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Born-Oppenheimer molecular dynamics and electronic properties of chlorophyll-c_2 in liquid methanol

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ABSTRACT

First principles Born-Oppenheimer molecular dynamics of chlorophyll-c_2 ($chlc_2$) 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 $chlc_2$. 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 $chlc_2$ 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 $chlc_2$ in liquid 2-methyl tetrahydrofuran (466 nm). Intramolecular hydrogen bonding involving the carboxyl and methoxycarbonyl moieties of $chlc_2$ leads to a blueshift of ~20 nm of the B band maximum.

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