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Dielectric tensor of the $Ce@C_{82}-C_{2v}$ crystal

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The structures and electronic properties of isomer-separated solids in metallofullerenes have attracted special attention in chemistry as new spherical molecules and in materials science because of their possibilities of applications toward materials with novel functionalities. In this work, the average dielectric tensor $(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})/3$ are theoretically calculated by using Su-Schrieffer-Heeger (SSH) model in conjunction with the local field method and Ewald method for the simple cubic phase of the $Ce@C_{82}$ crystal. The crystal structures of metallofullerenes have been determined by Rietveld analyses for X-ray powder diffraction data. The difference in the crystal phases and physical properties has never been clarified among isomers of any metallofullerene. Even in the most popular metallofullerenes, $M@C_{82}$, the crystal phases and their structures have been studied only for the major Isomer (isomer I). Subsequently, it was shown that crystals of solvent-free $Ce@C_{82}$ isomer I (C_{2v}) were isomorphous with those of the $Dy@C_{82}$ isomer I. The value of a was $15.78(1)$ Å for isomers I of $Dy@C_{82}$ and $Ce@C_{82}$. Our results show that the optical dielectric tensor elements vary depending on the $Ce@C_{82}$ molecular orientation relative to the electric field of light and the x , y and z components of the optical dielectric tensor are different for the C_{82} molecule. This is due to a strong anisotropy of the C_{82} molecule. The first dielectric tensor peak of our results is about 0.65 eV for the $Ce@C_{82}$ crystal in the Fig. 1. The large values of compared to C_{60} also indicate a higher static polarizability and reflect the fact that the onset of the inter band transition is at lower energy for the endohedral mono metallofullerenes. As regards the energy region of the loss function where the $\pi \rightarrow \pi$ transitions contribute (below ~ 6 eV), the general spectral shape is quite similar to that for C_{60} . Due to the relatively low symmetry of these endohedral molecules, the fine structure is less clear and an assignment of the features visible in to particular transitions between the occupied and unoccupied molecular orbitals is hardly possible. We also found that the spectral shapes of the total absorption are mainly determined by the geometrical distributions of the pentagons' in the fullerene structures.

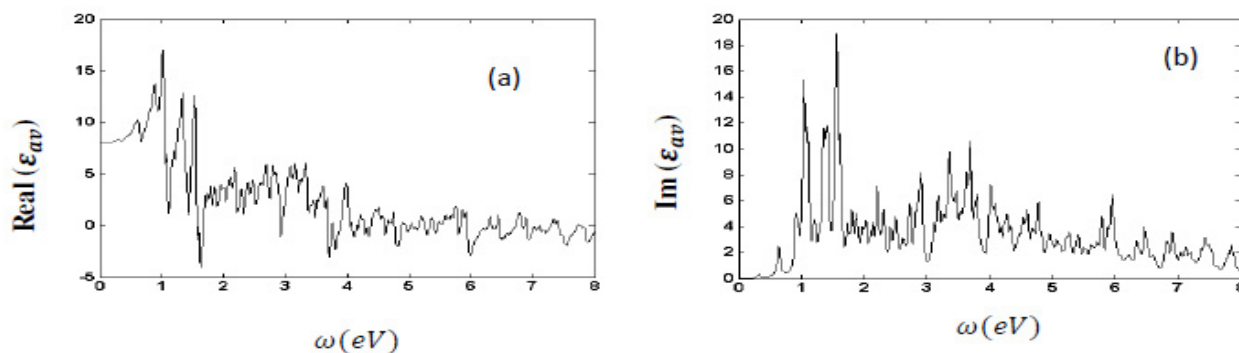


Figure 1: The (a) real and (b) imaginary parts of average elements of the dielectric tensor for the $Ce@C_{82}-C_{2v}$ crystal.

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