Octupolar molecules are of increasing interest in the field of nonlinear optics due to their potentially large twoor three-dimensional quadratic nonlinearities.[1] These molecules are non-dipolar species whose NLO response is related to multidirectional charge-transfer excitations, rather than to dipolar unidirectional excitations. A number of molecules with three-fold rotational symmetry, as well as molecular ions of D_{3h} , C_{3v} or D_3 symmetry, have been shown to display promising properties. In order to investigate new molecules that possess this type of structure, we have synthesized a new family of organic 1,3,5-triazine-2,4,6-trione derivatives.[2]



Albeit being known since the late 1890's, these simple octupolar structures have never been investigated for their optical properties. Straightforward syntheses of these derivatives, along with their full spectroscopic characterization (IR, UV–Vis) will be presented. Their linear optical (LO) and nonlinear optical (NLO) properties will then be discussed. In addition to good hyperpolarizabilities and good transparencies, some of these derivatives present also remarkable two photon absorption (TPA) properties. Structural modifications allowing improving this particular property in purely organic derivatives will be presented and their NLO activity will be rationalized with the help of DFT computations.

Organometallic derivatives have also been obtained from precursors possessing pendant alkyne groups (Scheme 1).[3] The syntheses of these organometallic derivatives, along with their spectroscopic characterization (UV–Vis), and including the molecular structure of one example, will be presented. The positive impact of the peripheral organometallic substituents on the NLO performances will finally be analyzed based on additional DFT calculations.

Finally, in the last part, part, the development of organic chromophores with large brightnesses and improved two-photons absorptions will be briefly related.

References :

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