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Plenary Lecture

Nuclear Quadrupole Interaction in Wide-line NMR*

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The atomic nucleus is the major component of the matter and its spin may be 0, 1/2, 1, and so on. While the zero-spin nuclei are not susceptible to NMR, the non-zero spin ones are applicable to the technique. Among them the 1/2-spin nuclei, such as ^{1}H, ^{13}C and ^{19}F, have the nuclear magnetic dipole moment in addition to their nuclear electric charge, the so-called the electric monopole. Thus the magnetic dipole interaction is the major part of the interaction, as demonstrated well in the wide range of application in the high resolution NMR. When the nuclei have their spins equal to or larger than one, they have another property, the nuclear electric quadrupole moment in addition to the magnetic dipole moment. This electric quadrupole moment of the nucleus interacts with its own atomic orbital electrons or the neighbouring ions surrounding the nucleus, thus this interaction produces rich information of the solid where the nucleus is embedded. The magnitude of this interaction may be in between 0 to 10^9 Hz in frequency depending on the circumstances. Therefore, this interaction may be much smaller than the usual Zeeman energy. However, it may be comparable to or even larger than the Zeeman Hamiltonian. The simplest case is, of course, $|H_Q| \ll |H_Z|$. Some examples of this case and $|H_Q| \sim |H_Z|$ are demonstrated in this talk. The method of determining the quadrupole interaction is to be discussed. The parameters of the nuclear quadrupole interaction are the nuclear quadrupole coupling constant, asymmetry parameter, and their three principal axes. These parameters are microscopic quantities which are related to the local chemical bondings.[1, 2] However, they may be related with the macroscopic physical quantity of the solid.[3] Some interesting results in mixed crystals are also shown and discussed.[4]

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