

# Calculation of Electric Field Gradients in Isolated Molecules Using the FPLAPW-Code WIEN95\*

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The full potential linearized augmented plane wave method as embodied in the program package WIEN95 was originally developed for crystalline solids and is based on crystal periodicity. The present work demonstrates that it is applicable to isolated molecules with the examples of  $\text{CdCl}_2$ ,  $\text{HgF}_2$ , and  $\text{HgCl}_2$  by investigating the required size of artificially enlarged unit cells and by calculating bond distances and vibrational frequencies in excellent agreement with experimental data. The dependence of electric field gradients at Cd and Hg, respectively, on bond angle is investigated. A point charge like behaviour of energetically low lying states is found, whereas large discrepancies from the point charge model occurred for the energetically high lying valence states.

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