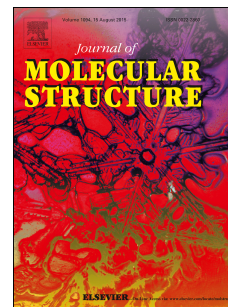


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Towards a better understanding of the parameters determining the competition between bromine halogen bonding and hydrogen bonding: An FTIR spectroscopic study of the complexes between bromodifluoromethane and trimethylamine

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Towards a better understanding of the parameters determining the competition between bromine halogen bonding and hydrogen bonding: an FTIR spectroscopic study of the complexes between bromodifluoromethane and trimethylamine.

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Abstract

Previous experimental and theoretical studies of various model compounds dissolved in liquid noble gases have shown that iodine halogen bonding can compete with hydrogen bonding and that experimental information on the thermodynamic equilibria present can be derived. To get a more general grasp of the competition between halogen bonding and hydrogen bonding, and to expand the set of experimental data to other, weaker, halogen donors, solutions in liquid krypton containing mixtures of bromodifluoromethane with trimethylamine or the fully deuterated trimethylamine- d_9 are studied using FTIR spectroscopy. Analysis of the experimental data obtained is supported by *ab initio* calculations, statistical thermodynamics and Monte Carlo-Free Energy Perturbation calculations. Careful comparison of the spectra of the monomers and of the mixtures studied, shows that for all solutions studied, only features due to a hydrogen-bonded complex are observed. The experimental complexation enthalpy for this species is determined to be $-14.2(4) \text{ kJ mol}^{-1}$.

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