FOURIER TRANSFORM MICROWAVE SPECTROSCOPIC AND AB INITIO STUDIES OF THE Kr-CH_4 AND Ar-CH_4 VAN DER WAALS COMPLEXES

YAQIAN LIU and WOLFGANG JÄGER, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada, T6G 2G2*.

Rotational spectra of various isotopomers of the Kr-CH_4 van der Waals complex were recorded using a pulsed molecular beam Fourier transform microwave spectrometer. Transitions corresponding to two excited internal rotor states, namely the j=1, K=0 and j=2, K=1 states, were measured and assigned, in addition to the previously reported ground state transitions.[a] The j=1, K=0 state was found to be Coriolis perturbed by a nearby j=1, K=1 state. The spectra of the isotopomers containing ^{83}Kr showed nuclear quadrupole hyperfine structure. Rotational, centrifugal distortion, and quadrupole coupling constants were determined and were used to obtain structural parameters. *Ab initio* potential energy surfaces of Kr-CH_4 and Ar-CH_4 were constructed at the CCSD(T) level of theory with the aug-cc-pVTZ basis set supplemented with bond functions. The dipole moments of the two complexes were also computed at various configurations. The obtained results from the *ab initio* calculations were compared with those from the experiment.

[a] Y. Liu and W. Jäger, 55th International Symposium on Molecular Spectroscopy, paper RE05 (2000).