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A Far-IR Absorbing Molecule Showing Highest Molecular Second Order Nonlinear Optical Response: A Computational Study

We report, till date the highest value of molecular first hyperpolarizability (Second order Nonlinear Optical response) for an organic molecule. Calculation shows that low energy absorption (Far-IR) and large ground to excited state dipole difference, are mainly responsible for such a high value first hyperpolarizability even at the molecular level.

Primary author: Dr SITHA, Sanyasi (University of the Witwatersrand)

Presenter: Dr SITHA, Sanyasi (University of the Witwatersrand)

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