THE ROTATIONAL SPECTRUM AND POTENTIAL ENERGY SURFACE OF AR-SIO: AN EXPERIMENTAL INVESTIGATION

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The rotational spectra of five isotopic species of the Ar–SiO complex have been observed at high-spectral resolution between 8 and 18 GHz using chirped Fourier transform microwave spectroscopy and a discharge nozzle source; follow-up cavity measurements have extended these measurements to as high as 35 GHz. The spectra of the normal species is dominated by a strong progression of a-type rotational transitions arising from increasing quanta in the Si–O stretch. A rotational analysis of these lines and a hyperfine analysis of Ar–Si$^{17}$O suggest that the complex is a highly fluxional prolate symmetric rotor with a vibrationally-averaged structure close to T-shaped in which the oxygen atom lies closer to argon than the silicon atom, much like Ar–CO. Newly performed calculations of the rovibrational level pattern are in good agreement with the experimentally-derived rotational constants of normal and isotopic Ar–SiO up to $v=12$ ($\sim$14,500 cm$^{-1}$) in the Si–O stretch suggesting that the present theoretical treatment well reproduces the salient properties of the intramolecular potential.