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A study of structural effects on linear and nonlinear response of bicompartmental Ni (II) Schiff base complexes

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Herein we investigate imaginary third order NLO activity, optical limiting capability and first hyperpolarizabilities of five Ni (II) salen complexes using experimental and theoretical methods. The complexes are tuned to have different NLO response by changing mainly the diimine spacer group. Out of the compounds reported, the one with *o*-phenylene spacer group exhibits the highest NLO activity comparable with that of polymers and semiconductors which is followed by the compound with ethylene spacer unit. The order of activity is a direct function of the degree of π-delocalization. Further all the tested compounds returned outstanding optical limiting capabilities making them excellent materials for fabrication of such devices. The experimental results were substantiated with frontier orbital calculations carried out using DFT at M06/6-31G* level of theory and complex with aromatic spacer group exhibits least energy gap and highest activity. The total dipole moment, polarizability and first hyperpolarizability were also calculated at the same level of theory which are also in line with the experimentally observed results.

KEYWORDS
crystal structure, DFT studies, nonlinear optical activity, optical limiting, Schiff base complexes

1 | INTRODUCTION

In recent years, intense research is going on so as to develop a simple and facile way to design efficient materials with novel architecture in the optoelectronic as well as photonic field.[1] Chemists from different area especially from organic[2] and polymeric[3] fields have reported a number of such materials which could show good nonlinear response (NLO). On the other hand, in order to show a good NLO response, a molecule should possess a suitable D-π-A system (Donor and acceptor separated by a π system). Generally, organic compounds having an extensive π delocalization have proved to be effective in this regard.[4] In recent years, synthetic inorganic chemists have prepared different inorganic compounds with transition metal ions or with various functionalities for satisfying the requirement in the field of nonlinear optics without compromising on the stability of materials.

Designing of a material to possess good second order or third order NLO response is a crucial task which includes the preparation of a molecule having high β value and to modify the material in order to possess a high χ^2 value. Inorganic compounds even though less used, have great potential in this field over the organic ligands since the complexation process may lead to the formation of geometrically constrained planar structure which enhances the optical nonlinearity.[5] Moreover, the transition metal can coordinate in different coordination mode with different oxidation state which may cause

Nithya Mohan and Sreejith S. S. have contributed equally to this work.

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