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Spectroscopy of diethyl carbonate a green solvent: An experimental and theoretical study

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Highlights

- Electronic photoabsorption spectrum (using synchrotron radiation) of diethyl carbonate (DEC) recorded in 7–11 eV region reported for the first time
- Gas phase infrared spectrum of DEC revisited in the 600–3100 cm⁻¹ region to obtain a comprehensive set of assignments for the vibrational modes
- Vertical excited state energies and nature of the transitions calculated using TDDFT methodology.
- Potential energy curves of the first few excited states studied to predict the photo-dissociation of the molecule
- Analysis of photoabsorption spectra of DEC in VUV region substantiated with quantum chemical calculations

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