

## Comprehensive DFT analysis on monosodium urate: Implications for gout pathophysiology

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This research employs advanced Density Functional Theory (DFT) techniques to conduct a comprehensive analysis of monosodium urate ( $\text{NaC}_5\text{H}_3\text{N}_4\text{O}_3$ ), a pivotal molecule in gout pathophysiology. The B3LYP/6-311G\*\* method is utilized to explore conformational stability, molecular structure, UV-Vis and IR spectra, as well as electronic properties of monosodium urate. The study reveals intricate information about electronic transitions, molecular vibrations, and orbital interactions, providing a profound understanding of molecular dynamics associated with monosodium urate. Additionally, Nuclear Magnetic Resonance (NMR) analysis predicts precise  $^1\text{H}$  and  $^{13}\text{C}$  chemical shifts, offering nuanced structural insights. Quantum calculations contribute to a thorough characterization of monosodium urate, enhancing our understanding of its molecular intricacies. The findings from this study significantly enhance our comprehension of the underlying molecular mechanisms of gout, shedding light on potential therapeutic interventions. The detailed insights into electronic properties and structural dynamics open new perspectives for the application of monosodium urate in environments influenced by electrical factors. In essence, this research not only expands our knowledge of gout pathophysiology but also presents innovative opportunities for targeted research and therapeutic development.

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