The Sign of the Electric Field Gradient at the ^{57}Fe Nucleus in *trans*- and *cis*-$FeCl_2(p\text{-}MeO\cdot C_6H_4\cdot NC)_4$

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Summary The signs of V_{zz} at the ^{57}Fe nucleus in *trans*- and *cis*-$FeCl_2(p\text{-}MeO\cdot C_6H_4\cdot NC)_4$ have been found to be positive and negative respectively.

THE 2:1 *trans*:*cis* quadrupole splitting ratio has been found to be widely applicable in the Mössbauer spectra of both Fe^{II} low spin and Sn^{IV} six-co-ordinate compounds. Several theoretical models[1,2] have predicted that the *trans* and *cis* quadrupole splittings are opposite in sign. Confirmation of this difference is essential for deriving partial quadrupole splitting values[1b] as well as for testing the validity of the models suggested.

The *trans*- and *cis*-compounds were prepared as reported previously.[3] These compounds have the largest quadrupole splittings yet reported for an Fe^{II} low spin *cis–trans* pair, and are thus very suitable for determining the sign of the electric field gradient using the magnetic field technique at 4°K.[4] Typical spectra of the *trans*- and *cis*-isomers at 4°K using longitudinal fields of 36 and 28 kG respectively are shown in the Figure. As discussed by Collins[4] the two-line zero-field spectrum splits into a doublet and a triplet in a magnetic field. If the doublet is at positive velocities, the sign of V_{zz} (and q) is positive; if the doublet is at negative velocities, the sign of V_{zz} is negative. Since the electric field gradient (EFG) equals $-V_{zz}$, and Q is positive for ^{57}Fe,[5] it is evident from the Figure that the sign of the EFG in the *trans*-compound is negative (V_{zz} is positive), whereas in the *cis*-isomer, the sign of the EFG is positive (V_{zz} is negative).

These signs are opposite to those previously assumed,[1b] and indicate that the $q_{lattice}$ term from the chloride does not dominate the magnitude of the quadrupole splitting. The signs of other Fe^{II} low spin six-co-ordinate compounds are now being investigated so that a large number of partial quadrupole splittings may be derived.

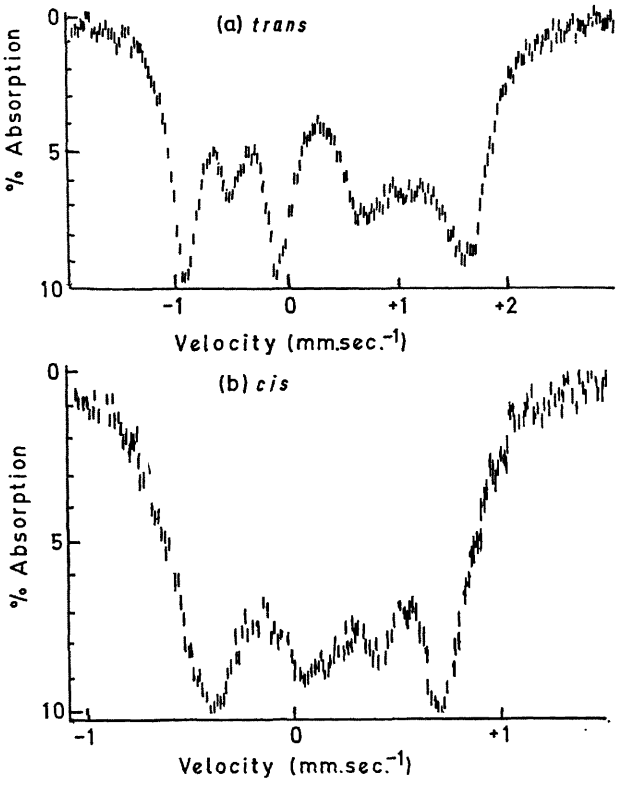

FIGURE. *Mössbauer spectra of*: (a) trans-$FeCl_2(p\text{-}MeO\cdot C_6H_4\cdot NC)_4$ *at* 4°K *in a longitudinal magnetic field of* 36 kG; (b) cis-$FeCl_2(p\text{-}MeO\cdot C_6H_4\cdot NC)_4$ *at* 4°K *in a longitudinal magnetic field of* 28 kG.

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