Supporting information (SI) for: How the Zundel ($H_5O_2^+$) potential elucidates the stretch and bend frequencies of the hydrated proton

Qi Yu and Joel M. Bowman*

Department of Chemistry and Cherry L. Emerson Center for Scientific Computation, Emory University, Atlanta, Georgia 30322, U.S.A.

E-mail: jmbowma@emory.edu

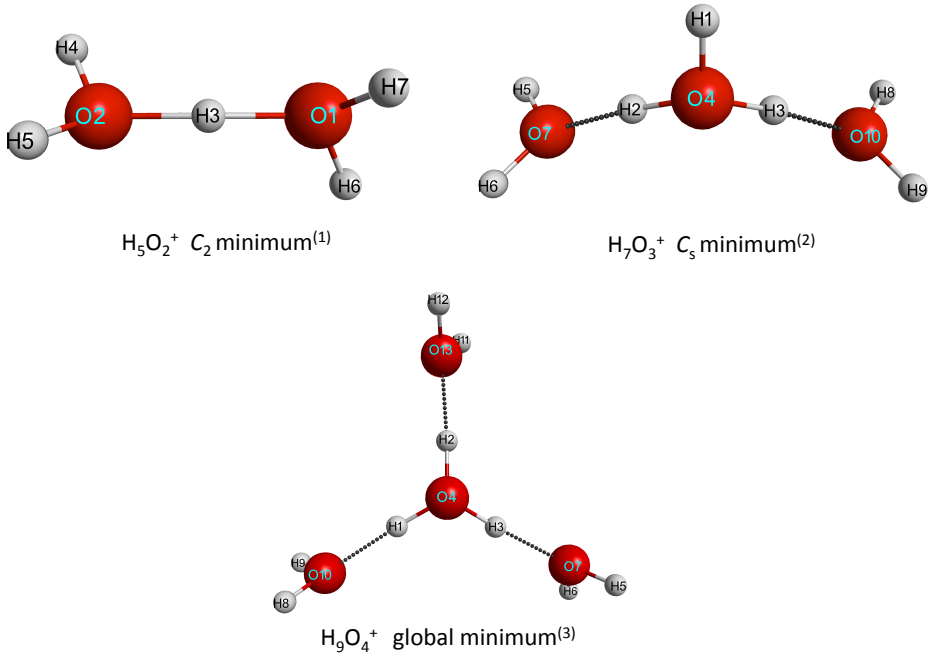

Figure S1: Optimized global minimum geometry of $H_5O_2^+$, $H_7O_3^+$ and $H_9O_4^+$. [(1)]PES calculation [(2)(3)]CCSD(T)-F12,aVTZ calculation

Table S1: Optimized geometry of $H_7O_3^+$ and $H_9O_4^+$ minimum

$H_7O_3^+$	MP2/aVTZ	CCSD(T)-F12/aVTZ	$H_9O_4^+$	MP2/aVTZ	CCSD(T)-F12/aVTZ
R(O_4-H_1) (Å)	0.967	0.964	R(O_4-H_1) (Å)	1.010	1.005
R(O_4-H_2) (Å)	1.038	1.029	R(O_{10}-H_1) (Å)	1.544	1.552
R(O_7-H_2) (Å)	1.452	1.464	R(O_4-O_{10}) (Å)	2.553	2.555
R(O_4-O_7) (Å)	2.487	2.491	R(O_{10}-H_8) (Å)	0.964	0.961
R(O_7-H_5) (Å)	0.964	0.961	$\angle H_1O_4H_2$ deg	112.5	113.1
$\angle H_1O_4H_2$ deg	112.2	112.4	$\angle O_{10}O_4O_7$ deg	114.0	114.6
$\angle O_7O_4O_{10}$ deg	113.0	114.2	$\angle O_{10}H_1O_4$ deg	175.2	175.4
$\angle O_7H_2O_4$ deg	174.4	175.1	$\angle H_8O_{10}H_9$ deg	106.1	106.4
$\angle H_5O_7H_6$ deg	106.9	107.3	$\angle O_4H_1H_3H_2$ deg	30.2	29.1
$\angle H_1O_4O_7H_5$ deg	45.3	50.3			
$\angle H_1O_4O_7H_6$ deg	104.7	107.0			

Table S2: *ab initio* **Harmonic frequencies (in cm^{-1}) of $H_7O_3^+$ and $H_9O_4^+$ minimum**

$H_9O_4^+$			$H_7O_3^+$		
Mode	MP2/aVTZ	CCSD(T)-F12/aVTZ	Mode	MP2/aVTZ	CCSD(T)-F12/aVTZ
1	64	56	1	76	76
2	65	61	2	82	100
3	72	63	3	126	124
4	104	76	4	238	192
5	106	121	5	252	209
6	119	130	6	351	342
7	241	147	7	369	366
8	261	162	8	402	392
9	265	175	9	403	394
10	286	271	10	481	479
11	341	306	11	614	589
12	342	308	12	1079	1054
13	376	343	13	1261	1242
14	378	345	14	1603	1625
15	417	372	15	1632	1654
16	737	712	16	1697	1699
17	963	944	17	1700	1709
18	966	948	18	**2462**	**2551**
19	1216	1186	19	**2618**	**2702**
20	1635	1644	20	3789	3818
21	1635	1645	21	3789	3818
22	1646	1654	22	**3812**	**3828**
23	1728	1731	23	3897	3914
24	1729	1733	24	3897	3914
25	**2928**	**2995**			
26	**2932**	**2998**			
27	**3024**	**3089**			
28	3797	3856			
29	3797	3858			
30	3798	3858			
31	3905	3955			
32	3906	3955			
33	3907	3956			

the bold text are stretching modes in hydronium part

Coordinates for $H_7O_3^+$ (in Å)

H	1.7491200611	-0.0796214950	-0.0000000000
H	0.3439059486	-0.2140113235	0.8689463747
H	0.3439059486	-0.2140113235	-0.8689463747
O	0.8513606628	-0.4310220136	-0.0000000000
H	-0.5625577669	0.8116970646	2.5631675028
H	-0.6119572769	-0.7283452143	2.7127202516
O	-0.4345874853	-0.0158831079	2.0923462443
H	-0.5625577669	0.8116970646	-2.5631675028
H	-0.6119572769	-0.7283452143	-2.7127202516
O	-0.4345874853	-0.0158831079	-2.0923462443

Coordinates for $H_9O_4^+$ (in Å)

H	-2.5042885607	-0.0886683874	-0.2749280329
H	-2.8661133680	-0.6906072983	1.2483490766
H	-1.2781610854	-0.6760414420	0.7079144092
O	-2.2496866456	-0.7313336709	0.4551079807
H	0.7562259336	-1.4858668951	1.0559952498
H	0.8092260973	0.0481979979	1.1646689663
O	0.2093151358	-0.7016040869	1.1505838047
H	-3.0420356836	0.4862456451	-2.3472777433
H	-3.2269671452	1.7085997555	-1.4310903499
O	-2.8277613673	0.8364399610	-1.4786220685
H	-3.8207598503	-0.2043184550	3.2330415854
H	-4.4930920687	-1.4172813483	2.5663649372
O	-3.9060510714	-0.6750215308	2.4002719735