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Evidence of structure dependence of hyperpolarizability in octupolar molecules CLAUDIA CARDOSO, CFC, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, PAULO ABREU, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, FERNANDO NOGUEIRA, CFC, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade de Coimbra — It was recently reported that second-order hyperpolarizability increases significantly upon introduction of positive charges at the pyridyl end groups in trispyridyl octopolar chromophores, when compared with the neutral species. We performed ab-initio and semi-empirical calculations for the geometries, electronic localization function and first hyperpolarizabilities of a series of 6 trispyridyl molecules in neutral and protonated forms. Ab-initio calculations correctly reproduce the large hyperpolarizability values of the protonated octopolar molecules. Semi-empirical calculations predict somehow smaller hyperpolarizability values but reproduce the trend of the experimental and ab-initio values. Linear response TDDFT calculations are in good agreement with the experimental absorption spectra, reproducing the red-shift of the peaks with protonation. A correlation between the molecular structures and the first hyperpolarizability was established.

Claudia Cardoso
CFC, Departamento de Física, Faculdade de Ciências e Tecnologia,
Universidade de Coimbra

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