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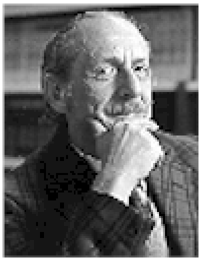

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Journal Citation Studies. 52. The Multifaceted Structure of Crystallography Research. Part 1. Core Journals, High Impact Papers, and Current Research Fronts

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Citation data for crystallography journals indexed in the 1988 *Science Citation Index®* were examined. Strong citation links with chemistry and physics journals were found, but the core journals studied showed little direct connection with the life sciences. *Acta Crystallographica* (Sections A, B, and C), the *Journal of Applied Crystallography*, the *Journal of Crystal Growth*, and *Molecular Crystals and Liquid Crystals* emerged as the leaders on various citation rankings.

I recently had the opportunity to participate in an international conference on "Advanced Methods in X-Ray and Neutron Structure Analysis of Materials." The conference was organized by the Czechoslovak Scientific and Technical Society and was held in Prague, August 20-24, 1990. Jaroslav Fiala, Central Research Institute Skoda, Pilzen, suggested in his invitation that a citation analysis of the crystallography literature would be an appropriate and interesting subject for the meeting. Indeed, previous journal citation studies have yielded interesting insights into various research specialties.[1-6] About 15 years ago, we examined *Acta Crystallographica*,[7] but we had not followed up with an analysis of a larger set of crystallography journals. Fiala's invitation gave us the opportunity to do so.

The presentation has been adapted for this two-part essay. In a sense the essays determine the "structure" of crystallography research from "citation diffraction" patterns in the literature. Part 1 continues our long-running series of journal citation studies and examines 11 crystallography journals indexed in the 1988 *Science Citation Index®* (*SCI®*). They are treated as if they constituted one large "Macrojournal of Crystallography" to determine the journals it cited most often, those it was most frequently cited by, its highest impact articles, and the specialty areas in which it dominates.

Part 2, which follows next week, will present an international perspective on crystallography and will identify leading nations in terms of productivity, citations, and impact in the literature. The overview also presents the highest impact articles from Czechoslovakia, not only in crystallography but in all of science.

It was exciting to be in Prague at a time when Czechoslovakia is undergoing such profound changes in its political, economic, social, and scientific life. Now that Czechoslovakia and other East European countries are free to go their independent ways, they are likely to sponsor even more international conferences as an effective means to renew personal scientific contacts and foster open communication and exchanges.

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4. ------------. Journal citation studies. 49. The diverse yet essential nutrients in the information diet of nutrition researchers. *Current Contents* (28):3-15, 11 July 1988.
5. ------------. Journal citation studies. 50. Part 1. The core journals of economics. Part 2. Most-cited economics papers and current research fronts. *Current Contents* (1):3-11, 2 January 1989; (2):3-8, 9 January 1989.
6. ------------. Journal citation studies. 51. Down to the sea again: probing the depths of marine biology literature. *Current Contents* (19):3-13, 8 May 1989.
7. ------------. Journal citation studies. 13. *Acta Crystallographica. Essays of an information scientist.* Philadelphia: ISI Press, 1977. Vol. 2. p. 128-33.

International Crystallography Research: Where It Is Published, What It Cites, and What Cites It

Back to Introduction

Crystallography: A Multifaceted, Multidisciplinary Field

Crystals have fascinated mankind since antiquity because of their brilliant colors and seemingly perfect geometric shapes. John G. Burke, emeritus professor of the history of science, University of California, Los Angeles, noted that these qualities inspired an ancient belief, which still persists today, that crystals possess magical and medicinal properties.[1] (p. 12) Crystals have apparently been used as tools or in rituals as early as the middle Pleistocene era some one million years ago. Burke traced the more rational examination of crystals as a part of natural philosophy to the Hellenic period, when Plato, Aristotle, and other classical Greek thinkers were developing various theories of matter.

According to Boris K. Vainshtein, Vladimir M. Fridkin, and Vladimir L. Indenbom, Institute of Crystallography, Academy of Sciences of the USSR, Moscow, crystallography emerged as an independent branch of science in the seventeenth and eighteenth centuries.[2] Indeed, the earliest treatise on crystallography was published in 1723 by the Swiss physician Maurice A. Cappeller.[1] (p. 56-7) Entitled *Prodromus crystallographiae, de crystallis improprie sic dictis commentarium*, the publication presented Cappeller's classification of crystals. Vainshtein summarized the major trends in crystallography research and the many scientific fields that benefited from these developments:

> From its very origin crystallography was intimately connected with mineralogy, whose most perfect objects of investigation were crystals. Later, crystallography became associated more closely with chemistry, because it was apparent that [crystal properties depend] directly on the composition of crystals and can only be described on the basis of atomic-molecular concepts. In the 20th century [it] also became more oriented towards physics, which found an ever-increasing number of new optical, electrical, and mechanical phenomena inherent in crystals. Mathematical methods began to be used...particularly the theory of symmetry (which achieved its classical completion in space-group theory at the end of the 19th century) and the calculus of tensors (for crystal physics).[2]

However, crystallography was completely changed—and had greater impact on an even wider range of scientific disciplines—by the development early in this century of X-ray diffraction analysis.[1] (p. 1-3),[2] This technology was discovered in 1912 by Max von Laue, University of Munich, Germany, and won him the 1914 Nobel Prize for physics. Also in 1912 William Henry Bragg, University of Leeds, UK, and his son, William Lawrence Bragg, then a graduate student at the University of Cambridge, UK, extended the application of X-ray diffraction to determine the internal structure of a variety of crystalline materials.[1] (p. 1-3) They shared the 1915 Nobel Prize for physics for this work.

As a result of X-ray diffraction and other techniques for structural analysis, crystallography no longer is focused on the external crystal form or its symmetry. Rather, it now concentrates on the internal atomic and molecular arrangement of crystals, which leads to a new understanding of the relationship between structure and physical, electronic, optical, acoustic, and other properties. In addition to giving birth to solid-state physics, X-ray diffraction and other crystallographic methods have become standard tools in materials science, metallurgy, mineralogy, organic and physical chemistry, molecular biology, quantum and semiconductor electronics, engineering, and allied fields.[2]

In summary, modern crystallography can be defined as the scientific investigation of the structure, growth, and properties of crystals. But, as Vainshtein *et al*. point out, crystallography is more than just the science of crystals: "At the same time, the general approach to the atomic structure of matter and the similarity of the various diffraction techniques make crystallography a science... also of the condensed state in general."[2]

A "Macrojournal" of Crystallography

The 1988 *SCI* listed 15 journals under the crystallography category. Using these as a starting point, we processed over 51,000 cited references in about 3,300 source articles to determine what they cited. This helped us to decide whether any other key journals in the field should be included or, conversely, whether any journals in the initial set should not be included. We also examined over 34,000 citations received by these journals to observe what cited them, for the same purposes. To be included in the final set, a journal had to rank among the 50 publications most cited *by* the *SCI*-categorized crystallography journals or the top 50 most frequently citing these journals.

As a result of this preliminary analysis, 11 *SCI*-indexed journals were selected to make up the crystallography "core" for the purpose of this study. They are listed in Table 1. The editor, publisher, and address are shown for each, as are its inaugural year of publication and 1988 impact factor. The latter is a simple ratio, the result of dividing the number of 1988 citations to a journal's 1987 and 1986 articles by the total number of articles it published in that two-year period. The median impact factor for the

Table 1: Core crystallography journals, 1988 *SCI*®, with their editors, years of origin (in parentheses), publishers, and 1988 impact factors.

Acta Crystallographica Section A: Foundations of Crystallography (1968) C.E. Bugg, ed. International Union of Crystallography Munksgaard International Copenhagen, Denmark	2.09
Acta Crystallographica Section B: Structural Science (1968) C.E. Bugg, ed. International Union of Crystallography Munksgaard International Copenhagen, Denmark	1.42
Acta Crystallographica Section C: Crystal Structure Communications (1972) C.E. Bugg, ed. International Union of Crystallography Munksgaard International Copenhagen, Denmark	0.47
Crystal Research and Technology (1966) H. Neels, ed. Akademie-Verlag Berlin, German Democratic Republic	0.32
Journal of Applied Crystallography (1968) M. Schlenker, ed. International Union of Crystallography Munksgaard International Copenhagen, Denmark	1.38
Journal of Crystal Growth (1967) M. Schieber, ed. Elsevier Amsterdam, The Netherlands	1.88
Journal of Crystallographic and Spectroscopic Research (1971) J.L. Atwood, S.F.A. Kettle, and M.F.C. Ladd, eds. Plenum Press New York, NY	0.42
Kristallografiya (1956) B.K. Vainshtein, ed. Academy of Sciences of the USSR Nauka Moscow, USSR	0.47
Liquid Crystals (1986) G.R. Luckhurst and E.T. Samulski, eds. Taylor & Francis London, United Kingdom	1.69
Molecular Crystals and Liquid Crystals (1966) M.M. Labes, ed. Gordon & Breach London, United Kingdom	0.86
Zeitschrift für Kristallographie (1877) H. Schulz & H.G. von Schnering, eds. R. Oldenbourg Verlag Munich, Federal Republic of Germany	0.78

Table 2: The 50 journals most cited by the core crystallography journals in the 1988 *SCI*®. Asterisks (*) indicate core journals. A=citations from core journals. B=citations from all journals. C=self-citations. D=percent of total citations that are core-journal citations (A/B). E=percent of total citations that are self-citations (self-citing rate, C/B). F=percent of core-journal citations that are self-citations (C/A). G=1988 impact factor. H=1988 immediacy index. I=total 1988 source items.

	A	B	C	D	E	F	G	H	I
*J. Cryst. Growth	2,343	7,018	2,114	33.4	30.1	90.2	1.88	0.36	704
*Acta Crystallogr. A—Found. Crys.	1,666	4,839	705	34.4	14.6	42.3	2.09	0.29	158
*Acta Crystallogr. B—Struct. Sci.	1,472	7,722	311	19.1	4.0	21.1	1.42	0.54	101
*Mol. Cryst. Liquid Cryst.	1,298	4,035	776	32.2	19.2	59.8	0.86	0.20	345
Appl. Phys. Lett.	1,200	28,589	---	4.2	---	---	4.06	0.88	1,627
J. Amer. Chem. Soc.	1,029	122,492	---	0.8	---	---	4.57	0.79	1,878
J. Appl. Phys.	1,025	33,787	---	3.0	---	---	1.75	0.32	2,507
J. Chem. Phys.	971	84,098	---	1.2	---	---	3.59	0.78	1,906
Acta Crystallogr.	965	5,252	---	18.4	---	---	N/A	N/A	N/A
*Acta Crystallogr. C—Cryst. Str.	947	2,493	744	38.0	29.8	78.6	0.47	0.21	893
Jpn. J. Appl. Phys.	713	14,435	---	4.9	---	---	2.23	1.15	1,327
*J. Appl. Cryst.	687	2,514	388	27.3	15.4	56.5	1.38	0.29	157
Phys. Rev. Lett.	661	73,497	---	0.9	---	---	8.21	2.10	1,430
Phys. Rev. B—Condensed Matter	645	68,179	---	1.0	---	---	3.82	0.94	3,508
*Kristallografiya SSSR	554	2,001	393	27.7	19.6	70.9	0.47	0.08	311
Inorg. Chem.	470	28,776	---	1.6	---	---	2.69	0.44	948
J. Electrochem. Soc.	456	13,073	---	3.5	---	---	1.54	0.23	679
J. Phys.—Paris	401	7,826	---	5.1	---	---	0.92	0.21	692
J. Phys. Chem.	371	34,856	---	1.1	---	---	3.14	0.49	1,250
Phys. Rev. A—Gen. Phys.	337	24,388	---	1.4	---	---	2.32	0.47	1,514
*Cryst. Res. Tech.	333	695	206	47.9	29.6	61.9	0.32	0.14	234
*Z. Kristallogr.	312	1,812	119	17.2	6.6	38.1	0.78	0.24	45
Phys. Status Solidi A—Appl. Res.	290	5,264	---	5.5	---	---	0.60	0.10	625
J. Chem. Soc. Chem. Commun.	278	23,515	---	1.2	---	---	2.42	0.38	978
J. Mol. Biol.	278	31,791	---	0.9	---	---	6.56	1.11	368
Macromolecules	275	11,241	---	2.5	---	---	2.40	0.43	580
Nature	274	167,897	---	0.2	---	---	15.76	4.42	1,119
Solid State Commun.	251	15,845	---	1.6	---	---	2.52	0.71	1,086
Phys. Rev.	250	25,842	---	1.0	---	---	N/A	N/A	N/A
J. Phys. Soc. Jpn.	235	10,281	---	2.3	---	---	1.80	0.82	422
J. Vac. Sci. Technol. A	219	4,826	---	4.5	---	---	1.92	0.56	566
J. Chem. Soc. Dalton Trans.	207	10,612	---	2.0	---	---	1.98	0.44	484
J. Org. Chem.	198	35,940	---	0.6	---	---	2.34	0.46	1,260
J. Electron. Mater.	192	949	---	20.2	---	---	1.42	0.38	81
Z. Anorg. Allg. Chem.	176	5,154	---	3.4	---	---	0.81	0.29	246
J. Phys. C—Solid State Phys.	173	11,980	---	1.4	---	---	1.98	0.58	501
Dokl. Akad. Nauk USSR	170	10,557	---	1.6	---	---	0.33	0.05	2,183
Mol. Phys.	170	8,238	---	2.1	---	---	1.96	0.41	252
Acta Metall. Mater.	160	7,912	---	2.0	---	---	1.84	0.43	295
J. Phys. Chem. Solids	160	4,796	---	3.3	---	---	0.92	0.22	215
Z. Naturforsch. Sect. A	159	3,433	---	4.6	---	---	0.90	0.30	181
Fiz. Tverd. Tela SSSR	155	5,553	---	2.8	---	---	0.45	0.08	743
Proc. Roy. Soc. London Ser. A	155	10,342	---	1.5	---	---	1.41	0.45	129
Tetrahedron	151	13,795	---	1.1	---	---	1.76	0.29	720
Amer. Mineral.	148	4,885	---	3.0	---	---	1.63	0.41	159
Inst. Phys. Conf. Ser.	146	1,505	---	9.7	---	---	N/A	N/A	N/A
Tetrahedron Lett.	139	31,910	---	0.4	---	---	2.08	0.36	1,770
Ferroelectrics	138	1,780	---	7.8	---	---	1.62	0.09	439
Chem. Phys. Lett.	137	22,653	---	0.6	---	---	2.29	0.45	1,179
Surface Sci.	135	20,444	---	0.7	---	---	2.92	0.07	646

crystallography core was 0.86, compared to 0.55 for the entire *SCI* file.

The eight publishers are an international group. Four journals are published in Denmark by Munksgaard International for the International Union of Crystallography (IUC). Two each are from the UK—Gordon & Breach and Taylor & Francis. The Federal Republic of Germany, German Democratic Republic, The Netherlands, US, and USSR account for one each.

These core journals will be treated as if they were a single "macrojournal" of crystallography. In 1988 it published 3,173 papers, which represent 0.6 percent of the approximately 500,000 papers covered in the *Journal Citation Reports®* (*JCR®*) section of the *SCI.* The macrojournal also cited 48,332 references, or 0.6 percent of the 8 million references included in the 1988 *JCR.* The average article from a core journal cited 15.4 references, compared to the *JCR* average of 15.9. Also, the core journals received 33,548 citations in 1988, or 0.4 percent of the total.

What the Macrojournal of Crystallography Cited

Table 2 lists the 50 journals that were most cited by the macrojournal in 1988, ranked by citations from the core (column A). Column G shows 1988 impact factors, followed by 1988 immediacy indexes in Column H. Immediacy is the average number of times a journal's 1988 articles were cited in 1988.

Nine core journals are listed, and they are indicated by asterisks. The four journals most-cited by the core are themselves core journals. They received 6,779 citations from the core, or 14.0 percent of all core references. Elsevier's *Journal of Crystal Growth* leads with over 2,300 core citations. However, as can be seen from column F, just over 90 percent of the core citations to this journal were *self*-citations. This would indicate that the *Journal of Crystal Growth* is not strongly connected with the broader crystallography literature since less than 10 percent of the citations it received were from other core journals. A possible reason for this may be that crystal growth research is a small and relatively self-contained specialty.

The next four core journals are the IUC's A, B, and C sections of *Acta Crystallographica* and Gordon & Breach's *Molecular Crystals and Liquid Crystals. Acta Crystallographica,* the parent journal that started in 1948, split into the A and B series in 1968. *Acta Crystallographica C* developed from *Crystal Structure Communications,* which began publication in 1972 and was renamed in 1983. The original *Acta Crystallographica* is *not* counted as a core journal since it no longer exists. It ranks ninth in Table 2 with 965 core citations. As is often the case, this demonstrates the continuing impact of older literature.

Strong Ties to Chemistry and Physics

Most of the noncore journals listed are chemistry and physics journals, such as the *Journal of the American Chemical Society,* the *Journal of Applied Physics,* and the *Journal of Chemical Physics.* Citations from the core typically represent no more than 5 percent of the total they receive per year, which can be seen in column D. That is, the macrojournal of crystallography is selectively citing that fraction of the general chemistry and physics literature that is relevant to its specific interests.

These citations represent a large proportion of the core's total and indicate that crystallographic methods and theories are strongly linked with chemical and physical research. This is to be expected since it is well known that crystallographic techniques are widely applied to analyze the structure and properties of organic and inorganic molecules, compounds, and materials. What is perhaps surprising is the virtual absence of life-sciences journals in Table 2.

Why So Few Signs of Life Sciences?

The *Journal of Molecular Biology* is the only life-sciences publication listed among the 50 journals most cited by the macrojournal of crystallography. It was cited 278 times (0.6 percent of total core citations), which represents just under 1 percent of all citations this journal received in the 1988 *SCI.* Even if the list were extended to the top 100, only four other life-sciences journals would appear: *Biochemistry* (128 core citations), *Biochimica et Biophysica Acta* (104), the *Journal of Biological Chemistry* (86), and the *Journal of Medicinal Chemistry* (65).

The lack of a stronger life-sciences presence is surprising in light of the profound contributions that crystallographic techniques have made to molecular biology, biochemistry, genetics, and other fields. Perhaps the most obvious example is the

1953 discovery of DNA's double-helix structure through X-ray crystallography, for which Francis H.C. Crick, James D. Watson, and Maurice H.F. Wilkins shared the 1962 Nobel Prize for physiology or medicine.[3,4]

The reviewers who refereed this essay suggested that a citation study of crystallography journals would not necessarily reveal a direct and obvious relationship with the life sciences. They noted that these journals are directed at professional crystallographers and focus on reports of improvements in methodology. While the core journals also publish a lot of crystallographic structure studies of interest to chemists and physicists, they very rarely contain reports on structural determinations of biological macromolecules. These latter studies are scattered widely in the life-sciences literature, notably the *Journal of Molecular Biology.*

Noncore Journal Articles Most cited by the Macrojournal of Crystallography

Another way to examine the areas of interest to crystallographers is to identify articles from *non*core journals that were most frequently cited by the macrojournal of crystallography in 1988. These are shown in Table 3 in alphabetic order by first author.

The highest impact article was published in the *Journal of Chemical Physics* by Robert F. Stewart, University of Washington, Seattle, *et al.* in 1965.[5] It is a *Citation Classic*®[6] on X-ray scattering and the hydrogen atom, which was cited 116 times by the core in 1988 and over 8,000 times total. The second-ranked paper is from the same journal and is on a related topic—relativistic calculations for X-ray scattering factors. It was published in 1970 by Don T. Cromer and David Liberman, Los Alamos Scientific Laboratory, New Mexico.[7]

Two are very recent papers on superconductivity. One is a 1986 *Zeitschrift für Physik B—Condensed Matter* article by 1987 Nobel Prize winners Johannes G. Bednorz and Karl A. Müller, IBM Zürich Research Laboratory, Rüschlikon, Switzerland.[8] The other is a 1987 *Physical Review Letters* article by M.K. Wu, University of Alabama, Huntsville, and colleagues.[9] Of the more than 2,700 citations these papers received in 1988, only 49 were from the crystallography core.

Table 3: Articles published in noncore journals cited at least 24 times by core crystallography journals in the 1988 *SCI*®. Articles are listed in alphabetic order by first author. A = 1988 citations from core journals. B = total 1945-1988 *SCI* citations. C = 1989 *SCI* citations. An asterisk (*) indicates the paper was the subject of a *Citation Classic*® commentary. The issue, year, and edition of *Current Contents*® in which the commentary appeared follow the bibliographic reference. *SCI/SSCI*® research-front numbers for 1988 also follow the reference.

A	B	C	Bibliographic Data
25	2,282	851	**Bednorz J G & Müller K A.** Possible high T_c superconductivity in the Ba-La-Cu-O system. *Z. Phys. B—Condens. Matter* 64:189-93, 1986. 88-2172
26	2,098	186	**Bondi A.** van der Waals volumes and radii. *J. Phys. Chem.* 68:441-51, 1964.
24	275	82	**Clark N A & Lagerwall S T.** Submicrosecond bistable electro-optic switching in liquid crystals. *Appl. Phys. Lett.* 36:899-901, 1980. 88-1585
33	867	96	**Cremer D & Pople J A.** A general definition of ring puckering coordinates. *J. Amer. Chem. Soc.* 97:1354-8, 1975. 88-0735
82	4,014	221	**Cromer D T & Liberman D.** Relativistic calculation of anomalous scattering factors for X-rays. *J. Chem. Phys.* 53:1891-8, 1970. 88-0653
43	248	96	**Nardelli M.** PARST: A system of FORTRAN routines for calculating molecular structure parameters from results of crystal structure analyses. *Comput. Chem.* 7:95-8, 1983. 88-7338
116	8,079	249	***Stewart R F, Davidson E R & Simpson W T.** Coherent X-ray scattering for the hydrogen atom in the hydrogen molecule. *J. Chem. Phys.* 42:3175-87, 1965. (48/77) 88-0653
24	2,043	692	**Wu M K, Ashburn J R, Torng C J, Hor P H, Meng R L, Gao L, Huang Z J, Wang Y Q & Chu C W.** Superconductivity at 93 K in a new mixed-phase Y-Ba-Cu-O compound system at ambient pressure. *Phys. Rev. Lett.* 58:908-10, 1987. 88-2172

What Journals Cite Crystallographers

Table 4 lists the 50 journals that most frequently cited the crystallography core in 1988, ranked by citations (column A). All 11 core journals are included, and they account for about 9,800 core citations, or 30.0 percent of citations the core received in 1988.

Once again, the *Journal of Crystal Growth* leads the list. However, of its 2,284 citations to core crystallography journals, about 93 percent were *self*-citations. As stated previously, this indicates that the journal is "self-contained" and not closely linked with the other crystallography journals in this study. Thus, while the journal may be par-

Table 4: The 50 journals that most frequently cited the core crystallography journals in the 1988 *SCI*®. Asterisks (*) indicate core journals. A=citations to core journals. B=citations to all journals. C=self-citations. D=percent of total citations that are core-journal citations (A/B). E=percent of total citations that are self-citations (self-cited rate, C/B). F=percent of core-journal citations that are self-citations (C/A). G=1988 impact factor. H=1988 immediacy index. I=total 1988 source items.

	A	B	C	D	E	F	G	H	I
*J. Cryst. Growth	2,284	11,947	2,114	19.1	17.7	92.6	1.88	0.36	704
*Acta Crystallogr. C—Cryst. Str.	2,164	9,701	744	22.3	7.7	34.3	0.47	0.21	893
*Acta Crystallogr. A—Found. Crys.	950	2,844	705	33.4	24.8	74.2	2.09	0.29	158
*Mol. Cryst. Liquid Cryst.	931	6,801	776	13.7	11.4	83.4	0.86	0.20	345
Inorg. Chem.	736	32,187	---	2.3	---	---	2.69	0.44	948
*Kristallografiya SSSR	712	3,212	393	22.2	12.2	55.2	0.47	0.08	311
J. Amer. Chem. Soc.	665	67,894	---	1.0	---	---	4.57	0.79	1,878
Phys. Rev. B—Condensed Matter	654	88,345	---	0.7	---	---	3.82	0.94	3,508
*Acta Crystallogr. B—Struct. Sci.	632	2,278	311	27.7	13.7	49.2	1.42	0.54	101
J. Appl. Phys.	626	42,777	---	1.5	---	---	1.75	0.32	2,507
*J. Appl. Cryst.	556	2,937	388	18.9	13.2	69.8	1.38	0.29	157
*Liq. Cryst.	511	3,183	80	16.1	2.5	15.7	1.69	0.19	146
J. Sol. State Chem.	502	6,177	---	8.1	---	---	1.21	0.37	313
*Cryst. Res. Tech.	465	2,955	206	15.7	7.0	44.3	0.32	0.14	234
Ferroelectrics	446	6,681	---	6.7	---	---	1.62	0.09	439
Appl. Phys. Lett.	445	19,937	---	2.2	---	---	4.06	0.88	1,627
Jpn. J. Appl. Phys.	412	14,266	---	2.9	---	---	2.23	1.15	1,327
J. Chem. Soc. Dalton Trans.	384	12,571	---	3.1	---	---	1.98	0.44	484
J. Phys. Chem.	373	44,519	---	0.8	---	---	3.14	0.49	1,250
J. Organometal. Chem.	365	26,246	---	1.4	---	---	1.93	0.33	910
Can. J. Chem.	349	14,018	---	2.5	---	---	1.02	0.20	486
Chem. Rev.	315	14,628	---	2.2	---	---	10.40	0.92	64
*Z. Kristallogr.	313	1,270	119	24.7	9.4	38.0	0.78	0.24	45
*J. Cryst. Spectrosc. Res.	309	1,204	68	25.7	5.6	22.0	0.42	0.44	79
Inorg. Chim. Acta	303	11,596	---	2.6	---	---	1.40	0.36	450
Phys. Status Solidi A—Appl. Res.	286	8,857	---	3.2	---	---	0.60	0.10	625
Coord. Chem. Rev.	275	11,414	---	2.4	---	---	3.21	0.69	45
Bull. Chem. Soc. Jpn.	273	16,218	---	1.7	---	---	0.91	0.21	830
Z. Naturforsch. Sect. B	261	5,417	---	4.8	---	---	1.14	0.35	284
J. Mol. Struct.	241	7,959	---	3.0	---	---	0.86	0.10	414
Organometallics	230	17,440	---	1.3	---	---	3.35	0.64	484
Z. Anorg. Allg. Chem.	214	4,279	---	5.0	---	---	0.81	0.29	246
J. Less-Common Metals	211	6,310	---	3.3	---	---	0.80	0.39	375
J. Mol. Biol.	210	17,956	---	1.2	---	---	6.56	1.11	368
J. Phys. C—Solid State Phys.	203	13,685	---	1.5	---	---	1.98	0.58	501
J. Chem. Phys.	202	17,956	---	0.3	---	---	3.59	0.78	1,906
Aust. J. Phys.	198	1,331	---	14.9	---	---	0.61	0.16	70
Solid State Commun.	188	15,929	---	1.2	---	---	2.52	0.71	1,086
Zh. Neorg. Khim. SSSR	185	6,974	---	2.7	---	---	0.26	0.07	718
J. Chem. Soc. Perkin Trans. II	183	9,413	---	1.9	---	---	1.11	0.27	341
Koord. Khim.	180	4,337	---	4.2	---	---	N/A	N/A	N/A
Angew. Chem. Int. Ed.	177	15,837	---	1.1	---	---	5.10	1.30	379
Mater. Res. Bull.	177	2,828	---	6.3	---	---	1.70	0.26	216
Macromolecules	176	16,551	---	1.1	---	---	2.40	0.43	580
Phys. Rev. A—Gen. Phys.	171	35,843	---	0.5	---	---	2.32	0.47	1,514
J. Mater. Sci.	169	12,360	---	1.4	---	---	0.78	0.11	659
J. Org. Chem.	159	39,692	---	0.4	---	---	2.34	0.46	1,260
Synthet. Metal.	149	3,696	---	4.0	---	---	1.99	0.28	216
J. Chem Soc. Chem. Commun.	148	12,506	---	1.2	---	---	2.42	0.38	978
Solid State Ionics	147	6,347	---	2.3	---	---	1.72	0.19	415

Table 5: The most-cited article from each core crystallography journal, 1945-1988 *SCI*®. Core journals that did not publish any article receiving at least 50 citations are excluded. A=1945-1988 citations. B=1989 citations. C=total number of papers from that journal cited at least 50 times. An asterisk (*) indicates that the paper was the subject of a *Citation Classic*® commentary. The issue, year, and edition of *Current Contents*® in which the commentary appeared follow the bibliographic reference. *SCI*® research-front numbers for 1988 also follow the reference.

A	B	C	Bibliographic Data
235	14	130	**Bachmann H G, Ahmed F R & Barnes W H.** The crystal structure of vanadium pentoxide. *Z. Kristallogr.* 115:110-31, 1961. 88-0955
79	8	1	**Boeyens J C A.** The conformation of six-membered rings. *J. Cryst. Mol. Struct.* 8:317-20, 1978. (Superseded title of *J. Cryst. Spectrosc. Res.*)
5,792	316	132	**Cromer D T & Mann J B.** X-ray scattering factors computed from numerical Hartree-Fock wave functions. *Acta Crystallogr. A—Found. Crys.* 24:321-5, 1968. 88-0653
4,112	45	1,119	**Cromer D T & Waber J T.** Scattering factors computed from relativistic Dirac-Slater wave functions. *Acta Crystallogr.* 18:104-9, 1965.
319	22	96	**deGennes P G.** Short range order effects in the isotropic phase of nematics and cholesterics. *Mol. Cryst. Liquid Cryst.* 12:193-214, 1971.
394	91	19	**Gerr R G, Yanovsky A I & Struchkov Yu T.** Improvements to the system of crystallographic programs at the X-Ray Structural Analysis Laboratory of the A.N. Nesmeyanov Institute of Heteroorganic Compounds of the Academy of Sciences of the USSR. *Sov. Phys.--Crystallogr.* 28:609-10, 1983. (Translated from *Kristallografiya SSSR* 28:1029-30, 1983.) 88-0474
260	113	102	**Matthews J W & Blakeslee A E.** Defects in epitaxial multilayers. I. Misfit dislocations. *J. Cryst. Growth* 27:118-25, 1974. 88-0921
1,105	152	72	**Rietveld H M.** A profile refinement method for nuclear and magnetic structures. *J. Appl. Cryst.* 2:65-71, 1969. 88-1410
2,522	136	269	***Shannon R D & Prewitt C T.** Effective ionic radii in oxides and fluorides. *Acta Crystallogr. B—Struct. Sci.* 25:925-46, 1969. (21/81/PC&ES) 88-7969
99	9	3	**Shoemaker C B, Shoemaker D P & Fruchart R.** The structure of a new magnetic phase related to the sigma phase: iron neodymium boride $Nd_2Fe_{14}B$. *Acta Crystallogr. C—Cryst. Str.* 40:1665-8, 1984.
79	4	5	**Voszka R, Tarjan I, Berkes L & Krajsovszky J.** Über die Herstellung besonders reiner Alkalihalogenid-Kristalle (On the production of exceptionally pure alkali halide crystals). *Krist. Tech.* 1:423-30, 1966. (Superseded title of *Cryst. Res. Tech.*)

ticularly influential in crystal growth research, its impact on crystallography as a whole is more limited.

As before, the noncore journals are dominated by chemistry and physics publications. They account for about 11,600 citations, or 35.1 percent of the 33,548 citations received by the core in 1988. Again, the *Journal of Molecular Biology* is the only life-sciences journal listed, with 210 citations to the core in 1988.

Most-Cited Articles from the Macrojournal of Crystallography

To give some indication of the specific topics of research in crystallography, it is useful to look at the titles of key articles in the field. Table 5 presents the most-cited articles from each of the core crystallography journals, in alphabetic order by first author. Total 1945-1988 *SCI* citations are given in column A, followed in column B by 1989 citations. Column C gives the number of articles from each journal that were cited at least 50 times.

Liquid Crystals is the only core journal not listed. It began in 1986, and none of its articles had achieved 50 citations through 1988 in the *SCI. Acta Crystallographica B* has produced the largest number (269), followed by *Acta Crystallographica A* (132). As stated earlier, both were started in 1968 when *Acta Crystallographica* was split.

The most-cited paper from *Acta Crystallographica* is included in the list although the journal is technically not considered a core journal in this study. It has published 1,119 articles cited at least 50 times in the 1945-1988 *SCI. Zeitschrift für Kristallographie*, founded in 1877, has produced 130 high impact articles, and the *Journal of Crystal Growth* (1967) has 102.

The highest impact article is by Cromer and Joseph B. Mann, Los Alamos Scientific Laboratory, published in 1968 in *Acta Crystallographica A.*[10] Cited about 5,800 times through 1988 and 316 times in 1989, it discusses computing X-ray scattering factors from Hartree-Fock wave functions. Another article by Cromer on scattering factors computed from Dirac-Slater wave functions is ranked second with over 4,100 citations. Coauthored with Los Alamos colleague J.T. Waber, it was published in 1965 in *Acta Crystallographica*. Next is a 1969 article on effective ionic radii in oxides and fluorides (over 2,600 citations) by R.D. Shannon and C.T. Prewitt, E.I. du Pont de Nemours & Company, Inc., Wilmington, Delaware.[11,12] The fourth-ranked paper, with 1,257 citations through 1989, is by H.M. Rietveld, Reactor Center of The Netherlands, Petten. It was published in 1969 in the *Journal of Applied Crystallography* and describes "A profile refinement method for nuclear and magnetic structures."[13]

Research Specialties in Crystallography

To get a broader view of recent areas of active research in crystallography, we can identify 1988 *SCI* research fronts that were cited by the core journals. Simply described, a research front is formed by the frequent co-citation of papers. The cited papers are defined as the "core" of the specialty, and the citing papers make up the research front and provide the terms that define the specialty's name.

Table 6 lists 12 1988 *SCI* research fronts in which there were at least 50 articles from the macrojournal of crystallography. The serial number is arbitrarily assigned to identify each research front among the 8,177 discrete research fronts in the 1988 database. Column A gives the number of citing papers published by the crystallography macrojournal, followed by the total number of citing articles in column B, and the number of cited core documents for each research front.

In terms of size, the four areas that attracted the greatest number of crystallography citing papers involved crown ether complexes (#88-6626, 435 papers); X-ray

Table 6: The 1988 *SCI*® /*SSCI*® research fronts that include at least 50 citing documents published in the core crystallography journals. A=number of articles from core crystallography journals citing the core of each front. B=total number of citing documents. C=total number of core documents.

Number	Name	A	B	C
88-0220	X-ray crystal structure, cluster bonding, transition-metal complexes, and nuclear magnetic resonance spectra	162	812	46
88-0483	Langmuir-Blodgett films, liquid crystalline side-chain polymers, optical second-harmonic generation, and monolayers at the air-water interface	72	486	60
88-0653	X-ray crystal structure, spirocyclic polyselenido complexes $[Na\text{-}15\text{-}Crown\text{-}5]_2[M(Se_4)_2]$, and heteronuclear cluster chemistry	256	792	26
88-1281	Semiconductor alloys, organometallic vapor-phase epitaxy, *ab initio* molecular-dynamics calculations, and electronic properties of amorphous silicon	56	207	57
88-1282	Metalorganic vapor-phase epitaxy of GaAs, MOVPE growth, and horizontal CVD reactor	69	198	27
88-1415	Thermotropic liquid crystalline copolyester, poly(etheretherketone) aromatic polymer composite, and reorientational motion model	53	420	52
88-1585	Ferroelectric liquid crystals, spontaneous polarization, low-frequency dielectric response of chiral smectics C*	60	236	35
88-2152	Red extinction model, intermolecular hydrogen bonding, and neutron diffraction data	107	261	19
88-3434	Heteronuclear cluster chemistry, X-ray crystal structure, group-1B metals, trimethylplatinum(IV) complexes, and dynamic behavior	76	355	10
88-4393	Hydrido acetate complexes, X-ray crystal, telluric acid adduct, and $Ph_2PCH_2PPh_2$(dppm) ligands	56	207	3
88-6626	Crown ether complexes of alkaline earth metal ions, barium thiocyanates, and tris(3-ethylpyridinium) decavanadate monohydrate	435	615	6
88-7292	Crystal structure of $ND_4D_2PO_4$, cadmium strontium tetranitrite tetrahydrate, and nucleoside analog 5-nitro-1-β-D-arabinofuranosyluracil	60	130	2

crystal structure of spirocyclic polyselenido and transition-metal complexes (#88-0653 with 256 papers and #88-0220, 162); and the red extinction model (#88-2152, 107 papers).

In terms of proportionate share, the research fronts with the highest concentration of crystallography citing papers are on crown ether complexes (70.7 percent); crystal structure of $ND_4D_2PO_4$ (#88-7292, 46.2 percent); red extinction model (41.0 percent); gallium-arsenide epitaxy (#88-1282, 34.8 percent); and X-ray crystal structure of polyselenido complexes (32.3 percent). Keep in mind that articles from the macro-journal of crystallography represent just 0.5 percent of the 1988 *SCI* database. But these articles constitute from 13 to 71 percent of the research fronts listed here, so the areas depicted are among the most active in the field.

Conclusion

In summary, this examination of 11 *SCI*-indexed crystallography journals indicated strong links with research in chemistry and physics but only weak ties to the life sciences, as indicated by journal citation patterns, high impact articles, and research front specialties. Taking a composite look at the data presented in Tables 2 and 4, as well as at impact factors and immediacy indexes, six core journals occupy an outstanding position—Sections A, B, and C of *Acta Crystallographica*, the *Journal of Applied Crystallography*, the *Journal of Crystal Growth*, and *Molecular Crystals and Liquid Crystals*.

However, it should be recalled that the *Journal of Crystal Growth* showed high self-cited and self-citing rates of 90.2 and 92.6 percent, respectively. While this journal may be influential within the specialty of crystal growth studies, its citation impact on mainstream crystallography is rather restricted.

* * * * *

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