ROTATIONAL FINE STRUCTURE IN THE FLUORESCENCE EXCITATION SPECTRUM OF TOLUENE

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Experimental measurements have been reported the $S_1 - S_0$ fluorescence excitation spectrum of toluene[1] which reveal forbidden bands corresponding to excited levels of the methyl internal rotation mode. We present theoretical predictions of the rotational fine structure of these bands, incorporating *ab initio* and least-squares-fitted geometrical structures for the S_0 and S_1 states. We particularly consider the coupling of overall and internal rotation, and the direct calculation of individual rovibronic line intensities.

[1] R. A. Walker, E. Richard, K.-T. Lu, E. L. Sibert III, and J. C. Weisshaar, J. Chem. Phys. **102** (1995) p. 8718, and references therein.