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On the Structure of the SF₆⁻ Anion JEFFREY STEILL, ROBERT COMPTON, The University of Tennessee Chemical Physics, K. BOWEN, SARAH STOKES, Johns Hopkins University Department of Chemistry — Negative ions of Sulfur hexafluoride have been studied in detail for decades; however, there remains much to be understood about this subject. The geometry of SF₆⁻ in its ground state is either of O_h symmetry like the parent molecule, or of a distorted C_{4v} symmetry. The lower symmetry form with an elongated axial S-F bond is predicted by Coupled-Cluster computational methods to be lower in energy by about 0.1 eV. The calculated frequencies for the two different geometries are significantly different, providing a possible means for a definitive structure determination. Photoelectron spectra of vibrationally relaxed SF₆⁻ give an EA of 1.0 (+/- 0.1) eV with a very broad energy spectrum, implying a significant geometry change from the neutral to the anion. This suggests the C_{4v} form may be the likely geometry. Quasi-equilibrium theory calculations of the lifetime of SF₆⁻ using the calculated frequencies for the anion combined with the known electron attachment rates gives a mean lifetime on the order of one millisecond. This lifetime is much larger than the lifetime derived from TOFMS methods, which is on the order of microseconds. The vibrational structure in the PES spectra is compared to the calculated frequencies for both of the possible geometries, but does not provide a completely unambiguous assignment. Therefore, we will also describe our recent attempts to measure the vibrational spectrum of gas-phase SF₆⁻.

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