Title:	Matrix Isolation Infrared and Ab Initio Study of the Interaction of N-Heterocyclic Carbene with Water and Methanol: A Case Study of a Strong Hydrogen Bond
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Abstract:	This study reports, for the first time, the experimental study of the hydrogen-bonded complexes of H2O and MeOH with 1,3-dimethylimidazol-2-ylidene, which is a dimethyl-substituted N-heterocyclic carbene, using matrix isolation infrared spectroscopy. The hydrogen bond was found to be established between the carbene carbon and the hydrogen in the O–H group of H2O or MeOH. The hydrogen-bonded complexes of N-heterocyclic carbenes are significantly stronger than many conventional hydrogen-bonded systems, as is evidenced by the large red shifts observed in the infrared frequencies of complexed H2O and MeOH. The experimental results were corroborated by computations performed at MP2 and M06-2X levels of theory, using 6-311++G(d,p) and aug-cc-pVDZ basis sets, which indicated large interaction energies (~9 kcal mol–1) for these complexes. Single-point calculations at the CCSD level of theory were also performed. Atoms-in-molecules (AIM), NBO, and LMOEDA analyses were also performed to understand the nature of the intermolecular interactions in these complexes. The dominant interaction was the electron delocalization from the carbene carbon to the σ* orbital of O–H of H2O or MeOH.
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