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

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The geometrical structure of potassium-doped Alq₃ [tris-(8-hydroxyquinoline) aluminum] and the interaction between the Alq₃ molecule and potassium were studied using infrared reflection absorption spectroscopy (IRRAS), surface-enhanced Raman scattering (SERS), and density functional theory calculations. A major aim of this study was to examine the theoretically predicted isomerization of Alq₃ molecules from the meridional form to the facial form upon alkali-metal doping. The observed spectra show significant changes with the deposition of potassium on a thin Alq₃ film. The calculated IR spectra of the K-Alq₃ complex differ significantly between the meridional and facial forms, and the calculation for the meridional form agrees fairly well with the observed spectrum. This demonstrates that (1) the Alq₃ molecule does not change to a facial isomer with the deposition of potassium, but retains the meridional form, in contrast to the reported theoretical prediction, and (2) the structure of the complex as evaluated from geometry optimization is reliable. We also found that the calculated IR spectrum of the K-Alq₃ complex with Alq₃ in its meridional form is significantly different from that of the isolated anion in the same isomeric form, which probably reflects nonuniform interaction between K and the three ligands of Alq₃. On the other hand, the calculated spectra of Alq₃ and the K-Alq₃ complex in the facial form are similar, possibly because the K atom in the suggested structure lies on the axis of threefold symmetry, leading to an equivalent effect on the three ligands. 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 without considering the presence of the counter ion. The observed SERS spectra and theoretical calculations of the Raman spectra show similar trends when compared to the IRRAS results. The present results show that vibrational spectroscopy can be used as a sensitive tool for discerning subtle differences between isomers as well as between complexes and isolated anions. ©2004 American Institute of Physics

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