

JAHN-TELLER EFFECT IN DIMETHYL AMINO PHENYL SUBSTITUTED SILVER PHTHALOCYANINE

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Breloy *et al.* [1] synthesized a new dimethyl amino phenyl substituted phthalocyanine (dmaphPcH₂) and its Ag(II) complex ([dmaphPcAg]⁰, see Fig. 1) used as a visible light-absorbing photoinitiator for free-radical and cationic polymerizations. Irradiation of the [dmaphPcAg]⁰ solutions led to the reduction of Ag(II) to Ag(I) and simultaneously generated the nitrogen-centered radical. In the next step, Ag nanoparticles and aromatic carbon-centered radicals were formed. The proposed photoinitiation mechanisms under light irradiation suppose the existence of [dmaphPc]⁰, Ag⁰ and [dmaphPcAg]^q, q = -1, 0 and + 1, entities.

The purpose of our recent study is the DFT study of complexes [dmaphPcAg]^q, q = -2 → +1. We have optimized their geometries and performed TD-DFT calculations within the D₄ symmetry group and its subgroups. The consequences of a Jahn-Teller effect with consecutive symmetry descent in these systems have been analyzed using a group-theoretical treatment

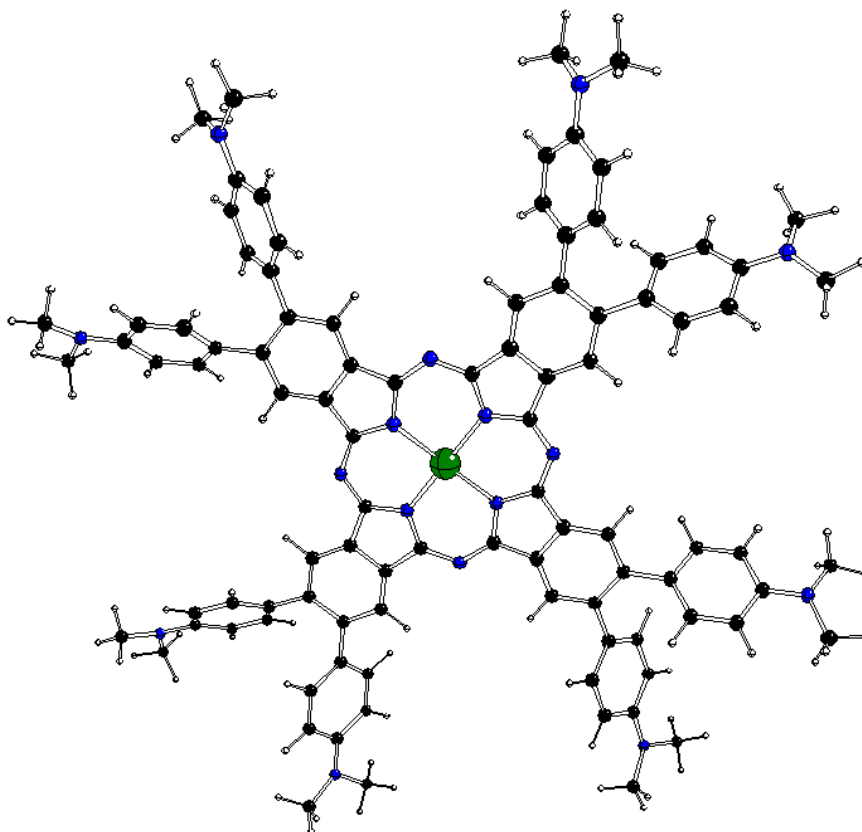


Figure 1. Structure of [dmaphPcAg]⁰ [1] (C – black, N – blue, H – white, Ag – green).

[1] L. Breloy, et al.; *Polym. Chem.* **12**, 1273 (2021).