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Born-Oppenheimer molecular dynamics and electronic properties of chlorophyll-c₂ in liquid methanol

J. Chem. Phys. **138**, 225102 (2013); <https://doi.org/10.1063/1.4808177>Benedito J. C. Cabral^{1,2, a)}, Kaline Coutinho³, and Sylvio Canuto³[View Affiliations](#)[View Contributors](#)

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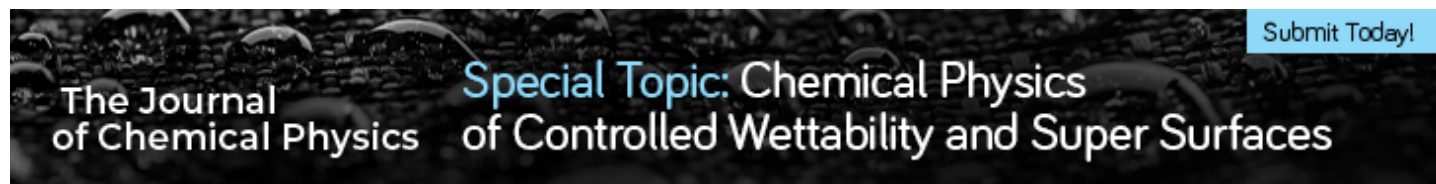
ABSTRACT

First principles Born-Oppenheimer molecular dynamics of chlorophyll- c_2 (chl c_2) in liquid methanol is reported. The structure of the chromophore-methanol solution is characterized by non-symmetric solvation and by the displacement of a pentacoordinated Mg atom from the π macrocycle plane of chl c_2 . Non-symmetrical solvation is in keeping with experimental data reported for chlorophyll-a and bacteriochlorophyll-a indicating a preferential side of the π macrocycle for binding a fifth ligand. The average displacement of the Mg atom (0.38 Å) is similar to X-ray data on magnesium phthalocyanine (~0.45 Å) and ethyl chlorophyllide-a dihydrate crystals (0.39 Å). The displacement of Mg from the macrocycle plane influences the orientational order of the methanol molecules in the axial region and the results indicate that the face defined by the methoxycarbonyl moiety exhibits a solvatophobic behavior. The maximum of the Soret (B) band for chl c_2 in liquid methanol (464 nm) is in good agreement with the experimental value (451 nm) and it is also very close to a recent result for chl c_2 in liquid 2-methyl tetrahydrofuran (466 nm). Intramolecular hydrogen bonding involving the carboxyl and methoxycarbonyl moieties of chl c_2 leads to a blueshift of ~20 nm of the B band maximum.

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