Title:	Discerning Near-Isoergic Isomers. A Matrix Isolation Infrared and ab Initio Study of the Propargyl Alcohol Dimers
Authors:	Saini, J. (/jspui/browse?type=author&value=Saini%2C+J.) Viswanathan, K.S. (/jspui/browse?type=author&value=Viswanathan%2C+K.S.)
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Abstract:	This study reports the first infrared spectroscopic investigation of the dimers of propargyl alcohol (PA) using matrix isolation infrared spectroscopy and ab initio computations. Computations indicated a number of isomers for the dimer, with the two most stable structures being nearly isoergic. Interestingly, our matrix isolation experiments were able to discern both of these isomers, which were corroborated by computations performed at the M06-2X/6-311++G(d,p) level. Identifying these two isomers was significant, since the two most stable and near-isoergic isomers can be expected to play an important role in the structure of the propargyl alcohol ices, an understanding of which is of significant importance in the study of astrochemical environments. The global minimum structure differed from its near-isoergic local minimum, in the dimer architecture; the former making a three-point hydrogen-bonded contact, O–H···O, O–H···π, and C–H···π, and the latter having two. The global minimum had been observed in molecular beam experiments, though not the near-isoergic local minimum. In both isomers, the propargyl alcohol monomer units were in their gauche conformation. AIM and NBO analyses were also performed to understand the nature of interaction in the dimers. The results of this study may well have significant implications in interpreting the PA spectra in astrochemical environments.
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