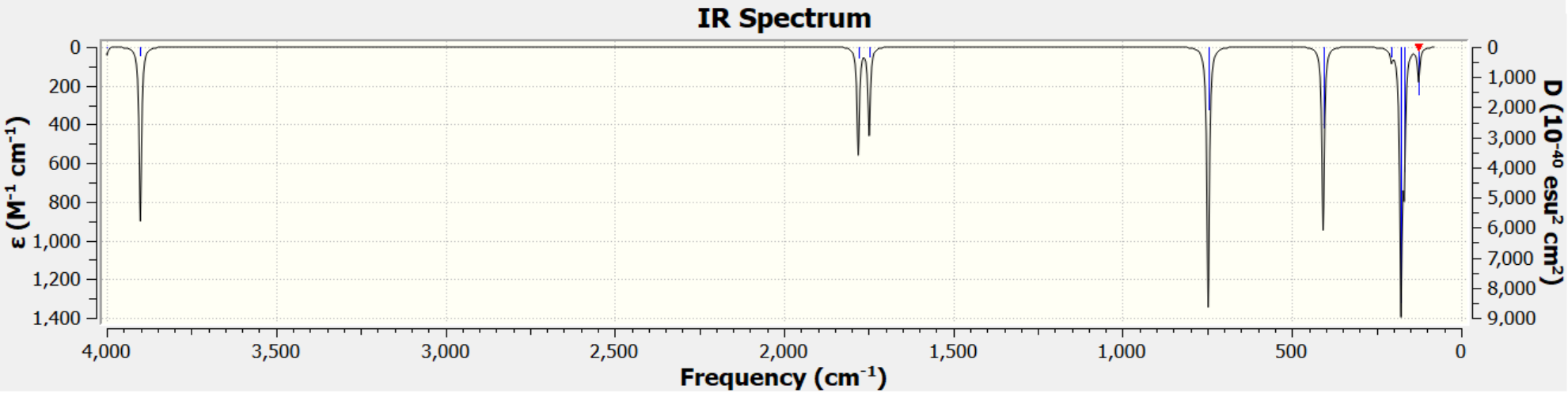
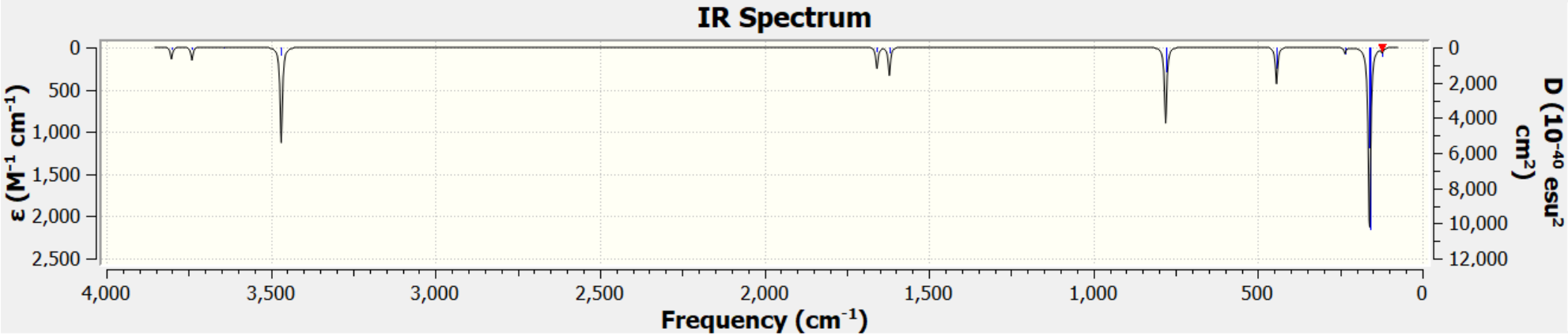
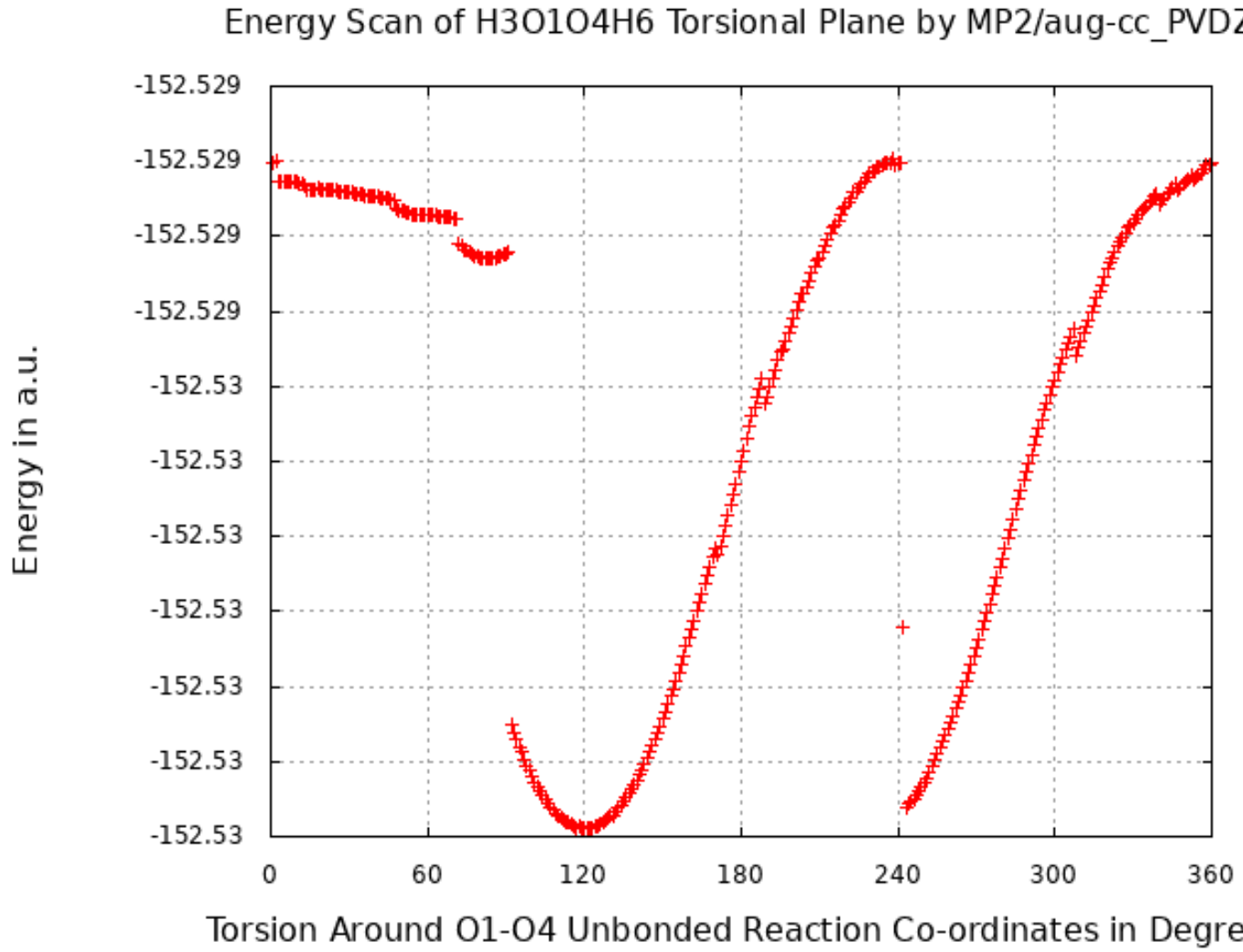
SUPPLEMENTARY FIGURES

SUP FIG.1. IR by HF/6-31G+ (top) and DFT/6-31G+ (bottom) computed by Gaussian 16.

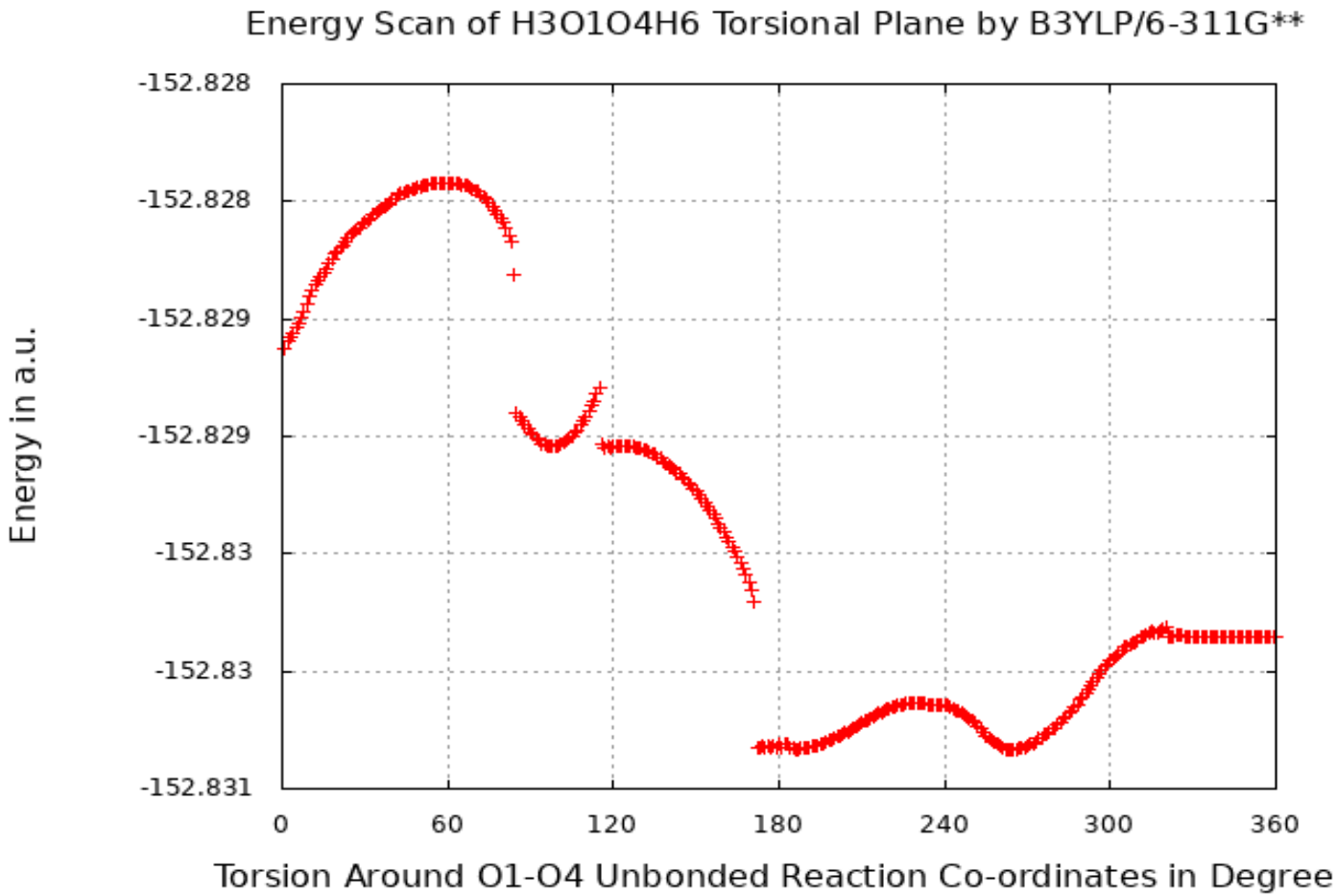




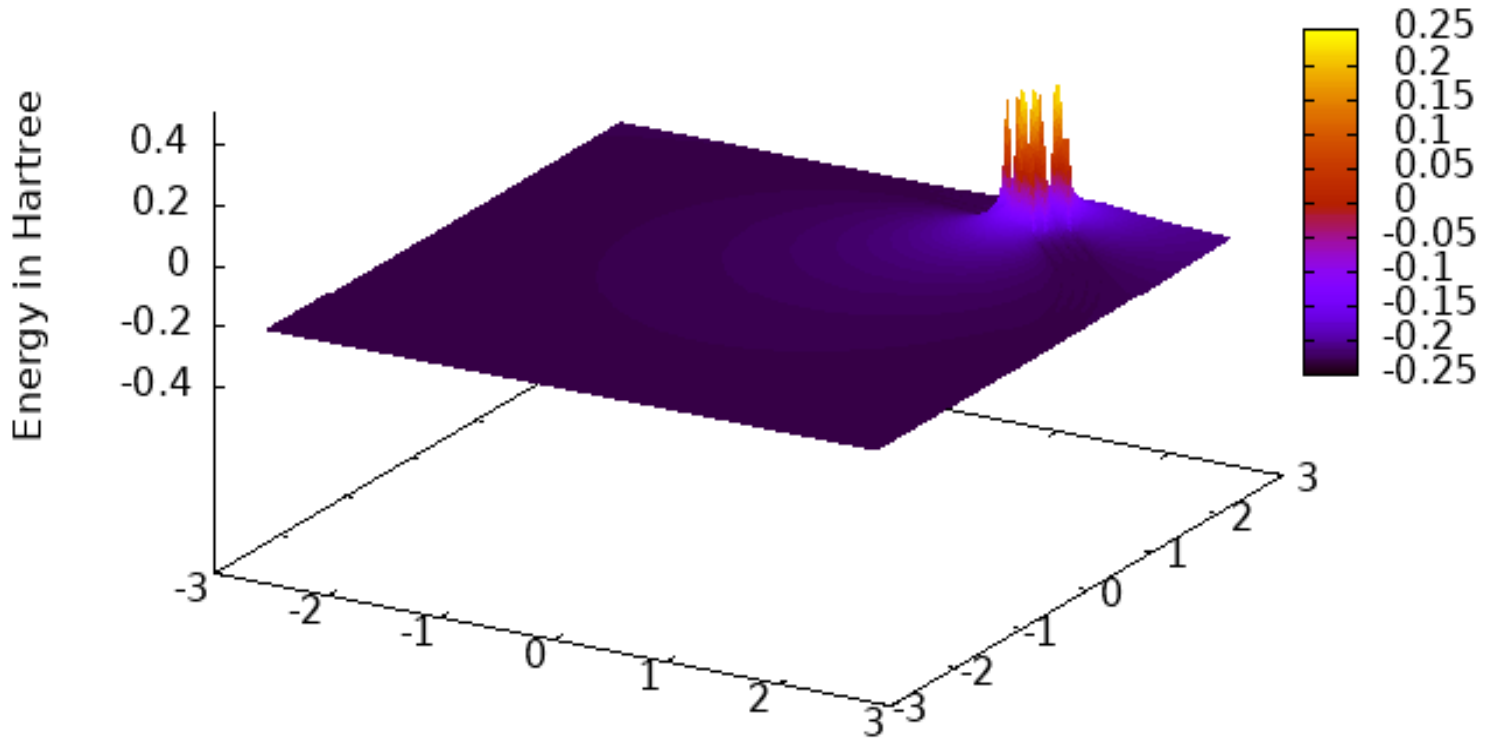
SUP FIG.2. First principle based torsion potential scan of water dimer around O1-O4 interaction by MP2/aug-cc PVDZ method.



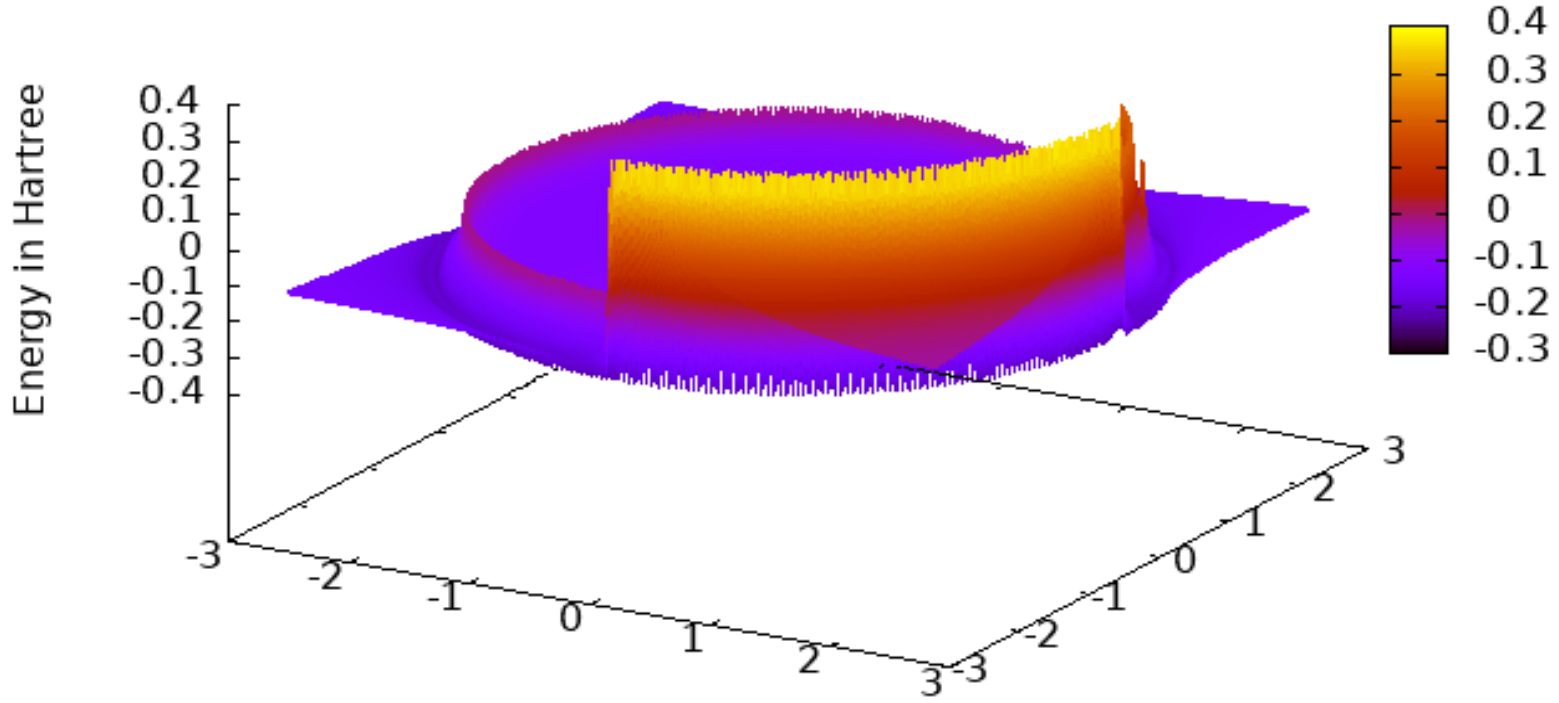
SUP FIG.3.


Energy Scan of H3O1O4H6 Torsional Plane by B3YLP/6-311G**
Energy in a.u.
-152.828
-152.828
-152.829
-152.829
-152.83
-152.83
-152.831
0
60
120
180
240
300
360
Torsion Around O1-O4 Unbonded Reaction Co-ordinates in Degree

SUP FIG.4. Anisotropic Singularities in Energy from Torsion of Unbonded O1-O4 Atoms Showing Signature of Water Dimer Break-up in Water Medium Computed by AM1 Method.



SUP FIG.5. Anisotropic Singularities in Energy from Torsion of Unbonded O1-O4 Atoms Showing Signature of Water Dimer Break-up in Water Medium Computed by PM3 Method.



Optimized geometry of water dimer in gas phase

(Gaussian 16 calculations) (Atoms are defined in Fig.1) [Supplementary Table 1]

Method	O1-O4 distance (Å)	O4-H2 dimeric H-bond distance (Å)	H2-O1-H3 angle (degree)	H5-O4-H6 angle (degree)	O1-H2-O4 angle (degree)
HF/6-31G	2.842	1.885	111.60	112.18	179.60
HF/6-311+G	2.833	1.870	112.78	112.71	179.12
DFT/B3LP-6-31G	2.777	1.794	108.99	109.61	173.65
DFT/ωB97X-D/6-31G	2.764	1.787	109.82	110.57	174.40
MP2/ cc-pVDZ	2.908	1.943	101.86	105.72	172.67
MP2/aug-cc-pVDZ	2.916	1.951	104.20	104.28	171.12