MICROWAVE SPECTROSCOPY AND INTERNAL DYNAMICS OF THE Ne-NO_2 VAN DER WAALS COMPLEX

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The rotational spectrum of the open-shell complex Ne-NO_2 in the 6 - 18 GHz region is reported. Both fine and hyperfine structure are observed. However, the spectrum does not fit a semi-rigid model as well as the related species Ar-NO_2 [a], Kr-NO_2 [b] and Xe-NO_2 [c]. This is almost certainly a result of the "floppy" nature of this species.

In order to model the dynamics of the complex and to reproduce the observed spectrum, we have obtained an accurate intermolecular potential surface using the RCCSD(T) method and aug-cc-pV(D/T)Z basis sets (extrapolated to the complete basis set limit). Full quantum dynamics calculations were then performed on this surface to give the rotational energy levels and the effective fine and hyperfine structure constants.

[a] R.J. Low, M.D. Brooks, C.J. Whitham and B.J. Howard *J. Chem. Phys.*, **105**, 6756 (1996).

[b] S. Blanco, C.J. Whitham, H. Qian and B.J. Howard, *PCCP.*, **3**, 3895 (2001).

[c] C.J. Whitham, R.J. Low and B.J. Howard, *Chem. Phys. Lett.*, **286**, 408 (1998).