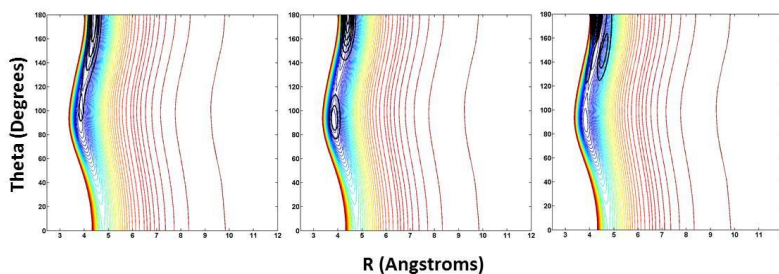


THE ROTATIONAL SPECTRUM AND POTENTIAL ENERGY SURFACE OF AR-SiO: A THEORETICAL INVESTIGATION

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The rotational spectra of five isotopic species of the Ar–SiO complex have been observed at high-spectral resolution, employing various techniques to obtain spectra between 8 and 35 GHz. Progressions of rotational transitions were recorded for a range of quanta in the Si–O stretch which correspond to resonance states of the complex since the vibrational frequency of the diatomic exceeds the binding energy of the complex. A complementary theoretical study was performed in which variational rovibrational calculations were performed using a series of potential energy surfaces (PESs) representing the SiO + Ar interaction and describing a range of vibrational quanta in the SiO($v=0,1,\dots,7$) fragment. As seen in the Figure, the global minimum ($V = -152.2 \text{ cm}^{-1}$) is nearly T-shaped, but a barrier of only 7.2 cm^{-1} leads to a second minimum in a long channel along the angular coordinate. The relative energy of the T-shaped minimum and the channel toward linearity, varies with the number of quanta in SiO (progressively favoring the more linear structure), and for SiO($v=7$), the T-shaped structure is no longer the global minimum. To compute the rovibrational levels and wavefunctions, the RV3 three-atom variational code of Wang and Carrington was used.



Probability density plots for some $J=0$ vdW vibrational states on the SiO($v=0$)–Ar PES. (left) ground state ($E = 0.0 \text{ cm}^{-1}$), (middle) first bend-excited state ($E = 2.63 \text{ cm}^{-1}$), (right) first stretch-excited state ($E = 33.57 \text{ cm}^{-1}$). Probability is delocalized along a low energy channel towards linearity.