

Singlet and triplet transitions in UV optical absorption spectra of pyrene

© Laysan Z. Khatymova,⁺ Olga G. Khvostenko,* and Rustem V. Khatymov

Laboratory of Negative Ion Mass Spectrometry and Molecular Spectroscopy.

Institute of Molecule and Crystal Physics. Ufa Research Center of Russian Academy of Sciences.

Prospekt Oktyabrya, 151. Ufa, 450075. Bashkortostan Republic. Russia.

Phone: +7 (347) 231-91-68. E-mail: lesya0706@ya.ru

*Supervising author; ⁺Corresponding author

Keywords: condensed aromatic compounds, pyrene, electronic structure, electron-excited singlet state, triplet states, UV optical absorption spectroscopy, photoelectron spectroscopy.

Abstract

Optical absorption UV–Vis spectra were obtained for pyrene. The survey UV-spectrum depicting the transitions into singlet electron-excited states in the range 1–6 eV was recorded using cyclohexane as solvent. With the aid of a cuvette with a large optical path length and by dissolving the pyrene sample in bromopropane, the spectrum was registered from which the direct vertical transitions into triplet states were distinguished. The experimental value 2.75 eV was determined for the energy of lowest vertical triplet transition, by ca. 0.6 eV lying higher than corresponding adiabatic transition energy measured by the other groups using phosphorescence technique. Assignment of the bands observed in UV spectra was accomplished using TD DFT B3LYP/6-31G level quantum chemical calculations. The pyrene molecular ground state electronic structure, namely the configuration of occupied and virtual molecular orbitals involved in electron excitation processes of interest, was considered on the basis of photoelectron spectrum taken from literature. The photoionization bands observed in this spectrum were attributed to the specific occupied molecular orbitals obtained from B3LYP/6-311G level calculations. The symmetries and electronic configurations of the studied singlet and triplet electron-excited states of pyrene were specified as well.