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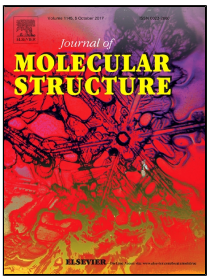

Vibrational studies of Thyroxine hormone: Comparative study with quantum Chemical calculations

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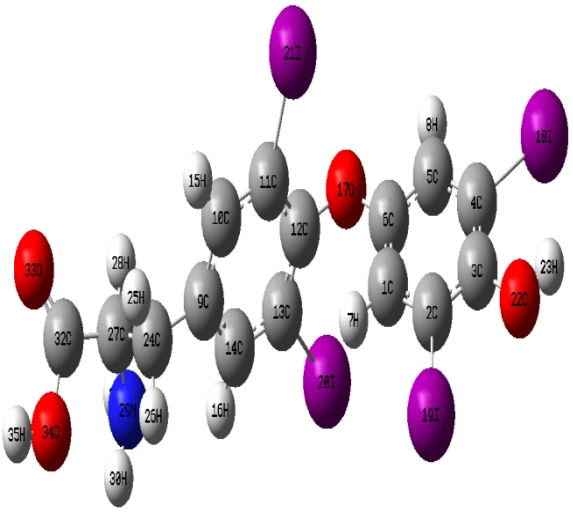
Raman and IR technique have been used to study the vibrational wave numbers. All the normal modes have been assigned and the scaled theoretical results found to be in a good agreement with the experimental findings. HOMO-LUMO energy gap is also calculated in order to study the electrical properties of the biomolecule. The study is extended to calculate the Natural Bond Orbital and different thermo-dynamical parameters.



Molecular structure of Thyroxine

Vibrational studies of Thyroxine hormone: Comparative study with quantum Chemical calculations

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