Title:	Matrix isolation and DFT study of the conformations of diethylcarbonate
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Abstract:	Conformations of diethylcarbonate (DEC) were studied using matrix isolation infrared spectroscopy. DEC was trapped in an Ar matrix at 12 K, using both an effusive source maintained at 298 and 423 K and a supersonic jet source. The experimental studies were supported by computations performed at the B3LYP/6-31++G** level of theory. The ground state conformer for DEC was found to have a "cc(tt)" geometry, where the 'c' refers to a cis orientation of the carbons attached to oxygen, while the 't' in parenthesis refers to the trans orientation of the terminal carbon. In addition to the ground state conformer, our computations also indicated local minima corresponding to conformers with cc(tg±), cc(g ±g∓) and cc(g±g ±) geometries, listed in increasing order of energy. Natural bond orbital analysis was also performed to understand the role of delocalization interactions and steric effect on conformational stability.
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