P-22

Calculations of EFG by the simple point charge model†

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Nuclei with the spin of $I \geq 1$ possess not only the nuclear magnetic moment but also the electric quadrupole moment which interacts with the electric field gradient (EFG). The EFG at the site of the nucleus in solid is caused by its own electron cloud and other surrounding atoms. This interaction is customary represented by the quadrupole coupling constant (QCC) and the asymmetry parameter (η). In order to calculate EFG, we have to consider the effects of own electrons and environmental atoms. Even if the effect of the first nearest neighbour is dominant, we often deliberate next nearest neighbour atoms for acquiring a meaningful value of EFG. By assuming the neighbour atoms are simple point charges and considering only the first nearest neighbour atoms, the EFG is easily calculated analytically. Although this simple point charge (SPC) model cannot provide the exact value of QCC, however, the principal axes and asymmetry parameter may easily be estimated. In the case of some crystals with ideal structures, the SPC method explains reasonably well the experimental results. The calculated EFG using this method for several structures will be presented.

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