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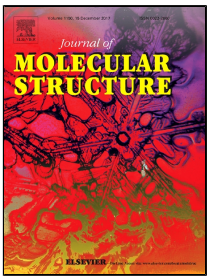

Spectroscopic investigation (FT-IR, FT-Raman), HOMO-LUMO, NBO, and molecular docking analysis of N-ethyl-N-nitrosourea, a potential anticancer agent

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Highlights

- N-ethyl-N-nitrosourea, also known as ENU, is a highly potent mutagen.
- Nitrosourea play an important role in the treatment of cancer.
- Vibrational and structural investigations have been carried out for most stable conformer of ENU molecule.
- All 39 normal modes of ENU have been assigned for the first time.
- In addition the experimental IR and Raman spectra have been recorded and analyzed in light of the computed fundamentals and the corresponding PEDs using GAR2PED software.
- HOMO–LUMO, total density plots, electrostatic potential (ESP) surface, and natural bond orbital (NBO) investigations have been carried out for the ENU molecule.
- The HOMO-LUMO energy gap supports the pharmacologically active property of the ENU molecule.
- To find out the anticancer activity of the title compound molecular docking investigations have been performed against protein 2JIU.