

Supplementary Information

Table 2. The Cartesian coordinates for the crystal structures and optimized [B3LYP/6-311+G(2d,2p)] structures of the two isomers of $H_{11}O_5^+$ (IYEPEH and BEXFEQ), and the $H_{15}O_7^+$ (NEBDII).

	IYEPEH						BEXFEQ						NEBDII					
	CRYSTAL			OPTIMIZED			CRYSTAL			OPTIMIZED			CRYSTAL			OPTIMIZED		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
O1	-2.688	-0.195	0.648	0.980	0.022	-0.715	-2.484	0.758	-0.340	-2.492	0.000	-0.517	-2.826	-1.128	-0.696	1.239	0.739	-1.389
H1a	-1.991	-0.087	0.174	1.858	0.026	-0.220	-1.825	0.913	0.066	-2.757	0.000	-1.447	-2.638	-0.192	-0.568	0.701	1.483	-0.916
H1b	-2.569	-0.801	1.232	0.420	-0.802	-0.497	-2.687	-0.331	-0.296	-1.899	0.846	-0.288	-3.679	-1.289	-0.294	1.950	0.404	-0.737
H1c	-2.889	0.475	1.127	0.403	0.833	-0.492	-3.319	1.397	0.086	-1.899	-0.846	-0.288	-2.204	-1.678	-0.207	0.614	-0.032	-1.561
O2	-0.820	-0.135	-0.957	3.280	-0.028	0.458	-0.215	1.711	0.036	-0.915	1.813	0.078	-2.363	1.363	-0.049	-0.192	2.406	-0.140
H2a	-0.370	0.557	-0.753	3.485	0.144	1.382	0.317	1.209	0.304	-0.145	1.366	0.491	-1.399	1.316	-0.179	-0.553	1.974	0.658
H2b	-0.335	-0.825	-0.859	4.101	0.049	-0.039	-0.019	2.329	0.467	-1.158	2.578	0.610	-2.455	1.908	0.744	0.077	3.302	0.086
O3	0.447	2.044	-0.399	-0.675	1.851	-0.069	1.536	-0.182	0.456	0.994	0.000	0.944	0.046	1.668	0.389	-1.236	0.602	1.703
H3a	-0.164	2.483	-0.008	-0.800	2.695	-0.514	1.557	-0.600	1.120	1.805	0.000	0.380	0.508	2.306	-0.180	-0.633	-0.162	1.773
H3b	0.904	2.571	-0.900	-1.547	1.438	0.052	2.250	-0.172	0.130	1.306	0.000	1.856	-0.129	2.186	1.187	-1.562	0.784	2.591
O4	2.262	0.254	0.969	-2.819	-0.022	0.369	4.182	-0.542	-0.281	3.163	0.000	-0.659	1.285	-0.293	-0.665	0.522	-1.627	1.232
H4a	2.016	-0.478	0.611	-3.60	-0.027	-0.192	4.338	-1.301	-0.395	3.685	-0.771	-0.901	1.145	0.617	-0.365	0.461	-2.429	1.763
H4b	1.831	0.897	0.620	-3.151	-0.029	1.276	4.663	-0.079	-0.675	3.685	0.771	-0.901	0.470	-0.453	-1.149	0.199	-1.856	0.341
O5	0.982	-1.958	-0.345	-0.631	-1.845	-0.078	-2.900	-1.682	-0.044	-0.915	-1.813	0.078	3.867	0.606	-0.451	-2.692	-0.520	-0.505
H5a	0.569	-2.450	0.206	-1.516	-1.460	0.040	-3.663	-1.684	0.111	-1.157	-2.578	0.610	3.305	-0.086	-0.061	-2.505	-0.015	0.303
H5b	1.544	-2.424	-0.783	-0.727	-2.697	-0.514	-2.565	-2.183	0.458	-0.145	-1.366	0.491	4.753	0.199	-0.389	-3.469	-0.135	-0.920
O6													5.628	-1.200	0.740	-0.372	-1.326	-1.466
H6a													4.758	-1.528	1.014	-0.408	-1.935	-2.212
H6b													6.042	-1.821	0.126	-1.305	-1.052	-1.254
O7													-5.261	-1.038	0.601	2.790	-0.156	0.421
H7a													-5.277	-0.073	0.712	2.273	-0.830	0.895
H7b													-6.209	-1.238	0.659	3.702	-0.454	0.351