

Supporting Information (Coordinates of DFT Optimized Structures)

Solvent-Dependent Transition from Concerted Electron-Proton to Proton Transfer in Photoinduced Reactions between Phenols and Polypyridine Ru Complexes with Proton- Accepting Sites

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Optimized Structures at M06 Level of Theory in CH₂Cl₂

p-MeO-PhOH (S=0)

C	0.31980	0.29384	0.00093
C	1.70503	0.36489	0.00140
C	2.35472	1.60189	0.00072
C	1.59350	2.77173	-0.00050
C	0.20201	2.69759	-0.00097
C	-0.44220	1.46459	-0.00022
H	-0.17671	-0.67744	0.00146
H	2.30907	-0.54126	0.00232
H	2.06902	3.74962	-0.00115
H	-0.39867	3.60595	-0.00193
O	-1.80280	1.45638	-0.00068
H	-2.11401	0.53636	-0.00015
O	3.71412	1.56176	0.00125
C	4.40403	2.78988	0.00096
H	4.17510	3.38757	0.89634
H	5.47047	2.54602	0.00130
H	4.17553	3.38686	-0.89501

p-MeO-PhOH⁺ (S=1/2)

C	0.33688	0.25797	0.00082
C	1.69624	0.34282	0.00088
C	2.33723	1.61982	0.00012
C	1.56792	2.81546	-0.00126
C	0.20594	2.72735	-0.00124
C	-0.42762	1.45362	0.00000
H	-0.16864	-0.70610	0.00145
H	2.32644	-0.54322	0.00160
H	2.05168	3.78765	-0.00235
H	-0.42263	3.61452	-0.00213
O	-1.74416	1.45536	0.00026
H	-2.10270	0.54326	0.00108
O	3.64608	1.58316	0.00090
C	4.41206	2.79833	0.00140
H	4.19275	3.38141	0.90220
H	5.45597	2.48386	0.00247
H	4.19457	3.38097	-0.90012

p-MeO-PhO⁻ (S=0)

C	0.32036	0.29437	0.00068
C	1.70409	0.36778	0.00140
C	2.36500	1.60040	0.00093
C	1.59492	2.76417	-0.00024
C	0.20218	2.69210	-0.00095
C	-0.53167	1.45779	-0.00047
H	-0.17030	-0.68242	0.00107
H	2.31241	-0.53998	0.00233
H	2.07366	3.74434	-0.00067
H	-0.38007	3.61748	-0.00190
O	-1.79753	1.39136	-0.00109
O	3.74713	1.55795	0.00160
C	4.41306	2.78625	0.00086

H	4.17745	3.39094	0.89354
H	5.48710	2.56873	0.00138
H	4.17805	3.38952	-0.89294

p-MeO-PhO[•] (S=1/2)

C	0.33964	0.26412	0.00081
C	1.70115	0.34762	0.00132
C	2.34375	1.61209	0.00069
C	1.58040	2.79913	-0.00053
C	0.20994	2.72241	-0.00104
C	-0.49152	1.45435	-0.00034
H	-0.16835	-0.69904	0.00130
H	2.33210	-0.54013	0.00223
H	2.07088	3.76968	-0.00110
H	-0.40002	3.62480	-0.00199
O	-1.73923	1.39077	-0.00080
O	3.67958	1.57307	0.00132
C	4.40561	2.79383	0.00097
H	4.18449	3.38628	0.89833
H	5.46217	2.51647	0.00154
H	4.18524	3.38533	-0.89719

p-Ph-PhOH (S=0)

C	-1.54302	0.04459	0.31426
C	-0.15424	0.05551	0.32030
C	0.57032	1.20646	-0.01345
C	-0.15857	2.35489	-0.35602
C	-1.54499	2.35912	-0.36518
C	-2.24576	1.19990	-0.02832
H	-2.08867	-0.86003	0.58577
H	0.37703	-0.84904	0.61570
H	0.37226	3.26164	-0.64549
H	-2.10410	3.25183	-0.64079
C	2.04818	1.21111	-0.00385
C	2.76407	2.36377	0.34830
C	2.77591	0.06295	-0.34643
C	4.15444	2.36920	0.35538
H	2.22261	3.26247	0.64364
C	4.16622	0.06571	-0.33330
H	2.24406	-0.83871	-0.65016
C	4.86336	1.21953	0.01614
H	4.68761	3.27629	0.63751
H	4.70884	-0.83803	-0.60810
H	5.95230	1.22278	0.02386
O	-3.59871	1.25413	-0.05006
H	-3.95941	0.38475	0.19226

p-Ph-PhOH⁺ (S=1/2)

C	-1.51572	-0.00739	0.20967
C	-0.14947	0.00270	0.20611
C	0.58596	1.20923	-0.00299
C	-0.15475	2.41143	-0.21746
C	-1.51957	2.41078	-0.23748
C	-2.21845	1.19868	-0.02028
H	-2.07153	-0.92557	0.39519
H	0.37974	-0.92446	0.40891

H	0.37092	3.34226	-0.41219
H	-2.09221	3.31589	-0.42507
C	2.02501	1.21185	0.00179
C	2.75106	2.41222	0.21816
C	2.75756	0.01487	-0.21192
C	4.13032	2.40874	0.23096
H	2.22195	3.34054	0.41890
C	4.13687	0.02503	-0.22012
H	2.23388	-0.91606	-0.41499
C	4.83043	1.21855	0.00649
H	4.67296	3.33229	0.41886
H	4.68458	-0.89585	-0.40650
H	5.91875	1.22122	0.00818
O	-3.53519	1.25807	-0.04461
H	-3.93339	0.37580	0.10237

***p*-Ph-PhO⁻ (S=0)**

C	-1.54802	0.04312	0.28652
C	-0.16812	0.05196	0.28090
C	0.57973	1.21503	0.00032
C	-0.16803	2.37800	-0.28087
C	-1.54792	2.38662	-0.28783
C	-2.34008	1.21481	-0.00103
H	-2.09023	-0.87501	0.52552
H	0.36277	-0.86947	0.53439
H	0.36295	3.29951	-0.53387
H	-2.09005	3.30469	-0.52729
C	2.04710	1.21509	0.00094
C	2.78520	2.37928	0.28801
C	2.78549	0.05094	-0.28557
C	4.17485	2.38116	0.28190
H	2.25470	3.29635	0.54506
C	4.17513	0.04913	-0.27836
H	2.25522	-0.86614	-0.54306
C	4.88516	1.21516	0.00204
H	4.70952	3.30295	0.51234
H	4.71002	-0.87263	-0.50840
H	5.97433	1.21519	0.00246
O	-3.59999	1.21473	-0.00161

***p*-Ph-PhO[•] (S=1/2)**

C	-1.52131	0.01966	0.29936
C	-0.15500	0.03042	0.29176
C	0.57578	1.21499	0.00019
C	-0.15483	2.39949	-0.29208
C	-1.52114	2.41012	-0.30100
C	-2.28889	1.21486	-0.00115
H	-2.08129	-0.88278	0.54055
H	0.38855	-0.87760	0.54907
H	0.38888	3.30756	-0.54888
H	-2.08097	3.31250	-0.54271
C	2.03896	1.21505	0.00092
C	2.76210	2.38540	0.29353
C	2.76249	0.04478	-0.29097
C	4.14980	2.38263	0.29866
H	2.23069	3.29950	0.55383

C	4.15019	0.04767	-0.29471
H	2.23143	-0.86937	-0.55181
C	4.85071	1.21518	0.00232
H	4.68910	3.29691	0.54083
H	4.68982	-0.86656	-0.53636
H	5.93944	1.21523	0.00285
O	-3.53477	1.21482	-0.00167

***p*-Cl-PhOH (S=0)**

C	0.31015	0.27793	0.00092
C	1.69982	0.32624	0.00141
C	2.33662	1.56030	0.00070
C	1.61026	2.74689	-0.00050
C	0.22336	2.69414	-0.00097
C	-0.43106	1.46059	-0.00023
H	-0.20141	-0.68480	0.00144
H	2.28059	-0.59396	0.00234
H	2.12407	3.70611	-0.00109
H	-0.36931	3.60697	-0.00191
O	-1.78397	1.47422	-0.00066
H	-2.11628	0.56055	-0.00012
Cl	4.09480	1.62365	0.00135

***p*-Cl-PhOH^{•+} (S=1/2)**

C	0.32382	0.23894	0.00074
C	1.68699	0.29583	0.00133
C	2.32737	1.56273	0.00074
C	1.59724	2.77721	-0.00065
C	0.23430	2.72595	-0.00115
C	-0.41836	1.45625	-0.00023
H	-0.20391	-0.71316	0.00112
H	2.28794	-0.61017	0.00221
H	2.12491	3.72750	-0.00128
H	-0.37832	3.62385	-0.00209
O	-1.72437	1.47941	-0.00034
H	-2.10939	0.57503	0.00034
Cl	4.02942	1.61948	0.00195

***p*-Cl-PhO⁻ (S=0)**

C	0.30921	0.28398	0.00090
C	1.69348	0.32996	0.00141
C	2.34659	1.56202	0.00071
C	1.61224	2.74766	-0.00046
C	0.22816	2.69991	-0.00096
C	-0.51981	1.46558	-0.00029
H	-0.20029	-0.68210	0.00150
H	2.27724	-0.59220	0.00238
H	2.13197	3.70723	-0.00102
H	-0.34449	3.63006	-0.00192
O	-1.78027	1.42365	-0.00071
Cl	4.12436	1.62081	0.00125

***p*-Cl-PhO[•] (S=1/2)**

C	0.31856	0.25550	0.00094
C	1.68770	0.30628	0.00141
C	2.32472	1.56140	0.00069

C	1.60478	2.77112	-0.00052
C	0.23541	2.72929	-0.00100
C	-0.48282	1.46680	-0.00026
H	-0.21213	-0.69480	0.00148
H	2.28766	-0.60164	0.00233
H	2.14165	3.71772	-0.00108
H	-0.35801	3.64187	-0.00193
O	-1.72867	1.42480	-0.00064
Cl	4.05954	1.61824	0.00136

***p*-MeOC(O)-PhOH (S=0)**

C	-1.03581	0.68782	0.00053
C	0.36137	0.73057	0.00030
C	1.01206	1.95429	-0.00100
C	0.28220	3.14760	-0.00206
C	-1.11688	3.08981	-0.00183
C	-1.77637	1.87470	-0.00058
H	0.93000	-0.19953	0.00116
H	2.09927	1.98452	-0.00117
H	-1.67966	4.02139	-0.00268
H	-2.86313	1.81695	-0.00040
O	-1.72508	-0.47050	0.00181
H	-1.10552	-1.22063	0.00269
C	0.92653	4.47486	-0.00355
O	0.32907	5.53326	-0.00441
O	2.26665	4.39406	-0.00389
C	2.95770	5.63967	-0.00557
H	2.70889	6.22615	0.88645
H	4.02206	5.39251	-0.00601
H	2.70769	6.22438	-0.89842

***p*-MeOC(O)-PhOH⁺ (S=1/2)**

C	-1.02344	0.69724	0.00197
C	0.40512	0.72425	-0.00112
C	1.03735	1.93324	-0.00469
C	0.27361	3.13357	-0.00510
C	-1.14340	3.09928	-0.00228
C	-1.79633	1.90190	0.00130
H	0.95603	-0.21477	-0.00026
H	2.12228	1.98748	-0.00700
H	-1.69071	4.03815	-0.00270
H	-2.88054	1.82173	0.00368
O	-1.69685	-0.41643	0.00494
H	-1.11371	-1.20949	0.00499
C	0.92498	4.47933	-0.00714
O	0.29025	5.51023	-0.01104
O	2.24604	4.38832	-0.00334
C	2.95876	5.63388	-0.00286
H	2.70546	6.21318	0.89089
H	4.01686	5.36889	-0.00039
H	2.70929	6.21192	-0.89849

***p*-MeOC(O)-PhO⁻ (S=0)**

C	-1.07508	0.61860	0.00103
C	0.36784	0.73936	0.00057
C	1.01117	1.95330	-0.00088

C	0.29162	3.17036	-0.00208
C	-1.11905	3.09132	-0.00180
C	-1.77596	1.88574	-0.00039
H	0.93881	-0.19159	0.00160
H	2.10129	1.98737	-0.00107
H	-1.68165	4.02671	-0.00281
H	-2.86728	1.84680	-0.00022
O	-1.66624	-0.48817	0.00254
C	0.92432	4.47334	-0.00367
O	0.35105	5.55449	-0.00455
O	2.28414	4.40043	-0.00414
C	2.95789	5.64559	-0.00563
H	2.71000	6.23768	0.88438
H	4.02703	5.41403	-0.00593
H	2.70914	6.23597	-0.89653

***p*-MeOC(O)-PhO[•] (S=1/2)**

C	-1.05583	0.65045	0.00098
C	0.39509	0.73553	0.00054
C	1.03232	1.94739	-0.00095
C	0.27868	3.14373	-0.00209
C	-1.13392	3.10351	-0.00174
C	-1.79171	1.90385	-0.00026
H	0.94771	-0.20227	0.00147
H	2.11836	2.00105	-0.00124
H	-1.67850	4.04559	-0.00267
H	-2.87876	1.84430	0.00003
O	-1.64164	-0.44886	0.00236
C	0.92699	4.47941	-0.00373
O	0.31483	5.52727	-0.00479
O	2.25931	4.39551	-0.00389
C	2.95857	5.64081	-0.00559
H	2.70882	6.22457	0.88706
H	4.02047	5.38703	-0.00562
H	2.70823	6.22245	-0.89945

***p*-NC-PhOH (S=0)**

C	0.32166	0.27357	0.00092
C	1.70463	0.32407	0.00140
C	2.36333	1.56130	0.00070
C	1.61525	2.74933	-0.00050
C	0.23442	2.69948	-0.00098
C	-0.41732	1.46133	-0.00023
H	-0.19489	-0.68598	0.00145
H	2.28436	-0.59681	0.00235
H	2.12838	3.70895	-0.00107
H	-0.36271	3.60887	-0.00193
O	-1.76266	1.47500	-0.00064
H	-2.10076	0.56227	-0.00010
C	3.78762	1.61126	0.00125
N	4.95166	1.65056	0.00171

***p*-NC-PhOH⁺ (S=1/2)**

C	0.33260	0.23320	0.00078
C	1.69381	0.29095	0.00133
C	2.34463	1.56148	0.00062

C	1.60667	2.77735	-0.00062
C	0.24461	2.73034	-0.00113
C	-0.40760	1.45576	-0.00024
H	-0.20010	-0.71610	0.00124
H	2.29326	-0.61553	0.00225
H	2.13725	3.72556	-0.00113
H	-0.37106	3.62604	-0.00207
O	-1.70791	1.48106	-0.00038
H	-2.10004	0.57781	0.00029
C	3.76139	1.61580	0.00137
N	4.92545	1.65950	0.00201

***p*-NC-PhO⁻ (S=0)**

C	0.32551	0.27914	0.00093
C	1.69678	0.32746	0.00142
C	2.38501	1.56507	0.00073
C	1.61725	2.75510	-0.00045
C	0.24583	2.71239	-0.00096
C	-0.49945	1.47008	-0.00028
H	-0.19262	-0.68138	0.00152
H	2.27802	-0.59648	0.00239
H	2.13608	3.71552	-0.00102
H	-0.33408	3.63701	-0.00193
O	-1.75180	1.42943	-0.00070
C	3.79495	1.60897	0.00121
N	4.96549	1.64454	0.00161

***p*-NC-PhO[•] (S=1/2)**

C	0.33013	0.25428	0.00097
C	1.69628	0.30520	0.00144
C	2.35038	1.56343	0.00069
C	1.61549	2.77572	-0.00049
C	0.24886	2.73736	-0.00100
C	-0.46720	1.47109	-0.00026
H	-0.20550	-0.69291	0.00153
H	2.29403	-0.60389	0.00238
H	2.15296	3.72174	-0.00101
H	-0.34745	3.64770	-0.00193
O	-1.71009	1.43040	-0.00067
C	3.77242	1.61013	0.00120
N	4.93667	1.64660	0.00162

***p*-O₂N-PhOH (S=0)**

C	0.33504	0.27050	0.00080
C	1.71695	0.31474	0.00135
C	2.35728	1.55177	0.00073
C	1.63667	2.74653	-0.00040
C	0.25687	2.70079	-0.00083
C	-0.39943	1.46312	-0.00021
H	-0.18560	-0.68659	0.00116
H	2.30449	-0.59885	0.00218
H	2.16433	3.69599	-0.00087
H	-0.33715	3.61195	-0.00163
O	-1.74165	1.48203	-0.00063
H	-2.08550	0.57097	-0.00016
N	3.80605	1.59819	0.00134

O	4.34899	2.69683	-0.00053
O	4.41984	0.53726	0.00343

***p*-O₂N-PhOH^{•+} (S=1/2)**

C	0.34567	0.22892	-0.01108
C	1.70865	0.28725	-0.01325
C	2.33237	1.55485	-0.00215
C	1.63177	2.77375	0.00830
C	0.26621	2.73220	0.01212
C	-0.39233	1.45602	0.00130
H	-0.18791	-0.71980	-0.01914
H	2.31565	-0.61316	-0.02275
H	2.17344	3.71463	0.01516
H	-0.34603	3.63022	0.02298
O	-1.68900	1.48745	0.00322
H	-2.08961	0.58628	-0.00237
N	3.80820	1.60081	0.00253
O	4.32676	2.69542	-0.10976
O	4.39334	0.54039	0.12060

***p*-O₂N-PhO⁻ (S=0)**

C	0.34352	0.26505	0.00064
C	1.71041	0.30919	0.00137
C	2.38300	1.55062	0.00089
C	1.63568	2.74890	-0.00024
C	0.26891	2.70904	-0.00085
C	-0.47727	1.46319	-0.00047
H	-0.18036	-0.69168	0.00093
H	2.30306	-0.60347	0.00224
H	2.17101	3.69638	-0.00055
H	-0.31190	3.63241	-0.00164
O	-1.72582	1.42540	-0.00101
N	3.79101	1.59442	0.00161
O	4.36067	2.69758	0.00055
O	4.43013	0.52991	0.00330

***p*-O₂N-PhO[•] (S=1/2)**

C	0.34536	0.24456	0.00057
C	1.71316	0.29303	0.00126
C	2.34213	1.54984	0.00087
C	1.63712	2.76586	-0.00018
C	0.26911	2.73009	-0.00079
C	-0.44878	1.46406	-0.00038
H	-0.19140	-0.70171	0.00075
H	2.31854	-0.60878	0.00201
H	2.18581	3.70319	-0.00043
H	-0.32484	3.64168	-0.00153
O	-1.69164	1.42576	-0.00095
N	3.80330	1.59473	0.00166
O	4.33870	2.69367	-0.00028
O	4.40551	0.53095	0.00418

[1]²⁺ (S=0)

Ru	-3.68272	-2.60074	0.09047
C	-4.76454	-4.91419	-1.36738
C	-5.10241	-5.18690	0.91717

C	-5.67648	-6.43446	0.73059
C	-5.78185	-6.93499	-0.56141
C	-5.32591	-6.16295	-1.62008
C	-4.31609	-3.99579	-2.42078
C	-3.49114	-1.87101	-2.88214
C	-3.57666	-2.08186	-4.24867
C	-4.02398	-3.31672	-4.70645
C	-4.40486	-4.27799	-3.78216
H	-5.00818	-4.75949	1.91395
H	-6.03167	-6.99645	1.5901
H	-6.22261	-7.91168	-0.74625
H	-5.41275	-6.53078	-2.63872
H	-3.11538	-0.93065	-2.48213
H	-3.28547	-1.29064	-4.93414
H	-4.08631	-3.52711	-5.77144
H	-4.77712	-5.24086	-4.12070
C	-3.68180	0.32538	0.00839
C	-3.22068	1.63871	0.02322
C	-1.86109	1.88223	0.15643
C	-0.98964	0.80532	0.27433
C	-1.50951	-0.47925	0.25164
C	-5.09458	-0.04916	-0.12650
C	-6.13381	0.86858	-0.24781
C	-7.44041	0.41265	-0.34676
C	-7.68104	-0.95636	-0.32498
C	-6.60466	-1.82125	-0.20503
H	-3.91668	2.46871	-0.06389
H	-1.48783	2.90328	0.17069
H	0.08154	0.94991	0.38549
H	-0.86835	-1.35394	0.34314
H	-5.92364	1.93441	-0.26462
H	-8.26056	1.12057	-0.43937
H	-8.68760	-1.35850	-0.40025
H	-6.74649	-2.90019	-0.18141
C	-2.74479	-3.37542	2.75678
C	-4.51969	-1.88184	2.91880
C	-4.51377	-1.95529	4.30274
C	-2.68843	-3.49200	4.14433
H	-5.23648	-1.25145	2.39634
H	-5.23202	-1.37235	4.87283
H	-1.94396	-4.12768	4.61470
N	-4.64488	-4.43896	-0.09996
N	-3.82492	-2.80949	-1.98024
N	-2.82298	-0.72232	0.11504
N	-5.33859	-1.38637	-0.10313
N	-3.66387	-2.57901	2.15337
C	-3.58311	-2.77719	4.92694
H	-3.54933	-2.85906	6.01049
C	-1.83612	-4.07361	1.84380
C	-0.91259	-5.03880	2.32735
C	-1.03189	-4.31405	-0.33073
C	-0.08438	-5.68167	1.46186
H	-0.89330	-5.28119	3.38534
C	-0.95191	-3.88982	-1.65401
C	-0.10349	-5.32728	0.08638
H	0.61369	-6.44921	1.78910

C	-0.05898	-4.49864	-2.53262
H	-1.56763	-3.06596	-2.00053
C	0.04365	-4.11859	-3.90042
C	0.77832	-5.55085	-2.02685
C	0.92001	-4.76265	-4.72676
H	-0.59546	-3.31510	-4.26782
C	1.67916	-6.19615	-2.91968
C	1.74320	-5.81203	-4.22990
H	0.99542	-4.47767	-5.77425
H	2.30557	-6.99225	-2.52111
H	2.43393	-6.30914	-4.90855
N	-1.93723	-3.75119	0.55163
N	0.75483	-5.92724	-0.74045

[1]²⁺ (S=1)

Ru	-3.64625	-2.59412	0.11757
C	-4.67560	-4.95587	-1.32464
C	-4.95363	-5.20795	0.97872
C	-5.51650	-6.46332	0.81647
C	-5.64428	-6.97611	-0.46862
C	-5.22294	-6.21398	-1.54951
C	-4.25162	-4.04363	-2.39098
C	-3.47780	-1.89868	-2.86705
C	-3.54059	-2.12970	-4.23143
C	-3.95563	-3.38014	-4.67624
C	-4.32369	-4.34347	-3.74787
H	-4.83359	-4.76791	1.96659
H	-5.84219	-7.02258	1.68885
H	-6.07465	-7.96120	-0.63167
H	-5.32562	-6.59633	-2.56095
H	-3.13250	-0.94535	-2.46978
H	-3.25840	-1.34225	-4.92444
H	-4.00125	-3.60344	-5.73939
H	-4.66789	-5.31918	-4.07922
C	-3.72600	0.35335	0.05930
C	-3.28574	1.67046	0.11358
C	-1.94234	1.92742	0.35527
C	-1.06688	0.86471	0.54335
C	-1.56394	-0.42763	0.47957
C	-5.11989	-0.04333	-0.17241
C	-6.16396	0.85505	-0.36089
C	-7.44941	0.36856	-0.55765
C	-7.66504	-1.00445	-0.56603
C	-6.58262	-1.84961	-0.37638
H	-3.98392	2.49060	-0.02942
H	-1.58468	2.95315	0.39982
H	-0.01063	1.02426	0.74041
H	-0.92756	-1.29886	0.62322
H	-5.97668	1.92515	-0.35103
H	-8.27590	1.05966	-0.70375
H	-8.65532	-1.42427	-0.71787
H	-6.69979	-2.93203	-0.38030
C	-2.68155	-3.32555	2.77414
C	-4.46422	-1.79754	2.94300
C	-4.44744	-1.84866	4.31936
C	-2.62541	-3.41061	4.17775

H	-5.18167	-1.17451	2.41221	C	-1.48235	-0.50164	0.21841
H	-5.15397	-1.25466	4.89167	C	-5.06724	-0.06015	-0.14999
H	-1.87583	-4.03848	4.65168	C	-6.10214	0.86103	-0.27842
N	-4.53810	-4.47163	-0.06378	C	-7.41249	0.41065	-0.35286
N	-3.80167	-2.83882	-1.96707	C	-7.66136	-0.95560	-0.29796
N	-2.85933	-0.67615	0.23372	C	-6.58902	-1.82462	-0.17206
N	-5.34283	-1.38176	-0.17538	H	-3.87454	2.44872	-0.16800
N	-3.61950	-2.52341	2.18294	H	-1.44254	2.87663	0.04358
C	-3.50521	-2.67974	4.94407	H	0.11708	0.92220	0.30829
H	-3.46057	-2.74031	6.02917	H	-0.84378	-1.37530	0.33285
C	-1.82450	-4.03138	1.87021	H	-5.88699	1.92515	-0.31845
C	-1.00540	-5.10081	2.27956	H	-8.22940	1.12153	-0.45069
C	-1.04578	-4.24390	-0.36760	H	-8.67113	-1.35286	-0.35154
C	-0.26441	-5.80250	1.36871	H	-6.73748	-2.90141	-0.12080
H	-0.98990	-5.38788	3.32836	C	-2.76805	-3.43001	2.76647
C	-0.87502	-3.74724	-1.64879	C	-4.50128	-1.88897	2.92756
C	-0.24778	-5.39426	-0.00026	C	-4.51673	-1.98880	4.31050
H	0.34839	-6.65395	1.65673	C	-2.73661	-3.57779	4.15152
C	-0.06877	-4.43256	-2.58096	H	-5.19251	-1.22883	2.40780
H	-1.34948	-2.81291	-1.94149	H	-5.22522	-1.39459	4.88102
C	0.09989	-3.99869	-3.91671	H	-2.02169	-4.24547	4.62344
C	0.59991	-5.61434	-2.14135	N	-4.68215	-4.43256	-0.07358
C	0.88348	-4.71765	-4.78943	N	-3.81569	-2.83966	-1.97009
H	-0.40963	-3.08959	-4.24065	N	-2.79744	-0.74153	0.09373
C	1.39593	-6.33331	-3.06231	N	-5.31977	-1.39452	-0.09613
C	1.53303	-5.89541	-4.35950	N	-3.65561	-2.59755	2.16233
H	1.00577	-4.38037	-5.81731	C	-3.62290	-2.85121	4.93323
H	1.89644	-7.23305	-2.70685	H	-3.61062	-2.95565	6.01509
H	2.14997	-6.45509	-5.06053	C	-1.86233	-4.12413	1.85298
N	-1.89408	-3.64483	0.54323	C	-0.93879	-5.09232	2.32717
N	0.51920	-6.05110	-0.85841	C	-1.03941	-4.33998	-0.31369
[1-H]³⁺ (S=0)				C	-0.08640	-5.72058	1.47106
Ru	-3.67237	-2.61767	0.10125	H	-0.92699	-5.35003	3.38127
C	-4.80082	-4.92008	-1.33638	C	-0.95212	-3.90657	-1.63862
C	-5.18588	-5.14406	0.94765	C	-0.11357	-5.32864	0.11872
C	-5.79970	-6.37422	0.77014	H	0.61226	-6.48316	1.80721
C	-5.89655	-6.89297	-0.51503	C	-0.05232	-4.47254	-2.53748
C	-5.39810	-6.15375	-1.57864	H	-1.58388	-3.08969	-1.97277
C	-4.32519	-4.02342	-2.39805	C	0.02273	-4.06286	-3.89594
C	-3.46391	-1.91652	-2.88153	C	0.82519	-5.50056	-2.08117
C	-3.54752	-2.14216	-4.24599	C	0.92033	-4.65713	-4.73841
C	-4.01514	-3.37446	-4.69042	H	-0.65402	-3.28103	-4.23818
C	-4.41500	-4.31899	-3.75638	C	1.74660	-6.09921	-2.95451
H	-5.10051	-4.70072	1.93832	C	1.78336	-5.67652	-4.26111
H	-6.19398	-6.90721	1.63100	H	0.98055	-4.35384	-5.78051
H	-6.36865	-7.85632	-0.69231	H	2.40954	-6.87944	-2.58650
H	-5.48524	-6.53352	-2.59285	H	2.49249	-6.13357	-4.94775
H	-3.07931	-0.97564	-2.49098	N	-1.95477	-3.79015	0.55998
H	-3.24410	-1.36292	-4.93971	N	0.75156	-5.86074	-0.77350
H	-4.08050	-3.59519	-5.75311	H	1.40554	-6.57042	-0.43506
H	-4.80614	-5.27759	-4.08549	[1-H]³⁺ (S=1)			
C	-3.65119	0.30771	-0.03550	Ru	-3.65258	-2.59399	0.11255
C	-3.18260	1.61802	-0.05974	C	-4.68297	-4.92541	-1.38384
C	-1.82123	1.85768	0.05997	C	-4.94024	-5.24709	0.91317
C	-0.95506	0.77985	0.20432	C	-5.50410	-6.49742	0.71768

C	-5.64527	-6.97015	-0.58105	H	-1.46489	-2.97078	-1.95508
C	-5.23351	-6.17534	-1.64221	C	-0.01310	-4.13863	-3.92307
C	-4.26209	-3.98507	-2.42583	C	0.65575	-5.64260	-2.14133
C	-3.47488	-1.83140	-2.85243	C	0.80007	-4.82832	-4.79728
C	-3.54062	-2.03107	-4.22145	H	-0.59610	-3.28039	-4.25732
C	-3.96743	-3.26675	-4.69503	C	1.47851	-6.33930	-3.02815
C	-4.33744	-4.25087	-3.78898	C	1.54619	-5.93118	-4.34885
H	-4.81688	-4.83873	1.91396	H	0.86700	-4.51899	-5.83802
H	-5.82406	-7.08168	1.57567	H	2.05740	-7.18881	-2.66894
H	-6.08029	-7.94843	-0.77051	H	2.18691	-6.46944	-5.04401
H	-5.34786	-6.52496	-2.66419	N	-1.91083	-3.72434	0.58112
H	-3.12321	-0.88886	-2.43715	N	0.57555	-6.00007	-0.81157
H	-3.25435	-1.22917	-4.89576	H	1.16647	-6.76462	-0.48803
H	-4.01970	-3.46353	-5.76305				
H	-4.69012	-5.21563	-4.14246				
C	-3.72811	0.34590	0.06274	[1-H] ²⁺ (S=1/2)			
C	-3.28351	1.66134	0.10354	Ru	-3.68465	-2.60721	0.09488
C	-1.93594	1.91438	0.32734	C	-4.75666	-4.93044	-1.34934
C	-1.06046	0.85065	0.51223	C	-5.10883	-5.18265	0.93546
C	-1.56191	-0.44037	0.46557	C	-5.67910	-6.43291	0.75673
C	-5.12171	-0.05339	-0.15790	C	-5.77436	-6.94652	-0.53136
C	-6.17268	0.83912	-0.32810	C	-5.31332	-6.18337	-1.59398
C	-7.45809	0.34611	-0.51084	C	-4.30659	-4.01871	-2.40740
C	-7.66689	-1.02778	-0.52284	C	-3.49124	-1.89267	-2.87835
C	-6.57910	-1.86974	-0.35252	C	-3.57413	-2.11090	-4.24395
H	-3.98035	2.48289	-0.03772	C	-4.01363	-3.35067	-4.69628
H	-1.57452	2.93913	0.36022	C	-4.39138	-4.30879	-3.76742
H	-0.00159	1.00970	0.69457	H	-5.02160	-4.74467	1.92825
H	-0.92520	-1.31110	0.61112	H	-6.03914	-6.98745	1.61916
H	-5.99063	1.90996	-0.31289	H	-6.21160	-7.92608	-0.70954
H	-8.29022	1.03333	-0.64167	H	-5.39272	-6.56053	-2.60990
H	-8.65708	-1.45197	-0.66201	H	-3.12056	-0.94849	-2.48248
H	-6.69291	-2.95213	-0.35735	H	-3.28645	-1.32156	-4.93317
C	-2.69357	-3.31791	2.80172	H	-4.07299	-3.56685	-5.76031
C	-4.47469	-1.80331	2.93625	H	-4.75899	-5.27518	-4.10134
C	-4.44731	-1.82006	4.31685	C	-3.67101	0.31844	0.01215
C	-2.61581	-3.36521	4.19524	C	-3.20377	1.62970	0.03265
H	-5.20102	-1.19868	2.39757	C	-1.84423	1.86676	0.17715
H	-5.15659	-1.21708	4.87612	C	-0.97915	0.78522	0.30152
H	-1.86001	-3.97503	4.68142	C	-1.50485	-0.49687	0.27280
N	-4.53372	-4.48012	-0.11023	C	-5.08466	-0.04928	-0.13180
N	-3.80673	-2.79060	-1.97420	C	-6.11878	0.87330	-0.26266
N	-2.86167	-0.68505	0.23709	C	-7.42677	0.42358	-0.37016
N	-5.33870	-1.39456	-0.16772	C	-7.67383	-0.94450	-0.34727
N	-3.62361	-2.53536	2.19288	C	-6.60237	-1.81393	-0.21745
C	-3.49684	-2.61578	4.95460	H	-3.89542	2.46301	-0.05848
H	-3.44040	-2.64630	6.04001	H	-1.46614	2.88601	0.19571
C	-1.82295	-4.05898	1.90486	H	0.09171	0.92467	0.42252
C	-0.97272	-5.06814	2.34921	H	-0.87108	-1.37634	0.37037
C	-1.05678	-4.30873	-0.31818	H	-5.90314	1.93808	-0.28036
C	-0.18806	-5.76588	1.44895	H	-8.24295	1.13509	-0.47035
H	-0.93482	-5.32821	3.40301	H	-8.68177	-1.34203	-0.42919
C	-0.93596	-3.86339	-1.63592	H	-6.74896	-2.89235	-0.19291
C	-0.21186	-5.38648	0.10667	C	-2.75961	-3.37738	2.77105
H	0.46128	-6.57657	1.77214	C	-4.52838	-1.86802	2.92091
C	-0.11069	-4.53166	-2.57142	C	-4.53379	-1.93203	4.30270
				C	-2.71485	-3.48162	4.16376

H	-5.23628	-1.23577	2.38817
H	-5.25047	-1.34091	4.86624
H	-1.97504	-4.11761	4.64204
N	-4.64552	-4.44315	-0.08549
N	-3.82097	-2.82813	-1.97195
N	-2.81813	-0.73399	0.12361
N	-5.33467	-1.38543	-0.10688
N	-3.67254	-2.57728	2.16305
C	-3.60892	-2.75927	4.93505
H	-3.58069	-2.83487	6.01954
C	-1.85740	-4.09187	1.87158
C	-0.96984	-5.05964	2.33658
C	-1.03742	-4.30381	-0.32119
C	-0.12355	-5.71120	1.45605
H	-0.94801	-5.32061	3.39044
C	-0.93327	-3.87127	-1.65074
C	-0.13870	-5.32995	0.11883
H	0.56061	-6.48667	1.79479
C	-0.05026	-4.49133	-2.56808
H	-1.52914	-3.02930	-1.98465
C	0.04104	-4.10532	-3.92191
C	0.78161	-5.54695	-2.11980
C	0.91159	-4.74459	-4.78238
H	-0.59523	-3.29202	-4.27211
C	1.66015	-6.19197	-2.99036
C	1.72189	-5.79053	-4.31621
H	0.97032	-4.43748	-5.82457
H	2.28780	-7.00028	-2.61689
H	2.40697	-6.29183	-4.99695
N	-1.93666	-3.75468	0.55263
N	0.70267	-5.90292	-0.78841
H	1.32702	-6.63329	-0.45337

[1]⁺ (S=1/2)

Ru	-3.69992	-2.60102	0.08399
C	-4.76058	-4.94528	-1.32493
C	-5.12447	-5.15560	0.96261
C	-5.68095	-6.41449	0.80478
C	-5.76123	-6.95620	-0.47358
C	-5.30225	-6.20936	-1.54789
C	-4.31734	-4.04714	-2.39577
C	-3.53118	-1.91632	-2.89460
C	-3.60954	-2.15374	-4.25665
C	-4.02899	-3.40677	-4.69337
C	-4.39576	-4.35665	-3.75239
H	-5.04437	-4.69645	1.94655
H	-6.03874	-6.95653	1.67613
H	-6.18355	-7.94536	-0.63395
H	-5.36835	-6.60809	-2.55658
H	-3.17146	-0.96313	-2.50998
H	-3.33127	-1.36997	-4.95622
H	-4.08097	-3.63856	-5.75454
H	-4.74783	-5.33333	-4.07348
C	-3.66216	0.32550	0.00817
C	-3.18181	1.63220	0.03849
C	-1.82014	1.85505	0.18451

C	-0.96627	0.76336	0.30119
C	-1.50413	-0.51336	0.26240
C	-5.07981	-0.02680	-0.13289
C	-6.10540	0.90663	-0.26076
C	-7.41782	0.47030	-0.36679
C	-7.67809	-0.89594	-0.34592
C	-6.61473	-1.77530	-0.21917
H	-3.86604	2.47261	-0.04501
H	-1.43170	2.87032	0.21110
H	0.10594	0.89063	0.42447
H	-0.88205	-1.40174	0.35541
H	-5.87931	1.96939	-0.27715
H	-8.22733	1.18987	-0.46457
H	-8.69016	-1.28339	-0.42705
H	-6.77017	-2.85285	-0.19562
C	-2.76145	-3.39653	2.74357
C	-4.53784	-1.87905	2.92110
C	-4.56156	-1.97290	4.29836
C	-2.74433	-3.53144	4.14496
H	-5.23792	-1.23215	2.39389
H	-5.28022	-1.39199	4.86996
H	-2.01424	-4.18268	4.61833
N	-4.66074	-4.43173	-0.06995
N	-3.84575	-2.84517	-1.97518
N	-2.81981	-0.73693	0.11003
N	-5.34207	-1.36049	-0.10952
N	-3.67998	-2.57476	2.15171
C	-3.64193	-2.82771	4.91868
H	-3.62695	-2.93198	6.00165
C	-1.86507	-4.07784	1.84605
C	-0.95137	-5.04803	2.29897
C	-1.03181	-4.26347	-0.35761
C	-0.10686	-5.67802	1.42498
H	-0.93155	-5.31299	3.35342
C	-0.92267	-3.82414	-1.67415
C	-0.10314	-5.30171	0.05208
H	0.59065	-6.44805	1.74901
C	-0.02693	-4.44285	-2.56994
H	-1.52810	-2.99288	-2.02143
C	0.08812	-4.05904	-3.92707
C	0.79126	-5.50343	-2.07611
C	0.96609	-4.70531	-4.76869
H	-0.53919	-3.24391	-4.29330
C	1.68090	-6.14877	-2.96410
C	1.76701	-5.76026	-4.28389
H	1.04377	-4.40348	-5.81226
H	2.29506	-6.95687	-2.56724
H	2.45794	-6.26627	-4.95677
N	-1.94629	-3.73065	0.51837
N	0.75196	-5.89468	-0.77550

[1]⁺ (S=3/2)

Ru	-3.65683	-2.58724	0.10550
C	-4.69804	-4.92645	-1.37955
C	-4.95340	-5.25076	0.91338
C	-5.51207	-6.50414	0.71880

C	-5.65184	-6.97670	-0.58049
C	-5.24337	-6.17944	-1.64044
C	-4.28197	-3.98284	-2.42353
C	-3.50551	-1.82670	-2.84810
C	-3.57254	-2.02438	-4.21799
C	-3.99239	-3.26197	-4.69269
C	-4.35928	-4.24795	-3.78754
H	-4.82608	-4.83885	1.91286
H	-5.82723	-7.09206	1.57623
H	-6.08142	-7.95743	-0.77055
H	-5.35468	-6.52930	-2.66284
H	-3.15751	-0.88635	-2.42422
H	-3.29120	-1.22030	-4.89213
H	-4.04239	-3.45834	-5.76105
H	-4.70601	-5.21456	-4.14227
C	-3.74937	0.33627	0.04906
C	-3.26817	1.66875	0.11844
C	-1.93701	1.91290	0.32752
C	-1.03634	0.82895	0.48562
C	-1.53829	-0.44864	0.41171
C	-5.10028	-0.04415	-0.12917
C	-6.19097	0.84687	-0.30067
C	-7.45997	0.36231	-0.46976
C	-7.68325	-1.03910	-0.48135
C	-6.60113	-1.87030	-0.31318
H	-3.96935	2.49398	0.01250
H	-1.57361	2.93727	0.38160
H	0.02355	0.98767	0.66230
H	-0.89826	-1.32323	0.52890
H	-6.00614	1.91904	-0.29744
H	-8.29315	1.05021	-0.59925
H	-8.67651	-1.45824	-0.61441
H	-6.71811	-2.95463	-0.31120
C	-2.69150	-3.31846	2.77360
C	-4.47102	-1.78376	2.91485
C	-4.46094	-1.81518	4.29289
C	-2.64090	-3.38189	4.17870
H	-5.17856	-1.16533	2.36537
H	-5.16654	-1.20941	4.85407
H	-1.89361	-4.00173	4.66687
N	-4.55113	-4.48064	-0.10727
N	-3.82804	-2.78925	-1.97206
N	-2.84118	-0.71024	0.17355
N	-5.34650	-1.41425	-0.12138
N	-3.62555	-2.52179	2.16948
C	-3.52283	-2.63870	4.93173
H	-3.48115	-2.68434	6.01794
C	-1.82000	-4.03274	1.88506
C	-0.95243	-5.05059	2.32698
C	-1.04117	-4.28306	-0.34208
C	-0.17031	-5.73660	1.43817
H	-0.92499	-5.30880	3.38303
C	-0.92343	-3.84186	-1.65331
C	-0.17360	-5.37274	0.05837
H	0.48646	-6.54499	1.75299
C	-0.08692	-4.51770	-2.56504

H	-1.46590	-2.96055	-1.98581
C	0.03167	-4.13839	-3.92289
C	0.66609	-5.63049	-2.08350
C	0.85054	-4.84161	-4.77677
H	-0.54347	-3.28103	-4.27768
C	1.49700	-6.33367	-2.98508
C	1.58670	-5.94921	-4.30447
H	0.93349	-4.54461	-5.82111
H	2.06297	-7.18046	-2.59818
H	2.23162	-6.49814	-4.98896
N	-1.90520	-3.69578	0.55249
N	0.62552	-6.01786	-0.78179

[1-(*p*-MeO-PhOH)]²⁺ (S=0)

Ru	-3.74622	-2.59357	0.06810
C	-4.92350	-4.82169	-1.44465
C	-5.26229	-5.14024	0.83430
C	-5.88384	-6.36012	0.61823
C	-6.01230	-6.82295	-0.68572
C	-5.53189	-6.04156	-1.72672
C	-4.44398	-3.89399	-2.47617
C	-3.51229	-1.80212	-2.88545
C	-3.61450	-1.97231	-4.25662
C	-4.13032	-3.16839	-4.74432
C	-4.55633	-4.13360	-3.84382
H	-5.14747	-4.74146	1.84068
H	-6.25697	-6.93065	1.46442
H	-6.49011	-7.77739	-0.89338
H	-5.63481	-6.37924	-2.75425
H	-3.08557	-0.89422	-2.46259
H	-3.28429	-1.18008	-4.92302
H	-4.21032	-3.34562	-5.81415
H	-4.98120	-5.06601	-4.20510
C	-3.64707	0.33305	0.04026
C	-3.14186	1.62960	0.07502
C	-1.77417	1.82452	0.20699
C	-0.93882	0.71714	0.30123
C	-1.50202	-0.54868	0.25854
C	-5.07201	0.00722	-0.09496
C	-6.08346	0.95823	-0.19178
C	-7.40410	0.54374	-0.29043
C	-7.68680	-0.81731	-0.29259
C	-6.63672	-1.71651	-0.19697
H	-3.81015	2.48374	0.00377
H	-1.36651	2.83198	0.23703
H	0.13710	0.82372	0.40958
H	-0.89034	-1.44615	0.32919
H	-5.84206	2.01740	-0.18819
H	-8.20299	1.27791	-0.36331
H	-8.70584	-1.18681	-0.36735
H	-6.81096	-2.79091	-0.19214
C	-2.83726	-3.43757	2.72609
C	-4.54907	-1.87369	2.90337
C	-4.53706	-1.95051	4.28710
C	-2.77711	-3.55960	4.11298
H	-5.24241	-1.21277	2.38720

H	-5.22707	-1.33992	4.86308	C	-3.50100	-1.80841	-2.88359
H	-2.05890	-4.22875	4.57748	C	-3.60433	-1.97767	-4.25481
N	-4.78031	-4.38540	-0.16578	C	-4.12390	-3.17197	-4.74282
N	-3.89286	-2.74531	-2.00724	C	-4.55203	-4.13649	-3.84254
N	-2.82319	-0.74464	0.12525	H	-5.14234	-4.74625	1.84187
N	-5.35747	-1.32170	-0.09691	H	-6.25562	-6.93339	1.46474
N	-3.72651	-2.60215	2.13060	H	-6.49110	-7.77831	-0.89346
C	-3.63659	-2.81086	4.90326	H	-5.63368	-6.38078	-2.75379
H	-3.59868	-2.89689	5.98631	H	-3.07210	-0.90161	-2.46053
C	-1.96286	-4.16811	1.80479	H	-3.27241	-1.18596	-4.92097
C	-1.08314	-5.17988	2.27745	H	-4.20535	-3.34827	-5.81269
C	-1.18382	-4.43532	-0.37535	H	-4.98002	-5.06735	-4.20415
C	-0.29179	-5.85815	1.40523	C	-3.64269	0.32885	0.03679
H	-1.06441	-5.42755	3.33422	C	-3.13790	1.62560	0.06945
C	-1.09081	-4.01241	-1.69916	C	-1.77045	1.82118	0.20286
C	-0.30669	-5.49319	0.03342	C	-0.93488	0.71425	0.30055
H	0.36799	-6.66101	1.72992	C	-1.49773	-0.55178	0.25988
C	-0.22768	-4.65090	-2.58673	C	-5.06731	0.00230	-0.09984
H	-1.67461	-3.16365	-2.04040	C	-6.07891	0.95289	-0.19890
C	-0.10823	-4.26207	-3.95038	C	-7.39935	0.53788	-0.29818
C	0.56462	-5.74161	-2.09543	C	-7.68169	-0.82322	-0.29865
C	0.74582	-4.93092	-4.78062	C	-6.63146	-1.72203	-0.20079
H	-0.71277	-3.42917	-4.30986	H	-3.80626	2.47943	-0.00462
C	1.44450	-6.41304	-2.98666	H	-1.36311	2.82880	0.23129
C	1.52735	-6.01492	-4.29218	H	0.14085	0.82151	0.41009
H	0.83620	-4.63827	-5.82462	H	-0.88595	-1.44899	0.33320
H	2.04053	-7.23902	-2.60075	H	-5.83778	2.01211	-0.19649
H	2.20289	-6.52933	-4.97293	H	-8.19837	1.27173	-0.37278
N	-2.05386	-3.83201	0.51514	H	-8.70056	-1.19310	-0.37374
N	0.51522	-6.12374	-0.80982	H	-6.80553	-2.79644	-0.19442
C	5.52408	-8.32662	1.46226	C	-2.83704	-3.43275	2.73284
C	5.87500	-6.97669	1.41128	C	-4.55195	-1.87168	2.90175
C	4.95154	-6.05215	0.91689	C	-4.54191	-1.94386	4.28582
C	3.70028	-6.46262	0.47911	C	-2.77856	-3.54987	4.12019
C	3.34477	-7.81597	0.52826	H	-5.24572	-1.21358	2.38258
C	4.26705	-8.73635	1.02189	H	-5.23408	-1.33262	4.85850
H	6.21919	-9.07227	1.84174	H	-2.05954	-4.21584	4.58808
H	5.23715	-5.00157	0.88034	N	-4.77539	-4.38961	-0.16452
H	2.99156	-5.72945	0.09190	N	-3.88394	-2.75085	-2.00562
H	3.98800	-9.78864	1.05785	N	-2.81866	-0.74836	0.12536
O	2.13792	-8.27568	0.11628	N	-5.35243	-1.32667	-0.10018
H	1.58808	-7.52345	-0.21058	N	-3.72677	-2.60114	2.13273
O	7.07237	-6.46971	1.81258	C	-3.64073	-2.80011	4.90655
C	8.02977	-7.37614	2.30854	H	-3.60435	-2.88212	5.98995
H	8.91240	-6.78453	2.56901	C	-1.96031	-4.16520	1.81559
H	7.67045	-7.89633	3.20957	C	-1.07934	-5.17353	2.29312
H	8.31215	-8.12460	1.55273	C	-1.17834	-4.44203	-0.36226
[1-(<i>p</i>-O₂N-PhOH)]²⁺ (S=0)				C	-0.28548	-5.85428	1.42523
Ru	-3.74115	-2.59770	0.07002	H	-1.06155	-5.41692	3.35090
C	-4.91935	-4.82511	-1.44359	C	-1.08558	-4.02410	-1.68763
C	-5.25814	-5.14428	0.83531	C	-0.29984	-5.49660	0.05152
C	-5.88165	-6.36308	0.61877	H	0.37381	-6.65379	1.75868
C	-6.01136	-6.82492	-0.68541	C	-0.22293	-4.66502	-2.57363
C	-5.52979	-6.04385	-1.72612	H	-1.66990	-3.17679	-2.03165
C	-4.43817	-3.89794	-2.47484	C	-0.10607	-4.27994	-3.93850
				C	0.57074	-5.75319	-2.07984

C	0.74672	-4.95059	-4.76846	H	-1.92538	3.12577	0.22617
H	-0.71184	-3.44842	-4.29890	H	-0.22596	1.29386	0.47884
C	1.44841	-6.42721	-2.97067	H	-1.01106	-1.07911	0.42998
C	1.52856	-6.03294	-4.27776	H	-6.29776	1.83554	-0.26622
H	0.83537	-4.66114	-5.81341	H	-8.55209	0.82429	-0.50115
H	2.04492	-7.25410	-2.58737	H	-8.77477	-1.67813	-0.49831
H	2.20242	-6.55017	-4.95801	H	-6.71153	-3.05846	-0.25810
N	-2.04983	-3.83518	0.52437	C	-2.55309	-3.16062	2.70724
N	0.52292	-6.12883	-0.79109	C	-4.44010	-1.77464	2.93656
C	5.52612	-8.29057	1.41404	C	-4.35184	-1.79410	4.31133
C	5.83981	-6.93058	1.39158	C	-2.41831	-3.20678	4.10552
C	4.92883	-5.98408	0.92617	H	-5.23180	-1.22465	2.43148
C	3.68861	-6.39892	0.47886	H	-5.07719	-1.24840	4.90770
C	3.35627	-7.76403	0.49675	H	-1.59768	-3.76194	4.55168
C	4.28750	-8.70369	0.96744	N	-4.40890	-4.48694	-0.05307
H	6.25544	-9.00757	1.78057	N	-3.92823	-2.79788	-1.98955
H	5.20119	-4.93244	0.91793	N	-2.99674	-0.57047	0.15163
H	2.96742	-5.67136	0.10864	N	-5.44867	-1.42365	-0.12610
H	4.01140	-9.75598	0.97126	N	-3.57439	-2.44361	2.14852
O	2.17319	-8.22168	0.08047	C	-3.31441	-2.52838	4.90243
H	1.59282	-7.47249	-0.22616	H	-3.20942	-2.55783	5.98457
N	7.13750	-6.49219	1.85984	C	-1.69351	-3.83145	1.77456
O	7.92399	-7.33990	2.26660	C	-0.80202	-4.84623	2.16270
O	7.39026	-5.29235	1.82898	C	-1.01537	-4.04514	-0.49363
[1-(<i>p</i>-MeO-PhOH)]²⁺ (S=1)				C	-0.07147	-5.53035	1.22751
Ru	-3.67882	-2.53329	0.08633	H	-0.72002	-5.11194	3.21404
C	-4.54357	-4.99210	-1.30568	C	-0.93792	-3.57044	-1.79399
C	-4.66905	-5.26720	1.00724	C	-0.14273	-5.14223	-0.14176
C	-5.05919	-6.58948	0.87145	H	0.58913	-6.35011	1.50389
C	-5.17021	-7.12478	-0.40601	C	-0.13415	-4.22397	-2.75206
C	-4.91311	-6.31735	-1.50544	H	-1.48847	-2.67755	-2.08390
C	-4.30157	-4.03665	-2.39004	C	-0.04952	-3.80656	-4.10040
C	-3.73954	-1.83510	-2.90390	C	0.62407	-5.35463	-2.32922
C	-3.88097	-2.06821	-4.26209	C	0.74168	-4.49103	-4.99417
C	-4.23697	-3.34398	-4.68496	H	-0.62462	-2.93452	-4.41506
C	-4.45648	-4.33595	-3.73976	C	1.42716	-6.04070	-3.26590
H	-4.56350	-4.80922	1.98823	C	1.48285	-5.61651	-4.57434
H	-5.26366	-7.18214	1.75846	H	0.80007	-4.16499	-6.03107
H	-5.45863	-8.16336	-0.54829	H	1.99685	-6.90393	-2.92092
H	-4.99798	-6.71824	-2.51129	H	2.10590	-6.14800	-5.29141
H	-3.44113	-0.85829	-2.52814	N	-1.84816	-3.47844	0.44845
H	-3.70876	-1.26072	-4.96790	N	0.61381	-5.77014	-1.03488
H	-4.34917	-3.56639	-5.74338	C	5.01189	-8.73595	1.59750
H	-4.75322	-5.33301	-4.05268	C	5.61563	-7.47844	1.55907
C	-3.93093	0.40652	0.02528	C	4.95494	-6.42582	0.92050
C	-3.56517	1.74694	0.05067	C	3.71291	-6.61916	0.33255
C	-2.22593	2.08107	0.20805	C	3.10012	-7.87807	0.37405
C	-1.28116	1.07162	0.34779	C	3.76338	-8.92709	1.00846
C	-1.70556	-0.24781	0.31999	H	5.50025	-9.57704	2.08464
C	-5.30908	-0.07388	-0.13068	H	5.43812	-5.44991	0.89282
C	-6.41659	0.75548	-0.26491	H	3.21033	-5.78986	-0.16670
C	-7.67715	0.18740	-0.39657	H	3.28538	-9.90550	1.03843
C	-7.80662	-1.19649	-0.39571	O	1.88795	-8.12312	-0.17527
C	-6.66475	-1.97059	-0.26275	H	1.49237	-7.27931	-0.51549
H	-4.31674	2.52493	-0.05103	O	6.82717	-7.18230	2.10532
				C	7.51415	-8.22044	2.76337

H	8.45333	-7.79159	3.12517
H	6.94452	-8.60680	3.62258
H	7.74322	-9.05445	2.08253

[1-(*p*-O₂N-PhOH)]²⁺ (S=1)

Ru	-3.69343	-2.55631	0.09726
C	-4.64200	-4.96768	-1.32786
C	-4.82650	-5.24210	0.98225
C	-5.32075	-6.52766	0.83369
C	-5.46612	-7.04190	-0.44869
C	-5.12779	-6.25306	-1.53965
C	-4.29918	-4.03108	-2.40188
C	-3.65645	-1.84393	-2.88577
C	-3.73501	-2.07413	-4.24945
C	-4.08809	-3.34475	-4.69016
C	-4.38049	-4.33086	-3.75852
H	-4.69890	-4.79835	1.96721
H	-5.58246	-7.10721	1.71429
H	-5.84551	-8.04918	-0.60196
H	-5.24968	-6.63684	-2.54828
H	-3.35357	-0.87502	-2.49321
H	-3.51124	-1.27042	-4.94507
H	-4.14197	-3.56779	-5.75298
H	-4.66880	-5.32490	-4.08909
C	-3.89178	0.38527	0.05093
C	-3.50339	1.71916	0.08949
C	-2.16295	2.02946	0.28118
C	-1.23937	1.00329	0.43970
C	-1.68553	-0.30840	0.39508
C	-5.27524	-0.06928	-0.13357
C	-6.36354	0.78249	-0.28350
C	-7.63272	0.24068	-0.43923
C	-7.78975	-1.14026	-0.44474
C	-6.66643	-1.93784	-0.29346
H	-4.23869	2.51045	-0.02771
H	-1.84505	3.06872	0.31132
H	-0.18417	1.20672	0.59819
H	-1.00857	-1.15216	0.51740
H	-6.22335	1.85978	-0.27591
H	-8.49270	0.89548	-0.55610
H	-8.76540	-1.60235	-0.56491
H	-6.73614	-3.02448	-0.29235
C	-2.61844	-3.23728	2.72804
C	-4.47351	-1.80816	2.94561
C	-4.41288	-1.85351	4.32141
C	-2.51173	-3.31078	4.12719
H	-5.24045	-1.22870	2.43530
H	-5.13544	-1.29922	4.91321
H	-1.71441	-3.89364	4.58003
N	-4.48957	-4.48014	-0.06986
N	-3.90972	-2.80318	-1.98341
N	-2.97773	-0.60823	0.19451
N	-5.44179	-1.41625	-0.13490
N	-3.61053	-2.48680	2.16301
C	-3.40707	-2.62467	4.91893
H	-3.32508	-2.67693	6.00219

C	-1.75526	-3.91102	1.79929
C	-0.88160	-4.93846	2.19012
C	-1.03303	-4.09851	-0.45653
C	-0.13539	-5.61436	1.26048
H	-0.82194	-5.22018	3.23860
C	-0.92341	-3.60415	-1.74719
C	-0.17448	-5.20625	-0.10279
H	0.51272	-6.44137	1.54375
C	-0.10115	-4.24472	-2.69814
H	-1.45921	-2.70130	-2.03253
C	0.01718	-3.80094	-4.03530
C	0.64131	-5.38684	-2.27967
C	0.82736	-4.47029	-4.92350
H	-0.54855	-2.92113	-4.34532
C	1.46305	-6.05789	-3.21035
C	1.55277	-5.60724	-4.50837
H	0.91250	-4.12365	-5.95178
H	2.02125	-6.93155	-2.87317
H	2.19116	-6.12738	-5.22020
N	-1.88150	-3.53807	0.47545
N	0.59820	-5.82391	-0.99163
C	4.97564	-8.77550	1.56772
C	5.55390	-7.50507	1.54187
C	4.90776	-6.42687	0.93836
C	3.66763	-6.61697	0.35902
C	3.06834	-7.88867	0.38120
C	3.73809	-8.96459	0.98808
H	5.50235	-9.59785	2.04370
H	5.38307	-5.44996	0.92964
H	3.15036	-5.78653	-0.11990
H	3.25892	-9.94138	0.99288
O	1.87148	-8.12626	-0.15359
H	1.45575	-7.27939	-0.49461
N	6.84875	-7.30316	2.15367
O	7.39161	-8.26171	2.69270
O	7.34499	-6.18217	2.10726

[1-(*p*-O₂N-PhOH)]²⁺ PT TS (S=1)

Ru	-3.74715	-2.53223	0.08212
C	-4.72998	-4.91569	-1.36301
C	-4.89457	-5.22228	0.94466
C	-5.40850	-6.49841	0.78158
C	-5.57482	-6.99077	-0.50670
C	-5.23617	-6.19039	-1.58935
C	-4.38304	-3.96878	-2.42646
C	-3.72063	-1.78069	-2.88715
C	-3.80898	-1.99399	-4.25286
C	-4.17713	-3.25564	-4.70696
C	-4.47373	-4.25068	-3.78602
H	-4.75160	-4.79597	1.93512
H	-5.66938	-7.08747	1.65608
H	-5.97077	-7.98987	-0.67111
H	-5.37417	-6.55640	-2.60252
H	-3.40577	-0.81968	-2.48540
H	-3.58112	-1.18405	-4.93980
H	-4.23933	-3.46502	-5.77209

H	-4.77385	-5.23769	-4.12693
C	-3.93264	0.40733	0.06590
C	-3.53757	1.73872	0.11455
C	-2.19288	2.04026	0.29068
C	-1.27163	1.00835	0.42375
C	-1.72459	-0.30062	0.37247
C	-5.31822	-0.04172	-0.10963
C	-6.40593	0.81350	-0.23893
C	-7.67785	0.27641	-0.38802
C	-7.83762	-1.10396	-0.40900
C	-6.71499	-1.90616	-0.27947
H	-4.27041	2.53498	0.01704
H	-1.86962	3.07761	0.32826
H	-0.21321	1.20532	0.56813
H	-1.04908	-1.14799	0.47653
H	-6.26238	1.89024	-0.22058
H	-8.53743	0.93451	-0.48784
H	-8.81532	-1.56275	-0.52458
H	-6.78878	-2.99211	-0.29117
C	-2.64158	-3.21002	2.70884
C	-4.50506	-1.80159	2.93948
C	-4.41963	-1.83011	4.31568
C	-2.50495	-3.26377	4.10213
H	-5.28743	-1.23693	2.43647
H	-5.13935	-1.27797	4.91288
H	-1.69356	-3.83149	4.54856
N	-4.55836	-4.44926	-0.09929
N	-3.97873	-2.74943	-1.99536
N	-3.02143	-0.59189	0.18835
N	-5.48728	-1.38905	-0.12663
N	-3.64532	-2.47668	2.15150
C	-3.39476	-2.57655	4.90363
H	-3.29093	-2.61359	5.98548
C	-1.78365	-3.89644	1.77099
C	-0.89404	-4.89781	2.16913
C	-1.10273	-4.11548	-0.48878
C	-0.14353	-5.58085	1.23884
H	-0.81229	-5.16171	3.22013
C	-1.03154	-3.66361	-1.80276
C	-0.22414	-5.19142	-0.11307
H	0.52343	-6.39254	1.52182
C	-0.21259	-4.30643	-2.75927
H	-1.59714	-2.78699	-2.10622
C	-0.13489	-3.89523	-4.10812
C	0.57252	-5.41345	-2.34305
C	0.67956	-4.56325	-4.99575
H	-0.73129	-3.04011	-4.42776
C	1.39870	-6.08864	-3.25562
C	1.44737	-5.66390	-4.56785
H	0.73403	-4.24031	-6.03345
H	1.98920	-6.93564	-2.90794
H	2.08868	-6.18192	-5.27813
N	-1.93503	-3.54756	0.44759
N	0.53774	-5.80078	-1.03232
C	4.96988	-8.37290	1.52826
C	5.54887	-7.09680	1.47154

C	4.88809	-6.04548	0.82363
C	3.65819	-6.26231	0.24521
C	3.03150	-7.54380	0.29043
C	3.74199	-8.58927	0.95050
H	5.50161	-9.17605	2.03244
H	5.35918	-5.06646	0.78448
H	3.15045	-5.44503	-0.26828
H	3.27433	-9.57229	0.98523
O	1.87318	-7.77534	-0.22811
H	1.19837	-6.69418	-0.68287
N	6.82360	-6.86733	2.07869
O	7.38351	-7.80588	2.64715
O	7.31467	-5.73885	2.01337

[1-H(*p*-MeO-PhO)]²⁺ (S=1)

Ru	-3.79786	-2.55743	0.06978
C	-4.84746	-4.90404	-1.35214
C	-5.18326	-5.14455	0.93652
C	-5.73576	-6.40445	0.77004
C	-5.83105	-6.92865	-0.51378
C	-5.38757	-6.16651	-1.58455
C	-4.41421	-3.99424	-2.41885
C	-3.63448	-1.85883	-2.90789
C	-3.71724	-2.08856	-4.27152
C	-4.13706	-3.33893	-4.71335
C	-4.49742	-4.29590	-3.77652
H	-5.09609	-4.69826	1.92567
H	-6.08147	-6.95855	1.63859
H	-6.25367	-7.91629	-0.68219
H	-5.46717	-6.55276	-2.59701
H	-3.27826	-0.90591	-2.51983
H	-3.44444	-1.29976	-4.96740
H	-4.19474	-3.56426	-5.77559
H	-4.84918	-5.27080	-4.10281
C	-3.81732	0.36735	-0.02701
C	-3.36432	1.68378	-0.01757
C	-2.00645	1.93657	0.11487
C	-1.12869	0.86522	0.23901
C	-1.64030	-0.42271	0.22149
C	-5.22796	-0.01607	-0.15831
C	-6.27272	0.89492	-0.28664
C	-7.57651	0.43089	-0.38315
C	-7.80880	-0.93966	-0.35208
C	-6.72729	-1.79703	-0.22511
H	-4.06583	2.50886	-0.10815
H	-1.63954	2.96003	0.12452
H	-0.05856	1.01736	0.35092
H	-0.99659	-1.29500	0.31926
H	-6.06872	1.96190	-0.31121
H	-8.40086	1.13316	-0.48143
H	-8.81292	-1.34833	-0.42569
H	-6.86198	-2.87692	-0.19445
C	-2.84153	-3.31034	2.73889
C	-4.62674	-1.82022	2.90156
C	-4.62155	-1.88268	4.28312
C	-2.78604	-3.41212	4.13221

H	-5.34649	-1.19779	2.37305	C	-4.40927	-3.96453	-2.43186
H	-5.34099	-1.29971	4.85161	C	-3.59451	-1.83620	-2.89249
H	-2.03619	-4.03978	4.60581	C	-3.67620	-2.04842	-4.25910
N	-4.73676	-4.40580	-0.09248	C	-4.11458	-3.28639	-4.71741
N	-3.94560	-2.79312	-1.99372	C	-4.49282	-4.24873	-3.79317
N	-2.95211	-0.67508	0.08343	H	-5.12910	-4.70809	1.89940
N	-5.46349	-1.35475	-0.12476	H	-6.14917	-6.94874	1.57968
N	-3.76843	-2.52034	2.13776	H	-6.31885	-7.87776	-0.75301
C	-3.68210	-2.69917	4.90909	H	-5.49651	-6.50475	-2.64683
H	-3.64503	-2.77364	5.99344	H	-3.22429	-0.89375	-2.49217
C	-1.94098	-4.01697	1.83411	H	-3.38849	-1.25585	-4.94461
C	-1.04326	-4.97936	2.29301	H	-4.17272	-3.49791	-5.78245
C	-1.13739	-4.22619	-0.36571	H	-4.85969	-5.21394	-4.13132
C	-0.20419	-5.63143	1.40747	C	-3.76583	0.35864	0.01728
H	-1.01077	-5.23629	3.34775	C	-3.29685	1.66909	0.05000
C	-1.03734	-3.79220	-1.69450	C	-1.93703	1.90307	0.19649
C	-0.23510	-5.25444	0.06604	C	-1.07339	0.81920	0.31070
H	0.48492	-6.40553	1.74063	C	-1.60078	-0.46183	0.26982
C	-0.14936	-4.40530	-2.61176	C	-5.18029	-0.00571	-0.12682
H	-1.63766	-2.95280	-2.02763	C	-6.21329	0.91916	-0.25015
C	-0.04614	-4.01020	-3.96248	C	-7.52223	0.47196	-0.35681
C	0.67783	-5.46494	-2.16256	C	-7.77123	-0.89588	-0.34073
C	0.83289	-4.64393	-4.81822	C	-6.70069	-1.76756	-0.21874
H	-0.67853	-3.19439	-4.31424	H	-3.98763	2.50408	-0.03234
C	1.56735	-6.10368	-3.03015	H	-1.55766	2.92163	0.22488
C	1.64086	-5.69285	-4.35155	H	-0.00240	0.95626	0.43335
H	0.90130	-4.33005	-5.85794	H	-0.96846	-1.34322	0.35921
H	2.19167	-6.91388	-2.65378	H	-5.99612	1.98370	-0.26240
H	2.33298	-6.18760	-5.03013	H	-8.33765	1.18518	-0.45099
N	-2.03311	-3.68080	0.51426	H	-8.77998	-1.29151	-0.42202
N	0.59494	-5.83510	-0.83927	H	-6.84872	-2.84587	-0.20000
C	5.48678	-8.66192	1.38202	C	-2.84525	-3.36667	2.74030
C	6.00441	-7.34866	1.45088	C	-4.59932	-1.84128	2.91368
C	5.21636	-6.24433	1.03093	C	-4.59285	-1.91092	4.29506
C	3.95199	-6.43796	0.55941	C	-2.78868	-3.47603	4.13253
C	3.38203	-7.76511	0.47746	H	-5.30649	-1.20100	2.38957
C	4.21615	-8.86227	0.90998	H	-5.29908	-1.31620	4.86789
H	6.08963	-9.50954	1.69758	H	-2.05103	-4.12044	4.60272
H	5.65730	-5.25147	1.10001	N	-4.74970	-4.39949	-0.11243
H	3.34076	-5.59584	0.23378	N	-3.92428	-2.77581	-1.99055
H	3.79262	-9.86294	0.84531	N	-2.91434	-0.69604	0.11826
O	2.21525	-7.97205	0.05189	N	-5.43201	-1.34163	-0.10928
H	1.20926	-6.60213	-0.50730	N	-3.75651	-2.55444	2.14496
O	7.22048	-7.04259	1.89506	C	-3.66891	-2.74878	4.91492
C	8.07965	-8.08548	2.34618	H	-3.63071	-2.82902	5.99879
H	9.00464	-7.59612	2.65776	C	-1.96014	-4.08589	1.82829
H	7.63818	-8.61333	3.20093	C	-1.09095	-5.07979	2.27434
H	8.29426	-8.79393	1.53648	C	-1.15797	-4.28489	-0.37310
[1-H(<i>p</i>-O₂N-PhO)]²⁺ (S=1)				C	-0.26930	-5.74204	1.37888
Ru	-3.78320	-2.56797	0.07680	H	-1.06650	-5.35503	3.32459
C	-4.86051	-4.88091	-1.37844	C	-1.04167	-3.82950	-1.69390
C	-5.21570	-5.14215	0.90482	C	-0.28735	-5.34473	0.04448
C	-5.78739	-6.39093	0.72010	H	0.39489	-6.54201	1.70181
C	-5.88119	-6.89924	-0.57022	C	-0.17204	-4.45387	-2.62156
C	-5.41822	-6.13212	-1.62915	H	-1.61461	-2.96514	-2.01143
				C	-0.05664	-4.03919	-3.96521

C	0.62314	-5.54510	-2.19142	H	-4.00508	2.43149	-0.04912
C	0.80363	-4.68377	-4.83213	H	-1.58259	2.88402	0.19410
H	-0.66458	-3.19913	-4.30244	H	-0.00073	0.94327	0.43532
C	1.49381	-6.19438	-3.06897	H	-0.93074	-1.36163	0.41185
C	1.58019	-5.76326	-4.38365	H	-6.00497	1.89732	-0.20339
H	0.88129	-4.35435	-5.86631	H	-8.33719	1.08319	-0.40563
H	2.09421	-7.02944	-2.70849	H	-8.76185	-1.39673	-0.39995
H	2.25775	-6.26665	-5.07044	H	-6.82259	-2.93751	-0.18266
N	-2.04046	-3.72933	0.51365	C	-1.76638	-3.91009	1.85177
N	0.52711	-5.93395	-0.87267	C	-1.23056	-4.28893	-0.36256
C	5.53110	-8.63650	1.36285	C	-0.12665	-5.02507	0.04749
C	5.94555	-7.29623	1.43202	C	-0.65092	-4.66137	2.22409
C	5.14633	-6.21595	1.01856	C	-2.69384	-3.27141	2.77751
C	3.89635	-6.47577	0.52809	C	-4.62497	-2.02268	2.99411
C	3.40316	-7.83962	0.43877	C	-4.48512	-2.07588	4.37455
C	4.28245	-8.91070	0.87393	C	-2.58528	-3.29793	4.16849
H	6.20009	-9.42466	1.69554	H	-1.46297	-4.14023	-1.41514
H	5.53111	-5.20340	1.09615	H	0.53433	-5.47276	-0.69290
H	3.24298	-5.67037	0.19498	H	-0.41847	-4.82014	3.27709
H	3.90782	-9.92906	0.79837	H	-5.45723	-1.50647	2.51966
O	2.25866	-8.09531	0.00618	H	-5.21918	-1.58966	5.01512
H	1.12380	-6.71034	-0.55426	H	-1.75269	-3.81282	4.64676
N	7.27857	-7.00709	1.96750	N	-4.74660	-4.44540	-0.10753
O	7.95001	-7.95095	2.35301	N	-3.70340	-2.86813	-1.92196
O	7.63454	-5.83932	1.99802	N	-2.89560	-0.74886	0.18368
[2]²⁺ (S=0)				N	-5.41480	-1.42383	-0.07953
Ru	-3.74951	-2.64213	0.14091	N	-3.73270	-2.62130	2.19218
C	-4.88962	-4.86891	-1.39038	N	-2.05157	-3.72801	0.53644
C	-5.25360	-5.18973	0.88812	N	-3.46985	-2.70877	4.96492
C	-5.93105	-6.37667	0.65881	N	0.16543	-5.21554	1.33505
C	-6.08972	-6.81268	-0.65132	[2]²⁺ (S=1)			
C	-5.56292	-6.05117	-1.68457	Ru	-3.78122	-2.62900	0.11310
C	-4.30171	-3.98717	-2.40681	C	-4.85798	-4.92844	-1.37510
C	-3.13386	-2.00722	-2.77979	C	-5.15926	-5.20681	0.92514
C	-3.12636	-2.21640	-4.14975	C	-5.78026	-6.43114	0.73672
C	-3.73225	-3.36100	-4.65390	C	-5.93601	-6.90848	-0.55886
C	-4.32481	-4.25450	-3.77282	C	-5.47011	-6.15070	-1.62528
H	-5.11283	-4.80914	1.89848	C	-4.33834	-4.03716	-2.41713
H	-6.32537	-6.94187	1.49884	C	-3.31859	-1.97913	-2.83606
H	-6.61964	-7.73689	-0.86913	C	-3.32156	-2.20907	-4.20262
H	-5.67907	-6.37551	-2.71480	C	-3.85376	-3.40206	-4.67711
H	-2.66549	-1.12791	-2.34181	C	-4.37017	-4.32464	-3.77681
H	-2.65019	-1.48939	-4.80186	H	-5.01348	-4.78891	1.91934
H	-3.74353	-3.55978	-5.72279	H	-6.13059	-6.99339	1.59759
H	-4.80133	-5.15503	-4.15037	H	-6.41927	-7.86522	-0.74162
C	-3.76045	0.29062	0.05677	H	-5.58678	-6.50793	-2.64434
C	-3.30617	1.60645	0.05636	H	-2.91093	-1.06158	-2.41471
C	-1.94893	1.86039	0.19265	H	-2.91174	-1.46123	-4.87533
C	-1.07096	0.79126	0.32585	H	-3.86966	-3.61585	-5.74303
C	-1.58384	-0.49612	0.31722	H	-4.79217	-5.26086	-4.13193
C	-5.17246	-0.08737	-0.08527	C	-3.76198	0.31795	0.13967
C	-6.21172	0.83089	-0.20248	C	-3.28793	1.62114	0.23633
C	-7.51709	0.37479	-0.31646	C	-1.93253	1.83688	0.44716
C	-7.75643	-0.99419	-0.31325	C	-1.07768	0.74725	0.55880
C	-6.67949	-1.85863	-0.19489	C	-1.60948	-0.52895	0.46347

C	-5.16647	-0.03043	-0.09964
C	-6.18848	0.90121	-0.24023
C	-7.48383	0.45780	-0.47098
C	-7.73164	-0.90646	-0.56641
C	-6.67094	-1.78662	-0.42277
H	-3.96875	2.46320	0.14651
H	-1.54883	2.85132	0.52264
H	-0.01128	0.87331	0.72243
H	-0.98261	-1.41419	0.54863
H	-5.97732	1.96412	-0.16625
H	-8.29322	1.17608	-0.57691
H	-8.73066	-1.29215	-0.74833
H	-6.81492	-2.86332	-0.49056
C	-1.79520	-3.90932	1.83284
C	-1.28527	-4.33481	-0.41651
C	-0.19720	-5.07382	-0.02528
C	-0.66335	-4.69002	2.17370
C	-2.67248	-3.27455	2.74123
C	-4.58726	-1.94429	2.99889
C	-4.42007	-1.97404	4.36071
C	-2.55136	-3.26578	4.15283
H	-1.52856	-4.19464	-1.46872
H	0.44973	-5.53901	-0.76545
H	-0.41840	-4.83912	3.22709
H	-5.41668	-1.41105	2.53630
H	-5.11797	-1.45770	5.01579
H	-1.71912	-3.79649	4.61865
N	-4.71397	-4.47211	-0.10519
N	-3.80527	-2.87377	-1.96393
N	-2.91797	-0.73884	0.25717
N	-5.42117	-1.36015	-0.18802
N	-3.73949	-2.59918	2.17525
N	-2.08688	-3.73290	0.49032
N	-3.38680	-2.64560	4.94811
N	0.11996	-5.25625	1.29008

[2-H]³⁺ (S=0)

Ru	-3.67011	-2.52047	0.11723
C	-4.52845	-4.73885	-1.59522
C	-4.71343	-5.33123	0.65433
C	-5.23018	-6.57515	0.32959
C	-5.40066	-6.89676	-1.01210
C	-5.04423	-5.97112	-1.98337
C	-4.12356	-3.68604	-2.53515
C	-3.27308	-1.52601	-2.74105
C	-3.29227	-1.60422	-4.12509
C	-3.74556	-2.77408	-4.72194
C	-4.16487	-3.82556	-3.91842
H	-4.56913	-5.02823	1.69013
H	-5.49488	-7.27130	1.12031
H	-5.80946	-7.86131	-1.30297
H	-5.17406	-6.20628	-3.03631
H	-2.92361	-0.62960	-2.23166
H	-2.95585	-0.75675	-4.71587
H	-3.77315	-2.87066	-5.80441
H	-4.51932	-4.74837	-4.36895

C	-4.24893	0.35483	0.25958
C	-4.05107	1.72699	0.38108
C	-2.76366	2.21866	0.54551
C	-1.69726	1.32835	0.58660
C	-1.95813	-0.02676	0.46452
C	-5.56434	-0.27269	0.08193
C	-6.75418	0.44120	-0.01136
C	-7.95265	-0.24525	-0.14890
C	-7.93527	-1.63367	-0.18560
C	-6.71676	-2.28856	-0.09647
H	-4.89615	2.40984	0.35355
H	-2.59650	3.28866	0.64163
H	-0.67383	1.67019	0.71353
H	-1.15368	-0.76042	0.48908
H	-6.74726	1.52695	0.01863
H	-8.88944	0.30123	-0.22448
H	-8.84921	-2.21218	-0.28654
H	-6.66270	-3.37523	-0.12205
C	-1.40948	-3.45637	1.64000
C	-0.99396	-3.64582	-0.65229
C	0.24905	-4.17567	-0.39960
C	-0.15662	-3.98235	1.90718
C	-2.37183	-3.06534	2.65968
C	-4.50331	-2.26714	3.04363
C	-4.26318	-2.34450	4.41164
C	-2.16884	-3.13408	4.03863
H	-1.33582	-3.50376	-1.67328
H	0.94177	-4.48013	-1.17593
H	0.23701	-4.14084	2.90587
H	-5.45428	-1.91896	2.64646
H	-5.03779	-2.04724	5.11618
H	-1.22606	-3.49271	4.45048
N	-4.37669	-4.43007	-0.28169
N	-3.67459	-2.54041	-1.95996
N	-3.20101	-0.50630	0.30397
N	-5.55444	-1.62963	0.02929
N	-3.55836	-2.62700	2.16720
N	-1.82686	-3.27706	0.34675
N	-3.10419	-2.77434	4.90946
N	0.63239	-4.32472	0.88226
H	1.55572	-4.71631	1.08206

[2-H]³⁺ (S=1)

Ru	-3.70182	-2.48130	0.07284
C	-4.45988	-4.77063	-1.61696
C	-4.57360	-5.32863	0.64947
C	-5.03460	-6.60137	0.35435
C	-5.20824	-6.95622	-0.97813
C	-4.91774	-6.03313	-1.97455
C	-4.12858	-3.70834	-2.56919
C	-3.45950	-1.47832	-2.78193
C	-3.47394	-1.56393	-4.16458
C	-3.82817	-2.77133	-4.75453
C	-4.15999	-3.85399	-3.95020
H	-4.42751	-5.00154	1.67692
H	-5.25418	-7.29373	1.16176

H	-5.57216	-7.94569	-1.24354
H	-5.05682	-6.29346	-3.02039
H	-3.18230	-0.55826	-2.27030
H	-3.20940	-0.69456	-4.75952
H	-3.84687	-2.87366	-5.83660
H	-4.43251	-4.80580	-4.39712
C	-4.26267	0.39602	0.29787
C	-4.04873	1.76184	0.43964
C	-2.75335	2.22956	0.62200
C	-1.69760	1.32655	0.66545
C	-1.97181	-0.02429	0.52464
C	-5.57800	-0.22154	0.10123
C	-6.76933	0.48992	0.04234
C	-7.96295	-0.19712	-0.13686
C	-7.94245	-1.58163	-0.25411
C	-6.72343	-2.23743	-0.19500
H	-4.88258	2.45817	0.40796
H	-2.57143	3.29600	0.73067
H	-0.67205	1.65526	0.80729
H	-1.18276	-0.77426	0.54747
H	-6.76736	1.57222	0.13374
H	-8.90217	0.34820	-0.18451
H	-8.85440	-2.15448	-0.39493
H	-6.65801	-3.31984	-0.28412
C	-1.43234	-3.50869	1.64167
C	-0.98333	-3.73427	-0.66365
C	0.21838	-4.31592	-0.39394
C	-0.22074	-4.09055	1.92806
C	-2.38439	-3.07580	2.63415
C	-4.47315	-2.12397	3.01296
C	-4.25774	-2.21209	4.37634
C	-2.21313	-3.14991	4.02833
H	-1.29964	-3.58758	-1.69413
H	0.90832	-4.66097	-1.15365
H	0.13763	-4.25913	2.93839
H	-5.39280	-1.71247	2.60384
H	-5.01301	-1.86146	5.07626
H	-1.30160	-3.57254	4.45045
N	-4.29756	-4.43407	-0.31184
N	-3.77182	-2.52610	-2.00411
N	-3.22162	-0.47369	0.33922
N	-5.56944	-1.57600	-0.01648
N	-3.54383	-2.56049	2.14685
N	-1.81982	-3.30409	0.31585
N	-3.12773	-2.72784	4.87998
N	0.58852	-4.47930	0.92680
H	1.48148	-4.91293	1.14735

[2-H]²⁺ (S=1/2)

Ru	-3.72236	-2.50522	0.07919
C	-4.49996	-4.77702	-1.60050
C	-4.69496	-5.33566	0.65142
C	-5.14703	-6.60868	0.34302
C	-5.28212	-6.96459	-0.99443
C	-4.95444	-6.03893	-1.97463
C	-4.12638	-3.72555	-2.55374

C	-3.37722	-1.53346	-2.78782
C	-3.38027	-1.63240	-4.17007
C	-3.76858	-2.83305	-4.75370
C	-4.14522	-3.88878	-3.93610
H	-4.57859	-5.01003	1.68399
H	-5.38886	-7.30208	1.14386
H	-5.63896	-7.95309	-1.27344
H	-5.05672	-6.29664	-3.02560
H	-3.07372	-0.61523	-2.28743
H	-3.08009	-0.77825	-4.77103
H	-3.77834	-2.94876	-5.83472
H	-4.44738	-4.83669	-4.37292
C	-4.22913	0.37503	0.29075
C	-4.00052	1.74132	0.43011
C	-2.69991	2.20654	0.55931
C	-1.65140	1.29380	0.54760
C	-1.94294	-0.05399	0.41046
C	-5.56256	-0.21946	0.13225
C	-6.74212	0.52026	0.10436
C	-7.95573	-0.13545	-0.04443
C	-7.96435	-1.52039	-0.16380
C	-6.75684	-2.19975	-0.13039
H	-4.83299	2.43966	0.43825
H	-2.50839	3.27151	0.66713
H	-0.61745	1.61358	0.64520
H	-1.15571	-0.80638	0.39533
H	-6.71522	1.60290	0.19602
H	-8.88401	0.43024	-0.06672
H	-8.89081	-2.07555	-0.28323
H	-6.71811	-3.28443	-0.21761
C	-1.43062	-3.45820	1.63512
C	-0.94666	-3.62478	-0.65940
C	0.28930	-4.12949	-0.38908
C	-0.19107	-3.96304	1.92956
C	-2.41487	-3.08681	2.62922
C	-4.56040	-2.29772	3.01009
C	-4.34778	-2.38993	4.37347
C	-2.24112	-3.16065	4.02079
H	-1.26117	-3.48545	-1.69203
H	1.00541	-4.41811	-1.14818
H	0.16317	-4.12660	2.94230
H	-5.50650	-1.94910	2.59993
H	-5.13293	-2.10853	5.07279
H	-1.29702	-3.50783	4.44107
N	-4.38300	-4.43264	-0.29178
N	-3.73526	-2.55261	-1.99063
N	-3.19919	-0.51035	0.28264
N	-5.57880	-1.57312	0.01680
N	-3.60239	-2.64360	2.13278
N	-1.83071	-3.26499	0.30682
N	-3.18387	-2.81982	4.88243
N	0.66167	-4.29118	0.93523
H	1.57494	-4.67140	1.16143

[2]⁺ (S=1/2)

Ru	-3.78603	-2.62472	0.10262
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C	-4.87572	-4.90679	-1.37667	N	-3.46297	-2.76059	4.95695
C	-5.29022	-5.14706	0.90178	N	0.20411	-5.13653	1.30959
C	-5.93199	-6.35860	0.70311				
C	-6.04350	-6.85347	-0.59209				
C	-5.51000	-6.11879	-1.64039	[2] ⁺ (S=3/2)			
C	-4.29840	-4.04270	-2.41198	Ru	-3.77805	-2.63405	0.12701
C	-3.21539	-2.02653	-2.83548	C	-4.86845	-4.88432	-1.38621
C	-3.18369	-2.27630	-4.19766	C	-5.17176	-5.20546	0.94579
C	-3.72830	-3.46489	-4.67267	C	-5.78471	-6.42083	0.75696
C	-4.29282	-4.35374	-3.76997	C	-5.94768	-6.89020	-0.57157
H	-5.17996	-4.71901	1.89666	C	-5.49424	-6.13593	-1.62003
H	-6.33361	-6.89992	1.55558	C	-4.35152	-4.02597	-2.38378
H	-6.54227	-7.80038	-0.78509	C	-3.26922	-1.95887	-2.80712
H	-5.58885	-6.48577	-2.66017	C	-3.28851	-2.15958	-4.16656
H	-2.79349	-1.11352	-2.41799	C	-3.86628	-3.35890	-4.65786
H	-2.73503	-1.54812	-4.86807	C	-4.39034	-4.27025	-3.78124
H	-3.71539	-3.69780	-5.73478	H	-5.02238	-4.79605	1.94484
H	-4.72578	-5.28636	-4.12194	H	-6.12943	-6.99485	1.61226
C	-3.75384	0.30558	0.10874	H	-6.42802	-7.84886	-0.75756
C	-3.27958	1.61343	0.18307	H	-5.60537	-6.49085	-2.64230
C	-1.91842	1.83960	0.32293	H	-2.83335	-1.05589	-2.37804
C	-1.05633	0.74955	0.38238	H	-2.86683	-1.41339	-4.83383
C	-1.58852	-0.52723	0.30472	H	-3.89708	-3.55271	-5.72826
C	-5.16896	-0.04405	-0.05788	H	-4.84331	-5.18891	-4.14869
C	-6.19376	0.89331	-0.16543	C	-3.76222	0.32248	0.09343
C	-7.50181	0.46145	-0.32615	C	-3.29842	1.63254	0.15480
C	-7.75843	-0.90460	-0.38214	C	-1.94767	1.86463	0.37567
C	-6.69651	-1.78714	-0.27003	C	-1.08738	0.78445	0.53224
H	-3.96914	2.45230	0.13556	C	-1.61104	-0.49733	0.46505
H	-1.53593	2.85564	0.38432	C	-5.16585	-0.04042	-0.14003
H	0.01713	0.87849	0.49215	C	-6.19009	0.88436	-0.31365
H	-0.95482	-1.41162	0.34672	C	-7.48457	0.43110	-0.52867
H	-5.97082	1.95594	-0.12396	C	-7.73013	-0.93616	-0.57058
H	-8.31046	1.18397	-0.40809	C	-6.66753	-1.80879	-0.39421
H	-8.76687	-1.28910	-0.50960	H	-3.98332	2.46682	0.03042
H	-6.85136	-2.86456	-0.30438	H	-1.57160	2.88365	0.42485
C	-1.77793	-3.86837	1.82493	H	-0.02416	0.92302	0.70689
C	-1.21724	-4.25473	-0.40677	H	-0.98021	-1.37698	0.58003
C	-0.10280	-4.95713	-0.00845	H	-5.98069	1.94979	-0.27922
C	-0.62104	-4.60237	2.17907	H	-8.29481	1.14373	-0.66299
C	-2.69028	-3.27308	2.73375	H	-8.72848	-1.33029	-0.73808
C	-4.66206	-2.05568	3.00510	H	-6.80357	-2.88852	-0.41753
C	-4.52027	-2.12486	4.37221	C	-1.78919	-3.92658	1.84456
C	-2.58978	-3.30837	4.14480	C	-1.29518	-4.34867	-0.40721
H	-1.45138	-4.11805	-1.46305	C	-0.20634	-5.09426	-0.02571
H	0.56933	-5.39551	-0.74357	C	-0.65832	-4.71203	2.17638
H	-0.38658	-4.74635	3.23651	C	-2.66263	-3.29678	2.76239
H	-5.51200	-1.54662	2.54989	C	-4.57273	-1.97485	3.04354
H	-5.25511	-1.66561	5.03061	C	-4.40993	-2.02991	4.40666
H	-1.73794	-3.81624	4.60291	C	-2.54217	-3.31693	4.17351
N	-4.77268	-4.42864	-0.10840	H	-1.55416	-4.20449	-1.45518
N	-3.74962	-2.88701	-1.95310	H	0.43167	-5.56424	-0.77079
N	-2.90555	-0.75466	0.17102	H	-0.40801	-4.86494	3.22831
N	-5.42789	-1.37734	-0.10487	H	-5.40157	-1.43189	2.59050
N	-3.77291	-2.61964	2.16524	H	-5.10882	-1.52580	5.07052
N	-2.06377	-3.69599	0.47924	H	-1.71169	-3.86001	4.62912
				N	-4.73865	-4.43560	-0.07487

N	-3.75898	-2.85307	-1.92347
N	-2.91382	-0.72420	0.24768
N	-5.41859	-1.37220	-0.17832
N	-3.72474	-2.60564	2.20663
N	-2.08560	-3.74517	0.50449
N	-3.37697	-2.71268	4.98294
N	0.11949	-5.27915	1.28748

Optimized Structures at M06 Level of Theory in MeCN

p-MeO-PhOH (S=0)

C	0.31900	0.29395	0.00091
C	1.70451	0.36465	0.00143
C	2.35505	1.60160	0.00080
C	1.59409	2.77197	-0.00037
C	0.20223	2.69816	-0.00089
C	-0.44257	1.46503	-0.00024
H	-0.17838	-0.67681	0.00140
H	2.30692	-0.54264	0.00234
H	2.07023	3.74957	-0.00092
H	-0.39699	3.60760	-0.00180
O	-1.80285	1.45534	-0.00076
H	-2.11160	0.53368	-0.00027
O	3.71405	1.56135	0.00136
C	4.40416	2.79046	0.00086
H	4.17442	3.38824	0.89574
H	5.47065	2.54693	0.00139
H	4.17507	3.38716	-0.89490

p-MeO-PhOH⁺ (S=1/2)

C	0.33640	0.25988	0.00090
C	1.69562	0.34324	0.00116
C	2.33620	1.61977	0.00042
C	1.56788	2.81610	-0.00080
C	0.20573	2.72920	-0.00106
C	-0.42708	1.45553	-0.00009
H	-0.17088	-0.70322	0.00146
H	2.32322	-0.54465	0.00197
H	2.05355	3.78730	-0.00161
H	-0.42049	3.61805	-0.00197
O	-1.74424	1.45226	-0.00022
H	-2.09538	0.53643	0.00039
O	3.64536	1.58254	0.00099
C	4.41119	2.79823	0.00110
H	4.19218	3.38148	0.90158
H	5.45514	2.48333	0.00203
H	4.19361	3.38074	-0.90020

p-MeO-PhO⁻ (S=0)

C	0.31998	0.29428	0.00069
C	1.70425	0.36750	0.00135
C	2.36546	1.60029	0.00083
C	1.59536	2.76431	-0.00033
C	0.20205	2.69216	-0.00101

C	-0.53227	1.45764	-0.00054
H	-0.17019	-0.68281	0.00118
H	2.31176	-0.54070	0.00232
H	2.07428	3.74419	-0.00076
H	-0.37964	3.61793	-0.00192
O	-1.79824	1.39067	-0.00094
O	3.74603	1.55785	0.00155
C	4.41325	2.78709	0.00090
H	4.17816	3.39155	0.89350
H	5.48684	2.56853	0.00140
H	4.17874	3.39029	-0.89270

p-MeO-PhO[•] (S=1/2)

C	0.33954	0.26434	0.00084
C	1.70126	0.34743	0.00136
C	2.34384	1.61192	0.00073
C	1.58040	2.79938	-0.00049
C	0.21005	2.72221	-0.00104
C	-0.49096	1.45431	-0.00032
H	-0.16718	-0.69954	0.00130
H	2.33021	-0.54172	0.00226
H	2.07125	3.76964	-0.00103
H	-0.39837	3.62566	-0.00200
O	-1.73918	1.39048	-0.00094
O	3.67869	1.57282	0.00131
C	4.40572	2.79498	0.00094
H	4.18398	3.38674	0.89823
H	5.46192	2.51632	0.00146
H	4.18464	3.38584	-0.89709

p-Ph-PhOH (S=0)

C	-1.54374	0.04385	0.31314
C	-0.15480	0.05504	0.31992
C	0.57029	1.20666	-0.01182
C	-0.15822	2.35586	-0.35302
C	-1.54489	2.35978	-0.36333
C	-2.24623	1.19992	-0.02894
H	-2.08907	-0.86157	0.58293
H	0.37540	-0.85074	0.61352
H	0.37185	3.26378	-0.64023
H	-2.10270	3.25363	-0.63830
C	2.04801	1.21113	-0.00256
C	2.76423	2.36459	0.34730
C	2.77551	0.06215	-0.34385
C	4.15485	2.36997	0.35323
H	2.22380	3.26451	0.64085
C	4.16610	0.06517	-0.33230
H	2.24411	-0.84082	-0.64448
C	4.86358	1.21971	0.01484
H	4.68817	3.27755	0.63353
H	4.70842	-0.83902	-0.60623
H	5.95255	1.22307	0.02141
O	-3.59899	1.25371	-0.05264
H	-3.95853	0.38288	0.18900

p-Ph-PhOH⁺ (S=1/2)

C	-1.51630	-0.00802	0.20461
C	-0.15020	0.00191	0.20339
C	0.58539	1.20929	-0.00120
C	-0.15442	2.41284	-0.21220
C	-1.51913	2.41242	-0.23330
C	-2.21796	1.19928	-0.02265
H	-2.07275	-0.92700	0.38409
H	0.37790	-0.92641	0.40311
H	0.37100	3.34468	-0.40215
H	-2.09026	3.31919	-0.41704
C	2.02454	1.21188	0.00348
C	2.75055	2.41273	0.21607
C	2.75680	0.01441	-0.20701
C	4.13015	2.40934	0.22695
H	2.22213	3.34191	0.41425
C	4.13648	0.02466	-0.21548
H	2.23359	-0.91744	-0.40653
C	4.83035	1.21872	0.00614
H	4.67256	3.33391	0.41088
H	4.68375	-0.89719	-0.39861
H	5.91869	1.22150	0.00680
O	-3.53521	1.25675	-0.05047
H	-3.92796	0.37144	0.09885

***p*-Ph-PhO⁻ (S=0)**

C	-1.54852	0.04395	0.28937
C	-0.16778	0.05266	0.28418
C	0.57962	1.21502	0.00034
C	-0.16766	2.37730	-0.28418
C	-1.54838	2.38579	-0.29085
C	-2.34089	1.21481	-0.00115
H	-2.08926	-0.87444	0.53114
H	0.36258	-0.86831	0.53999
H	0.36283	3.29835	-0.53941
H	-2.08901	3.30412	-0.53312
C	2.04815	1.21508	0.00098
C	2.78484	2.37899	0.29133
C	2.78514	0.05124	-0.28881
C	4.17491	2.38079	0.28539
H	2.25496	3.29585	0.55059
C	4.17521	0.04951	-0.28172
H	2.25553	-0.86565	-0.54853
C	4.88457	1.21517	0.00212
H	4.70986	3.30156	0.51848
H	4.71040	-0.87123	-0.51441
H	5.97366	1.21521	0.00255
O	-3.60105	1.21473	-0.00179

***p*-Ph-PhO[•] (S=1/2)**

C	-1.52115	0.01775	0.29098
C	-0.15486	0.02832	0.28368
C	0.57602	1.21501	0.00022
C	-0.15473	2.40162	-0.28392
C	-1.52102	2.41203	-0.29251
C	-2.28889	1.21484	-0.00113
H	-2.07978	-0.88723	0.52599

H	0.38786	-0.88205	0.53401
H	0.38811	3.31204	-0.53374
H	-2.07953	3.31694	-0.52803
C	2.03872	1.21507	0.00093
C	2.76180	2.38794	0.28491
C	2.76215	0.04226	-0.28238
C	4.14960	2.38502	0.29005
H	2.23087	3.30440	0.53750
C	4.14995	0.04528	-0.28620
H	2.23151	-0.87423	-0.53546
C	4.85054	1.21517	0.00225
H	4.68891	3.30106	0.52543
H	4.68954	-0.87073	-0.52109
H	5.93928	1.21521	0.00275
O	-3.53517	1.21477	-0.00171

***p*-Cl-PhOH (S=0)**

C	0.30970	0.27830	0.00093
C	1.69936	0.32598	0.00142
C	2.33596	1.56033	0.00070
C	1.61046	2.74736	-0.00050
C	0.22321	2.69500	-0.00097
C	-0.43129	1.46124	-0.00023
H	-0.20283	-0.68384	0.00147
H	2.27909	-0.59491	0.00234
H	2.12401	3.70674	-0.00108
H	-0.36768	3.60906	-0.00190
O	-1.78380	1.47269	-0.00068
H	-2.11351	0.55729	-0.00014
Cl	4.09495	1.62361	0.00132

***p*-Cl-PhOH[•] (S=1/2)**

C	0.32325	0.24048	0.00084
C	1.68628	0.29559	0.00136
C	2.32554	1.56216	0.00071
C	1.59701	2.77728	-0.00064
C	0.23400	2.72762	-0.00110
C	-0.41808	1.45791	-0.00021
H	-0.20688	-0.71005	0.00126
H	2.28504	-0.61168	0.00223
H	2.12519	3.72719	-0.00124
H	-0.37601	3.62734	-0.00201
O	-1.72446	1.47672	-0.00044
H	-2.10279	0.56845	0.00016
Cl	4.02955	1.61983	0.00176

***p*-Cl-PhO⁻ (S=0)**

C	0.30912	0.28393	0.00089
C	1.69375	0.32970	0.00140
C	2.34686	1.56200	0.00070
C	1.61242	2.74781	-0.00048
C	0.22795	2.70023	-0.00098
C	-0.52009	1.46560	-0.00028
H	-0.19960	-0.68259	0.00148
H	2.27684	-0.59278	0.00235
H	2.13219	3.70733	-0.00105

H	-0.34378	3.63094	-0.00193
O	-1.78049	1.42317	-0.00065
Cl	4.12322	1.62123	0.00133

***p*-Cl-PhO[•] (S=1/2)**

C	0.31849	0.25540	0.00096
C	1.68769	0.30599	0.00142
C	2.32412	1.56135	0.00069
C	1.60473	2.77126	-0.00053
C	0.23533	2.72934	-0.00101
C	-0.48269	1.46680	-0.00026
H	-0.21083	-0.69572	0.00149
H	2.28691	-0.60241	0.00232
H	2.14102	3.71815	-0.00108
H	-0.35670	3.64283	-0.00192
O	-1.72895	1.42493	-0.00064
Cl	4.05927	1.61864	0.00136

***p*-MeOC(O)-PhOH (S=0)**

C	-1.03633	0.68748	0.00052
C	0.36099	0.73120	0.00036
C	1.01078	1.95540	-0.00090
C	0.28039	3.14877	-0.00200
C	-1.11867	3.08981	-0.00182
C	-1.77760	1.87402	-0.00059
H	0.93024	-0.19854	0.00126
H	2.09805	1.98489	-0.00100
H	-1.68372	4.02012	-0.00268
H	-2.86455	1.81738	-0.00045
O	-1.72293	-0.47214	0.00172
H	-1.09922	-1.21947	0.00249
C	0.92510	4.47632	-0.00346
O	0.32640	5.53441	-0.00411
O	2.26432	4.39504	-0.00405
C	2.95964	5.63900	-0.00568
H	2.71312	6.22544	0.88653
H	4.02299	5.38906	-0.00605
H	2.71204	6.22369	-0.89872

***p*-MeOC(O)-PhOH^{•+} (S=1/2)**

C	-1.02499	0.69831	0.00218
C	0.40377	0.72417	-0.00082
C	1.03653	1.93279	-0.00474
C	0.27369	3.13273	-0.00546
C	-1.14346	3.09908	-0.00310
C	-1.79755	1.90270	0.00083
H	0.95392	-0.21513	0.00026
H	2.12141	1.98377	-0.00697
H	-1.69111	4.03755	-0.00400
H	-2.88185	1.82501	0.00303
O	-1.69692	-0.41687	0.00567
H	-1.10614	-1.20517	0.00616
C	0.92478	4.47810	-0.00729
O	0.29110	5.51032	-0.01130
O	2.24631	4.38824	-0.00317
C	2.95857	5.63332	-0.00265

H	2.70624	6.21266	0.89135
H	4.01683	5.36874	-0.00026
H	2.70992	6.21155	-0.89838

***p*-MeOC(O)-PhO⁻ (S=0)**

C	-1.07565	0.61736	0.00095
C	0.36727	0.73896	0.00058
C	1.01089	1.95344	-0.00080
C	0.29135	3.17017	-0.00198
C	-1.11899	3.09084	-0.00173
C	-1.77628	1.88470	-0.00041
H	0.94017	-0.19085	0.00155
H	2.10100	1.98647	-0.00097
H	-1.68285	4.02542	-0.00270
H	-2.86777	1.84727	-0.00026
O	-1.66684	-0.48956	0.00233
C	0.92483	4.47552	-0.00356
O	0.34753	5.55413	-0.00450
O	2.28175	4.40226	-0.00398
C	2.95970	5.64723	-0.00569
H	2.71297	6.23879	0.88459
H	4.02781	5.41241	-0.00592
H	2.71213	6.23676	-0.89709

***p*-MeOC(O)-PhO[•] (S=1/2)**

C	-1.05564	0.65009	0.00109
C	0.39512	0.73585	0.00075
C	1.03192	1.94797	-0.00088
C	0.27815	3.14417	-0.00225
C	-1.13445	3.10303	-0.00201
C	-1.79187	1.90323	-0.00042
H	0.94962	-0.20088	0.00188
H	2.11794	2.00040	-0.00106
H	-1.68088	4.04396	-0.00309
H	-2.87902	1.84507	-0.00022
O	-1.64129	-0.44965	0.00261
C	0.92636	4.48032	-0.00383
O	0.31320	5.52799	-0.00420
O	2.25801	4.39624	-0.00472
C	2.95950	5.64094	-0.00564
H	2.71134	6.22384	0.88788
H	4.02091	5.38555	-0.00625
H	2.71013	6.22321	-0.89922

***p*-NC-PhOH (S=0)**

C	0.32139	0.27387	0.00095
C	1.70413	0.32371	0.00143
C	2.36265	1.56146	0.00071
C	1.61533	2.75004	-0.00049
C	0.23439	2.70053	-0.00097
C	-0.41723	1.46199	-0.00023
H	-0.19639	-0.68496	0.00149
H	2.28349	-0.59738	0.00236
H	2.12878	3.70947	-0.00105
H	-0.36112	3.61105	-0.00191
O	-1.76209	1.47339	-0.00069

H	-2.09743	0.55878	-0.00015
C	3.78639	1.61126	0.00123
N	4.95066	1.65000	0.00165

***p*-NC-PhOH⁺ (S=1/2)**

C	0.33221	0.23467	0.00088
C	1.69328	0.29130	0.00140
C	2.34282	1.56143	0.00065
C	1.60615	2.77776	-0.00057
C	0.24412	2.73215	-0.00107
C	-0.40728	1.45739	-0.00022
H	-0.20278	-0.71300	0.00136
H	2.29261	-0.61505	0.00232
H	2.13770	3.72533	-0.00110
H	-0.36923	3.62949	-0.00199
O	-1.70796	1.47836	-0.00051
H	-2.09334	0.57108	0.00006
C	3.76041	1.61491	0.00129
N	4.92425	1.65739	0.00183

***p*-NC-PhO⁻ (S=0)**

C	0.32557	0.27887	0.00093
C	1.69703	0.32672	0.00142
C	2.38435	1.56500	0.00072
C	1.61736	2.75562	-0.00047
C	0.24573	2.71285	-0.00098
C	-0.49935	1.47011	-0.00027
H	-0.19200	-0.68195	0.00152
H	2.27812	-0.59718	0.00237
H	2.13655	3.71568	-0.00103
H	-0.33332	3.63800	-0.00193
O	-1.75159	1.42908	-0.00067
C	3.79400	1.60936	0.00122
N	4.96451	1.64470	0.00163

***p*-NC-PhO[•] (S=1/2)**

C	0.33004	0.25406	0.00098
C	1.69623	0.30481	0.00145
C	2.34952	1.56334	0.00070
C	1.61547	2.77585	-0.00049
C	0.24884	2.73745	-0.00100
C	-0.46697	1.47109	-0.00027
H	-0.20427	-0.69391	0.00153
H	2.29410	-0.60412	0.00238
H	2.15311	3.72169	-0.00100
H	-0.34612	3.64867	-0.00193
O	-1.71026	1.43066	-0.00069
C	3.77151	1.61032	0.00120
N	4.93577	1.64694	0.00161

***p*-O₂N-PhOH (S=0)**

C	0.33476	0.27098	0.00082
C	1.71647	0.31490	0.00131
C	2.35714	1.55217	0.00066
C	1.63672	2.74742	-0.00044
C	0.25691	2.70193	-0.00085

C	-0.39930	1.46374	-0.00021
H	-0.18688	-0.68544	0.00122
H	2.30218	-0.59981	0.00214
H	2.16344	3.69741	-0.00091
H	-0.33573	3.61407	-0.00162
O	-1.74102	1.48019	-0.00062
H	-2.08179	0.56695	-0.00014
N	3.80506	1.59786	0.00124
O	4.34990	2.69627	-0.00038
O	4.41932	0.53659	0.00348

***p*-O₂N-PhOH[•] (S=1/2)**

C	0.34547	0.23056	-0.00028
C	1.70835	0.28790	0.00044
C	2.33117	1.55477	0.00092
C	1.63101	2.77404	0.00089
C	0.26567	2.73397	0.00068
C	-0.39216	1.45787	-0.00007
H	-0.18993	-0.71672	-0.00112
H	2.31330	-0.61353	0.00016
H	2.17120	3.71541	0.00110
H	-0.34389	3.63390	0.00095
O	-1.68914	1.48489	-0.00056
H	-2.08283	0.57945	-0.00097
N	3.80656	1.59981	0.00117
O	4.32833	2.69955	-0.01283
O	4.39408	0.53337	0.01526

***p*-O₂N-PhO⁻ (S=0)**

C	0.34365	0.26494	0.00065
C	1.71072	0.30920	0.00136
C	2.38282	1.55091	0.00091
C	1.63574	2.74941	-0.00023
C	0.26869	2.70939	-0.00086
C	-0.47724	1.46313	-0.00044
H	-0.17950	-0.69221	0.00095
H	2.30287	-0.60390	0.00223
H	2.17073	3.69717	-0.00054
H	-0.31171	3.63305	-0.00168
O	-1.72576	1.42489	-0.00103
N	3.79111	1.59437	0.00163
O	4.36095	2.69731	0.00057
O	4.42898	0.52929	0.00324

***p*-O₂N-PhO[•] (S=1/2)**

C	0.34549	0.24445	0.00053
C	1.71317	0.29312	0.00116
C	2.34199	1.55001	0.00077
C	1.63707	2.76608	-0.00025
C	0.26916	2.73013	-0.00078
C	-0.44857	1.46401	-0.00035
H	-0.18959	-0.70281	0.00071
H	2.31722	-0.60949	0.00185
H	2.18407	3.70436	-0.00048
H	-0.32347	3.64255	-0.00144
O	-1.69168	1.42593	-0.00080

N	3.80244	1.59457	0.00167
O	4.33925	2.69332	-0.00044
O	4.40552	0.53072	0.00461

[1]²⁺ (S=0)

Ru	-3.67856	-2.60061	0.09250
C	-4.76647	-4.91424	-1.35615
C	-5.11585	-5.16986	0.92933
C	-5.69756	-6.41467	0.74758
C	-5.79955	-6.92296	-0.54167
C	-5.33421	-6.16097	-1.60367
C	-4.31280	-4.00249	-2.41295
C	-3.48577	-1.87930	-2.88132
C	-3.56726	-2.09710	-4.24708
C	-4.01284	-3.33422	-4.70009
C	-4.39724	-4.29157	-3.77295
H	-5.02483	-4.73585	1.92359
H	-6.06139	-6.96793	1.60913
H	-6.24582	-7.89799	-0.72230
H	-5.41972	-6.53373	-2.62063
H	-3.10886	-0.93810	-2.48449
H	-3.27297	-1.30945	-4.93532
H	-4.07124	-3.54965	-5.76432
H	-4.76835	-5.25614	-4.10804
C	-3.67635	0.32426	0.00217
C	-3.21589	1.63763	0.01162
C	-1.85607	1.88144	0.14144
C	-0.98434	0.80495	0.26170
C	-1.50375	-0.47990	0.24413
C	-5.08900	-0.05010	-0.13038
C	-6.12792	0.86718	-0.25644
C	-7.43426	0.40982	-0.35259
C	-7.67495	-0.95907	-0.32264
C	-6.59865	-1.82348	-0.19896
H	-3.91296	2.46633	-0.07878
H	-1.48289	2.90265	0.15091
H	0.08715	0.94972	0.36985
H	-0.86191	-1.35404	0.33669
H	-5.91825	1.93305	-0.27827
H	-8.25471	1.11689	-0.44916
H	-8.68146	-1.36199	-0.39466
H	-6.73995	-2.90239	-0.16905
C	-2.74821	-3.38668	2.75637
C	-4.51802	-1.88624	2.91785
C	-4.52019	-1.96917	4.30128
C	-2.70115	-3.51372	4.14312
H	-5.22996	-1.25055	2.39546
H	-5.23951	-1.38711	4.87094
H	-1.96518	-4.15901	4.61357
N	-4.64811	-4.43302	-0.09099
N	-3.82253	-2.81423	-1.97700
N	-2.81744	-0.72291	0.11155
N	-5.33298	-1.38693	-0.10115
N	-3.66011	-2.58160	2.15335
C	-3.59735	-2.80007	4.92503
H	-3.57115	-2.89073	6.00813

C	-1.83767	-4.08120	1.84319
C	-0.91237	-5.04679	2.32431
C	-1.03028	-4.31282	-0.33087
C	-0.08187	-5.68432	1.45745
H	-0.89211	-5.29248	3.38158
C	-0.95179	-3.88302	-1.65186
C	-0.10026	-5.32557	0.08281
H	0.61711	-6.45108	1.78492
C	-0.05807	-4.48708	-2.53301
H	-1.56726	-3.05797	-1.99500
C	0.04125	-4.10035	-3.89915
C	0.78155	-5.53876	-2.03216
C	0.91827	-4.73818	-4.73004
H	-0.60179	-3.29725	-4.26068
C	1.68298	-6.17739	-2.92921
C	1.74456	-5.78726	-4.23823
H	0.99114	-4.44871	-5.77651
H	2.31256	-6.97418	-2.53649
H	2.43581	-6.28020	-4.91959
N	-1.93729	-3.75444	0.55221
N	0.75994	-5.92078	-0.74656

[1]²⁺ (S=1)

Ru	-3.64521	-2.59156	0.11529
C	-4.67877	-4.95252	-1.32617
C	-4.96317	-5.19875	0.97683
C	-5.53390	-6.45068	0.81480
C	-5.66218	-6.96448	-0.46975
C	-5.23398	-6.20696	-1.55115
C	-4.25132	-4.04200	-2.39181
C	-3.47920	-1.89568	-2.86770
C	-3.53206	-2.13151	-4.23184
C	-3.94086	-3.38397	-4.67590
C	-4.31273	-4.34632	-3.74776
H	-4.84605	-4.75659	1.96413
H	-5.86724	-7.00510	1.68735
H	-6.10035	-7.94619	-0.63255
H	-5.34011	-6.58746	-2.56294
H	-3.13688	-0.94080	-2.47222
H	-3.24626	-1.34522	-4.92462
H	-3.97864	-3.61009	-5.73877
H	-4.65131	-5.32440	-4.07787
C	-3.72253	0.35296	0.05541
C	-3.27998	1.66942	0.10230
C	-1.93521	1.92401	0.33817
C	-1.06089	0.86054	0.52815
C	-1.56022	-0.43105	0.47148
C	-5.11667	-0.04360	-0.17114
C	-6.16103	0.85366	-0.36006
C	-7.44690	0.36540	-0.54948
C	-7.66275	-1.00741	-0.54815
C	-6.57978	-1.85213	-0.35997
H	-3.97724	2.48998	-0.04218
H	-1.57544	2.94927	0.37649
H	-0.00359	1.01920	0.72009
H	-0.92422	-1.30261	0.61499

H	-5.97333	1.92368	-0.35659	H	-3.08499	-0.96761	-2.49048
H	-8.27400	1.05553	-0.69679	H	-3.23992	-1.35894	-4.93905
H	-8.65357	-1.42860	-0.69218	H	-4.05406	-3.59894	-5.75248
H	-6.69835	-2.93415	-0.35502	H	-4.77296	-5.28579	-4.08582
C	-2.68651	-3.33565	2.77556	C	-3.65488	0.31265	-0.02159
C	-4.46246	-1.80057	2.93852	C	-3.18848	1.62366	-0.03309
C	-4.45290	-1.85584	4.31532	C	-1.82700	1.86298	0.08708
C	-2.63591	-3.42395	4.17799	C	-0.95953	0.78464	0.21897
H	-5.17525	-1.17402	2.40583	C	-1.48486	-0.49788	0.22180
H	-5.16092	-1.26112	4.88505	C	-5.06977	-0.05632	-0.14322
H	-1.89225	-4.05719	4.65415	C	-6.10508	0.86406	-0.27312
N	-4.53953	-4.46835	-0.06607	C	-7.41399	0.41130	-0.35679
N	-3.80799	-2.83443	-1.96811	C	-7.66092	-0.95574	-0.31034
N	-2.85700	-0.67689	0.23217	C	-6.58803	-1.82394	-0.18355
N	-5.33920	-1.38215	-0.16986	H	-3.88207	2.45405	-0.13300
N	-3.61473	-2.52579	2.18211	H	-1.44925	2.88249	0.07987
C	-3.51695	-2.69061	4.94203	H	0.11298	0.92610	0.32054
H	-3.47780	-2.75430	6.02723	H	-0.84492	-1.37213	0.32405
C	-1.82828	-4.04530	1.87297	H	-5.89113	1.92870	-0.30720
C	-0.99895	-5.10389	2.28547	H	-8.23174	1.12107	-0.45612
C	-1.04667	-4.25204	-0.36207	H	-8.66959	-1.35479	-0.37173
C	-0.24596	-5.79661	1.37567	H	-6.73453	-2.90151	-0.14057
H	-0.98175	-5.38953	3.33459	C	-2.76791	-3.41813	2.76507
C	-0.88664	-3.75602	-1.64601	C	-4.50804	-1.88420	2.92190
C	-0.23187	-5.39069	0.00724	C	-4.52274	-1.97998	4.30492
H	0.37661	-6.63964	1.66830	C	-2.73479	-3.56067	4.15041
C	-0.07435	-4.43459	-2.57810	H	-5.20264	-1.22958	2.39985
H	-1.37376	-2.82888	-1.93924	H	-5.23461	-1.38797	4.87356
C	0.08051	-4.00360	-3.91654	H	-2.01707	-4.22514	4.62246
C	0.61394	-5.60452	-2.13700	N	-4.67133	-4.43127	-0.07517
C	0.87043	-4.71372	-4.79179	N	-3.81416	-2.83514	-1.97108
H	-0.44624	-3.10410	-4.23988	N	-2.80005	-0.73642	0.09872
C	1.41601	-6.31385	-3.06001	N	-5.32032	-1.39128	-0.09851
C	1.54006	-5.87929	-4.36068	N	-3.65816	-2.59042	2.15922
H	0.98065	-4.37866	-5.82186	C	-3.62392	-2.83557	4.92994
H	1.93197	-7.20572	-2.70575	H	-3.61034	-2.93651	6.01221
H	2.16121	-6.43350	-5.06260	C	-1.86281	-4.11494	1.85261
N	-1.90098	-3.66528	0.54733	C	-0.94332	-5.08786	2.32611
N	0.54440	-6.03922	-0.85150	C	-1.04586	-4.33516	-0.31526
[1-H]³⁺ (S=0)				C	-0.09859	-5.72252	1.46748
Ru	-3.67265	-2.61182	0.09968	H	-0.92901	-5.34527	3.38044
C	-4.78351	-4.92164	-1.33719	C	-0.95685	-3.89922	-1.63861
C	-5.16584	-5.14697	0.94727	C	-0.12781	-5.33163	0.11473
C	-5.76618	-6.38388	0.77081	H	0.59636	-6.49017	1.80005
C	-5.85799	-6.90457	-0.51394	C	-0.06377	-4.47345	-2.53948
C	-5.36758	-6.16161	-1.57860	H	-1.57793	-3.07366	-1.97055
C	-4.31246	-4.02338	-2.39889	C	0.01504	-4.06126	-3.89694
C	-3.46605	-1.90969	-2.88123	C	0.80144	-5.51230	-2.08644
C	-3.54279	-2.13861	-4.24557	C	0.90294	-4.66664	-4.74218
C	-3.99745	-3.37550	-4.68985	H	-0.65055	-3.26795	-4.23479
C	-4.39381	-4.32235	-3.75672	C	1.71299	-6.12307	-2.96281
H	-5.08361	-4.70217	1.93755	C	1.75240	-5.69910	-4.26869
H	-6.15269	-6.92062	1.63284	H	0.96538	-4.36173	-5.78381
H	-6.31820	-7.87389	-0.69011	H	2.36482	-6.91278	-2.59460
H	-5.44854	-6.54333	-2.59255	H	2.45345	-6.16521	-4.95772
				N	-1.95587	-3.78118	0.56024

N	0.72865	-5.87221	-0.77950
H	1.37624	-6.58860	-0.44247

[1-H]³⁺ (S=1)

Ru	-3.65097	-2.58774	0.10787
C	-4.67580	-4.93253	-1.36953
C	-4.96100	-5.22009	0.92858
C	-5.52069	-6.47395	0.74413
C	-5.64285	-6.96678	-0.54900
C	-5.22042	-6.18701	-1.61701
C	-4.25171	-4.00147	-2.41797
C	-3.48057	-1.84362	-2.85699
C	-3.52994	-2.05835	-4.22453
C	-3.93838	-3.30316	-4.68968
C	-4.30940	-4.28223	-3.77848
H	-4.85330	-4.79448	1.92404
H	-5.85148	-7.04507	1.60678
H	-6.07237	-7.94925	-0.72909
H	-5.32269	-6.55041	-2.63542
H	-3.13976	-0.89477	-2.44722
H	-3.24337	-1.26063	-4.90358
H	-3.97560	-3.51136	-5.75616
H	-4.64649	-5.25484	-4.12557
C	-3.72252	0.35129	0.06120
C	-3.27663	1.66610	0.10078
C	-1.92808	1.91647	0.32062
C	-1.05370	0.85143	0.50237
C	-1.55650	-0.43912	0.45595
C	-5.11641	-0.04663	-0.15608
C	-6.16757	0.84556	-0.32488
C	-7.45285	0.35140	-0.50452
C	-7.66157	-1.02238	-0.51412
C	-6.57321	-1.86408	-0.34697
H	-3.97335	2.48800	-0.03849
H	-1.56504	2.94073	0.35233
H	0.00614	1.00847	0.68059
H	-0.91959	-1.31062	0.59597
H	-5.98527	1.91635	-0.31192
H	-8.28549	1.03814	-0.63494
H	-8.65169	-1.44768	-0.65017
H	-6.68674	-2.94632	-0.34983
C	-2.70255	-3.32889	2.79564
C	-4.47094	-1.80025	2.92994
C	-4.45318	-1.82967	4.31084
C	-2.63398	-3.38957	4.18857
H	-5.18904	-1.18589	2.39134
H	-5.16183	-1.22601	4.87018
H	-1.88778	-4.01218	4.67356
N	-4.54075	-4.46988	-0.10110
N	-3.81291	-2.79807	-1.97413
N	-2.85714	-0.68054	0.23281
N	-5.33306	-1.38740	-0.16689
N	-3.61988	-2.53189	2.18730
C	-3.51401	-2.63864	4.94794
H	-3.46583	-2.67941	6.03349
C	-1.83450	-4.07206	1.89785

C	-0.98727	-5.08484	2.33933
C	-1.06311	-4.30861	-0.32260
C	-0.20064	-5.77745	1.43647
H	-0.95395	-5.35023	3.39188
C	-0.93988	-3.85154	-1.63667
C	-0.22016	-5.38908	0.09694
H	0.44750	-6.59100	1.75536
C	-0.11337	-4.51448	-2.57485
H	-1.46483	-2.95385	-1.94768
C	-0.01326	-4.11203	-3.92357
C	0.65114	-5.62912	-2.15104
C	0.80147	-4.79645	-4.80162
H	-0.59748	-3.25219	-4.25198
C	1.47520	-6.32019	-3.04133
C	1.54580	-5.90291	-4.35968
H	0.86917	-4.48002	-5.84037
H	2.05107	-7.17306	-2.68460
H	2.18674	-6.43789	-5.05749
N	-1.91940	-3.73204	0.57714
N	0.56944	-5.99645	-0.82460
H	1.15729	-6.76564	-0.50642

[1-H]²⁺ (S=1/2)

Ru	-3.68174	-2.60504	0.09819
C	-4.75787	-4.93179	-1.33294
C	-5.12615	-5.16216	0.95218
C	-5.70294	-6.41038	0.77980
C	-5.79168	-6.93473	-0.50445
C	-5.31968	-6.18354	-1.57090
C	-4.30185	-4.02854	-2.39556
C	-3.48787	-1.90380	-2.87755
C	-3.56378	-2.13253	-4.24190
C	-3.99809	-3.37662	-4.68710
C	-4.37912	-4.32914	-3.75361
H	-5.04471	-4.71540	1.94167
H	-6.07305	-6.95464	1.64449
H	-6.23312	-7.91340	-0.67724
H	-5.39543	-6.56797	-2.58437
H	-3.11890	-0.95685	-2.48675
H	-3.27353	-1.34784	-4.93534
H	-4.05107	-3.60068	-5.74987
H	-4.74297	-5.29883	-4.08214
C	-3.66523	0.31913	0.00218
C	-3.19787	1.63027	0.01427
C	-1.83809	1.86740	0.15599
C	-0.97340	0.78616	0.28653
C	-1.49931	-0.49598	0.26527
C	-5.07907	-0.04782	-0.13810
C	-6.11216	0.87484	-0.27539
C	-7.42036	0.42460	-0.37846
C	-7.66864	-0.94307	-0.34409
C	-6.59793	-1.81257	-0.20894
H	-3.89006	2.46241	-0.08269
H	-1.45956	2.88665	0.16753
H	0.09771	0.92558	0.40554
H	-0.86508	-1.37475	0.36683

H	-5.89608	1.93943	-0.30094	H	-5.40069	-6.59212	-2.55534
H	-8.23624	1.13570	-0.48400	H	-3.15636	-0.96684	-2.50761
H	-8.67692	-1.34071	-0.42153	H	-3.31525	-1.37554	-4.95328
H	-6.74505	-2.89074	-0.17571	H	-4.07503	-3.64099	-5.75055
C	-2.76552	-3.39273	2.76988	H	-4.75327	-5.33139	-4.06881
C	-4.52445	-1.87146	2.92331	C	-3.66057	0.32266	0.00371
C	-4.54019	-1.95100	4.30429	C	-3.18383	1.63067	0.02777
C	-2.73266	-3.51421	4.16127	C	-1.82251	1.85749	0.17046
H	-5.22426	-1.22901	2.39228	C	-0.96552	0.76847	0.29024
H	-5.25661	-1.36079	4.86917	C	-1.50016	-0.50968	0.25713
H	-2.00348	-4.16382	4.63748	C	-5.07743	-0.03268	-0.13527
N	-4.65050	-4.43565	-0.07229	C	-6.10417	0.89869	-0.26645
N	-3.81988	-2.83409	-1.96678	C	-7.41574	0.45899	-0.37031
N	-2.81285	-0.73302	0.11906	C	-7.67373	-0.90750	-0.34372
N	-5.33010	-1.38335	-0.10396	C	-6.60896	-1.78490	-0.21435
N	-3.66808	-2.57891	2.16451	H	-3.87083	2.46831	-0.05959
C	-3.62720	-2.79348	4.93375	H	-1.43679	2.87394	0.19171
H	-3.60875	-2.88301	6.01746	H	0.10664	0.89924	0.41049
C	-1.86114	-4.10201	1.86870	H	-0.87450	-1.39553	0.35151
C	-0.97336	-5.07170	2.32998	H	-5.88021	1.96187	-0.28684
C	-1.03598	-4.29849	-0.32306	H	-8.22665	1.17657	-0.47091
C	-0.12471	-5.71658	1.44679	H	-8.68508	-1.29725	-0.42274
H	-0.95347	-5.33936	3.38224	H	-6.76311	-2.86254	-0.18685
C	-0.93048	-3.85689	-1.64972	C	-2.75954	-3.40186	2.74761
C	-0.13803	-5.32697	0.11181	C	-4.53579	-1.88577	2.92105
H	0.55982	-6.49395	1.78068	C	-4.56411	-1.98396	4.29840
C	-0.04729	-4.47255	-2.56970	C	-2.74688	-3.54200	4.14702
H	-1.52324	-3.01115	-1.97903	H	-5.23456	-1.23833	2.39318
C	0.04492	-4.07854	-3.92129	H	-5.28569	-1.40514	4.86850
C	0.78354	-5.53146	-2.12664	H	-2.02058	-4.19712	4.62084
C	0.91565	-4.71407	-4.78520	N	-4.66002	-4.43020	-0.06575
H	-0.59092	-3.26261	-4.26652	N	-3.84083	-2.84560	-1.97216
C	1.66184	-6.17264	-3.00064	N	-2.81561	-0.73719	0.10895
C	1.72457	-5.76364	-4.32459	N	-5.33734	-1.36660	-0.10741
H	0.97470	-4.40109	-5.82578	N	-3.67369	-2.57878	2.15399
H	2.28752	-6.98362	-2.62932	C	-3.64809	-2.83991	4.91981
H	2.40926	-6.26232	-5.00789	H	-3.63815	-2.94835	6.00242
N	-1.93715	-3.75589	0.55212	C	-1.85817	-4.08227	1.85004
N	0.70473	-5.89459	-0.79789	C	-0.94224	-5.04735	2.30340
H	1.32783	-6.62805	-0.46642	C	-1.02455	-4.26400	-0.35297
[1] ⁺ (S=1/2)				C	-0.09420	-5.67456	1.42752
Ru	-3.69346	-2.60295	0.08701	H	-0.91919	-5.31146	3.35807
C	-4.76806	-4.94047	-1.32136	C	-0.91892	-3.82283	-1.66989
C	-5.13133	-5.14944	0.96666	C	-0.09235	-5.29957	0.05586
C	-5.70355	-6.40118	0.80758	H	0.60616	-6.44119	1.75423
C	-5.79289	-6.93955	-0.47157	C	-0.02346	-4.43977	-2.56798
C	-5.32580	-6.19722	-1.54572	H	-1.52520	-2.99132	-2.01476
C	-4.31821	-4.04546	-2.39215	C	0.08635	-4.05511	-3.92511
C	-3.52025	-1.91876	-2.89141	C	0.79883	-5.49855	-2.07630
C	-3.59801	-2.15747	-4.25349	C	0.96420	-4.69838	-4.77063
C	-4.02278	-3.40879	-4.68946	H	-0.54499	-3.24189	-4.28879
C	-4.39585	-4.35647	-3.74832	C	1.68727	-6.14041	-2.96767
H	-5.04656	-4.69216	1.95121	C	1.76900	-5.75087	-4.28861
H	-6.06859	-6.93901	1.67854	H	1.03730	-4.39566	-5.81427
H	-6.22994	-7.92210	-0.63329	H	2.30545	-6.94777	-2.57479
				H	2.45949	-6.25530	-4.96325

N	-1.93981	-3.73468	0.52293
N	0.76401	-5.89083	-0.77479

[1]⁺ (S=3/2)

Ru	-3.65577	-2.58729	0.10225
C	-4.70331	-4.92974	-1.37200
C	-4.97016	-5.23578	0.92243
C	-5.53471	-6.48746	0.73387
C	-5.67038	-6.96898	-0.56257
C	-5.25368	-6.18154	-1.62680
C	-4.28367	-3.99261	-2.41981
C	-3.51053	-1.83613	-2.85199
C	-3.57156	-2.04120	-4.22101
C	-3.98506	-3.28287	-4.69075
C	-4.35364	-4.26551	-3.78246
H	-4.84789	-4.81663	1.91961
H	-5.85843	-7.06650	1.59413
H	-6.10476	-7.94858	-0.74748
H	-5.36441	-6.53678	-2.64741
H	-3.16498	-0.89322	-2.43183
H	-3.28924	-1.24010	-4.89823
H	-4.02946	-3.48491	-5.75829
H	-4.69619	-5.23490	-4.13359
C	-3.74215	0.33739	0.04921
C	-3.25897	1.66931	0.11852
C	-1.92727	1.91094	0.32786
C	-1.02822	0.82497	0.48549
C	-1.53265	-0.45196	0.41038
C	-5.09323	-0.04102	-0.13085
C	-6.18216	0.85159	-0.30523
C	-7.45177	0.36790	-0.47452
C	-7.67718	-1.03299	-0.48318
C	-6.59600	-1.86594	-0.31393
H	-3.95877	2.49566	0.01149
H	-1.56202	2.93474	0.38182
H	0.03223	0.98185	0.66111
H	-0.89349	-1.32760	0.52549
H	-5.99560	1.92353	-0.30452
H	-8.28399	1.05662	-0.60663
H	-8.67091	-1.45126	-0.61589
H	-6.71461	-2.94994	-0.31077
C	-2.69589	-3.32698	2.77188
C	-4.47271	-1.79110	2.91192
C	-4.46972	-1.83091	4.29024
C	-2.65159	-3.39955	4.17573
H	-5.17796	-1.16975	2.36283
H	-5.17861	-1.22876	4.85123
H	-1.91003	-4.02638	4.66380
N	-4.55807	-4.47619	-0.10224
N	-3.83452	-2.79548	-1.97290
N	-2.83594	-0.71089	0.17488
N	-5.34126	-1.41045	-0.12359
N	-3.62276	-2.52435	2.16751
C	-3.53674	-2.65897	4.92885
H	-3.50183	-2.71239	6.01494
C	-1.82202	-4.04087	1.88264

C	-0.94988	-5.05255	2.32484
C	-1.04029	-4.28343	-0.34319
C	-0.16083	-5.73221	1.43517
H	-0.92224	-5.31146	3.38067
C	-0.92665	-3.83952	-1.65441
C	-0.16465	-5.36724	0.05676
H	0.50053	-6.53620	1.75235
C	-0.08594	-4.50935	-2.56715
H	-1.47494	-2.96140	-1.98545
C	0.02671	-4.12848	-3.92501
C	0.67674	-5.61633	-2.08721
C	0.85029	-4.82412	-4.78159
H	-0.55851	-3.27717	-4.27792
C	1.51195	-6.31132	-2.99094
C	1.59656	-5.92528	-4.31109
H	0.92756	-4.52621	-5.82611
H	2.08585	-7.15462	-2.60738
H	2.24456	-6.46924	-4.99676
N	-1.90811	-3.70403	0.55104
N	0.64060	-6.00557	-0.78494

[1-(*p*-MeO-PhOH)]²⁺ (S=0)

Ru	-3.74528	-2.57739	0.07667
C	-4.87232	-4.86216	-1.38499
C	-5.24575	-5.11461	0.89749
C	-5.84853	-6.34839	0.70860
C	-5.94679	-6.85354	-0.58216
C	-5.45915	-6.09850	-1.63925
C	-4.39785	-3.95438	-2.43625
C	-3.53303	-1.84366	-2.89332
C	-3.61227	-2.05542	-4.26019
C	-4.07688	-3.28312	-4.71955
C	-4.48168	-4.23710	-3.79754
H	-5.15626	-4.68234	1.89273
H	-6.23088	-6.89584	1.56580
H	-6.40830	-7.82045	-0.76808
H	-5.54206	-6.46818	-2.65754
H	-3.14221	-0.91027	-2.49156
H	-3.30170	-1.27052	-4.94440
H	-4.13443	-3.49369	-5.78479
H	-4.86839	-5.19387	-4.13735
C	-3.68873	0.34818	0.00533
C	-3.20428	1.65273	0.02538
C	-1.84032	1.87039	0.15884
C	-0.98864	0.77717	0.27136
C	-1.53159	-0.49776	0.24266
C	-5.10807	0.00052	-0.12835
C	-6.13093	0.93649	-0.24752
C	-7.44536	0.50245	-0.34295
C	-7.71007	-0.86210	-0.31941
C	-6.64890	-1.74587	-0.20297
H	-3.88619	2.49462	-0.05886
H	-1.44840	2.88443	0.17717
H	0.08514	0.90128	0.38239
H	-0.90582	-1.38405	0.32895
H	-5.90252	1.99860	-0.26421

H	-8.25357	1.22426	-0.43387
H	-8.72371	-1.24682	-0.39092
H	-6.80888	-2.82225	-0.17865
C	-2.83302	-3.41382	2.73142
C	-4.55360	-1.85879	2.90940
C	-4.55348	-1.95138	4.29231
C	-2.78493	-3.55193	4.11699
H	-5.24683	-1.19751	2.39368
H	-5.25204	-1.35097	4.86868
H	-2.06905	-4.22451	4.58025
N	-4.75493	-4.38629	-0.11785
N	-3.88945	-2.77593	-1.99390
N	-2.84916	-0.71551	0.10684
N	-5.37563	-1.33180	-0.10602
N	-3.72042	-2.57516	2.13723
C	-3.65513	-2.81514	4.90694
H	-3.62788	-2.91398	5.98928
C	-1.94975	-4.13052	1.80882
C	-1.06590	-5.14295	2.27292
C	-1.15751	-4.36462	-0.37008
C	-0.27256	-5.81049	1.39415
H	-1.04958	-5.40214	3.32702
C	-1.05145	-3.91130	-1.68230
C	-0.28358	-5.42862	0.02672
H	0.38730	-6.61647	1.71150
C	-0.18532	-4.53684	-2.57638
H	-1.62356	-3.04813	-2.00742
C	-0.05531	-4.12029	-3.93083
C	0.59608	-5.64234	-2.10259
C	0.79796	-4.77849	-4.77080
H	-0.65368	-3.27653	-4.27511
C	1.47510	-6.30197	-3.00320
C	1.56798	-5.87830	-4.30035
H	0.89553	-4.46552	-5.80827
H	2.06298	-7.14030	-2.63108
H	2.24277	-6.38480	-4.98797
N	-2.03785	-3.78185	0.52272
N	0.53977	-6.04832	-0.82390
C	5.46519	-8.40542	1.43992
C	5.86090	-7.06794	1.38753
C	4.96734	-6.11349	0.89424
C	3.70211	-6.48202	0.45930
C	3.30128	-7.82322	0.50921
C	4.19398	-8.77329	1.00219
H	6.13584	-9.17359	1.81859
H	5.28532	-5.07227	0.85710
H	3.01740	-5.72497	0.07518
H	3.88145	-9.81618	1.04014
O	2.07992	-8.24122	0.09918
H	1.55844	-7.47039	-0.23632
O	7.07583	-6.60234	1.78674
C	8.00011	-7.54314	2.28353
H	8.90272	-6.98367	2.54628
H	7.62136	-8.05135	3.18327
H	8.25620	-8.30099	1.52774

[1-(<i>p</i> -O ₂ N-PhOH)] ²⁺ (S=0)			
Ru	-3.73875	-2.57878	0.07692
C	-4.86486	-4.86731	-1.37979
C	-5.23345	-5.11761	0.90376
C	-5.83538	-6.35219	0.71745
C	-5.93593	-6.85876	-0.57257
C	-5.45116	-6.10442	-1.63149
C	-4.39355	-3.96019	-2.43309
C	-3.53387	-1.84824	-2.89444
C	-3.61484	-2.06203	-4.26091
C	-4.07741	-3.29142	-4.71781
C	-4.47870	-4.24501	-3.79386
H	-5.14243	-4.68418	1.89836
H	-6.21549	-6.89906	1.57603
H	-6.39708	-7.82622	-0.75651
H	-5.53616	-6.47523	-2.64920
H	-3.14448	-0.91344	-2.49460
H	-3.30718	-1.27735	-4.94667
H	-4.13613	-3.50360	-5.78267
H	-4.86379	-5.20308	-4.13183
C	-3.68856	0.34672	0.00162
C	-3.20689	1.65233	0.01846
C	-1.84306	1.87319	0.14781
C	-0.98868	0.78200	0.25956
C	-1.52893	-0.49413	0.23425
C	-5.10745	-0.00413	-0.12825
C	-6.13256	0.92954	-0.24596
C	-7.44627	0.49263	-0.33805
C	-7.70804	-0.87245	-0.31277
C	-6.64475	-1.75388	-0.19785
H	-3.89083	2.49263	-0.06517
H	-1.45332	2.88811	0.16357
H	0.08513	0.90867	0.36739
H	-0.90095	-1.37889	0.32013
H	-5.90651	1.99212	-0.26411
H	-8.25619	1.21266	-0.42779
H	-8.72101	-1.25938	-0.38172
H	-6.80243	-2.83056	-0.17215
C	-2.81938	-3.40845	2.73146
C	-4.54526	-1.85962	2.91017
C	-4.54289	-1.95099	4.29319
C	-2.76885	-3.54527	4.11705
H	-5.24166	-1.20134	2.39490
H	-5.24288	-1.35260	4.86994
H	-2.04991	-4.21480	4.57998
N	-4.74546	-4.38991	-0.11341
N	-3.88683	-2.78009	-1.99319
N	-2.84640	-0.71496	0.10241
N	-5.37217	-1.33700	-0.10402
N	-3.71056	-2.57366	2.13751
C	-3.64067	-2.81092	4.90750
H	-3.61169	-2.90866	5.98988
C	-1.93521	-4.12305	1.80843
C	-1.04536	-5.12996	2.27237
C	-1.14677	-4.36028	-0.37132
C	-0.25071	-5.79625	1.39385

H	-1.02481	-5.38653	3.32702	C	-1.21989	1.00738	0.34570
C	-1.04697	-3.90898	-1.68456	C	-1.66736	-0.30419	0.32252
C	-0.26671	-5.41907	0.02524	C	-5.26593	-0.06951	-0.12776
H	0.41246	-6.59671	1.71730	C	-6.35917	0.77768	-0.26400
C	-0.18197	-4.53175	-2.58113	C	-7.62893	0.22965	-0.39002
H	-1.62385	-3.04869	-2.00868	C	-7.78113	-1.15164	-0.37988
C	-0.06192	-4.11536	-3.93644	C	-6.65239	-1.94479	-0.24675
C	0.60709	-5.63261	-2.10983	H	-4.22964	2.51278	-0.05882
C	0.79010	-4.76925	-4.78080	H	-1.82843	3.07200	0.21746
H	-0.66770	-3.27551	-4.27725	H	-0.16081	1.21129	0.47492
C	1.48433	-6.28788	-3.01484	H	-0.98782	-1.14748	0.43298
C	1.56787	-5.86425	-4.31290	H	-6.22134	1.85529	-0.27159
H	0.88040	-4.45698	-5.81906	H	-8.49334	0.88049	-0.49616
H	2.07971	-7.12423	-2.65059	H	-8.75722	-1.61834	-0.47589
H	2.24159	-6.36841	-5.00323	H	-6.71911	-3.03131	-0.23558
N	-2.02741	-3.77840	0.52165	C	-2.56031	-3.22241	2.70643
N	0.55693	-6.03583	-0.82886	C	-4.41153	-1.79137	2.93871
C	5.41938	-8.42893	1.42370	C	-4.33294	-1.82902	4.31427
C	5.80370	-7.08680	1.40049	C	-2.43496	-3.28815	4.10363
C	4.94829	-6.09577	0.92018	H	-5.18498	-1.21482	2.43529
C	3.69462	-6.44765	0.45761	H	-5.04804	-1.27097	4.91158
C	3.29206	-7.79447	0.47496	H	-1.63307	-3.87049	4.54916
C	4.16750	-8.77928	0.96200	N	-4.47404	-4.47666	-0.05010
H	6.10498	-9.18148	1.80299	N	-3.93575	-2.81382	-1.98780
H	5.27266	-5.05885	0.91295	N	-2.96426	-0.60375	0.15738
H	3.01637	-5.68460	0.07766	N	-5.42708	-1.41696	-0.11804
H	3.83770	-9.81607	0.96679	N	-3.55692	-2.47251	2.14996
O	2.09446	-8.19151	0.04324	C	-3.31951	-2.59584	4.90289
H	1.55810	-7.41239	-0.27672	H	-3.22321	-2.64146	5.98536
N	7.11379	-6.71667	1.88675	C	-1.70958	-3.90380	1.77034
O	7.84858	-7.60338	2.31028	C	-0.82107	-4.91990	2.15597
O	7.43293	-5.53220	1.85567	C	-1.02518	-4.10282	-0.49466
[1-(<i>p</i>-MeO-PhOH)]²⁺ (S=1)				C	-0.08178	-5.59431	1.21855
Ru	-3.67611	-2.55144	0.08639	H	-0.74398	-5.19335	3.20552
C	-4.64505	-4.97635	-1.30031	C	-0.95028	-3.62220	-1.79385
C	-4.80142	-5.22434	1.01479	C	-0.14656	-5.19722	-0.14659
C	-5.29749	-6.51142	0.88615	H	0.57961	-6.41368	1.49466
C	-5.45530	-7.04096	-0.38851	C	-0.13969	-4.26576	-2.75315
C	-5.13134	-6.26447	-1.49251	H	-1.50362	-2.73048	-2.07964
C	-4.32372	-4.04821	-2.38817	C	-0.05857	-3.84032	-4.09922
C	-3.69547	-1.86300	-2.90254	C	0.62877	-5.39092	-2.33493
C	-3.79037	-2.10881	-4.26261	C	0.74201	-4.51039	-4.99664
C	-4.14507	-3.38485	-4.68512	H	-0.64673	-2.97493	-4.40846
C	-4.42233	-4.36251	-3.73986	C	1.44182	-6.06080	-3.27432
H	-4.66681	-4.76757	1.99292	C	1.49576	-5.62856	-4.58134
H	-5.55160	-7.07963	1.77631	H	0.79663	-4.17849	-6.03199
H	-5.83627	-8.04995	-0.52604	H	2.02210	-6.91934	-2.93470
H	-5.26682	-6.65829	-2.49554	H	2.12642	-6.14958	-5.29974
H	-3.39038	-0.88859	-2.52549	N	-1.85984	-3.54451	0.44771
H	-3.57746	-1.31178	-4.96916	N	0.61818	-5.81541	-1.04229
H	-4.21265	-3.61891	-5.74480	C	5.06243	-8.65287	1.60551
H	-4.71305	-5.36056	-4.05558	C	5.64286	-7.38507	1.54478
C	-3.88093	0.38834	0.02627	C	4.96204	-6.35670	0.88743
C	-3.49191	1.72219	0.04661	C	3.72407	-6.58358	0.30251
C	-2.14715	2.03264	0.20316	C	3.13449	-7.85335	0.36536
				C	3.81794	-8.87774	1.01941

H	5.56542	-9.47588	2.10840
H	5.42479	-5.37148	0.84250
H	3.20676	-5.77228	-0.21099
H	3.35917	-9.86464	1.06844
O	1.93002	-8.13156	-0.18225
H	1.51153	-7.29740	-0.52580
O	6.84847	-7.05723	2.08577
C	7.55204	-8.07144	2.76522
H	8.48206	-7.61903	3.12173
H	6.98625	-8.45196	3.62922
H	7.79774	-8.91374	2.10073

[1-(*p*-O₂N-PhOH)]²⁺ (S=1)

Ru	-3.71516	-2.56328	0.10077
C	-4.78774	-4.86852	-1.39185
C	-5.16518	-5.11879	0.89723
C	-5.76370	-6.35345	0.70621
C	-5.85614	-6.85770	-0.58511
C	-5.36743	-6.10635	-1.64505
C	-4.29341	-3.96600	-2.43517
C	-3.41044	-1.85273	-2.86986
C	-3.43387	-2.07679	-4.23681
C	-3.88705	-3.30545	-4.70336
C	-4.32880	-4.25699	-3.79464
H	-5.07502	-4.68468	1.89053
H	-6.14530	-6.90233	1.56236
H	-6.31344	-7.82670	-0.77003
H	-5.44401	-6.47863	-2.66249
H	-3.03787	-0.91674	-2.45748
H	-3.09230	-1.29970	-4.91448
H	-3.90541	-3.52143	-5.76881
H	-4.70333	-5.21567	-4.14231
C	-3.64327	0.38609	0.02984
C	-3.13455	1.67812	0.07581
C	-1.78405	1.86442	0.34179
C	-0.97119	0.75914	0.56365
C	-1.53587	-0.50545	0.50718
C	-5.04784	0.05591	-0.23293
C	-6.04960	0.99801	-0.43257
C	-7.35155	0.56599	-0.64860
C	-7.62543	-0.79639	-0.66583
C	-6.58280	-1.68808	-0.46888
H	-3.78430	2.53203	-0.09574
H	-1.37185	2.86980	0.37801
H	0.08806	0.86499	0.77968
H	-0.94937	-1.40678	0.67625
H	-5.81623	2.05884	-0.41359
H	-8.14667	1.29169	-0.80094
H	-8.63082	-1.17323	-0.83032
H	-6.74650	-2.76410	-0.47818
C	-2.91021	-3.33080	2.81970
C	-4.61485	-1.71238	2.87487
C	-4.66274	-1.73534	4.25226
C	-2.91795	-3.38749	4.22265
H	-5.27330	-1.06362	2.30049
H	-5.36308	-1.09378	4.77900

H	-2.22384	-4.04178	4.74299
N	-4.68186	-4.39602	-0.12431
N	-3.80959	-2.78158	-1.98841
N	-2.83702	-0.68542	0.23799
N	-5.32745	-1.27124	-0.25134
N	-3.77267	-2.49383	2.17018
C	-3.79312	-2.59507	4.93463
H	-3.79886	-2.63356	6.02166
C	-2.04293	-4.09803	1.96887
C	-1.23534	-5.14311	2.44309
C	-1.20311	-4.39168	-0.23242
C	-0.45582	-5.87197	1.58075
H	-1.24576	-5.38985	3.50179
C	-1.00405	-3.94865	-1.53313
C	-0.41234	-5.52123	0.20351
H	0.15503	-6.70222	1.93139
C	-0.18412	-4.67292	-2.42426
H	-1.46821	-3.02712	-1.87395
C	-0.00080	-4.29636	-3.77474
C	0.48238	-5.83122	-1.93096
C	0.79984	-5.04632	-4.60695
H	-0.51294	-3.40565	-4.14245
C	1.29786	-6.58268	-2.80335
C	1.45090	-6.19759	-4.11798
H	0.93190	-4.75278	-5.64689
H	1.79820	-7.46952	-2.41435
H	2.08104	-6.78418	-4.78432
N	-2.06991	-3.76651	0.63315
N	0.37321	-6.20639	-0.62515
C	5.47199	-8.34370	1.16168
C	5.81241	-6.99644	1.02183
C	4.86496	-6.04685	0.64010
C	3.56571	-6.44513	0.39205
C	3.20646	-7.79949	0.52016
C	4.17452	-8.74061	0.91321
H	6.22826	-9.06373	1.46149
H	5.15482	-5.00447	0.54025
H	2.81572	-5.71362	0.09556
H	3.87940	-9.78339	1.01078
O	1.97396	-8.24094	0.28216
H	1.37848	-7.49292	-0.03461
N	7.17232	-6.57855	1.27338
O	7.99470	-7.43288	1.59011
O	7.44685	-5.38769	1.15791

[1-(*p*-O₂N-PhOH)]²⁺ PT TS (S=1)

Ru	-3.76888	-2.53986	0.10249
C	-4.82271	-4.82295	-1.43923
C	-5.18246	-5.13621	0.84474
C	-5.76278	-6.37498	0.62578
C	-5.85415	-6.84851	-0.67713
C	-5.38348	-6.06323	-1.72052
C	-4.34872	-3.88720	-2.46227
C	-3.49479	-1.75143	-2.84748
C	-3.52401	-1.94042	-4.21948
C	-3.96706	-3.16142	-4.71482

C	-4.39091	-4.14205	-3.82855
H	-5.09495	-4.72622	1.84843
H	-6.13131	-6.95070	1.46991
H	-6.29648	-7.82002	-0.88384
H	-5.45850	-6.41147	-2.74657
H	-3.13084	-0.82236	-2.41295
H	-3.19576	-1.14198	-4.87861
H	-3.99105	-3.34965	-5.78538
H	-4.75727	-5.09521	-4.19908
C	-3.72888	0.40851	0.10857
C	-3.23520	1.70454	0.18707
C	-1.88407	1.89919	0.44363
C	-1.05552	0.79789	0.62326
C	-1.60599	-0.47124	0.53793
C	-5.13086	0.06847	-0.15149
C	-6.14580	1.00231	-0.31884
C	-7.44335	0.55953	-0.53957
C	-7.69989	-0.80524	-0.59385
C	-6.64515	-1.68876	-0.42794
H	-3.89729	2.55485	0.04832
H	-1.48348	2.90802	0.50519
H	0.00489	0.91014	0.82998
H	-1.00610	-1.36893	0.67592
H	-5.92600	2.06511	-0.27118
H	-8.24855	1.27892	-0.66700
H	-8.70121	-1.19049	-0.76333
H	-6.79502	-2.76603	-0.46633
C	-2.93604	-3.35407	2.80573
C	-4.65339	-1.75766	2.89993
C	-4.68880	-1.80508	4.27848
C	-2.92633	-3.43437	4.20323
H	-5.32243	-1.10472	2.34313
H	-5.39177	-1.17995	4.82119
H	-2.22088	-4.08953	4.70663
N	-4.71572	-4.38102	-0.16069
N	-3.87780	-2.70776	-1.98858
N	-2.90825	-0.65909	0.27867
N	-5.39373	-1.26157	-0.20624
N	-3.80751	-2.51667	2.17705
C	-3.80530	-2.66267	4.93803
H	-3.80022	-2.71963	6.02409
C	-2.06209	-4.10416	1.93227
C	-1.23383	-5.13308	2.38734
C	-1.23937	-4.34637	-0.27520
C	-0.43781	-5.83310	1.50636
H	-1.22941	-5.39716	3.44129
C	-1.06608	-3.88642	-1.57864
C	-0.42337	-5.45272	0.15041
H	0.19445	-6.65468	1.83719
C	-0.23838	-4.57569	-2.49399
H	-1.55362	-2.97050	-1.89962
C	-0.08567	-4.17949	-3.84108
C	0.47435	-5.71488	-2.03573
C	0.73124	-4.89323	-4.69165
H	-0.63114	-3.30227	-4.19132
C	1.30541	-6.43263	-2.91076

C	1.42767	-6.02381	-4.22457
H	0.83976	-4.58364	-5.72936
H	1.84041	-7.30457	-2.53609
H	2.07039	-6.58038	-4.90408
N	-2.10721	-3.75504	0.60657
N	0.37014	-6.09161	-0.72334
C	5.34849	-8.19631	1.02914
C	5.75796	-6.86126	0.89805
C	4.84312	-5.87324	0.51260
C	3.53443	-6.21257	0.25648
C	3.08171	-7.56129	0.36943
C	4.04146	-8.53534	0.77285
H	6.07228	-8.94932	1.33111
H	5.17979	-4.84374	0.41862
H	2.82739	-5.43887	-0.04197
H	3.70586	-9.56728	0.86657
O	1.86524	-7.91764	0.12176
H	1.07916	-6.95391	-0.32155
N	7.11922	-6.50601	1.15430
O	7.91125	-7.39394	1.47576
O	7.45319	-5.32458	1.04298

[1-H(*p*-MeO-PhO)]²⁺ (S=1)

Ru	-3.77535	-2.57072	0.07488
C	-4.86193	-4.89526	-1.35057
C	-5.21739	-5.12599	0.93662
C	-5.79586	-6.37385	0.76713
C	-5.89227	-6.89775	-0.51679
C	-5.42599	-6.14654	-1.58572
C	-4.41125	-3.99182	-2.41526
C	-3.60299	-1.86565	-2.90050
C	-3.68301	-2.09492	-4.26448
C	-4.11571	-3.34023	-4.70792
C	-4.49223	-4.29307	-3.77296
H	-5.12948	-4.67936	1.92569
H	-6.16106	-6.91839	1.63373
H	-6.33511	-7.87619	-0.68733
H	-5.50777	-6.53067	-2.59884
H	-3.23444	-0.91796	-2.51112
H	-3.39677	-1.30979	-4.95912
H	-4.17115	-3.56486	-5.77044
H	-4.85494	-5.26370	-4.10003
C	-3.75711	0.35391	-0.01031
C	-3.28836	1.66457	0.00503
C	-1.92732	1.89976	0.13734
C	-1.06267	0.81701	0.25535
C	-1.58997	-0.46448	0.23147
C	-5.17245	-0.01092	-0.14062
C	-6.20566	0.91321	-0.26703
C	-7.51509	0.46458	-0.36103
C	-7.76444	-0.90299	-0.32909
C	-6.69352	-1.77390	-0.20524
H	-3.98056	2.49784	-0.08164
H	-1.54778	2.91861	0.15152
H	0.00946	0.95488	0.36683
H	-0.95608	-1.34457	0.32372

H	-5.98879	1.97768	-0.29121				
H	-8.33109	1.17681	-0.45789		[1-H(p-O ₂ N-PhO)] ²⁺ (S=1)		
H	-8.77370	-1.29940	-0.39991	Ru	-3.72210	-2.55778	0.09452
H	-6.84133	-2.85207	-0.17454	C	-4.79592	-4.85299	-1.41359
C	-2.83083	-3.36845	2.73367	C	-5.17037	-5.12130	0.87404
C	-4.58552	-1.84358	2.91131	C	-5.76982	-6.35399	0.67368
C	-4.58551	-1.92529	4.29205	C	-5.86354	-6.84813	-0.62133
C	-2.78212	-3.49147	4.12504	C	-5.37592	-6.08849	-1.67594
H	-5.29061	-1.19948	2.38921	C	-4.30370	-3.94164	-2.44969
H	-5.29438	-1.33521	4.86648	C	-3.41797	-1.82455	-2.86733
H	-2.04921	-4.14349	4.59210	C	-3.43866	-2.03927	-4.23576
N	-4.74719	-4.39955	-0.09041	C	-3.89418	-3.26325	-4.71202
N	-3.92938	-2.79659	-1.98840	C	-4.33818	-4.22146	-3.81117
N	-2.90486	-0.69968	0.09428	H	-5.08099	-4.69592	1.87115
N	-5.42442	-1.34635	-0.10873	H	-6.15132	-6.90892	1.52593
N	-3.73916	-2.55092	2.14113	H	-6.32142	-7.81542	-0.81340
C	-3.66594	-2.77040	4.90900	H	-5.45391	-6.45232	-2.69629
H	-3.63458	-2.86177	5.99229	H	-3.04562	-0.89186	-2.44796
C	-1.94123	-4.07926	1.82052	H	-3.09422	-1.25790	-4.90692
C	-1.05635	-5.05923	2.26734	H	-3.91201	-3.47104	-5.77907
C	-1.14411	-4.27429	-0.38252	H	-4.71348	-5.17698	-4.16653
C	-0.22892	-5.71307	1.37154	C	-3.66283	0.39079	0.03371
H	-1.02379	-5.32810	3.31911	C	-3.16026	1.68497	0.07618
C	-1.03881	-3.82300	-1.70557	C	-1.80936	1.87727	0.33652
C	-0.25846	-5.32178	0.03488	C	-0.99029	0.77615	0.55622
H	0.45160	-6.49897	1.69497	C	-1.54912	-0.49115	0.50372
C	-0.16312	-4.43964	-2.63232	C	-5.06534	0.05159	-0.22412
H	-1.62075	-2.96576	-2.02524	C	-6.07502	0.98616	-0.41634
C	-0.05554	-4.02773	-3.97767	C	-7.37473	0.54508	-0.62750
C	0.64735	-5.51865	-2.19869	C	-7.63875	-0.81915	-0.64653
C	0.81337	-4.66310	-4.84352	C	-6.58936	-1.70423	-0.45709
H	-0.67645	-3.19770	-4.31668	H	-3.81432	2.53578	-0.09406
C	1.52724	-6.15765	-3.07565	H	-1.40152	2.88450	0.36984
C	1.60635	-5.72965	-4.39199	H	0.06933	0.88716	0.76754
H	0.88497	-4.33605	-5.87906	H	-0.95597	-1.38818	0.67174
H	2.14096	-6.98109	-2.71024	H	-5.84915	2.04852	-0.39507
H	2.29131	-6.22514	-5.07744	H	-8.17583	1.26529	-0.77418
N	-2.02954	-3.72618	0.50539	H	-8.64206	-1.20318	-0.80664
N	0.55904	-5.90674	-0.88071	H	-6.74633	-2.78099	-0.46750
C	5.47361	-8.56784	1.41643	C	-2.91412	-3.32497	2.82171
C	5.93935	-7.23415	1.45785	C	-4.61810	-1.71578	2.86987
C	5.11891	-6.17311	0.99244	C	-4.66024	-1.73166	4.24965
C	3.87206	-6.42766	0.50369	C	-2.90999	-3.37424	4.21876
C	3.35362	-7.77740	0.44863	H	-5.28069	-1.07180	2.29560
C	4.22073	-8.82948	0.92684	H	-5.36157	-1.08932	4.77406
H	6.10238	-9.38204	1.76835	H	-2.21264	-4.02350	4.74041
H	5.51906	-5.16187	1.04118	N	-4.68727	-4.39110	-0.14226
H	3.23812	-5.61668	0.14505	N	-3.82115	-2.75948	-

C	-0.42706	-5.85552	1.59671
H	-1.22287	-5.36043	3.51762
C	-1.03461	-3.99563	-1.54595
C	-0.41362	-5.50911	0.23949
H	0.20335	-6.67045	1.94794
C	-0.20611	-4.71400	-2.44045
H	-1.51296	-3.08546	-1.89496
C	-0.04523	-4.35719	-3.79680
C	0.50255	-5.84134	-1.95520
C	0.77582	-5.09674	-4.62249
H	-0.58617	-3.48897	-4.17477
C	1.33795	-6.58646	-2.79559
C	1.46840	-6.21332	-4.12093
H	0.89042	-4.81629	-5.66766
H	1.86946	-7.44625	-2.38886
H	2.11515	-6.78887	-4.78022
N	-2.07813	-3.79145	0.63676
N	0.37544	-6.17321	-0.62922
C	5.46664	-8.37370	1.18114
C	5.87365	-7.03702	1.02250
C	4.93984	-6.05631	0.64920
C	3.62871	-6.40186	0.43475
C	3.16701	-7.75610	0.57382
C	4.15686	-8.72036	0.96642
H	6.20243	-9.11980	1.47250
H	5.27200	-5.02707	0.53416
H	2.90832	-5.63406	0.14878
H	3.82957	-9.75325	1.08356
O	1.95916	-8.10103	0.36366
H	0.98881	-6.95145	-0.24344
N	7.23257	-6.67711	1.23535
O	8.03989	-7.55760	1.55153
O	7.56516	-5.49490	1.09587

[2]²⁺ (S=0)

Ru	-3.75049	-2.64079	0.14951
C	-4.89160	-4.86512	-1.38249
C	-5.25648	-5.18487	0.89612
C	-5.93144	-6.37326	0.66679
C	-6.08612	-6.81155	-0.64299
C	-5.56034	-6.04982	-1.67668
C	-4.30767	-3.98068	-2.39859
C	-3.13981	-2.00036	-2.76984
C	-3.13592	-2.20734	-4.14027
C	-3.74490	-3.34985	-4.64529
C	-4.33586	-4.24496	-3.76486
H	-5.11813	-4.80226	1.90589
H	-6.32655	-6.93731	1.50721
H	-6.61277	-7.73770	-0.86059
H	-5.67334	-6.37567	-2.70684
H	-2.66947	-1.12220	-2.33159
H	-2.66000	-1.47957	-4.79174
H	-3.75959	-3.54616	-5.71465
H	-4.81423	-5.14478	-4.14175
C	-3.75967	0.28942	0.04833
C	-3.30451	1.60469	0.04155

C	-1.94804	1.85781	0.18712
C	-1.07252	0.78896	0.33802
C	-1.58621	-0.49816	0.33531
C	-5.17062	-0.08832	-0.10064
C	-6.20657	0.82980	-0.24370
C	-7.51173	0.37326	-0.35861
C	-7.75405	-0.99487	-0.32792
C	-6.67992	-1.85938	-0.18617
H	-4.00256	2.42876	-0.07649
H	-1.58050	2.88108	0.18268
H	-0.00310	0.94037	0.45605
H	-0.93572	-1.36399	0.44420
H	-5.99737	1.89565	-0.26360
H	-8.32986	1.08096	-0.46892
H	-8.75972	-1.39741	-0.41206
H	-6.82536	-2.93761	-0.15304
C	-1.76443	-3.91518	1.85010
C	-1.22941	-4.27622	-0.36722
C	-0.12302	-5.01126	0.03695
C	-0.64570	-4.66367	2.21666
C	-2.69206	-3.28430	2.78049
C	-4.61806	-2.02966	3.00515
C	-4.47893	-2.09405	4.38487
C	-2.58519	-3.32431	4.17092
H	-1.46141	-4.12018	-1.41864
H	0.53779	-5.45087	-0.70842
H	-0.41136	-4.82539	3.26862
H	-5.44785	-1.50581	2.53543
H	-5.21145	-1.60783	5.02718
H	-1.75557	-3.84836	4.64423
N	-4.74941	-4.44156	-0.09981
N	-3.70844	-2.86266	-1.91302
N	-2.89685	-0.74954	0.19087
N	-5.41538	-1.42391	-0.07370
N	-3.72831	-2.62654	2.19947
N	-2.05183	-3.72529	0.53648
N	-3.46774	-2.73742	4.97213
N	0.17215	-5.20963	1.32318

[2]²⁺ (S=1)

Ru	-3.78075	-2.63123	0.12059
C	-4.85883	-4.92565	-1.37720
C	-5.15510	-5.21349	0.92221
C	-5.77874	-6.43572	0.72967
C	-5.93636	-6.90786	-0.56761
C	-5.47166	-6.14670	-1.63186
C	-4.34448	-4.02809	-2.41561
C	-3.32304	-1.96895	-2.82482
C	-3.33056	-2.19130	-4.19270
C	-3.86711	-3.37989	-4.67265
C	-4.38195	-4.30724	-3.77655
H	-5.00900	-4.79871	1.91759
H	-6.13016	-6.99982	1.58885
H	-6.42083	-7.86338	-0.75355
H	-5.59015	-6.49917	-2.65242
H	-2.91105	-1.05514	-2.40030

H	-2.92023	-1.44021	-4.86146
H	-3.88739	-3.58708	-5.73981
H	-4.80659	-5.24077	-4.13525
C	-3.76132	0.31530	0.12802
C	-3.28536	1.61863	0.20881
C	-1.93100	1.83385	0.42601
C	-1.07915	0.74406	0.55843
C	-1.61244	-0.53225	0.47505
C	-5.16486	-0.03414	-0.11216
C	-6.18512	0.89668	-0.26755
C	-7.48061	0.45060	-0.49249
C	-7.73036	-0.91460	-0.56401
C	-6.67084	-1.79399	-0.40704
H	-3.96418	2.46000	0.10075
H	-1.54557	2.84849	0.48934
H	-0.01346	0.87016	0.72647
H	-0.98803	-1.41809	0.57131
H	-5.97202	1.96032	-0.21048
H	-8.28897	1.16792	-0.61175
H	-8.72966	-1.30268	-0.73903
H	-6.81616	-2.87143	-0.45608
C	-1.79133	-3.91357	1.84275
C	-1.28412	-4.33443	-0.40724
C	-0.19412	-5.07302	-0.01853
C	-0.65830	-4.69203	2.18199
C	-2.66874	-3.27950	2.75171
C	-4.58027	-1.94613	3.00682
C	-4.41589	-1.97807	4.36951
C	-2.54990	-3.27465	4.16287
H	-1.52956	-4.19233	-1.45866
H	0.45170	-5.53600	-0.76117
H	-0.41220	-4.83955	3.23534
H	-5.40630	-1.40875	2.54332
H	-5.11415	-1.45949	5.02255
H	-1.71994	-3.80970	4.62792
N	-4.70931	-4.47649	-0.10582
N	-3.81088	-2.86748	-1.95755
N	-2.92015	-0.74114	0.26430
N	-5.42093	-1.36430	-0.18134
N	-3.73255	-2.60066	2.18496
N	-2.08500	-3.73719	0.50139
N	-3.38561	-2.65388	4.95878
N	0.12547	-5.25692	1.29673

[2-H]³⁺ (S=0)

Ru	-3.67293	-2.51317	0.11525
C	-4.52037	-4.73887	-1.59267
C	-4.69783	-5.32995	0.65724
C	-5.20006	-6.58027	0.33368
C	-5.36832	-6.90514	-1.00718
C	-5.02367	-5.97647	-1.97965
C	-4.12448	-3.68462	-2.53437
C	-3.27883	-1.52344	-2.74416
C	-3.30211	-1.60302	-4.12800
C	-3.75528	-2.77396	-4.72265
C	-4.16979	-3.82572	-3.91725

H	-4.55520	-5.02627	1.69287
H	-5.45424	-7.27862	1.12598
H	-5.76519	-7.87501	-1.29711
H	-5.15123	-6.21387	-3.03223
H	-2.92652	-0.62726	-2.23673
H	-2.96743	-0.75556	-4.71974
H	-3.78511	-2.87174	-5.80508
H	-4.52200	-4.75059	-4.36514
C	-4.24690	0.36290	0.25894
C	-4.04729	1.73531	0.37234
C	-2.75834	2.22664	0.52444
C	-1.69276	1.33562	0.56154
C	-1.95510	-0.02007	0.44758
C	-5.56390	-0.26325	0.08864
C	-6.75573	0.44986	0.01091
C	-7.95364	-0.23767	-0.12529
C	-7.93459	-1.62561	-0.17727
C	-6.71476	-2.27941	-0.10118
H	-4.89198	2.41826	0.34459
H	-2.58988	3.29715	0.61304
H	-0.66769	1.67611	0.67807
H	-1.15035	-0.75305	0.46860
H	-6.75149	1.53528	0.05447
H	-8.89186	0.30819	-0.18747
H	-8.84795	-2.20509	-0.27841
H	-6.65804	-3.36559	-0.13724
C	-1.42322	-3.47321	1.64232
C	-0.99172	-3.63325	-0.64754
C	0.24761	-4.17160	-0.39153
C	-0.17583	-4.00989	1.91350
C	-2.38867	-3.08291	2.65908
C	-4.51065	-2.25885	3.03824
C	-4.27763	-2.34742	4.40597
C	-2.19085	-3.15987	4.03789
H	-1.32331	-3.47498	-1.66942
H	0.94601	-4.46683	-1.16603
H	0.20860	-4.18558	2.91263
H	-5.45517	-1.89582	2.63947
H	-5.05282	-2.04471	5.10767
H	-1.25158	-3.52773	4.44904
N	-4.37168	-4.42640	-0.27977
N	-3.67704	-2.53754	-1.96149
N	-3.19961	-0.49938	0.29934
N	-5.55338	-1.61949	0.02509
N	-3.56643	-2.62604	2.16396
N	-1.82906	-3.27701	0.34985
N	-3.12577	-2.79377	4.90752
N	0.61839	-4.34082	0.89013
H	1.53843	-4.73956	1.09203

[2-H]³⁺ (S=1)

Ru	-3.70572	-2.47821	0.07118
C	-4.45516	-4.77254	-1.61481
C	-4.55954	-5.32984	0.65177
C	-5.00888	-6.60703	0.35757
C	-5.18286	-6.96359	-0.97411

C	-4.90299	-6.03852	-1.97144
C	-4.13423	-3.70926	-2.56903
C	-3.46604	-1.47996	-2.78613
C	-3.48349	-1.56860	-4.16865
C	-3.83997	-2.77645	-4.75602
C	-4.17014	-3.85765	-3.94948
H	-4.41542	-5.00172	1.67909
H	-5.21897	-7.30088	1.16627
H	-5.53764	-7.95664	-1.23871
H	-5.04142	-6.29988	-3.01690
H	-3.18917	-0.55793	-2.27847
H	-3.21943	-0.70013	-4.76504
H	-3.86176	-2.88015	-5.83800
H	-4.44523	-4.81023	-4.39298
C	-4.26140	0.40293	0.30248
C	-4.04354	1.76774	0.44667
C	-2.74647	2.23139	0.62511
C	-1.69330	1.32545	0.66205
C	-1.97186	-0.02439	0.52077
C	-5.57775	-0.21029	0.10204
C	-6.76914	0.50184	0.05054
C	-7.96234	-0.18472	-0.13215
C	-7.94161	-1.56786	-0.26253
C	-6.72231	-2.22393	-0.21160
H	-4.87648	2.46491	0.41822
H	-2.56151	3.29719	0.73486
H	-0.66587	1.65020	0.79881
H	-1.18498	-0.77642	0.53985
H	-6.76766	1.58329	0.15272
H	-8.90189	0.36075	-0.17223
H	-8.85321	-2.14055	-0.40616
H	-6.65636	-3.30553	-0.31063
C	-1.44055	-3.51034	1.64112
C	-0.98369	-3.72506	-0.66222
C	0.21338	-4.31569	-0.38966
C	-0.23625	-4.10532	1.93077
C	-2.38921	-3.07332	2.63233
C	-4.48419	-2.13789	3.01271
C	-4.26571	-2.22502	4.37535
C	-2.20936	-3.13644	4.02557
H	-1.29223	-3.56774	-1.69324
H	0.90646	-4.65708	-1.14797
H	0.11064	-4.28582	2.94298
H	-5.40796	-1.73381	2.60531
H	-5.02562	-1.88420	5.07511
H	-1.28598	-3.53906	4.44165
N	-4.29346	-4.43402	-0.31046
N	-3.77809	-2.52619	-2.00671
N	-3.22372	-0.47007	0.34189
N	-5.56939	-1.56270	-0.02896
N	-3.55148	-2.56476	2.14594
N	-1.82368	-3.30083	0.31559
N	-3.12643	-2.72299	4.87921
N	0.57383	-4.49434	0.93186
H	1.46017	-4.94069	1.15418

[2-H] ²⁺ (S=1/2)			
Ru	-3.72376	-2.49635	0.08143
C	-4.49222	-4.77409	-1.59206
C	-4.70130	-5.32310	0.66112
C	-5.14950	-6.59804	0.35466
C	-5.27400	-6.96016	-0.98210
C	-4.94183	-6.03813	-1.96421
C	-4.11786	-3.72519	-2.54751
C	-3.37714	-1.53055	-2.78616
C	-3.37044	-1.63620	-4.16792
C	-3.74946	-2.84125	-4.74864
C	-4.12725	-3.89508	-3.92910
H	-4.59474	-4.99318	1.69333
H	-5.39628	-7.28795	1.15706
H	-5.62671	-7.95066	-1.25944
H	-5.03623	-6.30017	-3.01471
H	-3.08058	-0.60857	-2.28865
H	-3.06940	-0.78343	-4.77042
H	-3.75101	-2.96192	-5.82926
H	-4.42311	-4.84606	-4.36356
C	-4.23732	0.38230	0.28914
C	-4.01166	1.74924	0.42763
C	-2.71175	2.21667	0.55655
C	-1.66146	1.30586	0.54580
C	-1.95012	-0.04256	0.40920
C	-5.56898	-0.21573	0.13020
C	-6.75014	0.52093	0.09704
C	-7.96167	-0.13875	-0.05127
C	-7.96663	-1.52421	-0.16490
C	-6.75757	-2.20061	-0.12653
H	-4.84562	2.44594	0.43515
H	-2.52241	3.28213	0.66363
H	-0.62799	1.62726	0.64301
H	-1.16148	-0.79337	0.39380
H	-6.72590	1.60384	0.18461
H	-8.89122	0.42476	-0.07773
H	-8.89125	-2.08269	-0.28325
H	-6.71590	-3.28558	-0.20910
C	-1.43757	-3.47471	1.62705
C	-0.94525	-3.60167	-0.66789
C	0.28415	-4.12515	-0.40114
C	-0.20539	-4.00078	1.91740
C	-2.41599	-3.10245	2.62417
C	-4.54786	-2.28282	3.01655
C	-4.33298	-2.38852	4.37822
C	-2.23901	-3.18979	4.01465
H	-1.25146	-3.43621	-1.69921
H	1.00292	-4.40311	-1.16167
H	0.14107	-4.18736	2.92887
H	-5.48972	-1.91605	2.61278
H	-5.11243	-2.09930	5.08083
H	-1.29747	-3.55358	4.42661
N	-4.38289	-4.42448	-0.28407
N	-3.73585	-2.54805	-1.98724
N	-3.20552	-0.50095	0.28192
N	-5.58176	-1.56976	0.01980

N	-3.59844	-2.63853	2.13388
N	-1.83111	-3.25554	0.30084
N	-3.17427	-2.84172	4.88187
N	0.64618	-4.32031	0.92142
H	1.55428	-4.71515	1.14481

[2]⁺ (S=1/2)

Ru	-3.78388	-2.62576	0.10991
C	-4.87475	-4.90284	-1.37463
C	-5.29798	-5.14463	0.90224
C	-5.94187	-6.35445	0.69988
C	-6.04760	-6.84862	-0.59611
C	-5.50916	-6.11395	-1.64198
C	-4.29632	-4.03639	-2.40749
C	-3.20808	-2.02132	-2.82439
C	-3.17811	-2.26690	-4.18756
C	-3.72759	-3.45164	-4.66623
C	-4.29393	-4.34244	-3.76641
H	-5.19349	-4.71649	1.89784
H	-6.35023	-6.89444	1.54999
H	-6.54704	-7.79457	-0.79205
H	-5.58509	-6.47955	-2.66249
H	-2.78327	-1.11071	-2.40478
H	-2.72743	-1.53771	-4.85553
H	-3.71732	-3.68043	-5.72928
H	-4.73101	-5.27210	-4.12101
C	-3.75282	0.30350	0.09717
C	-3.27904	1.61224	0.15350
C	-1.91772	1.84031	0.28936
C	-1.05523	0.75139	0.36308
C	-1.58706	-0.52645	0.30218
C	-5.16817	-0.04785	-0.06364
C	-6.19271	0.88894	-0.17605
C	-7.50138	0.45519	-0.32763
C	-7.75863	-0.91118	-0.36822
C	-6.69651	-1.79324	-0.25224
H	-3.96890	2.44986	0.09308
H	-1.53546	2.85725	0.33570
H	0.01842	0.88211	0.46906
H	-0.95225	-1.40966	0.35325
H	-5.96961	1.95198	-0.14565
H	-8.31025	1.17693	-0.41418
H	-8.76759	-1.29694	-0.48749
H	-6.85244	-2.87078	-0.27481
C	-1.77766	-3.87392	1.83031
C	-1.21121	-4.24576	-0.40253
C	-0.09507	-4.94701	-0.00565
C	-0.61887	-4.60486	2.18348
C	-2.69269	-3.28387	2.74011
C	-4.66171	-2.06175	3.01117
C	-4.52475	-2.13882	4.37873
C	-2.59800	-3.33007	4.15102
H	-1.44263	-4.10290	-1.45856
H	0.57980	-5.37836	-0.74252
H	-0.38511	-4.75121	3.24070
H	-5.50841	-1.54704	2.55635

H	-5.26052	-1.67981	5.03638
H	-1.75106	-3.84628	4.60887
N	-4.77332	-4.42764	-0.10521
N	-3.74511	-2.88329	-1.94536
N	-2.90422	-0.75551	0.17256
N	-5.42735	-1.38136	-0.09771
N	-3.77182	-2.62391	2.17167
N	-2.06176	-3.69610	0.48462
N	-3.47237	-2.78360	4.96393
N	0.21015	-5.13245	1.31262

[2]⁺ (S=3/2)

Ru	-3.77290	-2.63337	0.11990
C	-4.87449	-4.91217	-1.39768
C	-5.16676	-5.24143	0.89337
C	-5.80294	-6.45450	0.68088
C	-5.97153	-6.89902	-0.62503
C	-5.50179	-6.12204	-1.67518
C	-4.34919	-4.00469	-2.42500
C	-3.29641	-1.95685	-2.80997
C	-3.30983	-2.15994	-4.18089
C	-3.86604	-3.33353	-4.67559
C	-4.39262	-4.26478	-3.79058
H	-5.01324	-4.84576	1.89603
H	-6.15676	-7.03271	1.52980
H	-6.46766	-7.84511	-0.82820
H	-5.62768	-6.45366	-2.70197
H	-2.87052	-1.05752	-2.36854
H	-2.88955	-1.40617	-4.84065
H	-3.89195	-3.52596	-5.74549
H	-4.83115	-5.18672	-4.16237
C	-3.77722	0.28961	0.08754
C	-3.26557	1.61061	0.17153
C	-1.92737	1.82303	0.36710
C	-1.04830	0.71639	0.49251
C	-1.58061	-0.54844	0.41070
C	-5.13659	-0.05265	-0.09937
C	-6.20370	0.86994	-0.25330
C	-7.48447	0.42137	-0.43489
C	-7.74479	-0.97265	-0.47745
C	-6.68453	-1.83526	-0.32691
H	-3.94926	2.45237	0.08238
H	-1.54068	2.83832	0.43085
H	0.01851	0.84842	0.64905
H	-0.95190	-1.43454	0.49803
H	-5.99263	1.93688	-0.22538
H	-8.29933	1.13359	-0.55009
H	-8.74835	-1.36266	-0.62157
H	-6.83014	-2.91576	-0.34839
C	-1.78352	-3.89764	1.86931
C	-1.25824	-4.35519	-0.36516
C	-0.16473	-5.08155	0.04162
C	-0.64758	-4.66194	2.23121
C	-2.67205	-3.25290	2.76232
C	-4.58979	-1.92505	2.98844
C	-4.43964	-1.94515	4.35391

C	-2.56726	-3.23595	4.17432
H	-1.50085	-4.23361	-1.42068
H	0.48811	-5.55600	-0.68781
H	-0.40604	-4.78784	3.28871
H	-5.41142	-1.39442	2.50886
H	-5.14579	-1.42358	4.99625
H	-1.74075	-3.76609	4.65170
N	-4.71807	-4.48742	-0.11938
N	-3.79807	-2.85830	-1.95400
N	-2.89287	-0.77998	0.19895
N	-5.41846	-1.41518	-0.12736
N	-3.73253	-2.58023	2.17947
N	-2.06997	-3.74968	0.52403
N	-3.41247	-2.61286	4.95913
N	0.14675	-5.23895	1.36235

