

Vibrational spectra and normal coordinate analysis of diamminemercury(II) chloride with $^{14}\text{N}/^{15}\text{N}$ and H/D isotopic substitution

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The IR and Raman spectra of solid diamminemercury(II) chloride with $^{14}\text{N}/^{15}\text{N}$ and H/D isotopic substitution have been measured. The spectra have been interpreted assuming D_{3d} symmetry for the $[\text{Hg}(\text{NH}_3)_2]^{2+}$ cations which have a linear framework structure. The skeletal metal-ligand modes $\nu_{\text{as}}(\text{HgN})$ and $\nu_{\text{as}}(\text{NHgN})$ in the IR spectra were confirmed by the observed isotopic shifts. A normal coordinate analysis for the three isotopic compounds has been carried out, based on a modified valence force field and on a modified Urey-Bradley force field. © 1981.