Title:	A Matrix Isolation Infrared and ab initio Study of the Conformers of 2-Nitrophenol: Hydrogen Bond Driven cis-trans Stabilization
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Abstract:	2-Nitrophenol can exist in cis and trans geometries, with the cis structure having the possibility of a hydrogen bond. The energy difference between the two geometries is large, being about 10 kcal mol-1, at the M06-2X/6-311++G(d,p) and MP2/6-311++G(d,p) levels of theory. However, the hydrogen bonds usually have interaction energies between 1-5 kcal mol-1 and the question therefore arises whether the energy difference between cis and trans geometries of 2-Nitrophenol is the result of an intramolecular hydrogen bond or if any other stabilising factor is also operating. Computations show that the trans nitrophenol is non-planar while the cis isomer is planar. The difference in the O-H stretching frequency between the cis and trans form is unusually large (~350 cm-1). Therefore, the various issues in the cis-trans isomers need to be understood. To study this problem further, we also studied a series of compounds: salicylic acid, salicylaldehyde and the salicylate. Matrix isolation infrared spectroscopy, is a powerful tool to study weak interactions and conformers, has been used to study in this work along with ab initio method. The technique offers higher spectral resolution, which is an important factor for separating complex spectral patterns in conformers and in weak hydrogen bond interactions. The ab initio computational calculation has been performed on all the molecules: 2-Nitrophenol, salicylaldehyde, salicylic acid and salicylate at MP2, M06-2X, and B3LYP level of theory and 6-311++G(d,p) and aug-cc-pVDZ basis sets. The computational results show that the stabilization energy between cis and trans conformer of all the molecules is about ~ 11 kcalmol-1. The non-planar conformer has been shown by trans 2-Nitrophenol and trans salicylate while all the conformers of all the molecules are planar. The matrix isolation experiment is also performed on 2-Nitrophenol in N2 and Ar matrix and salicylaldehyde in N2 matrix and all the modes have been assigned.
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