408162
C,0,1.1455280752,-0.002090848,-0.8560649512
O,0,1.6335903218,-0.0019526611,0.3263802975
O,0,-0.1293663585,-0.0011885554,-0.9605631241
F,0,-4.8880084263,1.0702444215,-0.9038143234
F,0,-5.143356729,0.016918486,0.9722654056
F,0,-4.8868846287,-1.0959275735,-0.8689353051

Sum of electronic and zero-point Energies= -2039.624475
Sum of electronic and thermal Energies= -2039.590368
Sum of electronic and thermal Enthalpies= -2039.589424
Sum of electronic and thermal Free Energies= -2039.693068

2c

Charge = 0 Multiplicity = 1
Ru,0,0.9642899972,0.5469215,-0.25410629
Cl,0,1.0489564965,-0.894122212,-2.1484271378
Cl,0,2.0566331669,-1.1391418071,1.024299006
C,0,0.0872040667,2.4416324623,-0.9583602592
C,0,0.0849885148,2.3921311498,0.4700281075
C,0,1.2789211602,2.1704041802,1.197392756
C,0,2.4837114041,1.9184096644,0.4772613123
C,0,2.5083632791,1.9394123344,-0.9345969711
C,0,1.292808857,2.1825041685,-1.6460462547
H,0,3.3655279367,1.5951253985,1.0201756449
H,0,3.4037467136,1.6491744302,-1.4714996714
H,0,1.2600785317,2.0786316247,2.2774880042
H,0,-0.8578631517,2.4704672037,1.004329289
H,0,-0.8401452828,2.5697168124,-1.5064101373
H,0,1.2785006074,2.0652195836,-2.7244212477
H,0,-1.5110173027,-0.3802600107,-1.718432782
C,0,-1.7733096566,-0.6846151922,-0.7115779751
C,0,-2.9944557548,-1.2717089443,-0.4252809982
C,0,-1.0687529104,-0.910859696,1.4740242635
C,0,-3.2646543958,-1.6942829987,0.8825425083
H,0,-3.7262054545,-1.4093234611,-1.2134614969
C,0,-2.262901005,-1.5071939367,1.8434684696
H,0,-0.2534686851,-0.7836177626,2.17733272
H,0,-2.4105622851,-1.8324344874,2.8672130291
N,0,-0.8286944972,-0.4905936468,0.2220831114
C,0,-4.5087050183,-2.2980420996,1.2207625784
C,0,-5.5658517489,-2.8088463335,1.5081463716
H,0,-6.497889313,-3.2641244985,1.7609962698

Sum of electronic and zero-point Energies= -1570.862813
Sum of electronic and thermal Energies= -1570.846443
Sum of electronic and thermal Enthalpies= -1570.845499
Sum of electronic and thermal Free Energies= -1570.908761

$2c^+$

Charge = 1 Multiplicity = 2
Ru,0,1.0108502232,0.4223725934,-0.1339051051
Cl,0,1.2376552968,-0.9838717509,-1.918276478
Cl,0,1.9335486733,-0.9437375261,1.4456866518
C,0,-0.0095280626,2.3743823298,-0.6786799177
C,0,0.2815926756,2.39093943,0.7261750973
C,0,1.6038259307,2.2289490803,1.1646269096
C,0,2.6419937878,1.9425086835,0.2283395331
C,0,2.3562435953,1.925677958,-1.1497440643
C,0,1.0301648921,2.1959022305,-1.6026925922
H,0,3.6382116656,1.6992097346,0.5826534477
H,0,3.130652495,1.6692146964,-1.8650804662
H,0,1.8203797436,2.1896376354,2.2279230375
H,0,-0.5230060492,2.5175009889,1.44332749
H,0,-1.0334416181,2.4884352115,-1.0197107443
H,0,0.8064791542,2.1311929569,-2.663265495
H,0,-1.3262506829,-0.6342867535,-1.7527021285
C,0,-1.6664054023,-0.8478185609,-0.7473151772
C,0,-2.9062728622,-1.417197294,-0.5270717549
C,0,-1.1968532188,-0.8283127934,1.5168185876
C,0,-3.3130950808,-1.7115043135,0.7824237454
H,0,-3.5505092899,-1.6392678732,-1.3703231594
C,0,-2.4201362283,-1.397004711,1.8171020863
H,0,-0.4858818533,-0.599188554,2.3004383674
H,0,-2.6752447771,-1.6028027121,2.8505440204
N,0,-0.8150270448,-0.5536761606,0.2544274566
C,0,-4.5745724338,-2.3017470283,1.0491795589
C,0,-5.6484757024,-2.8075452593,1.2765372137
H,0,-6.5976435571,-3.2573788126,1.4774860994

Sum of electronic and zero-point Energies= -1570.606187
Sum of electronic and thermal Energies= -1570.589680
Sum of electronic and thermal Enthalpies= -1570.588736
Sum of electronic and thermal Free Energies= -1570.652213

3a

Charge = 0 Multiplicity = 1
Ru,0,-4.6069658265,0.5224208084,-1.0707114079
C,0,-5.7973780951,1.1275717117,-2.2904588799
O,0,-6.5633574565,1.5172248878,-3.0796301094
C,0,-6.1234236394,-0.056766432,0.1534949672
C,0,-5.9157422148,-0.6665894385,1.341569223
H,0,-4.8847462068,-0.8555618399,1.6531635858
H,0,-7.1658874993,0.121804381,-0.133069507
P,0,-4.6245358415,-1.6245666883,-2.0153428472
P,0,-4.5882344466,2.5817021392,0.0509008132
C,0,-3.5668245534,3.8953156964,-0.7212762208
C,0,-6.2157987653,3.3900830109,0.2799904851
C,0,-3.9364836369,2.4777706035,1.7581770115

C,0,-3.5987671603,-1.8179905761,-3.5235603903
C,0,-3.9996518688,-2.9308397505,-0.8960432655
C,0,-6.2606023815,-2.2690382279,-2.5283206907
H,0,-4.0270524463,-3.9152647111,-1.3759863391
H,0,-2.9762499026,-2.6912335707,-0.5953580915
H,0,-4.6212394873,-2.941793057,0.0043558277
H,0,-3.5801379441,-2.8550582014,-3.8767618343
H,0,-3.997369061,-1.1735795425,-4.3135231048
H,0,-2.5809572202,-1.4818410332,-3.3053182899
H,0,-6.1839444797,-3.2818148459,-2.9386120724
H,0,-6.921345081,-2.2805587973,-1.6562093528
H,0,-6.6985159925,-1.606746179,-3.2817201606
H,0,-3.9442474088,3.4566116873,2.2504584913
H,0,-4.5564740177,1.7754012105,2.3235005431
H,0,-2.9177393399,2.0818185074,1.7337021068
H,0,-3.528967817,4.7993128688,-0.1031725792
H,0,-2.5549415861,3.5105244331,-0.8773825165
H,0,-3.9822211909,4.1455817036,-1.7026031127
H,0,-6.1240414142,4.3257785184,0.8419712875
H,0,-6.6654022026,3.5984247612,-0.6959130244
H,0,-6.8741548171,2.7040057473,0.8216990132
H,0,-0.8491273749,-0.6801981719,1.4923502252
C,0,-0.1296651868,-0.3383243068,0.7540990792
C,0,1.2329312613,-0.4345339879,0.9922071625
C,0,-0.5978432788,0.2053010383,-0.4454120083
H,0,1.5867592794,-0.8583112534,1.92977762
C,0,0.3294076867,0.6485597918,-1.3967727454
C,0,1.6889892478,0.5492574292,-1.1557087287
H,0,-0.0401182679,1.0742884951,-2.3251851383
H,0,2.3858808994,0.9057444441,-1.9093428202
C,0,-2.0503512872,0.3210039883,-0.7049261533
O,0,-2.476993099,0.8388272153,-1.7799914972
O,0,-2.8881930143,-0.0984501385,0.1619302787
C,0,2.1777149617,0.0028931517,0.046478791
C,0,3.6032426843,-0.1310336362,0.3638524999
C,0,4.6450000645,0.1695010583,-0.4415580532
H,0,3.8125824985,-0.5250878159,1.3602670884
Ru,0,6.545411706,-0.0846285599,0.143502877
H,0,4.4291904864,0.5563633658,-1.4407644358
C,0,7.0649839649,0.5686304844,-1.4641096522
P,0,6.4967854173,-2.3140025682,-0.6149993751
P,0,6.5366916547,2.0416979104,1.1563983512
O,0,7.4372436726,0.9849282959,-2.4870039549
C,0,8.0332897365,-3.2471788778,-0.2558631932
C,0,5.1904790459,-3.3325607641,0.1581475425
C,0,6.236530994,-2.5851685061,-2.4091737269
C,0,6.2371501578,3.4839944742,0.0661027493
C,0,5.2785956645,2.2411342421,2.4679416182
C,0,8.1053754843,2.4594742058,2.0085703254
H,0,7.9449999117,-4.2965999103,-0.5586012939
H,0,8.877273674,-2.7918644508,-0.7837914031

H,0,8.2255270304,-3.1899187484,0.8198650916
H,0,5.2314287332,-4.3659967089,-0.2028936958
H,0,5.3298301319,-3.3091230599,1.2426074966
H,0,4.2133609138,-2.8989265916,-0.0737894638
H,0,6.2303008448,-3.6524639357,-2.6556715661
H,0,5.2781034114,-2.1455166752,-2.7030716326
H,0,7.0277196115,-2.0895403755,-2.980199675
H,0,6.2439024011,4.4218097093,0.6319778294
H,0,7.0034823338,3.529118507,-0.7138882759
H,0,5.2631769709,3.3666402264,-0.4193018969
H,0,5.3366559337,3.2372358172,2.9202909097
H,0,4.284754837,2.0904352102,2.0365586947
H,0,5.4451332099,1.4743134646,3.2296148877
H,0,8.0385392724,3.4262375722,2.5201255159
H,0,8.3196128932,1.6731982745,2.7389955954
H,0,8.9256249475,2.4933359745,1.2844900651
Cl,0,6.6926388602,-1.0019288808,2.3822539359
C,0,-6.9284402463,-1.1225989558,2.3049437366
C,0,-6.5055618139,-1.7165084535,3.5054660717
C,0,-8.3139605441,-1.0023372034,2.0992145326
C,0,-7.4151857885,-2.1674353332,4.4560195181
H,0,-5.4378261906,-1.8223409579,3.6891713384
C,0,-9.2238840251,-1.4517905962,3.0469407011
H,0,-8.6838322957,-0.5512382723,1.1819993798
C,0,-8.783253084,-2.0379331855,4.2336200684
H,0,-7.0524233407,-2.6222129725,5.3747662443
H,0,-10.2895839847,-1.3448197428,2.8581498707
H,0,-9.4982943594,-2.3888201249,4.972853382

Sum of electronic and zero-point Energies= -3524.133910
Sum of electronic and thermal Energies= -3524.077462
Sum of electronic and thermal Enthalpies= -3524.076518
Sum of electronic and thermal Free Energies= -3524.230644

3a^{+}
Charge = 1 Multiplicity = 2
Ru,0,4.6570570457,0.2099824085,-1.1109146212
C,0,5.8807478536,0.3629753273,-2.4668887118
O,0,6.6601311276,0.4589684387,-3.3157442115
C,0,6.1080653594,-0.0436016857,0.1568001823
C,0,5.8137921837,-0.2498253254,1.499990301
H,0,4.7601535818,-0.2500277707,1.7846167709
H,0,7.1675286857,-0.0421055729,-0.1158635481
P,0,4.5684233003,2.5931049795,-0.8971155576
P,0,4.3619582451,-2.1137187184,-1.6121780461
C,0,3.6235316633,-2.3705549325,-3.2621574183
C,0,5.8886247885,-3.1181413437,-1.6280651478
C,0,3.2523256078,-2.9928710307,-0.459094419
C,0,3.8704343705,3.3862361292,-2.3861550489
C,0,3.5252379055,3.1844426636,0.4800930676
C,0,6.1744392423,3.4257758343,-0.6396254003

H,0,3.5316643583,4.2791886058,0.5166118574
H,0,2.497524452,2.8348698054,0.3515755635
H,0,3.902792599,2.7871155082,1.4263909641
H,0,3.7650736286,4.466143492,-2.2376790777
H,0,4.5250910701,3.2056070235,-3.2442211984
H,0,2.8930352247,2.9451987892,-2.6004377172
H,0,6.0452537411,4.5120389065,-0.5885643862
H,0,6.6232638325,3.0737324183,0.2937235974
H,0,6.8546793233,3.1876477978,-1.4631718118
H,0,3.180149639,-4.0505165195,-0.7346469364
H,0,3.641256651,-2.9072685067,0.5592696202
H,0,2.2539967164,-2.5474053789,-0.4792056793
H,0,3.4266282752,-3.4333099263,-3.4386992959
H,0,2.6894905625,-1.805610439,-3.3258108778
H,0,4.3037661422,-2.0000026073,-4.0351470088
H,0,5.6696089492,-4.1544213712,-1.9061977788
H,0,6.6012335056,-2.701183297,-2.3462769014
H,0,6.3482513761,-3.102653887,-0.6354725493
H,0,0.9489080185,-0.0942658009,1.7482278931
C,0,0.2345971545,0.0151830977,0.9374026719
C,0,-1.1238132695,-0.0300332857,1.1880447702
C,0,0.7056099176,0.2014819851,-0.3710523418
H,0,-1.4784483686,-0.1764132567,2.2053931685
C,0,-0.2257315145,0.3474820676,-1.413467694
C,0,-1.5809892906,0.2991331731,-1.1571987265
H,0,0.1364625554,0.4998550383,-2.4260673375
H,0,-2.276243523,0.4191078112,-1.9825915623
C,0,2.1368258324,0.2309740678,-0.6516359745
O,0,2.581166824,0.4055589335,-1.8410234589
O,0,3.0077173162,0.0701459429,0.2768631883
C,0,-2.0742551957,0.1010642141,0.1520137326
C,0,-3.4886940525,0.0230094123,0.4879492906
C,0,-4.5254291248,0.0320376334,-0.388519588
H,0,-3.7085146732,-0.0673703776,1.5519353991
Ru,0,-6.4188679659,-0.0927938249,0.1915652991
H,0,-4.2874731096,0.1074696032,-1.4534175346
C,0,-6.9012180083,-0.071972342,-1.5612250305
P,0,-6.5826845973,2.2527156547,0.4089917456
P,0,-6.3204783488,-2.453005976,0.2754637702
O,0,-7.2350407706,-0.0608320278,-2.6752468495
C,0,-8.1802999548,2.7858303351,1.1285889866
C,0,-5.3373133517,2.9951081735,1.5218723928
C,0,-6.4379296163,3.2497794795,-1.1216553644
C,0,-6.0620561408,-3.3394970507,-1.3075594234
C,0,-5.0071617197,-3.124375739,1.3551164558
C,0,-7.8532136706,-3.1970138287,0.947721972
H,0,-8.2060781682,3.8708680686,1.2778634444
H,0,-9.0036489652,2.4971670695,0.4675615472
H,0,-8.3125491263,2.2802871524,2.0899373289
H,0,-5.4760698039,4.0788590996,1.599577307
H,0,-5.434560073,2.5356374854,2.5095053116

H,0,-4.3364611688,2.7778634184,1.1373847382
H,0,-6.5382157226,4.3199614326,-0.9114503845
H,0,-5.4621821332,3.0669063426,-1.5827572718
H,0,-7.2119535198,2.9524008588,-1.8357812864
H,0,-6.0429630773,-4.4243050973,-1.1578221616
H,0,-6.8623503661,-3.0902211954,-2.0110746693
H,0,-5.111271967,-3.0234374729,-1.7485544689
H,0,-5.046325512,-4.2186712115,1.3820075147
H,0,-4.0314647828,-2.8003036335,0.9815279355
H,0,-5.1441940147,-2.7211455863,2.3623483846
H,0,-7.7640771476,-4.2859109847,1.0296947101
H,0,-8.0406197981,-2.7691972265,1.937248041
H,0,-8.7010776969,-2.9563113252,0.2985549724
Cl,0,-6.4830987098,-0.1639701542,2.6073054927
C,0,6.7462244176,-0.4734864298,2.5747509647
C,0,6.2304747101,-0.6808855032,3.8744457766
C,0,8.1495089736,-0.5012672342,2.4003417901
C,0,7.0738655738,-0.907794687,4.9493443413
H,0,5.1532168004,-0.661383154,4.0215722121
C,0,8.9882226207,-0.7273881458,3.4771694197
H,0,8.5789950128,-0.3442596006,1.4155730629
C,0,8.4560708354,-0.9321559626,4.7543215073
H,0,6.6607512007,-1.0662012224,5.940961406
H,0,10.063983873,-0.7460828106,3.32986607
H,0,9.1200087705,-1.109915911,5.59529171

Sum of electronic and zero-point Energies= -3523.924197
Sum of electronic and thermal Energies= -3523.867028
Sum of electronic and thermal Enthalpies= -3523.866084
Sum of electronic and thermal Free Energies= -3524.023213

3b

Ru,0,4.8457813142,0.0315730178,-0.8478111096
C,0,6.0941172382,0.05788248,-2.1587847203
O,0,6.8929913629,0.0757400466,-3.0077081761
C,0,6.2847061221,-0.0076543098,0.5711323995
C,0,5.9978492878,-0.0408873327,1.884261505
H,0,4.972500899,-0.0463076527,2.2542461112
H,0,7.3496820233,-0.0108424283,0.3196981034
P,0,4.840985072,2.373972951,-0.6985332215
P,0,4.8248990348,-2.3174885912,-0.7919310014
C,0,3.74461055,-3.1230711244,-2.0356217596
C,0,6.4411527868,-3.1453597886,-1.0330835911
C,0,4.2436556039,-3.0069699391,0.8005880175
C,0,3.8435826536,3.2430385491,-1.9683966536
C,0,4.1724414299,3.0016260627,0.8852548147
C,0,6.4750454688,3.1935177609,-0.811508073
H,0,4.2016822755,4.0961150012,0.9252130933
H,0,3.1440034781,2.6526190442,1.0101451229

H,0,4.7701929077,2.5873009953,1.7027759939
H,0,3.8175309702,4.3243688426,-1.7937356465
H,0,4.2686231397,3.046607069,-2.9577614273
H,0,2.8263297108,2.841627665,-1.9584895432
H,0,6.3852202973,4.2808206148,-0.7137188069
H,0,7.1204812259,2.8122600813,-0.0142627359
H,0,6.941458395,2.9556771979,-1.7726194877
H,0,4.2360313893,-4.1022997185,0.7804098612
H,0,4.9086676318,-2.6583272135,1.5965542228
H,0,3.2387938565,-2.6314908377,1.0117941763
H,0,3.7172735211,-4.2105957947,-1.9055855371
H,0,2.7336396432,-2.7149683109,-1.9491022619
H,0,4.1118489864,-2.8872638064,-3.0393496935
H,0,6.3482097427,-4.2348296305,-0.9662858155
H,0,6.8528716508,-2.8784531407,-2.0113978717
H,0,7.1360993014,-2.7962011291,-0.2630449525
C,0,7.0194476841,-0.1143866708,2.957272636
H,0,0.969121669,-0.0280576954,1.8202978419
C,0,0.2874885006,-0.0055555987,0.9750588876
C,0,-1.0851775169,-0.0102203269,1.1700870858
C,0,0.8143503752,0.0278768385,-0.319280938
H,0,-1.4845373092,-0.0368259802,2.1817399502
C,0,-0.0649902104,0.0572636652,-1.4091397
C,0,-1.4346701004,0.052656578,-1.209792867
H,0,0.3490989721,0.0834375563,-2.412906568
H,0,-2.093325526,0.0762975892,-2.0736899187
C,0,2.2767849737,0.0312708622,-0.5394297879
O,0,2.7560469443,0.0604865933,-1.7124584665
O,0,3.0739339281,0.0037911903,0.4580997261
F,0,6.8654275615,0.8728846119,3.8689748078
F,0,8.282302204,-0.0328823744,2.5032235938
F,0,6.9314169538,-1.2732778591,3.6541854819
C,0,-1.9824808722,0.0179108418,0.0870692844
C,0,-3.4217073226,0.0078202829,0.3667568076
C,0,-4.4238059317,0.0214472725,-0.5388731484
H,0,-3.6802660886,-0.0162673634,1.4272014045
Ru,0,-6.349795553,-0.0077472998,0.0107531022
H,0,-4.1598866092,0.0446075652,-1.5993124135
C,0,-6.7914331765,0.0330725108,-1.745696964
P,0,-6.3519372126,2.339993506,0.2062369686
P,0,-6.2951040367,-2.3618683453,0.0818877633
O,0,-7.1144043834,0.0586021155,-2.8651537821
C,0,-7.9391462301,3.0302372456,0.8099978181
C,0,-5.1267344005,2.9924229028,1.3959807862
C,0,-6.0125643892,3.3022491091,-1.3165173366
C,0,-5.8842927529,-3.2238985457,-1.4828095036
C,0,-5.0836070515,-3.048676614,1.2666494651
C,0,-7.8767551316,-3.129498636,0.6008397412
H,0,-7.8767639151,4.1152957645,0.9495165891
H,0,-8.7382071899,2.8062826129,0.0961534402
H,0,-8.181888018,2.5513378382,1.7635665008

H,0,-5.1936640971,4.0834332622,1.4700919028
H,0,-5.3150729635,2.538970848,2.3731734303
H,0,-4.1226033074,2.7062734583,1.0699593178
H,0,-6.0213468493,4.3797632339,-1.1197901171
H,0,-5.0302043031,3.018177162,-1.7069822476
H,0,-6.7618799909,3.0706815053,-2.0798726981
H,0,-5.8641186812,-4.3109534037,-1.3497387267
H,0,-6.6182371248,-2.9698037979,-2.2538605664
H,0,-4.9004131994,-2.8872527824,-1.8249100612
H,0,-5.121429261,-4.1435490537,1.2756547274
H,0,-4.0798899934,-2.7176328254,0.9846430519
H,0,-5.3091450927,-2.6580974979,2.2629439818
H,0,-7.785587708,-4.218537996,0.6796886015
H,0,-8.1578484103,-2.714696297,1.573803891
H,0,-8.6637009845,-2.8870765969,-0.1203313027
Cl,0,-6.6080311747,-0.0715185366,2.4186764863

Sum of electronic and zero-point Energies= -3630.160190
Sum of electronic and thermal Energies= -3630.104159
Sum of electronic and thermal Enthalpies= -3630.103215
Sum of electronic and thermal Free Energies= -3630.259639

3b^{+}

Charge = 1 Multiplicity = 2
Ru,0,-4.829569665,0.0547276759,-0.8305139543
C,0,-6.0447970588,0.1549774446,-2.1781538748
O,0,-6.8091280407,0.2192131224,-3.0480806709
C,0,-6.2960374246,-0.031646022,0.5435697293
C,0,-6.0105943356,-0.1120027599,1.8566669673
H,0,-4.9863104193,-0.1418803859,2.2276911348
H,0,-7.3563934906,-0.0016216474,0.279903635
P,0,-4.8832983964,-2.3153963968,-0.8867980027
P,0,-4.862462819,2.4104717615,-0.5279160663
C,0,-3.731144428,3.3419674179,-1.6280305753
C,0,-6.4826147805,3.218843128,-0.7846938983
C,0,-4.3803712716,2.9369776397,1.1552269933
C,0,-3.8721943473,-3.0729283267,-2.2133858005
C,0,-4.2662883305,-3.0886228395,0.6504007413
C,0,-6.5347108937,-3.0664553475,-1.1135498814
H,0,-4.3035737028,-4.1810465661,0.5823025055
H,0,-3.2392435096,-2.7650946319,0.839369282
H,0,-4.8868024472,-2.7557406276,1.4878035329
H,0,-3.8827582587,-4.1661788137,-2.1474625302
H,0,-4.264962349,-2.7678143656,-3.1882016776
H,0,-2.8431731875,-2.7104082295,-2.1391791728
H,0,-6.4742559022,-4.1598362572,-1.1026747737
H,0,-7.1954768165,-2.7373712381,-0.3058950553
H,0,-6.9664123345,-2.7421886241,-2.0654808894
H,0,-4.3764297902,4.0292645964,1.2346155202
H,0,-5.0885739301,2.5235177846,1.8793869367
H,0,-3.3862028614,2.5462780104,1.388986642

H,0,-3.7612825695,4.4150586717,-1.4105412971
H,0,-2.7093984601,2.9732965664,-1.5009756642
H,0,-4.0191553764,3.1770258843,-2.6706977612
H,0,-6.4211080949,4.2948743343,-0.5906073495
H,0,-6.8228761081,3.0600774396,-1.8125914514
H,0,-7.2187084894,2.7761369725,-0.1066242655
H,0,-0.9380634902,-0.0971922406,1.8035455392
C,0,-0.2679230311,-0.0556610478,0.9506851682
C,0,1.1017294727,-0.0669493821,1.119855929
C,0,-0.8144150465,0.0109954968,-0.3395471722
H,0,1.5246439885,-0.1175363011,2.1200717228
C,0,0.0391157406,0.0650462541,-1.4548859683
C,0,1.4074983498,0.0520083909,-1.2873104569
H,0,-0.4015304535,0.117672767,-2.4455436692
H,0,2.0470641459,0.0948700584,-2.1635512221
C,0,-2.2799551699,0.0258801548,-0.5272373332
O,0,-2.7745365055,0.0991668799,-1.693000526
O,0,-3.0558896142,-0.0337832209,0.4799396225
C,0,1.9792940264,-0.0140831865,0.0084068852
C,0,3.3942236215,-0.028425481,0.2647234717
C,0,4.4010972153,0.0083487216,-0.6840042751
H,0,3.6856630843,-0.0715003233,1.3134370543
Ru,0,6.2587295799,-0.0041504284,-0.1657639217
H,0,4.1009632617,0.0481247491,-1.7338482263
C,0,6.6990487375,0.0401197691,-1.9445546112
P,0,6.4505053312,-2.3809685351,-0.0409292111
P,0,6.4167400923,2.3672659072,0.0665209616
O,0,7.0061835849,0.0686877059,-3.0594088017
C,0,8.0677055786,-2.87076796,0.6557950429
C,0,5.2196512342,-3.1713403902,1.0498652679
C,0,6.3281864753,-3.3082431025,-1.6131427133
C,0,6.2695891878,3.3554648507,-1.4652070903
C,0,5.1772798076,3.0898328444,1.1942462076
C,0,8.0288137718,2.8540941043,0.7778358318
H,0,8.1310366667,-3.9601917849,0.7509399305
H,0,8.8794834309,-2.5241695378,0.008604058
H,0,8.1818578654,-2.410531966,1.6415958215
H,0,5.4083307747,-4.2476130104,1.1236212448
H,0,5.2842234977,-2.7160263971,2.0417912987
H,0,4.2142198922,-3.0068419538,0.651113647
H,0,6.4578494251,-4.3821386298,-1.4417381339
H,0,5.3479045358,-3.1389316102,-2.0693434751
H,0,7.0962818067,-2.9669837111,-2.3137563248
H,0,6.3671554794,4.4246306505,-1.2495893165
H,0,7.0473563823,3.0651795437,-2.1779765206
H,0,5.2946699097,3.1741671864,-1.9283418169
H,0,5.3558918457,4.1626566389,1.3227390573
H,0,4.1741201782,2.9367197761,0.7853628832
H,0,5.2434109537,2.5861828592,2.1625710438
H,0,8.0787267047,3.9401938376,0.9119856032
H,0,8.151625407,2.3613968562,1.7467170116

H,0,8.8437754651,2.5410345451,0.117698843
Cl,0,6.3569090528,-0.058707936,2.2331181711
C,0,-7.0368290819,-0.1077015859,2.9353362686
F,0,-6.9320947858,1.0072050432,3.6912612332
F,0,-8.2926994963,-0.1546734233,2.4696049688
F,0,-6.8754254398,-1.1520160364,3.7703982286

Sum of electronic and zero-point Energies= -3629.932856
Sum of electronic and thermal Energies= -3629.876401
Sum of electronic and thermal Enthalpies= -3629.875457
Sum of electronic and thermal Free Energies= -3630.032419

3c

Ru,0,-5.0508309008,-0.0056151049,0.1988807846
Cl,0,-4.6835532147,-1.5166565412,2.0073562089
Cl,0,-4.9886364825,-1.857664259,-1.3006803036
C,0,-5.4822943827,1.853858636,1.2996526687
C,0,-5.0488226896,2.1454804712,-0.0237374286
C,0,-5.7118353395,1.5993218925,-1.1578735897
C,0,-6.7645604894,0.6717202339,-0.9455493491
C,0,-7.2074956829,0.3441208494,0.3641023522
C,0,-6.5377188121,0.92187587,1.4762041327
H,0,-7.1669845245,0.1253998592,-1.7921197252
H,0,-7.9499882272,-0.4305621579,0.5137587248
H,0,-5.3455864232,1.7936382145,-2.1600027862
H,0,-4.1612820559,2.7549995191,-0.1700073998
H,0,-4.9422436162,2.2403059673,2.1569994329
H,0,-6.7676616986,0.5660384729,2.4750169505
H,0,-2.6493741439,0.1693274288,2.032964758
C,0,-2.1417227642,0.1448151068,1.0753195133
C,0,-0.7647827807,0.2081619398,0.9842626406
C,0,-2.3556075321,-0.0759922111,-1.2045855126
C,0,-0.1294297081,0.1160746554,-0.2665577374
H,0,-0.1927562196,0.3149425467,1.9001343592
C,0,-0.9841153938,-0.0177770175,-1.373031304
H,0,-3.025910283,-0.2291109116,-2.0429046357
H,0,-0.5726272983,-0.10242549,-2.3748853567
N,0,-2.9390461332,0.0074965643,0.0013857552
C,0,1.3155796727,0.1257082173,-0.471441549
C,0,2.2575158092,0.1081586086,0.5001015933
H,0,1.6345441819,0.1002727973,-1.5140661371
Ru,0,4.2048844192,0.0179709599,0.088216662
H,0,1.9174034235,0.1145700892,1.5392690353
C,0,4.5331410421,0.0351900443,1.8725310112
P,0,4.338574498,2.3649364106,-0.0944793011
P,0,4.0835683307,-2.3384344559,-0.0067185551
O,0,4.7825110238,0.0468795107,3.009788541
C,0,5.9907659853,2.9622989393,-0.615137677
C,0,3.2098524757,3.0818469929,-1.3406017651
C,0,3.9793639943,3.3420283281,1.4142735912

C,0,3.6151111,-3.2071615013,1.5369485821
C,0,2.8968204381,-2.9901024529,-1.2342677367
C,0,5.6669566676,-3.1257998963,-0.489361744
H,0,6.000563451,4.0502040041,-0.7455778904
H,0,6.7393808737,2.6848786568,0.1337965474
H,0,6.2500715201,2.477107907,-1.561074212
H,0,3.3247951144,4.1696590786,-1.3983565981
H,0,3.4324329303,2.6291966834,-2.3109513769
H,0,2.1784300796,2.8337868682,-1.0734585516
H,0,4.0748527596,4.4170139272,1.2268449321
H,0,2.9589047517,3.1266389752,1.7464331853
H,0,4.6653590335,3.0556697004,2.2174855848
H,0,3.58050262,-4.2918067485,1.389254304
H,0,4.3327210883,-2.9754632276,2.3300277098
H,0,2.627491374,-2.8613799843,1.8584589306
H,0,2.9262801272,-4.0848065658,-1.260248359
H,0,1.8869916724,-2.6596406931,-0.9752958538
H,0,3.1534633049,-2.5869069432,-2.2178377086
H,0,5.5587468778,-4.2125417955,-0.5772752466
H,0,5.9795100557,-2.7106308418,-1.4524001141
H,0,6.4393598407,-2.9022471268,0.253340201
Cl,0,4.5663906936,-0.0412174854,-2.3039491838

Sum of electronic and zero-point Energies= -3161.160738
Sum of electronic and thermal Energies= -3161.123121
Sum of electronic and thermal Enthalpies= -3161.122177
Sum of electronic and thermal Free Energies= -3161.234204

3c^{+}

Charge = 1 Multiplicity = 2
Ru,0,-5.0797734057,-0.0221333676,0.0487284645
Cl,0,-4.8025647726,-1.4037694684,1.8850942866
Cl,0,-4.9848623411,-1.7239990198,-1.5166089143
C,0,-5.246166113,2.1549588029,0.5004537119
C,0,-5.3791372487,1.9721545915,-0.9144751863
C,0,-6.3690727914,1.1083388674,-1.4117812697
C,0,-7.2180959654,0.3799992708,-0.5188529072
C,0,-7.086667641,0.5636595893,0.8650985748
C,0,-6.1120101546,1.4789049915,1.3759190445
H,0,-7.9055090311,-0.3614492743,-0.9105765207
H,0,-7.6695026364,-0.0396555295,1.5524330975
H,0,-6.4156714462,0.8991269035,-2.4755204968
H,0,-4.6890609096,2.4630183711,-1.5925931656
H,0,-4.4532893034,2.7828574058,0.893145221
H,0,-5.9637771449,1.5535540502,2.4481926203
H,0,-2.725479161,0.1150997405,1.9679260067
C,0,-2.2103441041,0.1044774382,1.0155515279
C,0,-0.8350839495,0.1445005706,0.9562804559
C,0,-2.3766284091,-0.0050433338,-1.2841500402
C,0,-0.1668781524,0.0966804687,-0.2864806321

H,0,-0.2876908672,0.208927857,1.8902754534
C,0,-1.0061564802,0.036169856,-1.4190942404
H,0,-3.019297679,-0.087227747,-2.1519863555
H,0,-0.5772660643,0.0055071109,-2.4161538643
N,0,-2.9917094277,0.0267677304,-0.0835186693
C,0,1.2643406718,0.0956129367,-0.4637232313
C,0,2.1955345496,0.0647417195,0.5433151728
H,0,1.6137920796,0.0896054621,-1.4946335477
Ru,0,4.1090738459,-0.0008306501,0.18638707
H,0,1.8203220886,0.0618061003,1.5708552481
C,0,4.3982325374,-0.0455027455,1.9915623072
P,0,4.3469088984,2.3618748733,0.073496887
P,0,4.1530876821,-2.3728189579,-0.0145729817
O,0,4.6048673439,-0.0725925961,3.1314540956
C,0,6.0219879462,2.8413071672,-0.4846109918
C,0,3.2263472229,3.1788506631,-1.1147402008
C,0,4.1053011935,3.2985160521,1.6274809048
C,0,3.8341530917,-3.3419469731,1.5045208324
C,0,2.9726692602,-3.0528036381,-1.2302065218
C,0,5.7869679643,-2.9588180525,-0.5908446081
H,0,6.1070236528,3.9299395386,-0.57312904
H,0,6.7726633698,2.484148042,0.2274614416
H,0,6.2148806605,2.3802585589,-1.4577849957
H,0,3.4310392215,4.2536245134,-1.1632650568
H,0,3.3712625825,2.7284223159,-2.1005768415
H,0,2.1887438158,3.0190863927,-0.8069728667
H,0,4.2537567237,4.37152504,1.4667283186
H,0,3.090785375,3.1320107392,2.0032810093
H,0,4.8113098903,2.9525835906,2.3886490078
H,0,3.9008683899,-4.4165054172,1.3041657357
H,0,4.5609369445,-3.0794070795,2.2793292797
H,0,2.8329628023,-3.1133841672,1.8831574886
H,0,3.0970471209,-4.1368926619,-1.3232106511
H,0,1.9497419036,-2.832350939,-0.9109089192
H,0,3.1484256953,-2.5752535086,-2.1980021482
H,0,5.7897899217,-4.0477494223,-0.7108398282
H,0,6.0135436912,-2.4853863301,-1.5507047093
H,0,6.5621356069,-2.6795455552,0.1296736416
Cl,0,4.3592547188,0.0379446744,-2.2067783317

Sum of electronic and zero-point Energies= -3160.919121
Sum of electronic and thermal Energies= -3160.880977
Sum of electronic and thermal Enthalpies= -3160.880032
Sum of electronic and thermal Free Energies= -3160.994564

3a^{2+}

Charge = 2 Multiplicity = 3
Ru,0,-4.70493,-0.84852,0.66879
C,0,-5.93686,-1.89573,1.52513
O,0,-6.71867,-2.55404,2.06173
C,0,-6.14665,0.16117,-0.13924
C,0,-5.86227,1.22733,-0.98968
H,0,-4.81072,1.45289,-1.17574
H,0,-7.20524,-0.05299,0.03249
P,0,-4.58662,0.57548,2.59489
P,0,-4.59518,-2.47168,-1.09509
C,0,-3.86964,-4.05445,-0.54422
C,0,-6.2044,-2.93496,-1.82375
C,0,-3.5845,-1.96338,-2.53005
C,0,-3.62482,-0.15598,3.96395
C,0,-3.80727,2.19648,2.27582
C,0,-6.20115,0.99075,3.34121
H,0,-3.78373,2.79535,3.1924
H,0,-2.78828,2.06012,1.90527
H,0,-4.37982,2.73064,1.51188
H,0,-3.53927,0.55064,4.79619
H,0,-4.12174,-1.06435,4.31826
H,0,-2.62887,-0.43146,3.60807
H,0,-6.0686,1.62583,4.22348
H,0,-6.82062,1.52054,2.61116
H,0,-6.72368,0.07685,3.64051
H,0,-3.5875,-2.75015,-3.29201
H,0,-3.99187,-1.04384,-2.95992
H,0,-2.55439,-1.76911,-2.22066
H,0,-3.78411,-4.75257,-1.38374
H,0,-2.88143,-3.87459,-0.11233
H,0,-4.50334,-4.50384,0.22661
H,0,-6.07351,-3.70522,-2.59105
H,0,-6.87173,-3.32118,-1.0471
H,0,-6.67101,-2.05555,-2.27714
H,0,-0.91772,1.33059,-1.11593
C,0,-0.21317,0.68467,-0.60174
C,0,1.15121,0.86608,-0.74793
C,0,-0.69627,-0.34204,0.21823
H,0,1.52567,1.66442,-1.38353
C,0,0.20498,-1.18516,0.88581
C,0,1.56746,-1.00485,0.74089
H,0,-0.18507,-1.97769,1.51659
H,0,2.24429,-1.66918,1.26892
C,0,-2.15752,-0.54388,0.3909
O,0,-2.59034,-1.47503,1.13515
O,0,-2.98949,0.21558,-0.20198
C,0,2.07445,0.02898,-0.08038
C,0,3.4821,0.28582,-0.27516
C,0,4.53617,-0.41741,0.2985
H,0,3.72654,1.11729,-0.93348

Ru,0,6.34286,0.09364,-0.06098
H,0,4.2907,-1.25361,0.95671
C,0,6.87425,-1.27255,1.06132
P,0,6.63707,1.74756,1.65754
P,0,6.74658,-1.22529,-2.02677
O,0,7.22548,-2.11934,1.75948
C,0,8.23086,2.60209,1.41102
C,0,5.37043,3.05786,1.64624
C,0,6.67844,1.13891,3.37869
C,0,6.8265,-3.03452,-1.79396
C,0,5.5282,-0.97119,-3.35833
C,0,8.35903,-0.76096,-2.74515
H,0,8.36361,3.37686,2.17425
H,0,9.06084,1.89237,1.48443
H,0,8.24261,3.06232,0.41899
H,0,5.6211,3.82803,2.38359
H,0,5.32554,3.5032,0.649
H,0,4.39429,2.62883,1.89051
H,0,6.8409,1.97102,4.07206
H,0,5.73108,0.65117,3.62779
H,0,7.48614,0.41217,3.50706
H,0,7.04479,-3.53033,-2.74594
H,0,7.61035,-3.29277,-1.07569
H,0,5.87077,-3.40681,-1.41269
H,0,5.8296,-1.5279,-4.25224
H,0,4.54481,-1.32077,-3.03091
H,0,5.46927,0.09502,-3.59185
H,0,8.54476,-1.34212,-3.65514
H,0,8.35103,0.3051,-2.98952
H,0,9.16665,-0.95745,-2.03313
Cl,0,6.23859,1.95196,-1.56228
C,0,-6.8051,2.08017,-1.65579
C,0,-6.30264,3.12145,-2.47401
C,0,-8.21039,1.93984,-1.53631
C,0,-7.15857,3.98109,-3.1387
H,0,-5.22624,3.23874,-2.5739
C,0,-9.06094,2.8013,-2.20301
H,0,-8.63056,1.15215,-0.91864
C,0,-8.54104,3.82415,-3.00528
H,0,-6.75914,4.77522,-3.7619
H,0,-10.13589,2.68503,-2.10464
H,0,-9.2154,4.49777,-3.52577

Sum of electronic and zero-point Energies= -3523.634914
Sum of electronic and thermal Energies= -3523.578011
Sum of electronic and thermal Enthalpies= -3523.577067
Sum of electronic and thermal Free Energies= -3523.733949

3b^{2+}
Charge = 2 Multiplicity = 3

Ru,0,5.0679870783,0.0327681094,-0.6097194754
C,0,6.4599431332,0.0685620112,-1.8165127663
O,0,7.3370279525,0.0919566978,-2.5612216377
C,0,6.3876819369,0.0204689565,0.829643714
C,0,5.9243580089,-0.0439984819,2.1120609262
H,0,4.8614059631,-0.0825834925,2.3433537776
H,0,7.4707135923,0.0564381028,0.6985819102
P,0,4.9029217894,2.4292345343,-0.836391756
P,0,4.9301469097,-2.355218653,-0.9367019459
C,0,4.4725495684,-2.7801010231,-2.6497684113
C,0,6.4919429682,-3.2415125519,-0.6142912553
C,0,3.6916059922,-3.1776201346,0.1208294557
C,0,4.4434890369,2.9185245569,-2.5317144074
C,0,3.6544589692,3.1945215187,0.2517041784
C,0,6.4543085787,3.3193053674,-0.4763623311
H,0,3.6710235724,4.2824457948,0.1248589744
H,0,2.6553757706,2.8251145791,0.0056171947
H,0,3.8689486537,2.9503493652,1.2957496421
H,0,4.312944328,4.0042704098,-2.592054615
H,0,5.2271717432,2.6180777736,-3.2338278849
H,0,3.5124792403,2.4201645856,-2.8152949238
H,0,6.3177035617,4.3951302579,-0.6301557823
H,0,6.7554606002,3.1414893646,0.560083544
H,0,7.2531389757,2.9677465169,-1.1364212159
H,0,3.7166422173,-4.2588786227,-0.0529739576
H,0,3.9074697306,-2.977306694,1.1739219987
H,0,2.6887478604,-2.8060700909,-0.105934958
H,0,4.3527505938,-3.8637660123,-2.7538629548
H,0,3.5359368727,-2.2801511198,-2.9113107225
H,0,5.2517378919,-2.443469856,-3.3403852116
H,0,6.3667453035,-4.3120207234,-0.8093585179
H,0,7.2855365328,-2.8558089214,-1.2614591813
H,0,6.7931239414,-3.1004544203,0.4277799164
C,0,6.8253108445,-0.0866959409,3.3140856034
H,0,1.1602626807,-0.0506423114,1.9539717445
C,0,0.4952984487,-0.0315423194,1.0964411633
C,0,-0.8779008569,-0.0412970525,1.2672472666
C,0,1.0367127197,0.0035519383,-0.1948155044
H,0,-1.2964755537,-0.0684899087,2.2698792172
C,0,0.184941251,0.0282491811,-1.3097873402
C,0,-1.1870971769,0.0190930008,-1.1387706568
H,0,0.6167899472,0.0546881541,-2.3053400305
H,0,-1.8265701363,0.038785376,-2.0156857421
C,0,2.5054923571,0.0147399134,-0.383195689
O,0,3.0171534603,0.0436732181,-1.5467154786
O,0,3.286894423,-0.0041385882,0.6231370757
F,0,6.5039342238,0.9005698206,4.157611664
F,0,8.1133399362,0.0385847805,2.9891176965
F,0,6.663983432,-1.2510943049,3.9556279612
C,0,-1.7516458533,-0.0155982379,0.1569516233
C,0,-3.1733736392,-0.025008188,0.4214474402

C,0,-4.1928992556,0.0024769878,-0.5226086806
H,0,-3.4563670976,-0.0550102713,1.4717930631
Ru,0,-6.0207930919,-0.0084933937,0.0438008821
H,0,-3.9128295839,0.0319708687,-1.5779012324
C,0,-6.4965085043,0.044283265,-1.7402929248
P,0,-6.3938132177,2.3497772756,0.3145784074
P,0,-6.4171597109,-2.3747833976,0.1771810991
O,0,-6.812595493,0.0768252973,-2.8475824065
C,0,-8.0153601864,2.6150711527,1.1081944412
C,0,-5.1755440046,3.1690398784,1.3941771343
C,0,-6.4356838617,3.3531557956,-1.210480764
C,0,-6.4674599951,-3.2884000062,-1.403062596
C,0,-5.2113529869,-3.2696273234,1.2099872785
C,0,-8.043509115,-2.6660489468,0.9516741304
H,0,-8.1898082612,3.6875210202,1.2496606679
H,0,-8.8182690949,2.2092492315,0.4848636329
H,0,-8.0286999434,2.1124882133,2.0793581404
H,0,-5.4697005145,4.209543504,1.5691754032
H,0,-5.1257587706,2.635614373,2.3470800935
H,0,-4.190123797,3.1485898041,0.9196850584
H,0,-6.654753401,4.3987671166,-0.9685698593
H,0,-5.4693609702,3.3039447379,-1.7215793747
H,0,-7.2073193936,2.981741647,-1.8914771331
H,0,-6.6962256458,-4.3440614199,-1.2212844058
H,0,-7.2356158593,-2.8713635692,-2.0612030856
H,0,-5.5008098493,-3.2191293395,-1.9111945484
H,0,-5.5141763146,-4.316947836,1.3161412098
H,0,-4.2225971317,-3.2266015232,0.7440548734
H,0,-5.1638144329,-2.7989511253,2.1954583888
H,0,-8.2305577234,-3.7426752497,1.0320637144
H,0,-8.053367473,-2.2188201893,1.9496085912
H,0,-8.8401910102,-2.2163547857,0.3508698322
Cl,0,-5.973285685,-0.0777170276,2.4322436349

Sum of electronic and zero-point Energies= -3629.628936
Sum of electronic and thermal Energies= -3629.572236
Sum of electronic and thermal Enthalpies= -3629.571292
Sum of electronic and thermal Free Energies= -3629.729695

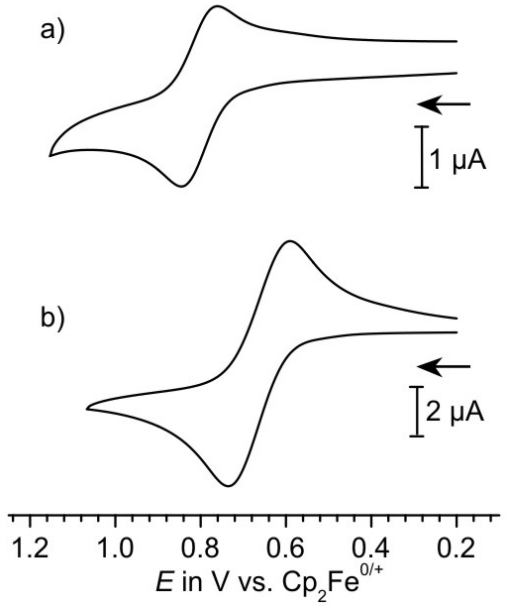

Figure S1. Cyclic voltammograms of a) **1b** and b) **2b** in CH_2Cl_2/NBu_4PF_6 (0.1 M) at a sweep rate of ν = 0.1 V/s.

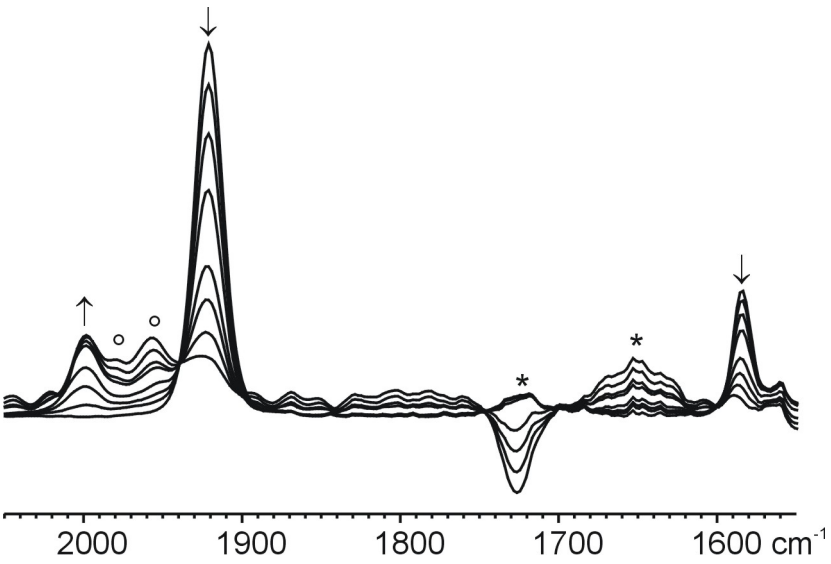

Figure S2. Spectroscopic changes in the infrared during electrochemical oxidation of complex **1b** (DCE/NBu_4PF_6 (0.2 M) at r. t.). The star symbol indicates artefacts due to solvent degradation; the circle symbols indicate the signals of decomposition products.

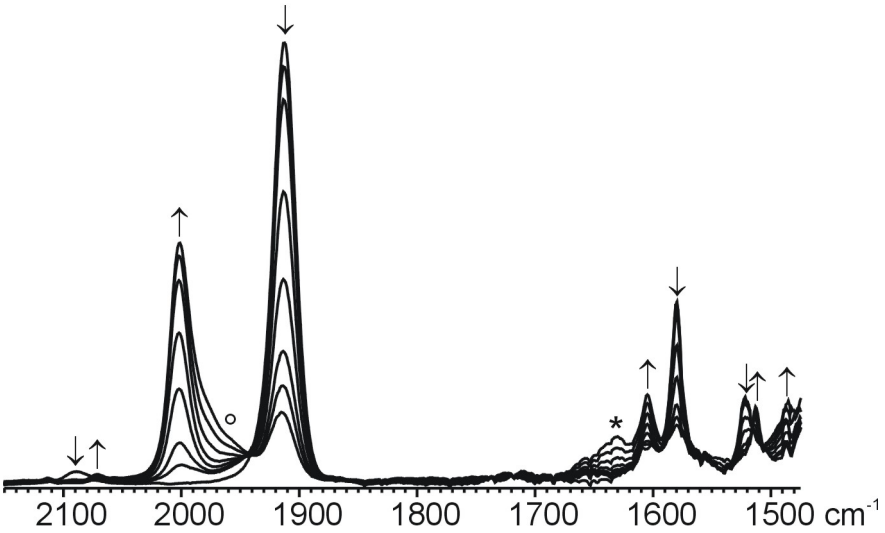

Figure S3. Spectroscopic changes in the infrared during electrochemical oxidation of complex **2b** (DCE/NBu_4PF_6 (0.2 M) at r. t.). The star symbol indicates artefacts due to solvent degradation; the circle symbols indicate the signals of a decomposition product.

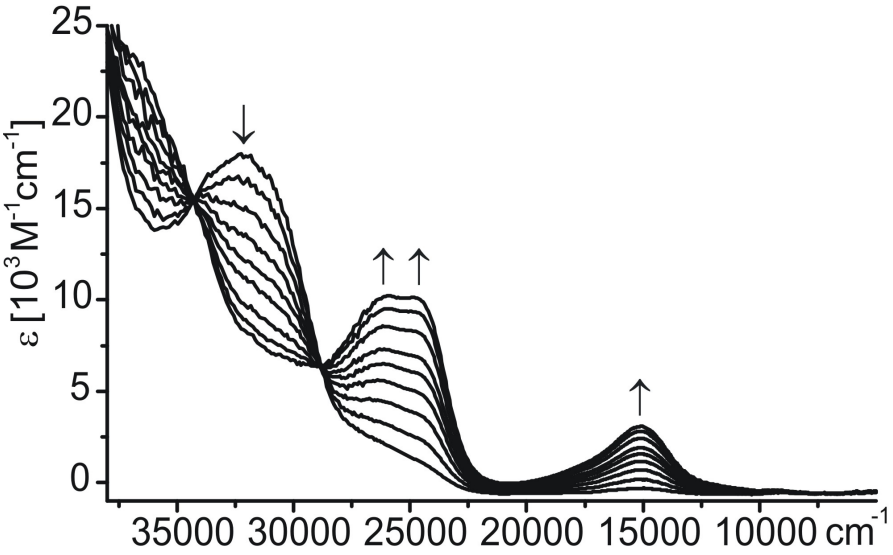

Figure S4. Changes in the UV/Vis/NIR spectra upon the oxidation of complex **2a** to **2a**$^{\bullet+}$ (DCE/NBu_4PF_6 (0.2 M) at r. t.).

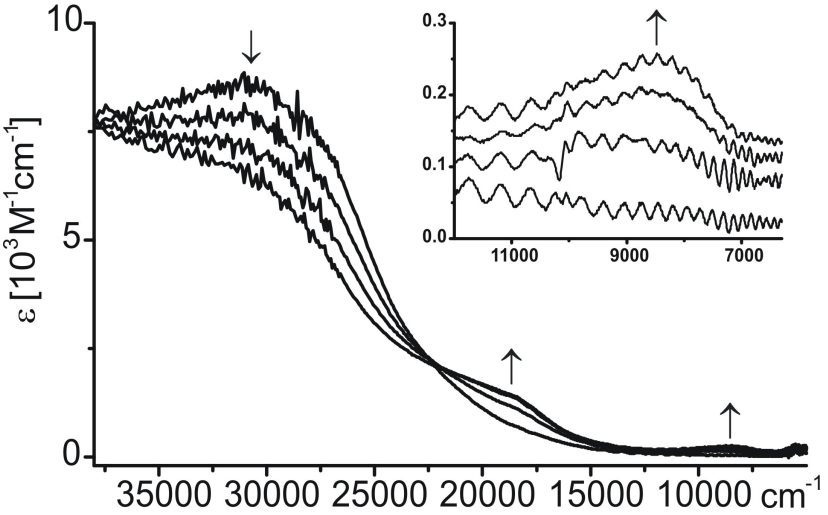

Figure S5. Changes in the UV/Vis/NIR spectra of complex **2b** upon oxidation to **2b**$^{\bullet+}$ (DCE/NBu_4PF_6 (0.2 M) at r. t.); inset: low energy region magnified.

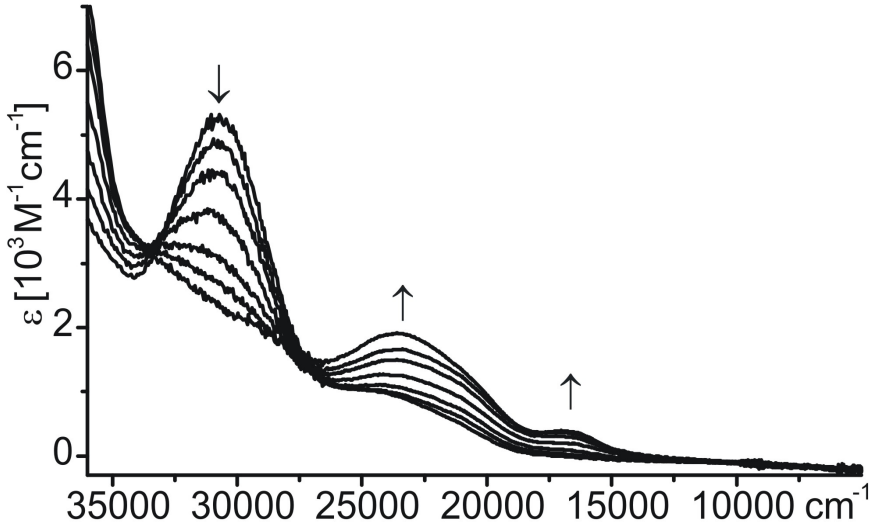

Figure S6. Changes in the UV/Vis/NIR spectra upon the oxidation of complex **2c** to **2c**$^{\bullet+}$ (DCE/NBu_4PF_6 (0.2 M) at r. t.).

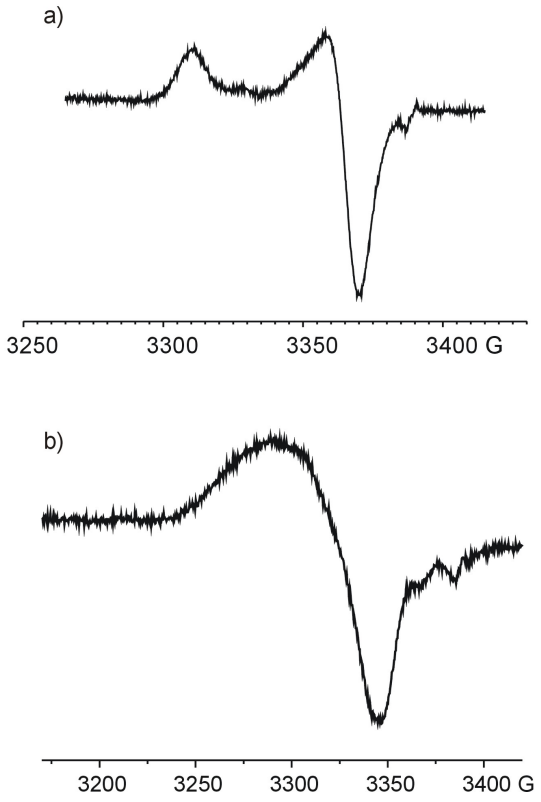

Figure S7. EPR spectra of electrogenerated radical cations a) $\mathbf{1b}^{\bullet+}$ and b) $\mathbf{2b}^{\bullet+}$ in CH_2Cl_2/NBu_4PF_6 (0.2 M) at T = 110 K.

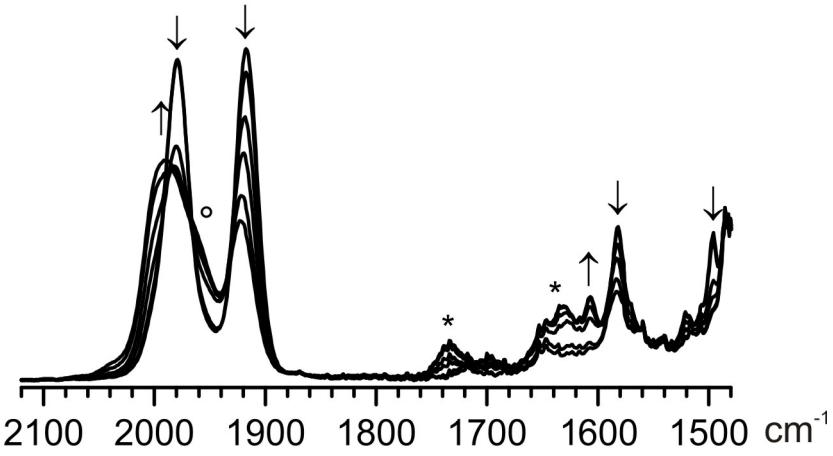

Figure S8. Spectroscopic changes in the infrared during electrochemical oxidation of complex $\mathbf{3b}^{\bullet+}$ to dioxidized $\mathbf{3b}^{2+}$ (DCE/NBu_4PF_6 (0.2 M)) at r. t. The star symbol indicates artefacts due to solvent degradation; the circle symbols indicate the signals of a decomposition product.

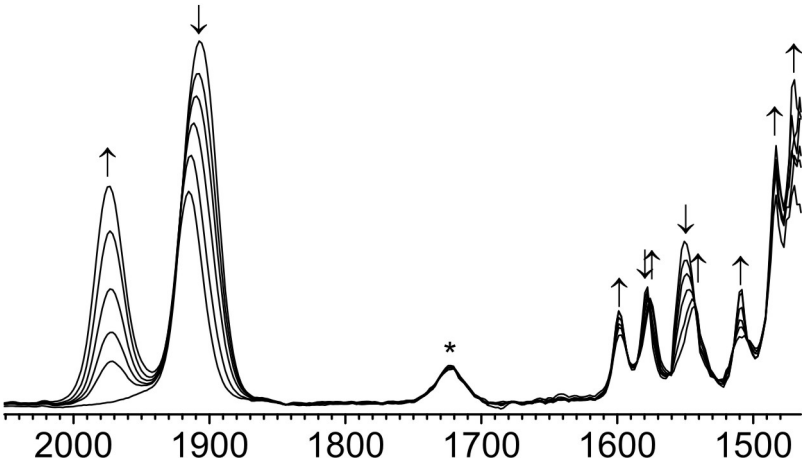

Figure S9. Spectroscopic changes in the infrared during electrochemical oxidation of complex **3a** to oxidized **3a**$^{\bullet+}$ (DCE, NBu_4PF_6 (0.2 M) at r. t.). The star symbol indicates artefacts due to solvent degradation.

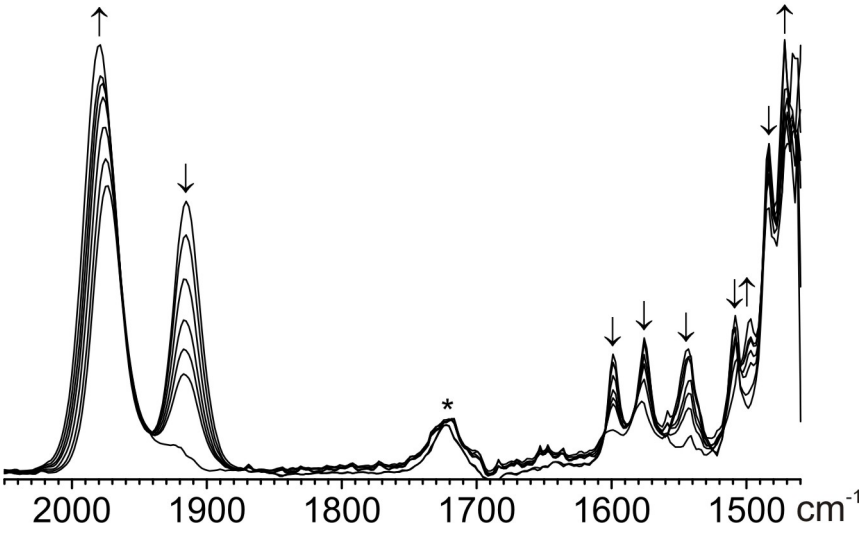

Figure S10. Spectroscopic changes in the infrared during electrochemical oxidation of complex **3a**$^{\bullet+}$ to dioxidized **3a**$^{2+}$ (DCE/NBu_4PF_6 (0.2 M) at r. t.). The star symbol indicates artefacts due to solvent degradation.

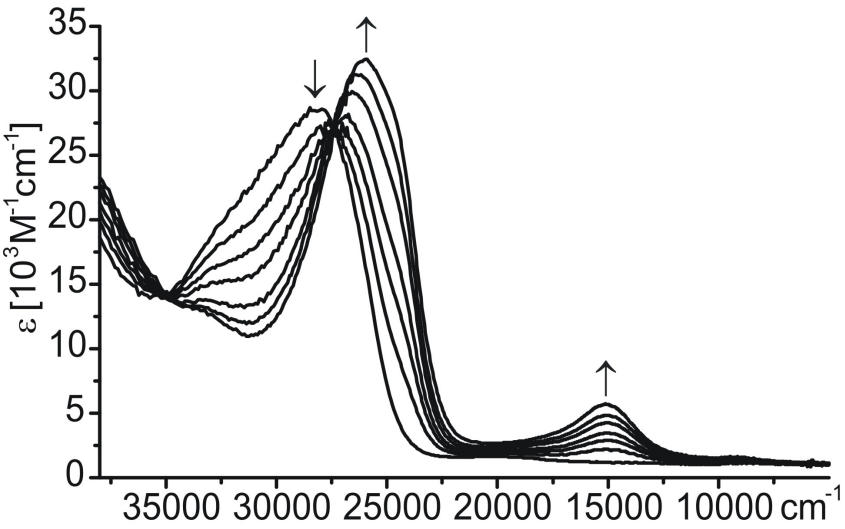

Figure S11. Changes in the UV/Vis/NIR spectra upon the oxidation of complex **3a** to **3a**$^{\bullet+}$ (DCE/NBu_4PF_6 (0.2 M) at r. t.).

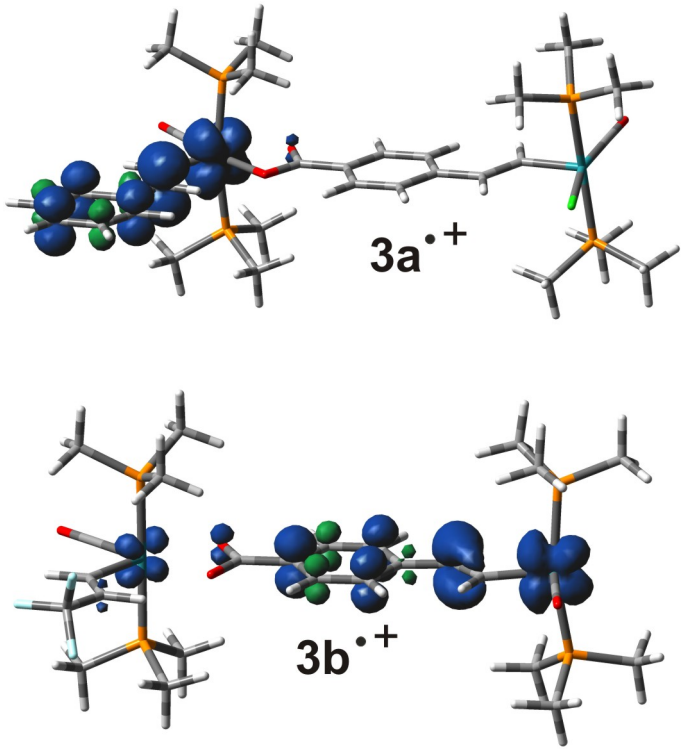

Figure S12. Calculated spin densities for radical cations **3a**$^{\bullet+}$ and **3b**$^{\bullet+}$.

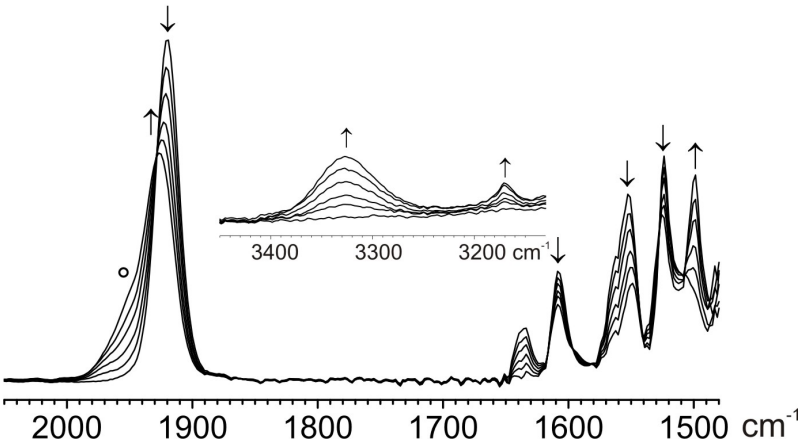

Figure S13. Spectroscopic changes in the infrared during electrochemical oxidation of complex **3c** to **3c**$^{\bullet+}$ (DCE/NBu_4PF_6 (0.2 M) at r. t.). The circle symbols indicate the signals of a decomposition product.

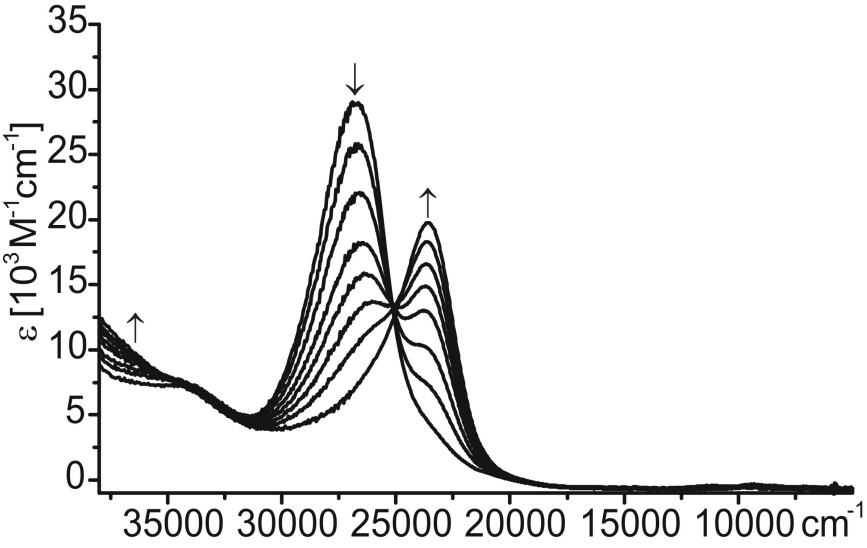

Figure S14. Changes in the UV/Vis/NIR spectra of complex **3c** upon oxidation to **3c**$^{\bullet+}$ (DCE/NBu_4PF_6 (0.2 M) at r. t.)

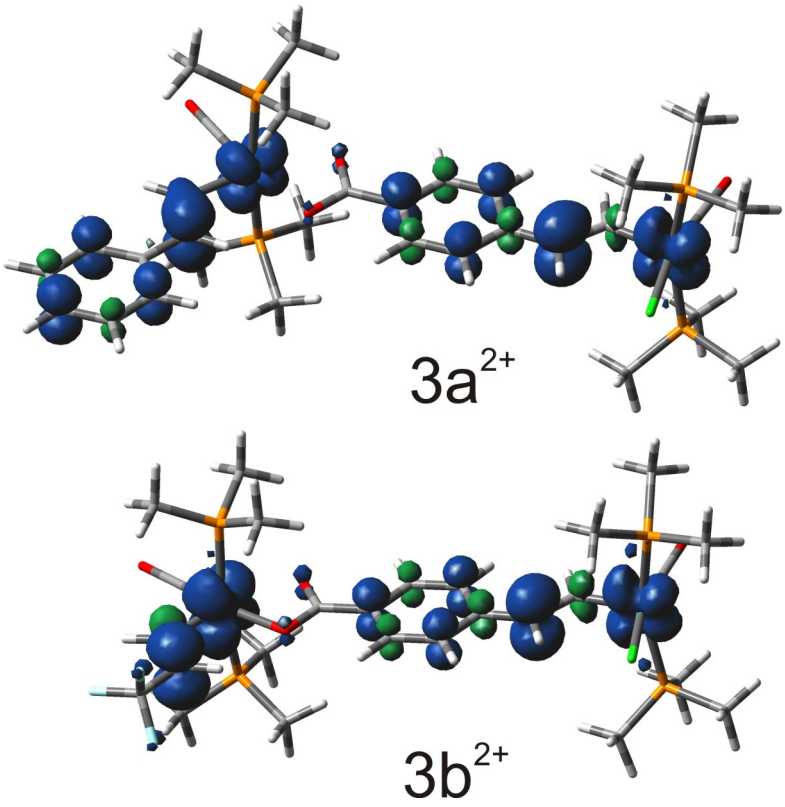

Figure S15. Calculated spin densities for dications **3a**$^{\bullet\bullet 2+}$ and **3b**$^{\bullet\bullet 2+}$.