

Table 3. The Cartesian coordinates for the optimized [B3LYP/6-311+G(2d,2p)] structure of  $\text{H}_{17}\text{O}_8^+$ .

Atom	X	Y	Z
O1	-1.278	-1.741	-0.729
H1a	-0.839	-1.10	-1.429
H1b	-1.785	-2.425	-1.179
O2	0.060	-0.013	2.115
H2a	0.089	-0.018	3.078
O3	0.884	-1.914	0.783
H3a	0.558	-1.152	1.485
H3b	0.082	-2.107	0.213
H3c	1.535	-1.451	0.177
O4	-2.062	0.204	0.873
H4a	-1.213	0.117	1.536
H4b	-1.853	0.987	0.281
H4c	-2.012	-0.601	0.276
O5	-0.906	1.964	-0.719
H5a	-0.601	1.253	-1.422
H5b	-1.267	2.737	-1.166
O6	1.245	1.696	0.794
H6a	1.792	1.118	0.183
H6b	0.497	2.049	0.226
H6c	0.774	1.009	1.490
O7	-0.057	0.011	-2.048
H7a	-0.085	0.017	-3.008
O8	2.120	-0.209	-0.814
H8a	1.323	-0.129	-1.483
H8b	2.949	-0.291	-1.298