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Vibronic coupling in the icosahedral C_{60}^{2+} Jahn-Teller cation: Repercussions of the nonsimple reducibility of the $H \otimes H$ product

Abstract References Citing Articles (3)

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Coulomb coupling between the two holes in the fullerene cation C_{60}^{2+} results in high- and low-spin terms. Vibronic coupling of the high-spin terms to a single mode of vibration of h_g symmetry can distort the lowest adiabatic potential-energy surface into wells of D_{3d}, D_{5d}, D_{2h}, or C_{2h} symmetry depending upon the precise nature of the coupling produced by different admixtures of the two sets of coupling coefficients arising from the two H-type irreducible representations appearing in the symmetric part of the $H \otimes H$ Kronecker product. The symmetry of dynamic distortions of C_{60}^{2+} ions when coupling to all eight of the possible h_g modes is taken into account depends very closely on both the vibronic coupling parameters and the splittings between different Coulomb terms. Using estimates for these parameters from the literature leads us to conclude that the distortional symmetry is most likely to be D_{2h}, but there is also the possibility that it could be D_{3d}.

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