

Experimental and Theoretical Study on the Structure of Nitramide H_2NNO_2

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Nitramide was investigated by multinuclear NMR spectroscopy, X-ray-diffraction and computational methods. The crystal structure analysis at various temperatures reveals a planar conformation of the molecule with a N-N bond length corresponding to a bond order between one and two. Hydrogen bonds connect the nitramide molecules side-on and end-on. This leads to the formation of layers in the crystal. Calculations were performed to explain the shorter N-N bond length in the crystal compared to the gas phase. The nitramide trimer is used as a model.