Survey of the EPR Community on the EPR Database and Related Projects

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I. Introduction

EPR studies provide a wealth of information, which can be best utilized if available in a computer-searchable form. Establishment of a computerized EPR-related database would require, among other things, standardization of notations and units. These proposals have been put forward to the International EPR (ESR) Society [**IES**] in the two submissions in August 1990 (1): *On Unification of Notations Used in EPR* and *On Establishment of a Computerized EPR-related Database* and the EPR community (2). A feasibility study of the EPR-related database project followed starting in early 1991. The objectives of the pilot study were: (i) to find out the opinions of the EPR community concerning the above two proposals, (ii) to investigate the users' requirements and identify the data needs, and (iii) to work out a Feasibility Study Report for consideration by the IES.

The present survey and the proposed EPR database project are perceived as a service to the EPR community under the auspices of IES. The idea of an EPR database has also been discussed at the EPR meetings held in Denver [EPR Newsletter [**EN**] **4**/3, 7 (1992); **5**/2, 5 (1993)]. A poster summarizing the preliminary results of this study has been presented at the EPR Symposium in Denver (3). In this paper the results of the analysis of the 70 plus valid responses received to date are presented.

II. Questionnaires and analysis of responses

For a meaningful analysis of responses the pertinent background on the stages of the project and working out of the questionnaires is important. The project started with the setting up of a namelist of EPR researchers working mainly in the area of transition-metal and rare-earth ion – EPR studies in early 1991. The namelist, complied using dBASE-IV, was based on an extensive survey of literature published since 1980 onwards and supplemented with addresses received from private contacts with EPR researchers. The questionnaire, *The Future of EPR Spectroscopy of Transition Ions* [**EPR-Q**] (1,2), has served as an initial test for working out the main questionnaire, *Planning EPR-database Structure* [**P-EPR**], in mid-1991. Included in the main set [**EPR-DB**], apart from **P-EPR**, were the additional questionnaires: *Mailing List for Future Issues* [**ML**] and *EPR-related Conferences* [**EPR-Con**]. The full set of questionnaires, i.e. **EPR-Q** and **EPR-DB**, and the two submissions, accompanied by an *Open letter to EPR community members*, have been dispatched to about 800 researchers in late 1991 and successively to over 100 more researchers thereafter. The paper (2), where the rationale for standardization of symbols in EPR was detailed and pertinent references were given, had also been enclosed. The analysis of responses began in mid-1992. In order to increase the number of responses a note on the project has been placed in EN [**3**/4, 6 (1991)] distributed in early 1992. However, it has generated but a few additional responses.

The geographical distribution of responses is presented in Table 1. There are two types of responses: (i) *Full*, i.e. responses to the full set of questionnaires (**EPR-Q** and **EPR-DB**), and (ii) *EPR-Q*, i.e. responses to **EPR-Q** only. The rate of response (%) is calculated including both (i) and (ii) with respect to the total number of **EPR-DB** sets sent. Some special cases are also indicated in Table 1. In several cases the envelopes with **EPR-DB** have been returned as *'undelivered'* mail or the person has indicated only that he/she has *'left the field'* of EPR in the meantime. In a few instances *'Mailing list only'* has been returned. The mailing of the **EPR-DB** questionnaires coincided with the major changes on the political map of Europe. Since it was difficult to accomodate these changes explicitly in our geographical listing, the new countries are considered jointly under the former name indicated by an asterisk, whereas the responses from the West and East Germany were merged. Several responses have been received after the analysis of data was completed. Including these responses would slightly increase the total response ratio in Table 1. The overall response ratio of about 8–9% is disappointingly low. We don't think, however, that this lack of attention is malicious; rather it is due to the natural tendency of (very busy) people to focus on their own immediate problems.

The results of the analysis of responses are organized into three parts concerned with (A) **EPR-Q** – in Figures 1 to 5, (B) **P-EPR** – in Figures 6 to 12 and Table 2 and 3, and (C) **ML** – only the aspects pertinent to the membership of the EPR community are included here.

A. EPR-Q: The Future of EPR Spectroscopy of Transition Ions

For the questions in Figure 1 the lack of answer (*no answer*) and the *no opinion* answer are merged, while the firm *no* answer is indicated explicitly. For the question A7.1 in Figure 2 the *of minor use* and *negligible use* answers are merged, yielding 6%, whereas the combined percentage of the *very useful* and *useful* answers is 91%. This indicates a very strong support for the **idea** of a comprehensive computerized EPR database. Financial viability of the EPR database looks promising gauging from the percentage of the potential subscribers: 14% *very likely* and 65% *probably*. Hence the end product of the EPR database project is likely to become a saleable commodity.

The overwhelming support by respondents for all other proposals dealt with in Figures 1 and 2 is evident, except for the financial commitments regarding development of an all-purpose user-friendly EPR computer package [Figure 2, A6.2(ii)]. The responses indicate that a strong need exists within the EPR community for (i) *the internationally accepted standards on EPR nomenclature and conventions* and (ii) *a glossary of terms used in EPR* (Figure 1) as well as (iii) *an EPR computer package* (Figures 1 and 2). The first two proposals can only be successfully dealt with if cooperation between ISMAR, IES and IUPAC, at a proper level, can be ensured. The author's attempts to bring about such cooperation have not been successful so far. Possibility of cooperation on these and related projects with AMPERE Society and regional EPR/ESR societies should also be investigated. The extension to the spin S>1/2 systems of the *Recommendations for EPR/ESR Nomenclature and Conventions for presenting experimental data in publications* [(4); cf also EN 3/1, 9 (1991)], dealing only with the S = 1/2 systems, is crucial for the EPR database project (2). To the best of our knowledge, the work on this extension, planned under the auspices of IUPAC Commission I.5 (5), has not continued. The lack of financial resources and manpower seems to be the major obstacle in pursuing these proposals.

The situation is better with regard to the EPR computer programs, due to efforts of Prof. R. Cammack, Chairman of the IES Computer Software Committee, who has complied a database of available EPR programs [EN **4**/3, 6 (1992)]. The names

Table 1: Geographical Distribution of Responses

GA	Country	No. Sent	Response Full	Response EPR-Q	%	Undelivered	Left the field	Mailing list only
AF	South Africa	1	0	0	0.0	0	0	0
	Zimbabwe	1	0	0	0.0	0	0	0
	subtotal	2	0	0	0.0	0	0	0
AP	Australia	27	3	1	14.8	1	0	0
	China	16	3	1	25.0	1	1	0
	Hong Kong	1	1	0	100.0	0	0	0
	India	34	3	2	14.7	0	0	0
	Israel	2	0	0	0.0	0	0	0
	Japan	78	2	1	3.8	7	0	1
	New Zealand	8	0	0	0.0	0	1	0
	South Korea	5	1	0	20.0	0	0	0
	Taiwan	5	0	0	0.0	0	0	0
	Vietnam	1	0	0	0.0	0	0	0
	subtotal	177	13	5	10.2	8	2	1
EU	Belgium	11	1	0	9.1	0	0	0
	Bulgaria	3	0	0	0.0	0	0	0
	CIS (f. USSR)*	128	12	1	10.2	7	0	1
	Czechoslovakia*	14	2	0	14.3	0	0	0
	Denmark	1	0	0	0.0	0	0	0
	France	69	1	0	1.4	1	1	1
	Germany*	65	1	4	7.7	0	1	0
	Greece	3	2	0	66.7	0	0	0
	Hungary	10	2	0	20.0	1	0	0
	Italy	26	1	0	3.8	0	0	0
	Netherlands	38	2	1	7.9	7	0	0
	Poland	28	4	1	17.9	0	0	0
	Portugal	1	0	0	0.0	0	0	0
	Romania	5	1	0	20.0	0	0	0
	Spain	28	3	0	10.7	0	0	0
	Sweden	2	0	0	0.0	0	0	0
	Switzerland	18	1	0	5.6	1	1	0
	Turkey	3	1	0	33.3	0	0	0
	UK	36	2	0	5.6	2	1	0
	Yugoslavia*	5	0	0	0.0	0	0	0
	subtotal	366	24	6	8.2	12	4	1
LA	Argentina	6	0	0	0.0	0	0	0
	Brazil	21	1	0	4.8	0	0	0
	Mexico	4	0	0	0.0	0	0	0
	Venezuela	6	0	0	0.0	0	0	0
	subtotal	37	1	0	2.7	0	0	0
NA	Canada	23	1	0	4.3	1	0	1
	USA	156	6	4	6.4	9	0	2
	subtotal	179	7	4	6.1	10	0	3
	total	889	57	16	8.2	37	6	6

Table 2: Compounds by Molecular Formula or Specific Ion

Compound	Freq.	Compound	Freq.
AMX_3	5	Co_2SiO_4	1
A_2MX_2	1	Cr^{3+} compounds	1
A_2MX_4	2	Fe^{2+} compounds	1
[A=alkaline; M=divalent; X=O,F]		Fe^{3+} compounds	2
$ABF_6 \cdot 6H_2O$	2	Gd^{3+} compounds	1
[A=Mn^{2+}, Ni^{2+}, Cu^{2+}, Co^{2+},		$LaGaO_3$	1
Fe^{2+}, Zn^{2+}, Cd^{2+}, Mg^{2+}, Ca^{2+};		$Li(RE)F_4$ [RE=Y, Yb, Dy, Er]	1
B=Si^{4+}, Ge^{4+}, Ti^{4+}, Zr^{4+}, Mg^{4+}]		LiH	1
BGO	1	$LiNbO_3$	3
$Bi_2Sr_2Ca_2Cr_3O_4$	1	LiOH	1
$BiVO_4$	3	Mn^{2+} compounds	2
BSO	1	MX_2	1
CaF_2, $Ca_{1-x}Sr_xF_2$	1	$NdGaO_3$	1
$Ca_2Fe_2O_5$	1	PbTe	1
$Ca_3Ga_2Ge_3O_{13}$	1	$PrGaO_3$	1
$Ca_3Ga_2Ge_4O_{14}$	1	$Rb_2Mn_xCr_{1-x}Cl_4$	1
CaO - systems	1	$RE_nX_mO_t$ [RE=Rare earth ions]	1
Ga_2O_3 - systems	1	$Sr_{1-x}Ba_xF_2$	1
GeO_2 - systems	1	X_mO_l [X=P, V, As, Al, Ti, Nb, Si, Bi]	1
CdTe	1	$Y_2Ba_2Cu_3O_{7-8}$	1
Co^{2+} compounds	1		

Table 3: Materials by Name of Specific Group

Material	Freq.	Material	Freq.
Apatites	1	Inorganic compounds	5
Biomolecular	6	Ionic crystals	2
Catalysts ceramics	1	Magnetic materials	1
Complex with chelate ligands	1	Minerals	2
Diamond like crystals	1	Optoelectronic materials	1
Disordered solid	2	Organic compound	1
Ferroelectric materials	3	Oxides	4
Fluorites	2	Paraelectric crystals	2
Garnets	1	Piezoelectric crystals	1
Germanium	1	Free radicals	4
Glasses	2	Spin traps	1
Graphite intercalation compounds	2	Superconducting materials	5
Halides	5	Transition-metal ion compounds	3

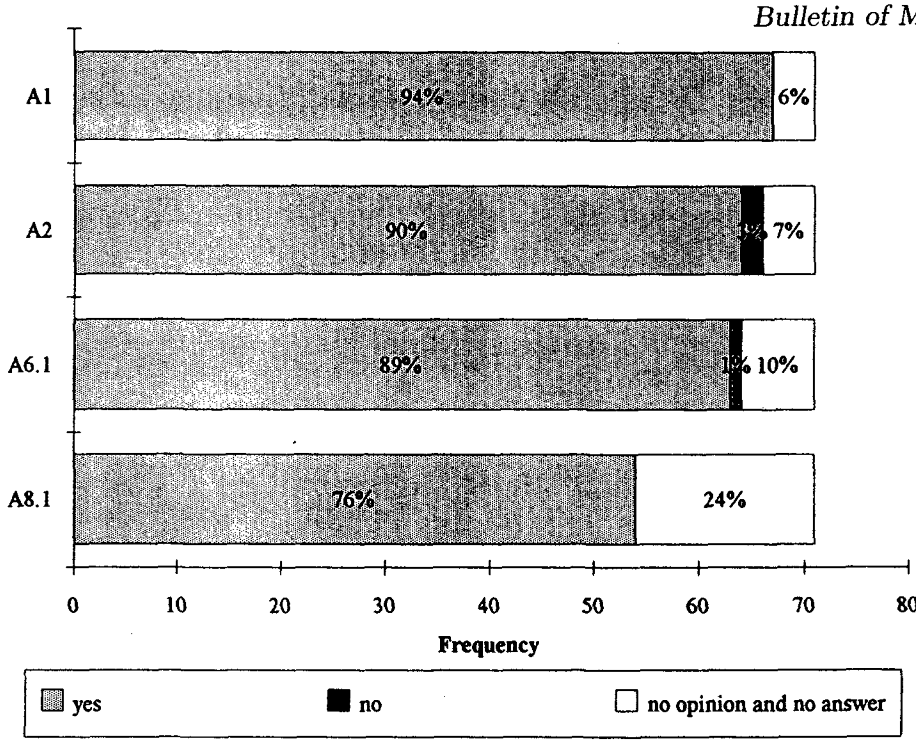


Figure 1: Answers to A1, A2, A6.1 and A8.1.
A1–Would you find it useful if there were **internationally accepted standards** on EPR nomenclature and conventions?
A2–Do you feel the need for a **glosary of terms** used in EPR, containing precise definitions of basic notions?
A6.1–Would you find it useful if an all-purpose user-friendly EPR computer programme package for analysis, simulation and fitting EPR spectra was available?
A8.1–Would you welcome establishment of an *EPR Documentation Center*?

of respondents who indicated some EPR/ESR programs developed in their groups (as revealed by the question C1 in **ML**), and which have not been listed in the 1991 edition of the ESR/EPR Software Database, have been passed on to Prof. Cammack. An EPR Documentation Center, whose establishment (Figure 1, A8.1) has received strong support (76%),.could take up a leading role in achieving the above goals, including development and on-going running of the EPR database.

The results of the inquiry on the preferred (i) notation for the zero-field splitting [**ZFS**] terms, (ii) axis system, and (iii) unit for the ZFS parameters are presented in Figures 3, 4 and 5, respectively. The extended Stevens (**ES**) operators (6,7) have received majority of *'votes'* (49%). There was quite a large proportion of *'undecided votes'* (27%), whereas the NS, BST, and KS/BCS operator notations (for definitions and references, see ref. 7) rated at or below 8%. Among other notations suggested, apart from a few ephemeral notations, several respondents indicated as a complementary one the conventional **S.D.S** (and a, F) notation. Question A4 (Figure 4) appears, in retrospect, to be poorly-constructed, since fully meaningful answers would require drawings of the crystal structures and axis systems. In *Remarks* several people mentioned the *crystallographic*, *principal*, and *magnetic* axis systems. Strong views that precise definitions should be always provided for the axis systems used in EPR studies were also expressed. This again reconfirms the need for a *glossary of terms used in EPR*.

Assuming that our sample of respondents is representative, these results are encouraging since they reveal that a much more coherent consensus on the ZFS notations (Figure 3) as well as on the unit for the ZFS parameters (Figure 5) exists within the EPR community, contrary to what could be expected judging by the messy situation prevailing in the literature in this regard (for a detailed review, see ref. 7). Nevertheless, the question of unification and standardization of notations used for the various spin Hamiltonian terms remains a thorny issue [EN **2**/3, 6 (1990); **5**/2, 6 (1993)], whose solution has been seriously attempted neither by the EPR community nor EPR organizations so far. Since

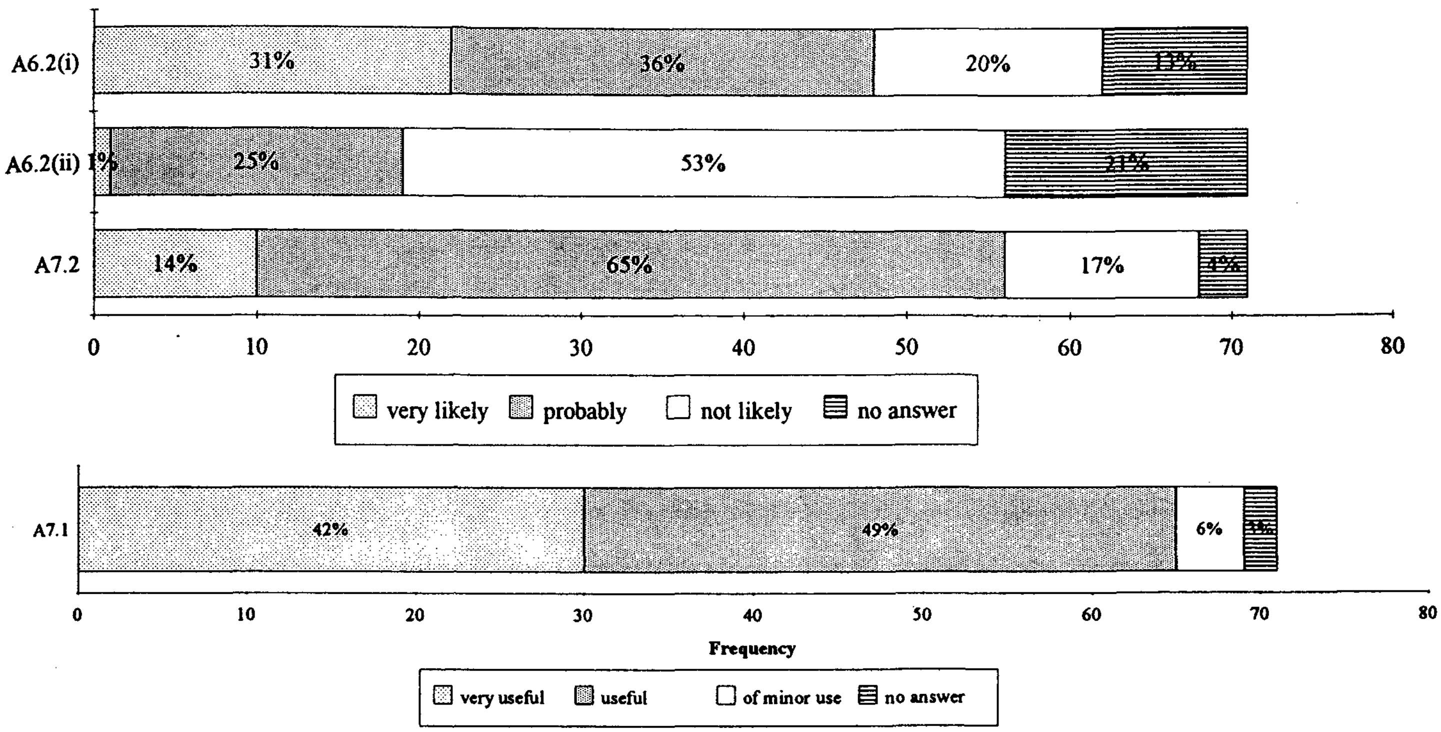


Figure 2: Answers to A6.2(i), A6.2(ii), A7.2 and A7.1.
A6.2–Would you be prepared to contribute to the development of such a package, (i) by working on the project? (ii) by obtaining financial assistance through your institution?
A7.2–If you would find a comprehensive EPR database useful or very useful, do you think your institution would subscribe to release of the EPR database information?
A7.1–How do you preceive the usefulness of a comprehensive computerized EPR database?

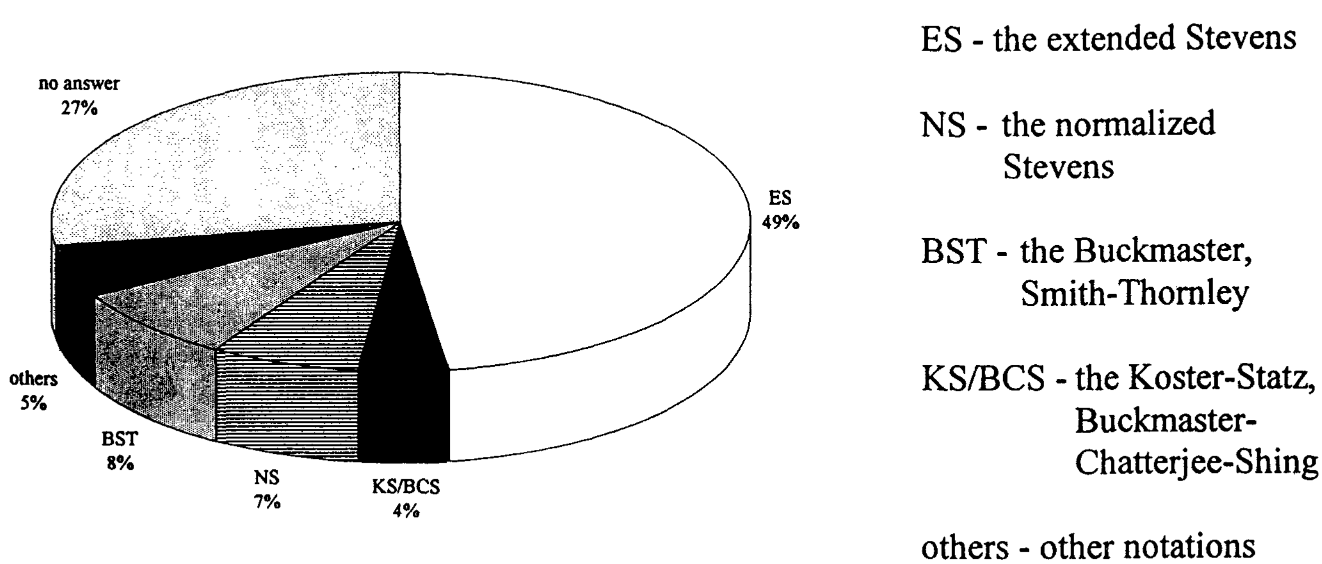


Figure 3: Answers to A3 – preferred notation for the ZFS Hamiltonian.

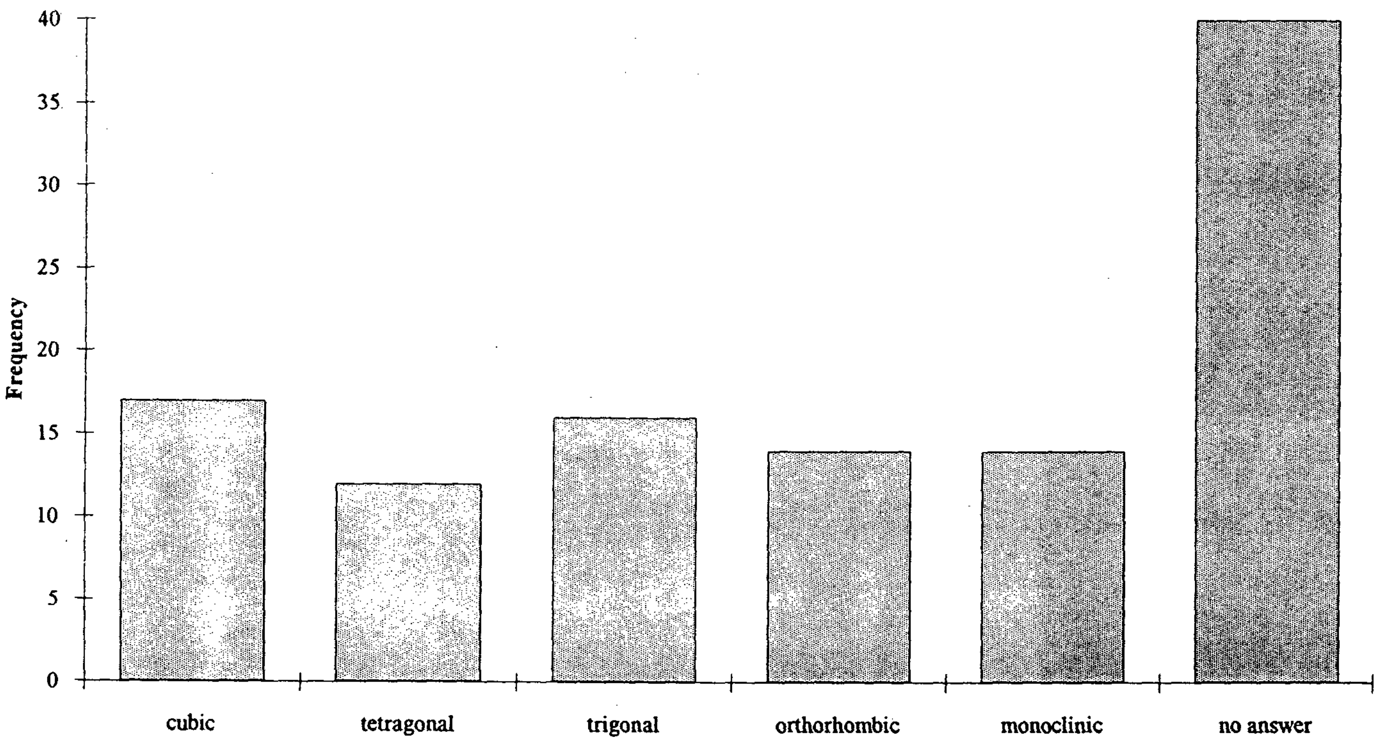


Figure 4: Answers to A4 – preferred axis system for presentation fo the ZFS data.

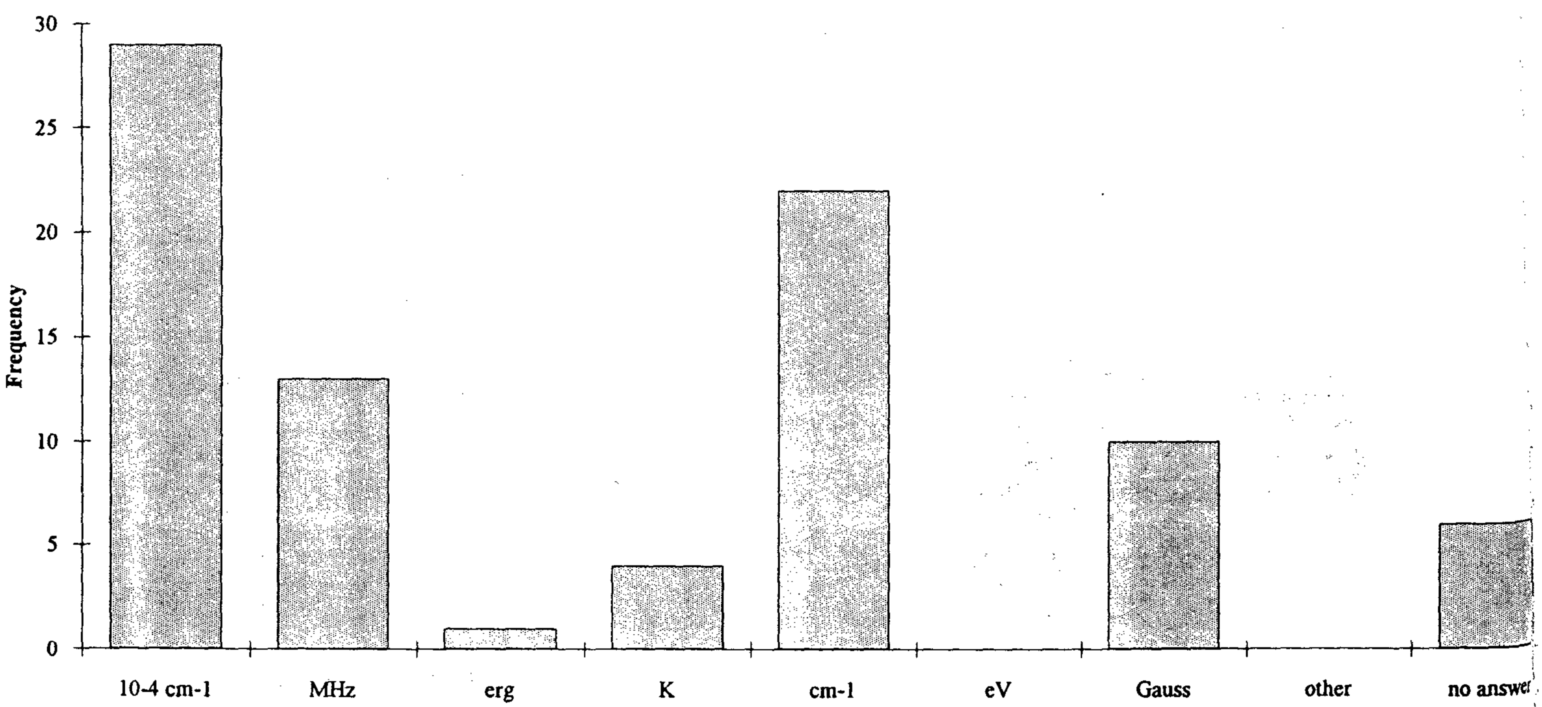


Figure 5: Answers to A5 – preferred unit for the ZFS parameters.

1990, when the question of setting up a nomenclature committee has first been put forward to IES, "this is a continuing problem" [EN **2**/3, 6 (1990)]. It should be realized that **the internationally accepted standards on EPR nomenclature and conventions** are essential for the future of the EPR field and thus a nomenclature committee should be established as soon as it is practically possible. However, only 9% of respondents declared willingness to become members of a pertinent committee (see Figure 10, B10c).

B. P-EPR: Planning EPR-database structure

Since most of the results are self-explanatory, we comment briefly on the findings presented in Figures 6 to 12 and Tables 2 and 3. Out of the 57 *full* responses, the majority of respondents indicated the chemical formula, paramagnetic ion/species and the values of the ZFS and Ze parameters, including the experimental errors, as the most useful data types (Figure 6). Other data types mentioned were: stress dependence of the ZFS parameters, isotopic composition, drawings of the structural formula of the species or the immediate environment of the magnetic site, hyperfine interactions for organic radicals, environment information like solvent of liquid radical solutions, EPR spectra (which could be electronically mailed to the database in a specific format if adopted internationally), protein concentration, values of the ZFS parameters in original notations, microwave power, modulation amplitude, sweep rate (powder spectra), preparation conditions, EPR linewidth, halfwidth and its isotropic properties, and magnetic exchange interactions. This reveals a wide range of options which should be taken into account during the planning phase of the development of a full-scale EPR database. However, including the drawings of structures and the actual EPR spectra in the EPR database would require graphical capabilities and a large-scale storage media, which would increase the costs significantly. Interestingly, out of the two options: (i) the actual EPR spectra database and (ii) the database of spin Hamiltonian parameters (as proposed here), the latter option was most favoured by the participants at the EPR 1992 meeting in Denver [EN **4**/3, 7 (1992)]. Most recently a discussion on these two options has been initiated by Dr P. Morse on the EPR LIST electronic network [EN **5**/3, 5 (1993)] starting in February 1994. Several useful ideas have been generated initially, however, quickly the interest in this topic has faded.

There is no uniformity on the most important compounds/materials or ions/species. The answers are grouped into *compounds by molecular formula or specific ion* in Table 2 and into *materials by name of specific group* in Table 3, whereas the frequency distribution of ions/species, transition-metal ions, and main group ions is presented in Figures 7, 8a, and 8b, respectively. Direct listing of ions may be more meaningful. The 52 responses indicating explicitly *ion/species* yield the following count: 3d ions (6), transition-metal ions (8), rare-earth ions (12); $V^{2+/4+}$ (2/2), $Cr^{2+/3+/5+}$ (4/15/2), $Mn^{2+/3+/4+}$ (25/4/3), $Fe^{2+/3+/4+}$ (7/25/1), Co^{2+} (5), Ni^{2+} (6), Cu^{2+} (17), Eu^{2+} (2), Gd^{3+} (13), Mo^{5+} (2), VO^{2+} (3). Paramagnetic species mentioned only once are not listed here. The results reflect the various widely spread research interests of the researchers, however, a definite focus on the transition-metal ions in technologically important materials may be noticed. The latter aspect may be helpful in searching for funds for the future development of a full-scale EPR database. Support from industrial companies, which use EPR techniques and/or utilize EPR data for materials characterization, could be sought. Out of the few commercial producers of EPR equipment, strong support for the EPR database has been declared by the Bruker, who could also help with marketing the product. Question B9 (Figure 10) is strongly related to the *'chemical content'* and hence is considered here. Although within the question B1 the researchers listed **particular** chemical structures (Table 2 and 3), the majority (70%) would like to have all chemical structures studied by EPR techniques listed in the EPR database (Figure 10, B9). Other suggestions were, e.g. *'initially crystalline systems, later all other chemical structures'* and *'inorganic compounds'*.

It is worthwhile to mentioned here that at the EPR 1992 meeting in Denver Prof. J. Weil volunteered to collect "inorganic" data, whereas Prof. H. Buckmaster agreed to assemble data from reprints in the way that he did in his reviews published in Mag. Reson. Rev. series [EN 4/3, 8 (1992)]. According to our informal information as of August 1993, no progress has been made in this regard be-

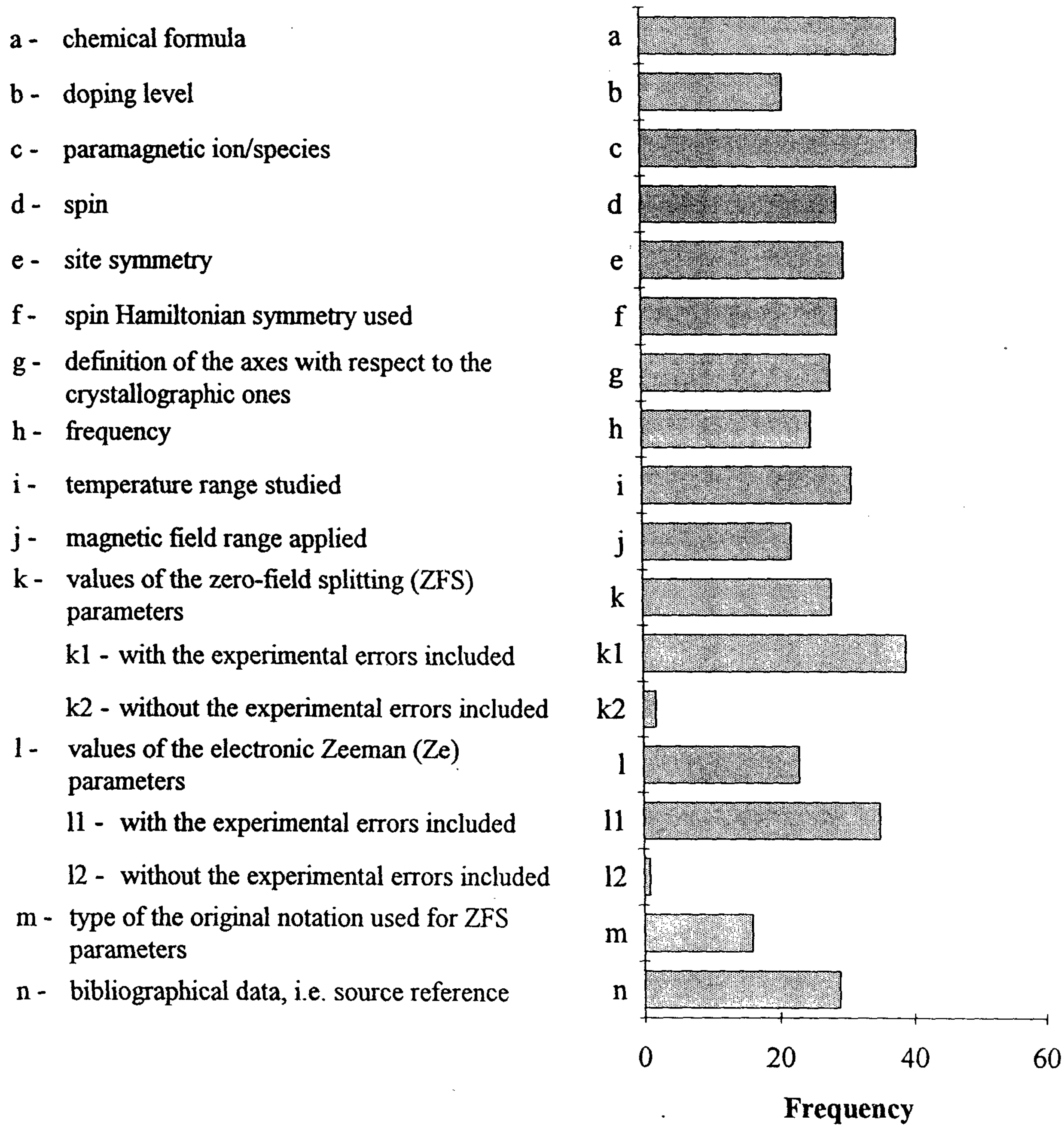


Figure 6: Answers to B1 – most useful data types.

cause of various other commitments. A more coordinated effort is needed to bring about substantial progress in the EPR database project.

From the suggested list of queries (Figure 9) the most useful seem to be (i) *References to EPR studies of the ion X in the compound Y*, (ii) *Papers on the ion X with spin Y in the site of symmetry Z*, and (iii) *Values of the ZFS parameter X for the ion Y at symmetry Z.* Other comments on the possible queries made include requests for information on the type of phase transition, type of ligand, crystallographic classes, values of the hyperfine interaction constants, name of starting material as well as desire for a large scientific state-of-the-art database system capable of flexible information searches.

Responses to questions concerning technical aspects of the database structure and organization are summarized in Figures 10 and 11. Most people (57%) want *all authors and full title* to be included in the bibliographical data (Figure 10, B3), whereas the minimal option is still satisfactory for some (25%). The *'votes'* on a **topical** (30%) versus **numerical** (35%) database are nearly equally split, with similar number of *'undecided votes'* (Figure 10,

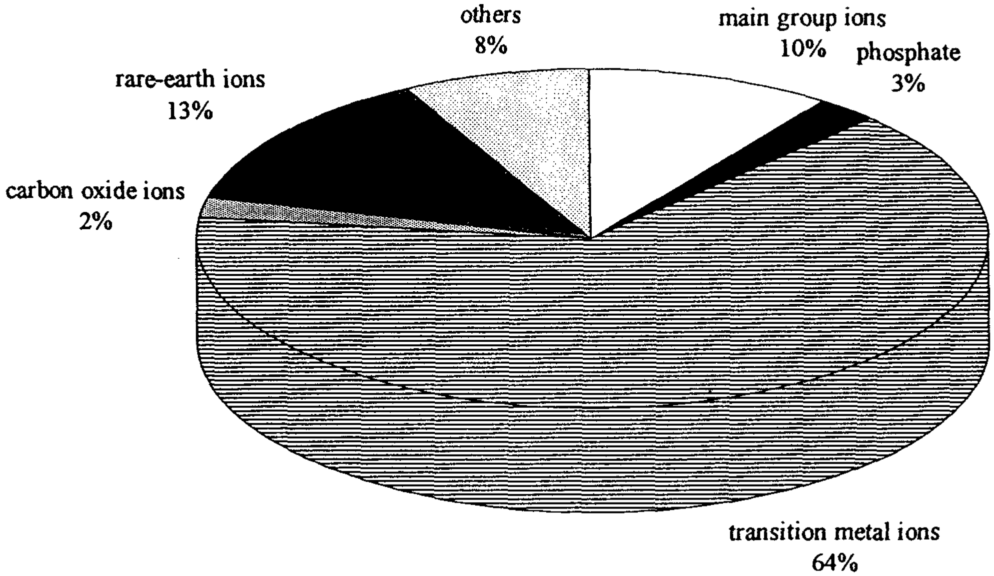


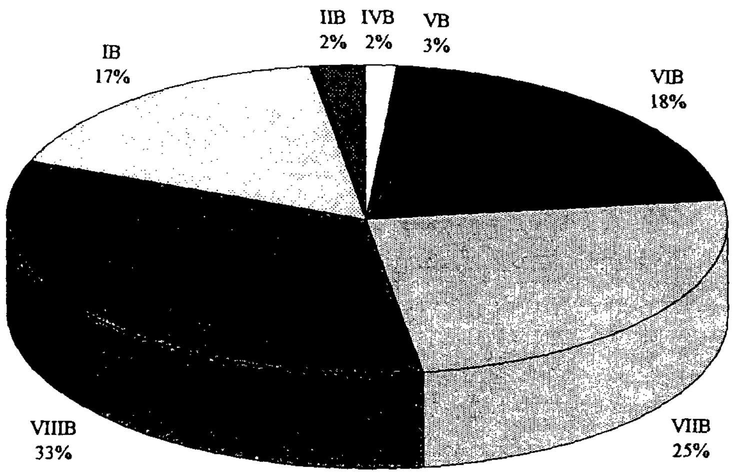
Figure 7: Frequency distribution of ions/species.

B4). The former option is less costly and easier to implement, whereas the latter one is much more *'labor intensive'*. Other comments on the database structure were, e.g. *"a simple topical database will be cheaper to establish and maintain, and more institutions will be able to afford the subscriptions", "small-scale, probably available on work stations or PC, high speed searches", "in order to keep the database size reasonable, the format of data storage should depend on the type of the paramagnetic species–for marketing purposes one would call this 'object oriented'", "EPR spectrum + spin Hamiltonian + Bibliographical details"*.

There is no special preference for the type of software to be used (Figure 10, B5), which indicates most probably a lack of sufficient knowledge on the technicalities of database systems among the respondents. This is confirmed by the answers to the question B6 regarding the database systems with which people have experience. The names specified by a handful of people (numbers in brackets) included either general purpose databases, e.g., dBASE (2), Fox-pro (2), Paradox (2), and Oracle (1) or large scientific databases, e.g., Chemical Abstracts (2), Cambridge Crystallographic (3), Inspec (2), SCI (1) and CCOD (1). Similarily the listing of the database systems available at the respondents' institution (question B7) included the same names as given in the answers to the question B6 and, additionally, Dialog, SQL, and Pascal (CNRS). The opinions on the scale of the EPR database are presented in Figure 11. A majority (54%) opted for a large full-scale database, comprehensive with regard to data types and literature sources.

Feasibility of the development of a full-scale EPR database hinges on several factors, among others, the existence of other EPR-related databases and the level of support from EPR community, which were probed in the question B10 (Figure 10) and B11 (Figure 12), respectively. The knowledge of other EPR-related databases (B11, Figure 12) is very low (7%). The items listed by this 7% of respondents include one EPR book (published in 1965), two review article series (*Mag. Reson. Rev.* and *Landolt-Börnstein*), STDB II, *'ESR/EPR in CAS-online'*, and *'Bruker'* (?). The only EPR-related computer database in this listing is STDB II, which is a database for spin trapping. This confirms that no EPR-related computer database exists at present. Concerning the level of support from the EPR community, the question of the low response rate in the EPR database survey aside, a tangible support for the EPR database project has been directly shown by about a quarter of respondents who declared their willingness to share the work and to take on some aspects of the development of the EPR database (Figure 10, B10a, b). Hence the numbers involved are enough for efficient multinational work on the project.

A



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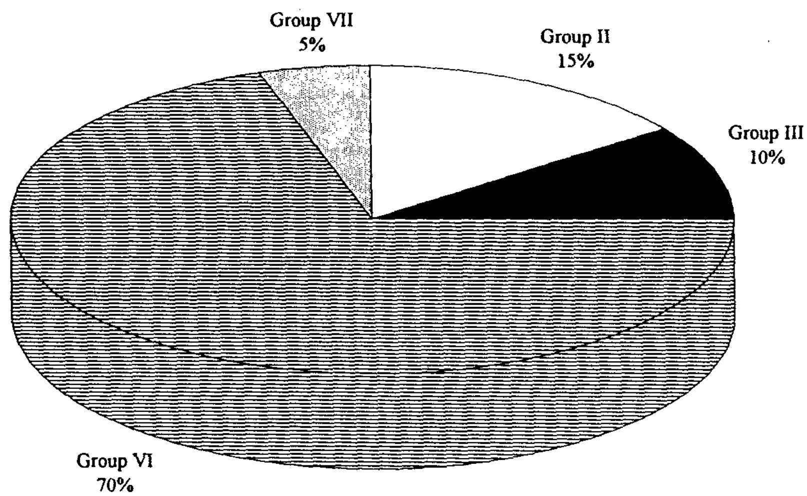

Figure 8: A) Frequency distribution of transition metal ions. B) Frequency distribution of main group ions.

C. ML: Membership aspects

The survey reveals the following pattern of membership of the EPR-related societies among the 25 respondents who provided answers to this question (numbers in brackets): (a) International EPR Society [20], (b) ISMAR [6], (c) Ampere Group [4], (d) ESR Group of the Royal Society of Chemistry [2], (e) Others [6]. Note that one person may be a member of more than one organization, while 48 respondents did not provide any indication on their membership or returned only the **EPR-Q**. The organizations specified under *others* are: the *'country related'* ones, which includes three national EPR/ESR groups (Poland, Hungary, Czechoslovakia) and two probably internal Russian ones (SMRM, ISDE – ?), as well as ESR Applied Metrology, ESR Dating and Dosimetry and American Institute of Ultrasound in Medicine.

The analysis of the brief description of the research interests given by the respondents provides suggestions for future amendments to the *fields-of-interest codes for members of IES* [cf EN **5**/2 (1993)]. We have tried to categorize the research interests revealed in our survey according to the 28 fields used by IES. The results are as follows (num-

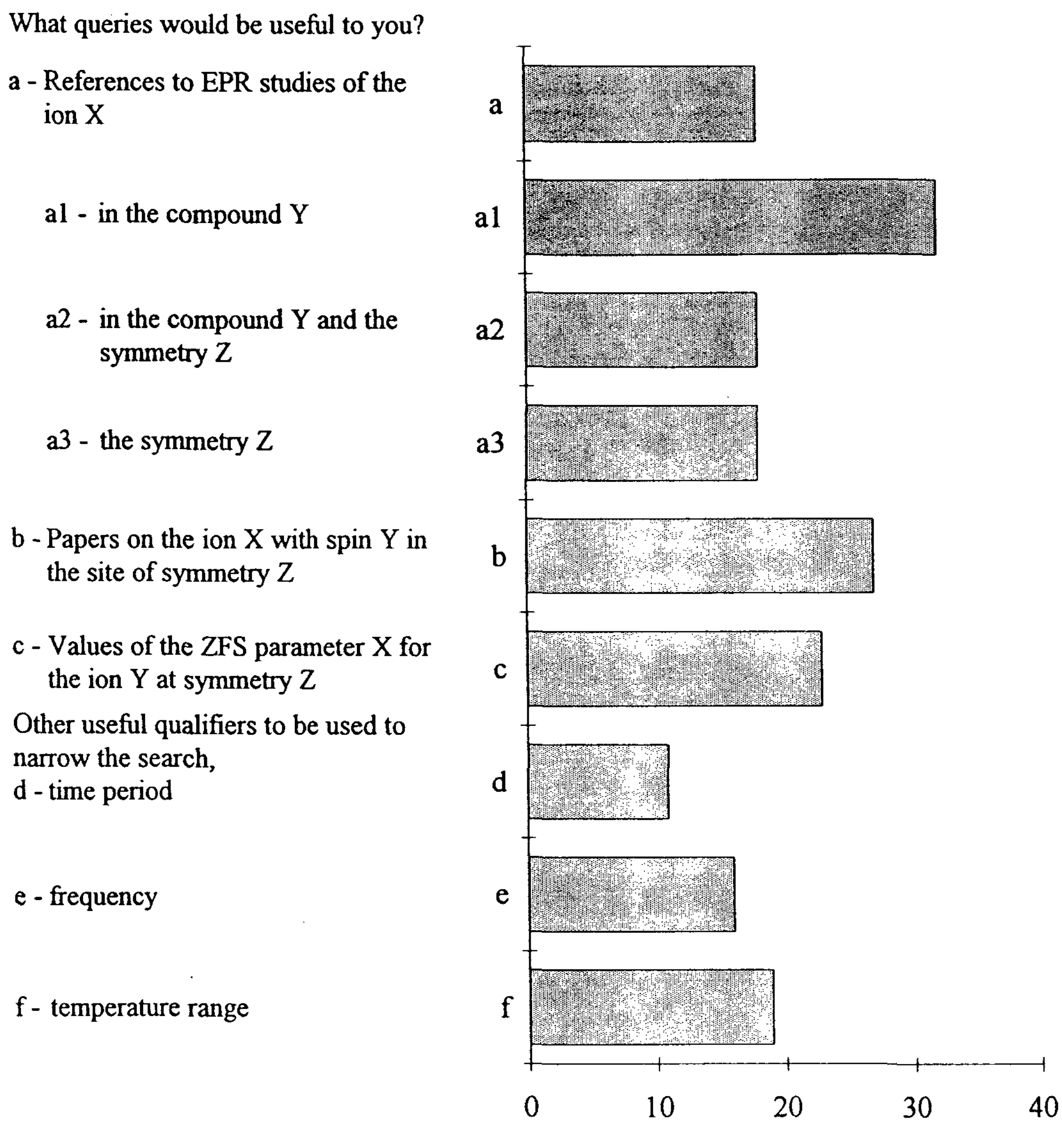

Figure 9: Answers to B2.

bers in brackets indicate no of occurences of research interests which fall within a given IES category): 1. BIOMED [8], 2. POLAR [0], 3. COAL [0], 4. COMP [14], 5. CRYST [15], 6. DMR [4], 7. FERR [2], 8. FREE [0], 9. GEOL [0], 10. EPRI [3], 11. INSTR [2], 12. LABEL [3], 13. LIQ [2], 14. MEMBR [2], 15. ION [5], 16. METALP [2], 17. OXY [0], 18. PEPR [1], 19. PHOTO [1], 20. POL [2], 21. RAD [4], 22. SOLID [20], 23. SUPERC [11], 24. SURFACE [1], 25. KINETICS [2], 26. TRAP [2], 27. VIVO [0], 28. CA [0].

The research interests, which do not fall within any IES code can be classified into five groups, namely, (a) EPR-related experimental techniques, (b) EPR-related theoretical aspects, (c) physical properties, (d) specific materials, and (e) other areas. The list compiled from the responses comprises: (a) APR [1], EPR dating [1], EPR dosimetry [3], ESE (ESEEM) [2]; (b) group theory [1], Jahn-Teller effect [2], ligand field theory [3], superposition model [2]; (c) defects and impurites [13], electron spin relaxation [1], exchange interactions [1], paramagnetic centers [2], phase transitions [12], spin-lattice coupling [2]; (d) high sensitivity scintilators [1], low dimensional conductors [1], metal films [1], semiconductors [3]; (e) catalysis [1], crystallography [1], FIR [1], magnetism [1], mesoscopic systems [1], Mössbauer spectroscopy [1], NMR [3], optical spectroscopy [2], susceptibility [2]. The distribution of fields within the IES list and the above list indicate the neccessity for a more adequate coding for the fields of interest as well as for a more precise specification of the content of each code. It would be worthwile to introduce, instead of the

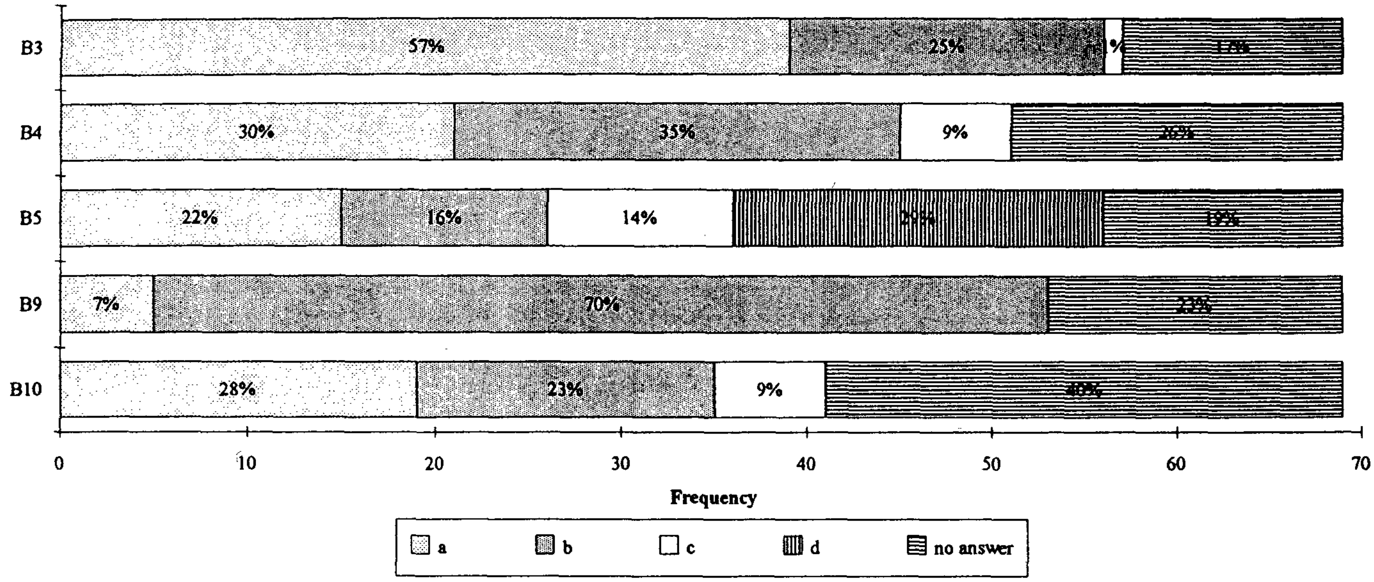

Figure 10: Answers to B3, B4, B5, B9 and B10.
B3–Should the bibliographical data include: [a] all authors and full title, [b] only the minimum information necessary to identify the reference, [c] no opinion.
B4–Would you be satisfied with [a] a **topical** database which would contain references on specific paramagnetic systems (i.e. compound/ion or species) and a **searchable** list of topics dealt with in a given source paper, **OR** [b] it is essential to retrieve from the database the **numerical** data on the parameters describing EPR spectra (i.e. ZFS and Ze parameters)? [c] no opinion.
B5–Preferred type of software to be used: [a] commercial, [b] specially developed, [c] adopted from a related database system, [d] no opinion.
B9–In your opinion should the EPR-database comprise data on [a] **particular** chemical structures only (at least at the initial stages of development)–then please name these structures **OR** [b] all chemical structures studied by the EPR technique?
B10–Would you like to become a member of [a] a panel of potential EPR-database users which will work out the User Requirements Report, [b] a group which will develop and test a prototype of EPR-database, [c] a committee which will work out "Recommendations for EPR Nomenclature and Conventions pertaining to spectra of spin $S>1/2$ systems".

present coding, a more comprehensive one based on the five groups (a-e) used above, provided it is technically feasible within the existing IES membership database.

III. Concluding remarks

It had been planned to produce and test a small-scale prototype at the second stage of the EPR database project. To this end a detailed study of alternative EPR database structures has been carried out using the results of the survey concerning the demands on the data structure and possible query systems. Since the present feedback has been insufficient, the project could not go beyond working out the framework of a small-scale prototype database, whereas its actual implementation has been postponed. The aspects arising from this survey and pertaining to the feasibility of a full-scale EPR database as well as the database structure and organization could be discussed in detail in the Feasibility Study Report. The alternative EPR database structures as well as several scientific and technical questions pertinent to the EPR database and related projects could also be dealt with therein.

The experience gained during this project can be utilized in future provided there is sufficient support

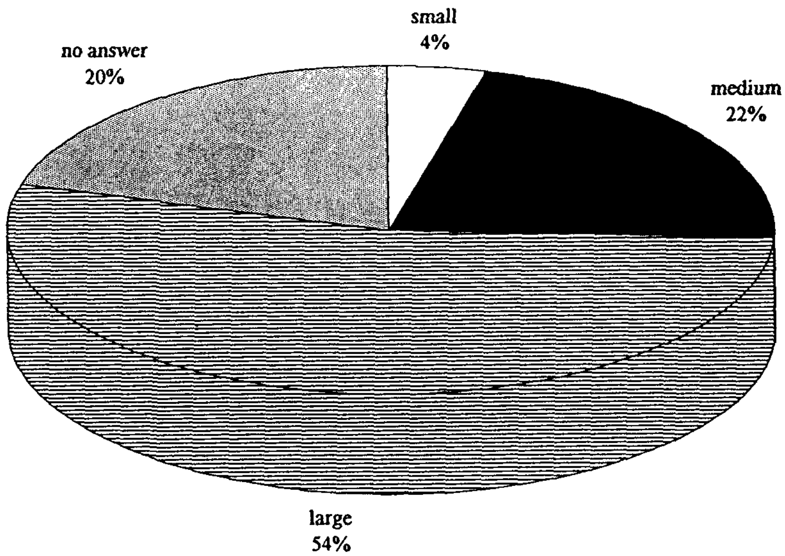

Figure 11: Answers to B8 – the scale of the EPR-database.

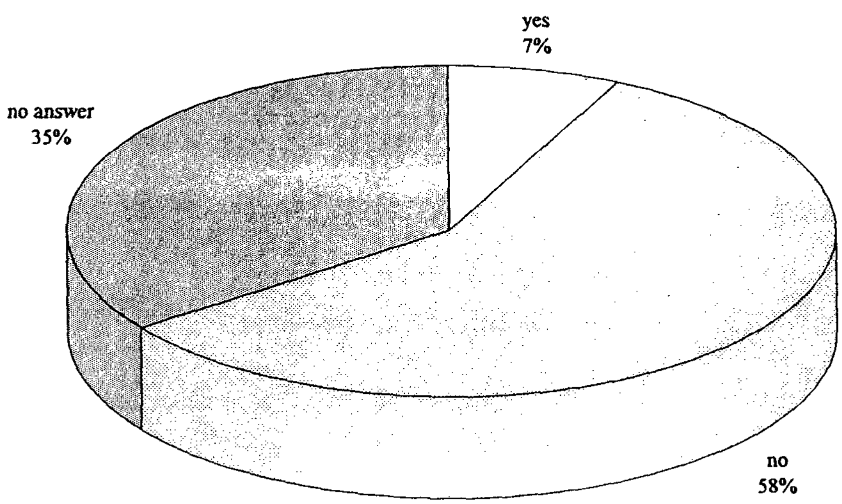

Figure 12: Answers to B11 – Do you know of any other EPR-related databases?

from the EPR community and EPR-related organizations for the continuation of the EPR database project to its full completion. The present situation in this regard has been succinctly evaluated by Prof. G. Eaton, who has suggested [EN **5**/2, 6 (1993)]: *"Greater support from the membership is needed to justify the effort involved, and there should be a committee to oversee the implementation"*. The author's personal and open interaction with EPR researchers was helpful and supportive for the project, while the questionnaires probably tended to generate a variety of negative feelings and annoyance at yet another time-consuming intrusion. Thus even though the response rate was low we believe that the views expressed represent those of the EPR community members as a whole. This survey has enabled us to learn about some qualitative trends. We ended up with the strong conviction that increases in support of the EPR database and the related projects from EPR organizations are vital for the continued health of the area. The grants must be made available, the tangible support by EPR organizations must be offered, if we expect more than the present efforts.

Finally, the author would welcome further responses as well as any comments on the EPR-database project and the related ones, their feasibility, resources available and/or required, and strategy for future development. Full set of the questionnaires and attachements is available from the author (FAX: 852 788-7830, Email: APCESLAW@CITYU.HK). It is hoped that this paper will encourage wide consultations within the EPR community.

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IV. References

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