supplementary

Structure of Imidazolium-N-phthalolylglycinate Salt Hydrate: Combined Experimental and Quantum Chemical Calculations Studies

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Received: 7 January 2020; Accepted: 30 January 2020; Published: date

Table S1. Bond Lengths in Å for **IM$^+$-NPG$^-$-HYD**.

Bond	DFT		X-Ray	Bond	DFT		X-Ray
	Conf. A	Conf. B			Conf. A	Conf. B	
O1-C1	1.20911	1.20774	1.207(3)	C1-C2	1.49332	1.49195	1.487(3)
O2-C8	1.21626	1.20817	1.213(3)	C2-C3	1.38389	1.38260	1.384(3)
O3-C10	1.24804	1.22823	1.243(3)	C2-C7	1.39069	1.39056	1.386(3)
O4-C10	1.25007	1.28972	1.264(3)	C3-C4	1.39878	1.39831	1.391(4)
N1-C1	1.38606	1.40023	1.392(3)	C4-C5	1.39823	1.39655	1.391(4)
N1-C8	1.40031	1.39845	1.381(3)	C5-C6	1.39897	1.39694	1.392(4)
N1-C9	1.44965	1.43814	1.448(3)	C6-C7	1.38346	1.38324	1.374(4)
N2-C11	1.37802	1.37584	1.373(3)	C7-C8	1.49368	1.49164	1.497(3)
N2-C13	1.32984	1.32155	1.325(3)	C9-C10	1.56229	1.53819	1.526(4)
N3-C12	1.37684	1.37268	1.370(3)	C11-C12	1.35969	1.36419	1.344(4)
N3-C13	1.32869	1.34207	1.322(3)				
IM$^+$··· NPG$^-$	3.23483		3.359(3)				
IM$^+$··· NPG$^-$		2.45662	2.665(3)				

Table S2: Bond Angles for **IM⁺-NPG⁻-HYD**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C8	N1	C1	112.5(2)	C7	C6	C5	117.5(2)
C9	N1	C1	123.7(2)	C6	C7	C2	121.6(2)
C9	N1	C8	123.8(2)	C8	C7	C2	107.6(2)
C13	N2	C11	108.7(2)	C8	C7	C6	130.8(2)
C13	N3	C12	109.2(2)	N1	C8	O2	125.5(2)
N1	C1	O1	124.8(2)	C7	C8	O2	128.6(2)
C2	C1	O1	129.5(2)	C7	C8	N1	105.9(2)
C2	C1	N1	105.7(2)	C10	C9	N1	113.6(2)
C3	C2	C1	130.1(2)	O4	C10	O3	126.6(2)
C7	C2	C1	108.3(2)	C9	C10	O3	118.7(2)
C7	C2	C3	121.6(2)	C9	C10	O4	114.8(2)
C4	C3	C2	116.9(2)	C12	C11	N2	107.1(2)
C5	C4	C3	121.4(2)	C11	C12	N3	106.8(2)
C6	C5	C4	120.9(2)	N3	C13	N2	108.2(2)

Table S3: Atomic Hirshfeld and atomic dipole moment[1] (ADC) corrected charges for **IM⁺-NPG⁻-HYD**.

Atom	Hirshfeld charges	ADC	Atom	Hirshfeld Charges	ADC
Configuration **A**			Configuration **B**		
1O	-0.436836	-0.533135	1O	-0.276766	-0.044037
2O	-0.252632	0.128721	2O	-0.276607	-0.585510
3O	-0.445521	-0.536577	3O	-0.319455	-0.326536
4N	-0.016426	0.272339	4O	-0.389215	-0.498113

5C	-0.010314	-0.467903	5N	-0.028787	0.147508
6C	-0.003277	0.569388	6C	0.178713	-0.316593
7C	0.175338	-0.243916	7C	-0.008358	0.096636
8C	-0.037872	-0.624922	8C	-0.016005	-0.148727
9C	-0.015505	-0.088443	9H	0.045717	0.043510
10C	0.167701	0.671080	10C	-0.021917	0.006269
11C	-0.035307	-0.360153	11H	0.039508	0.155367
12C	-0.028012	-0.133277	12C	-0.019714	-0.213489
13O	-0.274052	-0.952679	13H	0.040625	0.158399
14C	0.116003	0.271543	14C	-0.014897	-0.048699
15C	-0.036684	-0.002071	15H	0.046594	0.270199
16H	0.047600	-0.475733	16C	-0.005583	-0.207773
17H	0.037810	0.181409	17C	0.178716	0.490630
18H	0.031892	0.904718	18C	-0.032381	-0.111037
19H	0.034233	0.308591	19H	0.023850	0.078170
20H	0.030513	0.095246	20H	0.027493	0.090340
21H	0.029413	0.093841	21C	0.153076	0.255353
22N	0.039169	-0.261540	22N	0.036922	0.014871
23N	0.025685	-0.025810	23H	0.098325	0.248230
24C	0.066254	-0.007189	24N	0.011084	-0.150037
25C	0.161480	0.056616	25H	0.163241	0.274496
26C	0.052073	-0.100346	26C	0.050589	-0.096990
27H	0.169483	0.363499	27H	0.080201	0.143832
28H	0.165504	0.313496	28C	0.029513	-0.054891
29H	0.086350	0.254978	29H	0.073797	0.228534
30H	0.092053	0.202388	30C	0.160248	0.005282
31H	0.081042	0.142999	31H	0.100210	0.245246
32O	-0.308787	-0.750929	32O	-0.344340	-0.739504
33H	0.149049	0.373840	33H	0.130293	0.363397
34H	0.142523	0.359874	34H	0.085184	0.225540

[1]Tian Lu, Feiwu Chen, Atomic dipole moment corrected Hirshfeld population method, *J. Theor. Comput. Chem*., 11, (2011), 163.

Table S4. TD-DFT calculation for **IM$^+$-NPG$^-$-HYD** at the CAM-B3LYP/cc-PVTZ theoretical level; calculated wavelength (λ), oscillator strength (f), transition energy (E), and contributing orbitals to the transitions.

ES	E (eV)	f	λ (nm)	Main contributing transitions
2	1.7285	0.001	534.38	HOMO⟶ LUMO
4	1.7981	0.003	513.69	HOMO-2⟶ LUMO
5	2.0674	0.004	446.79	HOMO⟶ LUMO+1
6	2.1441	0.0024	430.78	HOMO-1⟶ LUMO+1
7	2.7269	0.0041	338.73	HOMO⟶ LUMO+4
8	2.7443	0.0013	336.58	HOMO⟶ LUMO+3
9	3.0800	0.0047	299.89	HOMO-1⟶ LUMO+4
10	3.0922	0.0374	298.70	HOMO-2⟶ LUMO+4
11	3.1039	0.013	297.59	HOMO-1⟶ LUMO+3
12	3.1154	0.0045	296.48	HOMO-2⟶ LUMO+3
13	3.5583	0.01	259.58	HOMO⟶ LUMO+5

[a]The states whose oscillator strengths are less than 0.001 are not included.

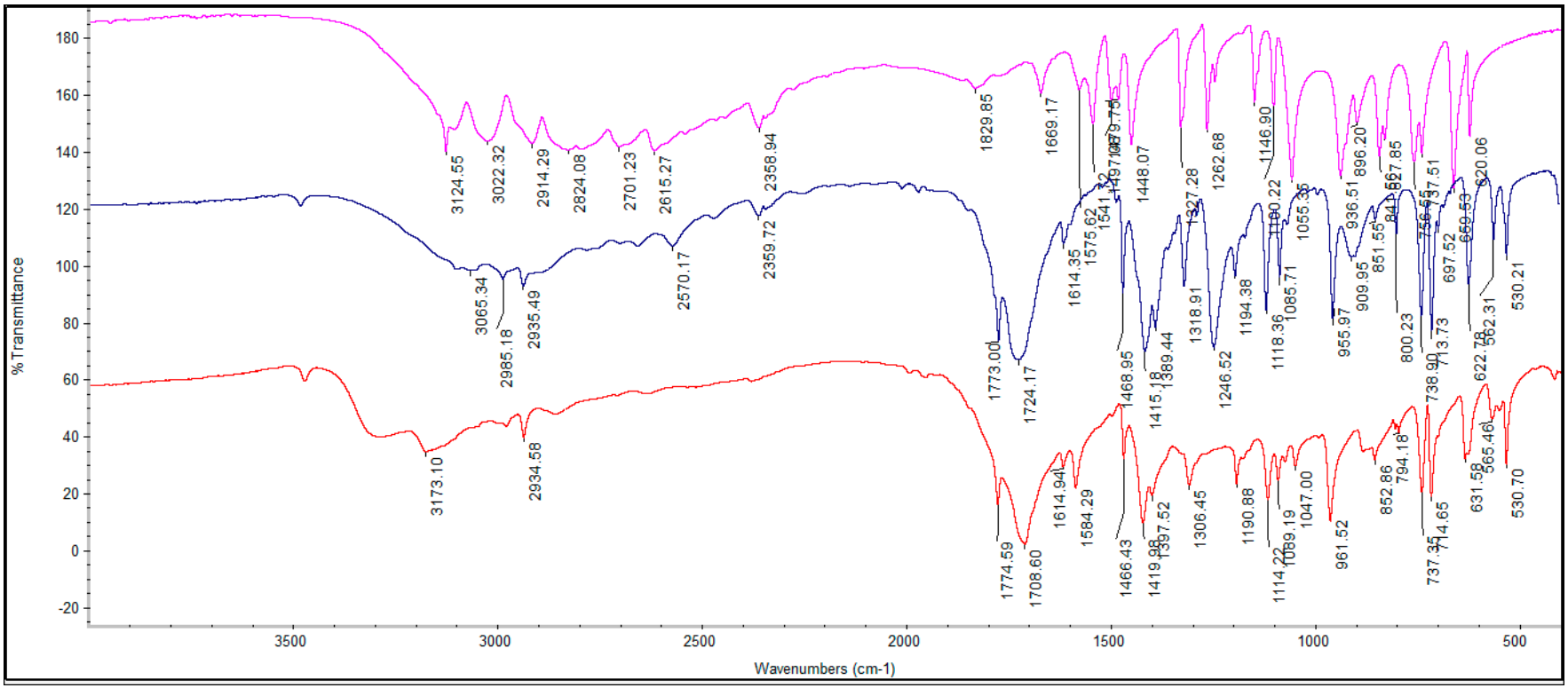

Figure S1. IR spectra of solid polycrystalline samples of imidazole (Purple), NPG (Blue) and **IM^{+}-NPG^{-}-HYD (**Red).

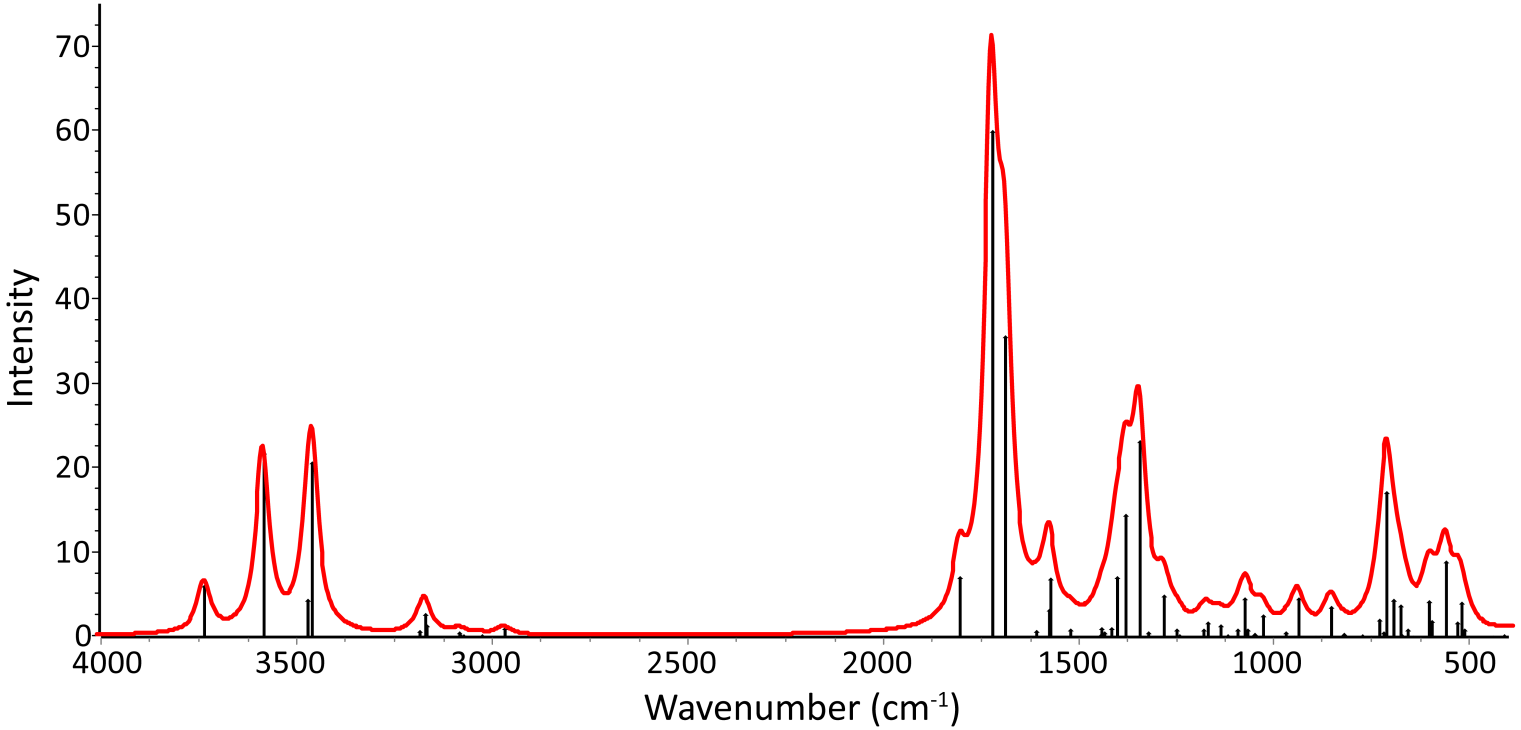

Figure S2. DFT/ M062X/ 6-31G** simulated IR spectrum of **IM^{+}-NPG^{-}-HYD**.

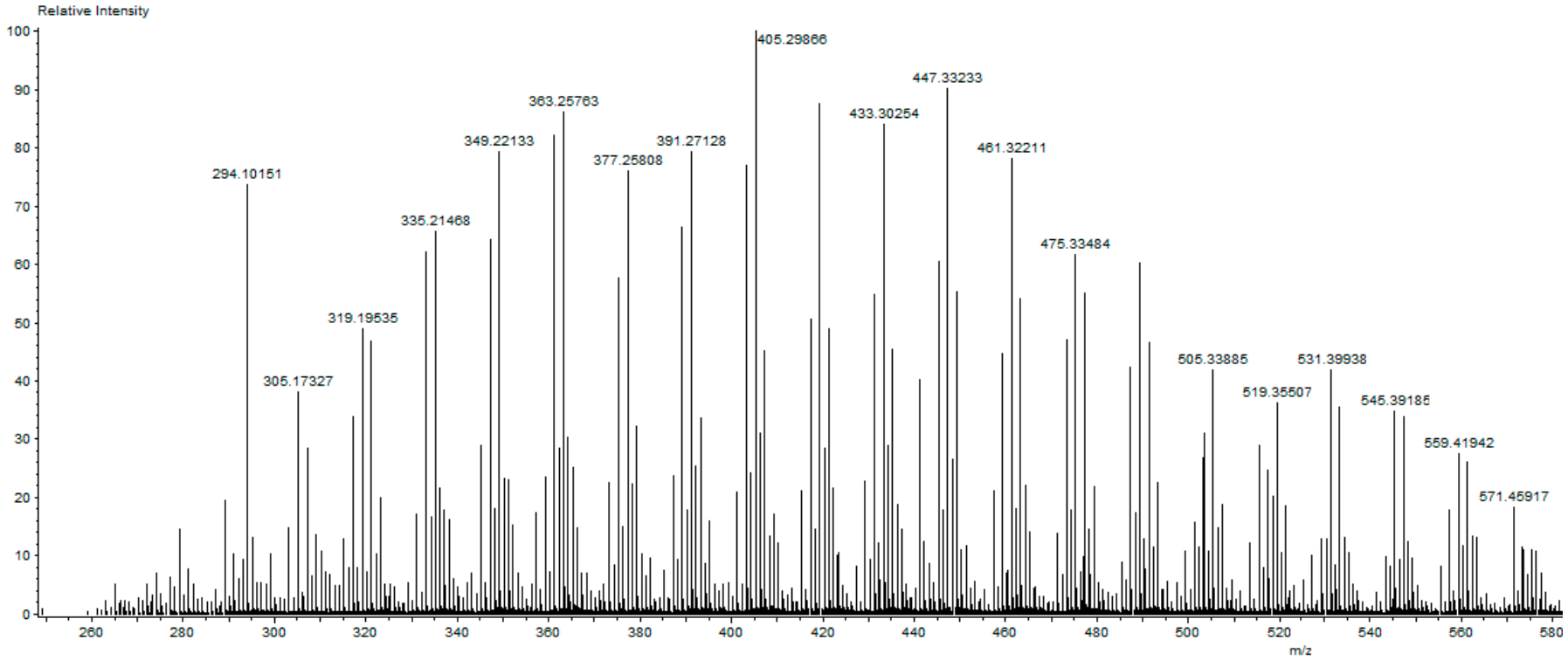

Figure S3. ESI-MS spectrum of polycrystalline samples of **IM^{+}-NPG^{-}-HYD**.

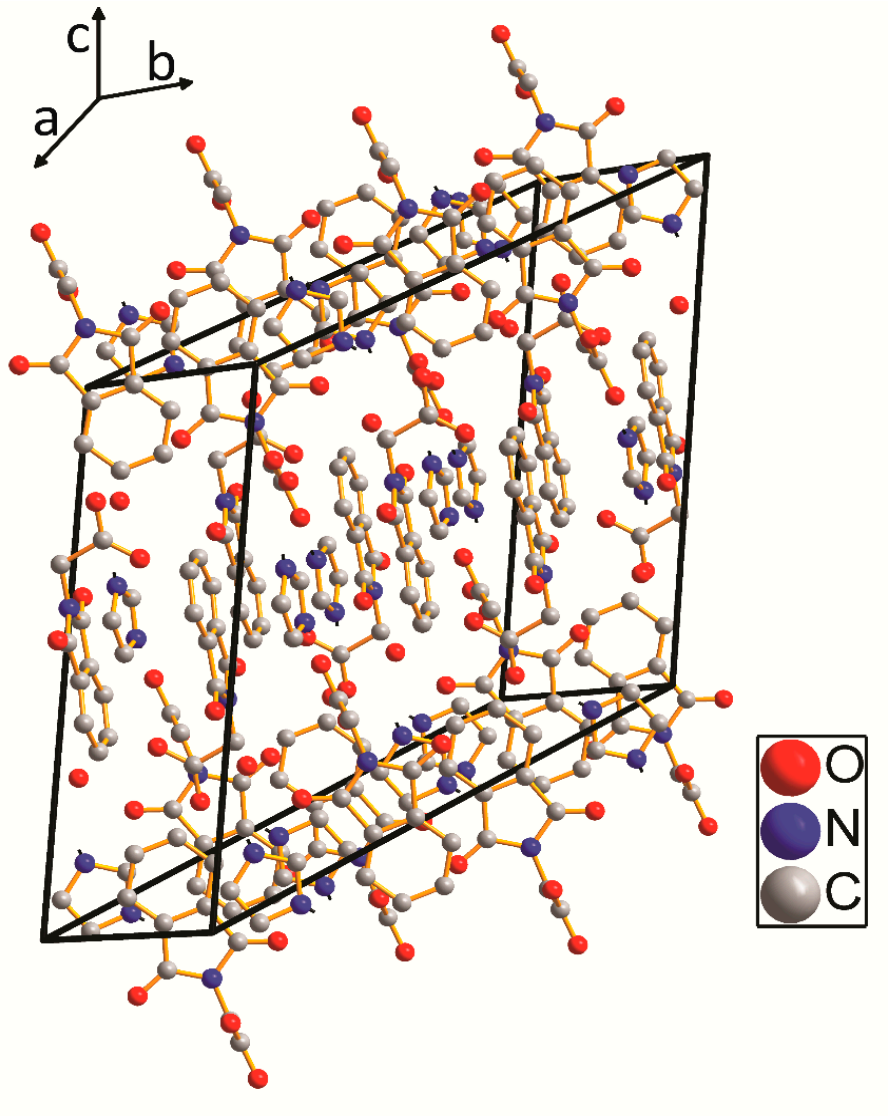

Figure S4. Diagram illustrating the packing of **IM^{+}-NPG^{-}-HYD** in the unit cell at 100 K (H atoms have been omitted for clarity).

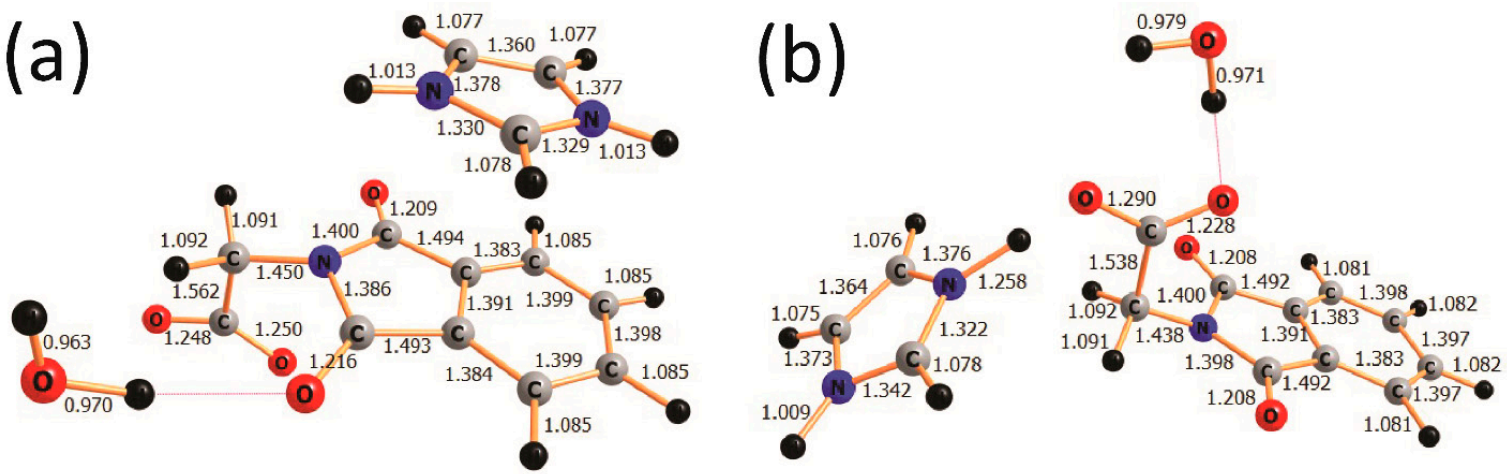

Figure S5. DFT optimized structures in EtOH of both the configuration (a) **A** and (b) **B** of the **IM⁺-NPG⁻-HYD** at the M062X/6-31G** level of theory. Bond distances given in angstrom (Å).

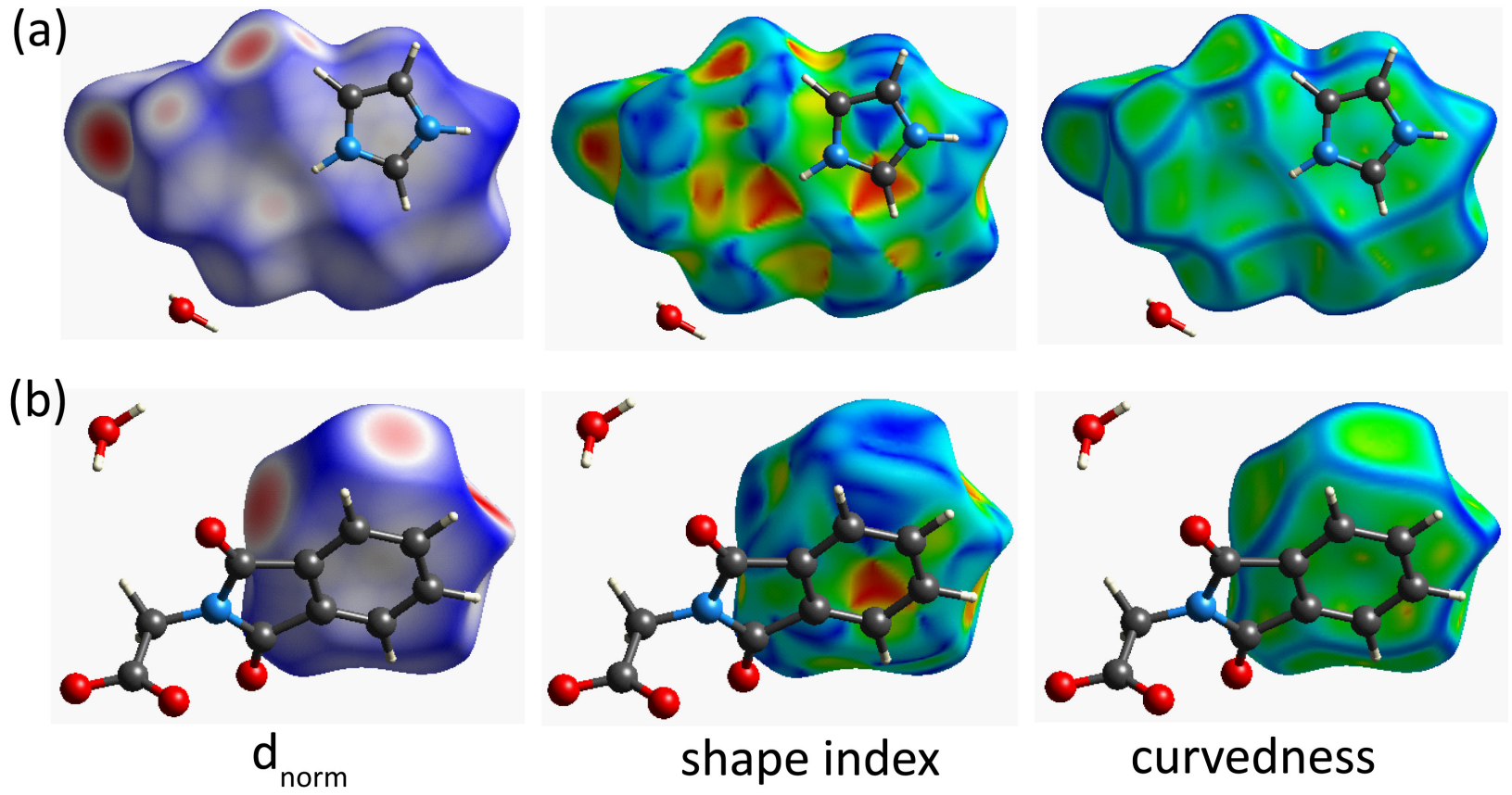

Figure S6. Hirshfeld surface mapped with dnorm (left), shape index (middle), and curvedness (right) for the **IM^{+}-NPG^{-}-HYD**.

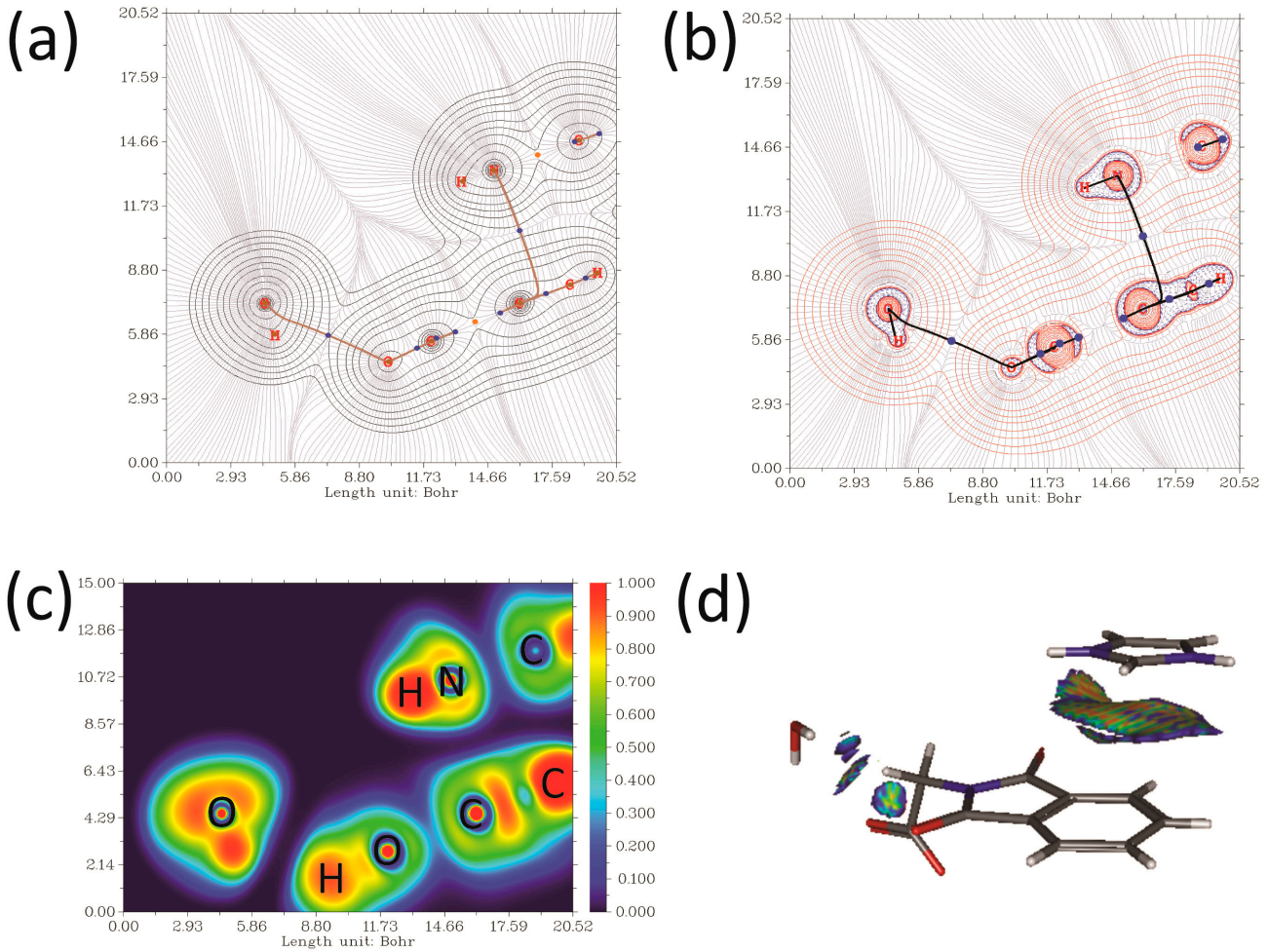

Figure S7. QTAIM analysis of N···C, and O···O interactions in **IM⁺-NPG⁻-HYD** (configuration **A**): (**a**) contour line plots of the electron density ρ, (**b**) contour line plots of the Laplacian distribution of electron density $\nabla^2\rho(r)$, the solid (red) and dashed (blue) lines corresponds to positive and negative values of $\nabla^2\rho(r)$ respectively, (**c**) surface maps of electron localization function (ELF), and (**d**) NCI surface between IM^+ and NPG^- showing electron density for π-π stacking

interaction. Bond paths are shown as black lines, selected zero-flux surfaces, bond critical points, and BCPs, (3, −1) are shown in blue.

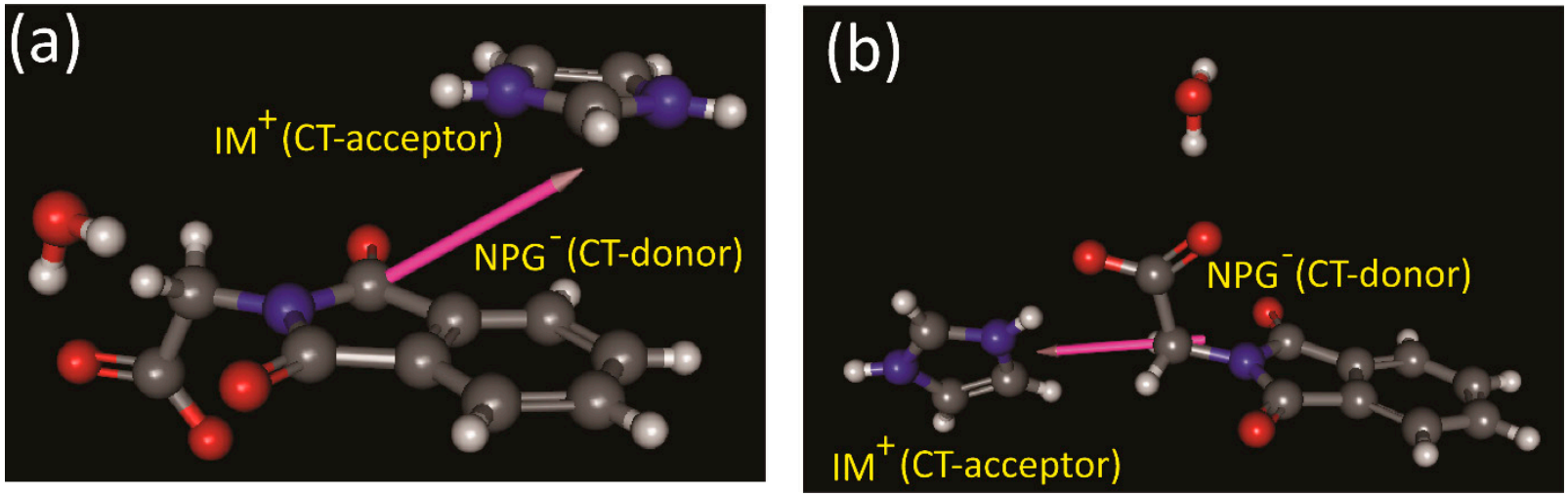

Figure S8. Showing charge transfer donor-acceptor moieties of both the configuration (**a**) **A** and (**b**) **B** of the **IM⁺-NPG⁻-HYD.** Pink arrow represents the dipole moment vector.

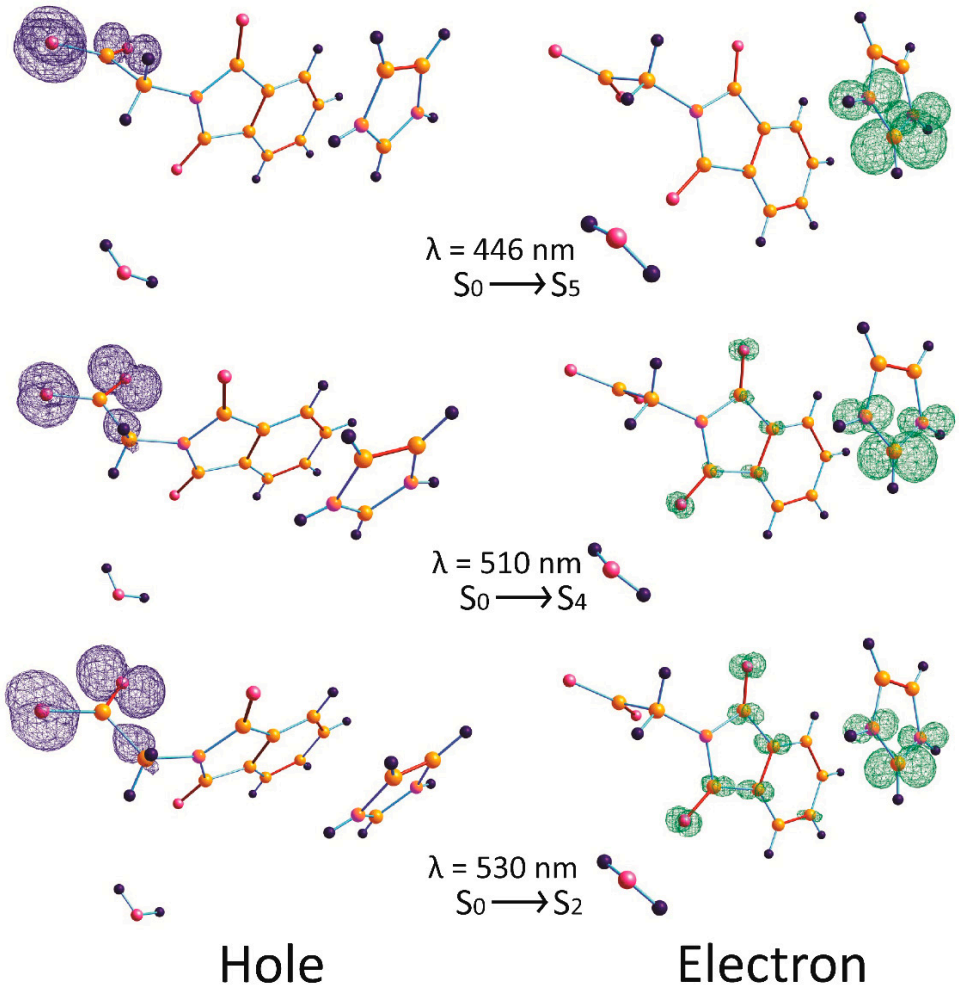

Figure S9. Electron (green isosurface) and hole (blue isosurface) distribution between excited state and ground state of **IM$^+$-NPG$^-$-HYD** for the absorptions at 297, 336, 427, and 443 nm. Value of contour envelopes is 0.002 au.

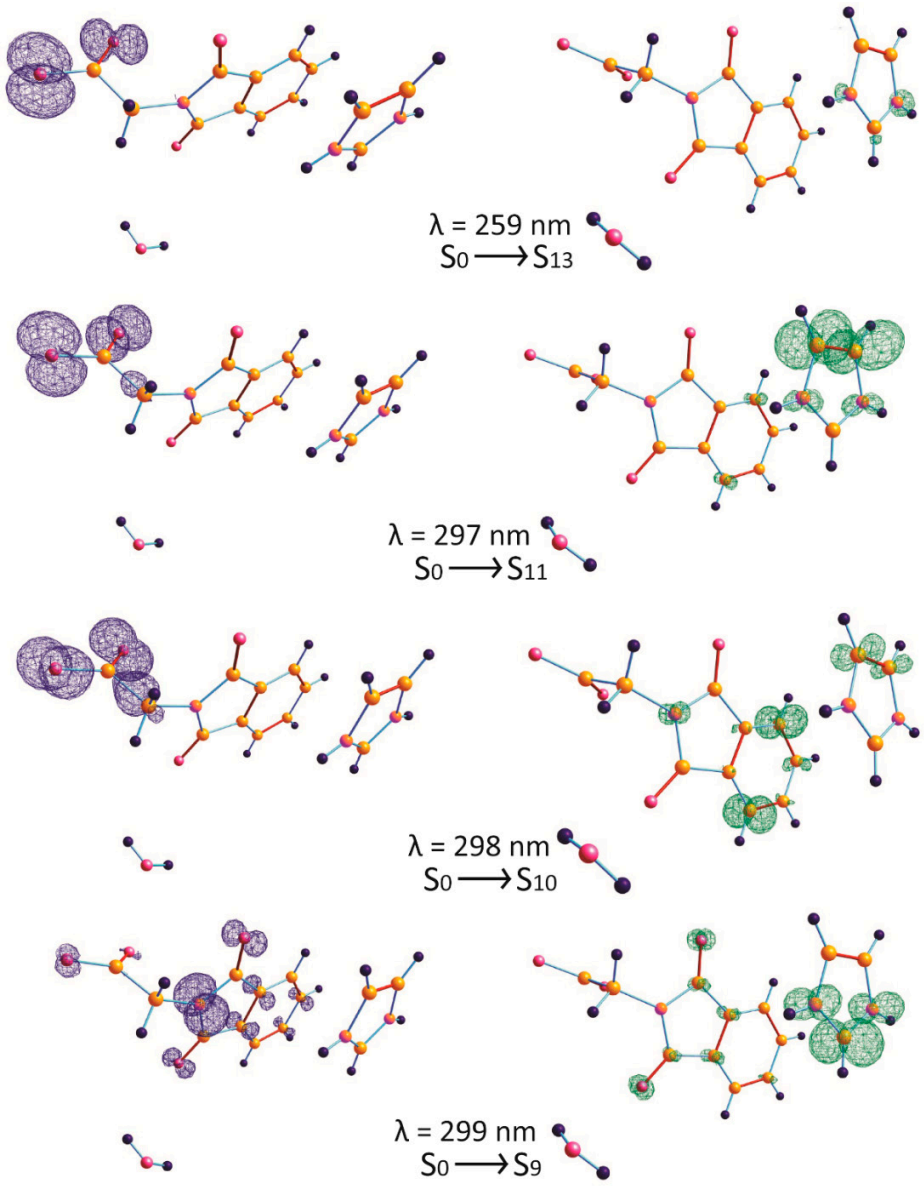
λ = 259 nm
S0 ⟶ S13
λ = 297 nm
S0 ⟶ S11
λ = 298 nm
S0 ⟶ S10
λ = 299 nm
S0 ⟶ S9
Hole
Electron

Figure S10. Electron (green isosurface) and hole (blue isosurface) distribution between excited state and ground state of **IM⁺-NPG⁻-HYD** for the absorptions at 510, 530, 427, and 652 nm. Value of contour envelopes is 0.002 au.

Coordinates of the DFT optimized structure of IM⁺-NPG⁻-HYD

Configuration A				Configuration B			
O	7.595307000	5.902375000	10.678643000	O	10.696753000	6.980409000	9.837611000
O	10.606163000	7.075186000	9.482335000	O	6.437098000	8.562329000	10.202451000
O	7.870231000	6.208031000	12.902763000	O	7.728058000	5.458355000	10.856994000
N	8.673902000	8.228721000	10.040961000	O	7.990569000	5.561764000	13.058598000
C	7.751162000	8.376464000	7.920250000	N	8.649092000	7.911146000	10.371853000
C	9.006323000	7.790664000	7.796061000	C	9.654467000	7.485385000	9.495155000
C	9.562840000	7.617203000	9.170908000	C	9.153861000	7.786681000	8.122376000
C	7.508279000	8.360022000	5.559385000	C	9.769001000	7.637765000	6.893146000
C	9.548096000	7.480554000	6.560969000	H	10.778724000	7.259318000	6.814169000
C	7.499741000	8.601691000	9.375288000	C	9.029727000	7.997985000	5.762223000
C	6.972595000	8.668113000	6.814472000	H	9.471375000	7.899423000	4.779467000
C	8.774407000	7.779996000	5.434775000	C	7.724846000	8.482377000	5.876218000
O	6.512986000	9.050220000	9.911086000	H	7.180545000	8.751543000	4.980214000
C	7.961296000	6.524874000	11.699048000	C	7.112191000	8.624651000	7.123551000
C	8.644572000	7.908374000	11.454471000	H	6.102064000	8.998155000	7.220121000
H	10.529553000	7.026979000	6.473485000	C	7.853665000	8.266721000	8.235062000
H	9.159880000	7.556386000	4.445860000	C	7.492785000	8.289303000	9.682208000
H	6.932563000	8.572956000	4.664980000	C	8.613053000	7.493806000	11.747631000
H	5.993374000	9.123807000	6.918899000	H	9.624699000	7.538192000	12.155094000
H	9.667025000	7.883942000	11.836142000	H	7.979278000	8.186348000	12.303983000
H	8.090634000	8.692441000	11.973359000	C	8.072378000	6.059101000	11.871438000
N	9.551485000	11.105668000	8.869217000	N	8.611758000	7.104286000	14.866837000
N	9.118447000	11.247815000	6.777988000	H	8.293566000	6.314157000	13.940600000
C	8.298364000	11.669844000	8.767591000	N	8.498295000	8.640896000	16.399330000
C	10.034794000	10.854446000	7.656049000	H	8.110180000	9.349815000	17.003278000
C	8.024568000	11.760099000	7.438809000	C	9.863242000	7.249512000	15.419684000
H	10.041405000	10.910386000	9.734572000	H	10.700979000	6.657736000	15.095390000
H	9.217830000	11.167869000	5.772847000	C	9.803683000	8.216837000	16.379757000

H	7.719794000	11.943517000	9.633733000	H	10.551792000	8.619248000	17.038867000
H	10.994601000	10.419914000	7.426735000	C	7.806933000	7.960024000	15.472189000
H	7.158808000	12.129292000	6.915546000	H	6.756522000	8.093623000	15.272585000
O	11.926699000	7.122270000	12.041767000	O	6.706861000	3.078136000	12.020008000
H	11.510934000	7.008385000	11.172488000	H	6.816727000	3.298367000	12.967372000
H	12.308140000	8.005694000	11.998118000	H	7.056032000	3.892008000	11.622341000