Title:	Conformational Landscape of Tri-n-butyl Phosphate: Matrix Isolation Infrared Spectroscopy and Systematic Computational Analysis
Authors:	Ramanathan, N. (/jspui/browse?type=author&value=Ramanathan%2C+N.) Sundararajan, K. (/jspui/browse?type=author&value=Sundararajan%2C+K.) Viswanathan, K.S. (/jspui/browse?type=author&value=Viswanathan%2C+K.S.)
Keywords:	Conformation Energy Polarity Molecular structure
Issue Date:	2017
Publisher:	ACS Publications
Citation:	Journal of Physical Chemistry A, 121 (32)
Abstract:	The conformations of tri-n-butyl phosphate (TBP) were studied using matrix isolation infrared spectroscopy and density functional theory (DFT) calculations. TBP was trapped in a N2 matrix using both effusive and supersonic sources, and its infrared spectra were recorded. The computational exploration of TBP is a very demanding problem to confront, due to the presence of a large multitude of conformations in TBP. To simplify the problem, computations were done on model compounds, dimethyl butyl phosphate (DMBP) and dibutyl methyl phosphate (DBMP), to systematically arrive at the conformations of TBP that are expected to contribute to its chemistry at room temperature. Some predictive rules seem to simplify this complex conformational landscape problem. The predictive rules that were formulated enabled us to search the relevant portion of the conformational topography of this molecule. The computations were performed at the B3LYP level of theory using the 6-31++G(d,p) basis set. Vibrational wavenumber calculations were also performed for the various conformers to assign the infrared features of TBP, trapped in solid N2 matrix.
URI:	https://pubs.acs.org/doi/10.1021/acs.jpca.7b05006 (https://pubs.acs.org/doi/10.1021/acs.jpca.7b05006) http://hdl.handle.net/123456789/1854 (http://hdl.handle.net/123456789/1854)
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