Metal-Formamide Complexes and their Role in Prebiotic Chemical Catalysis

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The possibility that formamide represents a key building block for the prebiotic syntheses of nucleobases, amino acids, carboxylic acids, and sugars has been recently put forward by Saladino et al. [1]. The role of minerals and mineral surfaces in catalyzing the chemical reactions of formamide also have been considered experimentally. Because such minerals dissolve themselves in water at temperatures close to or above 100 °C, it is important to investigate the interaction of formamide with hydrated metal cations as well as the structures of the corresponding metal-formamide complexes. A search of the Cambridge Structural Database (CSD) indicates that only a limited number of complexes which are relevant to the coordination chemistry of formamide has been so far crystallographically characterized. In contrast, a large number of transition metal-formamide complexes has been characterized with Raman spectroscopy [2].

With this information in mind, we decided to investigate the neutral and charged complexes of formamide with alkali earth metal ions, particularly Mg(2+) and Ca(2+), with the aid of computational quantum chemistry methods. The calculations provide important information not only about the molecular geometry of such complexes but also on the intramolecular interactions that take place once the formamide molecules are coordinated to the metal center. In general, the coordination of the substrate to the metal center is important for its activation for it represents the initial step of metal-based catalytic processes [3].

[1] Saladino et al., 2012, Chem. Soc. Rev., 41, 5526.
[2] Powell et al., Spectrochim. Acta A, 1985, 41, 1023.
[3] Pichierri et al., 2007, J. Org. Chem., 72, 861.

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