Study on the Second Order Optical Properties of *N*-(2,4-Dichloro)-salicylaldimine

Aslı Karakaş[a], Hüseyin Ünver[b], Ayhan Elmali[c], and Ingrid Svoboda[d]

[a] Selçuk University, Faculty of Arts and Sciences, Department of Physics, TR-42049 Campus, Konya, Turkey
[b] Ankara University, Faculty of Sciences, Department of Physics, TR-06100 Tandoğan, Ankara, Turkey
[c] Ankara University, Faculty of Engineering, Department of Engineering Physics, TR-06100 Tandoğan, Ankara, Turkey
[d] Institute for Material Science, Darmstadt University of Technology, Petersenstraße 23, D-64287 Darmstadt, Germany

Reprint requests to Prof. A. E.; E-mail: elmali@eng.ankara.edu.tr

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N-(2,4-Dichloro)-salicylaldimine was synthesized, characterized by elemental analysis, FT-IR, and UV-visible spectroscopy, and its crystal structure was determined. The title compound is almost planar and contains short intramolecular O-H…N hydrogen bonds [O1-N1 2.601(1) Å]. It remains transparent in the visible region and has solvatochromic behavior in the UV region in the range 198 – 349 nm, implying non-zero microscopic first hyperpolarizability. The *ab-initio* quantum mechanical calculations (finite field second-order Møller Plesset perturbation theory) of the studied compound have been carried out to compute the electric dipole moment ($\boldsymbol{\mu}$) and the first hyperpolarizability ($\boldsymbol{\beta}$) values. The *ab-initio* results also show that this ligand might have microscopic nonlinear optical behavior with non-zero values.

Key words: Nonlinear Optics; First Hyperpolarizability; UV-visible Spectroscopy; Crystal Structure; *Ab-initio* Calculation.