THE Ar-CO POTENTIAL ENERGY SURFACE DETERMINED THROUGH FITTING OF MICROWAVE DATA

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The Ar-CO complex is very challenging theoretically since it is a floppy molecule displaying two large amplitude motions: A vdW stretching mode corresponding to a low frequency mode of 18 cm^{-1} and a bending mode corresponding to an even lower frequency of 12 cm^{-1}. As the A rotational constant of the complex is only 5 times smaller than the frequency of the bending mode, one expects a strong coupling between the two large amplitude motions and the overall rotation of the molecule. Subband by subband analyses[a] of the large body of infrared[a] and microwave[b] data available now for the complex showed that this was indeed the case. However, although theses data include several values of the vibrational quantum numbers, no global analysis of the high-resolution data pertaining to the complex has been carried out yet.

In the present paper, a new theoretical approach aimed at accounting for the rovibrational energy of the complex will be presented. In this variational approach, the 2-dimensional Schrödinger equation for the two large amplitude vdW modes is solved and all the terms arising in the the Hamiltonian are taken into account. For instance, the new approach allows us to reproduce the variation, evidenced in the subband by subband analyses,[a] of the effective B-values upon the K rotational quantum number and the two vibrational quantum numbers.

In the paper, the new submillimeter-wave measurements carried out in Cologne will also be presented. With a view towards determining the vdW potential energy surface, the new theoretical approach has been used to perform a preliminary global analysis of these new data along with the already available ones[b] and its results will also be discussed.

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[a] S. König, G. Hilpert, and M. Havenith, *Molec. Physics* **86,** 1233. (1995). Y. Xu, S. Civiš, A. R. W. McKellar, S. König, M. Haverlag, G. Hilpert, and M. Havenith, *Molec. Physics* **87,** 1071. (1996). Y. Xu and A. R. W. McKellar, *Molec. Physics* **88,** 859 (1996).

[b] *See for instance:* R. Gendriesch, I. Pak, F. Lewen, L. Surin, D. A. Roth, and G. Winnewisser, *J. Molec. Spectrosc.* **196,** 139 (1999) *and earlier references therein.*