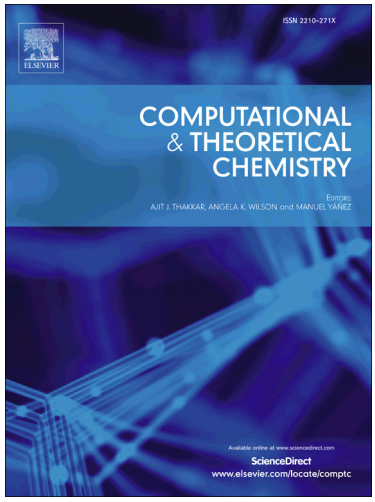

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PII: S2210-271X(17)30097-X
DOI: http://dx.doi.org/10.1016/j.comptc.2017.02.031
Reference: COMPTC 2427

To appear in: *Computational & Theoretical Chemistry*

Received Date: 14 February 2017
Revised Date: 28 February 2017
Accepted Date: 28 February 2017

Please cite this article as: A. Karpfen, On the structure of the H_2CO-HNO dimer: Planar or orthogonal?, *Computational & Theoretical Chemistry* (2017), doi: http://dx.doi.org/10.1016/j.comptc.2017.02.031

On the structure of the H_2CO-HNO dimer: Planar or orthogonal?

Alfred Karpfen[1]

Abstract:

The potential energy surface of the dimer formed between formaldehyde and nitrosyl hydride has been investigated theoretically at the MP2 and CCSD(T) levels using several extended basis sets. Six low-lying minima, all with Cs symmetry, were detected. Two of them are planar, four are non-planar. All dimers display geometry changes and vibrational frequency shifts characteristic for a formyl group engaged in hydrogen bonding: red shifts of C=O stretches and blue shifts of C-H stretches. In five of the dimers the N-H stretching frequency is also blue-shifted, but in one structure the blue shift vanishes, when applying harmonic vibrational analysis. Including anharmonic effects, all N-H stretches are blue shifted. The two most stable structures are nearly equienergetic and are reminiscent of the minima encountered in the formaldehyde dimer.

Keywords: ab initio; hydrogen bond; blue shift; formaldehyde, nitrosyl hydride.

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