Title:	Matrix isolation infrared and DFT study of the trimethyl phosphite-hydrogen chloride interaction: Hydrogen bonding versus nucleophilic substitution
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Abstract:	Trimethyl phosphite (TMPhite) and hydrogen chloride (HCl), when separately codeposited in a N2 matrix, yielded a hydrogen bonded adduct, which was evidenced by shifts in the vibrational frequencies of the TMPhite and HCl submolecules. The structure and energy of the adducts were computed at the B3LYP level using 6-31++G* and aug-cc-pVDZ basis sets. While our computations indicated four minima for the TMPhite-HCl adducts, only one adduct was experimentally identified in the matrix at low temperatures, which interestingly was not the structure corresponding to the global minimum, but was the structure corresponding to the first higher energy local minimum. The Onsager self-consistent reaction field model was used to explain this observation. In an attempt to prepare the hydrogen bonded adduct in the gas phase and then trap it in the matrix, TMPhite and HCl were premixed prior to deposition. However, in these experiments, no hydrogen bonded adduct was observed; on the contrary, TMPhite reacted with HCl to yield CH3Cl, following a nucleophilic substitution, a reaction that is apparently frustrated in the matrix.
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