ANHARMONIC VIBRATIONAL SPECTROSCOPY CALCULATIONS FOR RARE GAS CONTAINING HYDRIDES

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A number of rare gas containing hydrides with a common formula HRgX, where X represents a strongly electronegative species and Rg is Xe, Kr or Ar, have been prepared and identified in rare gas matrices [1, 2, 3] and in the gas phase [4]. Anharmonic vibrational calculations for various HRgX molecules [5, 6, 7] have been performed using the vibrational self-consistent field (VSCF) method, and its extension the correlation-corrected VSCF (CC-VSCF). The computational approach combines the electronic structure codes with algorithms that compute vibrational states including anharmonic effects and coupling between vibrational modes. The most intense bands of the HRgX molecules, the H-Rg stretching modes, are found to be highly anharmonic. In general, the other fundamental modes present anharmonic effects to a lesser extent. New predictions of overtone and combination vibrations, based on the CC-VSCF calculations, are made to help experimental investigations of several rare gas hydrides.

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