Title: Quantum Signature in Anisotropic Singularities of Dihedral Energy in Hydrogen Bond Breaking of Water Dimer

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FIGURES AND CAPTIONS

Fig.1. Atomic Labelling of Water Dimer. The Hydrogen Bond is Formed between O4 and H2 atoms; O1 and O4 Atoms are not Under Chemical Bonding Interaction.

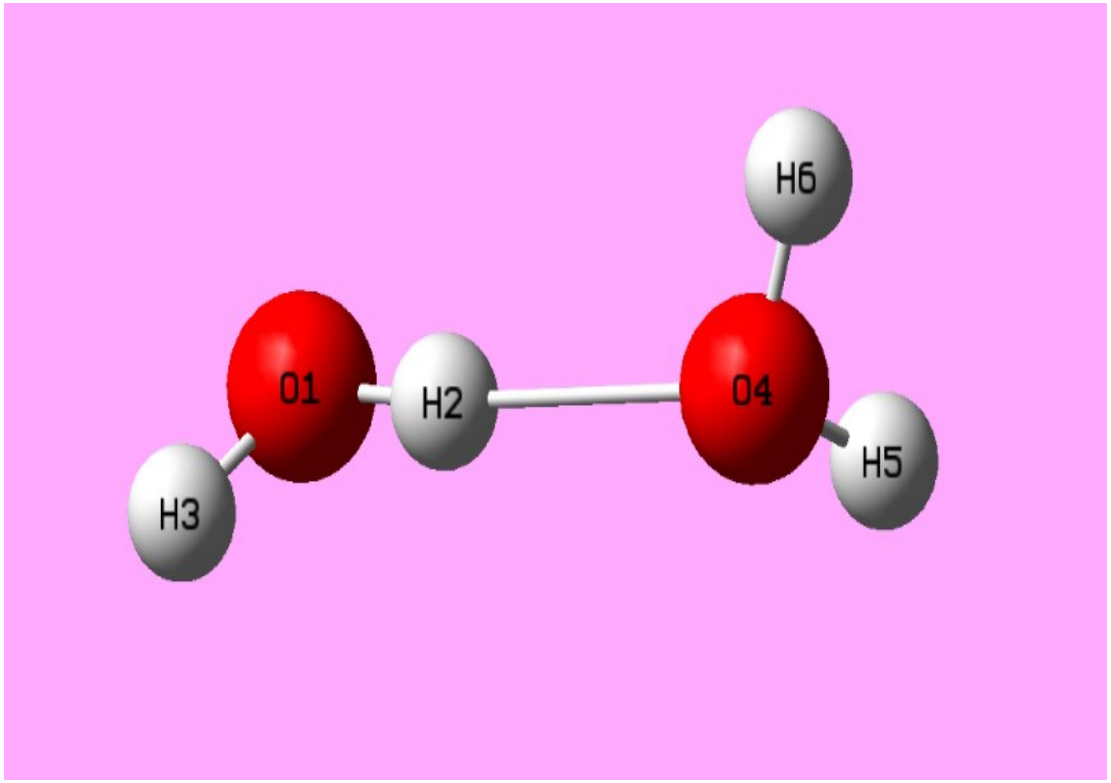

Fig.2. HOMO-LUMO Energy gap and Orbitals of Water Dimer and Electrostatics Potential Map of Water Dimer as computed by B3YLP/6-31G* basis are show below.

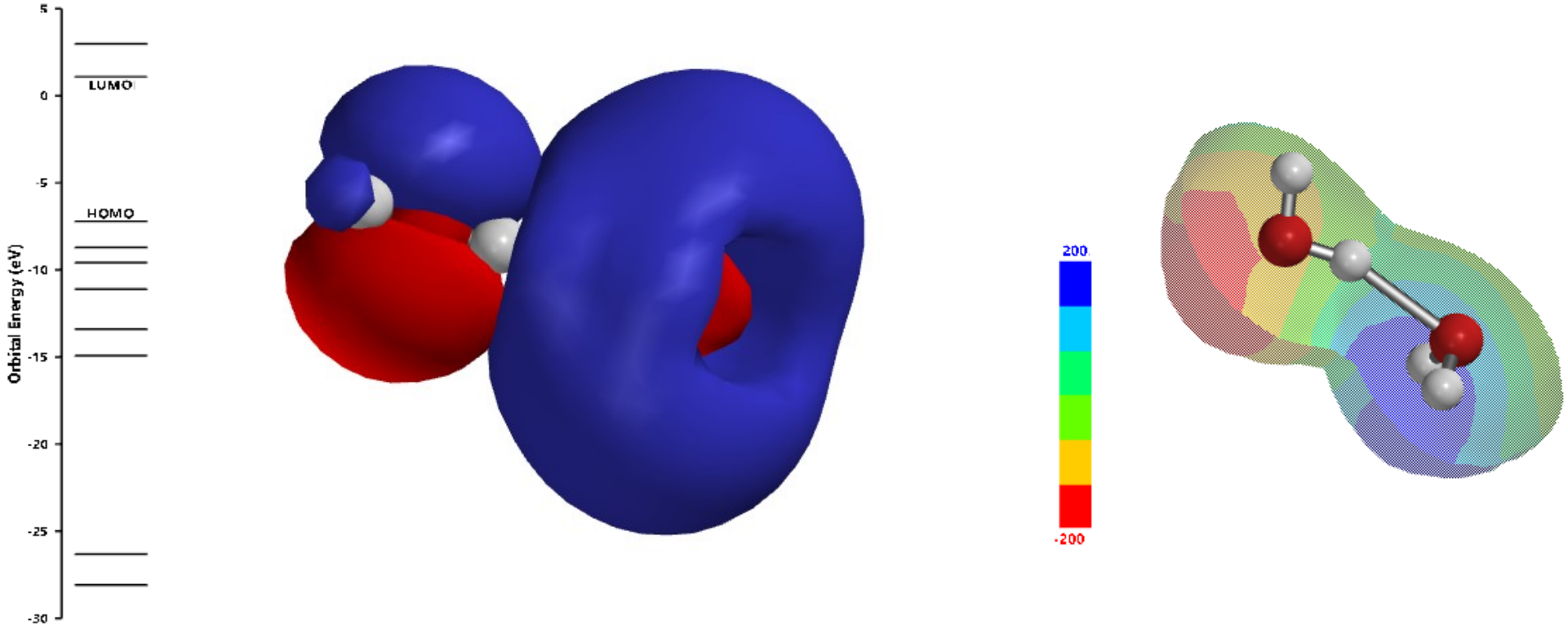

FIG. 3 Estimation of Water Dimer Binding Energy from O4-H2 Bond via HF/6-31G* Basis

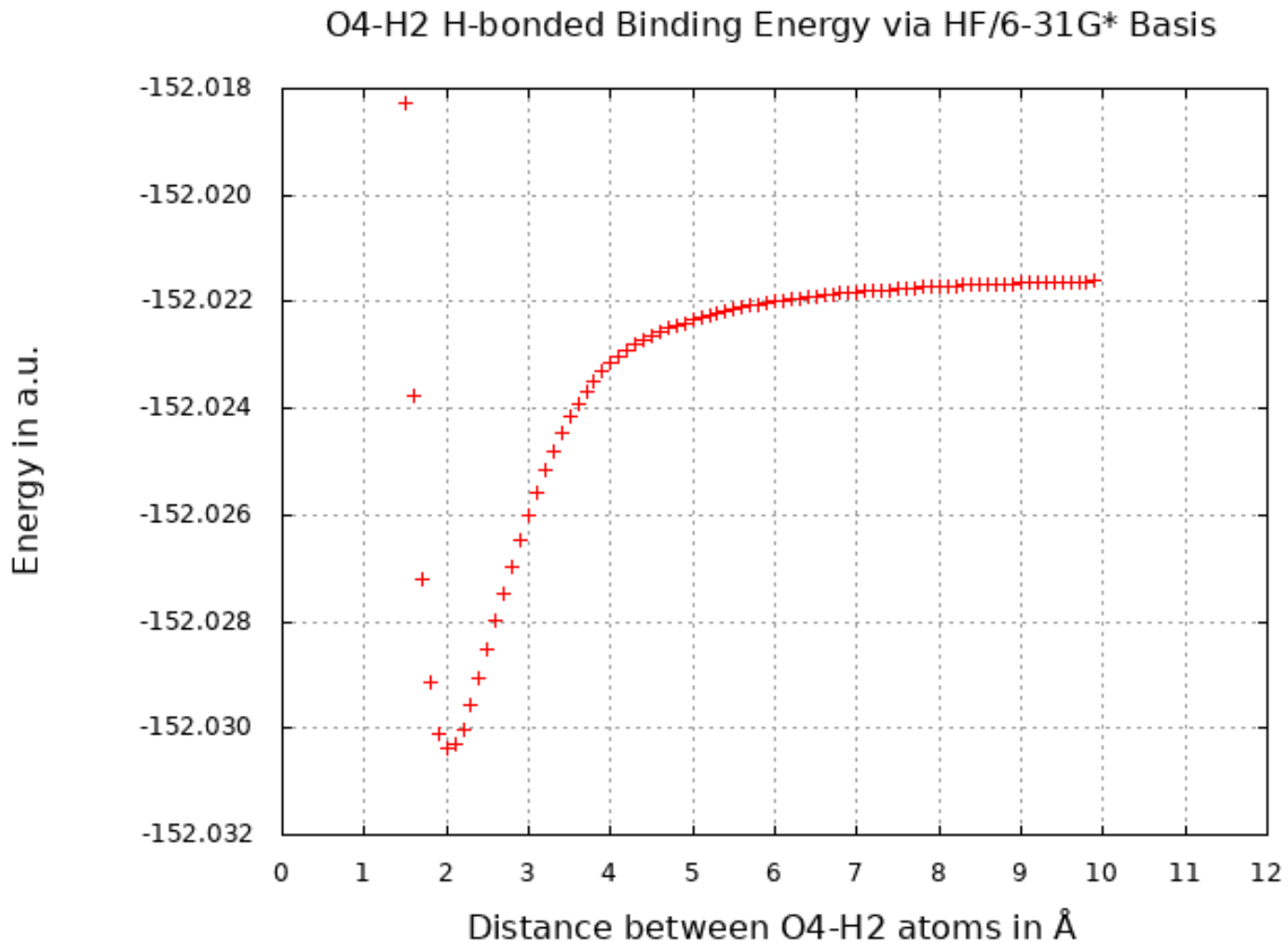

FIG. 4. Estimation of Water Dimer Binding Energy from O4-H2 Bond via MP2/ccDVPZ Basis

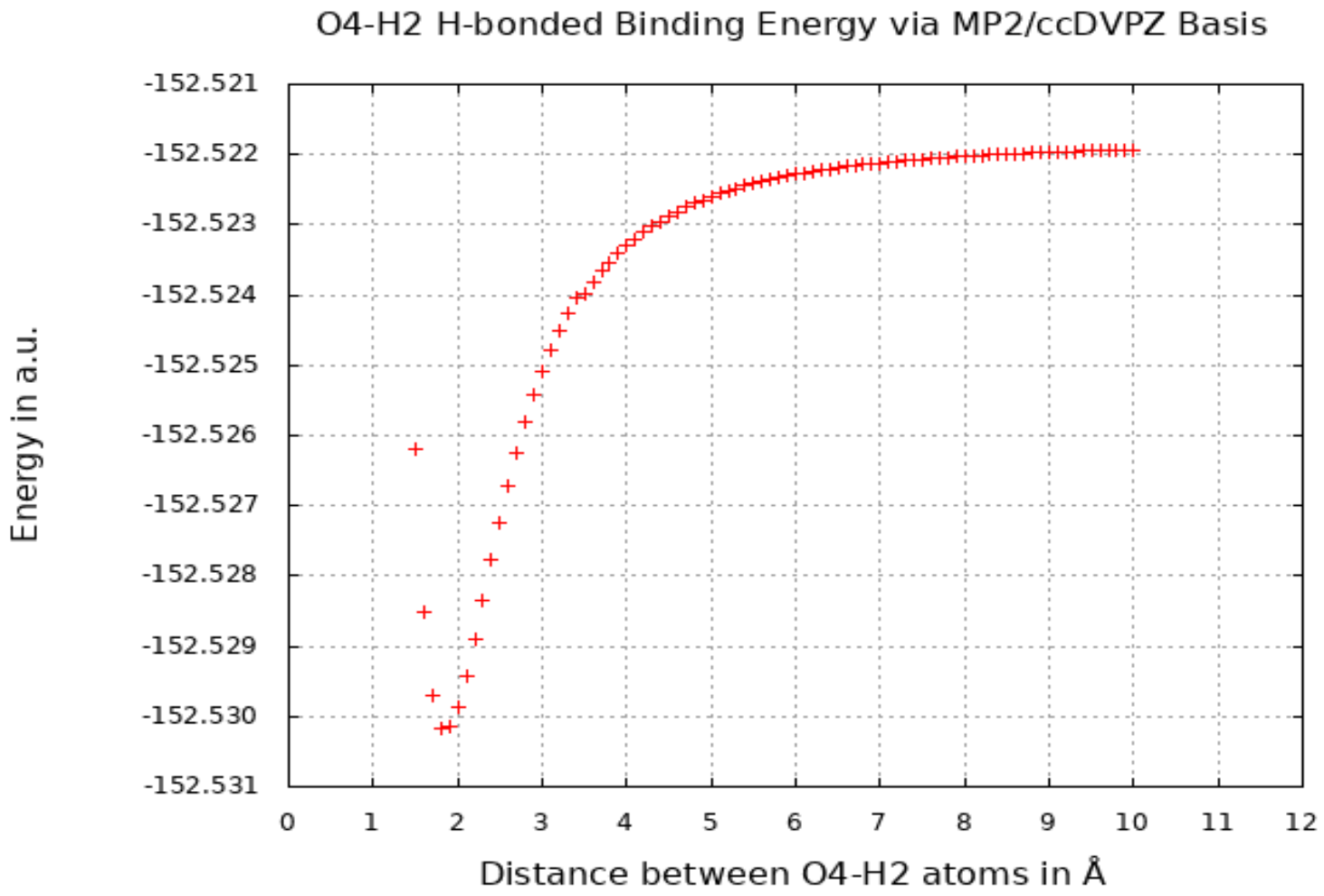

FIG. 5. Estimation of Water Dimer Binding Energy from O1-O4 Interaction Distance via HF/6-31G* Basis

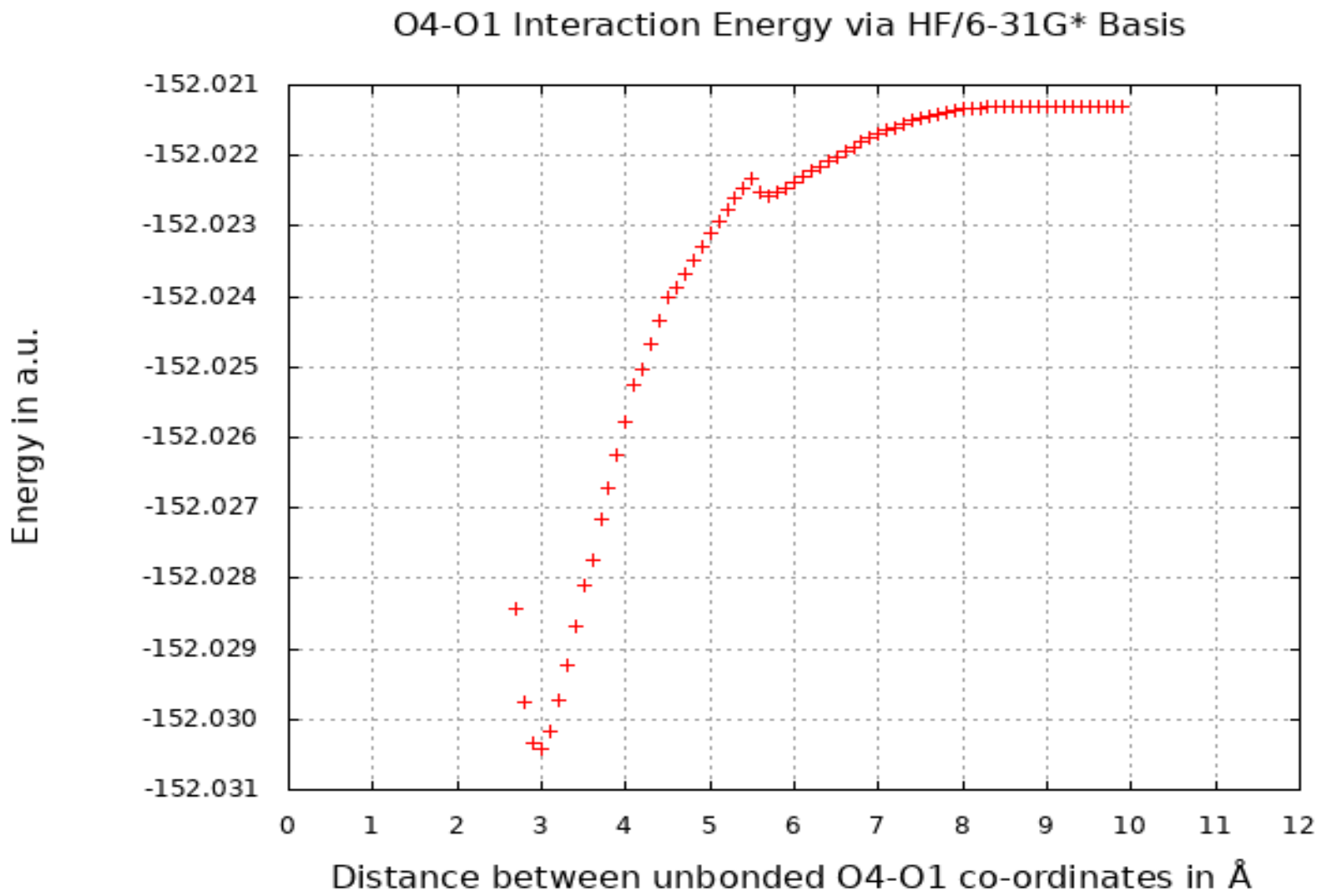

FIG. 6. Estimation of Water Dimer Binding Energy from O1-O4 Interaction Distance via MP2/ccDVPZ Basis

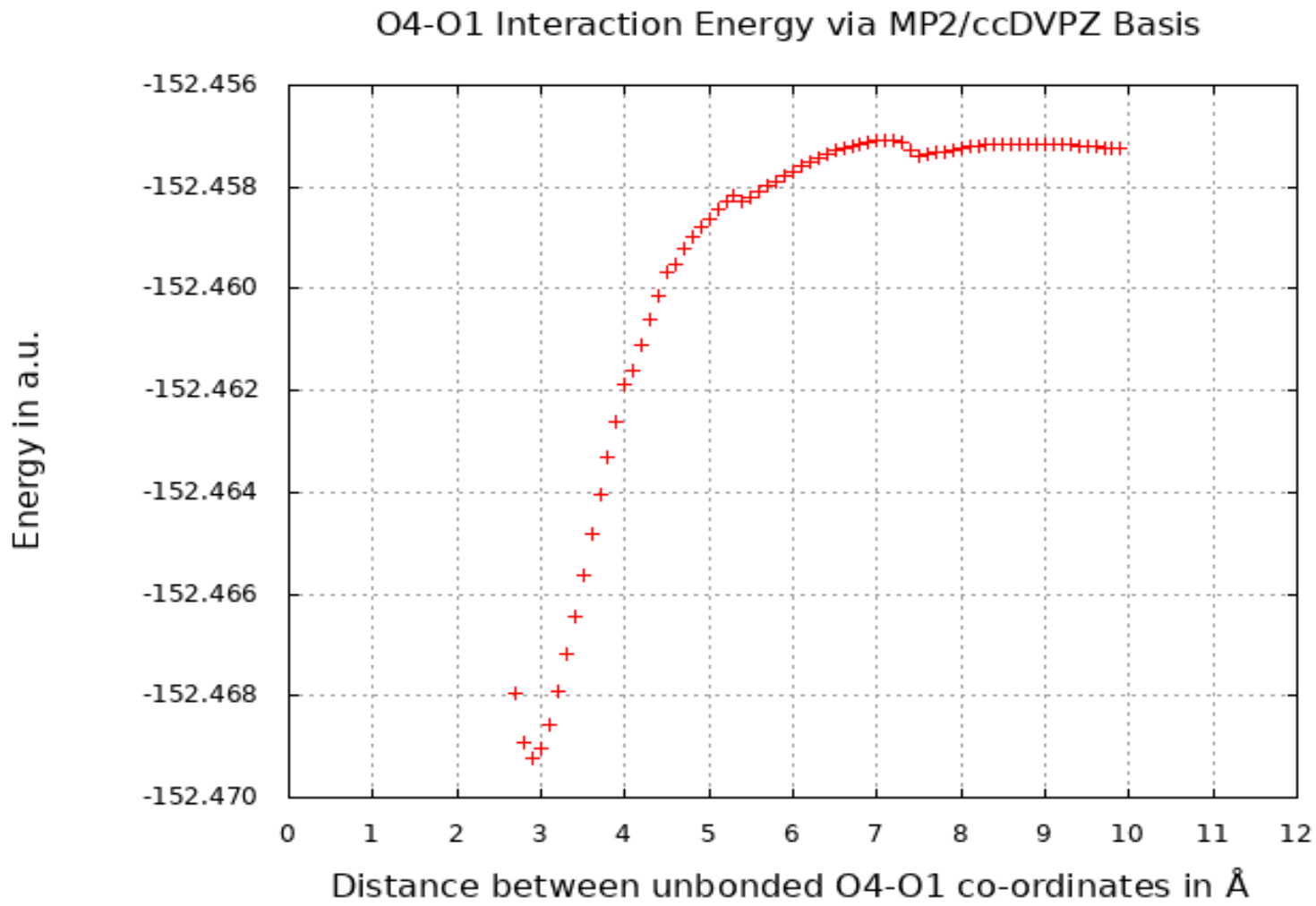

FIG. 7. Water Dimer Donor (O4) and Acceptor (H2) Atoms Give Two Separate Split in O-H Vibration Mode of IR as Computed via EDF2/6-31G* in Spartan 18.

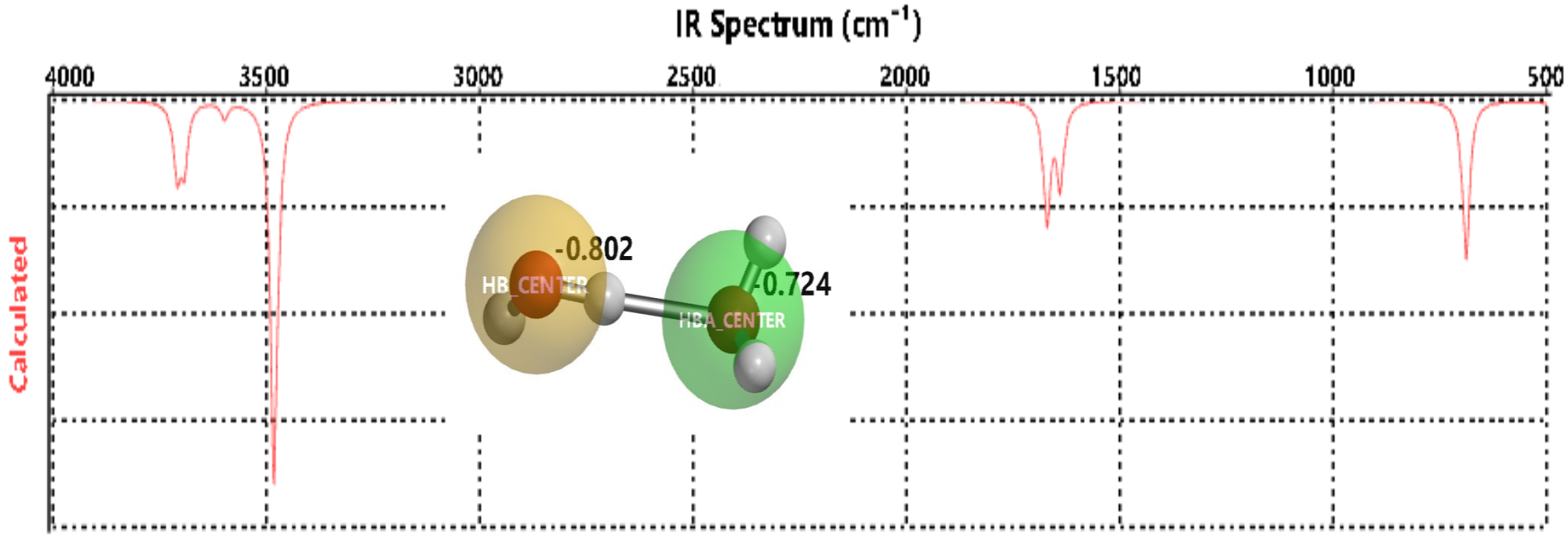

Fig.8. IR Spectra Computed via DFT/wB97/6-31G* (Top) and MP2/ccPVDZ (bottom) as Implemented in Spartan 18.

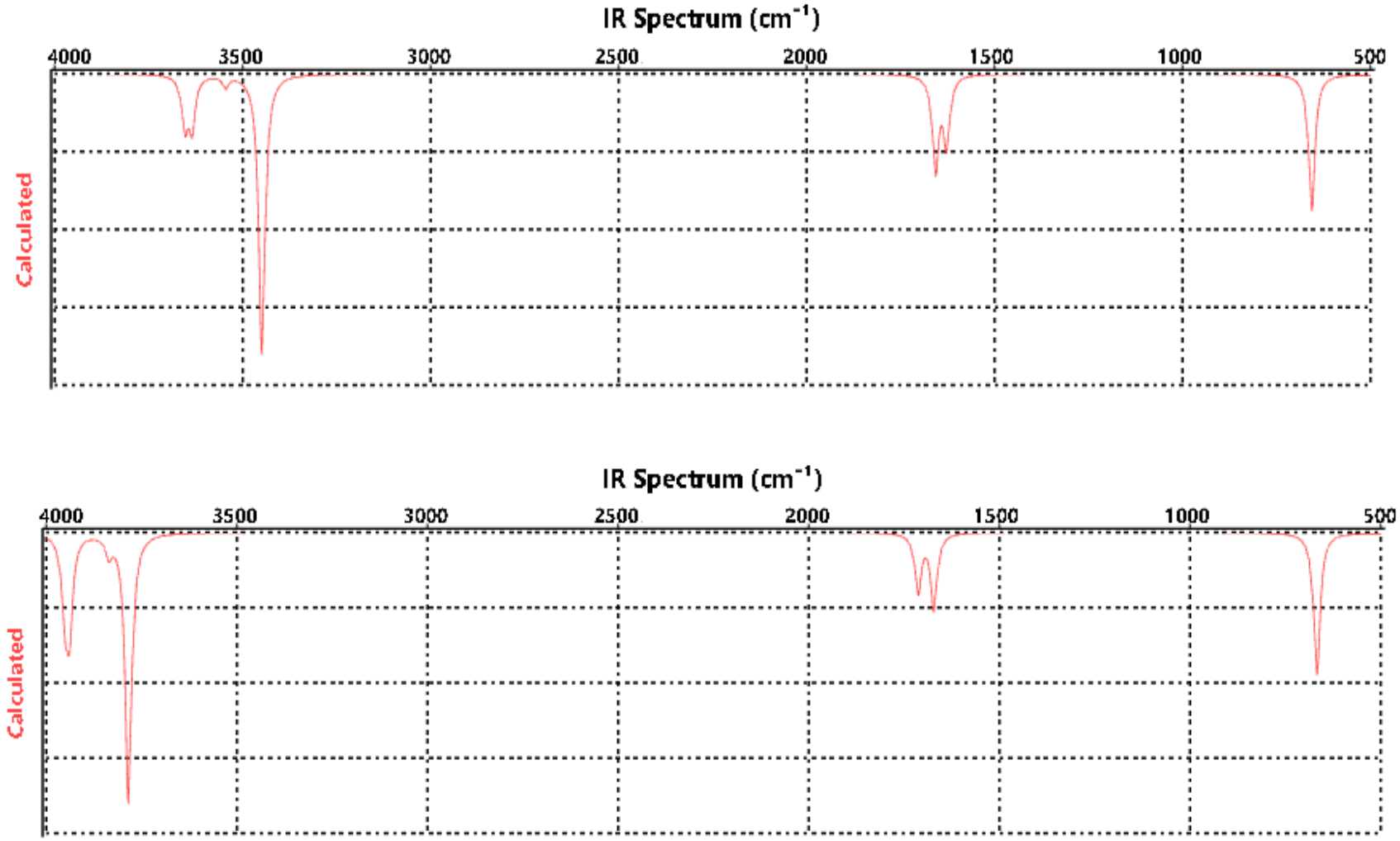

Fig.9. Water Dimer Dihedral Plane H5O4H2O1 of Rotation for MM and QM based Torsion around H-bond Linking Water Monomers.

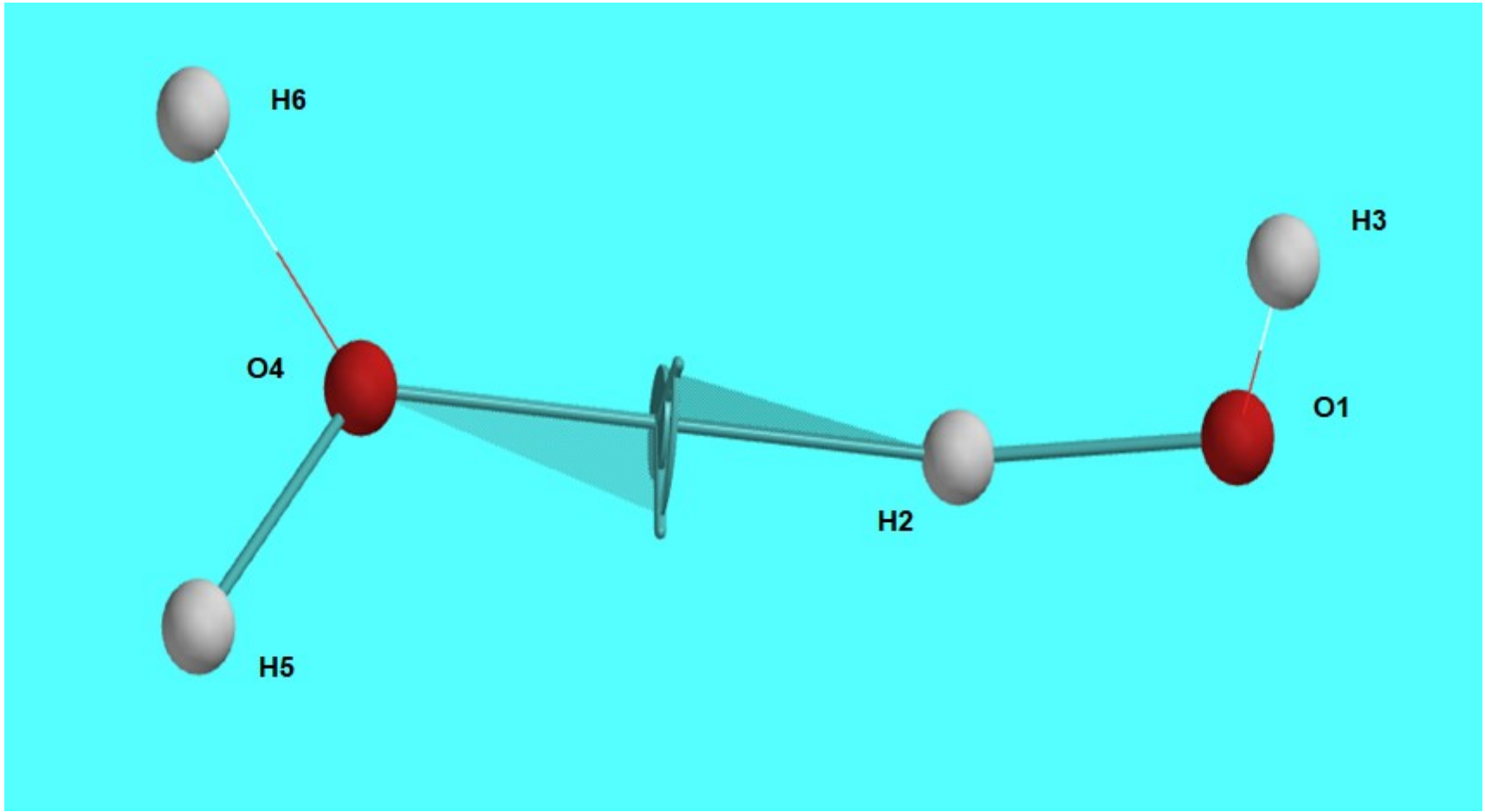

Fig.10. Molecular mechanics based dihedral energy of water dimer around O4H2 H-bond by MMFF method.

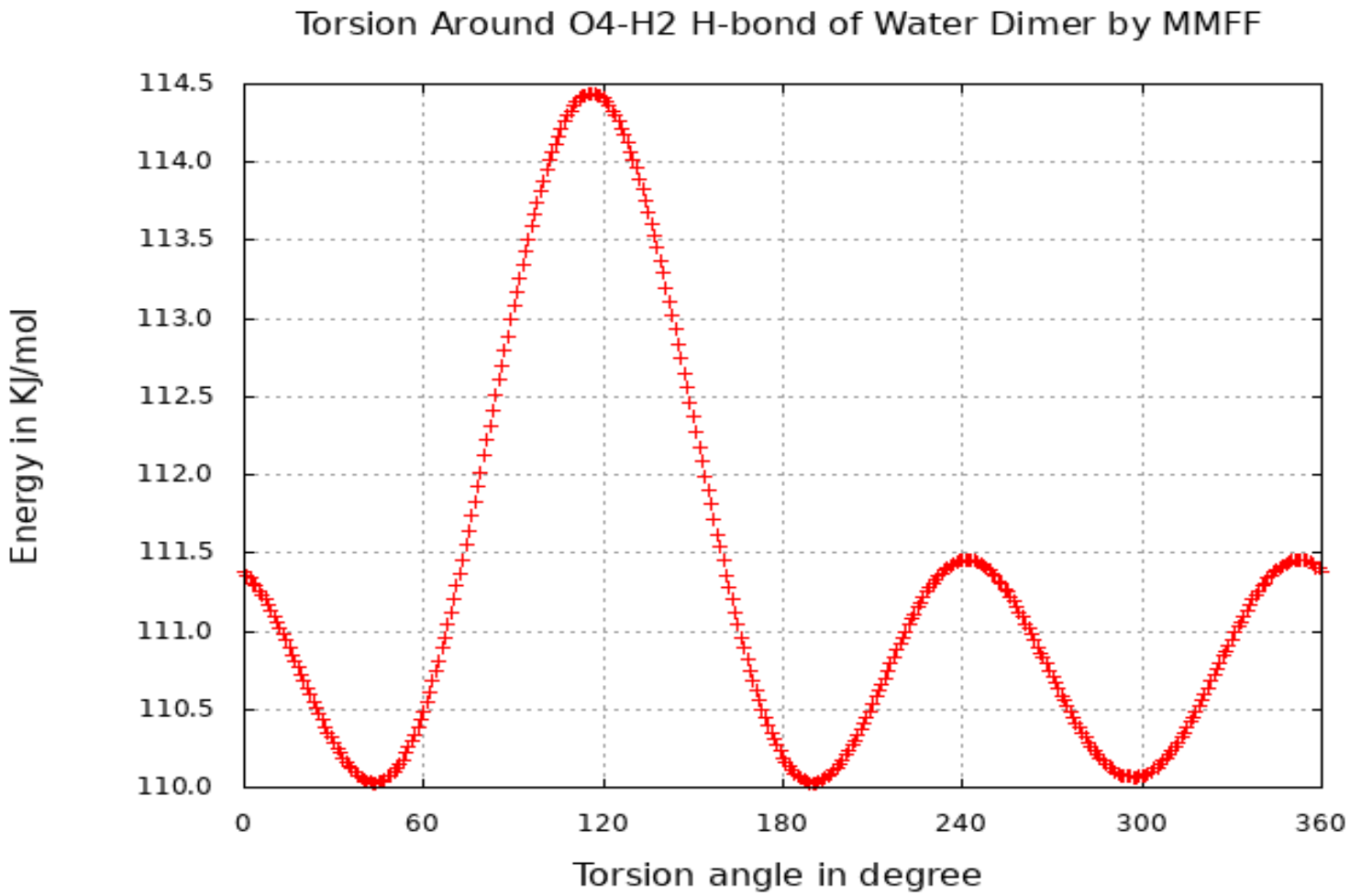

Fig.11. First principle based dihedral energy of water dimer around O4H2 H-bond by HF/6-31G* method.

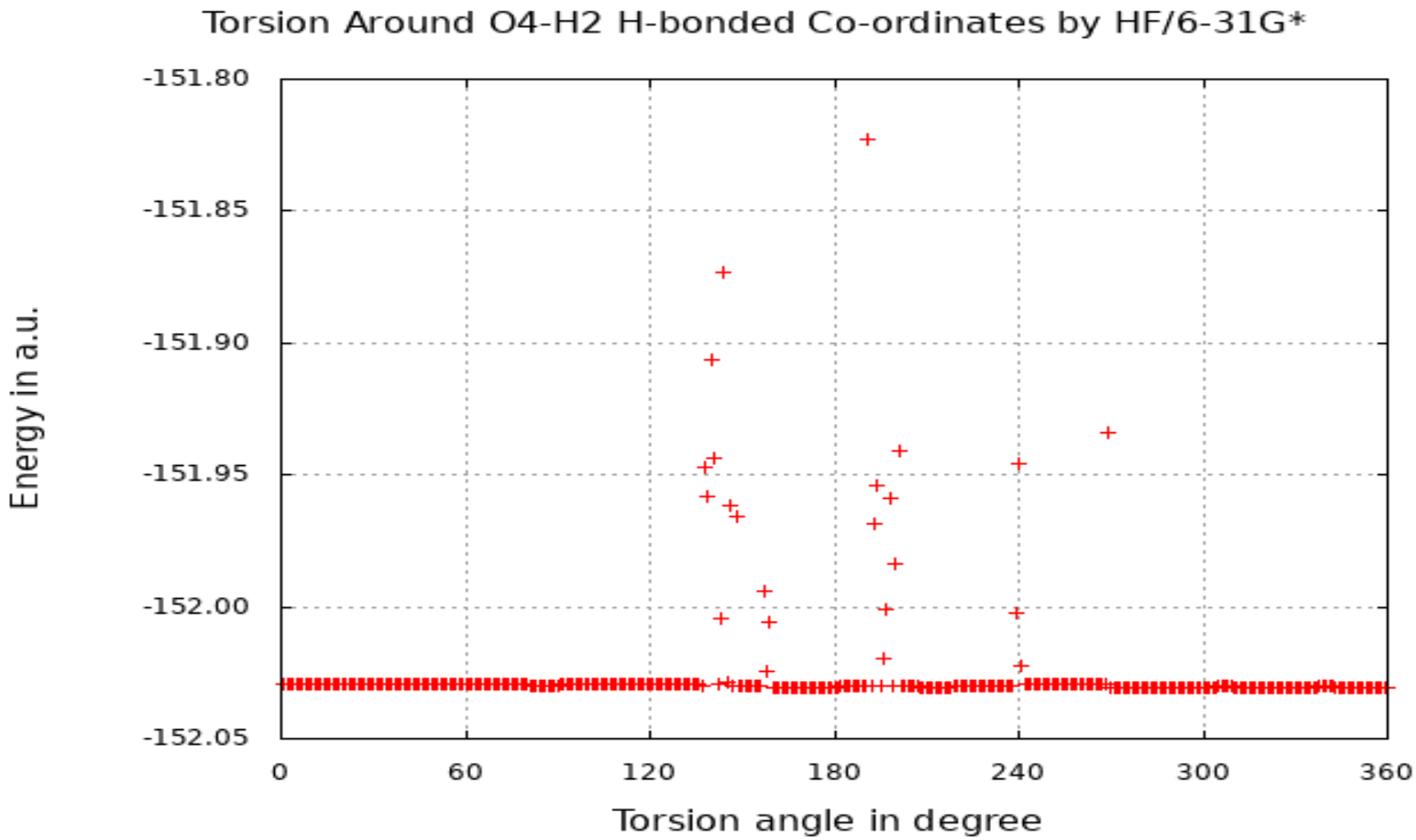

Fig.12. First principle based dihedral energy of water dimer around O4H2 H-bond by B3YLP/6-31G* method.

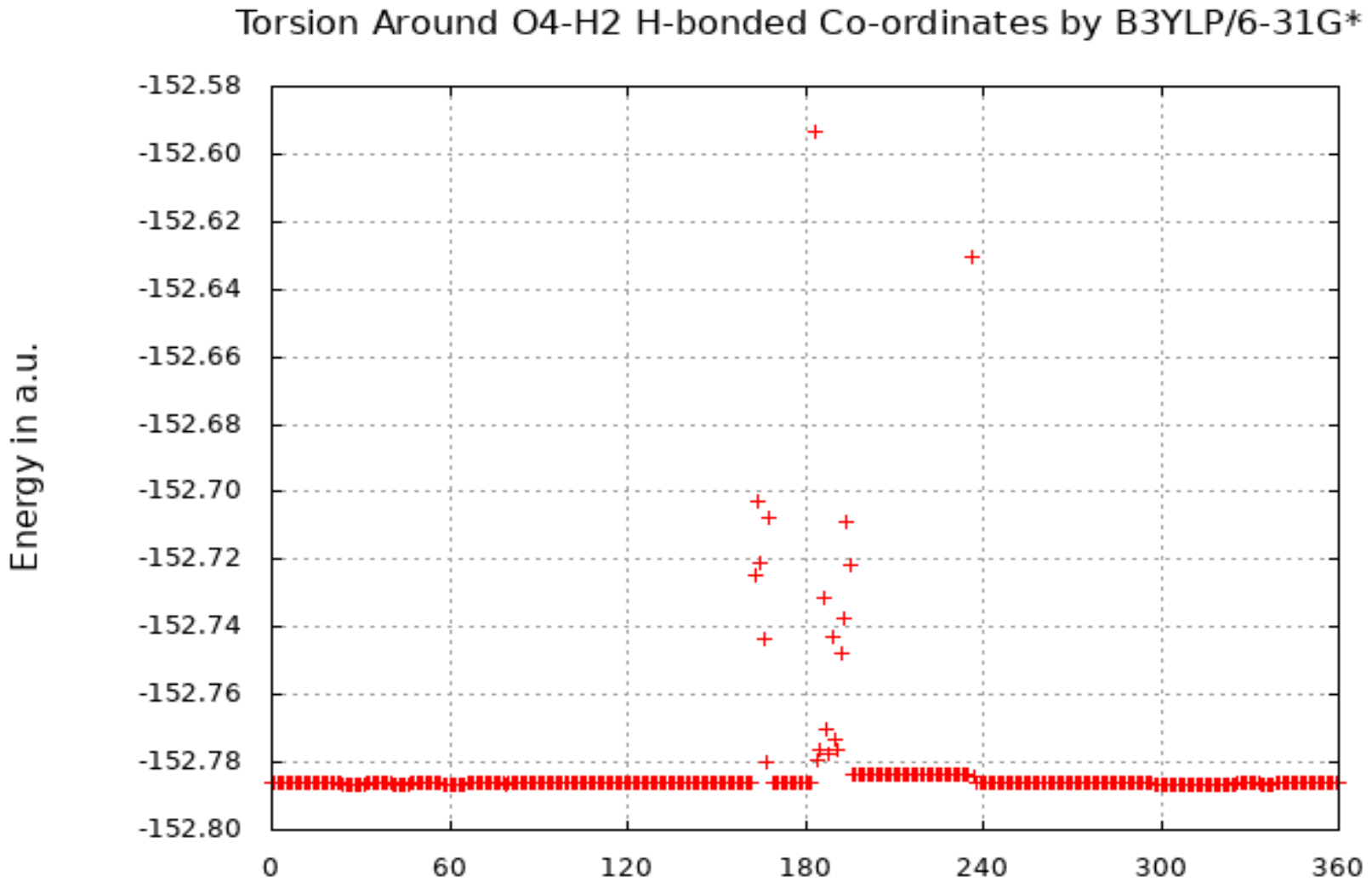

Fig.13. First principle based dihedral energy of water dimer around O4H2 H-bond by MP2/aug-ccPVDZ method.

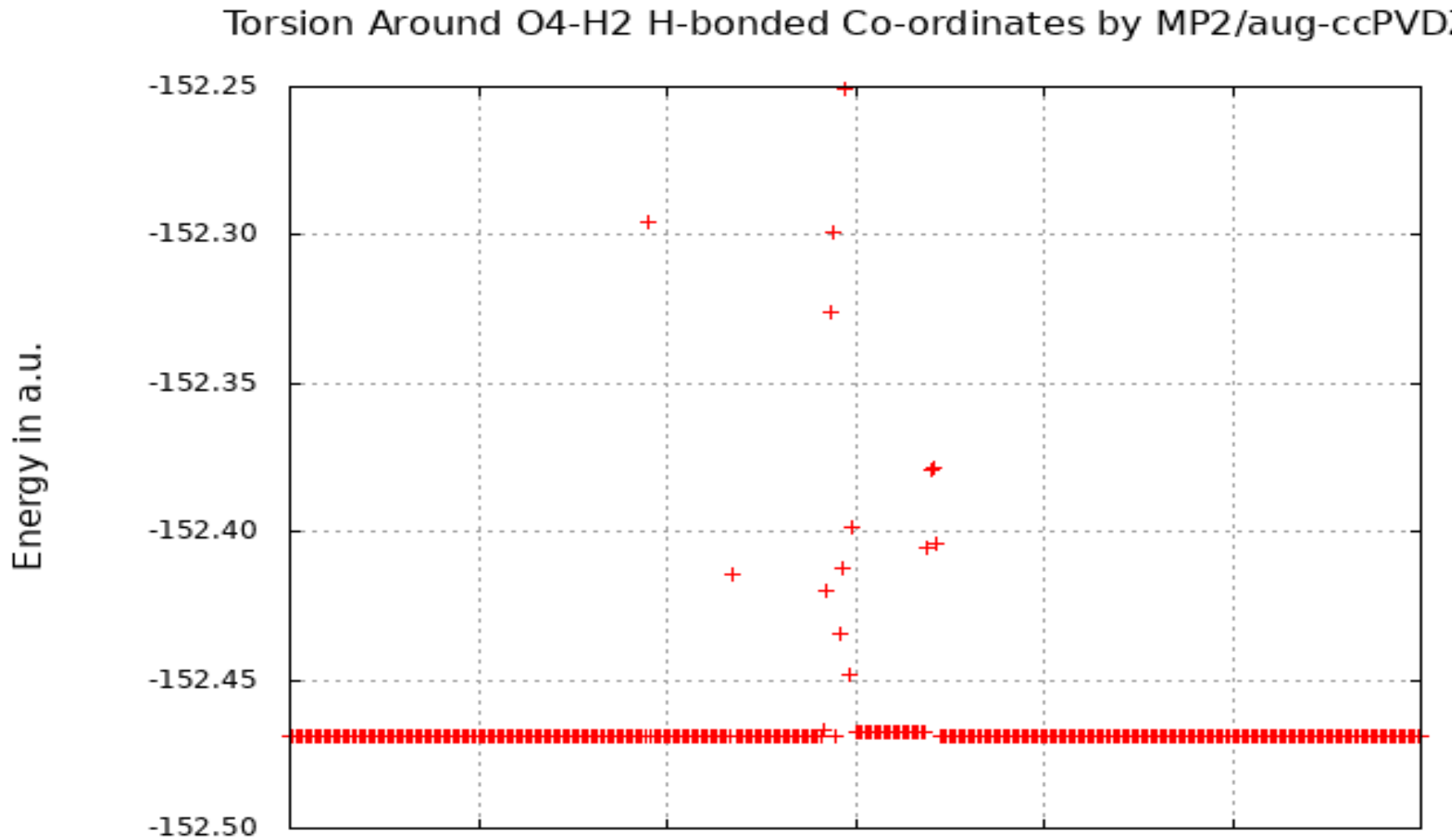

Fig. 14. Anisotropic Singularities in Dihedral Energy Due to Water Dimer's Weak H-Bond Breaking Computed in Critical Range for Gas Phase by AM1 Method.

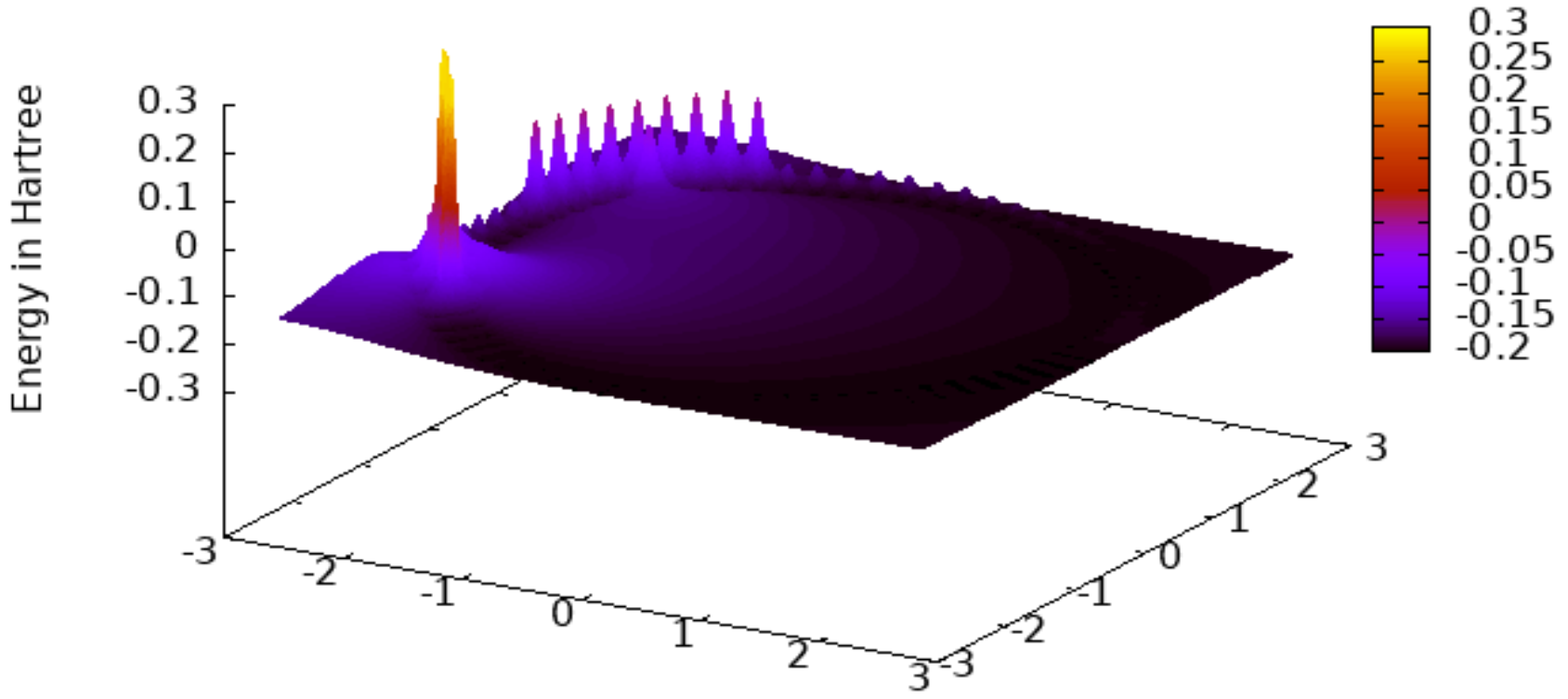

Fig. 15. Anisotropic Singularities in Dihedral Energy Due to Water Dimer's Weak H-Bond Breaking Computed in Critical Range for Gas Phase by PM3 Method.

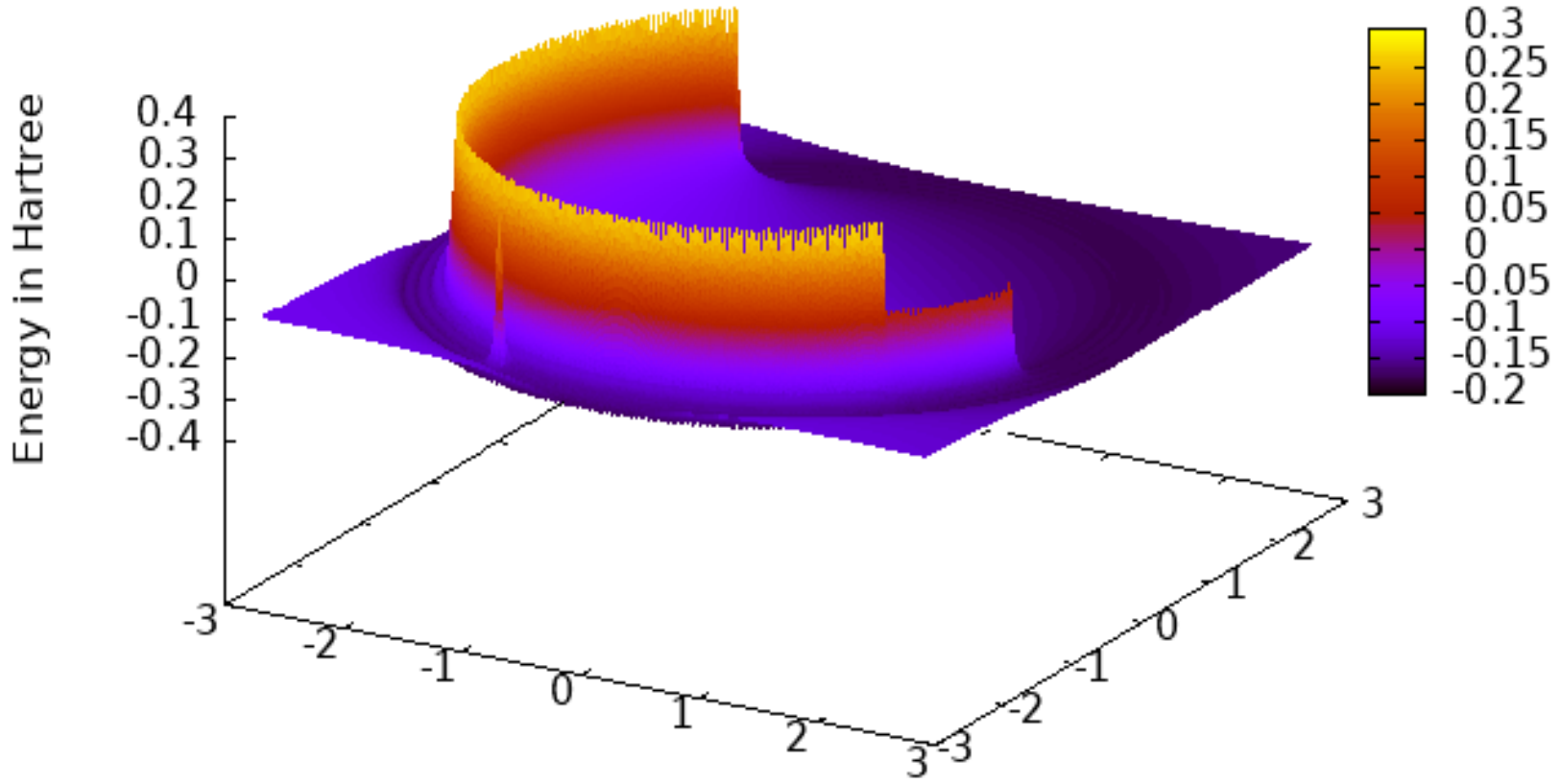

Fig. 16. Molecular mechanics based dihedral energy of water dimer around O1-O4 interaction co-ordinates by MMFF method.

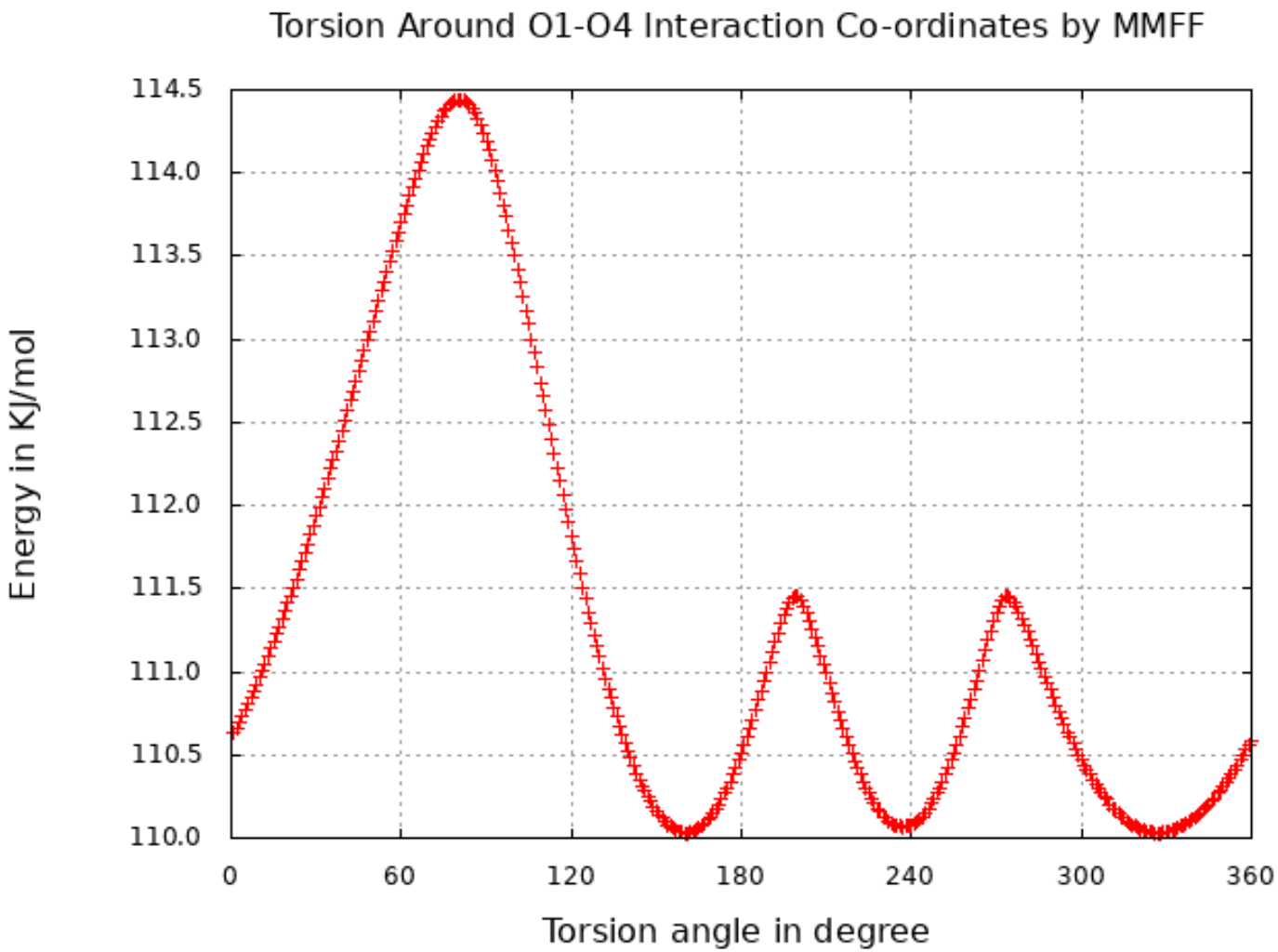

Fig. 17. Dihedral Energy via Torsion Around O1-O4 by DFT B3YLP/6-31G* Basis as Applied in Gaussian 16.

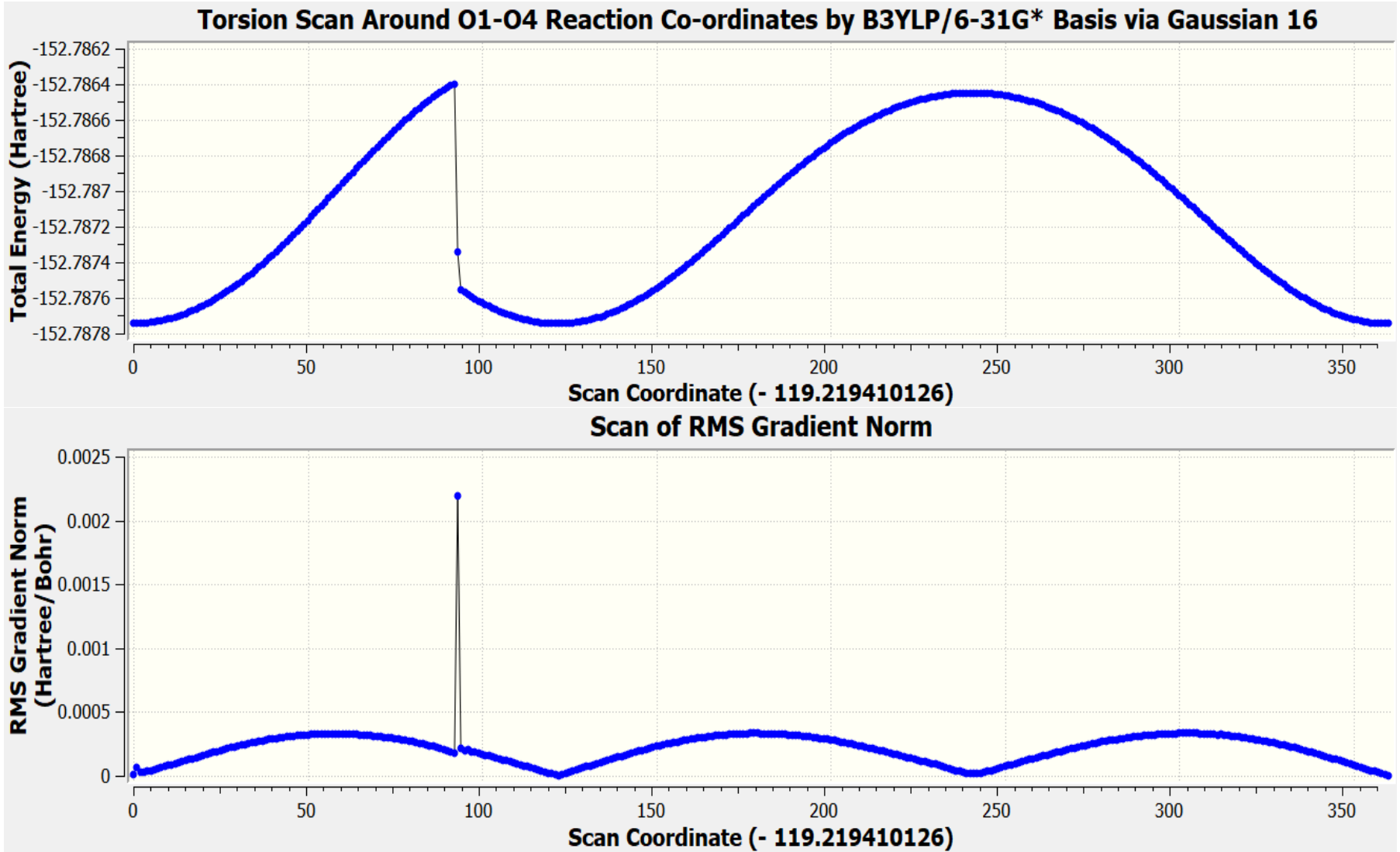

Fig. 18. Dihedral Energy via Torsion Around O1-O4 by DFT wB97xd/6-31G* Basis as Applied in Gaussian 16.