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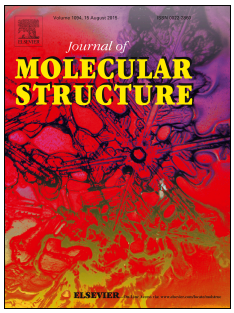

Molecular structure of tryptamine in gas phase according to gas electron diffraction method and quantum chemistry calculations

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Molecular structure of tryptamine in gas phase according to gas electron diffraction method and quantum chemistry calculations

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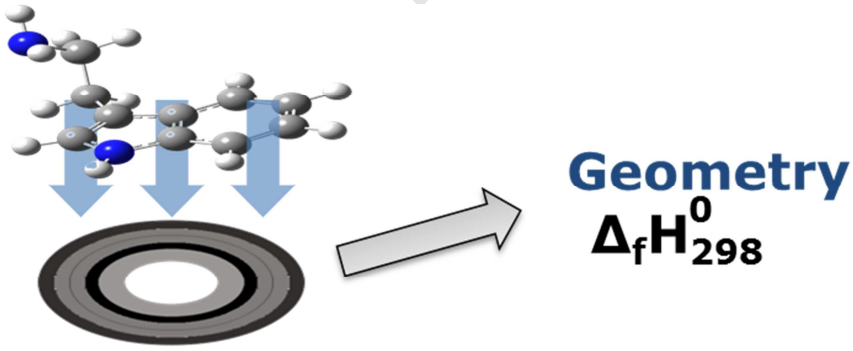
Abstract

The molecular structure of tryptamine was studied by gas-phase electron diffraction (GED) and quantum chemical calculations (DFT/B3LYP and MP2 methods with cc-pVTZ basis set). The best fit of the experimental scattering intensities (R-factor = 3.8%) was obtained for the four-conformer model. The experimental structural parameters are found to be in good agreement with the results of theoretical calculations. The geometric parameters of gaseous tryptamine are compared with those in the crystal phase. The standard enthalpy of formation of tryptamine in the gas phase was calculated using Gaussian-4 theory, yielding value of 133.6 ± 3.3 kJ/mol.

Graphical abstract



Highlights

- Equilibrium molecular structure of tryptamine in gas phase.
- The $A^+G^-G^+$ and $A^+G^-G^-$ conformers are the most abundant.
- Standard heat of formation estimation for tryptamine by Gaussian-4 calculations.

Keywords Tryptamine / Molecular equilibrium structure/ Gas electron diffraction / Standard enthalpy of formation

1. Introduction