TROPYL RADICAL: A JAHN-TELLER SYSTEM WITH SEVEN-FOLD SYMMETRY

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The laser induced fluorescence (LIF) spectrum of the $\widetilde{A}^2E_3'' \leftarrow \widetilde{X}^2E_2''$ transition of the tropyl, C_7H_7, radical has been recorded and found to be in good agreement with the recently recorded REMPI spectrum.[b] Dispersed fluorescence (DF) spectra, pumping several different transitions, have also been observed and yield the first experimental information on the ground-state vibronic levels. In order to analyze these spectra extensive *ab inito* calculations were carried out to determine the parameters of both the ground- and excited-state Jahn-Teller potential energy surfaces (PESs). Efforts to simulate both the LIF and DF spectra, and to refine the *ab inito* parameters by the aid of the SOCJT program will be discussed.[c]

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[b] T. Pino, F. Guthe, H. Ding, J. P. Maier *J. Phys. Chem. A* **106**, 10022, 2002.

[c] T. A. Barkholtz, T. A. Miller *Int. Rev. Phys. Chem.* **17**, 435, 1998.