Crystal and nonlinear optical properties of triphenylguanidine: theory and experiments\textsuperscript{1} CLÁUDIA CARDOSO, CFC, Departamento de Fisica, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, PEDRO SILVA, CEMDRX, Departamento de Fisica, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, FERNANDO Nogueira, CFC, Departamento de Fisica, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, JOSÉ ANTÓNIO PAIXÃO, CEMDRX, Departamento de Fisica, Faculdade de Ciências e Tecnologia, Universidade de Coimbra — Guanidine compounds have attracted much interest due to the donor and acceptor abilities of the nitrogen and their potential nonlinear optical properties. Octupolar molecules are particularly interesting from the point of view of nonlinear optics. Their null dipole moment does not stand as a drawback for its crystallization and still allows the crystal to present large third order susceptibilities if some symmetry requirements are fulfilled. In the present work we focused on the triphenylguanidine (TPG) octupolar molecule and its crystalline forms. We present computational and experimental results both for the isolated molecule and TPG crystals. The structural properties as well as optical spectra and response properties will be presented from the point of view of the requirements to obtain octupolar molecules-based materials with enhanced nonlinear optical properties.

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