solve the difficulties inherent in the correlations between the quartets themselves. These are problems of a theoretical nature that need to be resolved.

A logical extension to these applications of four- and five-phase invariants is to include them in both an active and passive way in the magic integer/ψ map program *MAGIC* and the random phase set/linear equation system *YZARC* where they offer the potential of further enhancing these techniques.

Quartets and quintets can be expensive to calculate in terms of computer time especially when the third-neighbourhood formulae are used. The search for these invariants and their neighbourhoods lends well to the parallel techniques of vector and array processors. The advent of cheaper processors of this kind may well make fully exhaustive searches for quartets and quintets a routine computer operation. We intend to explore this line of development.

We wish to thank the Computing Service of the University of Glasgow for the provision of facilities for carrying out this work.

References

COLLENS, A., DECLERCQ, J. P., GERMAIN, G., PUTZEYS, J. P. & VAN MEERSSCHE, M. (1974). *Cryst. Struct. Commun.* **3**, 119–122.

DECLERCQ, J. P., GERMAIN, G. & WOOLFSON, M. M. (1979). *Acta Cryst.* A**35**, 622–626.

DE TITTA, G. T., EDMONDS, J. W., LANGS, D. A. & HAUPTMAN, H. (1975). *Acta Cryst.* A**31**, 472–479.

DE TITTA, G. T., EDMONDS, J. W., LANGS, D. A. & HAUPTMAN, H. (1976). Am. Crystallogr. Assoc. Summer Meeting, Pennsylvania State Univ., Abstract D3.

FORTIER, S. & HAUPTMAN, H. (1977). *Acta Cryst.* A**33**, 829–833.

FREER, A. A. & GILMORE, C. J. (1980). In preparation.

GIACOVAZZO, C. (1976*a*). *Acta Cryst.* A**32**, 91–99.

GIACOVAZZO, C. (1976*b*). *Acta Cryst.* A**32**, 100–104.

GIACOVAZZO, C. (1980). *Acta Cryst.* A**36**, 74–82.

GILMORE, C. J. (1977). *Acta Cryst.* A**33**, 712–716.

GILMORE, C. J., HARDY, A. D. U., MACNICOL, D. D. & WILSON, D. R. (1977). *J. Chem. Soc. Perkin Trans.* 2, pp. 1427–1434.

HAUPTMAN, H. (1977*a*). *Acta Cryst.* A**33**, 556–564.

HAUPTMAN, H. (1977*b*). *Acta Cryst.* A**33**, 565–568.

HAUPTMAN, H. (1977*c*). *Acta Cryst.* A**33**, 553–555.

HEINERMAN, J. J. L. (1978). In *Direct Methods in Crystallography*, edited by H. A. HAUPTMAN, pp. 177–194. Pittsburgh: Polycrystal.

LESSINGER, L. (1976). *Acta Cryst.* A**32**, 538–550.

PUTTEN, N. VAN DER & SCHENK, H. (1977). *Acta Cryst.* A**33**, 856–858.

PUTTEN, N. VAN DER & SCHENK, H. (1979). *Acta Cryst.* A**35**, 381–387.

Acta Cryst. (1980). A**36**, 475–482

Crystallographic Literature: A Bibliometric and Citation Analysis*

BY DONALD T. HAWKINS

Bell Laboratories, Murray Hill, New Jersey 07974, *USA*

(*Received* 2 *April* 1979; *accepted* 17 *January* 1980)

Abstract

The literature of crystallography was studied by bibliometric analysis using the Lockheed DIALOG® on-line information retrieval system and the *Chemical Abstracts* database. In the period 1972 to 1976, the publication of journal articles on crystallography remained approximately constant at 9550 papers per year. Major journals publishing articles on crystallography were identified and ranked; ten journals devote more than half their contents to the subject. Twenty journals account for half the papers on crystallography. Use of Bradford's Law along with ranking by percentage of crystallographic papers showed that there are 22 core journals. The 18 that had citation data available were ranked on an 'influence' basis. The most influential journals, as identified by citation data, are large well known chemistry and physics journals. The citation linkages between the field of crystallography and other closely related fields of

---

* *Editorial note:* A preliminary investigation of the extent to which *Acta Crystallographica* attracts and publishes the most important papers on crystallography was made at the request of the Chairman of the Commission on Journals for presentation at an Open Meeting of the Commission in Warsaw, 11 August 1978. Objective examination, from time to time, of how well a journal serves its community of readers, authors and subscribers may be beneficial both to that community and to its publishers. Interest in the relationships discerned among the various journals publishing crystallographic papers led to subsequent analysis. The present paper, following its subjection to the usual acceptance process, makes the results of this analysis available to the crystallographic community and also provides a basis for future assessment.

0567-7394/80/030475-08$01.00

science show that links to chemistry and physics are about an order of magnitude stronger than those to metallurgy, materials science, mineralogy and biology.

Introduction

A large number of papers on crystallography are published each year. The role of crystallography in scientific research can be determined by examining its published literature. Because crystallography is interdisciplinary, its literature might be expected to be rather widely dispersed. However, there are also several sources whose primary focus is crystallography. This study examines the relationship of these 'exclusive' sources to other sources, their influence among crystallographers, and how well they cover the subject.

Garfield (1974) published the results of a citation study of *Acta Crystallographica*. He listed the journals citing and those cited by *Acta Crystallographica*. Six journals accounted for 50% of the references made by this journal, and its self-citing rate was 36%. Garfield also listed 45 papers published in *Acta Crystallographica*, each of which was cited more than 100 times between 1961 and 1972, and concluded that *Acta Crystallographica* is a very significant journal, not only to crystallographers, but to scientists in general. Garfield's motivation for his study came from a private communication noting that 19 of the 100 most cited chemical articles from 1961 to 1972 were concerned with crystallography. His 1974 citation study was based on data from 1972; more recent data (Garfield, 1976) appear in *Journal Citation Reports* (JCR). JCR also includes data on the two separate sections of *Acta Crystallographica*, *Acta Crystallographica A* and *Acta Crystallographica B*.

In the present study, both bibliometric and citation analyses were applied to the crystallographic literature. Bibliometrics is the quantitative study of a body of literature and can be used to identify major sources, trends with time, types of publications, and so on. Citation studies are useful for determining the influence of the various sources upon one another and the patterns of use of the information.

Bibliometric analysis

The Lockheed DIALOG® on-line information retrieval system was used to gather the data for the bibliometric analysis in the manner used in previous studies of this type (Hawkins, 1976, 1977). Data were taken from the *Chemical Abstracts* (CA) database for 1972 through 1976 (Lockheed's File 3). (This section of the database contains articles *abstracted* between 1972 and 1976. Because of the time lag in the abstracting process, there are small differences between the number of items published and those abstracted in any given time period.) Although there are several sources of crystallographic data and also several possible definitions of crystallography, the CA database was chosen because it is widely available in both printed and online versions and also because of its convenient section classification scheme. In this study, 'crystallography' was defined to include the study of crystals and crystal structures. Specifically excluded are the materials-science aspects of crystals, such as nucleation, techniques of crystal growth, *etc.*

After experimenting with a keyword search, it was found that the CA section classification codes adequately retrieved papers on crystallography, and many irrelevant or marginally relevant papers were being retrieved by the additional keyword terms in the profile. The keyword terms were therefore omitted, and the set of all papers in CA Section 75 (entitled *Crystallization and Crystal Structure*, and called Section 70 before 1975), was formed. This set contained 65 637 papers. Table 1, from the Chemical Abstracts Subject Coverage manual (1975), shows the subsection breakdown of Section 75. According to our definition, Section 75, Subsection 1, entitled *Crystallization*, should be omitted from this study. The set of crystallographic papers was therefore taken to be those classified by CA in Section 75, Subsections 0, 2, 3, 4 and 5. This set contained 57 419 papers. It is important to note that CA and similar databases cover the 'primary' literature (journals, conference proceedings, *etc.*); the 'secondary' literature, such as abstracts and indexes, is generally not included. Well known sources of crystallographic information, such as *Structure Reports* and the Landolt–Börnstein compilations are therefore not covered by CA and are not included in this study.

A list of 176 chemistry and physics journals likely to publish papers on crystallography was taken from the following sources: Kiehlmann's (1972) list of journals covered by the major abstracting services, the

Table 1. *Subsection breakdown of Chemical Abstracts Section* 75

0. Reviews
1. Crystallization
    Methods and theory
    Nucleation
    Growth (including twinning)
    Effect of impurities
2. Order–disorder and dislocations
3. Phase transformation of crystals
4. Physical properties of crystals
5. Crystal structure determinations
    Methods and theory, elements, metals
    Inorganic compounds
    Minerals
    Organic compounds
    Mesomorphic (liquid crystalline) phases
    Liquids
    Gases

journal hierarchy studies of Carpenter & Narin (1973), and Narin, Carpenter & Berlt (1972), the *Science Citation Index* journal lists (1976), Garfield's (1976) *Journal Citation Reports*, Garfield's (1974) citation study of *Acta Crystallographica*, and Pinski's (1977) study of citation interrelationships of chemistry journals. These journals were then matched against the modified set of papers from CA Section 75 to yield the number of papers appearing in each journal. For each journal, the total number of papers it published during the five-year period under study was recorded, as well as the number of crystallographic papers. The percentage of crystallographic papers was calculated for each journal. Table 2 lists these data for the top 35 journals, ranked by the percentage of crystallographic papers.*

Table 2. *Top* 35 *journals ranked by percentage of crystallographic papers published,* 1972–1976

Journal	Total no. of papers	% Crystallographic
Cryst. Struct. Commun.	746	99·9
Acta Cryst. B	3369	98·7
J. Cryst. Mol. Struct.	174	91·4
Acta Cryst. A	617	89·3
Z. Kristallogr. KKK	111	89·2
J. Appl. Cryst.	493	85·0
Cryst. Lattice Defects	132	79·5
Kristallografiya	1268	68·1
Mol. Cryst. Liq. Cryst.	597	63·3
J. Solid State Chem.	862	58·8
Mater. Res. Bull.	1092	48·5
Kristall. Tech.	694	48·1
Philos. Mag.	1041	46·1
Rev. Chim. Mineral.	321	45·8
Bull. Soc. Fr. Minéral. Cristallogr.	377	44·6
J. Struct. Chem.	1149	34·4
J. Less-Common Met.	974	32·4
Phys. Status Solidi A	3428	30·1
Z. Anorg. Allg. Chem.	1417	29·5
Am. Mineral.	700	29·4
J. Phys. Chem. Solids	1170	28·7
Izv. Akad. Nauk SSR, Neorg. Mater. [*Inorg. Mater.* (*USSR*)]	2881	27·4
Ferroelectrics	362	26·2
J. Chem. Soc. Dalton Trans.	2730	26·1
Fiz. Tverd. Tela (*Leningrad*) (*Sov. Phys.-Solid State*)	3881	25·2
J. Phys. C.	1975	24·4
Phys. Kondens. Mater.	70	24·3
J. Electron Mater.	206	23·3
Phys. Status Solidi B	2978	23·0
Acta Chem. Scand.	1430	21·7
Inorg. Chem.	3683	21·2
Surface Sci.	1677	20·7
J. Cryst. Growth	1431	20·6
Acta Metall.	730	20·5
Jpn. J. Appl. Phys.	1900	20·4

Ten journals devote more than half their contents to crystallography. The journals were also ranked by number of crystallographic papers published. Fig. 1 is a plot of cumulative percentage of crystallographic papers against the number of journals, and it shows that 20 journals contain half of the papers on crystallography.

One might expect some of the percentages in Table 2 to be higher for the 'exclusively' crystallographic journals. For example, *Acta Crystallographica A* contains about 90% crystallographic papers, and *Kristallografiya* contains only 68% of such papers. The remaining 10 and 32%, respectively, represent papers whose subject lies outside our definition of crystallography, or indexing errors. Examination of many of these residual papers showed that few of them are indexed incorrectly. Most of them deal with crystal-growth techniques and hence were classified by CA in Section 75, Subsection 1. (In fact, this paper, which is appearing in *Acta Crystallographica A*, will undoubtedly be classified by CA in Section 20, dealing with documentation, rather than in Section 75. It will therefore fall into the 10% of the 'non-crystallographic' papers published in *Acta Crystallographica A*.)

Since the DIALOG system allows a search on publication type and date, the type of papers abstracted in CA Section 75 could be determined (Table 3), as well as the time distribution (Table 4). Not surprisingly, the overwhelming majority of the 57 419 papers in crystal-

Table 3. *Types of literature on crystallography*

Type	No. of papers	Percent of total
Books	105	0·2
Conference presentations	4120	7·2
Journal articles	49757	86·7
Patents	1290	2·2
Reports	1168	2·0
Theses	979	1·7
Total	57419	100·0

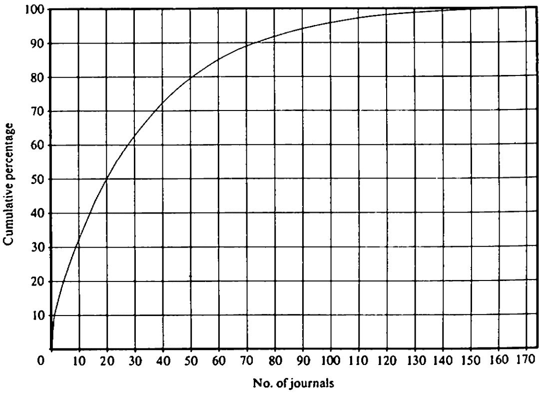

Fig. 1. Cumulative percentage of crystallographic journals.

---

* The data for the full list of 176 journals have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35046 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

lography appeared as journal articles. The yearly production of papers abstracted between 1972 and 1976 remained approximately constant at 9950 papers per year.

Bradford (1948) observed that a collection of journals on a given subject, when ranked by the number of relevant articles they contained, could be partitioned into 'zones' of productivity. This observation has come to be known as Bradford's Law. Brookes (1968, 1973) and other authors have described various derivations and applications of Bradford's Law. Bradford's Law was applied to the crystallographic literature by plotting the cumulative number of publications against the logarithm of the journal rank. The resulting elongated S-shaped curve is shown in Fig. 2. This curve has the classic shape, showing that the data fit the Bradford distribution well. The core, determined by the number of journals up to the point where the curve becomes linear, contains about 15 journals. It is slightly larger than one obtains for many fields because the crystallographic literature is somewhat dispersed. Table 5 lists the 15 core journals derived from Bradford's Law. The number of crystallographic papers published and the rank of the journal on a percentage basis (from Table 2) are also listed. The top journal in Table 5, *Acta Crystallographica B*, published about 2½ times as many papers as the next journal. If the two sections of *Acta Crystallographica* are combined, the ratio is nearly 3 to 1.

Table 4. *Yearly publication rate of journal articles*

Year	No. of articles published
1972	9799
1973	10310
1974	10123
1975	9892
1976	9633
Average	9950 (±360)

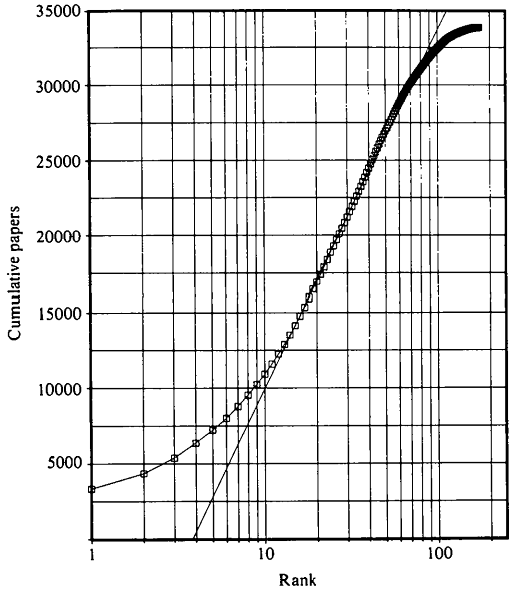

Fig. 2. Bradford plot for crystallographic journals.

Table 5. *Top 15 journals in crystallography, as derived from Bradford's law*

Journal	No. of crystallographic papers	Rank from Table 2
Acta Cryst. B	3325	2
Phys. Status Solidi A	1031	18
Phys. Rev. B	1022	39
Fiz. Tverd. Tela (Leningrad)	979	25
Kristallografiya	863	8
Izv. Akad. Nauk SSSR, Neorg. Mater.	788	22
Inorg. Chem.	782	31
Cryst. Struct. Commun.	745	1
J. Chem. Soc. Dalton Trans.	713	24
Phys. Status Solidi B	686	29
C. R. Acad. Sci. Ser. C	667	46
J. Chem. Phys.	651	77
J. Am. Chem. Soc.	640	88
J. Chem. Soc. Chem. Commun.	632	59
Solid State Commun.	630	44

Table 2 shows that the 'exclusively' crystallographic journals do indeed cover their subject well. They all rank within the top nine and contain over 60% of their contents on crystallography; all have the word 'crystal' or some variant of it in their titles. However, only two of these 'exclusive' journals are in the Bradford's Law-core. The majority of the journals listed in Table 5 rank well down in Table 2 because they tend to be large physics or chemistry journals. For example, the *Journal of the American Chemical Society*, which is a highly significant and important journal ranking near the top of many lists of journals (including those in JCR), ranks 88th in percentage of crystallographic papers even though it contains 640 such papers. The Bradford distribution, depending on the absolute number of papers published, tends to give weight to large journals. The percentage distribution, on the other hand, allows smaller but still significant journals to rank high. So, for example, the *Journal of Crystal and Molecular Structure*, publishing only 174 papers in five years, is highly significant to crystallography since 91% of its papers were so classified by CA in Section 75. A unified list of core journals for crystallography, consisting of the Bradford's Law core plus the journals with half or more of their contents on crystallography, contains the 22 journals listed in Table 6.

Citation analysis

Bibliometric data reveal publication patterns and trends for a field and can identify major sources of information on the subject. They do not, however,

Table 6. *Core journals in crystallography* (*listed alphabetically*)

Acta Cryst. A
Acta Cryst. B
C. R. Acad. Sci. Ser. C
Cryst. Lattice Defects
Cryst. Struct. Commun.
Fiz. Tverd. Tela (*Leningrad*)
Inorg. Chem.
Izv. Akad. Nauk SSSR, Neorg. Mater.
J. Am. Chem. Soc.
J. Appl. Cryst.
J. Chem. Phys.
J. Chem. Soc. Chem. Commun.
J Chem. Soc. Dalton Trans.
J. Cryst. Mol. Struct.
J. Solid State Chem.
Kristallografiya
Mol. Cryst. Liq. Cryst.
Phys. Rev. B
Phys. Status Solidi A
Phys. Status Solidi B
Solid State Commun.
Z. Kristallogr. KKK

reveal its patterns of use or the influence an article may have on its readers. Although such information can be subjective and hard to determine, one concrete measure of the usage of an article or a journal is its citation record. A citation often indicates that an author has read an article, and that it has influenced his research. The primary source of citation data is the *Science Citation Index*, from which is derived *Journal Citation Reports* (JCR), with data on citations from one journal to another over a period of time. Using JCR one can easily determine, for example, which journals cite *Acta Crystallographica*, and which journals are cited by *Acta Crystallographica*. The use of citation data is not without its problems, however. The absolute number of citations cannot be used as a measure of a journal's influence because of the wide variation in the sizes of journals. Journals publishing a large number of review papers receive more citations than other journals because of the nature of their contents. Garfield's impact factor, which is the ratio of the number of citations a journal receives to the number of papers it publishes, helps to overcome these difficulties somewhat. In the present case, however, the population of crystallographers is considerably smaller than that of chemists or physicists, for example. Crystallographic journals will understandably rank lower in influence among chemists considered as a whole than among crystallographers. Attempts to normalize citations based on memberships in professional societies were unsuccessful; not all publishing scientists are members of a professional society, and many are members of several.

An 'influence' measure was developed by Pinski and Narin to take these factors into account. Their methodology, involving the construction of a 'citation matrix' and an iterative process to find weighting factors has been published elsewhere (Pinski, 1977; Pinski & Narin, 1976; Narin, 1976), and will not be discussed in detail here. Briefly, the citation matrix has as its elements the number of citations each journal makes to the others represented in the matrix. The influence of each journal on the others is therefore taken into account. Size-independent weighting factors for each journal can be derived from the citation matrix. The first approximation to the weighting factors is the ratio of the number of citations *to* the journal to the number of citations *from* the journal, which is simply the ratio of the individual column sums to the row sums of the matrix. Further approximations of the influence per publication are calculated by iteration to find the eigenvalues of the citation matrix. Convergence usually occurs after several iterations.

Pinski and Narin's influence methodology was applied to those journals in Table 6 for which citation data were available in the 1976 JCR. (The 1976 JCR contains data on citations made in 1975.) *Crystal Structure Communications* is a well known crystallographic journal which is not covered by the 1976 JCR. Citation data for this journal were obtained privately from Garfield and included in this study. Adjustments were made to the data to account for journals which have been divided into sections by allocating the citations to the earlier unified journal in the same proportion as the number of citations made to the respective sections. Citations to Soviet journals and their cover-to-cover translations were added together. From these citation data, influence weights for 18 of the 22 journals in Table 6 were calculated and are given on a logarithmic scale in Fig. 3.

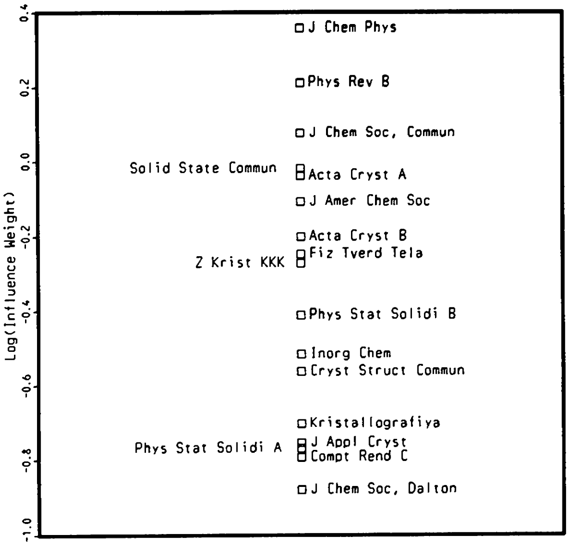

Fig. 3. Influence weights for crystallographic journals. (The value for *Cryst. Lattice Defects*, with a log (influence weight) value of −1·47, is off the scale of the figure.)

If we accept citations as one measure (among several) of the influence and importance of a journal, then citation analysis can provide a basis for ranking the core journals in crystallography. It is of interest to note that the most influential journals on this basis are large, well known and heavily cited, chemistry and physics journals. The 'exclusively' crystallographic journals are somewhat lower in this ranking. These findings agree well with Pinski's (1977) 'influence maps' for chemistry journals. (Pinski assumed crystallography to be part of physical chemistry.) Garfield's (1974) citation results also agree well with this study. The dominant position of *Acta Crystallographica* has not changed in the five years since Garfield's work. The bibliometric data yield a somewhat different ranking of journals in the core than the citation data. This is not unexpected; publication patterns and citation patterns focus on different aspects of the information transfer process. For the same reason, some journals heavily cited by crystallographic journals (*i.e.* those of high influence) rank rather low on the basis of percentage of contents devoted to crystallography.

Citation data can be analyzed in other ways besides the influence method of Pinski and Narin. Hirst (1978) has discussed the 'discipline impact factor' (DIF), which is the number of citations received by a journal from the other journals in the core, divided by the number of citable items published by the journal over a certain time period. The DIF is slightly different from Garfield's impact factor in that it uses citations only from a given core. The DIF's for the 18 core journals having citation data were calculated and are shown on a logarithmic scale in Fig. 4. Large and well known chemistry and physics journals again rank among the most influential journals; however, the two sections of *Acta Crystallographica* rank very high. *Acta Crystallographica* is, without doubt, the most influential crystallographic journal for which citation data are available. We note that the results from the DIF's differ somewhat from the influence values shown in Fig. 3.

The percentage of the citations to core journals and the self-citing rate of each journal are readily available in the JCR, which lists the citations each journal makes and receives, ranked by number, as well as the total number of citations to and from each journal. Many times, but not always, the journal cited most often by a given journal is itself. Table 7 lists the self-citation percentage and percentage of citations to the 18 core journals, along with Garfield's 'impact factor', the ratio of citations received by the journal to the number of citable items published. The average self-citation rate for the 18 core journals is 21%, and about 37% of the total citations, on average, are to other journals in the core. The remaining 63% of the over 258 000 citations are widely dispersed over a large number of journals. Crystallographic journals are not significantly different from other core journals in these respects.

Citation linkages between journals and disciplines are perhaps even more illuminating than the simple influence rankings of Figs. 3 and 4. They show which journals are cited heavily and which are on the periphery of a discipline. Citation maps for several disciplines have been published since the advent of the JCR; a paper which also explains their construction was published recently (Cawkell, 1978) for the field of acoustics.

Fig. 5 is a citation map showing only the links between the five major crystallographic journals in the core. Linkages both to and from each journal are

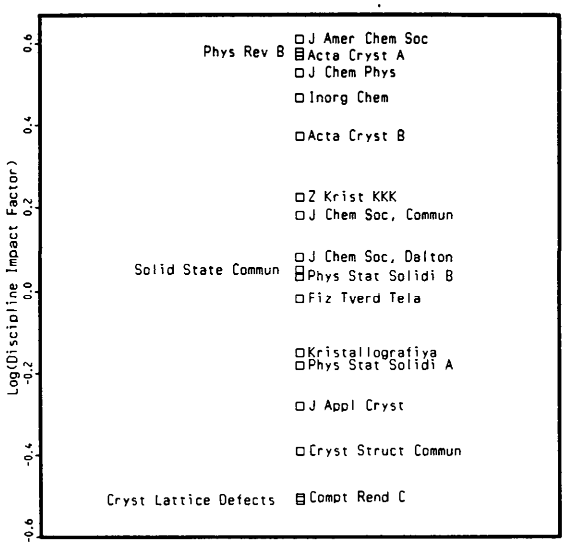

Fig. 4. Discipline impact factors for crystallographic journals.

Table 7. *Journal citation data*

Journal	Self-citation percentage	Core citation percentage*	Impact factor
Acta Cryst. A	21·2	44·4	1·521
Acta Cryst. B	27·2	50·5	1·316
C. R. Acad. Sci. Ser. C	12·2	24·6	0·528
Cryst. Lattice Defects	1·6	27·0	1·133
Cryst. Struct. Commun.	8·1	43·8	0·485
Fiz. Tverd. Tela (Leningrad)	15·8	32·1	0·632
Inorg. Chem.	18·5	49·2	2·347
J. Am. Chem. Soc.	30·0	43·1	4·671
J. Appl. Cryst.	8·1	32·6	1·045
J. Chem. Phys.	33·3	39·1	2·931
J. Chem. Soc. Chem. Commun.	11·9	36·9	2·077
J. Chem. Soc. Dalton Trans.	9·9	43·5	1·924
Kristallografiya	14·4	32·1	0·524
Phys. Rev. B	26·3	34·9	2·710
Phys. Status Solidi A	8·6	23·7	0·763
Phys. Status Solidi B	10·2	38·2	1·116
Solid State Commun.	7·6	32·9	1·903
Z. Kristallogr. KKK	13·3	43·1	0·722
Averages	20·9	37·1	

* Percentage of citations to 18 core journals.

shown, and the strength of each link (*i.e.* the number of citations) is indicated by the thickness of the line joining the two journals. An arrowhead indicates the direction of each link. The two sections of *Acta Crystallographica* are very strongly bound together, and the *Journal of Applied Crystallography* is strongly bound to *Acta Crystallographica A*. The Soviet journal, *Kristallografiya*, is strongly bound to *Acta Crystallographica B*. *Zeitschrift fuer Kristallographie KKK* has only weak links to the other four journals. Interestingly, all of the other four journals cite it, but *Zeitschrift fuer Kristallographie KKK* cites only *Kristallografiya*. This map clearly shows that there are four central crystallographic journals closely linked together: the three journals published by the International Union of Crystallography, and one Soviet journal.

Fig. 6 is a citation map of the linkages between crystallographic journals and the other journals in the core. For clarity, links between the five major crystallographic journals in the core have been omitted, and only one link is shown for each pair of journals (the direction of the link is not indicated). Some of the weaker links not involving crystallographic journals are also omitted. Chemistry journals are shown on the left, physics journals on the upper right, and materials science journals on the lower right. Fig. 6 shows that crystallographic journals are more strongly bound to chemistry journals than to physics journals. *Acta Crystallographica B*, for example, has very strong links to three chemical journals and strong links to two others. In contrast, all links from crystallography to physics are of moderate strength or weaker. *Zeitschrift fuer Kristallographie KKK* has only very weak links to all journals. Fig. 6 therefore confirms Fig. 5 in showing that this journal, while in the core, is less central than the other four journals of Fig. 5.

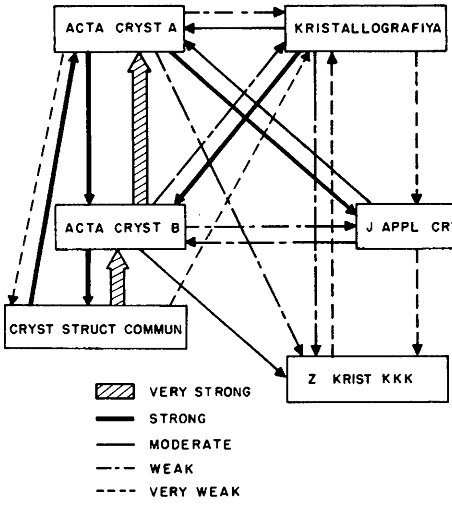

Fig. 5. Citation map for crystallographic journals.

In looking at the citation maps of Figs. 5 and 6, it must be emphasized that they depend on data taken from JCR and are subject to the limitations discussed therein. The reader is referred to pages 1 and 3 of the JCR introduction for a full discussion of the caution which must be used in interpreting citation data. In particular, it must be remembered that Figs. 5 and 6 deal with only a small fraction of all the journals that could have been included (although most of the major journals probably appear).

Finally, we can examine the citation linkages between crystallography and other disciplines in more detail. Each journal (not only those in the core) that cited or was cited by a crystallographic journal was classifed by subject, and the citations were totalled. Each discipline was therefore treated as equivalent to one merged journal. The subject classification was made along commonly used lines, such as those in the introduction to the *Science Citation Index.** A large

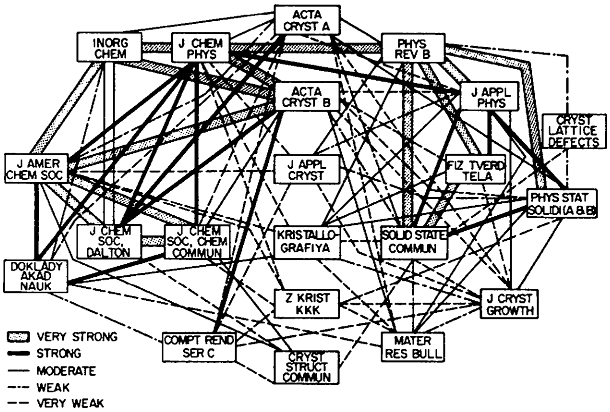

Fig. 6. Citation map for journals in crystallography, chemistry, physics, and materials science.

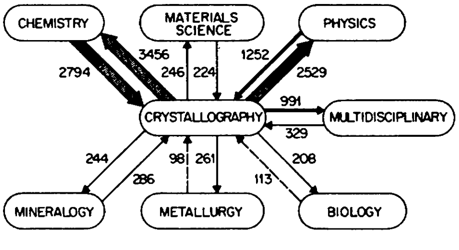

Fig. 7. Citation map for crystallography and other disciplines with the number of citations between these shown.

---

* The only two somewhat arbitrary decisions that were made concerned the *Journal of Physical Chemistry* (JPC) and the *Journal of Chemical Physics* (JCP). JPC, published by the American Chemical Society, was classifed as a chemistry journal, and JCP, published by the American Institute of Physics, was classified as a physics journal.

Table 8. *Strength of linkage between journals in crystallography and other disciplines*

Link to	Strength
Chemistry	Strong
Physics	↓
Multidisciplinary	
Materials science	
{Mineralogy	
Metallurgy}	
Biology	Weak

number of journals with only a few citations each could not be classified because they were not listed separately by JCR, but were combined into an 'all others' category.

Fig. 7 shows the citation linkages between crystallography and six other disciplines. The linkage to multidisciplinary journals, such as *Science* and *Nature*, is also shown. The number of citations associated with each link is also indicated. Table 8 ranks the linkages shown in Fig. 7, from the strongest (to chemistry) to the weakest (to biology). The links to chemistry are about an order of magnitude stronger than those to mineralogy, materials science, metallurgy, and biology, confirming the conclusions of Fig. 6.

Bibliometric and citation data usually do not change rapidly with time; brief checks of available 1978 data show that this is the case with the crystallographic literature.

I am heavily indebted to S. C. Abrahams for his guidance and much helpful advice throughout this study. I also thank Eugene Garfield for reviewing the manuscript, and for providing the citation data for *Crystal Structure Communications*.

References

BRADFORD, S. C. (1948). *Documentation*. London: Crosby Lockwood, Ltd.

BROOKES, B. C. (1968). *J. Doc.* **24**, 247–265.

BROOKES, B. C. (1973). *Libr. Trends*, **22**, 18–43.

CARPENTER, M. P. & NARIN, F. (1973). *J. Am. Soc. Inf. Sci.* **24**, 425–436.

CAWKELL, A. E. (1978). *J. Am. Soc. Inf. Sci.* **29**, 42–46.

Chemical Abstracts (1975). Subject Coverage and Arrangement of Abstracts by Sections. Columbus, Ohio: Chemical Abstracts Service.

GARFIELD, E. (1974). *Current Contents* No. 37, September 11. (Also appears in GARFIELD, E. (1977). *Essays of an Information Scientist*, Vol. 2, pp. 128–133. Philadelphia: Institute for Scientific Information.)

GARFIELD, E. (1976). *Journal Citation Reports*. Philadelphia: Institute for Scientific Information.

HAWKINS, D. T. (1976). *J. Chem. Inf. Comput. Sci.* **16**, 21–23.

HAWKINS, D. T. (1977). *J. Chem. Inf. Comput. Sci.* **17**, 41–45.

HIRST, G. (1978). *J. Am. Soc. Inf. Sci.* **29**, 171–172.

KIEHLMANN, E. (1972). *J. Chem. Doc.* **12**, 157–163.

NARIN, F. (1976). Report PB-252339. Computer Horizons, Inc., Cherry Hill, NJ.

NARIN, F., CARPENTER, M. P. & BERLT, N. (1972). *J. Am. Soc. Inf. Sci.* **23**, 323–331.

PINSKI, G. (1977). *J. Chem. Inf. Comput. Sci.* **17**, 67–74.

PINSKI, G. & NARIN, F. (1976). *Inf. Process. Manage.* **12**, 297–312.

Science Citation Index (1976). Yearly Guide and Journal Lists. Philadelphia: Institute for Scientific Information.

Acta Cryst. (1980). A**36**, 482–490

Anharmonic Temperature Factors of Zinc Selenide Determined by X-ray Diffraction from an Extended-Face Crystal

BY G. J. MCINTYRE,* G. MOSS† AND Z. BARNEA

University of Melbourne, School of Physics, Parkville 3052, *Australia*

(*Received* 29 *January* 1979; *accepted* 11 *December* 1979)

Abstract

Generalized structure factor expressions are derived for the zinc blende structure. Inclusion of dispersion corrections is shown to give rise to the breakdown of Friedel's law for all-even-index reflections, an effect due to the presence of bonding or anharmonicity. X-ray intensity measurements from an extended-face crystal are interpreted within the generalized structure factor formalism to yield the B factors $B_{\rm Zn} = 1{\cdot}020 \pm 0{\cdot}005$ Å^2 and $B_{\rm Se} = 0{\cdot}739 \pm 0{\cdot}008$ Å^2 and an effective cubic anharmonic thermal parameter $\mathscr{B}_{\rm ZnSe} = \beta_{\rm Zn}/\alpha^3_{\rm Zn} -$

---

* Present address: Department of Physics, University of Edinburgh, Edinburgh, Scotland.

† Present address: Chemistry Department, SUNY Buffalo, NY 14214, USA

0567-7394/80/030482-09$01.00