

Full normal coordinate analysis and molecular dynamic parameters for the Cr(CN)₆³⁻ ion

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A full normal coordinate analysis for the Cr(CN)₆³⁻ ion, in octahedral symmetry, has been carried out on the basis of new experimental data, using three different force fields. Consistent sets of force constants have been obtained and utilized to evaluate mean amplitudes of vibration (\bar{a}), perpendicular amplitude correction coefficients (K) and Shrinkage effects (δ). The capability of the force fields to reproduce the observed vibrational frequencies is discussed in detail. © 1986, Taylor & Francis Group, LLC. All rights reserved.