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Second-order NonLinear Optical Properties of Λ-Shaped Pyrazine Derivatives Enlarged with 2,5-Thiophene Groups

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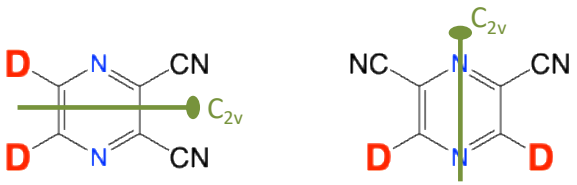
The linear and nonlinear optical (NLO) properties of two new series of pyrazine derivatives have been investigated by means of density functional theory [1]. The derivatives comprise cyano groups as acceptor units, methoxy groups as donor units, and 2,5-thiophene groups as π-conjugated linkers that systematically enlarge the Λ shape of the chromophores. The two series of compounds differ in the relative position of the donor and acceptor groups in the pyrazine, forming 2,3- or 2,6-isomers. Both series of isomers present potential C_{2v} symmetry with a different orientation of the C_2 axis and the σ_v plane of the symmetry point group: in the pyrazine plane but perpendicular to the N-N pyrazine's axis for the 2,3-isomers, and in the pyrazine plane and containing the N-N pyrazine's axis for the 2,6-isomers (Figure 1). Focusing on the different orientation of the C_{2v} symmetry elements and how these structural changes affect the electronic structure and the characterization of the electronic excited states of the chromophores, a rationalization of the second-order nonlinear responses (mainly Hyper-Rayleigh Scattering (HRS) hyperpolarizabilities) will be done from a fundamental point of view [2].



2,3-isomer **2,6-isomer**

D = MeO, Thiophene $(Th)_n$ (where n=1-2), MeO-$(Th)_n$ (where n=1,2)

Figure 1. Pyrazine derivatives investigated in this work.

References:

[1] Castet, F.; Gillet, A.; Bures, F.; Plaquet, A.; Rodriguez, V. Second-order nonlinear optical properties of Λ-shaped pyrazine derivatives. *Dyes and Pigments*, **2021**, *184*, 108850.

[2] Boyd, R.W. Nonlinear Optics, 3rd edition; Academic Press, Inc.: Orlando, FL, United States, 2008; 1-640.