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Unravelling hydrogen bonding interactions of tryptamine-water dimer from neutral to cation

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(Supporting Information)

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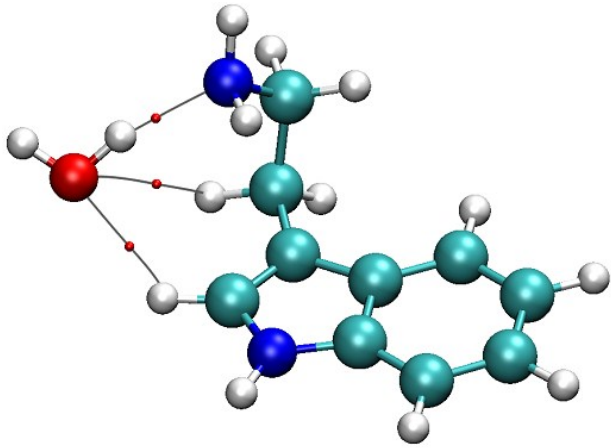
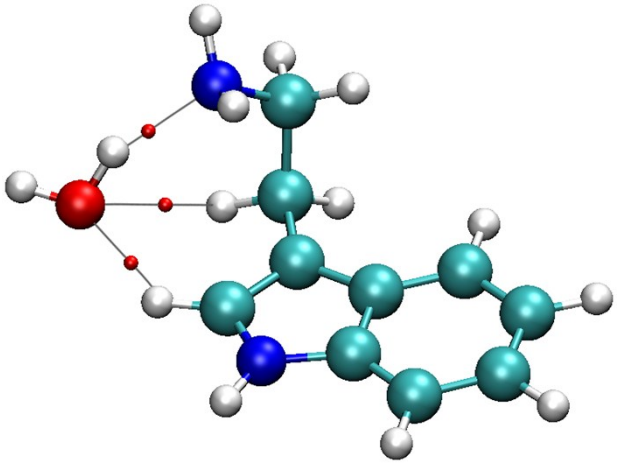
(a)

A-H_2O



(b)

A^+-H_2O



(c)

H^+-H_2O

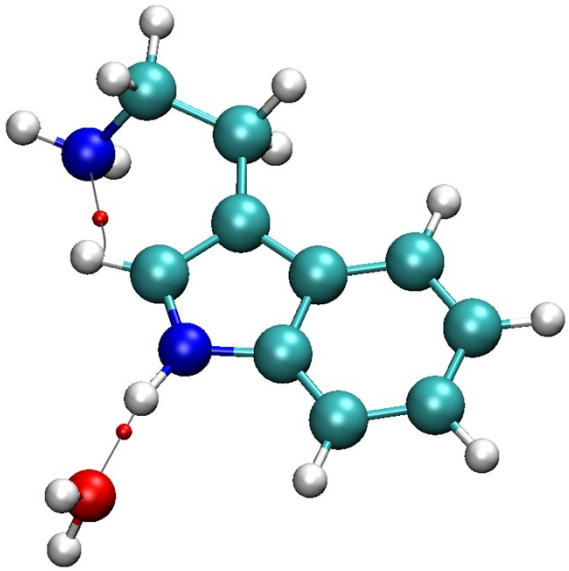


Figure S1. Display of the bond critical points (BCPs) and bond paths from AIM analysis for **A-H_2O**, **A^+-H_2O**, and **H^+-H_2O** complexes. The little red points stand for the (3, -1) BCPs associated with the inter- and intramolecular H-bonds.

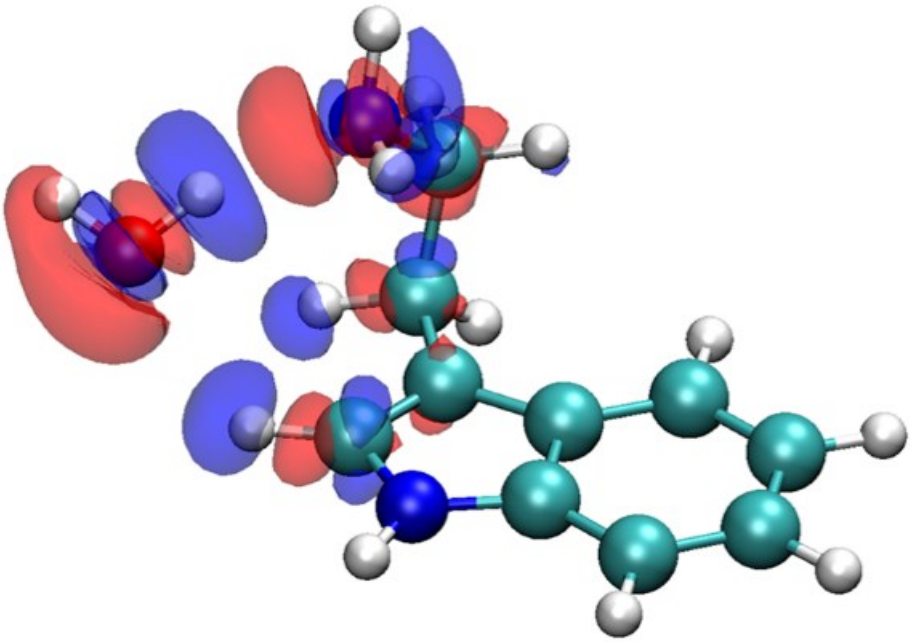


Figure S2. Electron density difference map (EDDM) for **A-H_2O** dimer. Red and blue parts respectively denote the increase and decrease of the electron density from monomer to dimer. Geometric calculations were done with M06-2X/aug-cc-pVDZ with the iso-density value set at 0.001 a.u..

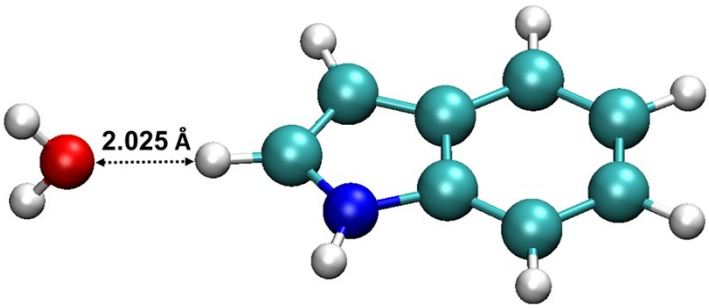


Figure S3. Optimized geometries of indole$^+$-water complex by M06-2X/aug-cc-pVDZ.

Table S1. Natural population analysis (NPA) charges and the ChelpG charges of **A-H_2O** and **A^+-H_2O** dimers by M06-2X/aug-cc-pVDZ.

Atom	**A-H_2O**		**A^+-H_2O**	
	NPA	ChelpG	NPA	ChelpG
C1	-0.002	0.037	0.172	0.223
C2	-0.147	-0.178	0.237	0.087
C3	-0.105	0.101	-0.113	-0.096
C4	0.162	0.265	0.111	0.302
H5	0.233	0.151	0.126	0.148
H6	0.262	0.152	0.149	0.146
C7	-0.216	-0.232	0.039	-0.015
C8	-0.259	-0.253	-0.100	-0.234
C9	-0.242	-0.085	0.012	0.047
C10	-0.259	-0.123	-0.149	-0.149
H11	0.236	0.128	0.134	0.180
H12	0.234	0.092	0.129	0.126
H13	0.234	0.090	0.134	0.139
N14	-0.604	-0.533	-0.198	-0.470
H15	0.436	0.366	0.234	0.408
C16	-0.469	0.095	-0.261	-0.040
H17	0.241	-0.032	0.140	0.039
H18	0.259	-0.002	0.146	0.059
C19	-0.227	0.334	-0.096	0.250
H20	0.201	-0.096	0.106	-0.061
H21	0.219	-0.036	0.124	0.037
N22	-0.948	-0.500	-0.474	-0.425
H23	0.399	0.202	0.197	0.188
H24	0.394	0.216	0.208	0.237
O25	-1.024	-0.711	-0.516	-0.737
H26	0.511	0.189	0.257	0.188
H27	0.482	0.366	0.253	0.424