



Study of the interaction of tris-(8-hydroxyquinoline) aluminum (Alq₃) with potassium using vibrational spectroscopy: Examination of the possible isomerization upon K-doping

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
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Abstract

The geometrical structure of potassium doped Alq₃ (tris-(8-hydroxyquinoline) aluminum) and its interaction with potassium were studied using infrared reflection-absorption spectroscopy (IRRAS), surface enhanced Raman scattering and DFT calculations. The major aim of this study was to examine the isomerization of Alq₃ molecules from the meridional to the facial form upon alkali-metal doping, which has been theoretically predicted by other researchers. The observed spectra showed significant changes after potassium deposition. The calculated IR spectra of the K-Alq₃ complex for the meridional and facial forms were very different, and that the meridional form is in reasonable agreement with the observed spectrum. This demonstrates that the Alq₃ molecule is not converted to a facial isomer by potassium deposition, but retains the meridional form, in contrast to reported theoretical predictions. We also found that the calculated IR spectrum of the K-Alq₃ complex with Alq₃ in its meridional form is much different from that of the isolated anion in the same isomeric form. We consider that the observed significant changes of spectra are due to the modification of electron distribution by the complexation with the K atom. Even though vibrational spectra of alkali-metal doped organic materials are usually interpreted on the basis of an isolated anion, the results presented here show that care should be taken in interpreting the spectra of doped organic materials, and that the presence of the counter ion needs to be taken into account. The observed Raman spectra and theoretical calculations of the Raman spectra show similar trends when compared to the IRRAS results. The present study demonstrates that vibrational spectroscopy can be used as a sensitive tool for discriminating subtle differences between isomers as well as between complexes and isolated anions.

Keywords: Infrared and Raman spectroscopy; Organic/inorganic interfaces

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