THE HIGH RESOLUTION SPECTRUM OF THE $Ar-C_2H_2$ COMPLEX

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New spectra of the $Ar-C_2H_2$ van der Waals complex have been recorded using FANTASIO+, a new experimental setup with improved signal to noise and measurement accuracy[a] over the previous one, FANTASIO.[b] The spectra span the 6500–6600 cm^{-1} region corresponding to the $\nu_1 + \nu_3$ band of isolated acetylene. Several bands of the complex were observed. The strongest one connects the two ground van der Waals states and could be rotationally assigned. The yet unassigned weaker bands are combination bands involving changes in the van der Waals modes quantum numbers.

The new experimental data have first been used to refine an *ab initio* potential energy surface (PES) obtained at CCSD(T) level with large basis sets including bond functions. Combination differences involving rotational levels of the strongest band lower state were calculated up to $J = 9$ and $K_a = 1$ and fitted together with microwave[c] and infrared data.[d] The approach used in the analysis treats exactly the large amplitude bending and stretching modes and the overall rotation of the complex. The parameters involved in the expansion[e] of the PES were fitted to the line positions yielding RMS values of 0.021 MHz and 0.6×10^{-3} cm^{-1} for the microwave and infrared data, respectively.

The new experimental data have also been used to refine the PES of the complex for the $v_1 = v_3 = 1$ vibrational state of acetylene. Using the results of the previous analysis, rotational energies were retrieved for the strongest band upper state and analyzed. The results of this second analysis are not as satisfactory as the previous one. This may be due to perturbations or to the fact that the PES for the upper vibrational state differs from that of the ground vibrational state.

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[a] Didriche, Lauzin, Foldès, De Ghellinck D'Elseghem Vaernewijck, and Herman, *Molec. Phys.* **108** (2010) 2155.

[b] Lauzin, Didriche, Macko, Demaison, Liévin, and Herman, *J. Phys. Chem. A* **113** (2009) 2359.

[c] DeLeon and Muenter, *J. Chem. Phys.* **72** (1980) 6020; and Liu and Jäger, *J. Molec. Spec.* **205** (2001) 177.

[d] Bemish *et al.*, *J. Chem. Phys.* **99** (1993) 8585; and Hu *et al.*, *J. Molec. Spec.* **153** (1992) 486.

[e] Munteanu and Fernandez, *J. Chem. Phys.* **123** (2005) 014309.