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# Optimization and Vibrational Study of 2-propylpyridine-4-carbothioamide by DFT- A theoretical study

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**Abstract:** The molecular structure and simulated vibrational spectra of 2-propylpyridine -4-carbothioamide have been calculated using the different density functional theoretical methods. The comparative performance of different DFT methods at various basis sets has been examined and predicted molecular structure and vibrational spectra of the molecule. The calculated results show that DFT/B3LYP functional and 6-31 G basis set gives the highest certainty in predicting the structure and vibrational spectra of 2-propylpyridine -4-carbothioamide.
**Keywords**: 2-propylpyridine-4-carbothioamide, DFT, molecular structure, vibrational spectra.

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