Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis and Electronic Structure Determination of Uranium(VI) Ligand Radical Complexes

Supporting Information

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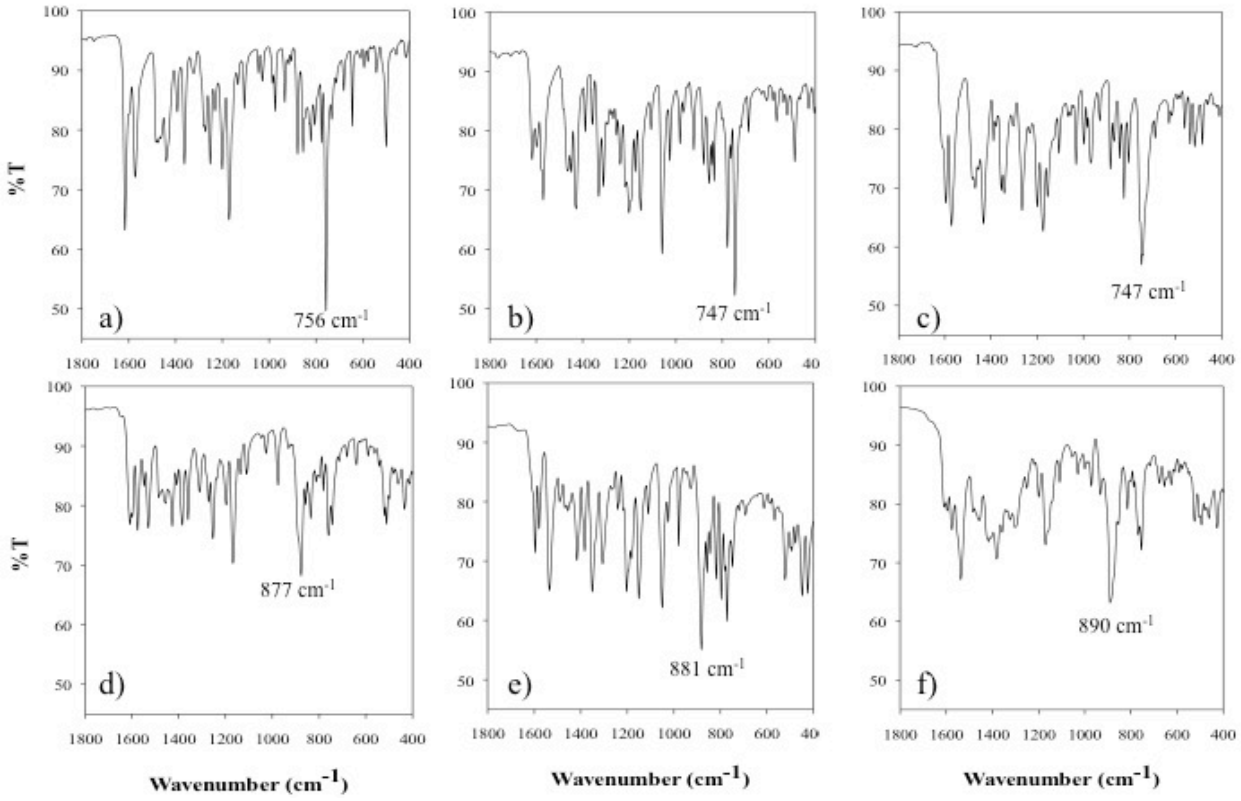

Figure S1. IR spectra of salophen ligands (a-c), and complexes **1a-c** (d-f), respectively.

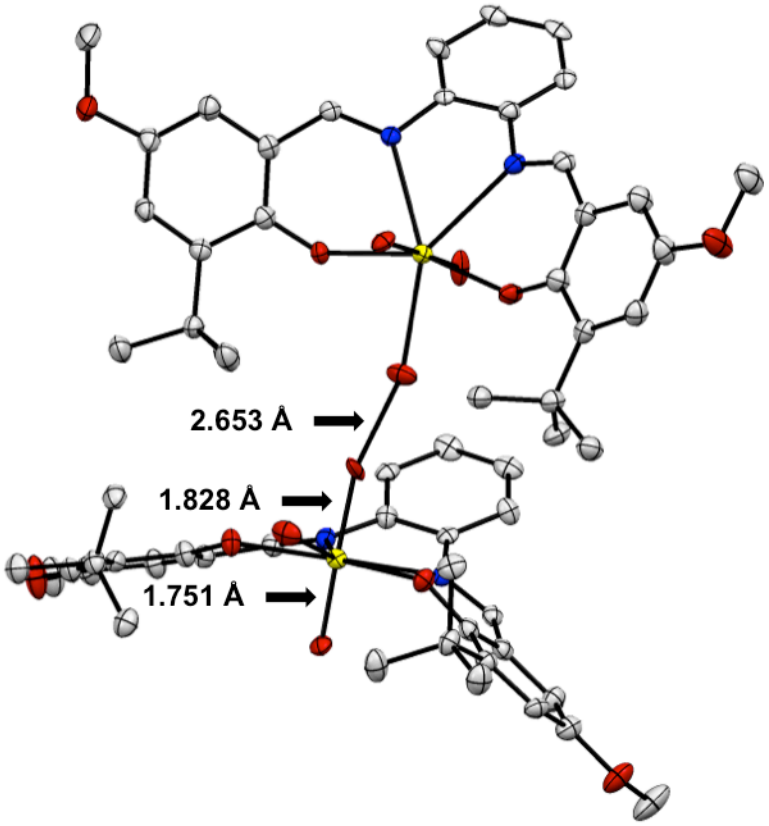

Figure S2. POV-Ray representation (50% probability) of **1b,** depicting intermolecular interaction.

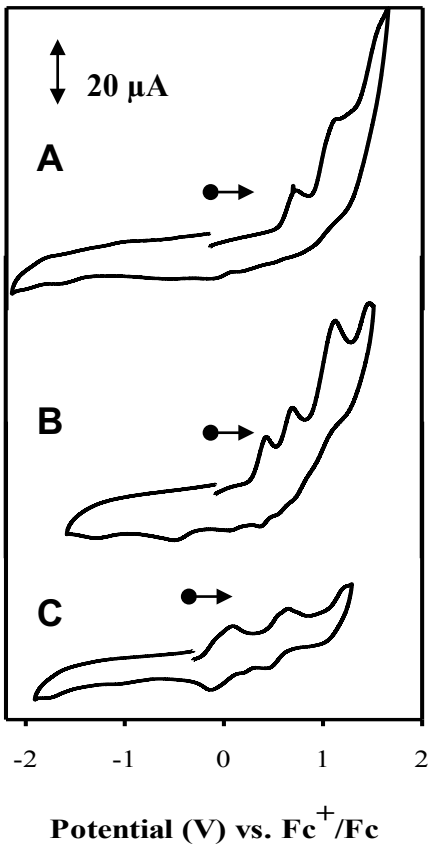

Figure S3. Cyclic voltammograms of **1a** (A), **1b** (B) and **1c** (C) *versus* Fc^+/Fc. Conditions: 1.0 mM solutions in CH_2Cl_2, 0.1 M nBu$_4$NClO$_4$, T = 298 K.

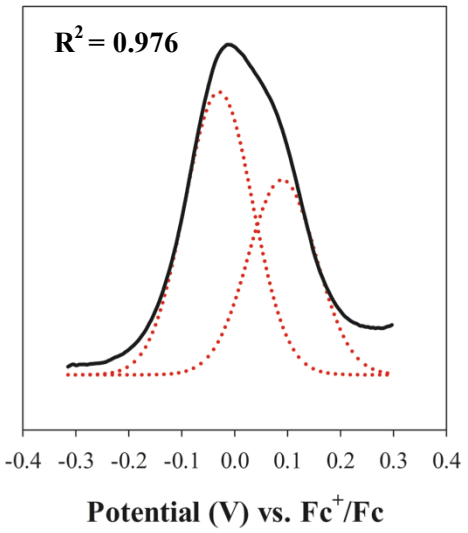

Figure S4. Differential pulse voltammetry (DPV) of **1c** (black solid line); fitted gaussian curves using PeakFit (red dotted lines). Conditions: 1.0 mM solutions in CH_2Cl_2, 0.1 M nBu$_4$NClO$_4$, T = 298 K.

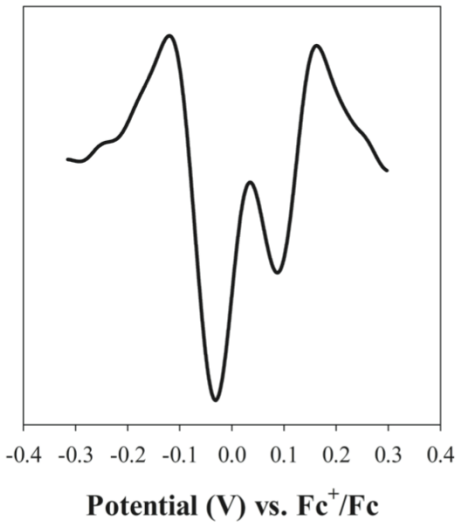

Figure S5. Second derivative of the DPV

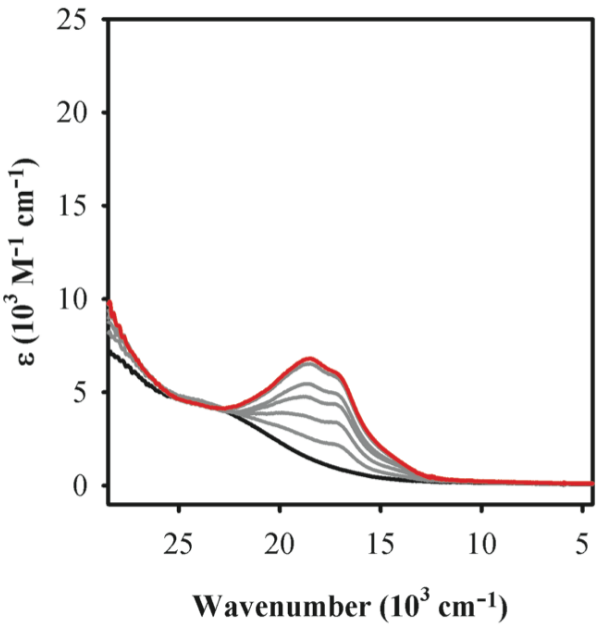

Figure S6. Electronic spectra of chemical oxidation of **1c** (black) to **[1c]**$^{+}$ (red). Oxidation was done through the titration (grey lines) with acetylferrocenium hexafluoroantimony. Conditions: 1.0 mM solution in CH_2Cl_2, T = 193 K. Spectra were corrected for solvent contraction at low temperature.

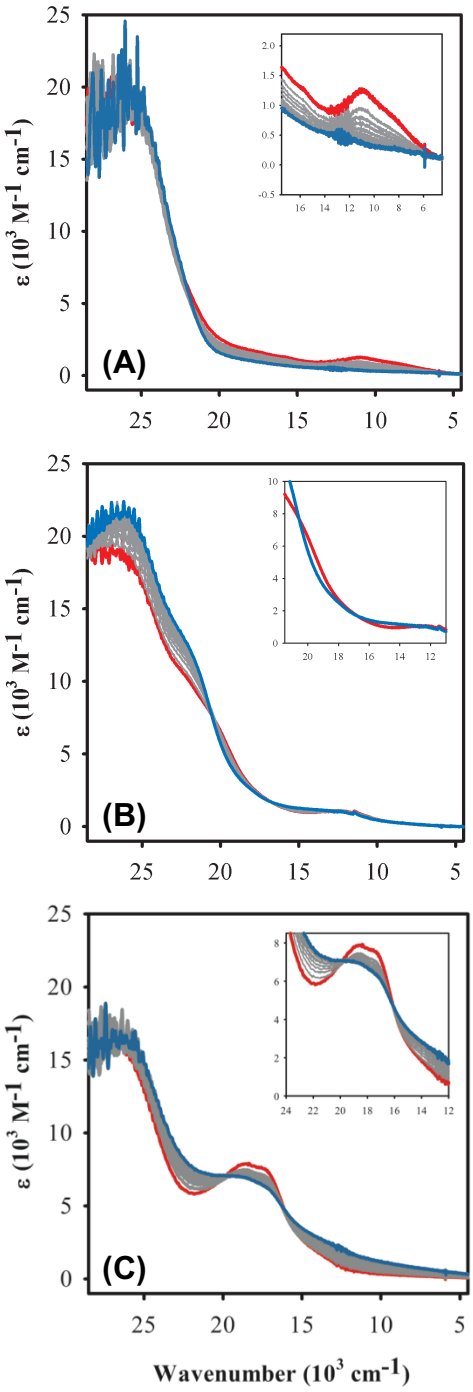

Figure S7. Electronic spectra of the decay study of **[1a-c]**$^{+}$ shown in **A-C**, respectively. (t = 0 min - red; t = 5 hr - blue; 30 min scans (grey lines). Conditions: 1.0 mM solution in CH_2Cl_2, T = 298 K.

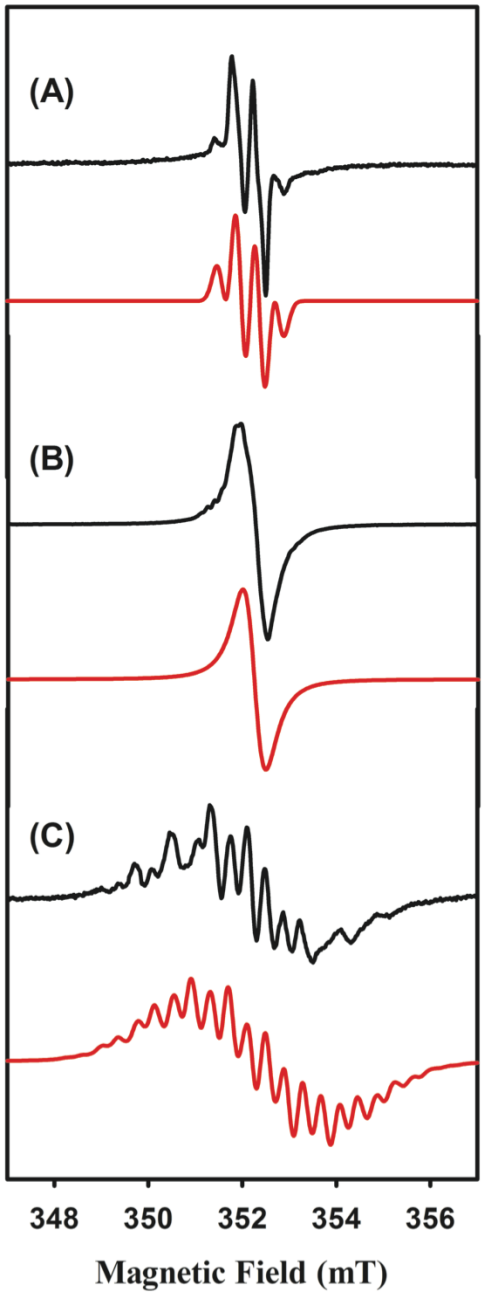

Figure S8. X-Band EPR spectra for oxidation of **1a** (A), **1b** (B), and **1c** (C) in CH_2Cl_2 with 0.5 equiv. of $[N(C_6H_3Br_2)_3^{\bullet}]^+[SbF_6]^-$; Experimental data (black); Simulation (red): (A) g = 2.001, AH_1 = 10.6 MHz, AH_2 = 10.9 MHz, AH_3 = 11.0 MHz; (B) g = 2.000; (C) g = 1.999, AN_1 = 23.5 MHz, AN_2 = 10.5 MHz, AH_1 = 21.3 MHz, AH_2 = 8.6 MHz, AH_3 = 8.9 MHz, AH_4 = 4.4 MHz; Conditions: 1.0 mM; frequency, 9.86 GHz; power, 2.00 mW; modulation frequency, 100 kHz; amplitude, 0.2 mT; T = 298 K.

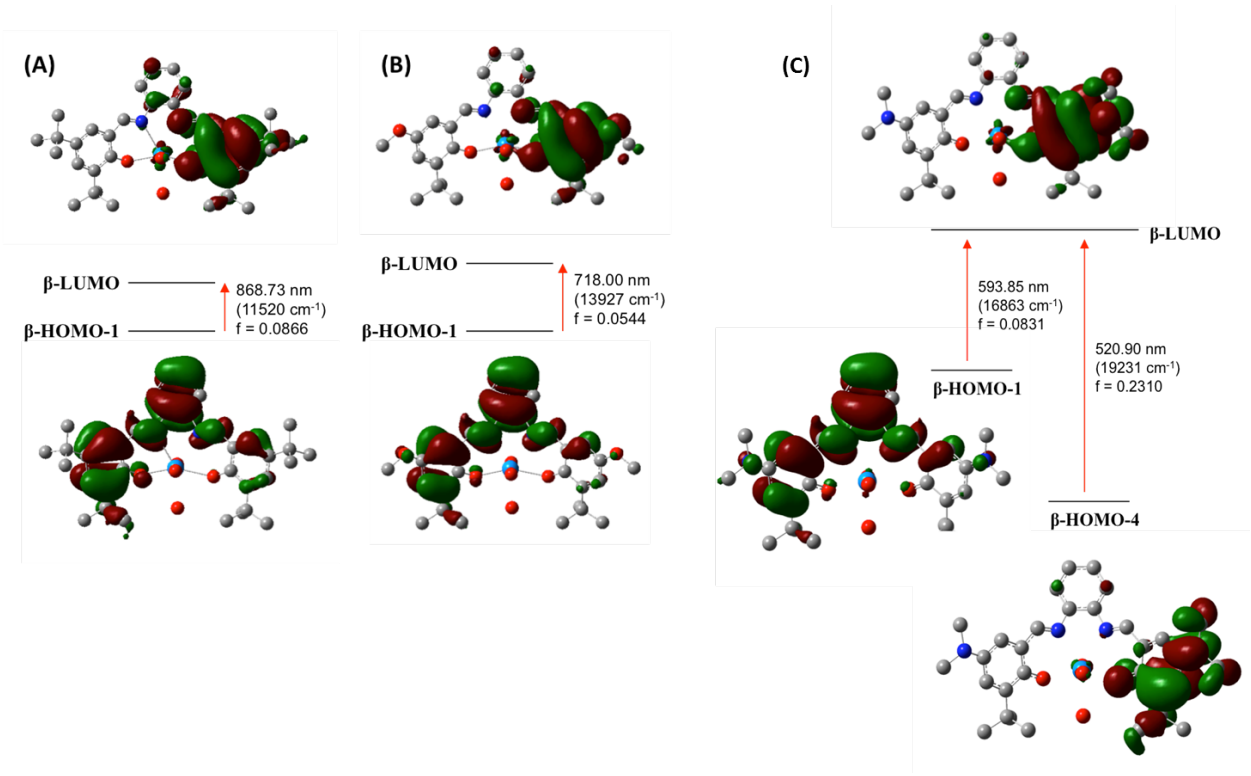

Figure S9. TD-DFT assignment of the calculated NIR transitions for **[1a-c]**$^{+}$ (β-HOMO-1 → β-LUMO)

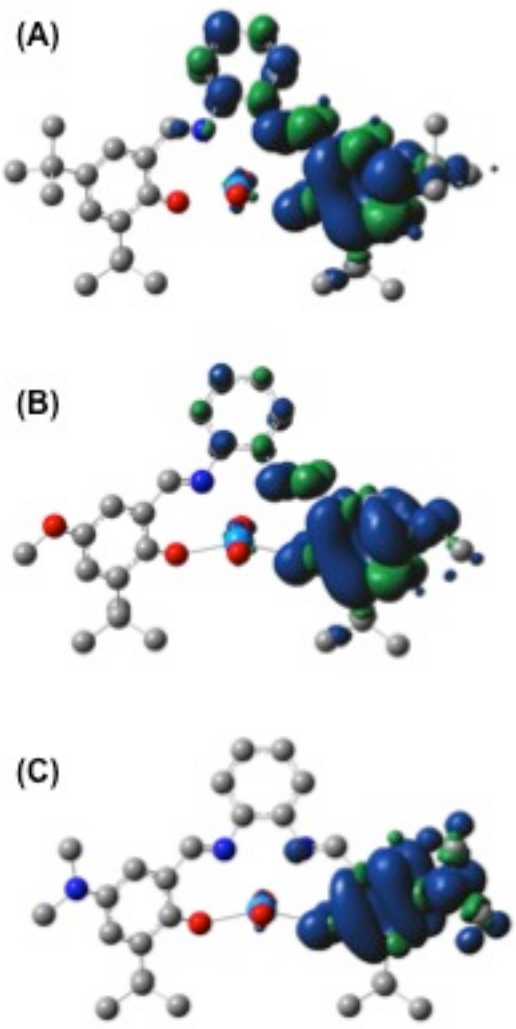

Figure S10. Predicted spin density of **[1a]**$^{+}$ (A), **[1b]**$^{+}$ (B) and **[1c]**$^{+}$ (C) without H_2O coordinated in the equatorial plane.

Computational Data

A) Optimized coordinates (Å) for **1a**

U	0.01147	-0.257423	-0.803698
O	2.216472	-0.751599	-0.815472
N	-1.368104	1.878125	-0.593048
C	0.695221	3.06997	-1.00999
N	1.349724	1.892662	-0.577486
O	-2.188913	-0.796115	-0.750327

C	1.380559	4.203499	-1.471485
H	2.464703	4.190783	-1.52041
O	-0.006628	-0.057837	-2.58551
C	0.681763	5.324997	-1.915522
H	1.228511	6.188952	-2.281297
O	0.03168	-0.393309	0.980097
C	-0.714975	5.315877	-1.930135
H	-1.265047	6.172588	-2.307783
O	-0.047796	-2.813796	-1.270604
H	-0.915479	-3.093226	-1.610454
H	0.603511	-3.114046	-1.927312
C	-1.40895	4.186242	-1.499138
H	-2.491645	4.161771	-1.569666
C	-2.544452	1.9698	-0.03768
H	-2.919407	2.972236	0.188893
C	2.513468	1.988681	0.003288
H	2.871828	2.990976	0.256451
C	-3.453104	0.910373	0.314955
C	-4.622205	1.303364	1.012442
H	-4.713279	2.349742	1.28579
C	-5.617625	0.401629	1.338127
C	-5.418377	-0.934634	0.917464
H	-6.19544	-1.649918	1.157812
C	-4.306007	-1.396382	0.217922
C	-3.272148	-0.450823	-0.085069
C	3.427222	0.930648	0.346878
C	3.282733	-0.414772	-0.118368
C	4.335277	-1.349532	0.150926
C	5.417786	-0.90048	0.903503
H	6.207032	-1.60889	1.123182
C	5.573518	0.414668	1.402479
C	4.569886	1.312723	1.092694
H	4.632822	2.346376	1.417769
C	-6.89691	0.783427	2.102906
C	-4.181302	-2.880339	-0.188896
C	4.269812	-2.805759	-0.35817
C	6.821068	0.780138	2.225511
C	-6.926941	2.279652	2.469043
H	-7.850686	2.507689	3.012654
H	-6.901101	2.918095	1.5783
H	-6.085732	2.557479	3.114615
C	-6.981573	-0.03484	3.413561
H	-7.895233	0.220367	3.964496

H	-6.123252	0.176237	4.061941
H	-7.000041	-1.113155	3.221696
C	-8.135731	0.476209	1.227335
H	-9.056227	0.73834	1.763242
H	-8.196186	-0.585148	0.963039
H	-8.108768	1.0532	0.295561
C	-5.441699	-3.696577	0.167504
H	-6.338088	-3.308734	-0.330079
H	-5.628755	-3.721249	1.247018
H	-5.302214	-4.732083	-0.162802
C	-3.983705	-3.007433	-1.719883
H	-3.858906	-4.061873	-1.996638
H	-3.113953	-2.445999	-2.067579
H	-4.860825	-2.623608	-2.254659
C	-2.994567	-3.525695	0.568387
H	-3.181553	-3.520412	1.648646
H	-2.056878	-2.995689	0.392795
H	-2.867075	-4.569889	0.255419
C	3.080582	-3.542891	0.304552
H	2.127066	-3.057863	0.091157
H	3.208358	-3.577495	1.393109
H	3.029303	-4.576947	-0.059878
C	5.545314	-3.604215	-0.015402
H	5.698145	-3.699148	1.065806
H	6.444128	-3.15476	-0.453258
H	5.451936	-4.617614	-0.421739
C	4.123837	-2.827177	-1.899832
H	4.055684	-3.863071	-2.255199
H	4.997893	-2.366921	-2.376415
H	3.234833	-2.286127	-2.228868
C	6.794803	2.247147	2.695212
H	5.926387	2.454492	3.331234
H	6.776241	2.946206	1.851065
H	7.694762	2.462175	3.282332
C	6.898786	-0.124434	3.47867
H	6.958118	-1.18557	3.213952
H	6.01764	0.014222	4.115771
H	7.789182	0.120636	4.070591
C	8.090629	0.570868	1.365197
H	8.187753	-0.466207	1.025995
H	8.989034	0.816607	1.944697
H	8.072412	1.2136	0.477227
C	-0.71976	3.061328	-1.022279

B) Optimized coordinates (Å) for **1b**

U	0.009027	-0.077264	-0.606977
O	2.20878	-0.562619	-0.655057
N	-1.365797	2.040556	-0.190413
C	0.699767	3.262002	-0.488349
N	1.349324	2.047829	-0.163358
O	-2.188576	-0.604216	-0.614243
C	1.389471	4.431196	-0.840816
H	2.473788	4.42101	-0.885252
O	-0.000295	0.302065	-2.360676
C	0.693909	5.589316	-1.184461
H	1.243361	6.481907	-1.468105
O	0.021667	-0.383545	1.156145
C	-0.70287	5.584423	-1.205282
H	-1.249716	6.473122	-1.505695
O	-0.060558	-2.571719	-1.341287
H	-0.92875	-2.798725	-1.716938
H	0.591452	-2.800624	-2.025495
C	-1.40089	4.422204	-0.880732
H	-2.483378	4.406463	-0.956148
C	-2.538839	2.081699	0.372744
H	-2.916057	3.057633	0.691972
C	2.505948	2.08591	0.433163
H	2.868555	3.057604	0.781165
C	-3.446224	0.988926	0.627862
C	-4.601248	1.314764	1.369376
H	-4.730127	2.318119	1.76521
C	-5.580805	0.36553	1.599143
C	-5.418577	-0.921516	1.057287
H	-6.195755	-1.652577	1.230554
C	-4.302232	-1.296713	0.303059
C	-3.27156	-0.328192	0.09207
C	3.412075	0.991581	0.68596
C	3.271175	-0.303379	0.088481
C	4.314357	-1.26328	0.275157
C	5.397926	-0.910351	1.085709
H	6.182154	-1.636573	1.246496
C	5.521183	0.349592	1.697841
C	4.538622	1.297937	1.477929
H	4.642323	2.284451	1.920754

C	-4.18651	-2.730777	-0.257432
C	4.254491	-2.658943	-0.383702
H	-2.058965	-2.918475	0.29078
C	-0.714796	3.257476	-0.506815
O	-6.662769	0.764899	2.341229
O	6.57081	0.724454	2.497034
C	7.612102	-0.214399	2.731876
H	8.327111	0.29013	3.384143
H	7.239408	-1.116038	3.234774
H	8.115621	-0.502969	1.800116
C	-7.697308	-0.177544	2.590908
H	-7.328909	-1.043705	3.155558
H	-8.442986	0.349361	3.188872
H	-8.162406	-0.525264	1.659399
C	5.52405	-3.492593	-0.109775
H	6.429654	-3.002053	-0.485168
H	5.661214	-3.703256	0.957207
H	5.435494	-4.456916	-0.622762
C	4.129272	-2.516909	-1.920696
H	3.247706	-1.938175	-2.201789
H	5.012475	-2.015295	-2.334503
H	4.060336	-3.509276	-2.383738
C	3.055488	-3.457102	0.183047
H	3.16371	-3.59743	1.265192
H	2.105945	-2.952865	0.000233
H	3.012628	-4.450648	-0.281269
C	-2.999186	-3.456237	0.422503
H	-2.883376	-4.465542	0.007314
H	-3.177425	-3.555553	1.499639
C	-5.448522	-3.575732	0.016832
H	-5.62805	-3.718882	1.088527
H	-6.34646	-3.132258	-0.428753
H	-5.317014	-4.569352	-0.426177
C	-3.996144	-2.69639	-1.794102
H	-3.130192	-2.097952	-2.084302
H	-3.868312	-3.715837	-2.178986
H	-4.877466	-2.263479	-2.282431

C) Optimized coordinates (Å) for **1c**

U	0.016945	-0.238548	-0.685594
O	2.218041	-0.711608	-0.719206

N	-1.370522	1.900068	-0.458582
C	0.691137	3.096091	-0.867791
N	1.344387	1.919024	-0.435775
O	-2.179334	-0.77371	-0.622641
C	1.376319	4.232048	-1.323614
H	2.460757	4.221054	-1.367363
O	-0.008006	-0.021146	-2.468255
C	0.677215	5.352972	-1.768766
H	1.223688	6.218727	-2.130813
O	0.04709	-0.393599	1.098986
C	-0.719516	5.34106	-1.78924
H	-1.269609	6.197344	-2.16796
O	-0.068173	-2.789626	-1.181667
H	-0.979635	-3.07831	-1.360913
H	0.454535	-3.062503	-1.954684
C	-1.413231	4.209585	-1.362408
H	-2.495677	4.183377	-1.436645
C	-2.546469	1.990177	0.097048
H	-2.922851	2.992273	0.323331
C	2.503445	2.012656	0.153909
H	2.860061	3.013745	0.414827
C	-3.453454	0.927787	0.451252
C	-4.619217	1.326923	1.148789
H	-4.711224	2.373427	1.414997
C	-5.615851	0.413416	1.482021
C	-5.427161	-0.919912	1.032634
H	-6.203554	-1.63832	1.250339
C	-4.310281	-1.366161	0.330089
C	-3.268382	-0.427654	0.042908
C	3.413388	0.949797	0.498926
C	3.277738	-0.382624	0.001371
C	4.339011	-1.309038	0.254191
C	5.411266	-0.883786	1.035201
H	6.200834	-1.593346	1.232866
C	5.542414	0.418523	1.585723
C	4.540197	1.330779	1.266789
H	4.596806	2.360689	1.599489
C	-4.196052	-2.84455	-0.101139
C	4.305007	-2.745831	-0.312292
H	-2.085463	-2.961498	0.526053
C	-0.724016	3.084773	-0.885046
C	7.826649	-0.076301	2.351618
H	8.56879	0.333714	3.039771

H	7.615595	-1.100642	2.676314
H	8.276176	-0.121354	1.345561
C	-7.921002	-0.087805	2.175846
H	-7.704322	-1.081119	2.582962
H	-8.705696	0.350377	2.796008
H	-8.31792	-0.214936	1.154876
C	5.58373	-3.542584	0.022377
H	6.485166	-3.066247	-0.380243
H	5.717559	-3.679735	1.101686
H	5.510122	-4.539719	-0.426223
C	4.187612	-2.704835	-1.856074
H	3.297226	-2.161416	-2.176792
H	5.065179	-2.216092	-2.296759
H	4.137272	-3.725878	-2.254976
C	3.112249	-3.52412	0.293679
H	3.207017	-3.585974	1.384538
H	2.157115	-3.052976	0.059588
H	3.09516	-4.548705	-0.099933
C	-3.020714	-3.509007	0.657535
H	-2.876052	-4.540239	0.310655
H	-3.230305	-3.544283	1.732999
C	-5.463958	-3.660495	0.227951
H	-5.662432	-3.703758	1.304856
H	-6.352796	-3.258954	-0.272214
H	-5.326415	-4.690777	-0.119217
C	-3.985101	-2.944739	-1.632388
H	-3.106825	-2.385338	-1.960793
H	-3.869563	-3.99455	-1.929886
H	-4.853345	-2.540875	-2.166892
N	6.627683	0.750372	2.408991
N	-6.745087	0.771454	2.231907
C	6.832357	2.15653	2.721092
H	7.022044	2.777305	1.828532
H	5.958497	2.566938	3.238995
H	7.68704	2.251479	3.394091
C	-6.995157	2.189312	2.441171
H	-6.155021	2.654596	2.96836
H	-7.159074	2.746141	1.502512
H	-7.880974	2.305933	3.069019

D) Optimized coordinates (Å) for **[1a]**$^{+}$

U	-0.072633	-0.314675	-0.799639
O	2.268203	-0.842934	-0.62207
N	-1.32643	1.858724	-0.576446
C	0.739215	3.004853	-1.089463
N	1.393484	1.846571	-0.611407
O	-2.250279	-0.714428	-0.825527
C	1.42765	4.10851	-1.621803
H	2.508713	4.081178	-1.707383
O	0.020853	-0.111523	-2.566235
C	0.728597	5.211711	-2.099383
H	1.271464	6.048822	-2.526348
O	-0.078838	-0.470191	0.97384
C	-0.670454	5.220034	-2.067376
H	-1.220059	6.067474	-2.465038
O	0.050839	-2.784282	-1.44149
H	-0.206665	-3.502585	-0.839064
H	-0.336569	-3.006641	-2.305701
C	-1.367019	4.122791	-1.567247
H	-2.451157	4.109381	-1.603587
C	-2.476296	1.990822	0.033388
H	-2.798322	3.00422	0.286315
C	2.577247	1.982971	-0.091146
H	2.955383	2.993529	0.07589
C	-3.406259	0.958801	0.393235
C	-4.525502	1.354007	1.167029
H	-4.556825	2.37979	1.519162
C	-5.545357	0.471267	1.467812
C	-5.434704	-0.83182	0.925915
H	-6.240854	-1.523445	1.135701
C	-4.377751	-1.290027	0.140721
C	-3.30815	-0.376339	-0.106062
C	3.50703	0.945984	0.298693
C	3.328159	-0.465444	-0.039948
C	4.394534	-1.417723	0.287927
C	5.496158	-0.920465	0.952096
H	6.287168	-1.607831	1.218637
C	5.672533	0.446327	1.315054
C	4.662258	1.354599	0.956318
H	4.775438	2.40658	1.190174
C	-6.768238	0.843312	2.323737
C	-4.366814	-2.726924	-0.424736
C	4.267497	-2.902762	-0.082748
C	6.939195	0.872152	2.056465

C	-6.697272	2.295766	2.832147
H	-7.580133	2.514291	3.442902
H	-6.680278	3.01731	2.00716
H	-5.812379	2.465932	3.456378
C	-6.842472	-0.094854	3.552304
H	-7.715755	0.155009	4.166633
H	-5.947104	0.005748	4.176557
H	-6.932569	-1.146555	3.260086
C	-8.057363	0.687671	1.481466
H	-8.937162	0.940434	2.085332
H	-8.187988	-0.337305	1.118136
H	-8.03968	1.353401	0.610764
C	-5.660376	-3.496877	-0.085299
H	-6.551665	-3.004295	-0.490285
H	-5.796227	-3.626034	0.994529
H	-5.60631	-4.496834	-0.529455
C	-4.245619	-2.692249	-1.968428
H	-4.242009	-3.715376	-2.363908
H	-3.32998	-2.193656	-2.292375
H	-5.099	-2.165106	-2.411114
C	-3.188195	-3.525179	0.182227
H	-3.274139	-3.580479	1.273542
H	-2.230142	-3.063096	-0.061587
H	-3.187469	-4.549866	-0.209483
C	3.07224	-3.530024	0.681082
H	2.12728	-3.051806	0.419775
H	3.216655	-3.449907	1.764481
H	2.999685	-4.594016	0.427987
C	5.533166	-3.696888	0.300778
H	5.717862	-3.687685	1.380776
H	6.426862	-3.321528	-0.210471
H	5.397692	-4.741394	0.002634
C	4.064492	-3.0558	-1.612971
H	4.031314	-4.121539	-1.86601
H	4.89883	-2.606526	-2.163821
H	3.134726	-2.595163	-1.949492
C	6.969711	2.383039	2.355738
H	6.133526	2.692598	2.992597
H	6.950977	2.98279	1.438827
H	7.894936	2.625919	2.887672
C	7.016076	0.102821	3.401765
H	7.047235	-0.981856	3.258706
H	6.157143	0.338654	4.039427

H	7.927526	0.39556	3.934666
C	8.175879	0.51912	1.188332
H	8.247297	-0.553508	0.98348
H	9.086946	0.818688	1.717816
H	8.148067	1.049502	0.230321
C	-0.676412	3.009666	-1.065666

E) Optimized coordinates (Å) for **[1b]**$^{+}$

U	-0.052214	0.121315	-0.609012
O	2.302919	-0.602435	-0.571682
N	-1.358382	2.010622	-0.175886
C	0.697119	3.226484	-0.544793
N	1.359742	2.027129	-0.180072
O	-2.211212	-0.570035	-0.598956
C	1.382831	4.380715	-0.951704
H	2.465913	4.370929	-1.016816
O	0.00272	0.25054	-2.352023
C	0.678721	5.520971	-1.330139
H	1.219924	6.402144	-1.659686
O	-0.002263	-0.455544	1.13966
C	-0.719045	5.511855	-1.325033
H	-1.272185	6.3882	-1.64826
O	0.05058	-2.538462	-1.405316
H	-0.389298	-3.254478	-0.916079
H	-0.172013	-2.677064	-2.341956
C	-1.41118	4.363191	-0.946605
H	-2.494443	4.343035	-1.003297
C	-2.513822	2.075033	0.42555
H	-2.861723	3.058793	0.750769
C	2.513177	2.116028	0.401277
H	2.870318	3.102314	0.706083
C	-3.431485	0.998198	0.697889
C	-4.566528	1.32597	1.46612
H	-4.673572	2.320124	1.889793
C	-5.55848	0.383876	1.682971
C	-5.429762	-0.88708	1.095076
H	-6.219811	-1.607083	1.254041
C	-4.332797	-1.260529	0.31032
C	-3.291579	-0.3049	0.126721
C	3.447853	1.039655	0.687936
C	3.332438	-0.295365	0.106534

C	4.42579	-1.257218	0.298034
C	5.479313	-0.882287	1.107172
H	6.285755	-1.577901	1.287482
C	5.550814	0.39811	1.711006
C	4.541658	1.357803	1.467582
H	4.654631	2.344599	1.905242
C	-4.25819	-2.673003	-0.309072
C	4.388175	-2.638946	-0.372404
H	-2.145669	-2.915015	0.229956
C	-0.715453	3.214652	-0.54305
O	-6.616895	0.776126	2.45384
O	6.540061	0.804044	2.502359
C	7.634871	-0.077176	2.819848
H	8.277192	0.497007	3.485293
H	7.269384	-0.972007	3.330708
H	8.181916	-0.348522	1.912785
C	-7.672934	-0.15044	2.684467
H	-7.317307	-1.044188	3.212278
H	-8.395688	0.373703	3.311577
H	-8.15793	-0.450573	1.747158
C	5.671512	-3.446425	-0.089147
H	6.570375	-2.937626	-0.455664
H	5.800138	-3.661323	0.977852
H	5.604249	-4.407974	-0.607973
C	4.269927	-2.473843	-1.909941
H	3.35256	-1.957895	-2.197039
H	5.124907	-1.915383	-2.308168
H	4.268766	-3.464323	-2.378664
C	3.190054	-3.456711	0.174713
H	3.261026	-3.571665	1.262373
H	2.235241	-2.99156	-0.069809
H	3.206718	-4.457908	-0.271136
C	-3.08852	-3.454771	0.336296
H	-2.985613	-4.44113	-0.133018
H	-3.26512	-3.607036	1.407138
C	-5.543335	-3.49094	-0.063036
H	-5.727012	-3.668673	1.002647
H	-6.427616	-3.005504	-0.491566
H	-5.440386	-4.470645	-0.542583
C	-4.064508	-2.581555	-1.842686
H	-3.144628	-2.057797	-2.107078
H	-4.026313	-3.590245	-2.271873
H	-4.905612	-2.052588	-2.30614

F) Optimized coordinates (Å) for **[1c]**$^{+}$

U	-0.030372	-0.275239	-0.725788
O	2.302774	-0.712022	-0.695496
N	-1.359231	1.880601	-0.486992
C	0.683955	3.068832	-0.977513
N	1.350594	1.911962	-0.500679
O	-2.195601	-0.732672	-0.663082
C	1.36261	4.182125	-1.493028
H	2.445975	4.170638	-1.557
O	-0.004231	-0.061494	-2.498575
C	0.651575	5.278898	-1.975732
H	1.187479	6.128212	-2.387762
O	0.035402	-0.448159	1.049628
C	-0.745761	5.262973	-1.966366
H	-1.304408	6.101924	-2.369801
O	0.051926	-2.756071	-1.374214
H	-0.35369	-3.434912	-0.808662
H	-0.262454	-2.937529	-2.276478
C	-1.430833	4.151313	-1.478728
H	-2.514264	4.120289	-1.529314
C	-2.513605	1.992752	0.111766
H	-2.869069	3.00172	0.337909
C	2.497042	2.05592	0.084092
H	2.846146	3.068513	0.302177
C	-3.415315	0.940648	0.5018
C	-4.545004	1.33692	1.253589
H	-4.61767	2.377493	1.546988
C	-5.536667	0.42045	1.603709
C	-5.382311	-0.901455	1.107316
H	-6.160757	-1.615044	1.331752
C	-4.300105	-1.341352	0.347023
C	-3.263471	-0.404599	0.055025
C	3.42637	1.009853	0.475672
C	3.32219	-0.353339	-0.012242
C	4.417199	-1.280001	0.265072
C	5.442015	-0.843842	1.070218
H	6.245343	-1.527221	1.297774
C	5.517064	0.478774	1.617753
C	4.499163	1.399861	1.262017
H	4.54646	2.427055	1.602263

C	-4.229342	-2.804849	-0.141968
C	4.414704	-2.705152	-0.318096
H	-2.098575	-2.99078	0.345013
C	-0.728284	3.049207	-0.970517
C	7.59037	-0.114883	2.79986
H	8.255238	0.353556	3.522724
H	7.153532	-1.007607	3.256803
H	8.177164	-0.40996	1.923125
C	-7.788524	-0.110473	2.438402
H	-7.52661	-1.093093	2.84593
H	-8.538297	0.325756	3.10088
H	-8.248706	-0.260849	1.44839
C	5.699915	-3.477748	0.044436
H	6.601685	-2.980166	-0.330875
H	5.805655	-3.625836	1.125395
H	5.656863	-4.469859	-0.416547
C	4.333743	-2.639976	-1.864551
H	3.426275	-2.138357	-2.204269
H	5.200383	-2.109912	-2.276797
H	4.3381	-3.657541	-2.271963
C	3.214715	-3.505265	0.247191
H	3.258494	-3.551749	1.341613
H	2.26132	-3.067635	-0.04904
H	3.251732	-4.532393	-0.134792
C	-3.035297	-3.516921	0.538515
H	-2.945145	-4.545851	0.168206
H	-3.175346	-3.56052	1.624748
C	-5.498469	-3.608449	0.211367
H	-5.654974	-3.685162	1.293317
H	-6.398347	-3.174642	-0.239355
H	-5.39427	-4.62808	-0.175699
C	-4.074767	-2.852542	-1.681942
H	-3.166775	-2.346353	-2.013707
H	-4.036838	-3.895637	-2.019712
H	-4.932108	-2.374012	-2.170054
N	-6.627276	0.768866	2.400389
N	6.542953	0.842934	2.429379
C	-6.856011	2.179863	2.672419
H	-7.046192	2.76991	1.760434
H	-7.719071	2.280125	3.33307
H	-5.994074	2.619268	3.1872
C	6.63939	2.21317	2.944577
H	5.762518	2.46062	3.551301

H	7.527906	2.294896	3.567205
H	6.722594	2.931242	2.122483

G) TD-DFT excitation energies and oscillator strengths for **[1a]**$^{+}$

Excited State 1: 2.289-A 1.4272 eV 868.73 nm f=0.0866 <S**2>=1.060
174A ->176A 0.10277
170B ->175B -0.36788
172B ->175B -0.51971
173B ->175B 0.54044
173B ->176B 0.10202
174B ->175B -0.43765
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2361.98690811
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.186-A 1.9818 eV 625.61 nm f=0.0029 <S**2>=0.945
170B ->175B -0.30709
172B ->175B -0.31999
173B ->175B 0.15075
174B ->175B 0.85703

Excited State 3: 3.406-A 2.1721 eV 570.81 nm f=0.0018 <S**2>=2.650
171A ->187A -0.13755
173A ->177A -0.10332
173A ->181A -0.12943
174A ->176A 0.14762
174A ->177A -0.16342
174A ->179A -0.12173
174A ->181A -0.18958
175A ->176A -0.15226
175A ->177A 0.39365
175A ->181A 0.28475
175A ->188A 0.11057
170B ->175B 0.17867
172B ->177B 0.11239
172B ->181B -0.14960
173B ->176B 0.15665
173B ->177B 0.14359
173B ->179B -0.15685
173B ->181B -0.15873
174B ->175B 0.18521
174B ->176B -0.19254
174B ->177B -0.32378
174B ->179B 0.13400

174B ->181B 0.23800
174B ->188B -0.11993

Excited State 4: 2.190-A 2.3837 eV 520.12 nm f=0.0013 <S**2>=0.949
148B ->175B 0.18062
152B ->175B 0.17148
159B ->175B 0.11066
168B ->175B 0.77812
168B ->176B -0.11976
169B ->175B -0.16394
170B ->175B -0.27169
172B ->175B -0.10571
173B ->175B -0.23380

Excited State 5: 2.917-A 2.4779 eV 500.36 nm f=0.0179 <S**2>=1.877
172A ->176A -0.12380
173A ->176A -0.12359
174A ->176A 0.17330
175A ->177A -0.27793
168B ->175B 0.25978
170B ->175B 0.49407
172B ->176B -0.17454
173B ->175B 0.30508
173B ->176B 0.17641
174B ->177B 0.26581
174B ->181B -0.10677

Excited State 6: 3.500-A 2.5996 eV 476.93 nm f=0.0000 <S**2>=2.812
153A ->176A -0.24452
153A ->178A 0.27494
153A ->179A -0.23787
161A ->176A 0.12312
161A ->178A -0.13618
161A ->179A 0.11871
168A ->176A 0.10756
168A ->178A -0.11580
168A ->179A 0.10504
175A ->176A 0.20831
175A ->178A -0.20648
175A ->179A 0.17985
151B ->176B -0.25365
151B ->178B -0.12553
151B ->179B -0.19109
151B ->180B 0.10066
152B ->176B 0.14164
152B ->179B 0.10257

153B ->176B -0.15489
153B ->179B -0.11316
154B ->176B 0.10179
160B ->176B 0.13699
160B ->179B 0.10472
167B ->176B 0.13334
167B ->179B 0.10139
174B ->176B 0.23415
174B ->179B 0.16168

Excited State 7: 2.706-A 2.6391 eV 469.80 nm f=0.0161 <S**2>=1.580
153A ->177A -0.17712
173A ->176A 0.12069
174A ->176A -0.13100
175A ->176A 0.10147
175A ->177A 0.15134
151B ->177B 0.14145
168B ->175B 0.18531
171B ->175B 0.14415
172B ->175B 0.30960
172B ->176B 0.12794
173B ->175B 0.65376
174B ->175B 0.12163
174B ->177B -0.14242

Excited State 8: 3.329-A 2.6933 eV 460.34 nm f=0.0012 <S**2>=2.520
153A ->177A 0.31830
153A ->181A -0.16525
154A ->177A 0.10037
161A ->177A -0.15306
168A ->177A -0.11671
173A ->176A 0.11072
174A ->176A -0.10503
175A ->181A 0.22858
151B ->177B -0.25366
151B ->181B -0.13196
152B ->177B 0.14348
153B ->177B -0.16673
160B ->177B 0.13268
167B ->177B 0.11049
170B ->175B -0.15081
172B ->175B 0.20826
172B ->176B 0.15330
173B ->175B 0.24516
174B ->181B 0.20947

Excited State 9: 3.470-A 2.8882 eV 429.27 nm f=0.0059 <S**2>=2.760

153A ->179A	-0.12998
174A ->177A	0.26342
174A ->179A	0.11217
174A ->181A	0.26757
174A ->188A	-0.10425
175A ->177A	0.18078
175A ->178A	0.15603
175A ->179A	0.29026
175A ->181A	0.14090
175A ->187A	0.10430
175A ->188A	-0.12292
170B ->175B	0.14160
173B ->177B	-0.23532
173B ->179B	0.13739
173B ->181B	0.24637
174B ->176B	-0.11800
174B ->177B	-0.23141
174B ->178B	-0.19585
174B ->179B	0.26502
174B ->181B	0.16303
174B ->188B	0.11379

Excited State 10: 3.355-A 3.0368 eV 408.28 nm f=0.0150 <S**2>=2.564

153A ->177A	0.11875
153A ->178A	0.23815
153A ->179A	0.20000
153A ->181A	-0.12428
161A ->178A	-0.12759
161A ->179A	-0.10940
168A ->178A	-0.11947
168A ->179A	-0.10899
174A ->177A	0.16116
174A ->181A	0.13536
175A ->178A	-0.29003
175A ->179A	-0.25148
175A ->181A	0.16232
151B ->178B	-0.21204
152B ->178B	0.11639
153B ->178B	-0.12862
160B ->178B	0.11835
167B ->178B	0.12079
170B ->175B	0.13529
172B ->175B	-0.12399
173B ->177B	-0.12335
173B ->181B	0.12712

174B ->176B -0.18733
174B ->177B -0.21365
174B ->178B 0.24238
174B ->181B 0.16820

Excited State 11: 2.332-A 3.0761 eV 403.06 nm f=0.0370 <S**2>=1.109
175A ->176A -0.25792
175A ->177A 0.57723
167B ->177B 0.10834
170B ->175B -0.14211
172B ->175B 0.17233
174B ->176B 0.20865
174B ->177B 0.51252
174B ->178B 0.15624

Excited State 12: 2.582-A 3.1197 eV 397.43 nm f=0.0741 <S**2>=1.417
173A ->176A -0.14363
174A ->176A 0.18054
174A ->187A 0.10931
175A ->176A -0.10808
175A ->177A -0.27480
175A ->178A -0.12880
175A ->180A -0.10981
170B ->175B -0.44316
171B ->175B 0.26477
172B ->175B 0.47795
173B ->187B -0.10067
174B ->176B -0.17848
174B ->177B -0.18435
174B ->179B 0.10278

Excited State 13: 3.425-A 3.1937 eV 388.21 nm f=0.0048 <S**2>=2.683
153A ->180A -0.33033
161A ->180A 0.18296
168A ->180A 0.17948
175A ->178A 0.10120
175A ->179A -0.12260
175A ->180A 0.44569
175A ->181A 0.16814
151B ->180B 0.22330
152B ->180B -0.12721
153B ->180B 0.13869
160B ->180B -0.13326
167B ->180B -0.14094
170B ->175B -0.12171
172B ->175B 0.14273

174B ->178B -0.10124
174B ->179B -0.14775
174B ->180B -0.34112

Excited State 14: 2.149-A 3.2135 eV 385.82 nm f=0.0057 <S**2>=0.905
175A ->176A -0.45596
175A ->177A -0.17979
175A ->178A 0.24295
175A ->179A -0.31964
175A ->180A -0.10909
174B ->176B 0.48292
174B ->177B -0.28379
174B ->179B 0.27202
174B ->181B -0.13086

Excited State 15: 3.184-A 3.2739 eV 378.70 nm f=0.0456 <S**2>=2.285
170A ->176A 0.19937
171A ->177A -0.13654
171A ->181A -0.16401
172A ->176A -0.14644
172A ->185A -0.13484
173A ->185A -0.11121
174A ->176A 0.14395
174A ->187A -0.15612
175A ->181A -0.11081
175A ->188A 0.12547
154B ->175B -0.10703
164B ->175B 0.39023
170B ->176B -0.15997
171B ->177B -0.14120
171B ->181B 0.17221
172B ->175B 0.10722
172B ->184B 0.10892
172B ->185B -0.14377
173B ->176B 0.10971
173B ->186B 0.12381
173B ->187B 0.14426
174B ->176B -0.19919
174B ->188B -0.14153

Excited State 16: 2.140-A 3.3626 eV 368.71 nm f=0.0211 <S**2>=0.895
153A ->178A -0.11405
153A ->179A -0.13691
168A ->178A 0.10014
175A ->177A -0.12732
175A ->178A 0.42710

175A ->179A 0.35057
175A ->180A -0.13835
151B ->178B -0.19249
152B ->178B 0.10702
153B ->178B -0.12025
160B ->178B 0.12624
167B ->178B 0.14686
174B ->178B 0.47207
174B ->179B -0.31443
174B ->180B -0.13088

Excited State 17: 2.128-A 3.4277 eV 361.71 nm f=0.0173 <S**2>=0.883
153A ->180A -0.15329
168A ->180A 0.12433
175A ->178A 0.28747
175A ->179A -0.11680
175A ->180A 0.46479
151B ->178B -0.11558
151B ->180B -0.13234
160B ->180B 0.10196
167B ->180B 0.12875
174B ->176B -0.11873
174B ->178B 0.27365
174B ->179B 0.36878
174B ->180B 0.42053

Excited State 18: 2.964-A 3.4575 eV 358.60 nm f=0.0601 <S**2>=1.946
153A ->176A 0.10428
153A ->178A -0.10192
153A ->179A 0.11291
172A ->176A -0.17173
173A ->176A 0.13883
174A ->176A -0.13547
175A ->176A 0.29928
175A ->178A -0.12413
175A ->179A 0.18584
151B ->175B -0.10122
151B ->176B 0.10408
154B ->175B -0.12869
164B ->175B 0.45896
171B ->175B 0.12381
174B ->176B 0.35509
174B ->179B 0.11877
174B ->180B -0.14471

Excited State 19: 3.082-A 3.4967 eV 354.57 nm f=0.0480 <S**2>=2.125

153A ->178A 0.15289
173A ->176A 0.28720
174A ->176A -0.18695
174A ->177A -0.12472
175A ->176A -0.26487
175A ->177A -0.13137
175A ->178A 0.23488
175A ->179A -0.14019
175A ->180A -0.21963
164B ->175B 0.19958
171B ->175B 0.28328
172B ->175B -0.15379
174B ->176B -0.28430
174B ->177B 0.21010
174B ->178B -0.22599
174B ->181B 0.14215

Excited State 20: 2.445-A 3.5433 eV 349.91 nm f=0.0025 <S**2>=1.244
175A ->177A 0.10113
175A ->181A -0.13878
164B ->175B -0.15917
170B ->175B 0.13062
171B ->175B 0.79965
172B ->175B -0.27401
173B ->175B -0.14442
174B ->177B -0.14841
174B ->178B 0.15262

Excited State 21: 3.413-A 3.5942 eV 344.96 nm f=0.0089 <S**2>=2.662
153A ->177A 0.18306
153A ->179A -0.10666
171A ->181A 0.10088
174A ->176A -0.10033
175A ->177A 0.35620
175A ->178A 0.11162
175A ->179A -0.26555
175A ->181A -0.34616
151B ->177B -0.14005
164B ->175B 0.11482
171B ->175B -0.10719
171B ->181B -0.10336
174B ->176B -0.12378
174B ->177B -0.35245
174B ->179B -0.26387
174B ->181B -0.26019

Excited State 22: 3.035-A 3.7046 eV 334.68 nm f=0.0664 <S**2>=2.053

153A ->178A	-0.16912
153A ->179A	-0.14356
153A ->181A	0.10702
172A ->176A	-0.10729
173A ->176A	0.16050
174A ->176A	-0.20736
174A ->177A	0.12460
175A ->178A	-0.20196
175A ->179A	-0.33319
151B ->178B	0.17394
152B ->178B	-0.10549
173B ->176B	0.12039
173B ->177B	-0.16610
174B ->177B	0.10892
174B ->178B	0.36380
174B ->179B	0.10142
174B ->180B	-0.23965
174B ->181B	0.28473

Excited State 23: 2.704-A 3.7384 eV 331.65 nm f=0.1028 <S**2>=1.578

153A ->178A	-0.10579
153A ->179A	-0.17338
174A ->177A	0.11619
175A ->176A	-0.20222
175A ->178A	-0.22897
175A ->181A	0.48929
151B ->178B	0.11446
164B ->175B	0.12519
173B ->176B	-0.19944
174B ->178B	0.21597
174B ->179B	-0.35321
174B ->180B	0.24256
174B ->181B	-0.20573

Excited State 24: 2.713-A 3.8487 eV 322.14 nm f=0.0976 <S**2>=1.590

153A ->178A	-0.11382
153A ->179A	-0.14057
170A ->176A	0.10052
172A ->176A	0.17334
173A ->176A	-0.23090
174A ->176A	0.29201
174A ->177A	-0.34492
175A ->178A	-0.12658
175A ->179A	-0.18103
175A ->181A	-0.17665

175A ->188A -0.10078
164B ->175B 0.11202
172B ->176B 0.13816
173B ->176B -0.28679
173B ->177B 0.10121
174B ->181B 0.38456
174B ->188B 0.12161

Excited State 25: 3.391-A 3.8964 eV 318.21 nm f=0.0182 <S**2>=2.624
153A ->180A -0.27482
161A ->180A 0.10635
173A ->176A 0.12222
174A ->177A -0.16981
175A ->178A -0.19122
175A ->180A -0.33139
175A ->188A -0.11126
151B ->178B 0.12623
151B ->180B 0.18584
152B ->180B -0.10391
173B ->176B 0.23206
173B ->177B 0.12599
174B ->178B 0.26709
174B ->179B 0.15629
174B ->180B 0.27772
174B ->181B -0.17818
174B ->188B 0.10890

Excited State 26: 3.175-A 3.9200 eV 316.28 nm f=0.0378 <S**2>=2.270
153A ->180A 0.21398
174A ->177A -0.18038
175A ->180A 0.20882
175A ->181A 0.27606
175A ->188A -0.16004
151B ->179B -0.14072
151B ->180B -0.14716
164B ->175B -0.14830
173B ->176B 0.33229
173B ->177B 0.16086
173B ->188B 0.11646
174B ->179B -0.17347
174B ->180B -0.26323
174B ->188B 0.15066

Excited State 27: 2.885-A 4.0135 eV 308.92 nm f=0.0700 <S**2>=1.831
153A ->179A -0.14306
170A ->176A -0.14906

171A ->176A -0.12022
172A ->176A -0.14287
173A ->176A 0.31731
174A ->176A 0.19500
174A ->177A -0.25838
174A ->185A -0.11199
175A ->176A -0.28125
175A ->178A -0.22761
175A ->179A 0.12037
175A ->180A 0.21617
151B ->176B 0.10296
151B ->178B -0.10830
170B ->176B 0.10132
171B ->175B -0.14454
173B ->177B -0.24245
174B ->180B -0.17903

Excited State 28: 2.309-A 4.0449 eV 306.52 nm f=0.2247 <S**2>=1.082
174A ->176A 0.11218
174A ->177A 0.56008
175A ->176A -0.16092
175A ->178A -0.12824
175A ->180A 0.12526
175A ->181A -0.13517
173B ->176B 0.15681
173B ->177B 0.58362
173B ->181B -0.10486

Excited State 29: 2.403-A 4.0803 eV 303.86 nm f=0.0292 <S**2>=1.194
153A ->176A 0.10202
153A ->178A 0.16781
153A ->179A 0.30379
161A ->179A -0.13509
172A ->184A -0.10242
174A ->176A 0.26871
175A ->178A 0.14872
175A ->179A 0.23057
175A ->181A -0.11513
151B ->178B 0.21304
151B ->179B -0.14931
152B ->178B -0.12519
153B ->178B 0.12832
164B ->175B 0.14127
170B ->176B 0.10853
172B ->176B 0.11041
173B ->177B -0.11665

174B ->176B -0.12805
174B ->178B 0.27243

Excited State 30: 2.296-A 4.0873 eV 303.34 nm f=0.0520 <S**2>=1.068
153A ->176A 0.15405
153A ->178A -0.32559
161A ->178A 0.14598
172A ->176A 0.26319
173A ->176A -0.19160
175A ->176A 0.20404
175A ->178A -0.12517
175A ->179A -0.11993
175A ->181A 0.13496
151B ->176B -0.12866
151B ->178B -0.19723
152B ->178B 0.11669
153B ->178B -0.11103
164B ->175B 0.14596
170B ->176B 0.10081
173B ->176B 0.28870
173B ->178B 0.14138
174B ->176B -0.13655
174B ->178B -0.13328
174B ->181B -0.13985

H) TD-DFT excitation energies and oscillator strengths for **[1b]**$^{+}$

Excited State 1: 2.609-A 1.7268 eV 718.00 nm f=0.0544 <S**2>=1.452
156A ->160A 0.17292
158A ->160A 0.19424
151B ->159B -0.13459
154B ->159B -0.33088
156B ->159B 0.41910
156B ->160B 0.11100
157B ->159B 0.51438
157B ->160B 0.18396
157B ->163B -0.11383
158B ->159B -0.39665
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2276.60176400
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.243-A 2.0611 eV 601.55 nm f=0.0071 <S**2>=1.008
154B ->159B -0.20390
156B ->159B 0.23243
157B ->159B 0.18933

158B ->159B 0.87838
158B ->161B 0.10914

Excited State 3: 3.351-A 2.0890 eV 593.50 nm f=0.0063 <S**2>=2.558
155A ->171A 0.10529
157A ->161A -0.12024
157A ->165A 0.12126
158A ->161A -0.16308
158A ->165A 0.13862
159A ->160A -0.13108
159A ->161A 0.45163
159A ->165A -0.24953
159A ->172A 0.10973
154B ->159B 0.15774
156B ->159B -0.11699
156B ->165B 0.10060
157B ->159B -0.14036
157B ->160B 0.13231
157B ->161B 0.15030
157B ->163B -0.11521
157B ->165B -0.15354
158B ->159B 0.20822
158B ->160B -0.25452
158B ->161B -0.36703
158B ->163B 0.11936
158B ->165B 0.23076
158B ->172B -0.12243

Excited State 4: 3.165-A 2.4896 eV 498.00 nm f=0.0085 <S**2>=2.254
156A ->160A 0.18275
156A ->169A -0.11388
158A ->160A 0.28894
158A ->163A -0.11236
158A ->165A 0.13073
159A ->161A -0.28852
159A ->171A -0.10911
154B ->159B 0.41082
156B ->159B -0.14539
156B ->160B 0.12600
156B ->165B 0.10950
157B ->159B -0.12427
157B ->160B 0.23740
157B ->163B -0.17079
158B ->160B 0.10998
158B ->161B 0.28719

Excited State 5: 3.465-A 2.5556 eV 485.14 nm f=0.0003 <S**2>=2.752

137A ->162A	0.13759
139A ->162A	0.16328
142A ->162A	-0.14239
144A ->160A	-0.16939
144A ->162A	0.29674
144A ->163A	-0.15572
148A ->162A	-0.12309
152A ->162A	-0.15446
159A ->160A	0.21409
159A ->162A	-0.28139
159A ->163A	0.13321
139B ->160B	-0.13028
139B ->163B	-0.10372
142B ->160B	-0.24153
142B ->162B	-0.15894
142B ->163B	-0.18987
143B ->160B	-0.13201
143B ->163B	-0.10244
152B ->160B	0.11634
158B ->160B	0.25163
158B ->161B	-0.10512
158B ->162B	0.13792
158B ->163B	0.16196

Excited State 6: 3.475-A 2.6268 eV 472.00 nm f=0.0000 <S**2>=2.768

137A ->161A	0.11693
139A ->161A	0.14010
142A ->161A	-0.13212
144A ->161A	0.27062
144A ->163A	-0.12183
144A ->165A	0.13097
148A ->161A	-0.10839
152A ->161A	-0.13716
158A ->161A	0.13127
159A ->163A	0.26865
159A ->164A	-0.13014
159A ->165A	-0.29719
139B ->161B	-0.12751
142B ->161B	-0.24859
142B ->163B	-0.12763
142B ->165B	-0.11987
143B ->161B	-0.13382
152B ->161B	0.11546
158B ->162B	-0.12157
158B ->163B	0.27887

158B ->165B 0.29119

Excited State 7: 3.259-A 2.6984 eV 459.48 nm f=0.0067 <S**2>=2.405
144A ->161A -0.12420
156A ->160A 0.18709
157A ->161A 0.13727
157A ->165A -0.11074
158A ->160A 0.15280
158A ->161A 0.18230
158A ->165A -0.19130
158A ->171A 0.10624
159A ->161A 0.17024
159A ->163A 0.12787
159A ->172A -0.18263
142B ->161B 0.11923
150B ->159B 0.24834
151B ->159B -0.13846
154B ->159B 0.24263
156B ->160B 0.18013
156B ->163B -0.11417
157B ->161B -0.22610
157B ->165B 0.23243
158B ->161B -0.13016
158B ->163B 0.13105
158B ->171B 0.10517
158B ->172B 0.16646

Excited State 8: 2.201-A 2.7328 eV 453.70 nm f=0.0030 <S**2>=0.961
138B ->159B 0.21201
150B ->159B 0.75778
150B ->160B -0.11556
153B ->159B -0.17792
154B ->159B -0.33501
157B ->159B -0.20727

Excited State 9: 2.092-A 2.8975 eV 427.89 nm f=0.0640 <S**2>=0.844
157A ->160A -0.10344
158A ->160A 0.16756
159A ->160A -0.16738
159A ->161A 0.49095
150B ->159B -0.17853
154B ->159B -0.25084
156B ->159B 0.12995
157B ->159B -0.39014
158B ->160B 0.34640
158B ->161B 0.42003

Excited State 10: 2.234-A 2.9261 eV 423.72 nm f=0.0678 <S**2>=0.998

157A ->160A	0.11411
158A ->160A	-0.14361
159A ->161A	0.40329
150B ->159B	0.21298
151B ->159B	-0.17821
154B ->159B	0.29170
156B ->159B	-0.18274
157B ->159B	0.52781
158B ->160B	0.18055
158B ->161B	0.33811

Excited State 11: 3.401-A 2.9560 eV 419.44 nm f=0.0017 <S**2>=2.642

139A ->163A	-0.10803
142A ->163A	0.10789
144A ->162A	-0.15809
144A ->163A	-0.21627
144A ->165A	-0.12621
152A ->162A	0.10020
152A ->163A	0.15017
158A ->161A	-0.11454
159A ->160A	0.11976
159A ->162A	0.25178
159A ->163A	0.36517
159A ->165A	0.19915
139B ->162B	0.11379
142B ->162B	0.22472
142B ->163B	-0.10218
143B ->162B	0.11874
151B ->159B	0.10266
152B ->162B	-0.12697
157B ->159B	0.16057
158B ->162B	-0.30352
158B ->163B	0.17151
158B ->165B	-0.16301

Excited State 12: 2.676-A 3.0645 eV 404.58 nm f=0.1009 <S**2>=1.541

153A ->160A	0.18442
156A ->160A	-0.10667
156A ->169A	-0.10342
157A ->160A	-0.17434
158A ->160A	0.11955
159A ->164A	-0.14386
159A ->172A	-0.10269
151B ->159B	0.55422

152B ->159B -0.10707
154B ->159B -0.10323
154B ->160B 0.10454
156B ->159B -0.28415
157B ->159B 0.31774
157B ->170B -0.10260
158B ->162B 0.11772

Excited State 13: 2.055-A 3.0823 eV 402.25 nm f=0.0065 <S**2>=0.806
159A ->160A -0.41074
159A ->161A -0.16507
159A ->162A 0.36870
159A ->163A -0.29085
158B ->160B 0.41956
158B ->161B -0.34427
158B ->162B 0.11465
158B ->163B 0.30061
158B ->165B -0.14189

Excited State 14: 3.439-A 3.1075 eV 398.98 nm f=0.0069 <S**2>=2.707
137A ->164A -0.10984
139A ->164A -0.13810
142A ->164A 0.13599
144A ->164A -0.27607
148A ->164A 0.11565
152A ->164A 0.18742
159A ->164A 0.45235
159A ->165A -0.21885
139B ->164B 0.12080
142B ->164B 0.24495
143B ->164B 0.13579
151B ->159B 0.14544
152B ->164B -0.15664
158B ->162B -0.10730
158B ->163B -0.15460
158B ->164B -0.41519
158B ->165B 0.11112

Excited State 15: 2.890-A 3.2304 eV 383.80 nm f=0.0483 <S**2>=1.838
153A ->160A -0.10796
155A ->161A 0.12734
155A ->165A -0.13238
157A ->160A -0.30696
157A ->169A -0.11651
158A ->160A 0.41927
158A ->161A 0.15092

158A ->171A -0.14171
159A ->162A -0.15138
159A ->172A 0.14127
151B ->159B 0.14519
155B ->161B -0.11985
155B ->165B 0.13635
156B ->159B -0.22323
157B ->161B -0.13701
157B ->165B 0.10687
157B ->170B 0.12198
157B ->171B -0.11110
158B ->160B -0.12460
158B ->162B -0.19090
158B ->165B -0.13900
158B ->172B -0.14115

Excited State 16: 2.129-A 3.2515 eV 381.31 nm f=0.0326 <S**2>=0.883
144A ->163A -0.14843
152A ->163A 0.12864
159A ->162A 0.32375
159A ->163A 0.41756
159A ->164A -0.17425
159A ->165A 0.14348
142B ->162B -0.15234
152B ->162B 0.11825
158B ->161B -0.12009
158B ->162B 0.41254
158B ->163B -0.39135
158B ->164B -0.20793

Excited State 17: 2.081-A 3.3103 eV 374.54 nm f=0.0038 <S**2>=0.833
144A ->164A -0.14944
152A ->164A 0.14661
159A ->160A 0.11717
159A ->162A 0.26811
159A ->164A 0.52438
142B ->162B -0.12340
142B ->164B -0.14268
152B ->164B 0.13512
158B ->160B -0.14610
158B ->162B 0.34807
158B ->163B 0.20701
158B ->164B 0.45708

Excited State 18: 3.430-A 3.3680 eV 368.12 nm f=0.0015 <S**2>=2.692
137A ->162A -0.11681

139A ->162A -0.12612
144A ->160A 0.10817
144A ->162A -0.18983
157A ->160A -0.16318
159A ->160A 0.41190
159A ->161A 0.12875
159A ->162A -0.32251
159A ->163A 0.12759
142B ->160B 0.11492
142B ->161B -0.10725
158B ->160B 0.39881
158B ->161B -0.29983
158B ->162B 0.23261
158B ->163B 0.12021

Excited State 19: 3.017-A 3.4227 eV 362.24 nm f=0.0162 <S**2>=2.026
153A ->160A 0.15016
158A ->160A -0.19236
159A ->161A 0.25462
159A ->163A -0.25141
159A ->165A 0.26510
142B ->161B -0.10720
142B ->163B -0.10969
151B ->159B 0.28136
154B ->159B 0.25084
155B ->159B -0.14925
156B ->159B 0.38292
158B ->160B -0.12974
158B ->161B -0.17344
158B ->163B -0.17633
158B ->165B -0.17121

Excited State 20: 2.982-A 3.5037 eV 353.87 nm f=0.0010 <S**2>=1.973
144A ->161A -0.13137
155A ->161A 0.11391
155A ->165A -0.10087
157A ->160A -0.11184
159A ->161A -0.24636
159A ->165A -0.19702
151B ->159B 0.23819
154B ->159B 0.30576
155B ->159B -0.19059
156B ->159B 0.42193
158B ->161B 0.24981
158B ->163B 0.20246
158B ->165B 0.26393

Excited State 21: 2.085-A 3.5676 eV 347.53 nm f=0.1308 <S**2>=0.837

159A ->160A	0.15827
159A ->163A	-0.24905
159A ->165A	0.53254
154B ->159B	-0.10002
156B ->159B	-0.13636
157B ->161B	-0.12446
158B ->160B	-0.10804
158B ->163B	0.32411
158B ->164B	-0.27287
158B ->165B	0.47071

Excited State 22: 2.978-A 3.6154 eV 342.94 nm f=0.0486 <S**2>=1.966

144A ->162A	-0.10019
144A ->163A	-0.12576
156A ->160A	0.16383
157A ->160A	0.39470
157A ->161A	0.13063
157A ->162A	0.12001
158A ->160A	-0.20796
158A ->161A	0.15298
159A ->160A	-0.17418
159A ->162A	-0.28686
159A ->165A	-0.19314
139B ->162B	0.10678
142B ->162B	0.15422
151B ->159B	0.13709
154B ->159B	-0.16774
156B ->159B	-0.18736
157B ->160B	0.12510
157B ->161B	-0.19368
158B ->162B	0.30343

Excited State 23: 3.172-A 3.7018 eV 334.93 nm f=0.0408 <S**2>=2.265

137A ->163A	-0.13138
139A ->163A	-0.14300
144A ->162A	-0.12582
144A ->163A	-0.22570
144A ->165A	-0.10283
156A ->160A	-0.13473
157A ->160A	-0.27305
158A ->160A	0.13849
159A ->162A	-0.16849
159A ->163A	-0.30119
139B ->162B	0.10568

142B ->162B 0.15315
142B ->163B -0.12832
151B ->159B -0.18811
157B ->160B -0.20654
158B ->162B 0.27859
158B ->163B -0.18423
158B ->165B 0.23697

Excited State 24: 3.332-A 3.8318 eV 323.57 nm f=0.0076 <S**2>=2.526
137A ->164A 0.15154
139A ->164A 0.16899
142A ->164A -0.11280
144A ->164A 0.27219
148A ->164A -0.10999
157A ->160A -0.11046
158A ->160A -0.10503
158A ->161A 0.16033
159A ->160A 0.28371
159A ->162A 0.25543
159A ->163A -0.10251
159A ->164A 0.20714
159A ->165A -0.27506
139B ->164B -0.14425
142B ->163B -0.11809
142B ->164B -0.21273
143B ->164B -0.11428
156B ->159B -0.12925
158B ->162B -0.14114
158B ->163B -0.13967
158B ->164B -0.28432

Excited State 25: 3.216-A 3.8435 eV 322.58 nm f=0.0286 <S**2>=2.335
153A ->160A -0.12853
156A ->169A 0.15969
157A ->160A 0.13346
157A ->166A -0.15971
158A ->161A -0.27913
159A ->164A 0.10371
159A ->165A -0.10532
159A ->171A 0.13593
159A ->172A -0.19922
151B ->159B 0.23141
156B ->159B 0.11748
156B ->168B -0.13520
156B ->169B 0.11260
157B ->160B 0.29043

157B ->161B 0.16587
157B ->172B 0.11617
158B ->163B -0.11545
158B ->164B -0.13290
158B ->171B 0.12298
158B ->172B 0.17835

Excited State 26: 2.856-A 3.8751 eV 319.95 nm f=0.0512 <S**2>=1.789
144A ->164A 0.10553
153A ->160A 0.11777
157A ->160A 0.20412
157A ->166A 0.11173
158A ->160A 0.17880
159A ->160A -0.39464
159A ->162A -0.20896
159A ->163A 0.19560
159A ->164A 0.42004
159A ->165A 0.15319
139B ->164B -0.10764
142B ->162B -0.11071
142B ->164B -0.15952
155B ->159B 0.10370
156B ->159B 0.10123
157B ->160B -0.15273
158B ->162B -0.16445
158B ->164B -0.16871

Excited State 27: 2.383-A 3.9437 eV 314.39 nm f=0.0144 <S**2>=1.170
153A ->160A 0.10814
156A ->160A -0.17989
157A ->166A 0.16042
159A ->160A 0.12320
155B ->159B 0.64983
155B ->160B 0.10743
156B ->159B 0.20794
157B ->159B -0.13373
157B ->160B 0.26184
158B ->162B 0.14387
158B ->164B -0.11490
158B ->165B -0.11372

Excited State 28: 2.216-A 4.0137 eV 308.90 nm f=0.2190 <S**2>=0.978
156A ->160A -0.10440
158A ->161A 0.50852
158A ->162A 0.14188
159A ->160A -0.19191

159A ->163A 0.11333
159A ->164A 0.14938
159A ->165A 0.19223
142B ->162B 0.12631
155B ->159B -0.28651
157B ->160B 0.29500
157B ->161B 0.42544
157B ->165B -0.10383
158B ->162B 0.10797

Excited State 29: 2.179-A 4.0424 eV 306.71 nm f=0.1645 <S**2>=0.937
137A ->163A -0.12236
139A ->163A -0.13553
144A ->162A -0.11036
144A ->163A -0.22580
148A ->163A 0.10751
157A ->160A -0.15185
157A ->163A 0.10848
157A ->166A -0.11281
158A ->160A -0.17983
158A ->161A 0.32926
158A ->163A -0.16876
159A ->162A -0.10148
159A ->163A -0.19811
139B ->162B -0.14174
142B ->162B -0.21857
142B ->163B 0.15243
143B ->162B -0.12699
155B ->159B 0.31546
157B ->160B 0.14252
157B ->161B 0.20769
158B ->162B -0.23946

Excited State 30: 2.531-A 4.0692 eV 304.69 nm f=0.0119 <S**2>=1.352
137A ->162A 0.10763
139A ->162A 0.12365
144A ->162A 0.19837
144A ->163A 0.11139
153A ->160A -0.16564
157A ->166A -0.19656
158A ->160A -0.11268
158A ->162A 0.12392
158A ->166A 0.10763
159A ->160A -0.10883
159A ->162A 0.10877
159A ->163A 0.12698

159A ->165A 0.10072
139B ->162B 0.11314
142B ->162B 0.18844
143B ->162B 0.10369
151B ->159B 0.15397
155B ->159B 0.36906
157B ->160B -0.28128
158B ->160B 0.14565
158B ->163B -0.15033
158B ->164B 0.13372
158B ->165B 0.22828

I) TD-DFT excitation energies and oscillator strengths for **[1c]**$^{+}$

Excited State 1: 3.321-A 1.8044 eV 687.13 nm f=0.0062 <S**2>=2.507
165A ->169A -0.13211
165A ->173A 0.11069
167A ->168A -0.13897
167A ->169A 0.44554
167A ->171A 0.10793
167A ->173A -0.25118
164B ->167B 0.11284
165B ->167B 0.15917
165B ->168B -0.17668
165B ->171B 0.11425
166B ->167B 0.32284
166B ->168B -0.36614
166B ->169B -0.29843
166B ->171B 0.15955
166B ->173B 0.24140
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2315.45568017
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.412-A 1.9510 eV 635.49 nm f=0.0123 <S**2>=1.205
167A ->169A -0.24214
167A ->173A 0.13295
160B ->167B 0.10702
164B ->167B 0.13774
165B ->167B 0.20574
166B ->167B 0.84659
166B ->168B 0.16641
166B ->169B 0.13791
166B ->173B -0.12353

Excited State 3: 2.815-A 2.0878 eV 593.85 nm f=0.0831 <S**2>=1.732

164A ->168A 0.21495
165A ->168A 0.16038
166A ->168A 0.21430
167A ->169A -0.14661
160B ->167B 0.25370
163B ->167B 0.12670
164B ->167B 0.34907
164B ->168B -0.11073
164B ->169B 0.12569
165B ->167B 0.42024
165B ->168B -0.18992
165B ->171B 0.12420
166B ->167B -0.39216
166B ->169B 0.14795

Excited State 4: 2.206-A 2.3802 eV 520.90 nm f=0.2310 <S**2>=0.967
161A ->168A -0.13493
166A ->168A 0.18251
162B ->167B 0.89565

Excited State 5: 3.054-A 2.4940 eV 497.13 nm f=0.0512 <S**2>=2.082
165A ->169A 0.24853
165A ->173A -0.21136
166A ->168A -0.25778
166A ->169A 0.10619
167A ->171A 0.15261
167A ->179A 0.10904
160B ->167B 0.31032
162B ->167B 0.10062
164B ->167B 0.24742
164B ->173B 0.11184
165B ->167B 0.30340
165B ->168B 0.23898
165B ->169B 0.12680
165B ->171B -0.16146
165B ->173B -0.17842
166B ->168B -0.13116
166B ->169B -0.12629
166B ->171B 0.14852
166B ->173B 0.10664
166B ->178B -0.10578
166B ->181B -0.10836

Excited State 6: 3.448-A 2.5081 eV 494.33 nm f=0.0005 <S**2>=2.723
148A ->168A 0.14958
148A ->170A -0.28452

148A ->171A 0.12136
153A ->170A 0.12696
154A ->170A 0.11720
155A ->170A -0.16424
156A ->170A 0.11013
162A ->170A -0.10804
166A ->168A -0.10399
167A ->168A 0.27486
167A ->170A -0.33001
167A ->171A 0.11394
148B ->168B 0.14749
148B ->169B -0.10643
148B ->170B 0.10957
148B ->171B 0.11895
155B ->168B 0.10089
166B ->168B 0.23406
166B ->169B -0.21798
166B ->170B 0.15220
166B ->171B 0.15070

Excited State 7: 3.407-A 2.5517 eV 485.88 nm f=0.0085 <S**2>=2.651
148A ->169A -0.25395
148A ->171A 0.12632
148A ->173A -0.14043
153A ->169A 0.11414
154A ->169A 0.10769
155A ->169A -0.15027
156A ->169A 0.10694
162A ->169A -0.10406
166A ->168A 0.12112
166A ->169A 0.10428
167A ->169A -0.17536
167A ->171A 0.26811
167A ->172A -0.13241
167A ->173A -0.24190
148B ->168B 0.12111
148B ->169B 0.14409
148B ->171B 0.11324
148B ->173B 0.10261
153B ->169B -0.10084
155B ->169B 0.10143
160B ->167B -0.11273
165B ->167B -0.11610
166B ->169B 0.17590
166B ->171B 0.28219
166B ->173B 0.22316

Excited State 8: 2.194-A 2.6511 eV 467.67 nm f=0.0361 <S**2>=0.954

166A ->168A	0.17785
167A ->168A	-0.17320
167A ->169A	0.64939
165B ->168B	0.10306
166B ->168B	0.48661
166B ->169B	0.32994

Excited State 9: 3.008-A 2.7112 eV 457.30 nm f=0.0685 <S**2>=2.012

148A ->169A	0.11158
164A ->168A	0.14692
165A ->169A	0.15798
165A ->173A	-0.11846
165A ->179A	0.11822
166A ->168A	0.42167
167A ->169A	-0.13362
167A ->180A	-0.11480
167A ->181A	0.11682
148B ->169B	-0.11172
160B ->167B	-0.19904
164B ->167B	-0.11179
164B ->168B	-0.15952
164B ->171B	0.10530
165B ->167B	-0.19377
165B ->169B	0.14687
165B ->173B	-0.19097
165B ->178B	0.10185
166B ->168B	-0.19028
166B ->169B	-0.26961
166B ->171B	0.11872
166B ->181B	-0.13622

Excited State 10: 2.899-A 2.8570 eV 433.97 nm f=0.0059 <S**2>=1.851

148A ->171A	0.13168
155A ->171A	0.10487
162A ->171A	0.10725
166A ->168A	-0.12630
167A ->168A	0.39397
167A ->169A	0.10964
167A ->171A	0.47769
167A ->173A	0.21598
148B ->170B	-0.11126
165B ->168B	-0.10215
166B ->168B	-0.15950
166B ->169B	0.27957

166B ->170B -0.33059
166B ->172B 0.10235

Excited State 11: 2.721-A 2.8696 eV 432.05 nm f=0.0002 <S**2>=1.601
148A ->170A 0.10615
166A ->168A -0.10381
167A ->168A -0.25783
167A ->169A -0.12364
167A ->170A 0.47888
165B ->169B -0.12450
166B ->168B 0.31161
166B ->169B -0.35014
166B ->170B -0.11589
166B ->171B 0.33120
166B ->173B -0.21155

Excited State 12: 3.450-A 3.0021 eV 412.99 nm f=0.0018 <S**2>=2.726
148A ->172A 0.19387
153A ->172A -0.10132
155A ->172A 0.13986
162A ->172A 0.12429
163A ->172A -0.10583
166A ->168A 0.10241
166A ->172A -0.11322
167A ->168A 0.16487
167A ->170A 0.10662
167A ->172A 0.50362
167A ->173A -0.24083
148B ->172B -0.13349
153B ->172B 0.10170
155B ->172B -0.11084
161B ->172B -0.11110
166B ->168B 0.10279
166B ->169B -0.11663
166B ->170B -0.17887
166B ->171B -0.14536
166B ->172B -0.44437

Excited State 13: 2.873-A 3.0471 eV 406.90 nm f=0.0336 <S**2>=1.814
158A ->168A 0.10536
165A ->168A -0.18374
165A ->179A -0.13205
166A ->168A 0.48149
166A ->179A -0.11459
167A ->168A 0.13506
167A ->170A -0.16429

167A ->171A -0.13774
167A ->180A 0.11109
167A ->181A -0.11229
160B ->167B 0.13525
163B ->173B 0.10680
164B ->177B -0.10124
165B ->178B -0.15255
166B ->170B -0.21774
166B ->171B 0.14239
166B ->172B 0.15747
166B ->173B -0.15800
166B ->181B 0.13146

Excited State 14: 2.201-A 3.0720 eV 403.59 nm f=0.0423 <S**2>=0.961
162A ->171A 0.10564
166A ->168A 0.20267
167A ->170A 0.20004
167A ->171A 0.45956
167A ->172A -0.22431
167A ->173A 0.15943
166B ->169B -0.15736
166B ->170B 0.31335
166B ->171B -0.45826
166B ->172B -0.21782

Excited State 15: 2.389-A 3.1241 eV 396.86 nm f=0.0095 <S**2>=1.177
148A ->170A 0.14335
167A ->168A 0.35459
167A ->170A 0.19699
167A ->172A 0.37976
166B ->170B 0.53219
166B ->171B 0.24951
166B ->172B 0.29997
166B ->173B 0.12470

Excited State 16: 3.226-A 3.1439 eV 394.37 nm f=0.0018 <S**2>=2.352
148A ->168A 0.14050
148A ->170A -0.20230
148A ->171A 0.14138
148A ->172A 0.11278
167A ->168A -0.27197
167A ->170A 0.38801
167A ->172A 0.27701
148B ->168B 0.12277
148B ->171B 0.11178
166B ->168B -0.36192

166B ->169B 0.29092
166B ->172B 0.24723

Excited State 17: 3.343-A 3.2334 eV 383.45 nm f=0.0096 <S**2>=2.544
148A ->169A -0.23101
148A ->171A 0.10482
148A ->173A -0.11764
164A ->168A 0.10674
165A ->168A 0.11964
166A ->168A -0.21844
167A ->169A 0.34134
167A ->171A -0.19486
167A ->173A 0.33293
148B ->169B 0.14909
166B ->168B -0.12903
166B ->169B -0.29229
166B ->171B -0.18533
166B ->173B -0.27584

Excited State 18: 2.166-A 3.2714 eV 379.00 nm f=0.0025 <S**2>=0.923
158B ->167B -0.48401
159B ->167B 0.25369
160B ->167B -0.33095
163B ->167B -0.14236
164B ->167B -0.28201
165B ->167B 0.59314

Excited State 19: 2.066-A 3.2981 eV 375.93 nm f=0.1102 <S**2>=0.817
167A ->168A 0.13468
167A ->170A 0.15341
167A ->171A -0.25185
167A ->172A -0.10893
167A ->173A 0.55140
166B ->171B 0.25248
166B ->172B -0.34934
166B ->173B 0.49456

Excited State 20: 2.939-A 3.3676 eV 368.17 nm f=0.0155 <S**2>=1.909
164A ->168A 0.11363
165A ->168A 0.21086
165A ->169A 0.13547
166A ->168A -0.19577
166A ->170A -0.11017
166A ->176A 0.12396
167A ->168A -0.12390
167A ->170A -0.24486

158B ->167B 0.30661
160B ->167B -0.23550
162B ->167B 0.11820
163B ->167B -0.10884
164B ->167B -0.21684
165B ->167B 0.20982
165B ->169B 0.19736
165B ->173B -0.11225
166B ->170B 0.13897
166B ->171B 0.13210
166B ->181B 0.10547

Excited State 21: 2.403-A 3.4010 eV 364.56 nm f=0.0037 <S**2>=1.194
164A ->168A -0.12241
165A ->168A -0.15545
166A ->168A 0.14328
167A ->170A 0.12369
147B ->167B 0.10182
158B ->167B 0.62741
158B ->179B -0.10128
159B ->167B -0.17570
163B ->167B -0.10147
164B ->167B -0.17901
165B ->167B 0.39887
166B ->170B -0.10984

Excited State 22: 3.239-A 3.5119 eV 353.04 nm f=0.0180 <S**2>=2.373
148A ->170A 0.17141
148A ->171A 0.28552
153A ->171A -0.10352
155A ->171A 0.13262
161A ->168A -0.12148
164A ->168A -0.10391
165A ->168A -0.10757
166A ->168A 0.11287
166A ->171A -0.11468
166A ->176A -0.11339
167A ->168A -0.29956
167A ->170A -0.32189
167A ->171A -0.15562
145B ->170B -0.10589
148B ->170B -0.18276
148B ->171B 0.10392
153B ->170B 0.10371
166B ->170B 0.28931
166B ->171B -0.10718

166B ->173B 0.14451

Excited State 23: 2.961-A 3.5745 eV 346.86 nm f=0.0158 <S**2>=1.942
148A ->171A 0.15619
167A ->168A 0.45211
167A ->170A 0.26950
167A ->171A -0.35189
167A ->172A -0.35143
167A ->173A -0.36389
148B ->170B -0.10245
148B ->171B 0.11644
166B ->169B 0.10153
166B ->170B 0.14058
166B ->171B -0.12267

Excited State 24: 3.167-A 3.6943 eV 335.61 nm f=0.0001 <S**2>=2.258
148A ->172A -0.12149
161A ->168A 0.25603
164A ->176A -0.10523
165A ->168A 0.12809
165A ->169A -0.18644
165A ->176A -0.11990
166A ->169A -0.23710
166A ->170A -0.18494
166A ->176A 0.17399
167A ->172A 0.11562
167A ->180A -0.14369
167A ->181A 0.14108
167A ->182A 0.11380
160B ->167B 0.12710
160B ->169B 0.10357
164B ->167B -0.20539
164B ->177B -0.10255
165B ->168B -0.10224
165B ->169B -0.16960
166B ->171B -0.14447
166B ->180B 0.11138
166B ->181B -0.17462

Excited State 25: 3.384-A 3.6999 eV 335.10 nm f=0.0004 <S**2>=2.613
148A ->172A 0.34371
148A ->173A -0.18230
153A ->172A -0.11411
154A ->172A -0.10503
155A ->172A 0.14571
158A ->172A -0.11942

166A ->170A -0.11632
166A ->172A -0.16416
167A ->172A -0.36521
167A ->173A 0.13603
145B ->172B -0.13922
148B ->172B -0.24787
149B ->172B 0.10486
153B ->172B 0.13746
154B ->172B 0.11417
155B ->172B -0.12783
166B ->170B 0.13907
166B ->172B 0.25967
166B ->173B -0.10758

Excited State 26: 2.771-A 3.8478 eV 322.22 nm f=0.0088 <S**2>=1.670
148A ->171A 0.11240
166A ->170A -0.10761
166A ->171A -0.16548
166A ->172A -0.10686
148B ->170B 0.10667
160B ->167B -0.15058
165B ->167B 0.11393
165B ->168B 0.26481
165B ->171B -0.10313
166B ->168B 0.24337
166B ->169B -0.22672
166B ->170B -0.30639
166B ->171B -0.22316
166B ->172B 0.35423
166B ->173B 0.35708

Excited State 27: 2.263-A 3.8592 eV 321.27 nm f=0.1103 <S**2>=1.030
158A ->169A 0.10710
166A ->169A 0.73732
166A ->171A -0.20682
166A ->173A 0.20268
148B ->169B -0.10242
160B ->167B 0.12915
164B ->167B -0.15773
165B ->168B -0.10168
165B ->169B -0.20047
166B ->173B 0.11305

Excited State 28: 2.472-A 3.8863 eV 319.03 nm f=0.0028 <S**2>=1.278
148A ->170A -0.14980
158A ->170A 0.11571

165A ->168A -0.14259
166A ->168A -0.13877
166A ->170A 0.49806
145B ->170B -0.10940
148B ->170B -0.19759
153B ->170B 0.10982
155B ->170B -0.11030
160B ->167B -0.19274
164B ->167B 0.13914
165B ->168B -0.25658
166B ->168B 0.16831
166B ->171B -0.13922
166B ->172B 0.14942
166B ->173B 0.20060

Excited State 29: 2.375-A 3.9255 eV 315.84 nm f=0.0807 <S**2>=1.160
148A ->171A -0.21710
164A ->168A 0.12592
165A ->168A 0.22345
166A ->171A 0.30819
166A ->172A 0.13813
167A ->171A 0.14140
148B ->170B -0.17647
148B ->171B 0.11303
153B ->170B 0.10394
155B ->170B -0.10214
160B ->167B 0.21177
161B ->167B -0.11491
164B ->167B -0.27541
165B ->168B 0.26618
166B ->171B -0.17171
166B ->172B 0.16691
166B ->173B 0.21436

Excited State 30: 2.248-A 3.9360 eV 315.00 nm f=0.0215 <S**2>=1.013
148A ->171A 0.13762
166A ->170A 0.45897
166A ->171A -0.27419
148B ->171B -0.11178
160B ->167B 0.32939
161B ->167B -0.16460
163B ->167B -0.16597
164B ->167B -0.36518
165B ->169B 0.23456

J) Optimized coordinates (Å) for **[1a]**$^{+}$ without H_2O

U	-0.077918	-0.274211	-0.878529
O	2.238034	-0.836697	-0.75393
N	-1.332869	1.851758	-0.543332
C	0.739941	3.033154	-0.939931
N	1.389162	1.840569	-0.544766
O	-2.238165	-0.711314	-0.971419
C	1.434216	4.176038	-1.372508
H	2.51636	4.157262	-1.445207
O	0.040443	0.030445	-2.628323
C	0.739996	5.313993	-1.768041
H	1.287604	6.18347	-2.116997
O	-0.109638	-0.456089	0.888955
C	-0.659493	5.319821	-1.754963
H	-1.20423	6.19729	-2.088908
C	-1.362054	4.185708	-1.355733
H	-2.445654	4.175525	-1.406774
C	-2.48786	1.93002	0.067539
H	-2.822052	2.920849	0.384484
C	2.571899	1.927349	-0.009646
H	2.958776	2.919466	0.230233
C	-3.399364	0.862946	0.368628
C	-4.512812	1.187145	1.182925
H	-4.564603	2.192376	1.587513
C	-5.499042	0.259572	1.462236
C	-5.362259	-1.014242	0.85913
H	-6.140219	-1.740729	1.058009
C	-4.312272	-1.400883	0.02691
C	-3.282906	-0.441286	-0.202269
C	3.486847	0.854163	0.316086
C	3.293294	-0.526375	-0.122955
C	4.328589	-1.523499	0.155964
C	5.428742	-1.095851	0.868376
H	6.201628	-1.815485	1.101178
C	5.626503	0.240575	1.324003
C	4.639828	1.193873	1.015244
H	4.77034	2.224083	1.324412
C	-6.711153	0.553857	2.36295
C	-4.26562	-2.80468	-0.615012
C	4.17269	-2.975751	-0.319307
C	6.891594	0.585031	2.108011
C	-6.677336	1.987378	2.926127
H	-7.552625	2.15161	3.564092

H	-6.704133	2.739987	2.129646
H	-5.784593	2.164299	3.53713
C	-6.720049	-0.433056	3.555168
H	-7.585065	-0.237502	4.199968
H	-5.812676	-0.324481	4.160432
H	-6.781579	-1.47546	3.22456
C	-8.016326	0.384739	1.54846
H	-8.887133	0.581963	2.185076
H	-8.121424	-0.629414	1.14834
H	-8.046258	1.084356	0.705115
C	-5.509848	-3.64522	-0.259622
H	-6.437637	-3.17215	-0.600996
H	-5.591725	-3.831606	0.817354
H	-5.435764	-4.619108	-0.755744
C	-4.224295	-2.677592	-2.158011
H	-4.186952	-3.674865	-2.613085
H	-3.353931	-2.112286	-2.49661
H	-5.12563	-2.174104	-2.527206
C	-3.028406	-3.587471	-0.10905
H	-3.056886	-3.6959	0.9815
H	-2.091647	-3.094263	-0.378588
H	-3.019842	-4.592854	-0.547299
C	2.934937	-3.623179	0.356286
H	2.006766	-3.107058	0.103556
H	3.04293	-3.624007	1.446717
H	2.846889	-4.664107	0.025479
C	5.401492	-3.830815	0.052495
H	5.546109	-3.899471	1.136488
H	6.322597	-3.447291	-0.400568
H	5.250031	-4.848224	-0.321551
C	4.028219	-3.017261	-1.863418
H	3.938137	-4.059779	-2.188585
H	4.913782	-2.590304	-2.347575
H	3.14839	-2.473177	-2.211095
C	6.950606	2.068929	2.5169
H	6.110268	2.351002	3.161021
H	6.962814	2.734338	1.646367
H	7.871208	2.249656	3.080873
C	6.936268	-0.281995	3.393993
H	6.946481	-1.353524	3.171836
H	6.075353	-0.073947	4.038394
H	7.847723	-0.048762	3.955191
C	8.130504	0.267865	1.228435

H	8.182357	-0.788927	0.948773
H	9.04129	0.509704	1.786944
H	8.124409	0.864718	0.30996
C	-0.6769	3.036541	-0.936197

K) Optimized coordinates (Å) for **[1b]**$^{+}$ without H_2O

U	-0.067999	0.096563	-0.685498
O	2.255017	-0.650247	-0.648548
N	-1.335922	1.984338	-0.124657
C	0.724066	3.205634	-0.435019
N	1.377763	1.980416	-0.143232
O	-2.223236	-0.532297	-0.789522
C	1.41473	4.376517	-0.780165
H	2.49676	4.363382	-0.858288
O	0.029322	0.39926	-2.394224
C	0.715083	5.542548	-1.080369
H	1.259651	6.437883	-1.362624
O	-0.075128	-0.489884	1.050986
C	-0.682683	5.545013	-1.057479
H	-1.23144	6.444456	-1.318521
C	-1.380745	4.380921	-0.742252
H	-2.464754	4.371443	-0.785418
C	-2.481705	2.000508	0.498873
H	-2.829977	2.957011	0.896427
C	2.543829	2.020017	0.419023
H	2.927859	2.984915	0.757473
C	-3.376349	0.893025	0.720464
C	-4.466843	1.131584	1.580324
H	-4.562146	2.08295	2.094744
C	-5.423833	0.150343	1.780945
C	-5.31149	-1.064927	1.081246
H	-6.075059	-1.814612	1.232421
C	-4.265406	-1.344677	0.19439
C	-3.256662	-0.353765	0.029688
C	3.45637	0.911574	0.653815
C	3.290492	-0.405689	0.048144
C	4.331368	-1.422287	0.230651
C	5.412572	-1.099692	1.025299
H	6.188092	-1.83277	1.193108
C	5.549679	0.17438	1.632438
C	4.573459	1.175997	1.419942
H	4.729606	2.149702	1.872783

C	-4.22016	-2.684441	-0.573041
C	4.21048	-2.799491	-0.439529
H	-2.039397	-2.955348	-0.444365
C	-0.689026	3.205406	-0.420505
O	-6.434065	0.451368	2.649935
O	6.569031	0.533908	2.406036
C	7.634947	-0.391989	2.696107
H	8.314235	0.153725	3.348522
H	7.244559	-1.273049	3.212333
H	8.149467	-0.680907	1.775692
C	-7.455954	-0.515489	2.87043
H	-7.04927	-1.442596	3.293066
H	-8.141634	-0.063225	3.588465
H	-7.999807	-0.744905	1.945608
C	5.431688	-3.691243	-0.13523
H	6.366919	-3.248812	-0.496459
H	5.533652	-3.903216	0.935189
H	5.304438	-4.650422	-0.64689
C	4.128219	-2.627904	-1.978989
H	3.257437	-2.043947	-2.281531
H	5.028049	-2.134675	-2.363763
H	4.060504	-3.616019	-2.447575
C	2.95315	-3.538058	0.0894
H	3.007084	-3.670969	1.175711
H	2.031882	-3.0036	-0.147773
H	2.900419	-4.531644	-0.369481
C	-2.955533	-3.486461	-0.17895
H	-2.950722	-4.452285	-0.69851
H	-2.939215	-3.683434	0.89939
C	-5.438986	-3.576805	-0.258246
H	-5.48397	-3.860003	0.799758
H	-6.384998	-3.0943	-0.52903
H	-5.363763	-4.501384	-0.84088
C	-4.227657	-2.416614	-2.098341
H	-3.380412	-1.800552	-2.405718
H	-4.180444	-3.367594	-2.642784
H	-5.150723	-1.905171	-2.395751

L) Optimized coordinates (Å) for **[1c]**$^{+}$ without H_2O

U	-0.047755	-0.248703	-0.789369
O	2.253761	-0.774937	-0.750534
N	-1.345276	1.866082	-0.448511

C	0.709344	3.064764	-0.867066
N	1.36845	1.873163	-0.466424
O	-2.199882	-0.724561	-0.830104
C	1.394995	4.203908	-1.311464
H	2.477729	4.188261	-1.383652
O	0.015924	0.042315	-2.549977
C	0.691178	5.337611	-1.712287
H	1.232788	6.208159	-2.06861
O	-0.037686	-0.415124	0.986142
C	-0.70622	5.335477	-1.692609
H	-1.258639	6.206404	-2.031519
C	-1.399499	4.199537	-1.278369
H	-2.483598	4.181845	-1.321573
C	-2.492555	1.932391	0.171923
H	-2.847865	2.921856	0.471382
C	2.525318	1.963061	0.110077
H	2.898125	2.956663	0.370244
C	-3.378362	0.847778	0.508131
C	-4.479867	1.172832	1.332464
H	-4.548861	2.186184	1.709673
C	-5.446002	0.218409	1.654122
C	-5.306657	-1.059445	1.047182
H	-6.071064	-1.795309	1.247763
C	-4.257705	-1.425369	0.20563
C	-3.240898	-0.458861	-0.04672
C	3.434438	0.881236	0.453741
C	3.284848	-0.467563	-0.057759
C	4.336672	-1.443567	0.202161
C	5.390536	-1.056997	0.995058
H	6.165148	-1.776295	1.212362
C	5.523896	0.257304	1.552498
C	4.531603	1.219038	1.231225
H	4.62328	2.237741	1.586989
C	-4.20828	-2.830893	-0.434147
C	4.256471	-2.861954	-0.392584
H	-2.028764	-3.088264	-0.248798
C	-0.704296	3.058799	-0.853744
C	7.623514	-0.41058	2.643269
H	8.366474	0.048148	3.292284
H	7.200748	-1.280618	3.15552
H	8.118088	-0.739581	1.723749
C	-7.642308	-0.412519	2.565527
H	-7.341935	-1.414486	2.891688

H	-8.361645	-0.035644	3.294598
H	-8.153414	-0.506544	1.5939
C	5.49049	-3.710377	-0.02311
H	6.421882	-3.267507	-0.394084
H	5.581357	-3.862943	1.058482
H	5.391814	-4.698285	-0.484411
C	4.198981	-2.777093	-1.939403
H	3.327324	-2.21968	-2.286569
H	5.099968	-2.293667	-2.334701
H	4.149716	-3.788916	-2.357829
C	3.007691	-3.601351	0.151941
H	3.042375	-3.672693	1.245108
H	2.079339	-3.102622	-0.131913
H	2.984554	-4.620286	-0.251327
C	-2.949844	-3.595332	0.046178
H	-2.937615	-4.602803	-0.387529
H	-2.950781	-3.69866	1.137701
C	-5.43255	-3.690082	-0.054999
H	-5.492772	-3.874449	1.023814
H	-6.373619	-3.233237	-0.381828
H	-5.351556	-4.664262	-0.549665
C	-4.198128	-2.704138	-1.977641
H	-3.343557	-2.123512	-2.330037
H	-4.152167	-3.700571	-2.434147
H	-5.114529	-2.215789	-2.329906
N	-6.500041	0.490789	2.523618
N	6.578118	0.575224	2.346832
C	-6.726526	1.871733	2.922122
H	-6.96132	2.532183	2.071151
H	-7.560161	1.907546	3.625615
H	-5.845774	2.277098	3.433314
C	6.705467	1.919591	2.92103
H	5.815356	2.174459	3.503761
H	7.570107	1.941469	3.581109
H	6.846744	2.66686	2.132796

M) TD-DFT excitation energies and oscillator strengths for **[1a]**$^{+}$ without H_2O

Excited State 1: 2.282-A 1.3997 eV 885.79 nm f=0.0849 <S**2>=1.052
169A ->171A -0.10247
165B ->170B 0.37614
167B ->170B 0.52419
168B ->170B 0.53835

168B ->171B 0.10205
169B ->170B 0.43190
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2285.59403423
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.173-A 1.9455 eV 637.29 nm f=0.0027 <S**2>=0.930
165B ->170B -0.30003
167B ->170B -0.31339
168B ->170B -0.14753
169B ->170B 0.86553

Excited State 3: 3.400-A 2.1678 eV 571.93 nm f=0.0015 <S**2>=2.640
166A ->182A -0.13421
168A ->172A 0.10358
168A ->176A 0.13213
169A ->171A 0.16353
169A ->172A -0.16031
169A ->174A 0.10821
169A ->176A -0.20314
170A ->171A -0.17495
170A ->172A 0.37476
170A ->176A 0.29458
170A ->184A -0.10003
165B ->170B 0.20385
167B ->172B 0.11174
167B ->176B -0.15301
168B ->171B -0.17179
168B ->172B -0.13908
168B ->174B 0.13301
168B ->175B -0.10709
168B ->176B 0.16506
169B ->170B 0.16561
169B ->171B -0.21237
169B ->172B -0.30648
169B ->176B 0.24329

Excited State 4: 2.405-A 2.4209 eV 512.15 nm f=0.0128 <S**2>=1.196
170A ->172A -0.17046
147B ->170B -0.10325
161B ->170B -0.29322
162B ->170B 0.18069
163B ->170B -0.38964
164B ->170B 0.12144
165B ->170B 0.48192
167B ->170B 0.16390

168B ->170B -0.42688
169B ->172B 0.16537

Excited State 5: 2.746-A 2.4790 eV 500.13 nm f=0.0088 <S**2>=1.635
167A ->171A -0.10473
168A ->171A 0.12792
169A ->171A 0.15754
170A ->172A -0.23384
143B ->170B 0.15654
147B ->170B 0.14788
161B ->170B 0.33145
162B ->170B -0.18434
163B ->170B 0.46635
164B ->170B -0.10135
165B ->170B 0.28812
167B ->171B -0.16239
168B ->171B -0.14609
169B ->172B 0.21581

Excited State 6: 3.497-A 2.5917 eV 478.39 nm f=0.0001 <S**2>=2.807
148A ->171A -0.25173
148A ->173A 0.17717
148A ->174A 0.32688
156A ->171A 0.12310
156A ->174A -0.15996
162A ->174A -0.11637
170A ->171A 0.21350
170A ->173A -0.12753
170A ->174A -0.24119
146B ->171B -0.22964
146B ->174B -0.19086
146B ->175B 0.10785
147B ->171B 0.13919
147B ->174B 0.11198
148B ->171B -0.14444
148B ->174B -0.11905
149B ->171B 0.10572
155B ->171B 0.12865
155B ->174B 0.10869
162B ->171B 0.10346
169B ->171B 0.23214
169B ->174B 0.17516

Excited State 7: 2.607-A 2.6097 eV 475.08 nm f=0.0134 <S**2>=1.449
148A ->172A 0.13662
168A ->171A 0.13375

169A ->171A 0.14028
170A ->172A -0.14642
161B ->170B -0.15592
163B ->170B -0.22017
166B ->170B -0.14920
167B ->170B -0.33183
167B ->171B -0.14963
168B ->170B 0.65295
169B ->170B -0.10847
169B ->172B 0.13571

Excited State 8: 3.396-A 2.6775 eV 463.06 nm f=0.0017 <S**2>=2.633
148A ->172A 0.35340
148A ->176A -0.19279
156A ->172A -0.16460
162A ->172A -0.10475
170A ->172A -0.11600
170A ->176A 0.24959
145B ->172B 0.10361
146B ->172B -0.24981
146B ->176B -0.13363
147B ->172B 0.15462
148B ->172B -0.16759
149B ->172B 0.11380
155B ->172B 0.13455
165B ->170B -0.16053
167B ->170B 0.16738
167B ->171B 0.13108
168B ->170B -0.15133
169B ->176B 0.21917

Excited State 9: 3.473-A 2.8631 eV 433.04 nm f=0.0049 <S**2>=2.766
148A ->173A -0.15138
148A ->174A 0.11142
169A ->172A 0.24068
169A ->176A 0.26108
170A ->172A 0.18488
170A ->173A 0.27661
170A ->174A -0.22010
170A ->176A 0.16906
170A ->183A -0.11007
146B ->173B 0.11934
165B ->170B 0.12989
168B ->172B 0.21260
168B ->176B -0.23695
169B ->171B -0.11940

169B ->172B -0.22865
169B ->173B -0.27250
169B ->174B 0.19286
169B ->176B 0.18457
169B ->183B 0.10631

Excited State 10: 3.364-A 2.9939 eV 414.12 nm f=0.0158 <S**2>=2.579
148A ->172A 0.12359
148A ->173A 0.29343
148A ->174A -0.10405
156A ->173A -0.15397
162A ->173A -0.12060
169A ->172A 0.18750
169A ->176A 0.17531
170A ->173A -0.34069
170A ->174A 0.13501
170A ->176A 0.15031
146B ->173B -0.20200
147B ->173B 0.12107
148B ->173B -0.12664
155B ->173B 0.11932
162B ->173B 0.10113
165B ->170B 0.15635
167B ->170B -0.14146
168B ->172B 0.14665
168B ->176B -0.15838
169B ->171B -0.18597
169B ->172B -0.19273
169B ->173B 0.25365
169B ->176B 0.16606

Excited State 11: 2.324-A 3.0516 eV 406.30 nm f=0.0369 <S**2>=1.100
169A ->171A 0.11064
170A ->171A -0.29932
170A ->172A 0.54613
170A ->175A -0.10816
165B ->170B -0.17335
166B ->170B 0.11258
167B ->170B 0.20628
169B ->171B 0.23388
169B ->172B 0.48430
169B ->173B 0.12764

Excited State 12: 2.555-A 3.0869 eV 401.65 nm f=0.0692 <S**2>=1.382
168A ->171A 0.14651
169A ->171A 0.17617

169A ->182A 0.10031
170A ->172A -0.31011
170A ->173A -0.12230
165B ->170B -0.42755
166B ->170B 0.25911
167B ->170B 0.46176
169B ->171B -0.21372
169B ->172B -0.22111
169B ->174B 0.10637

Excited State 13: 3.424-A 3.1625 eV 392.05 nm f=0.0042 <S**2>=2.682
148A ->175A -0.33718
156A ->175A 0.18540
162A ->175A 0.15137
170A ->174A 0.15778
170A ->175A 0.46580
170A ->176A 0.10717
146B ->174B 0.11890
146B ->175B 0.18903
147B ->175B -0.11757
148B ->175B 0.12164
155B ->175B -0.11844
162B ->175B -0.10389
165B ->170B -0.11880
167B ->170B 0.13992
169B ->174B -0.20489
169B ->175B -0.32852

Excited State 14: 2.138-A 3.1850 eV 389.28 nm f=0.0029 <S**2>=0.893
170A ->171A -0.43606
170A ->172A -0.20447
170A ->174A 0.39410
170A ->175A -0.11059
169B ->171B 0.47369
169B ->172B -0.31116
169B ->174B 0.27445
169B ->176B -0.12602

Excited State 15: 3.174-A 3.2607 eV 380.24 nm f=0.0507 <S**2>=2.269
165A ->171A 0.20811
165A ->174A 0.10785
166A ->172A -0.13541
166A ->176A -0.17376
167A ->171A -0.14295
167A ->180A -0.14039
168A ->180A 0.11878

169A ->171A 0.12709
169A ->182A -0.15655
169A ->183A 0.11200
170A ->176A -0.10757
170A ->184A -0.12560
149B ->170B -0.12328
159B ->170B 0.40495
165B ->171B -0.16065
165B ->174B 0.10228
165B ->175B -0.10347
166B ->170B 0.10311
166B ->172B -0.13756
166B ->176B 0.17915
167B ->179B 0.10132
167B ->180B -0.15226
168B ->171B -0.10168
168B ->181B -0.11824
168B ->182B -0.14961
169B ->171B -0.19492
169B ->183B -0.11753

Excited State 16: 2.146-A 3.3234 eV 373.07 nm f=0.0213 <S**2>=0.902
148A ->173A -0.15688
156A ->173A 0.10879
162A ->173A 0.10968
170A ->171A -0.11700
170A ->172A -0.15668
170A ->173A 0.53606
170A ->174A -0.14864
170A ->175A -0.13106
146B ->173B -0.19085
147B ->173B 0.11525
148B ->173B -0.12332
155B ->173B 0.13403
162B ->173B 0.13108
169B ->172B -0.11457
169B ->173B 0.53589
169B ->174B -0.16729
169B ->175B -0.10776

Excited State 17: 2.116-A 3.3928 eV 365.44 nm f=0.0073 <S**2>=0.870
148A ->175A -0.15321
156A ->175A 0.10677
162A ->175A 0.10695
170A ->173A 0.22083
170A ->174A 0.22342

170A ->175A 0.48121
146B ->174B -0.10188
146B ->175B -0.11070
169B ->171B -0.10374
169B ->173B 0.16851
169B ->174B 0.46292
169B ->175B 0.40111

Excited State 18: 3.169-A 3.4307 eV 361.40 nm f=0.0358 <S**2>=2.261
148A ->171A 0.12522
148A ->174A -0.16296
165A ->171A 0.10322
167A ->171A -0.13812
170A ->171A 0.36275
170A ->174A -0.26328
146B ->171B 0.11213
149B ->170B -0.11445
159B ->170B 0.38136
166B ->170B 0.11668
169B ->171B 0.40391
169B ->172B -0.15722
169B ->173B 0.11537
169B ->174B 0.18377
169B ->175B -0.13407

Excited State 19: 2.691-A 3.4669 eV 357.62 nm f=0.0540 <S**2>=1.561
167A ->171A -0.10170
168A ->171A -0.28084
169A ->171A -0.18303
169A ->172A -0.11920
170A ->171A -0.14842
170A ->172A -0.11233
170A ->173A 0.13681
170A ->174A 0.14407
170A ->175A -0.16976
159B ->170B 0.20343
166B ->170B 0.57390
167B ->170B -0.22698
168B ->170B 0.11021
169B ->171B -0.14877
169B ->172B 0.14921
169B ->173B -0.11111
169B ->176B 0.11941

Excited State 20: 2.681-A 3.5046 eV 353.78 nm f=0.0189 <S**2>=1.546
167A ->171A 0.12675

168A ->171A 0.12973
169A ->171A 0.11847
170A ->172A 0.14125
170A ->173A -0.10890
170A ->176A -0.17372
159B ->170B -0.27459
165B ->170B 0.11977
166B ->170B 0.63680
167B ->170B -0.21736
168B ->170B 0.10963
169B ->171B 0.11098
169B ->172B -0.20001
169B ->173B 0.19624
169B ->176B -0.15478

Excited State 21: 3.417-A 3.5668 eV 347.60 nm f=0.0099 <S**2>=2.669
148A ->172A -0.18661
148A ->176A 0.10767
166A ->176A -0.10093
170A ->172A -0.35870
170A ->174A -0.23345
170A ->176A 0.37984
146B ->172B 0.12769
159B ->170B -0.12300
166B ->176B 0.10087
169B ->171B 0.12248
169B ->172B 0.35372
169B ->174B 0.22073
169B ->175B -0.13433
169B ->176B 0.29099

Excited State 22: 3.378-A 3.6460 eV 340.06 nm f=0.0173 <S**2>=2.602
148A ->173A -0.28636
148A ->174A 0.15103
167A ->171A -0.10388
168A ->171A -0.12609
169A ->171A -0.16976
169A ->172A 0.10540
170A ->173A -0.37056
170A ->174A 0.24589
146B ->173B 0.21878
147B ->173B -0.14481
148B ->173B 0.12363
149B ->173B -0.11256
168B ->172B 0.10775
169B ->173B 0.45014

169B ->175B -0.11391
169B ->176B 0.13925

Excited State 23: 2.280-A 3.7138 eV 333.84 nm f=0.1523 <S**2>=1.050
169A ->171A 0.12376
170A ->171A -0.18209
170A ->174A -0.14693
170A ->175A 0.13779
170A ->176A 0.47604
159B ->170B 0.13357
167B ->171B 0.12837
168B ->171B 0.24089
169B ->173B 0.11672
169B ->174B -0.31101
169B ->175B 0.36380
169B ->176B -0.31163

Excited State 24: 2.537-A 3.8204 eV 324.53 nm f=0.1113 <S**2>=1.359
148A ->173A -0.12341
165A ->171A 0.10150
167A ->171A 0.18877
168A ->171A 0.24633
169A ->171A 0.33106
169A ->172A -0.31587
170A ->173A -0.11598
170A ->174A 0.10958
170A ->176A -0.24288
159B ->170B 0.12279
167B ->171B 0.15011
168B ->171B 0.32635
169B ->176B 0.38483
169B ->183B 0.10109

Excited State 25: 3.499-A 3.8473 eV 322.26 nm f=0.0021 <S**2>=2.810
148A ->175A -0.35163
156A ->175A 0.11411
170A ->173A -0.16716
170A ->174A -0.14981
170A ->175A -0.39449
146B ->174B 0.16569
146B ->175B 0.19835
147B ->174B -0.10571
147B ->175B -0.12893
148B ->175B 0.10795
149B ->175B -0.10356
169B ->173B 0.16957

169B ->174B 0.29065
169B ->175B 0.32990

Excited State 26: 3.167-A 3.9021 eV 317.74 nm f=0.0298 <S**2>=2.257
148A ->175A -0.10054
167A ->180A 0.10417
168A ->180A -0.13034
169A ->172A 0.26462
169A ->183A 0.10365
170A ->176A -0.19589
170A ->182A -0.10317
170A ->183A 0.18059
170A ->184A -0.13766
159B ->170B 0.14344
167B ->180B 0.12661
168B ->171B 0.39225
168B ->172B 0.19490
168B ->183B 0.13068
169B ->173B -0.16050
169B ->175B 0.13168
169B ->176B 0.11233
169B ->183B -0.18256
169B ->184B 0.10914

Excited State 27: 2.724-A 3.9822 eV 311.35 nm f=0.0393 <S**2>=1.605
148A ->173A 0.19717
148A ->174A -0.17811
165A ->171A 0.13077
166A ->171A 0.11350
167A ->171A 0.15383
168A ->171A 0.31160
169A ->171A -0.14610
169A ->172A 0.19255
170A ->171A 0.28465
170A ->173A 0.25430
170A ->174A 0.13863
170A ->175A -0.16935
146B ->173B 0.16421
147B ->173B -0.10432
148B ->173B 0.10012
166B ->170B 0.12522
168B ->172B -0.15281
169B ->173B 0.16479
169B ->175B 0.14010
169B ->176B 0.10939

Excited State 28: 2.475-A 4.0305 eV 307.61 nm f=0.0596 <S**2>=1.281

148A ->173A	0.31187
148A ->174A	-0.15064
156A ->173A	-0.11970
166A ->171A	-0.10429
168A ->171A	-0.15771
169A ->171A	0.27913
170A ->171A	-0.15627
170A ->173A	0.17455
170A ->174A	-0.27815
170A ->175A	0.14601
170A ->176A	-0.20980
146B ->173B	0.23180
147B ->173B	-0.14875
148B ->173B	0.13902
149B ->173B	-0.11829
167B ->171B	0.11285
169B ->173B	0.26178

Excited State 29: 2.237-A 4.0337 eV 307.37 nm f=0.2606 <S**2>=1.001

169A ->172A	0.60219
170A ->171A	-0.11893
170A ->173A	-0.10973
170A ->176A	-0.11294
168B ->171B	-0.19759
168B ->172B	-0.58628
168B ->176B	0.12623

Excited State 30: 2.489-A 4.0718 eV 304.49 nm f=0.0172 <S**2>=1.299

148A ->171A	0.18226
148A ->173A	-0.19355
148A ->174A	-0.18748
165A ->171A	-0.10149
167A ->171A	0.24916
168A ->171A	0.13554
169A ->171A	0.17602
169A ->174A	-0.12311
170A ->171A	0.20438
146B ->171B	-0.13626
159B ->170B	0.17913
165B ->171B	0.13828
168B ->171B	-0.23258
168B ->172B	0.16386
168B ->173B	-0.10795
169B ->171B	-0.17547
169B ->176B	-0.13509

N) TD-DFT excitation energies and oscillator strengths for **[1b]**$^{+}$ without H_2O

Excited State 1: 2.602-A 1.7200 eV 720.84 nm f=0.0528 <S**2>=1.442
151A ->155A 0.17378
153A ->155A 0.19527
146B ->154B -0.13915
149B ->154B -0.33298
151B ->154B -0.42123
151B ->155B -0.12161
151B ->160B -0.10031
152B ->154B 0.51038
152B ->155B 0.18228
152B ->158B -0.11529
153B ->154B -0.40107
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2200.20860125
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.216-A 2.0287 eV 611.14 nm f=0.0068 <S**2>=0.978
153A ->155A 0.10386
149B ->154B -0.19405
151B ->154B -0.22310
152B ->154B 0.18158
153B ->154B 0.89131

Excited State 3: 3.365-A 2.0978 eV 591.03 nm f=0.0069 <S**2>=2.581
150A ->166A 0.10076
152A ->156A 0.11508
152A ->160A -0.12761
153A ->156A 0.16256
153A ->160A -0.15456
154A ->155A -0.14538
154A ->156A 0.44233
154A ->160A -0.28427
154A ->168A -0.11995
149B ->154B -0.17625
151B ->154B -0.13338
151B ->160B 0.10122
152B ->154B 0.15006
152B ->155B -0.11931
152B ->156B -0.15828
152B ->160B 0.15829
153B ->154B -0.13740
153B ->155B 0.23269
153B ->156B 0.38071

153B ->160B -0.25385
153B ->168B -0.11442

Excited State 4: 3.163-A 2.4718 eV 501.59 nm f=0.0086 <S**2>=2.251
151A ->155A 0.18197
151A ->164A -0.11635
153A ->155A 0.29746
153A ->158A -0.10877
153A ->160A 0.14579
154A ->156A 0.29351
154A ->166A 0.11197
149B ->154B 0.41511
151B ->154B 0.14623
151B ->155B -0.13655
151B ->160B -0.11363
152B ->154B -0.12529
152B ->155B 0.23241
152B ->158B -0.16055
152B ->159B 0.10729
153B ->156B 0.30178
153B ->160B -0.11872

Excited State 5: 3.468-A 2.5553 eV 485.20 nm f=0.0001 <S**2>=2.757
132A ->157A -0.11539
132A ->158A 0.11758
134A ->157A -0.12574
134A ->158A 0.12404
139A ->155A 0.18681
139A ->157A -0.24929
139A ->158A 0.24937
147A ->157A 0.11544
147A ->158A -0.12146
154A ->155A 0.21669
154A ->157A -0.21950
154A ->158A 0.21110
134B ->155B 0.13949
134B ->158B 0.12881
136B ->155B 0.11871
136B ->158B 0.11058
137B ->155B 0.22120
137B ->158B 0.20614
138B ->155B -0.14451
138B ->158B -0.13076
147B ->155B -0.11537
147B ->158B -0.10966
153B ->155B -0.25851

153B ->158B -0.19689

Excited State 6: 3.473-A 2.6219 eV 472.88 nm f=0.0001 <S**2>=2.766
132A ->156A -0.12421
134A ->156A -0.13557
139A ->156A -0.28252
139A ->158A 0.10749
139A ->160A -0.15610
147A ->156A 0.13181
153A ->156A -0.14249
154A ->157A 0.15050
154A ->158A 0.21985
154A ->160A -0.31303
134B ->156B 0.13494
136B ->156B 0.12211
137B ->156B 0.22615
137B ->160B 0.11441
138B ->156B -0.14168
147B ->156B -0.11222
152B ->156B 0.10914
153B ->157B 0.20692
153B ->158B -0.20181
153B ->160B -0.28862

Excited State 7: 3.309-A 2.6771 eV 463.14 nm f=0.0080 <S**2>=2.487
139A ->156A -0.15885
139A ->160A -0.10408
151A ->155A 0.18662
152A ->156A 0.13492
152A ->160A -0.11453
153A ->155A 0.15604
153A ->156A 0.17242
153A ->160A -0.20913
153A ->166A 0.10875
154A ->156A -0.18241
154A ->158A -0.12964
154A ->167A 0.15740
154A ->168A -0.12829
137B ->156B 0.12029
138B ->156B -0.10470
146B ->154B -0.13219
149B ->154B 0.30386
151B ->155B -0.17808
151B ->158B 0.11205
152B ->156B -0.21663
152B ->160B 0.24472

153B ->156B -0.14770
153B ->157B -0.10248
153B ->166B 0.10561
153B ->167B 0.13743
153B ->168B -0.12090

Excited State 8: 2.128-A 2.7832 eV 445.48 nm f=0.0089 <S**2>=0.882
133B ->154B 0.19712
145B ->154B 0.71479
145B ->155B -0.10946
148B ->154B -0.17293
149B ->154B -0.33125
151B ->154B -0.14251
152B ->154B -0.37564

Excited State 9: 2.108-A 2.8831 eV 430.04 nm f=0.0584 <S**2>=0.861
147A ->156A -0.10201
153A ->155A -0.13162
154A ->155A -0.17831
154A ->156A 0.52176
154A ->157A 0.14081
145B ->154B 0.24972
146B ->154B -0.10375
149B ->154B 0.18105
152B ->154B 0.25859
153B ->155B -0.34490
153B ->156B -0.47161

Excited State 10: 3.034-A 2.9032 eV 427.06 nm f=0.0278 <S**2>=2.051
139A ->157A 0.16230
139A ->158A 0.13254
154A ->155A 0.15421
154A ->156A -0.27752
154A ->157A 0.22266
154A ->158A 0.23670
154A ->160A 0.12649
134B ->157B -0.10739
137B ->156B -0.10689
137B ->157B -0.18339
138B ->157B 0.11428
145B ->154B 0.18769
146B ->154B -0.19796
147B ->157B 0.12192
149B ->154B 0.18507
152B ->154B 0.23801
152B ->156B -0.11196

153B ->156B 0.24205
153B ->157B 0.32490
153B ->160B 0.10804

Excited State 11: 2.686-A 2.9163 eV 425.15 nm f=0.0365 <S**2>=1.553
139A ->157A -0.16226
139A ->158A -0.10389
152A ->155A 0.11703
153A ->155A -0.14891
153A ->156A -0.10058
154A ->156A -0.20871
154A ->157A -0.25369
154A ->158A -0.17222
154A ->160A -0.10131
137B ->157B 0.13229
145B ->154B 0.31905
149B ->154B 0.21482
151B ->154B 0.18329
152B ->154B 0.49074
153B ->155B 0.12867
153B ->156B 0.18369
153B ->157B -0.18755

Excited State 12: 2.173-A 3.0427 eV 407.48 nm f=0.0104 <S**2>=0.930
154A ->155A 0.37575
154A ->156A 0.16823
154A ->157A -0.23855
154A ->158A 0.37833
146B ->154B -0.18999
153B ->155B 0.44122
153B ->156B -0.32042
153B ->158B 0.24382
153B ->159B -0.12413
153B ->160B -0.15123

Excited State 13: 2.643-A 3.0483 eV 406.73 nm f=0.0838 <S**2>=1.496
139A ->159A 0.11356
148A ->155A 0.14682
151A ->155A -0.10058
152A ->155A -0.15461
153A ->155A 0.14182
154A ->155A 0.20447
154A ->159A 0.23424
146B ->154B 0.47990
151B ->154B 0.29221
152B ->154B 0.31826

153B ->158B 0.20290
153B ->159B 0.10031

Excited State 14: 3.356-A 3.0818 eV 402.31 nm f=0.0199 <S**2>=2.566
132A ->159A 0.10644
134A ->159A 0.12472
139A ->159A 0.27324
147A ->159A -0.17423
154A ->159A 0.45367
154A ->160A -0.15956
134B ->159B -0.10928
137B ->158B -0.11399
137B ->159B -0.19017
138B ->159B 0.12555
146B ->154B -0.23532
147B ->159B 0.13333
151B ->154B -0.10461
152B ->154B -0.10517
153B ->158B 0.20916
153B ->159B 0.40086

Excited State 15: 2.167-A 3.2077 eV 386.51 nm f=0.0062 <S**2>=0.924
139A ->157A -0.10158
147A ->157A 0.11335
152A ->155A 0.14067
153A ->155A -0.17778
154A ->156A 0.12567
154A ->157A -0.47336
154A ->158A -0.25616
154A ->159A 0.15461
137B ->157B -0.18196
138B ->157B 0.11976
147B ->157B 0.15518
151B ->154B -0.12997
153B ->157B 0.53632
153B ->159B -0.15471

Excited State 16: 2.911-A 3.2229 eV 384.69 nm f=0.0656 <S**2>=1.868
139A ->158A -0.15564
148A ->155A -0.10035
150A ->156A -0.11884
150A ->160A 0.13617
152A ->155A -0.26158
152A ->164A -0.11065
153A ->155A 0.35640
153A ->156A 0.15632

153A ->160A -0.11097
153A ->166A -0.13863
154A ->155A 0.13542
154A ->157A -0.14541
154A ->158A -0.12605
154A ->160A -0.10956
154A ->167A -0.11067
154A ->168A 0.11271
146B ->154B 0.10157
150B ->156B 0.11987
150B ->160B -0.13881
151B ->154B 0.18545
152B ->165B 0.11703
152B ->166B -0.11514
153B ->155B -0.16310
153B ->157B 0.15845
153B ->158B -0.27768
153B ->160B -0.10723
153B ->167B -0.10716
153B ->168B 0.11467

Excited State 17: 2.112-A 3.2637 eV 379.89 nm f=0.0034 <S**2>=0.865
139A ->159A 0.15253
147A ->159A -0.14375
154A ->157A 0.27865
154A ->158A -0.11942
154A ->159A 0.52841
137B ->158B 0.10271
137B ->159B 0.10121
147B ->159B -0.11965
153B ->155B 0.16211
153B ->157B -0.21430
153B ->158B -0.35958
153B ->159B -0.43575

Excited State 18: 3.391-A 3.2991 eV 375.81 nm f=0.0062 <S**2>=2.624
139A ->155A -0.11052
139A ->157A 0.16846
139A ->158A -0.11374
152A ->155A 0.19490
153A ->155A -0.13125
154A ->155A 0.40323
154A ->156A 0.11687
154A ->157A -0.23397
154A ->158A 0.24445
137B ->155B -0.10702

153B ->155B -0.40123
153B ->156B 0.26028
153B ->157B -0.22146
153B ->158B -0.21028

Excited State 19: 3.271-A 3.3879 eV 365.96 nm f=0.0093 <S**2>=2.424
132A ->156A -0.10037
139A ->156A -0.14655
148A ->155A -0.11137
153A ->155A 0.16324
154A ->156A 0.33551
154A ->158A -0.23119
154A ->160A 0.35921
134B ->156B 0.10224
137B ->156B 0.12428
146B ->154B -0.19378
149B ->154B -0.16229
151B ->154B 0.24683
153B ->156B 0.28848
153B ->158B 0.18915
153B ->160B 0.27047

Excited State 20: 2.801-A 3.4696 eV 357.34 nm f=0.0031 <S**2>=1.711
139A ->156A 0.10079
154A ->156A -0.16452
154A ->160A -0.12405
146B ->154B -0.32201
149B ->154B -0.34271
150B ->154B -0.21196
151B ->154B 0.47241
152B ->156B 0.10447
153B ->156B -0.18011
153B ->158B -0.13225
153B ->159B 0.10590
153B ->160B -0.22173

Excited State 21: 2.079-A 3.5372 eV 350.51 nm f=0.1320 <S**2>=0.831
154A ->155A 0.12656
154A ->158A -0.23466
154A ->160A 0.56422
149B ->154B 0.10748
151B ->154B -0.14948
152B ->156B 0.10054
153B ->158B -0.25880
153B ->159B 0.35089
153B ->160B -0.46062

Excited State 22: 3.220-A 3.5455 eV 349.69 nm f=0.0120 <S**2>=2.342

132A ->157A	-0.12163
132A ->158A	-0.10762
134A ->157A	-0.12489
134A ->158A	-0.10669
139A ->157A	-0.21709
139A ->158A	-0.19296
151A ->155A	0.10770
152A ->155A	0.23363
152A ->157A	0.10560
153A ->155A	-0.12193
154A ->155A	0.15273
154A ->157A	0.34875
154A ->158A	0.12474
154A ->160A	0.17161
132B ->157B	0.12292
134B ->157B	0.16334
136B ->157B	0.12625
137B ->157B	0.21390
138B ->157B	-0.14057
149B ->154B	-0.17125
150B ->154B	-0.10792
151B ->154B	0.20963
153B ->157B	0.40468

Excited State 23: 2.860-A 3.6485 eV 339.82 nm f=0.0637 <S**2>=1.795

139A ->157A	0.10793
139A ->158A	0.11807
151A ->155A	0.19784
152A ->155A	0.41857
152A ->158A	-0.10690
153A ->155A	-0.21873
153A ->156A	0.13475
154A ->158A	-0.21937
146B ->154B	0.23073
149B ->154B	-0.12486
151B ->154B	0.14842
151B ->155B	-0.13949
152B ->155B	0.26011
152B ->156B	-0.16523
152B ->160B	0.10329
153B ->157B	-0.16361
153B ->158B	0.14142
153B ->160B	-0.17854

Excited State 24: 3.445-A 3.7547 eV 330.21 nm f=0.0021 <S**2>=2.717

132A ->159A	0.19100
133A ->159A	-0.11267
134A ->159A	0.19296
139A ->159A	0.34229
143A ->159A	-0.12088
154A ->155A	-0.13031
154A ->157A	-0.15539
154A ->158A	0.10882
154A ->159A	-0.35554
154A ->160A	0.17099
132B ->159B	-0.12992
134B ->158B	-0.11600
134B ->159B	-0.17574
136B ->159B	-0.13919
137B ->158B	-0.15854
137B ->159B	-0.23164
138B ->159B	0.14989
153B ->158B	-0.22721
153B ->159B	-0.31851

Excited State 25: 2.861-A 3.8309 eV 323.64 nm f=0.0291 <S**2>=1.797

150A ->155A	-0.10758
151A ->164A	0.10450
152A ->155A	0.24214
153A ->155A	0.19442
153A ->156A	-0.22056
154A ->155A	0.43730
154A ->157A	0.23854
154A ->158A	-0.24909
154A ->159A	-0.28211
154A ->160A	-0.17751
150B ->154B	-0.13715
151B ->154B	-0.19230

Excited State 26: 3.028-A 3.8397 eV 322.90 nm f=0.0477 <S**2>=2.043

148A ->155A	-0.13660
151A ->164A	0.15079
152A ->162A	-0.16433
153A ->156A	-0.21829
154A ->155A	-0.19759
154A ->158A	0.17180
154A ->160A	0.13141
154A ->166A	-0.14483
154A ->167A	0.16034
154A ->168A	-0.13024

146B ->154B 0.21425
151B ->163B 0.13123
152B ->155B 0.37144
152B ->156B 0.17581
153B ->157B 0.13252
153B ->166B 0.11809
153B ->167B 0.13451
153B ->168B -0.12035

Excited State 27: 2.359-A 3.9025 eV 317.70 nm f=0.0059 <S**2>=1.142
139A ->158A -0.13796
151A ->155A 0.15508
152A ->157A 0.10662
152A ->162A -0.14873
153A ->156A -0.14085
153A ->157A -0.11058
154A ->157A 0.10595
137B ->157B -0.12994
150B ->154B 0.64246
151B ->154B 0.20178
152B ->154B 0.11526
152B ->155B -0.15693
153B ->157B -0.13783

Excited State 28: 2.185-A 3.9512 eV 313.79 nm f=0.0211 <S**2>=0.943
132A ->157A 0.10325
132A ->158A 0.10181
134A ->157A 0.10612
134A ->158A 0.10217
139A ->157A 0.20525
139A ->158A 0.19037
153A ->156A 0.12492
153A ->157A 0.14744
153A ->158A 0.11625
154A ->155A 0.18259
154A ->158A -0.26762
154A ->159A -0.14549
154A ->160A -0.19925
132B ->157B 0.12864
134B ->157B 0.17837
136B ->157B 0.14350
137B ->157B 0.25321
138B ->157B -0.16256
150B ->154B 0.43078
151B ->154B 0.11379
152B ->156B 0.18063

153B ->157B 0.21641
153B ->160B 0.11440

Excited State 29: 2.135-A 4.0039 eV 309.65 nm f=0.3366 <S**2>=0.890
139A ->158A -0.11874
151A ->155A -0.16487
152A ->155A -0.24305
153A ->155A -0.25878
153A ->156A 0.51548
153A ->157A 0.10880
153A ->158A -0.13890
154A ->155A 0.18543
154A ->157A 0.10005
154A ->160A -0.10133
152B ->155B 0.36105
152B ->156B 0.38922
152B ->160B -0.11092

Excited State 30: 2.627-A 4.0392 eV 306.95 nm f=0.0105 <S**2>=1.475
132A ->157A -0.10863
134A ->157A -0.10986
139A ->157A -0.20134
148A ->155A 0.15263
152A ->155A 0.10413
152A ->162A 0.17103
153A ->155A 0.24683
153A ->156A 0.12243
153A ->157A -0.18699
153A ->158A 0.16724
154A ->155A -0.13112
154A ->157A 0.11078
137B ->157B -0.10242
146B ->154B -0.14229
149B ->155B 0.11415
150B ->154B 0.33588
152B ->155B 0.21084
153B ->155B -0.19911
153B ->158B 0.13273
153B ->159B -0.11558
153B ->160B -0.19568

O) TD-DFT excitation energies and oscillator strengths for **[1c]**$^{+}$ without H_2O

Excited State 1: 3.330-A 1.7903 eV 692.55 nm f=0.0043 <S**2>=2.523
160A ->164A -0.12463
160A ->168A 0.11465

162A ->163A -0.15821
162A ->164A 0.45027
162A ->168A -0.28364
160B ->162B 0.13757
160B ->163B -0.15745
160B ->166B 0.10267
161B ->162B 0.32650
161B ->163B -0.31541
161B ->164B -0.36496
161B ->166B 0.14177
161B ->168B 0.25159
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2239.06347019
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.358-A 1.9299 eV 642.44 nm f=0.0068 <S**2>=1.140
162A ->164A -0.22546
162A ->168A 0.13940
159B ->162B 0.10645
160B ->162B 0.16091
161B ->162B 0.88147
161B ->163B 0.13583
161B ->164B 0.15260
161B ->168B -0.12837

Excited State 3: 2.896-A 2.0840 eV 594.93 nm f=0.0811 <S**2>=1.846
158A ->163A 0.11833
159A ->163A 0.22154
160A ->163A 0.16418
161A ->163A -0.23694
162A ->164A -0.15517
155B ->162B 0.25502
158B ->162B 0.13391
159B ->162B 0.34931
159B ->163B -0.14281
159B ->164B 0.10772
159B ->168B -0.10743
160B ->162B 0.42460
160B ->163B -0.22184
160B ->166B 0.14581
161B ->162B -0.30548
161B ->164B 0.16042

Excited State 4: 2.218-A 2.3819 eV 520.52 nm f=0.2428 <S**2>=0.980
156A ->163A -0.13403
161A ->163A -0.19701

156B ->162B -0.10450
157B ->162B 0.88968
157B ->163B 0.10738

Excited State 5: 3.030-A 2.4818 eV 499.57 nm f=0.0414 <S**2>=2.046
160A ->164A 0.22686
160A ->168A -0.21025
161A ->163A 0.25112
162A ->166A 0.19327
162A ->177A 0.10474
155B ->162B 0.31390
157B ->162B 0.14869
159B ->162B 0.25176
160B ->162B 0.31232
160B ->163B 0.19929
160B ->164B 0.15310
160B ->166B -0.11356
160B ->168B -0.17032
161B ->164B -0.18308
161B ->165B -0.14360
161B ->166B 0.13414
161B ->177B -0.10518

Excited State 6: 3.458-A 2.5040 eV 495.15 nm f=0.0018 <S**2>=2.739
143A ->163A 0.13924
143A ->165A -0.21477
143A ->166A 0.18213
150A ->163A -0.10927
150A ->165A 0.16246
150A ->166A -0.14229
160A ->164A -0.11949
160A ->168A 0.10360
162A ->163A 0.28357
162A ->165A -0.28459
162A ->166A 0.17957
143B ->163B 0.14486
143B ->166B 0.13667
150B ->163B -0.13455
150B ->166B -0.13412
160B ->164B -0.12917
160B ->166B 0.10041
161B ->163B 0.27648
161B ->164B -0.15176
161B ->166B 0.17279
161B ->168B -0.10492

Excited State 7: 3.389-A 2.5541 eV 485.43 nm f=0.0106 <S**2>=2.622

143A ->164A	-0.24093
143A ->166A	0.10777
143A ->168A	-0.15779
150A ->164A	0.18690
150A ->168A	0.11239
161A ->163A	-0.13593
161A ->164A	-0.10369
162A ->164A	-0.15852
162A ->165A	0.10267
162A ->166A	0.22495
162A ->167A	-0.11447
162A ->168A	-0.27162
143B ->164B	0.15191
143B ->168B	0.10462
145B ->164B	0.10065
150B ->164B	-0.15257
155B ->162B	-0.12649
160B ->162B	-0.13018
161B ->164B	0.18402
161B ->165B	-0.18182
161B ->166B	0.21278
161B ->168B	0.22431

Excited State 8: 2.187-A 2.6221 eV 472.85 nm f=0.0352 <S**2>=0.945

161A ->163A	-0.15887
162A ->163A	-0.20812
162A ->164A	0.64621
161B ->163B	0.43830
161B ->164B	0.39687

Excited State 9: 3.020-A 2.6848 eV 461.80 nm f=0.0624 <S**2>=2.030

143A ->164A	-0.12151
159A ->163A	-0.13603
160A ->164A	-0.13209
160A ->168A	0.10719
160A ->174A	-0.11289
161A ->163A	0.41651
161A ->168A	-0.10163
162A ->164A	0.11164
162A ->166A	-0.14356
162A ->168A	-0.10400
162A ->177A	-0.13682
143B ->164B	0.11181
150B ->164B	-0.10990
155B ->162B	0.20837

159B ->162B 0.12281
159B ->163B 0.14965
160B ->162B 0.20641
160B ->164B -0.12468
160B ->168B 0.17693
161B ->163B 0.12425
161B ->164B 0.29772
161B ->165B 0.18011
161B ->168B 0.10061
161B ->177B 0.13025

Excited State 10: 3.046-A 2.8083 eV 441.49 nm f=0.0071 <S**2>=2.070
143A ->165A 0.15021
150A ->165A -0.11335
150A ->166A -0.11170
157A ->166A 0.10258
160A ->164A -0.11390
161A ->163A 0.16972
161A ->164A 0.11378
162A ->163A 0.34613
162A ->164A 0.12834
162A ->165A 0.21296
162A ->166A 0.44981
162A ->168A 0.17700
143B ->165B -0.10993
150B ->165B 0.12135
160B ->163B -0.10598
161B ->163B -0.14654
161B ->164B 0.22134
161B ->165B -0.31140
161B ->166B -0.12570

Excited State 11: 2.531-A 2.8268 eV 438.60 nm f=0.0012 <S**2>=1.352
150A ->165A -0.10748
161A ->163A 0.11525
162A ->163A -0.32858
162A ->164A -0.16529
162A ->165A 0.43255
162A ->166A -0.14301
160B ->164B -0.14125
161B ->163B 0.38329
161B ->164B -0.33246
161B ->165B -0.23597
161B ->166B 0.23157
161B ->168B -0.18364

Excited State 12: 3.440-A 2.9601 eV 418.85 nm f=0.0026 <S**2>=2.708

143A ->167A	0.16901
150A ->167A	-0.17194
157A ->167A	0.12732
158A ->167A	0.10703
161A ->163A	-0.13775
161A ->167A	0.11367
162A ->163A	0.17994
162A ->167A	0.54040
162A ->168A	-0.17656
143B ->167B	-0.11111
150B ->167B	0.13827
156B ->167B	-0.10877
161B ->163B	0.13937
161B ->164B	-0.11893
161B ->166B	-0.22115
161B ->167B	-0.44990

Excited State 13: 2.320-A 3.0186 eV 410.73 nm f=0.0275 <S**2>=1.096

161A ->163A	0.21965
162A ->163A	-0.11054
162A ->164A	-0.10875
162A ->165A	0.43667
162A ->166A	0.27064
150B ->165B	-0.13405
156B ->165B	0.11194
158B ->165B	-0.10324
161B ->165B	0.55335
161B ->166B	-0.13170
161B ->167B	-0.22225

Excited State 14: 2.841-A 3.0501 eV 406.50 nm f=0.0428 <S**2>=1.768

143A ->165A	-0.12154
153A ->163A	-0.10312
160A ->163A	0.18638
160A ->174A	0.10999
161A ->163A	0.43879
161A ->164A	0.10576
161A ->174A	-0.10383
162A ->163A	-0.17622
162A ->165A	-0.12642
162A ->166A	-0.24878
162A ->167A	0.16483
162A ->168A	-0.14435
162A ->177A	0.11119
155B ->162B	-0.10156

160B ->173B 0.13092
161B ->164B 0.21670
161B ->165B -0.29555
161B ->177B -0.11970

Excited State 15: 2.482-A 3.0739 eV 403.34 nm f=0.0051 <S**2>=1.290
143A ->165A 0.10335
143A ->166A -0.11051
162A ->163A 0.30472
162A ->165A 0.11763
162A ->167A 0.40583
161B ->163B 0.12820
161B ->165B 0.24343
161B ->166B 0.53209
161B ->167B 0.30848
161B ->168B 0.16094

Excited State 16: 3.115-A 3.0885 eV 401.44 nm f=0.0061 <S**2>=2.175
143A ->163A -0.13054
143A ->165A 0.12053
143A ->166A -0.18892
150A ->166A 0.11287
161A ->163A 0.12914
162A ->163A 0.22717
162A ->165A -0.32949
162A ->166A 0.15298
162A ->167A -0.33006
143B ->163B -0.12688
143B ->166B -0.13563
150B ->166B 0.11042
161B ->163B 0.36313
161B ->164B -0.18876
161B ->167B -0.29384

Excited State 17: 3.378-A 3.1917 eV 388.46 nm f=0.0068 <S**2>=2.602
143A ->164A -0.23239
143A ->168A -0.15082
150A ->164A 0.10411
160A ->163A 0.10126
161A ->163A 0.19871
162A ->164A 0.34442
162A ->166A -0.15864
162A ->168A 0.37849
143B ->164B 0.16072
143B ->168B 0.10803
161B ->164B -0.30674

161B ->166B -0.16939
161B ->168B -0.29582

Excited State 18: 2.059-A 3.2515 eV 381.31 nm f=0.1074 <S**2>=0.810
162A ->163A 0.12414
162A ->166A -0.26611
162A ->167A -0.11351
162A ->168A 0.56933
161B ->165B -0.10638
161B ->166B 0.21544
161B ->167B -0.41525
161B ->168B 0.45797

Excited State 19: 2.179-A 3.2981 eV 375.92 nm f=0.0017 <S**2>=0.937
161A ->163A -0.10864
153B ->162B -0.27901
154B ->162B 0.17541
155B ->162B -0.35047
158B ->162B -0.19045
159B ->162B -0.33535
160B ->162B 0.70150

Excited State 20: 3.156-A 3.3532 eV 369.75 nm f=0.0117 <S**2>=2.240
143A ->165A -0.18948
143A ->166A -0.12626
159A ->163A -0.13314
160A ->163A -0.21712
160A ->164A -0.14693
161A ->163A -0.21505
161A ->165A -0.14592
161A ->171A 0.12029
162A ->163A 0.17635
162A ->165A 0.31075
162A ->177A 0.11296
143B ->165B 0.15710
150B ->165B -0.11124
155B ->162B 0.18574
157B ->162B -0.11652
159B ->162B 0.13191
160B ->164B -0.19044
160B ->168B 0.12551
161B ->165B -0.17718
161B ->166B -0.16132
161B ->177B -0.11294

Excited State 21: 3.205-A 3.4468 eV 359.71 nm f=0.0123 <S**2>=2.318

143A ->165A 0.22411
143A ->166A 0.23138
150A ->165A -0.12231
150A ->166A -0.13527
156A ->163A -0.10622
160A ->163A -0.15783
161A ->163A -0.12829
161A ->171A 0.10491
162A ->165A -0.20044
162A ->166A -0.19612
139B ->165B -0.11171
143B ->165B -0.21283
145B ->165B -0.13130
147B ->165B -0.10904
150B ->165B 0.14903
153B ->162B -0.27476
155B ->162B 0.11223
159B ->162B 0.12664
160B ->163B 0.10841
161B ->165B 0.29989

Excited State 22: 2.320-A 3.4679 eV 357.52 nm f=0.0053 <S**2>=1.096
160A ->163A -0.10207
162A ->166A -0.11902
142B ->162B 0.11965
153B ->162B 0.75367
153B ->163B 0.12437
153B ->174B -0.11322
154B ->162B -0.22644
159B ->162B -0.12227
160B ->162B 0.25339

Excited State 23: 2.806-A 3.5110 eV 353.13 nm f=0.0222 <S**2>=1.718
162A ->163A 0.52999
162A ->165A 0.27120
162A ->166A -0.44082
162A ->167A -0.29528
162A ->168A -0.34447

Excited State 24: 3.418-A 3.6379 eV 340.81 nm f=0.0001 <S**2>=2.671
143A ->167A 0.39154
143A ->168A -0.13817
145A ->167A 0.14133
147A ->167A 0.11409
148A ->167A -0.11812
150A ->167A -0.21609

153A ->167A -0.13420
161A ->167A 0.19660
162A ->167A -0.35882
162A ->168A 0.10352
139B ->167B -0.13020
143B ->166B -0.14289
143B ->167B -0.25636
144B ->167B 0.10648
145B ->167B -0.16015
147B ->167B -0.13138
148B ->167B 0.10596
150B ->166B 0.10050
150B ->167B 0.18547
161B ->166B 0.17281
161B ->167B 0.25962

Excited State 25: 3.132-A 3.6928 eV 335.74 nm f=0.0002 <S**2>=2.203
156A ->163A 0.26643
159A ->171A -0.10945
160A ->163A 0.14989
160A ->164A -0.18839
160A ->171A -0.12606
161A ->164A 0.25886
161A ->165A 0.21041
161A ->171A -0.17595
162A ->175A -0.12992
162A ->177A 0.18585
155B ->162B 0.13333
159B ->162B -0.19960
160B ->164B -0.18468
161B ->166B -0.13264
161B ->175B 0.10050
161B ->176B 0.10680
161B ->177B -0.19002

Excited State 26: 2.645-A 3.8050 eV 325.85 nm f=0.0030 <S**2>=1.499
143A ->166A 0.16796
150A ->166A -0.10248
161A ->165A 0.15466
161A ->166A 0.23574
162A ->166A -0.10730
139B ->165B 0.10223
143B ->165B 0.19756
145B ->165B 0.11945
147B ->165B 0.10537
150B ->165B -0.14782

155B ->162B -0.11537
160B ->163B 0.20332
161B ->163B 0.26688
161B ->164B -0.17386
161B ->165B -0.17915
161B ->166B -0.29936
161B ->167B 0.24741
161B ->168B 0.33643

Excited State 27: 2.439-A 3.8401 eV 322.86 nm f=0.0100 <S**2>=1.237
143A ->165A -0.18050
150A ->165A 0.10892
161A ->164A -0.22283
161A ->165A -0.29633
161A ->166A -0.10208
162A ->168A 0.10136
139B ->165B -0.11419
143B ->165B -0.22465
145B ->165B -0.14234
147B ->165B -0.11734
150B ->165B 0.17705
160B ->164B -0.13160
161B ->163B 0.26017
161B ->165B 0.13388
161B ->166B -0.26410
161B ->167B 0.22490
161B ->168B 0.40913

Excited State 28: 2.256-A 3.8603 eV 321.18 nm f=0.1196 <S**2>=1.023
153A ->164A -0.10457
161A ->164A 0.68523
161A ->165A -0.20367
161A ->166A -0.18161
161A ->168A 0.23644
143B ->164B 0.10977
143B ->165B -0.10925
155B ->162B -0.13773
159B ->162B 0.13443
160B ->164B 0.19932

Excited State 29: 2.435-A 3.8879 eV 318.89 nm f=0.0370 <S**2>=1.232
143A ->166A -0.16905
159A ->163A 0.12147
160A ->163A 0.24097
161A ->163A -0.16132
161A ->165A 0.32837

161A ->166A -0.35673
161A ->167A -0.10798
162A ->166A 0.11900
162A ->177A -0.11862
143B ->163B 0.11539
155B ->162B 0.12483
159B ->162B -0.12965
160B ->163B 0.39826
161B ->177B 0.11348

Excited State 30: 2.398-A 3.9337 eV 315.19 nm f=0.0608 <S**2>=1.188
160A ->163A -0.23203
161A ->165A 0.33752
161A ->166A -0.21568
155B ->162B -0.41703
156B ->162B 0.20911
158B ->162B 0.20070
159B ->162B 0.44071
160B ->164B -0.21355