

# Valence and Rydberg excitations of 4-fluorotoluene in the VUV photoabsorption energy range

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The electronic state spectroscopy of 4-fluorotoluene in the gas phase has been investigated for the first time using high-resolution vacuum ultraviolet photoabsorption (VUV) experiments in the 4.4–10.8 eV energy range, with absolute cross-section measurements obtained. Additionally, we also present a set of ab initio calculations (vertical excitation energies and oscillator strengths) at time-dependent density functional theory (TD-DFT) [1] theory level with GAMESS (The General Atomic and Molecular Electronic Structure System) [2] package. These are used in the assignment of valence, mix valence-Rydberg and Rydberg transitions, with the associated vibronic series analyzed. We compare our results with the other two conformers of fluorotoluene, namely 2-fluorotoluene [3] and 3-fluorotoluene (submitted to Journal of Quantitative Spectroscopy and Radiative Transfer).

**Keywords:** Fluorotoluene, parafluorotoluene, 4-fluorotoluene, photoabsorption, VUV, cross section, valence states, Rydberg states.

## Referências

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