Electronically excited state of neutral/protonated, Indole/5-Hydroxyinodole-water clusters: a theoretical study

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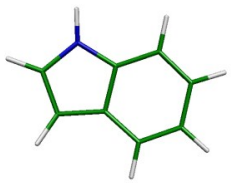
This supplementary file contains 2 Tables:

Table SM1: xyz coordinates revealed to the ground optimized geometry of neutral/protonated of indole and hydroxyl indole water clusters

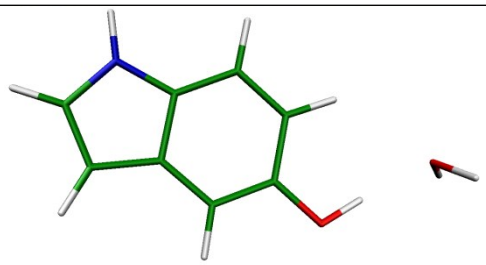
Table SM2: Vertical transition energies of neutral and protonated of indole and 5-Hydroxy indole , computed at the CC2/aug-cc-pVDZ level of theory.

SM1

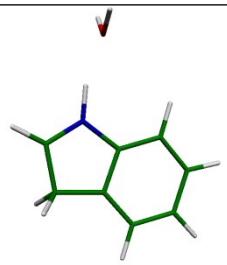
Indole-W			
C	-2.79303	2.26047	-0.08005
C	-2.96990	1.25178	-1.02010
C	-1.95117	0.27022	-0.76932
C	-1.18599	0.75007	0.34444
N	-1.72345	1.95535	0.73490
C	-1.59220	-0.96766	-1.35922
C	-0.50777	-1.67753	-0.83758
C	0.23724	-1.18276	0.26781
C	-0.09130	0.03416	0.87155
H	0.47604	0.42371	1.72304
H	-1.35703	2.50702	1.51223
H	-3.35650	3.18222	0.06924
H	-3.73902	1.22643	-1.79213
H	-2.15711	-1.36153	-2.21162
H	-0.22224	-2.63505	-1.28619
H	1.08182	-1.76489	0.65185
O	-0.16813	2.92946	2.99088
H	-0.16611	2.24370	3.67289
H	0.75985	2.96283	2.72039



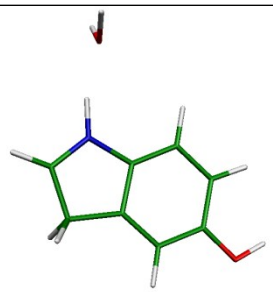
HydroxyIndole-W			
C	-2.80925	2.59826	0.00467
C	-3.10575	1.24257	0.03434
C	-1.85205	0.53754	0.02074
C	-0.82131	1.53030	-0.01776
N	-1.43792	2.76671	-0.02658
H	-3.47410	3.46253	0.00336
H	-0.96041	3.65914	-0.05180
H	-4.10643	0.81121	0.06252
C	-1.49491	-0.83207	0.03720
C	-0.14136	-1.18194	0.01540
C	0.86914	-0.17689	-0.02293
C	0.54317	1.18229	-0.03983
H	1.33090	1.94347	-0.06928
H	1.91919	-0.48776	-0.03919
O	0.17746	-2.51340	0.03199
H	1.15085	-2.58483	0.01414
H	-2.24992	-1.62436	0.06654
O	2.97626	-2.86049	-0.01321
H	3.23753	-3.39225	0.75138
H	3.21190	-3.42603	-0.76173



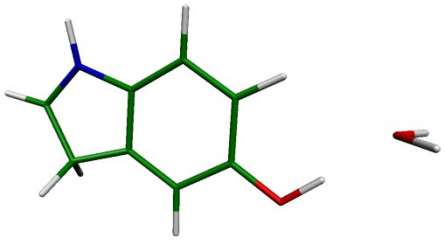
Protonated Indole-W			
C	-2.30594	2.74165	0.01868
C	-3.01229	1.42352	0.02904
C	-1.86350	0.44625	0.02993
C	-0.66647	1.18772	0.02078
N	-1.01214	2.56795	0.01438
C	0.61463	0.62552	0.01862
C	0.66294	-0.77766	0.02641
C	-0.52162	-1.54911	0.03577
C	-1.79709	-0.95275	0.03766
H	-2.70192	-1.56779	0.04497
H	-0.44363	-2.64061	0.04168
H	1.63332	-1.28245	0.02520
H	1.51553	1.24519	0.01126
H	-0.28549	3.32998	0.00701
H	-2.74566	3.74265	0.01479
H	-3.67237	1.33795	-0.85526
H	-3.66544	1.34808	0.91937
O	1.11691	4.21495	-0.00619
H	1.50400	4.67799	0.75137
H	1.49424	4.66998	-0.77346



Protonated HydroxyIndole(NH)-W			
C	-3.33375	2.29019	0.16255
C	-3.57693	0.81308	0.17978
C	-2.17725	0.25773	0.07481
C	-1.28718	1.34970	0.00929
N	-2.05336	2.53873	0.06732
H	-4.06791	3.09789	0.21798
H	-1.61182	3.49267	0.03501
C	-1.67980	-1.04354	0.03665
C	-0.27968	-1.21513	-0.06794
C	0.59357	-0.09703	-0.13213
C	0.10176	1.21318	-0.09440
H	0.76560	2.08064	-0.14322
H	1.67334	-0.26394	-0.21283
O	0.16066	-2.49088	-0.10187
H	1.12798	-2.49484	-0.17411
H	-2.32157	-1.92797	0.08376
H	-4.23576	0.52370	-0.66082
H	-4.10268	0.52312	1.10931
O	-0.55590	4.78004	-0.04375
H	-0.29522	5.34205	0.70073
H	-0.40911	5.34160	-0.81911



Protonated HydroxyIndole(OH)-W			
C	-2.47453	2.85920	0.11240
C	-2.99877	1.46093	0.05504
C	-1.73454	0.63692	0.00721
C	-0.63589	1.52435	0.03720
N	-1.16305	2.83355	0.09993
H	-3.02769	3.80011	0.15901
H	-0.58614	3.67998	0.13259
C	-1.51153	-0.73543	-0.05591
C	-0.17085	-1.19841	-0.08821
C	0.91701	-0.27495	-0.05627
C	0.70107	1.10426	0.00695
H	1.53977	1.80670	0.03110
H	1.93695	-0.66928	-0.08234
O	0.00636	-2.52028	-0.14881
H	0.97231	-2.73144	-0.16829
H	-2.32420	-1.46708	-0.08154
H	-3.64772	1.33496	-0.83278
H	-3.63117	1.25655	0.94027
O	2.65643	-3.03420	-0.20164
H	3.03019	-3.54617	0.53094
H	3.01200	-3.47629	-0.98686



SM2

state	Energy (eV)	oscillator strengths	configuration
Indole-W			
S1 ($\pi\pi^*$)	4.86	0.0328	(H-1- L) 70.5% (H-L+2) 24%
S2 ($\pi\pi^*$)	5.08	0.0930	(H-L) 78% (H-1-L+2) 8%
S3 ($\pi\pi^*$)	6.46	0.7108	(H-L+2) 58% (H-1-L) 17.5%
S4 ($\pi\pi^*$)	6.72	0.0818	(H-1-L+2) 53% (H-2-L) 23%
Hydroxy Indole-W			
S1 ($\pi\pi^*$)	4.45	0.0786	(H-L) 85%
S2 ($\pi\pi^*$)	5.24	0.1182	(H-1-L) 79%
S3 ($\pi\pi^*$)	6.46	0.5360	(H-L+3) 66% (H-2-L) 7%
S4 ($\pi\pi^*$)	6.75	0.1798	(H-1-L+3) 67% (H-2-L) 11%

Protonated Indole-W			
S1 ($\pi\pi^*$)	4.28	0.0351	(H-1-L) 61% (H-L) 32%
S2 ($\pi\pi^*$)	4.43	0.1713	(H-L) 70% (H-1-L) 24%
S3 ($\pi\pi^*$)	5.64	0.0407	(H-L+1) 56% (H-1-L+2) 34%
S4 ($\pi\pi^*$)	6.75	0.1148	(H-1-L+1) 69% (H-L+2) 22%
Protonated Hydroxy Indole(NH)-W			
S1 ($\pi\pi^*$)	3.71	0.2488	(H–L) 96%
S2 ($\pi\pi^*$)	4.43	0.0048	(H-1– L) 74% (H-L+1) 23%
S3 ($\pi\pi^*$)	5.14	0.0913	(H-L+1) 61% (H-1-L) 23.5%
S4 ($\pi\pi^*$)	6.41	0.0117	(H-L+3) 65% (H-1- L+1) 23%
Protonated Hydroxy Indole(OH)-W			
S1 ($\pi\pi^*$)	3.23	0.2776	(H-L) 96%
S2 ($\pi\pi^*$)	4.19	0.0055	(H-1-L) 88%
S3 ($\pi\pi^*$)	4.95	0.0771	(H-L+1) 75% (H-1-L+3) 11%
S4 ($\pi\pi^*$)	6.21	0.0341	(H-L+3) 71% (H-1-L+1) 15%