

The *ab initio* intermolecular potential of Ar-C₂H₂ refined using high-resolution spectroscopic data

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The high-resolution infrared spectra of the $\nu_1 + \nu_3$ (2CH) band of the Ar-C₂H₂ complex has been recorded from 6544 to 6566 cm⁻¹. The previously reported [1] $K_a=1-0$, 2-1, and 0-1 sub-bands were observed and the $K_a=1-2$, 2-3 and 3-2 sub-bands were assigned for the first time. The intermolecular potential energy surface of this complex has been calculated *ab initio* and optimized fitting the new high-resolution data. Refined intermolecular potential energy surfaces have been obtained for the ground vibrational state and for the excited $\nu_1 = \nu_3 = 1$ stretching state. For the former state, the results of the analysis are satisfactory and the microwave transitions of the complex are reproduced with a root mean square deviation of 5MHz. For the latter state, systematic discrepancies arise in the analysis.

[1] C. Lauzin, K. Didriche, P. Macko, J. Demaison, J. Liévin, M. Herman *J. Phys. Chem. A* **2009**, *113*, 2359.