ELECTRON ENERGY STRUCTURE OF THE TETRACYANOQUINODIMETHANE MOLECULE IN THE NEUTRAL AND ANION-RADICAL STATES

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S u m m a r y

The absorption spectra of tetracyanoquinodimethane (TCNQ) solutions and TCNQ films have been studied in the spectral range of 1.4—5.6 eV at room temperature. Making use of the results obtained and the literature data, the energy structures of the electronic levels of a neutral molecule TCNQ° and an anion-radical $TCNQ^{\div}$ have been analyzed. Their excited states have been ascertained to belong mainly to the $\pi\pi^*$-type. In a condensed state, the absorption bands at 2.85 and 3.65 eV are caused by $TCNQ^{\div}$, the band at 3.08 eV by TCNQ°, and the band 5.25 eV by both $TCNQ^{\div}$ and TCNQ°. The absorption spectra of the TCNQ solutions in water and acetic acid in the range of 1.4—4.1 eV consist of dimer bands only, while they are a superposition of the absorption bands of TCNQ°, $TCNQ^{\div}$, and $TCNQ^{\div}$ dimers for the solutions in ethanol and dimethylformamide.