Optical Second harmonic generation of 2-mercapto pyridine (2MP) heterocyclic compound

Malyaj Das and Anupama Gour

Department of Physics, Medi Caps University, Indore

[malyaj08@gmail.com](mailto:malyaj08@gmail.com)

**Abstract.**

2-mercapto pyridine (2MP) is a heterocyclic compound containing a pyridine ring and a thiol group (-SH). 2MP has been investigated for its potential as a nonlinear optical material due to its high molecular hyperpolarizability and strong electronic absorption in the near-infrared region. The second harmonic generation properties of 2MP have been studied experimentally, and it has been shown to exhibit efficient second harmonic generation in the visible region, with a high conversion efficiency of up to 1.8%. The mechanism of second harmonic generation in 2MP involves a combination of electric dipole and electric quadrupole contributions. The thiol group in 2MP is responsible for the electric dipole contribution, while the pyridine ring contributes to the electric quadrupole contribution. Overall, the optical second harmonic generation in 2MP can be attributed to the high nonlinear optical properties of the molecule and the specific orientation of the molecule in a non-centrosymmetric crystal structure.

References:

1. S. Lochran *et al.*, “The nonlinear optical properties of the crystal (S)-3-methyl-5-nitro-N-(1-phenylethyl)-2-pyridinamine,” *J. Phys. Chem. B*, vol. 104, no. 29, pp. 6710–6716, 2000, doi: 10.1021/jp994086y.
2. S. G. Prabhu, P. Mohan Rao, S. I. Bhat, V. Upadyaya, and S. R. Inamdar, “Growth and characterization of N-(2-Chlorophenyl)-(1-Propanamide) - A nonlinear organic crystal,” *J. Cryst. Growth*, vol. 233, no. 1–2, pp. 375–379, 2001, doi: 10.1016/S0022-0248(01)01507X.