AB INITIO AND EXPERIMENTAL STUDIES OF THE *E* INTERNAL ROTOR STATE OF He-CH_3F

KELLY J. HIGGINS, ZHENHONG YU, and WILLIAM KLEMPERER, *Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02138.*

The excited *E* internal rotor state of He-CH_3F is studied using microwave spectroscopy and *ab initio* calculations. Bound state calculations on a high-level *ab initio* intermolecular potential surface[a] predict a T-shaped ground state and two low-lying excited states with the He localized either at the C end ("linear") or the F end ("anti-linear") of the C-F bond, similar to that found for the *A* internal rotor state presented previously.[b] There are several distinct differences between the *A* and *E* states. Whereas the ground state rotational transitions of the *A* state could be fit with a standard asymmetric rotor Hamiltonian, the *E* state exhibits a much more complex energy level structure due to the internal rotation of the CH_3F. In addition, the *E* state is calculated to be bound by 11.709 cm^{-1}, 0.249 cm^{-1} greater than the *A* state relative to their respective dissociation products, $K = 1$ or $K = 0$ CH_3F, and the ground state to linear state energy gap is predicted to be 4.148 cm^{-1}, 0.156 cm^{-1} greater than in the *A* state. At present six rotational transitions between five different energy levels have been observed and assigned with the aid of double resonance experiments and the *ab initio* calculations.

[a] 54th International Symposium on Molecular Spectroscopy (1999)
[b] 55th International Symposium on Molecular Spectroscopy (2000)