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The electric field gradient in mercuric chloride

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The temperature dependence of the

^{35}Cl quadrupolar resonance frequency has been measured in a high purity sample of mercuric chloride (HgCl_2) over the temperature range 4 K - 460 K. The results allow the temperature dependence of the electric field gradient (efg) at the two inequivalent sites of the chlorine atoms to be determined. Several models were considered to describe the experimental observations, including both librational and vibrational modes. The Bayer model for librational modes provides a satisfactory description of the changes in the efg over the entire temperature range, when the temperature variation of the lattice modes is taken into account, while the other mechanisms considered provide less convincing descriptions. A single librational mode with a wavenumber of approximately 26 cm^{-1} can account for the variation of the electric field gradient over the temperature range investigated. Our conclusions are consistent with the results of optical spectroscopy investigations.

Level (Hons, MSc, PhD, other)?

other

Consider for a student award (Yes / No)?

No

**Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?**

Yes

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