

AB INITIO AND EXPERIMENTAL STUDIES OF THE *E* INTERNAL ROTOR STATE OF He-CH<sub>3</sub>F

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The excited *E* internal rotor state of He-CH<sub>3</sub>F is studied using microwave spectroscopy and *ab initio* calculations. Bound state calculations on a high-level *ab initio* intermolecular potential surface<sup>a</sup> 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.<sup>b</sup> 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<sub>3</sub>F. In addition, the *E* state is calculated to be bound by 11.709 cm<sup>-1</sup>, 0.249 cm<sup>-1</sup> greater than the *A* state relative to their respective dissociation products, *K* = 1 or *K* = 0 CH<sub>3</sub>F, and the ground state to linear state energy gap is predicted to be 4.148 cm<sup>-1</sup>, 0.156 cm<sup>-1</sup> 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.

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