

Table A1. Cartesian coordinates, energies (in Hartrees) of all complexes reported herein in standard xyz format. The xyz format lists the total number of atoms on the first line, a descriptive title on the second line that contains: the charge and multiplicity, structure descriptor and the total energy in Hartrees. The subsequent lines list the atom by atomic number followed by the Cartesian coordinates (in angstroms).

Solvent Calculations

Indole Ring

16
Neutral singlet indole -363.839546867
1 -0.552026 -1.428045 -1.727001
6 -1.350653 -1.249711 -1.018718
6 -1.225682 -0.620270 0.197451
6 -2.734023 -1.618940 -1.160637
1 -0.354728 -0.194518 0.676968
7 -2.455446 -0.575634 0.824573
6 -3.402004 -1.178439 0.020801
1 -2.629631 -0.164955 1.731246
6 -3.482384 -2.274539 -2.159146
6 -4.775232 -1.375347 0.222862
1 -5.266956 -1.032358 1.129568
6 -5.486431 -2.026755 -0.782381
1 -6.552969 -2.195524 -0.657431
6 -4.846207 -2.472296 -1.962551
1 -2.999506 -2.620774 -3.070127
1 -5.432386 -2.976980 -2.726511

16
Cationic doublet indole -363.633534396
1 -0.578039 -1.435934 -1.732367
6 -1.383644 -1.263627 -1.031942
6 -1.247663 -0.609224 0.229958
6 -2.740138 -1.620541 -1.161179
1 -0.362114 -0.190731 0.688218
7 -2.434376 -0.567225 0.832859
6 -3.407481 -1.179939 0.020304
1 -2.608150 -0.153565 1.743576
6 -3.481732 -2.280281 -2.170974
6 -4.752800 -1.366814 0.230549
1 -5.254450 -1.028763 1.131101
6 -5.473772 -2.032358 -0.798899
1 -6.538196 -2.194905 -0.662680
6 -4.851389 -2.477589 -1.970781
1 -2.993143 -2.622855 -3.077525
1 -5.439176 -2.980733 -2.731251

5-hydroxyindole solvent

17
Neutral singlet 5-HOI -439.062412021
1 -0.452051 0.925161 -0.145235
6 -1.250836 1.141341 0.552169
6 -1.134371 1.873570 1.712566
6 -2.623783 0.726758 0.453003
1 -0.270103 2.359167 2.145200
7 -2.357043 1.940346 2.344676
6 -3.294222 1.247159 1.598555
1 -2.536047 2.423578 3.213643
6 -3.351430 -0.029799 -0.487384
6 -4.658522 1.028603 1.817809
1 -5.164823 1.427957 2.692437
6 -5.359375 0.278054 0.876133
1 -6.421423 0.090530 1.018845
6 -4.706447 -0.243957 -0.264102
1 -2.875897 -0.443302 -1.372768
8 -5.394970 -0.990525 -1.203310
1 -6.325793 -1.072864 -0.940323

17
Cationic doublet 5-HOI -438.860765078
1 -0.433497 0.925713 -0.153477
6 -1.230373 1.141365 0.543924
6 -1.129492 1.865487 1.698100
6 -2.615743 0.719698 0.436456
1 -0.282960 2.358873 2.152320
7 -2.379154 1.916238 2.315010
6 -3.295412 1.240453 1.588033
1 -2.563750 2.398403 3.189047
6 -3.325298 -0.018800 -0.483028
6 -4.676378 1.028628 1.823289
1 -5.162498 1.437084 2.703236
6 -5.385860 0.287424 0.900137
1 -6.445684 0.099144 1.039994
6 -4.725554 -0.234601 -0.241077
1 -2.876682 -0.442451 -1.375576
8 -5.351540 -0.959625 -1.166374
1 -6.297260 -1.081257 -0.958100

4-Fluoro-5-hydroxyindole solvent

17
Neutral singlet 4F5-HOI -538.300363174
1 -0.457526 0.924179 -0.141469
6 -1.252371 1.143126 0.557668
6 -1.137191 1.875807 1.717779
6 -2.625480 0.735125 0.468397
1 -0.271761 2.360433 2.148559
7 -2.358592 1.944376 2.350605
6 -3.300754 1.253644 1.611165
1 -2.535748 2.428864 3.219487
6 -3.377614 -0.011557 -0.444880
6 -4.665966 1.037452 1.833552
1 -5.170036 1.438059 2.707907
6 -5.367838 0.287331 0.893811
1 -6.429581 0.099627 1.035889
6 -4.732112 -0.243191 -0.251565
9 -2.765226 -0.526309 -1.554176
8 -5.398245 -0.988509 -1.197534
1 -6.331094 -1.076680 -0.943282

17
Cationic doublet 4F5-HOI -538.095235317
1 -0.438429 0.930604 -0.143379
6 -1.236290 1.144786 0.552534
6 -1.135315 1.876170 1.718770
6 -2.612226 0.731738 0.456231
1 -0.282028 2.366027 2.164140
7 -2.366858 1.926990 2.326786
6 -3.295274 1.245361 1.595177
1 -2.552887 2.408946 3.200964
6 -3.353175 -0.005728 -0.446695
6 -4.667032 1.036725 1.830331
1 -5.153626 1.445441 2.709634
6 -5.392876 0.289710 0.905035
1 -6.452116 0.109952 1.057690
6 -4.762713 -0.238050 -0.230713
9 -2.804046 -0.525773 -1.538048
8 -5.362794 -0.965737 -1.171343
1 -6.309450 -1.095384 -0.975203

6-Fluoro-5-hydroxyindole solvent

17
Neutral singlet 6F5-HOI -538.301490237
1 -0.435694 0.929897 -0.145052
6 -1.234286 1.145648 0.552477
6 -1.119813 1.876600 1.711989
6 -2.607225 0.730061 0.450833
1 -0.257828 2.363067 2.147591
7 -2.345902 1.942037 2.342987
6 -3.278164 1.250264 1.596795
1 -2.526671 2.422887 3.212993
6 -3.330610 -0.027190 -0.492485
6 -4.644555 1.035138 1.821417
1 -5.175027 1.422197 2.685539
6 -5.302988 0.287588 0.865732
9 -6.646339 0.030709 1.010995
6 -4.684892 -0.249191 -0.282557
1 -2.853277 -0.440027 -1.376801
8 -5.404856 -0.986380 -1.192960
1 -6.329009 -1.051528 -0.897580

17
Cationic doublet 6F5-HOI -538.092556535
1 -0.417712 0.930104 -0.155319
6 -1.213643 1.145488 0.542862
6 -1.115938 1.865225 1.692033
6 -2.600011 0.719845 0.430492
1 -0.273494 2.360816 2.151293
7 -2.375472 1.915280 2.313820
6 -3.284516 1.243615 1.589596
1 -2.560300 2.396831 3.188126
6 -3.299843 -0.019205 -0.493371
6 -4.668666 1.037484 1.834177
1 -5.175909 1.435898 2.705894
6 -5.332313 0.300566 0.897487
9 -6.652128 0.033433 1.012961
6 -4.691982 -0.239277 -0.262231
1 -2.846425 -0.440675 -1.384186
8 -5.363509 -0.954411 -1.150572
1 -6.305276 -1.049243 -0.901149

NO SOLVENT

Indole ring no solvent

16

Neutral singlet indole -363.831837620

1	-0.555176	-1.428605	-1.726375
6	-1.352454	-1.249325	-1.017322
6	-1.223759	-0.620967	0.195515
6	-2.735574	-1.617945	-1.158445
1	-0.350297	-0.196201	0.671437
7	-2.455568	-0.575002	0.824923
6	-3.403556	-1.178732	0.020225
1	-2.631163	-0.166520	1.730365
6	-3.482353	-2.273042	-2.156126
6	-4.775361	-1.375721	0.221627
1	-5.270773	-1.034226	1.127568
6	-5.485309	-2.026721	-0.782973
1	-6.551751	-2.195853	-0.658643
6	-4.844693	-2.471190	-1.961075
1	-2.998479	-2.618998	-3.066447
1	-5.429998	-2.976039	-2.725286

16

Cationic doublet indole -363.556328747

1	-0.577337	-1.435787	-1.732003
6	-1.383029	-1.262419	-1.030417
6	-1.243096	-0.609296	0.227996
6	-2.739110	-1.618317	-1.158001
1	-0.354331	-0.191920	0.683946
7	-2.433528	-0.565106	0.835823
6	-3.407861	-1.178075	0.023189
1	-2.605010	-0.151547	1.746660
6	-3.482954	-2.279915	-2.169852
6	-4.753801	-1.366651	0.230576
1	-5.263084	-1.031796	1.129382
6	-5.475562	-2.033756	-0.801238
1	-6.540373	-2.196769	-0.664877
6	-4.852688	-2.478321	-1.971913
1	-2.995102	-2.623406	-3.077243
1	-5.439398	-2.982006	-2.733060

5-hydroxyindole no solvent

17

Neutral singlet 5-HOI -439.050329156

1	-0.456790	0.923566	-0.144899
6	-1.253652	1.141159	0.553629
6	-1.133162	1.872689	1.709826
6	-2.626730	0.727163	0.455312
1	-0.266130	2.356871	2.138652
7	-2.357647	1.941412	2.345383
6	-3.296529	1.247020	1.599249
1	-2.537067	2.422212	3.213465
6	-3.351227	-0.028210	-0.484607
6	-4.658950	1.028608	1.818190
1	-5.168795	1.426569	2.692123
6	-5.357272	0.278156	0.875425
1	-6.420141	0.091218	1.018732
6	-4.705653	-0.243727	-0.264182
1	-2.879067	-0.442812	-1.370365
8	-5.389653	-0.988669	-1.203568
1	-6.318672	-1.071447	-0.940451

17

Cationic doublet 5-HOI -438.782703583

1	-0.433141	0.925457	-0.151185
6	-1.231871	1.141147	0.544968
6	-1.126863	1.868183	1.698855
6	-2.617148	0.720328	0.440269
1	-0.275081	2.359951	2.146879
7	-2.374602	1.920000	2.316887
6	-3.296529	1.241287	1.589826
1	-2.556713	2.403395	3.190620
6	-3.328118	-0.019442	-0.479719
6	-4.675485	1.028645	1.825419
1	-5.166627	1.434784	2.705016
6	-5.388252	0.286233	0.902364
1	-6.448618	0.101112	1.047932
6	-4.731154	-0.235405	-0.239171
1	-2.884287	-0.446210	-1.374016
8	-5.347138	-0.957916	-1.169994
1	-6.295510	-1.089772	-0.983038

4-fluoro-5-hydroxyindole no solvent

17			
Neutral singlet 4F5-HOI -538.286413173			
1	-0.467913	0.919093	-0.145087
6	-1.256809	1.142329	0.558697
6	-1.135678	1.874368	1.714117
6	-2.630477	0.735707	0.471946
1	-0.267133	2.357424	2.140663
7	-2.359267	1.945637	2.352248
6	-3.303962	1.253738	1.613073
1	-2.536062	2.428373	3.219923
6	-3.373660	-0.012205	-0.447353
6	-4.667392	1.037558	1.834915
1	-5.176641	1.435842	2.708032
6	-5.364284	0.287108	0.891589
1	-6.427084	0.099767	1.033089
6	-4.729658	-0.243108	-0.252999
9	-2.759466	-0.519583	-1.544858
8	-5.395882	-0.986369	-1.197282
1	-6.325769	-1.073902	-0.938798

17			
Cationic doublet 4F5-HOI -538.015107010			
1	-0.444012	0.925076	-0.144839
6	-1.240622	1.142759	0.552634
6	-1.133147	1.878208	1.718631
6	-2.614862	0.733573	0.461965
1	-0.273035	2.365572	2.156049
7	-2.361907	1.932315	2.330393
6	-3.296997	1.247266	1.598959
1	-2.544004	2.416200	3.203764
6	-3.353736	-0.007952	-0.448189
6	-4.667265	1.036551	1.833162
1	-5.160692	1.442171	2.711526
6	-5.393879	0.288253	0.906948
1	-6.453754	0.110756	1.064197
6	-4.767124	-0.240122	-0.231162
9	-2.803148	-0.521327	-1.528964
8	-5.360091	-0.964585	-1.174433
1	-6.308862	-1.102936	-0.998726

6-fluoro-5-hydroxyindole no solvent

17			
Neutral singlet 6F5-HOI -538.291222227			
1	-0.438387	0.928866	-0.143531
6	-1.235852	1.145750	0.554428
6	-1.117652	1.876611	1.709785
6	-2.608858	0.730349	0.452967
1	-0.253160	2.361834	2.141873
7	-2.346188	1.943791	2.343019
6	-3.279932	1.249955	1.596401
1	-2.527765	2.421709	3.212328
6	-3.329626	-0.026422	-0.490568
6	-4.645373	1.034050	1.820309
1	-5.182419	1.418022	2.682040
6	-5.302720	0.285951	0.864489
9	-6.643837	0.026961	1.007624
6	-4.683440	-0.249512	-0.283152
1	-2.854662	-0.440008	-1.375180
8	-5.402672	-0.984223	-1.190584
1	-6.324590	-1.041907	-0.890336

17			
Cationic doublet 6F5-HOI -538.013838280			
1	-0.414488	0.928832	-0.151703
6	-1.212896	1.145081	0.544257
6	-1.112772	1.866068	1.690185
6	-2.599510	0.719436	0.432134
1	-0.266157	2.360278	2.145123
7	-2.375450	1.919264	2.314926
6	-3.286952	1.245528	1.591562
1	-2.558579	2.402765	3.188175
6	-3.298922	-0.020705	-0.492573
6	-4.671717	1.037896	1.836740
1	-5.187297	1.432635	2.706491
6	-5.335390	0.299692	0.900756
9	-6.647834	0.027682	1.009856
6	-4.691782	-0.239679	-0.262215
1	-2.847419	-0.444851	-1.384526
8	-5.362968	-0.950406	-1.149492
1	-6.307004	-1.047738	-0.907782