Accurate Calculations of Second-Order Vibronic Reduction Factors for C_{60} ions

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Abstract. An effective Hamiltonian containing Jahn-Teller (JT) first- and second-order vibronic reduction factors (RFs) is a convenient way of modelling the spectroscopic properties of solids and molecules in which vibronic interactions are important. It can act as a bridge between experimental data and basic theory. In particular, second-order RFs can give valuable information on many of the fundamental properties of strongly coupled systems. As interest in the icosahedral fullerene molecules and ions has grown over the last few years, it has become necessary to be able to calculate values for second-order RFs in icosahedral symmetry in terms of more fundamental vibronic coupling parameters. Following on from earlier work on the icosahedral $T \otimes h$ JT system, we present here results of such calculations of the second-order vibronic RFs for the icosahedral $G \otimes g$, $G \otimes h$, $H \otimes g$ and $H \otimes h$ JT systems. These systems are relevant for the ground and excited states of C_{60} anions and cations. The calculations are based on the Franck-Condon approximation followed by additional non-Condon corrections. Previous work has demonstrated that such an approach can give values for the RFs close to those deduced from experiments.
(In the electronic version of this article, the figures are in colour.)

1. Introduction

The electronic properties of individual fullerene ions are often much influenced by the vibrations of the fullerene molecule, due to the Jahn-Teller (JT) coupling [1, 2] between the electrons and the nuclear cage. This is particularly true when the electrons are in a degenerate orbital state [3]. Icosahedral symmetry gives rise to orbital triplet (T_1, T_2), quadruplet (G) and quintuplet (H) states (in additional to singlet A states). This means that the ground and/or the excited states of fullerene molecules and ions can be subject to various different JT effects. There are many ways in which the JT coupling can influence the data obtained during an experimental investigation and it is important to find out the nature of the physical principles involved in these influences.