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Dynamics of polar guest molecules contained in cryptophane molecular crystals ERICK WINSTON, ROBERT HORANSKY, MATTHEW MYERS, JOHN PRICE, The University of Colorado, Boulder, JAROSLAV VACEK, Academy of Sciences of the Czech Republic — Cryptophanes are a class of molecules with an interior cavity which can be occupied by smaller guest molecules non-covalently. In cases where the guest molecules are free to tumble within the cryptophane, and where the cryptophanes can be crystalized, it is possible to create ordered arrays of reorienting guest molecules. By using dipolar guests such as the methyl halides, the guest motions can be observed by dielectric spectroscopy and guests may order via strain or dipole-dipole interactions. We will present the results of dielectric spectroscopy experiments on single crystals of iodomethane in cryptophane-A. The observed rotational barriers are compared to computational molecular mechanics calculations based on the X-ray structure of the complex.

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