

## THE POSITION OF DEUTERIUM IN THE HOD – N<sub>2</sub>O AS DETERMINED BY STRUCTURAL AND NUCLEAR QUADRUPOLE COUPLING CONSTANTS

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A recent investigation of the HOD – N<sub>2</sub>O complex measuring the OH + OD excited band in the near-IR was completed by Foldes *et al.*<sup>a</sup> During this study, one of us (WAK) was contacted about the position of deuterium in the HOD – N<sub>2</sub>O complex, as his group completed the original microwave study of H<sub>2</sub>O – N<sub>2</sub>O and its deuterated isotopologues<sup>b</sup> in 1992. The results of this microwave study did not give the orientation of HOD in the complex, however, we present here a supplementary study to the original microwave work using a Balle-Flygare cavity instrument, attempting to determine the orientation of HOD relative to the N<sub>2</sub>O. In addition to a Kraitchman and a least-squares inertial structure fit of the molecule, we present the nuclear quadrupole coupling tensor of deuterium to determine the position of HOD in the complex.

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<sup>a</sup>Földes, T.; Lauzin, C.; Vanfleteren, T.; Herman, M.; Lièvin, J.; Didriche, K. High-resolution, near-infrared CW-CRDS and ab initio investigations of N<sub>2</sub>O – HDO. *Mol. Phys.* **2015**, *113*(5),473-482.

<sup>b</sup>Zolanz, D.; Yaron, D.; Peterson, K.I.; Klemperer, W. Water in weak interactions: The structure of the water-nitrous oxide complex. *J. Chem. Phys.* **1992**, *97*,2861.