Magnetic Hyperfine Interaction in ^{119}Sn Mössbauer Spectra

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Summary An applied magnetic field has been used to determine the sign of the quadrupole interaction in Me_2SnMoO_4 and Me_2SnCl_2.

THE quadrupole interaction in ^{119}Sn Mössbauer spectroscopy has attracted considerable attention in recent years and there have been several interpretations of the origins or absence of the quadrupole splittings, Δ, in terms of chemical bonding theory.[1] Further progress has been hampered by a lack of information concerning the sign of the principal component of the electric field gradient tensor. We have accordingly determined this sign for two key compounds by recording the Mössbauer spectra of samples within the field of a superconducting magnet.

The magnitude of the nuclear magnetic moment of the ^{119}Sn nucleus in its excited state is not precisely known, but by using the values[2] of $\mu_g = -1{\cdot}046$ nuclear magnetons and $\mu_{ex} = +0{\cdot}70$ nuclear magnetons the Zeeman hyperfine levels will be as in Figure 1. For magnetic fields which are conveniently attainable (⩽50 kgauss) three types of Mössbauer spectral patterns are expected from compounds exhibiting small or zero asymmetry parameters; (i) Δ zero or small so that the electric quadrupole interaction is effectively a small perturbation on the magnetic spectrum, (ii) Δ intermediate (*e.g.* 1·5—3 mm./sec.) when the electric quadrupole and magnetic interactions are of the same order of magnitude, (iii) Δ large (⩾4 mm./sec.) whereby the magnetic interaction may be considered as a perturbation on the electric quadrupole interaction. Examples of (i) and (iii) are shown in Figure 2, where the compounds are SnO_2

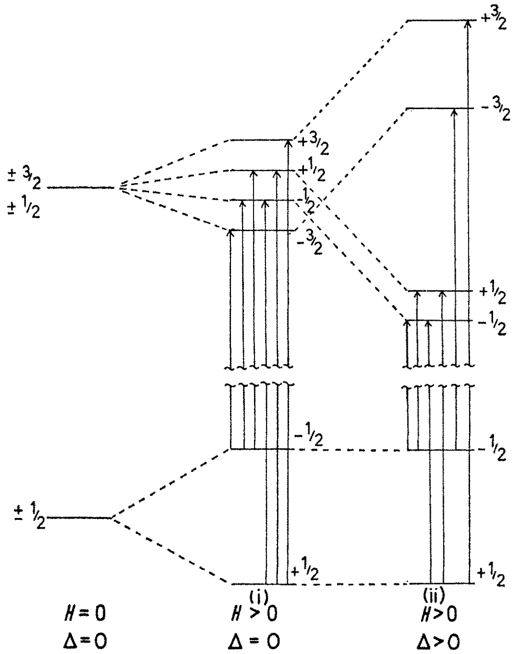

FIGURE 1. *Energy level of the* ^{119}Sn *nucleus for* (i) *magnetic and* (ii) *combined magnetic and quadrupolar interactions.*

($\Delta \leqslant 0{\cdot}2$ mm./sec., H_{appl} = 45 kgauss), and Me_2SnMoO_4 ($\Delta = 4{\cdot}2$ mm./sec., H_{appl} = 20, 30 kgauss), respectively, and the applied magnetic field is perpendicular to the direction of propagation of the γ-ray.

It is clear that a completely resolved six-line spectrum can be obtained for ^{119}Sn in an applied magnetic field of approximately 30 kgauss provided that the quadrupole splitting is sufficiently large. In the case of Me_2SnMoO_4 the sign of V_{zz} is shown to be positive. When Δ is smaller complete resolution is not possible, *e.g.* Me_2SnCl_2, Δ = $3{\cdot}4$ mm./sec., Figure 2 (d), but in this case the pattern of lines also unequivocally establishes the sign of the electric field gradient as positive. Both compounds presumably have a polymeric *trans*-octahedral structure and the positive V_{zz} indicates a greater electron density around tin in the *xy* plane than in the *z*(Me) direction.

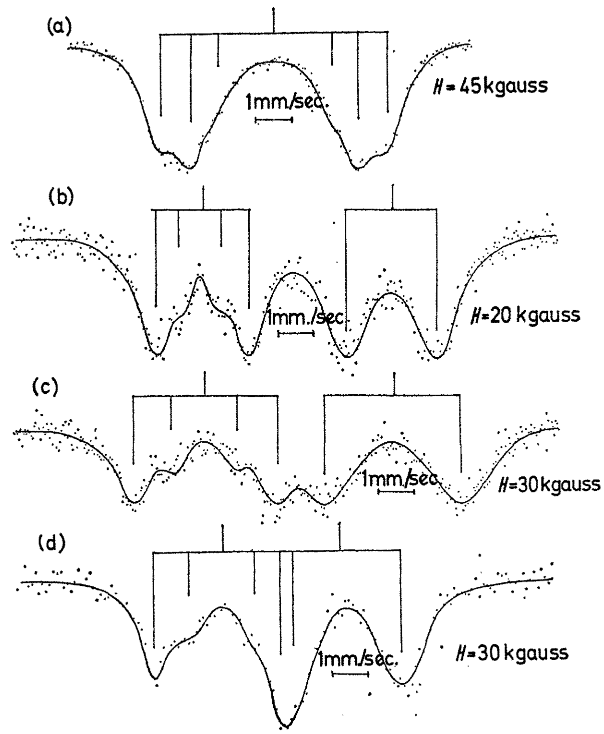

FIGURE 2. *Mössbauer spectra of* (a) SnO_2, (b) *and* (c) Me_2SnMoO_4, *and* (d) Me_2SnCl_2, *in external magnetic fields.*

In addition to the establishment of the sign of V_{zz} an applied magnetic field can also be used to determine the presence or absence of small quadrupole interactions. In the absence of a magnetic field any quadrupole splitting less than the natural Heisenberg linewidth (*ca.* $0{\cdot}63$ mm./sec.) will be unresolved and will appear only as line broadening. However, in the presence of a magnetic field the degeneracies are removed and any quadrupole interaction is manifested by an uneven separation of the lines in the spectrum. Figure 2 (a) shows the virtual absence of any quadrupole interaction ($\leqslant 0{\cdot}2$ mm./sec.) in SnO_2.

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