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LETTER TO THE EDITOR

On the relations between the zero-field splitting parameters in the extended Stevens operator notation and the conventional ones used in EMR for orthorhombic and lower symmetry

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Abstract. Electron magnetic resonance (EMR) studies of paramagnetic species with the spin $S \geqslant 1$ at orthorhombic symmetry sites require an axial zero-field splitting (ZFS) parameter and a rhombic one of the second order ($k = 2$), whereas at triclinic sites all five ZFS ($k = 2$) parameters are expressed in the crystallographic axis system. For the spin $S \geqslant 2$ also the higher-order ZFS terms must be considered. In the principal axis system, instead of the five ZFS ($k = 2$) parameters, the two principal ZFS values can be used, as for orthorhombic symmetry; however, then the orientation of the principal axes with respect to the crystallographic axis system must be provided. Recently three serious cases of incorrect relations between the extended Stevens ZFS parameters and the conventional ones have been identified in the literature. The first case concerns a controversy concerning the second-order rhombic ZFS parameters and was found to have lead to misinterpretation, in a review article, of several values of either E or b_2^2 published earlier. The second case concerns the set of five relations between the extended Stevens ZFS parameters b_k^q and the conventional ones D_{ij} for triclinic symmetry, four of which turn out to be incorrect. The third case concerns the omission of the scaling factors f_k for the extended Stevens ZFS parameters b_k^q. In all cases the incorrect relations in question have been published in spite of the earlier existence of the correct relations in the literature. The incorrect relations are likely to lead to further misinterpretation of the published values of the ZFS parameters for orthorhombic and lower symmetry. The purpose of this paper is to make the spectroscopists working in the area of EMR (including EPR and ESR) and related spectroscopies aware of the problem and to reduce proliferation of the incorrect relations.

During recent work on a comparative survey of the conventional and tensor–operator notations used in the up-to-now EMR-related literature to express zero-field splitting (ZFS) Hamiltonian $\mathrm{H}_{\mathrm{ZFS}}$, a number of pitfalls awaiting unaware spectroscopists have been revealed. Among others, three potentially serious cases concerning sets of incorrect relations between the extended Stevens ZFS parameters and the conventional ones, which have recently appeared in the literature, have been identified. In all cases the incorrect relations in question have been published in spite of the earlier existence of the correct relations in the literature. The incorrect relations may lead to further misinterpretation of the published values of the ZFS parameters for orthorhombic and lower symmetry. Hence these problems require immediate action to bring it to the attention of the EMR community. The purpose of this Letter is to make the spectroscopists working in the area of EMR (including EPR and ESR) and related spectroscopies aware of these problems and to reduce proliferation of the incorrect relations. Below, firstly the background theory is briefly outlined and then each of the three cases is discussed.

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The *conventional* form of H_{ZFS} *most widely* used in the literature, which is suitable for paramagnetic species with spin $S \geqslant 1$ at sites with triclinic symmetry, is given by (Abragam and Bleaney 1970, Altshuler and Kozyrev 1974, Rudowicz 1987, Stevens 1997, Pilbrow 1990):

$$H_{ZFS} = \boldsymbol{S} \cdot \boldsymbol{D} \cdot \boldsymbol{S} \tag{1a}$$

whereas for the spin $S \geqslant 2$ the higher-order ZFS terms are required. For H_{ZFS} expressed in the principal axis system for monoclinic and triclinic symmetry as well as for orthorhombic symmetry, H_{ZFS} is given by (Abragam and Bleaney 1970, Altshuler and Kozyrev 1974, Rudowicz 1987, Pilbrow 1990):

$$H_{ZFS} = D\left[S_z^2 - \tfrac{1}{3}S(S+1)\right] + E[S_x^2 - S_y^2]. \tag{1b}$$

Here the axes (x, y, z) may be chosen in different ways for orthorhombic symmetry (see Rudowicz and Bramley 1985, Rudowicz 1987), whereas for monoclinic and triclinic symmetry the orientation of the principal axes (x, y, z) with respect to the crystallographic axis system (X, Y, Z) must be provided.

On the other hand, in the last several decades, the Stevens operators (Stevens 1952) have been used more often. Two types of the Stevens operators exist, namely (i) the *usual* (or *conventional*) Stevens operators, which were originally defined only for $q \geqslant 0$ (Stevens 1952) and are listed, e.g. by Orbach (1961), Abragam and Bleaney (1970), (1986) and Newman and Urban (1975), and (ii) the *extended* Stevens (ES) operators, O_k^q, which were introduced more recently (Rudowicz 1985) as an extension of the former operators and which comprise in a unified way also the components O_k^q with negative q (Newman and Urban 1975, Rudowicz 1985). The set of operators listed in appendix V of Altshuler and Kozyrev (1974), albeit using two separate symbols (O_k^q for the positive q components of the ES operators and Ω_k^q for the negative ones) is equivalent, in fact, to the set of the ES operators (Rudowicz 1985, 1987). The general reference form of the ZFS Hamiltonian in terms of the ES operators (Abragam and Bleaney 1970, 1986, Altshuler and Kozyrev 1974) is written in the *compact* form (as defined by Rudowicz 1987; to be distinguished from the *expanded* form also used in the literature) as:

$$H_{ZFS} = \sum_{kq} B_k^q O_k^q(S_x, S_y, S_z) = \sum_{kq} f_k b_k^q O_k^q(S_x, S_y, S_z). \tag{2}$$

The uniform 'scaling' of ZFS parameters b_k^q requires the factors f_k to be taken as (Abragam and Bleaney, 1970, 1986, Rudowicz 1987, Altshuler and Kozyrev 1974):

$$f_2 = 1/3 \qquad f_4 = 1/60 \qquad f_6 = 1/1260. \tag{3}$$

For numerical convenience, the second form of H_{ZFS} shown in equation (2) has been more often used in EMR studies of transition ions. Relations between the orthorhombic ZFS parameters in equation (1*b*) and (2) are then obtained as (Abragam and Bleaney, 1970, 1986, Rudowicz 1987):

$$D = b_2^0(\mathrm{ES}) = 3B_2^0(\mathrm{ES}) \qquad 3E = b_2^2(\mathrm{ES}) = 3B_2^2(\mathrm{ES}). \tag{4}$$

Concerning the relations for triclinic symmetry, using the explicit definitions of the operators involved (Altshuler and Kozyrev 1974, Newman and Urban 1975, Rudowicz 1985), the following relations between the D_{ij} components in equation (1*a*) and the ZFS parameters equation (2) are obtained (Yeom *et al* 1996, see also McGavin 1987):

$$\begin{aligned} &B_2^0(\mathrm{ES}) = D_{zz}/2 \qquad B_2^1(\mathrm{ES}) = 2D_{xz} \qquad B_2^{-1}(\mathrm{ES}) = 2D_{yz} \\ &B_2^2(\mathrm{ES}) = (D_{xx} - D_{yy})/2 \qquad B_2^{-2}(\mathrm{ES}) = D_{xy}. \end{aligned} \tag{5}$$

Keeping in mind the background theory outlined above, the readers can more easily understand the nature of the inconsistencies and/or problems occurring in each of the three cases discussed below.

Case 1. Controversy concerning the rhombic ZFS parameters: $3E = b_2^2 = 3B_2^2$ or $E = b_2^2 = 3B_2^2$?

In a recent review Misra (1999a) writes in his equation (9) the second-order conventional H_{ZFS} as in equation (1*b*) above with the ZFS parameters replaced by: $D \rightarrow b_2^0$ and $E \rightarrow b_2^2$. While the first substitution yields the usual relation as in equation (4), the second one yields a relation *inconsistent* with the well established one, i.e. $b_2^2(\mathrm{ES}) = 3E$. For spin $S = 2$ in tetragonal symmetry Misra (1999a) writes in his equation (11) the same *inconsistent* rhombic term, which should *not* appear at all for this case, and the ZFS axial terms: second-order with $D \rightarrow b_2^0$ and fourth-order (Rudowicz 1987) with $F/180$ replaced by b_4^0 and the constant part omitted, which again yields a relation *inconsistent* with the well established ones, i.e. $B_4^0(\mathrm{ES}) = a/120 + F/180$ and $b_4^0(\mathrm{ES}) = a/2 + F/3$, plus the abbreviated cubic term expressed in the cubic axes. The second-order ZFS terms, i.e. the axial term and the same *inconsistent* rhombic term, appear also in equation (21) (and on p 107—the axial term only) of Misra (1999a) for spin $S = 1/2$, whereas there should be no ZFS terms for $S = 1/2$. On p 110 of Misra (1999a) three symbols, B_k^m, B_k^q, and B_n^m, are used to denote the same ES parameters B_k^q as defined in equation (2), whereas no relationships are provided between the parameters B_2^q ($q = 0, 2$) and b_2^0 and b_2^2 introduced earlier in equation (9) of Misra (1999a).

In order to exclude the possibility that different conventions for the operators and parameters have been adopted by Misra (1999a, c) we have analysed the definitions used in the parallel reviews Misra (1999b), based on Misra *et al* (1996), and Misra (1999d). Apart from the confusion between the properties of the tesseral-tensor operators (TTO) and those of the spherical-tensor operators (STO) and inappropriate nomenclature, discussed below, it has been verified that the same definitions as for the operators defined in equations (1)–(3) have been adopted in the reviews Misra (1999a, b, c, d) and Misra *et al* (1996). Using the definitions of the operators O_n^m in Misra (1999b), which are found to be identical with O_k^q in Rudowicz (1985) (see also Abragam and Bleaney, 1970, 1986, Rudowicz 1987, Altshuler and Kozyrev 1974) and the conventions in equation (3), which are mentioned explicitly in Misra (1999d, p 287), the same relations as in equation (4) are obtained. This proves that the relation: $E = b_2^2$ used by Misra (1999a, c) is incorrect.

Moreover, there are two other practical *negative* implications of the *inconsistent* substitution $E \rightarrow b_2^2$ (Misra 1999a, c). *Firstly*, the maximum rhombicity limit, $0 \leqslant b_2^2/b_2^0 \leqslant 1/3$, (Misra 1999a, p 112) is incorrect (besides which the definition of the ratio λ is misprinted—b_2^2 appears twice) if the well established meaning of $b_2^0(\mathrm{ES})$ and $b_2^2(\mathrm{ES})$ is adopted as in equation (4), since then we have (Rudowicz and Bramley 1985) $0 \leqslant b_2^2(\mathrm{ES})/b_2^0(\mathrm{ES}) \leqslant 1$. *Secondly*, the relations $b_2^2(= E)$ and E $(=b_2^2)$ are explicitly used in the extensive tabulation of transition ion data in Misra (1999c), being a compilation of data mostly taken from other review articles and a few original papers. Since in the majority of the original sources the well established meaning of $b_2^2(\mathrm{ES}) = 3E$ is used, the inconsistent substitution $E \rightarrow b_2^2$ in Misra (1999a, c) renders the tabulation of the rhombic second-order ZFS parameters unreliable. This can be verified by comparing the original data expressed in terms of either b_2^2 or E with those quoted by Misra (1999c) after other reviews.

Two examples suffice to illustrate the seriousness of the problem. (i) The original data from Bielecki *et al* (1987) for Cr^{3+} in $KAl(SO_4)_2.12H_2O$: '$|E|(10^{-4}\mathrm{cm}^{-1}) = 80 \pm 5$' appearing in the source review (Jain 1990) as '$E(\mathrm{cm}^{-1}) = 0.0080$' are listed by Misra (1999c; p 177) under the heading '$b_2^2(= E)(\mathrm{cm}^{-1})$' as '0.008'—here for the well established relation $b_2^2(\mathrm{ES}) = 3E$ the value $b_2^2 = 0.024$ should appear. (ii) The original data from Jain *et al* (1979) for Mn^{2+} in $CaCd(CH_3COO)_4.12H_2O$: '$b_2^2(\equiv 3E) = 468.0 \pm 2.0$ G' (note the original explicit use of the relation $b_2^2(\equiv 3E)$) appearing in the source review (Misra and Sun 1991) as: '$b_2^2 = 468$ G' are listed by Misra (1999c, p 184) under the heading '$b_2^2 (= E)(10^{-4}\mathrm{cm}^{-1})$' as '468 G'—here for the well established relation $E = \mathrm{b}_2^2(\mathrm{ES})/3$ the value '156' should appear. Interestingly, the correct relation '$E = \mathrm{b}_2^2/3$' was used earlier, e.g. in the review by Misra and Sun (1991). Hence it is hard to understand why the incorrect relation: $E = \mathrm{b}_2^2 = 3\mathrm{B}_2^2$ has been used later in Misra *et al* (1996), Misra (1999a, c), as well as in table 2 of Misra (1999b).

The author must admit that only during later stages of the work on the review (Rudowicz *et al* 2000) a possible origin of the *inconsistent* substitution $E \rightarrow \mathrm{b}_2^2$ in Misra (1999a, b, c) and Misra *et al* (1996) has been found. On checking Altshuler and Kozyrev—both in the Russian (1972) and English (1974) versions—the relation in equation (3.127), $E = \mathrm{b}_2^2 = 3\mathrm{B}_2^2$, has been spotted. Checking the definitions of the operators in Altshuler and Kozyrev (1974) it can be verified that it is an obvious misprint, i.e. a factor 3 is missing—*'E' should read '3E'!* It remains a mystery why such a basic mistake has escaped being noticed and corrected for so long. Correct relations, $3E = \mathrm{b}_2^2$ and $E = \mathrm{B}_2^2$, can be found, e.g. in Abragam and Bleaney (1970), (1986, p 152) and Rudowicz (1987). However, the consequence of such inconsistent, so presumably inadvertent, usage of the well established symbols in Misra (1999a, b, c) and Misra *et al* (1996), as well as misleading forms of SH as discussed above, are very serious since they appear in a source (Poole and Farach 1999) which potentially may serve as a major reference. Hence there is a high risk of proliferation of such confusion on a wider scale in the follow-up EMR literature.

Another drawback of the series of reviews Misra (1999a, b, c, d) is the usage of a variety of symbols, correlated neither mutually nor with the existing notation for the ES operators (Rudowicz 1985, 1987), as well as the confusion between the properties of the tesseral-tensor operators (TTO) and those of the spherical-tensor operators (STO), and inappropriate nomenclature. In spite of the widely adopted symbol 'O', e.g. O_k^q, (Abragam and Bleaney 1970, 1986, Altshuler and Kozyrev 1974, Rudowicz 1985, 1987), 'the Stevens operator equivalents' are denoted by Misra (1999b) and Misra *et al* (1996) as '$\mathrm{Y}_n^m(|m| \leqslant n)$', which resembles the spherical harmonics. The explicit forms of Y_n^m listed in Misra *et al* (1996) and Misra (1999b) in an appendix are apparently adapted from Altshuler and Kozyrev (1974), where these operators were denoted originally as O_n^{+m} and O_n^{-m}. Recently Ryabov (1999) has pointed out that the list of operator equivalents in Misra *et al* (1996) '*is found to contain a number of errors*'. Regrettably, Ryabov (1999) provides no explicit examples of such errors.

It is important to keep in mind two points regarding the operators O_n^{+m} and O_n^{-m} (Altshuler and Kozyrev 1974) alias $Y_n^m(|m| \leqslant n)$ (Misra *et al* 1996, Misra 1999b). (i) These operators should not to be confused with the ES operators O_k^q defined in equation (2)—for details see, Rudowicz (1985, 1987). (ii) These operators are not the 'Stevens operator equivalents', as stated in Misra *et al* (1996) and Misra (1999b), since they are the STO type operators. In fact, the linear combinations of these operators (Rudowicz 1985, 1987) are directly related (apart from normalization factors) to the operators $\mathrm{O}_k^q(\mathrm{ES})$ defined in equation (2). Only the operators $\mathrm{O}_k^q(\mathrm{ES})$, which are the TTO type operators, can properly be named the 'Stevens operator equivalents'. Usage of a separate symbol Ω_n^m (Misra *et al* 1996, Misra 1999b) or R_n^m (Misra 1999d) for the ES operators O_k^q with negative q, whereas C_n^m for the associated ZFS parameters, although it follows the notation of Altshuler and Kozyrev (1972, 1974), is no longer justified in view of the existing consistent notation introduced in Newman and Urban (1975) and Rudowicz (1985, 1987). Full discussion of the intricacies and interrelations between various notations used in the area of EMR (including EPR and ESR) and related spectroscopies will be provided in the review (Rudowicz *et al* 2000).

Case 2. Incorrect relations between the parameters: b_k^q(ES) and D_{ij} for triclinic symmetry

Recently Baker *et al* (1995) and Kuriata *et al* (1998) have used the second-order H_{ZFS} in the form:

$$\boldsymbol{S} \cdot \boldsymbol{D} \cdot \boldsymbol{S} = \sum_m \mathrm{b}_2^m \mathrm{O}_2^m(S) \tag{6}$$

where $\mathrm{O}_2^m(S)$ were defined in Baker *et al* (1995) as 'second-order Stevens operators (Stevens 1952)', whereas the 'coefficients of the $\boldsymbol{D}$-matrix' were given by

$$\mathrm{b}_2^0 = (3/2)D_{zz} \qquad \mathrm{b}_2^{\pm 1} = (1/2)(D_{zx} \pm \mathrm{i}D_{zy}) \qquad \mathrm{b}_2^{\pm 2} = (1/4)(D_{xx} - D_{yy} \pm 2\mathrm{i}D_{xy}). \tag{7}$$

Note that the negative components of the Stevens operators cannot be referred to Stevens (1952), since they were not defined therein, as discussed briefly above (for details, see Rudowicz 1985, 1987, Rudowicz *et al* 2000). Moreover, major problems arise concerning the form of equation (6) (see, case 3 below) and the relations in equation (7). The relations in equation (7), apart from the first one (see, case 3 below), turn out to be *incorrect* since they imply that the ZFS parameters with $q(m) \neq 0$, expressed in the ES notation defined in equation (2), are complex. This is contrary to the fact that the parameters b_k^q(ES) are all real (Altshuler and Kozyrev 1974, Newman and Urban 1975, Rudowicz 1985, 1987, Rudowicz *et al* 2000). It appears that the authors (Baker *et al* 1995 and Kuriata *et al* 1998) might have confused the properties of the tesseral-tensor operators (TTO) and those of the spherical-tensor operators (STO)—see Rudowicz (1987), Rudowicz *et al* (2000). The derivation of the relations in equation (7) must be re-considered by the authors (Baker *et al* 1995 and Kuriata *et al* 1998), while conforming to the standard definitions of the operators and parameters used.

It turns out that the relations in equation (7) have not been used for any actual parameter conversions by Baker *et al* (1995) and Kuriata *et al* (1998), although they might have been used implicitly by the authors for the superposition model calculations. One more problem in Baker *et al* (1995) concerns the ambiguity of the numerical values of the ZFS parameters, which were provided only as the principal values D_i. Since the labelling of the axes $i = x, y, z$ in table 3 of Baker *et al* (1995) is not explicitly provided, hence it is impossible to recalculate unambiguously the values D_{ij} by transforming them back into the crystallographic axis system. The values D_{ij} are necessary if one wants to utilize either the incorrect relations in equation (7) or the correct ones in equation (5). Similar ambiguity concerning the labelling of D_i and the axes $i = x, y, z$ appears in table 1 of Kuriata *et al* (1995). This illustrates an important point that for low symmetry cases the complete and clear definitions of the axis systems used are indispensable for meaningful comparison of EMR data taken from various sources. In view of the above problem and its consequences, there is an urgent imperative for adoption of unified guidelines for presentation of ZFS parameters in the EMR-related literature as discussed briefly below. Our recent search of the SCI database concerning the papers Baker *et al* (1995) and Kuriata *et al* (1998) indicates no applications of the incorrect relations in equation (7) by other authors as yet, since only a few self-citations have been revealed by the search.

Case 3. Missing 'scaling' factors f_k at the ZFS parameters b_k^q(ES)

It should be noted that omitting in equation (6) the factors f_k at b_k^q(ES) defined in the second form of H_{ZFS} in equation (2), as done e.g. in Baker *et al* (1995) and Kuriata *et al* (1998), introduces a serious ambiguity about the meaning of the parameters 'b_2^m' used by the authors. Two different options are possible: (i) the authors did in fact mean the 'B' parameters B_k^q defined in equation (2) or (ii) they meant the 'b' parameters b_k^q actually appearing in their equation, whereas the factors f_k were inadvertently omitted. Although in most such cases the option (ii), i.e. an unintentional omission or a misprint may be suspected, the only way to verify this is via comparison with data from other sources for the same ion/host system, which may be expressed in other notations. In the present case of Baker *et al* (1995) and Kuriata *et al* (1998), as well as of Baker (1998)—where the (apparently Stevens) operators denoted $\mathrm{O}_n^m(S)$ are referred to Abragam and Bleaney (1970), one must conclude, based on the definitions of the operators provided by the authors, that the b_2^m's in equations (6) and (7) should be in one to one correspondence with the b_2^q's conforming to the standard definition in equation (2), i.e. the option (ii) above applies. Then the first relation in equation (7) appears to be correct, whereas the other four relations involving $q(m) \neq 0$ are incorrect.

Other recent examples (for earlier cases, see Rudowicz 1987) of the omission of the scaling factors f_k at b_k^q(ES) in equation (2) have been identified in the literature. This includes, e.g., Rettori *et al* (1993), (where also the confusion between the crystal field (CF) Hamiltonian and the ZFS Hamiltonian (Rudowicz 1987) is evident), Martins *et al* (1995) and Rettori *et al* (1996) (where the Stevens operators are denoted O_{nm}). In the case of Keeble *et al* (1995), although the scaling factor $1/3$ is missing in the general SH form, the correct explicit SH form and relations between (b_2^0, b_2^2) and $D_i (i = x, y, z)$ are provided. This leaves no doubt that the Stevens operators were meant by Keeble *et al* (1995), in spite of naming them (so inappropriately, see Rudowicz (1987), Rudowicz *et al* (2000)) '*normalized* spin operators' without providing any reference for the definitions of the operators.

In summary, in view of the above problems/errors and their consequences, there is an urgent imperative for adoption of unified guidelines for presentation of ZFS parameters in the EMR-related literature. In the words of an anonymous referee: '*Poorly defined notation and lack of any universally accepted definitions of spin-Hamiltonian forms has been a long standing confusing feature of EPR*'. Suitable options for unified guidelines in this regard have been, to a certain extent, put forward by the author earlier. This includes adoption of (i) the extended Stevens operators and the parameters b_k^q (ES) as the standard reference notation and (ii) units of $10^{-4}\mathrm{cm}^{-1}$ or cm^{-1} (Rudowicz 1987, 1991, 1994). Additionally, for orthorhombic and lower symmetry cases, (iii) it seems useful to adopt in a uniform way the axis system conforming to the standard range of the ratio $0 \leqslant \lambda' \equiv \mathrm{b}_2^2(\mathrm{ES})/\mathrm{b}_2^0(\mathrm{ES}) \leqslant 1$ (see, e.g., Rudowicz and Bramley 1985, Rudowicz and Madhu 1999). It is worth noting that the guideline (i), and partially (ii), have been adopted, e.g., in several reviews dealing with EMR data for Mn^{2+} (Jain and Lehmann 1990, Misra and Sun 1991, Heming *et al* 1984), and Fe^{3+} and Cr^{3+} in minerals (Buscher *et al* 1987). These guidelines have also received firm support, especially the first one, from Professor Stevens who recommended adopting the authors' (Rudowicz 1985, 1987) '*proposals for future standardization in the definitions and notations*' (Stevens 1997, p 103). Updated and more detailed unified guidelines for presentation of ZFS parameters will presented in the forthcoming paper.

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References

Abragam A and Bleaney B 1970 *Electron Paramagnetic Resonance of Transition Ions* (Oxford: Clarendon Press)

——1986 *Electron Paramagnetic Resonance of Transition Ions* (New York: Dover)

Altshuler S and Kozyrev B M 1972 *Electron Paramagnetic Resonance in Compounds of Transition Elements* (Moscow: Nauka) (in Russian)

——1974 *Electron Paramagnetic Resonance in Compounds of Transition Elements* (New York: Wiley)
Baker J M 1998 in *Foundations of Modern EPR* ed G R Eaton, S S Eaton and K M Salikhov (Singapore: World Scientific) p 171
Baker J M, Kuriata J, O'Connell A C and Sadlowski L 1995 *J. Phys.: Condens. Matter* **7** 2321
Bielecki K, Kruczynski Z and Fârcaş S I 1987 *Phys. Status Solidi* b **141** K67
Buscher R, Such K P and Lehmann G 1987 *Phys. Chem. Minerals* **14** 553
Heming M, Remme S and Lehmann G 1984 *Ber. Bunsnege Phys. Chem.* **88** 946
Jain A K, Saraswat R S and Upreti G C 1979 *J. Chem. Phys*. **70** 4424
Jain V K 1990 *Magn. Reson. Rev.* **14** 261
Jain V K and Lehmann G 1990 *Phys. Status Solidi* b **159** 495
Keeble D J, Li Z and Poindexter E H 1995 *J. Phys.: Condens. Matter* **7** 6327
Kuriata J, Baker J M, Sadlowski L, Stefaniuk I and Bodziony T 1998 *J. Phys. : Condens. Matter* **10** 407
Kuriata J, Sadlowski L, Stefaniuk I and Waplak S 1995 *J. Phys.: Condens. Matter* **7** 2333
Martins G B *et al* 1995 *Phys. Rev.* B **51** 11909
McGavin D G 1987 *J. Magn. Reson.* **74** 19
Misra S K 1999a *Handbook of Electron Spin Resonance* vol 2, ed C P Poole Jr and H A Farach (New York: AIP) ch VI
——1999b *Handbook of Electron Spin Resonance* vol 2, ed C P Poole Jr and H A Farach (New York: AIP) ch VII
——S K 1999c *Handbook of Electron Spin Resonance* vol 2, ed C P Poole Jr and H A Farach (New York: AIP) ch VIII
——S K 1999d *Handbook of Electron Spin Resonance* vol 2, ed C P Poole Jr and H A Farach (New York: AIP) ch IX
Misra S K, Poole C P Jr and Farach H A 1996 *Appl. Magn. Reson.* **11** 29
Misra S K and Sun J S 1991 *Magn. Reson. Rev.* **16** 57
Newman D J and Urban W 1975 *Adv. Phys.* **24** 793
Orbach R 1961 *Proc. R. Soc.* A **264** 458
Pilbrow J R 1990 *Transition-Ion Electron Paramagnetic Resonance* (Oxford: Clarendon)
Poole C P Jr and Farach H A (ed) 1999 *Handbook of Electron Spin Resonance* vol 2, (New York: AIP)
Rettori C *et al* 1993 *Phys. Rev.* B **47** 8156
——1996 *Phys. Rev.* B **54** 1123
Rudowicz C 1985 *J. Phys. C: Solid State Phys.* **18** 1415
——1985 *J. Phys. C: Solid State Phys.* **18** 3837 (erratum)
——1987 *Magn. Reson. Rev.* **13** 1
——1988 *Magn. Reson. Rev.* **13** 335 (erratum)
——1991 *Bull. Magn. Reson*. **12** 174
——1994 *Bull. Magn. Reson*. **16** 224
Rudowicz C and Bramley R 1985 *J. Chem. Phys*. **83** 5192
Rudowicz C and Madhu S B 1999 *J. Phys.: Condens. Matter* **11** 273
Rudowicz C, Galeev A and Chung T C Y 2000 to be submitted
Ryabov I D 1999 *J. Magn. Reson.* **140** 141
Stevens K W H 1952 *Proc. Phys. Soc.* **65** 209
——1997 *Magnetic Ions in Crystals* (Princeton: Princeton University Press)
Yeom T H, Rudowicz C, Choh S H and McGavin D G 1996 *Phys. Status Solidi* b **198** 839