

60 years of IUCr journals

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In the 60 years since its birth in 1948, the number of journals published by the International Union of Crystallography has risen from one to eight. A brief account of the history of the forerunner of the IUCr journals, *Zeitschrift für Kristallographie*, is given. The context of the birth of the IUCr and the first of its journals, *Acta Crystallographica*, is recalled. The circumstances which led to the growth of *Acta* into several sections, at first *A* and *B* then, successively, *C*, *D*, *E* and *F*, and the launch of two new journals, the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation*, are described. The transition from print-on-paper to electronic journals is also remembered.

1. Introduction

The year 2008 saw the 60th anniversary of the establishment of the International Union of Crystallography, brilliantly celebrated during its Twenty-First General Assembly and Congress, which was held in Osaka, Japan, 23–31 August 2008. It saw also the 60th birthday of *Acta Crystallographica*. Until the late 1930s, all major articles on crystallography and X-ray structure determination had been published in *Zeitschrift für Kristallographie*, but the journal lost its international nature at the outbreak of World War II. In 1944, when the end of the war was still uncertain, Paul Ewald gave a lecture full of foresight in Oxford in which he stressed the pressing need for an international journal of crystallography and laid the basis for the International Union of Crystallography (see §3.2).

After many discussions and a preliminary gathering of crystallographers in London in 1946, the establishment of the International Union of Crystallography and the launch of its journal, *Acta Crystallographica*, took place in 1948 (Kamminga, 1989; Cruickshank, 1998). The Union grew very rapidly; the first edition of the *World Directory of Crystallographers*, compiled by W. Parrish in 1957, listed 2240 entries and the third edition, compiled in 1964, had 5037 entries. The directory now numbers over 10 000 entries. At the same time, the number of fields covered by crystallography and its applications, which was already quite large in 1948, as noted by Ewald in his editorial for the first issue of *Acta*, expanded very rapidly. With the development of theory and faster and faster computers, structure determination became an easy task and the number of structures solved grew exponentially, including the number of biologically important substances; new techniques such as synchrotron radiation revolutionized the discipline. The number of papers submitted to the journal grew in the same way. This led to the expansion of *Acta* into a number of journals. First, in 1968, came the split of *Acta* into two sections, *A* and *B*, and the establishment of a new journal, the *Journal of Applied Crystallography*; then came the crea-

tion in 1983 of *Section C*, in 1993 of *Section D*, in 1994 of the *Journal of Synchrotron Radiation* and, more recently, of *Sections E* and *F* in 2001 and 2005, respectively. The fascinating development of the IUCr journals will be described here, starting with the story of *Zeitschrift für Kristallographie*.

2. The forerunner: *Zeitschrift für Kristallographie*2.1. 1824–1877: *Poggendorffs Annalen*

Crystallography developed rapidly in the first half of the 19th century, following the founding works of R.-J. Haüy and Ch. S. Weiss. At that time, the journal in which many of the important crystallographic and crystallography-oriented mineralogical papers were published was the *Annalen der Physik und Chemie*, whether from German authors or authors of other nationalities (Berzelius, Des Cloizeaux, Brewster, Fresnel, Groth and his students, Mitscherlich, Naumann, von Neumann, Sohncke, ...). The Editor of '*Poggendorffs Annalen*', as they were called, was J. C. Poggendorff (1796–1877), who took over after the death of the preceding Editor, L. W. Gilbert, in 1824.

2.2. 1877: Establishment of *Zeitschrift für Kristallographie*

Zeitschrift für Kristallographie was founded in 1877 by Paul Heinrich von Groth (Fig. 1), then Professor of Mineralogy at the University of Strasbourg, as the *Zeitschrift für Kristallographie und Mineralogie*. He started thinking about establishing a crystallography journal in 1875. As Poggendorff was nearing retirement age, Groth feared that his successor would not be so open as to continue including mineralogy and crystallography in the *Annalen der Physik und Chemie*, and they would find themselves without a home. In fact, when Poggendorff's successor, G. Wiedemann, took over the Editorship, the *Annalen*, published in cooperation with the German Physical Society, became more specifically oriented towards physics. Groth's motivations are explained in the

'Prospectus', or announcement, he wrote for the first number of the *Zeitschrift* (January 1877) and in his retrospective paper on the history of the journal, written at the end of his life (Groth, 1928) – see also Kraus (1928a,b) and Steinmetz & Weber (1938). He pointed out that crystallography was the only field for which a dedicated journal did not exist. Of course, if one restricted crystallography to the simple geometric description of the crystal forms, that would be justified and it could not be separated from mineralogy. However, the knowledge of crystal forms and of the physical properties of solids in relation to their chemical composition, namely the theoretical, physical and chemical aspects of crystallography, together with mineralogy, constitute a scientific field in its own right, in the same way as for the neighbouring fields of physics, chemistry and geology. At the time, there were no Chairs of Crystallography and no Institutes of Crystallography, and the number of crystallographers would have been too small to ensure the viability of such a journal, even taking into account the participation of authors from abroad. It was therefore necessary to widen the scope of the field, and the only way to do this was to include mineralogy, inasmuch as it concerned the study of minerals, and not petrology, which belongs to geology. For that reason, Groth included mineralogy in the title. Indeed, at the start, the majority of papers concerned the more mineralogical and geological aspects of crystallography, but after a few relatively thin issues, the journal grew rapidly and attained international fame with seminal crystallographic papers by, among others, Fedorov, Barlow and Sohncke. Groth himself, together with his numerous students from all over the world, contributed



Figure 1
P. von Groth (1843–1927) [after Steinmetz & Weber (1938), reproduced with permission from Oldenbourg Wissenschaftsverlag].

many important crystallographic papers. That the period was timely for launching the *Zeitschrift* is confirmed by the fact that it coincided with the establishment of the British Mineralogical Society in June 1876, with W. H. Miller as President, and that of the *Société Minéralogique de France* in 1878 by A. Des Cloizeaux; the journal published by the latter (*Bulletin de la Société Minéralogique de France*) was regularly abstracted in the *Zeitschrift*.

From the start, Groth wanted to develop an international following for the journal. In order to do so he obtained, as indicated under the title of the journal (Fig. 2), the collaboration of a number of well known foreign crystallographers and mineralogists, for example E. S. Dana in the United States. Each issue contained a large section of notes, letters and abstracts of articles published elsewhere; the abstracts were a very important feature of the journal. Groth wanted them to give a representation as complete as possible of all research in the field of crystallography and mineralogy. Ewald (1944, 1977) recalls that 'the aim was to make the abstracts so informative that for the subscriber to the *Zeitschrift* there was no need to look up the originals in order to find out whether he

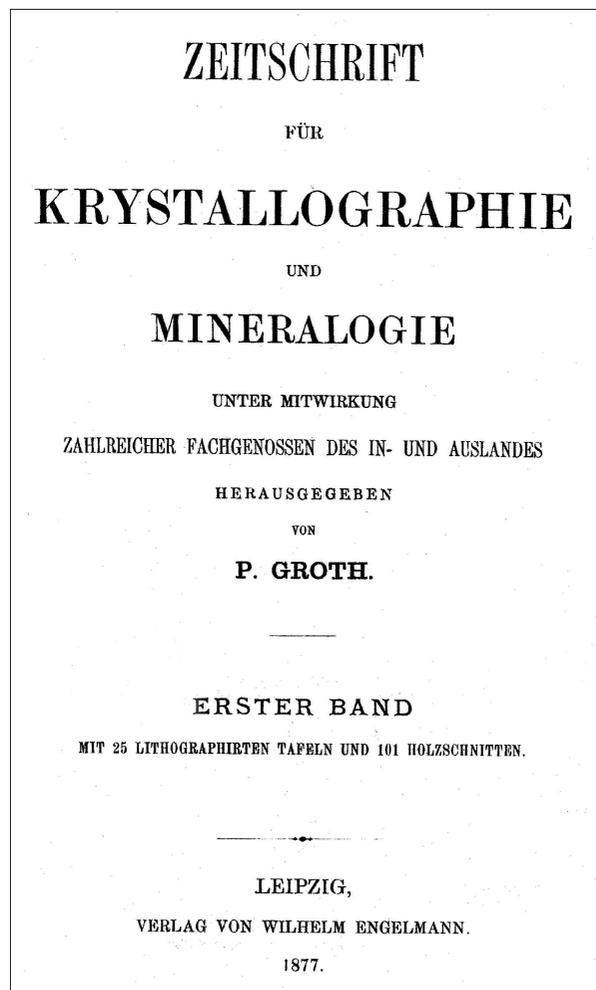


Figure 2
The first issue of *Zeitschrift für Kristallographie*. Reproduced with permission from Oldenbourg Wissenschaftsverlag.

would be interested in the details'. An important point is that Groth asked his assistants, Gossner and Steinmetz, to repeat those measurements that he doubted were correct. This critical aspect of the work added great value to the abstracting and was a precursor of the checking which is now done routinely by the IUCr Editorial Office in Chester.

In 1883, Groth moved to Munich, where he became Director of the Institute of Mineralogy and of the State Collections. He continued to edit the journal until his retirement at the age of 78, publishing 52 volumes as sole Editor and three more with E. Kaiser as Joint Editor. From the material he collected in these 55 volumes of the *Zeitschrift für Kristallographie*, he produced the *Chemische Kristallographie*, which appeared in five volumes between 1906 and 1919, as a complete dictionary of the physical and chemical properties of crystalline substances.

When Groth retired in 1921, he handed over the Editorship to Paul Niggli (1888–1953) in Zürich, who remained Chief Editor until 1940. A new era opened up for crystallography after the discovery of X-ray diffraction in 1912. The number of crystallographic papers increased rapidly and 'Mineralogy' could now be dropped from the title of the journal, which now read *Zeitschrift für Kristallographie (Kristallgeometrie, Kristallphysik, Kristallchemie)*. The first publisher, Wilhelm Engelmann, ceased trading during the period of high inflation in Germany in the 1920s and a new publisher acquired the *Zeitschrift für Kristallographie, Akademische Verlagsgesellschaft*, also in Leipzig.

In 1923, three Co-editors were appointed: Paul Ewald and Max von Laue to cover physical aspects of crystallography and Kasimir Fajans to cover chemical aspects. Niggli continued publishing the abstracts and, when Ewald became Co-editor, he felt that the abstracts should be restricted to papers containing structure determinations. This was the origin of the *Strukturbericht*, of which P. P. Ewald and C. Hermann were the first Editors (1913 to 1928) and which replaced the abstracts. Eight volumes, for the years 1933 to 1939, were published as supplements to the *Zeitschrift für Kristallographie*, thanks to financial aid from the *Notgemeinschaft der Deutschen Wissenschaft* (Ewald, 1944). It was continued as *Structure Reports* when the IUCr was founded in 1948.

2.3. Internationalization of *Zeitschrift für Kristallographie*

Since there was no international journal dedicated to crystallography, many papers submitted to the *Zeitschrift*, especially on structure determinations, came from abroad. At the suggestion of Ewald during a meeting held in Romanshorn on Lake Constance in 1927, it was decided to accept papers in French and English as well as in German, instead of translating them, as Groth had done; 'The unique role the *Zeitschrift* had gained in the pre-X-ray days as the specialized journal of crystallography was preserved by this step' (Ewald, 1962, p. 698). From 1928 onwards, the front page of the journal showed the collaboration of a number of prominent crystallographers from all over the world, such as, among others, the Braggs, G. Friedel, V. M. Goldschmidt, A. Joffé and R. W. G. Wyckoff.

The *Zeitschrift* became a widely recognized international journal of crystallography where the most important results on structure determinations were published, for instance, W. L. Bragg's 1930 paper on the structure of silicates and many others. In 1931 it published the reports of the committees appointed at the Conference of Crystallographers held at the instance of Sir William Bragg at the Royal Institution in London in 1929 to consider (1) a standard scheme for abstracting structural papers, (2) the preparation of tables and (3) nomenclature. The Tables Committee met in Zürich in 1930, at P. Niggli's invitation. There, in a 12-day meeting, the Tables Committee organized the work of the international group of authors who prepared the two volumes of the *Internationale Tabellen zur Bestimmung von Kristallstrukturen (International Tables for the Determination of Crystal Structures)*, edited by C. Hermann and published in 1935 by G. Bornträger, the publisher of Niggli's famous book, *Geometrische Kristallographie des Diskontinuums* (1919). They incorporated the recommendation by the Nomenclature Committee to replace the Schoenflies notation of space groups by Hermann–Mauguin notation.

This international character of the *Zeitschrift* helped the journal to keep a certain freedom in editing during the 1930s, which was often difficult for the other scientific journals in Germany to achieve at that time (Ewald, 1962). The *Zeitschrift* was very successful scientifically, but not financially. The journal was privately owned and the scientific editors had no say on the financial policy. Prices rose steadily due to inflation. As physics and crystallography developed rapidly in the 1930s, the number of volumes also increased and, since the journal was billed per volume and not per year, the cost of subscribing became too high for foreign libraries. The number of subscriptions therefore rose only slightly, and the circulation of the *Zeitschrift* remained limited and was not sufficient to balance the rapid increase in the price of production; this created very important difficulties for the journal in the pre-war days. During the war years, the *Zeitschrift* lost its international following and, in 1940, Paul Niggli wrote several letters to Maurice L. Huggins in the United States (newly elected President of the American Society for X-ray and Electron Diffraction) to express his concern that the *Zeitschrift für Kristallographie* and also the *Strukturbericht* might have to be discontinued. The *Zeitschrift* finally closed down in 1945 (the last issue was No. 1, Volume 106, February 1945) and its publication was only resumed in October 1954 with issue No. 2 of Volume 106, under the Editorship of G. Menzer, M. J. Buerger, F. Laves and I. N. Stranski.

3. Plans for a new crystallography journal – the war years

3.1. United States

In the late 1930s and early 1940s, several groups in the United States gave serious thought to the need for a society that would represent American crystallographers and organize meetings; they also considered the possibility of starting a

new journal just for crystallography. One of these groups, an association of chemists and crystallographers, led to the formation of the American Society for X-ray and Electron Diffraction; another group, of mineralogists and crystallographers from the Boston–Cambridge area in Massachusetts, led to the organization of the Crystallographic Society of America.

3.1.1. American Society for X-ray and Electron Diffraction (ASXRED). The American Society for X-ray and Electron Diffraction was founded in 1941, following discussions between the members of the Committee on Application of X-rays to Chemistry and Chemical Technology and the National Research Council Committee on X-ray and Electron Diffraction (McLachlan, 1983*a*). At the start it had 135 members, Maurice L. Huggins (Eastman Kodak) as President, Bert Warren (MIT) as Vice-President and George Tunell (the Geophysical Laboratory) as Secretary and Treasurer; its first official meeting was held in July 1941, at Gibson Island, Maryland. It then met every year until 1949. The American crystallographers were very conscious of the need for a vehicle for the publication of articles on crystallography (Buerger, 1983). They considered two types of publication, one for monographs and the other an ordinary journal devoted to crystallography. In 1943, when he was President of ASXRED, Martin Buerger appointed a small Monograph Subcommittee consisting of José Donnay, George Tunell and himself. On 16 October 1944, he wrote to Henry Lipson in Cambridge, UK, who was at the time Secretary of the British X-Ray Analysis Group (XRAG), to inform him that American crystallographers were interested in establishing a journal of crys-

tallography and expressing the hope that XRAG would join with the Americans on this project (Buerger, 1983).

3.1.2. Crystallographic Society of America (CSA). The Crystallographic Society of America was organized in the fall of 1939 (Fron del, 1983) by a group of crystallographers and mineralogists who felt ‘*that the future of mineralogy lays in understanding the roles of crystal structures in the properties, genesis and relations between minerals*’ (Buerger, 1983). The President was Martin Buerger (MIT), with Harry Berman (Harvard University) as Vice-President and Clifford Fron del (Harvard University) as Secretary and Treasurer. The Society held several meetings until 1942, when its activities were suspended by World War II. After the war, in March 1946, the Society held a large meeting at Smith College (Northampton, Massachusetts), with William Parrish as Secretary; from then on it assumed a national status. The two societies, ASXRED and CSA, merged on 1 January 1950 to form the American Crystallographic Association.

3.2. United Kingdom: X-Ray Analysis Group (XRAG)

From October 1939 to September 1943, W. L. Bragg, the Director of the Cavendish Laboratory in Cambridge, UK, was President of the Institute of Physics (Phillips, 1979). During the war, he organized several meetings on the applications of X-ray methods to industrial problems. The first two Conferences on X-rays and Industry were held in Cambridge in April 1942 and in April 1943. The success of these conferences led to the establishment of the X-Ray Analysis Group with a membership of about 350 drawn from both universities and industry. The committee of this new group met in July 1943 and elected Lawrence Bragg as Chairman and Henry Lipson as Secretary. The inaugural meeting was held in Manchester in October of that year. From then on, XRAG met biannually. Bragg remained Chairman until 1947, after which he was Vice-Chairman until his death.

At the First Annual Conference of XRAG held in March 1944 in Oxford, P. P. Ewald (Fig. 3), who was then Professor at the University of Belfast in Ireland, gave an important evening lecture in which he made a vibrant plea for an international journal of crystallography edited by an international union of crystallography (Ewald, 1944). First he stressed the rejuvenation of crystallography since the discovery of X-ray diffraction [what he later called (Ewald, 1962) the ‘new crystallography’]. He then deplored the dispersion of the results of crystallographic research among many journals (physical, chemical, physico-chemical, mineralogical *etc.*) and the absence of any learned society devoted solely to the promotion and the knowledge of crystallography. He maintained that the common laws and methods of observation of the various sides of pure and applied crystallography made it a field of science in its own right that ‘*would gain much by being clearly outlined as such and by being provided for by a Crystallographic Society with its own Journal*’. Ewald recalled the experience of the *Zeitschrift für Kristallographie* as the privileged international medium for crystallographic papers before the war, and predicted that the desire for international



Figure 3
P. P. Ewald (1888–1985), the first Editor of *Acta Crystallographica*.

cooperation would soon return after the war. He outlined the following list of what should be, in his view, the aims of a future international union of crystallography:

(a) *Publication*. Structural and other crystallographic papers should be concentrated in a single journal, but a situation such as that of the privately owned *Zeitschrift für Kristallographie* should be avoided. It would be preferable to have a journal owned and edited by an international union of crystallography.

(b) *Archives*. Details of structural or other work not of immediate interest to the general reader should be deposited in archives.

(c) *Abstracts and summaries* of crystallographic work should be published in conjunction with the journal and the archives.

(d) *International Tables*. Ewald noted that the first edition was exhausted and a second edition should be prepared taking into account the experience gained by the various laboratories that used it. The Tables should be prepared by an international committee and owned by the union.

(e) *Analytical Tables of Crystals*. Systems for determining unknown crystalline substances from geometrical, optical and X-ray data were being developed and a scheme of wide applicability should emerge.

(f) *General tasks*. The union should coordinate the research on the structure and properties of solid-state matter; cooperate with the Unions of Physics and Chemistry; make recommendations in matters of instruction and of planning of research; and act as a juridical person in matters requiring handling of money.

In the last part of his talk, Ewald discussed the use of the term 'crystallography', noting that the British and American societies that had recently been founded had avoided it and had adopted titles that stressed instead the method of observation. He suggested that this implied a restriction which need not be. 'Crystallography' in its original meaning did not include all the applications of the diffraction methods but, nevertheless, it covered the entire field. Ewald noted that it should include the less perfect crystals that depart from the perfect regularity of 'old-time' crystals. He also suggested that it might be preferable to use the expression 'leptology' coined by the German crystallographer Friedrich Rinne (1917) of the Mineralogy Institute in Leipzig after the Greek *λεπτός*, meaning small, fine, thin, slight. Rinne used the term *Leptonenkunde*, literally the science of leptons, or *Feinbaulehre*, to designate the science of the inner structure of crystals. The term, however, was not generally adopted. In fact, Ewald was later happy this term was not chosen since it actually means 'talking winding stuff' (Ewald, 1977). According to Webster's Revised Unabridged Dictionary (copyright 1996, 1998 MICRA, Inc.), it describes a 'tedious discourse on trifling matters'. (Of course, 'lepton' now represents a fundamental particle, a term coined in 1948 by L. Rosenfeld.) In his talk, Ewald showed tremendous foresight and it is quite remarkable how closely the International Union of Crystallography turned out to fit Ewald's original ideas.

Following Ewald's lecture in March 1944 and Martin Buerger's letter to him of 16 October 1944, the Secretary of XRAG, Henry Lipson, called a meeting of that group on 18 November 1944 to consider the formation of an international union of crystallography and the possibility of publishing a journal. A Publications Subcommittee was set up, which first met on April 1945 (for details, see Kamminga, 1989).

At the Second Annual Conference of the X-Ray Analysis Group, held on 12–13 April 1945 at the Royal Institution in London, Sir Lawrence Bragg reported on the discussions of the Publications Subcommittee (Parker *et al.*, 1945). The Subcommittee concluded that there were enough papers written by British crystallographers to fill a quarterly journal and was of the opinion that the scope of the journal should be the structure of matter, rather than the methods used. It suggested that it might be possible to cooperate with the American Society for X-ray and Electron Diffraction, which was discussing a similar project. Cooperation with workers on the European continent was also under consideration. The conference authorized the Subcommittee to continue with the project. At the July 1945 XRAG Committee meeting, it was decided to take advantage of the summer 1946 meeting of XRAG to hold international discussions. W. A. Wooster reported to XRAG the content of discussions he had had in Moscow with A. V. Shubnikov, Director of the Institute of Crystallography of the USSR Academy of Sciences (Kamminga, 1989). The crystallographers there were also considering an international journal to replace the *Zeitschrift* and had several possibilities in mind, including a journal published in triplicate, in Russian, English and French.

In October 1945, F. A. Bannister, who had replaced H. Lipson as Secretary of XRAG, wrote on behalf of XRAG to A. V. Shubnikov in the USSR and to J. D. H. Donnay (ASXRED) in the USA proposing to hold an international conference in London in July 1946. There was also correspondence between W. L. Bragg and a number of eminent crystallographers in different countries: P. P. Ewald, Ch. Mauguin and J. Wyart in France, J. A. A. Ketelaar in The Netherlands, A. Westgren in Sweden *etc.* The XRAG Publications Subcommittee held several further meetings, in December 1945, January 1946 and May 1946, to crystallize the plans for the July conference. The Institute of Physics strongly favoured an international journal based in London and the Publications Subcommittee finally resolved in its January 1946 meeting to propose a single international journal, the centre of publication of which should be in the UK or the USA. This was communicated to Donnay in the USA and Shubnikov in the USSR, as well as to the prominent crystallographers in Belgium, France, The Netherlands, South Africa, Switzerland and Sweden.

4. The 1946 XRAG meeting in London (*X-ray Analysis during the War Years*). Foundation of *Acta Crystallographica*

A lively and detailed account of the conference is given by McLachlan (1983b). It took place at the Royal Institution in

London on 9, 10 and 11 July 1946. There were 330 participants, out of which 68 were from abroad. The American delegation was led by D. Harker, President of ASXRED, and M. J. Buerger, President of the CSA. The Russian delegation arrived late but did attend meetings that took place later in Cambridge. M. von Laue, who was at the time interned at Madingley, near Cambridge, England, was allowed to attend the conference. The talks were essentially devoted to accounts of the work done during the war in the various countries.

The delegates to the conference agreed to form a Provisional International Crystallographic Committee which met at Brown's Hotel on 12 and 13 July. Sir Lawrence Bragg was Chair on the first day and David Harker was Chair on the second. Robert C. Evans acted as Secretary. Bragg, Bannister and the XRAG Publications Subcommittee had prepared a provisional agenda which was distributed to the participants. Regarding the journal, the agenda included: (a) Scope of the journal; (b) Title of the journal; (c) Location of the centre of publications; (d) Financial responsibility; (e) Editorial arrangements *etc.*

The scope of the journal was discussed along the basis of proposals submitted by J. D. Bernal. Concerning the title of the journal, Bragg had thought of something like *Atomic Architecture*, Ewald proposed, as we have seen, *Journal of Leptology* and W. T. Astbury proposed *Journal of Structure Analysis*. After a vote by the Committee members, the name *Structural Crystallography* was favoured. Eventually, the name *Acta Crystallographica* was chosen, at Shubnikov's insistence (Belov & Vainshtein, 1970). Bragg then suggested that there should be some organization to assume responsibility for the journal and unanimous agreement was reached in favour of forming a separate union of crystallography on the same level as the other Unions, such as those of Physics and Chemistry, and Bragg was asked to explore that possibility further.

As a result of the meeting of the Provisional Committee, three subcommittees were formed:

(a) A *Journals Subcommittee* composed of Bragg, Buerger, Harker, Ketelaar, Shubnikov (Fig. 4), Taylor and Wyart, with Ewald as Chairman and Evans as Secretary, which would serve

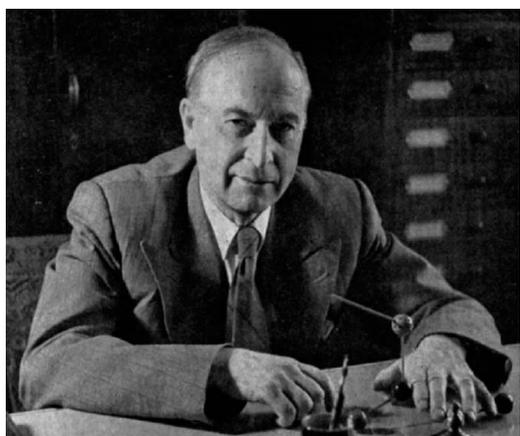


Figure 4
A. V. Shubnikov (1887–1970).

as a provisional Executive Committee. The Subcommittee met on 17 July at the Cavendish Laboratory in Cambridge. By that time the Russian crystallographers had arrived and the name *Acta Crystallographica* was adopted for the journal. It was decided to have an Advisory Board composed of W. L. Bragg, V. M. Goldschmidt, A. Joffé, M. von Laue, C. Mauguin, P. Niggli and R. W. G. Wyckoff, and to invite P. P. Ewald to be the Editor and R. C. Evans, I. Fankuchen, A. V. Shubnikov and J. Wyart to be Co-editors. It was agreed that papers could be published in English, French, German and Russian, with all abstracts in English.

The Subcommittee also had the task of looking into the possibility of founding an international union. The International Union of Pure and Applied Physics (IUPAP) was not happy with this idea and Ewald (1977) reports that his loyalties were divided, since he was at the time the General Secretary of IUPAP. However, since the interests of the crystallographers were as close to chemistry and mineralogy as to physics, it was decided to form an independent union. Bragg had asked F. M. Stratton, an astronomer in Cambridge, who was at the time the Secretary of the International Council of Scientific Unions (ICSU), to attend the meeting in Cambridge. Stratton was very much in favour of the idea and ultimately helped to get the case for a union of crystallography successfully through ICSU. The established Unions had the feeling that they were there to tie together wide fields of science and that more restricted domains should not be permitted to create a Union. Stratton's view that the smaller Unions were more active and more tightly knit carried the decision and the IUCr really owes its existence to him. He also helped the Subcommittee draw up the draft Statutes and By-Laws of the proposed union of crystallography – see P. P. Ewald's biographical note (Ewald, 1961), written after Stratton's death in 1960.

(b) A *Strukturbericht Subcommittee* consisting of Bernal, Wyckoff and Wyart, with Ewald as Secretary. This committee decided to continue the *Strukturbericht* as *Structure Reports*. A. J. C. Wilson undertook the organization of *Structure Reports* and edited the first ten volumes.

(c) An *International Tables Subcommittee* consisting of Hermann, Nowacki, Patterson, Robertson and Wyart, with Kathleen Lonsdale as President and Martin Buerger as Secretary.

5. 1947: Admission of the International Union of Crystallography into ICSU

On 31 March 1947, the Provisional International Crystallographic Committee approved the Statutes and By-Laws drafted by the Journals Subcommittee and, on 7 April 1947, the IUCr was formally admitted to ICSU (Evans, 1983). The draft Statutes and By-Laws were published in the second (May) issue of *Acta Crystallographica* [*Acta Cryst.* (1948), **1**, 93–95] and their final version, as adopted by the First General Assembly, were published in the November issue [*Acta Cryst.* (1948), **1**, 275–276].

The IUCr's admission into ICSU was of particular importance for the journal, since it helped ensure financial support by UNESCO for the activities of the Union. This support was vital during the early years of the existence of *Acta Crystallographica*.

6. 1946–1948: Preparations for the journal

The Journals Subcommittee asked Ewald and Evans (Fig. 5) to find a suitable printer and publisher (Ewald, 1977, 1983). Together, Ewald and Evans prepared a crystallographic text and contacted several printing establishments in France, England, Sweden, Denmark, The Netherlands and Austria, and also the American Institute of Physics. They got prices and specimen settings from seven. The most attractive were from Cambridge University Press (CUP) and the American Institute of Physics. CUP was finally chosen for the printing and distribution of *Acta*, with the American Institute of Physics being responsible for the distribution and collection of subscriptions in North America. Ewald (1977) recalls that when the decision was taken by the Journals Subcommittee to have an international journal, the American delegates insisted that American spelling should be used for American papers. This raised some problems with CUP when they were chosen for the production of the journal! It was finally agreed that the compositors at CUP would not change spellings in the manuscripts and that the responsibility for the spelling would rest with the Technical Editor of the journal. Evans decided on the typeface and specified the design and colour of the cover, which remained the same until 1968. He also assumed the role of Technical Editor. Evans was at the time Lecturer in the Department of Mineralogy and Petrology at Cambridge and attached to the Crystallography Laboratory of the Cavendish Laboratory. His office was across the street from the offices of CUP; it was therefore easy for him to stay in close touch with



Figure 5
R. C. Evans (1909–2005) and J. M. Bijvoet (1892–1980), respectively Secretary and President of the IUCr, at the Third General Assembly and Congress in Paris in 1954. Courtesy A. Jeanne-Michaud, IMPMC, Paris.

them. According to Ewald, '*he was a very accurate proof reader and there are hardly any misprints in the first Volumes of Acta*'.

7. 1948: The First General Assembly

On 15 July 1947, Elizabeth Wood, Secretary of the American Society for X-Ray and Electron Diffraction, and William Parrish, Secretary of the Crystallographic Society of America, wrote to R. C. Evans inviting the International Union of Crystallography to hold its first international conference in the United States in the summer of 1948 (Evans, 1983). The provisional Executive Committee gladly accepted the invitation and, in October, Evans received an invitation from J. B. Conant, President of Harvard University, to hold the Union's first meeting at that University from Wednesday 28 July to Tuesday 3 August 1948. The Congress was organized by a local committee under C. Frondel and a programme committee under B. E. Warren of MIT. Details of the meeting can be found in Evans (1983). The total number of participants was 310, of which 265 were from the USA, 20 were from the UK, 14 were from Canada and lesser numbers were from Belgium, France, Germany, Italy, The Netherlands, Spain, Sweden and Switzerland. Max von Laue gave a memorable after-dinner speech describing the history of the discovery of X-ray diffraction (Laue, 1983) and P. P. Ewald spoke of his life as a student in Munich during the first decade of the 20th century. The titles of the papers presented are given in *Acta Cryst.* (1948), **1**, 342–343.

Three sessions of the General Assembly were held during the Conference [*Acta Cryst.* (1948), **1**, 340–342]. Ewald (1977) recalls that at the First General Assembly where the Statutes and By-Laws were to be adopted there was some uncertainty as to '*who is going to vote?*' (from the floor): '*you, the Assembly* (Ewald) – '*by what authority?*' (from the floor). Thanks to Evans, the matter was sorted out and the Statutes and By-Laws were adopted. W. L. Bragg was elected the first President, M. von Laue was elected Honorary President, A. R. Westgren and R. W. G. Wyckoff were elected Vice-Presidents, R. C. Evans was elected General Secretary and Treasurer, and M. J. Buerger, A. L. Patterson and J. Wyart were ordinary members. The editorial and other arrangements for *Acta Crystallographica* were confirmed, with Ewald as Editor, Evans as Technical Editor and Evans, I. Fankuchen and J. Wyart as Co-editors. Ewald remained as Editor until 1960.

Six commissions were established: *Acta Crystallographica*, chaired by Ewald; *Structure Reports*, chaired by A. J. C. Wilson (Fig. 6); *International Tables*, chaired by Kathleen Lonsdale; *Crystallographic Data*, chaired by F. W. Matthews; *Crystallographic Apparatus*, chaired by I. Fankuchen; and *Crystallographic Nomenclature*, to be nominated by the Adhering Bodies.

The *Commission on Structure Reports* decided that the *Reports* should be divided into three sections: Inorganic Materials (with J. M. Bijvoet as Sub-editor), Metals and Alloys (with C. S. Barrett as Sub-editor), and Organic Structures

(with J. M. Robertson as Sub-editor), A. J. C. Wilson being the first General Editor. *Structure Reports* for 1947–1948 were published in 1951 by N. V. A. Oosthoek in The Netherlands. *Structure Reports* for the years 1945–1946, 1942–1944 and 1940–1941 were published in 1953, 1955 and 1956, respectively. Since A. J. C. Wilson replaced Ewald as Editor of *Acta* on 1 January 1960, the successive Editors of *Structure Reports* have been W. B. Pearson (1960–1972), J. Trotter (1972–1981) and G. Ferguson (1981–1993), all of them from Canada. *Structure Reports* were published for organic compounds up to 1985 and for inorganic materials and metals up to 1990 inclusive, at which point data and manuscripts were starting to be submitted as Crystallographic Information Files (CIFs) (see §10). The Commission was disbanded in 1993.

The *Commission on International Tables* proposed that the *Tables* would be issued in three volumes: Vol. I, *Theory of Crystallographic Groups*, with N. F. M. Henry as Editor; Vol. II, *Mathematical Tables not subject to revision*, with A. L. Patterson as Editor; and Vol. III, *Physical and Crystallographical Tables subject to periodic revision*, with C. H. MacGillivray as Editor. Volume I was published in October 1952 by Kynoch Press, Birmingham, England; Volume II was published at the end of 1959 and Volume III was published in June 1962. A Volume IV, *Revised and Supplementary Tables to Volumes II and III*, was published in October 1974, edited by J. A. Ibers and W. C. Hamilton. At the Sixth General Assembly held in Rome in 1963, N. F. M. Henry succeeded Dame Kathleen Lonsdale as Chairman of the Commission and General Editor. It was then decided to consider the possibility of a new edition of the *International Tables*. In meetings held in Marburg in January 1965 and in Aachen in January 1966 and April 1967, plans for a pilot edition were discussed. Two series were considered: Series A (*Symmetry Tables*) and Series B (*Diffraction Tables*). At the Ninth General Assembly, held in Kyoto in 1972, Th. Hahn succeeded N. F. M. Henry as Editor. Several parts of the pilot project were distributed to



Figure 6
A. J. C. Wilson (1914–1995) at the Third General Assembly and Congress in Paris in 1954. Courtesy A. Jeanne-Michaud, IMPMC, Paris.

the participating laboratories in 1969, 1972 and 1973, and the proposals for the new series were finalized at a meeting in Grenoble in September 1972. The final production of the various volumes took time and the plan for the series changed over the years as the new volumes were planned. Volume A, *Space-Group Symmetry*, Editor Th. Hahn, was published in 1983 and its Teaching Edition was published in 1985; Volume A1, *Symmetry Relations between Space Groups*, Editors H. Wondratschek and U. Müller, was published in 2004; Volume B, *Reciprocal Space*, Editor U. Shmueli, was published in 1993; Volume C, *Mathematical, Physical and Chemical Tables*, Editor A. J. C. Wilson, was published in 1992; Volume D, *Physical Properties of Crystals*, Editor A. Authier, was published in 2003; Volume E, *Subperiodic Groups*, Editors V. Kopský and D. B. Litvin, was published in 2002; Volume F, *Crystallography of Biological Macromolecules*, Editors M. G. Rossmann and E. Arnold, was published in 2001; and Volume G, *Definition and Exchange of Crystallographic Data*, Editors S. R. Hall and B. McMahon, was published in 2005. The eight volumes were made available online in 2006. H. Fues replaced Th. Hahn as General Editor in 2005.

8. 1948–1968: A single journal

The first issue of *Acta Crystallographica* is dated March 1948; it had 48 pages and contained an editorial preface by Ewald, six full papers and three short communications. In his editorial, Ewald begins by listing recent major developments achieved with X-ray diffraction and giving examples of new areas of research opening up in the field. He then states the goal of *Acta Crystallographica*: ‘[It] is intended to offer a central place for publication and discussion of all research in this vast and ever-expanding field. It borders, naturally, on pure physics, chemistry, biology, mineralogy, technology and also on mathematics, but is distinguished by being concerned with the methods and results of investigating the arrangement of atoms in matter, particularly when that arrangement has regular features. . . . *Acta*, in trying to reassemble the crystallographic work now scattered through a great variety of journals . . . should fulfil an important function in the general mechanism of scientific publication’. *Acta Crystallographica* has indeed fulfilled this centripetal role remarkably well and has become the vehicle *par excellence* for publishing crystallographic papers. However, it is striking that, maybe as a victim of its own success, a mere 20 years after its launch it started to be subjected to the same centrifugal forces as the whole field of crystallography, at first splitting up into *Sections A* and *B* and the *Journal of Applied Crystallography*, later with the successive creation of *Sections C* and *D* and the *Journal of Synchrotron Radiation*, more recently with *Sections E* and *F*.

The launch of *Acta Crystallographica* could not have taken place without considerable financial help. As stated above, the admission of the IUCr into ICSU played a crucial role in this respect. The support from UNESCO encouraged support from private enterprises, mainly from sources in Great Britain and the United States. The audited accounts of *Acta* for 1947, the year before the launch, show a subvention of GBP 654

Table 1No. of pages published in *Acta Crystallographica*.

Year	No. of pages
1948	348
1949	425
1950	490
1951	583
1952	869
1953	888

from UNESCO and support from British sources up to GBP 1936; for 1948, the subvention from UNESCO was GBP 656, that from British sources was GBP 1642 and that from American sources was GBP 420, to be compared with a total income of GBP 2957 from subscriptions and trade [*Acta Cryst.* (1949), **2**, 195]. Lists of private donors are given in *Acta Cryst.* (1948), **1**, 45 and 340. The support from UNESCO continued through 1949, up to GBP 1323, as well as support from American sources, for an amount of GBP 166. There was no outside support to the *Acta* account in 1950.

The journal was an immediate success and the number of submitted papers increased steadily, as did the number of printed pages per year, as shown in Table 1. From 1 January 1953, *Acta* was published monthly, and it remained so until 1968 when it was split into *Sections A* and *B* and the *Journal of Applied Crystallography*.

This increase became, however, a cause for concern when the number of sheets grudgingly granted by Cambridge University Press became insufficient and a new printer had to be found. After the Second General Assembly of the IUCr, which took place in Stockholm, Sweden, from 27 June to 3 July 1951, Ewald visited Copenhagen, where he had discussions with Ejnar Munksgaard to find out whether his firm would be

willing and in a position to take over the production of *Acta* (Ewald, 1977). This is indeed what happened, starting with Volume 4 (1952).

The success of *Acta* was the source of another kind of difficulty. The increasing number of pages entailed an increase in expenditure and *Acta* was published at a loss. This, in turn, endangered the finances of the Union. The subscription rate, which had started at USD 10, was increased to USD 15 in 1952 and to USD 25 in 1953. Outside help, from UNESCO and private sources, had to be found. J. M. Bijvoet (Fig. 5), who had been elected President at the Second General Assembly in Stockholm, wanted to change publisher again, to Oosthoek in Utrecht, The Netherlands, which was already publishing the *Structure Reports* and had offered to publish *Acta* more cheaply. Evans, as Technical Editor, and Ewald, as General Editor, strongly resented this because they did not want to go through another change of publisher, and they threatened to resign. This situation brought about a serious crisis in the Union (Kamminga, 1989), which was finally solved in 1955 when R. W. G. Wyckoff, elected President at the Third General Assembly held in Paris in 1954, decided that any change of publisher should be delayed. In order to bring in some money, *Acta Crystallographica* carried advertisements from 1955.

R. C. Evans remained Technical Editor until March 1958, when he was replaced by R. W. Asmussen, Professor at the Technical University of Denmark in Copenhagen. The workload had, however, become so great that it required a professional Technical Editor. S. A. Bryant, who had studied crystallography in Oxford, was appointed in 1962, starting his work on 15 November. Before that, he had been working as Senior Technical Editor at the Shell Thornton Research Centre. For a long time the sole full-time employee of the Union, he worked at first from his home in Chester; this is how the Union's Offices happen to be located in Chester. After his retirement at the end of 1975, he was succeeded by D. W. Penfold (1976–1985), who was then Assistant Technical Editor. M. H. Dacombe, who was appointed Editorial Assistant from 1 October 1975, replaced D. W. Penfold as Technical Editor from 1985 to 1993, when he was appointed Executive Secretary following J. N. King's death. The Editorial Office was reorganized and P. Strickland became Managing Editor.

P. P. Ewald was General Editor until the end of 1959. The successive Editors since then have been A. J. C. Wilson (1960–1978), S. C. Abrahams (1978–1987), C. E. Bugg (1987–1996), J. R. Helliwell (1996–2005) and G. Kostorz (2005–).

Looking back now at some of the editorial problems which arose in the early days, one is tempted to smile. For instance, in 1957, the Commission on *Acta Crystallographica* worried about the 'increasing number of manuscripts dealing with computational methods. [...] The technical language is usually forbidding. Discussion of rules of acceptance of such papers is still actively going on' [*Acta Cryst.* (1958), **11**, p. 567]. A decision was finally taken during the Fifth General Assembly held in 1960 in Cambridge, UK, by sorting computing papers into two classes: brief descriptions of programs and papers giving new computing methods for a

**Figure 7**

J. Wyart (1902–1992), Alice Bragg and W. L. Bragg (1890–1971) at the Third General Assembly and Congress in Paris in 1954. Courtesy A. Jeanne-Michaud, IMPMC, Paris.

general class of computers. At the same General Assembly, it was decided to set up a Commission on Crystallographic Computing.

The Third General Assembly and Congress of the IUCr was the first one I attended. I was at the time a student at the Laboratoire de Minéralogie–Cristallographie of Paris University, in the old and memorable Sorbonne. Our laboratory organized the Congress, under the direction of Jean Wyart (Fig. 7). My own minute contribution to the organization was to head a small group of interpreters. This gave me the unique opportunity of approaching the pioneers of our field. Many are the crystallographers with whom I started then a friendship which has lasted ever since: Paul Ewald, Bert Warren, Theo Hahn, Andrew Lang, Nikolay Belov and many more.

9. 1968: *Acta Crystallographica* is split up into Sections A and B; the *Journal of Applied Crystallography* is established

The desirability of having a journal of applied crystallography was first discussed in 1963 and a committee of three, W. Parrish (Chair), H. P. Rooksby and A. J. C. Wilson, was appointed by the Executive Committee to study this possibility. The committee reported at the Sixth General Assembly held in 1963 in Rome that there was indeed a need for such a journal and made some specific proposals about the scope of the journal and its editorial policy. A further committee was designated to analyse these proposals. Some of the members of this committee had mixed feelings about the idea. They

were of the opinion that most of the papers that were intended to go into a journal of applied crystallography would fit in the present *Acta Crystallographica* and also feared that, after the split, *Acta* would consist essentially of structure papers. Besides, it was not certain that the financial situation was sound enough. After further discussion in the General Assembly, it was nevertheless decided to proceed with the plans for the new journal. Unfortunately, W. Parrish informed the Executive Committee in 1965 that he was unable to continue. The matter arose again at the Seventh General Assembly held in Moscow in 1966. The number of pages published per year in *Acta* had risen above 2000 (Fig. 8) with a very large proportion of structural papers. The Editor of the journal, A. J. C. Wilson, reported that the Commission on *Acta Crystallographica* felt that there was a need for a journal of applied crystallography but was not very keen on the idea of a journal on crystal physics, which had also been suggested. During the General Assembly, Professor A. Guinier (Fig. 9) was asked whether he would be willing to serve as Editor of a journal of applied crystallography, should such a journal be launched, which he agreed to. The Executive Committee set up a Publications Subcommittee to consider the publication policy of the Union with the newly elected Treasurer, D. W. J. Cruickshank, as convener and J. M. Cowley, A. Guinier and A. J. C. Wilson as members (this was an ancestor of the present Finance Committee of the Union, which was established in 1981). After several discussions and consultations, the Subcommittee suggested in June 1967 that *Acta Crystallographica* should be split into two sections, A and B, and that the *Journal of Applied Crystallography* should be launched (Cruickshank, 1998). *Section A* was devoted to crystal physics, diffraction, and theoretical and general crystallography, published as one volume, six parts per year, and *Section B* was devoted to structural crystallography and crystal chemistry,

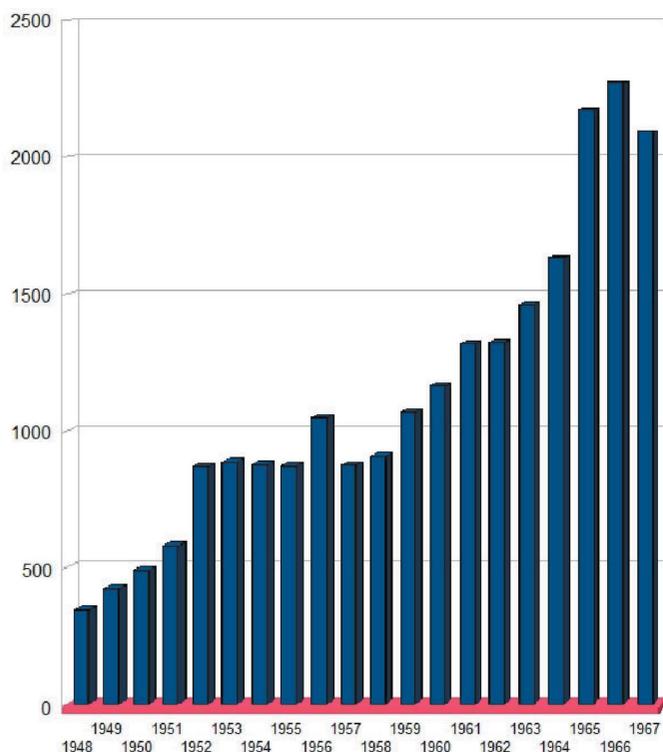


Figure 8
No. of pages published per year in *Acta Crystallographica*, 1948–1967.



Figure 9
A. Guinier (1911–2000), the first Editor of the *Journal of Applied Crystallography*.

published as one volume, twelve parts per year. *Sections A* and *B* started in January 1968 with an issue dedicated to P. P. Ewald for his 80th birthday.

The *Journal of Applied Crystallography (JAC)*, launched in April 1968, was concerned with new methods, apparatus, problems and discoveries in applied crystallography. The successive Editors have been A. Guinier (1968–1969), R. A. Young (1970–1978), M. Hart (1978–1984), M. Schlenker (1984–1990), A. M. Glazer (1990–1999), G. Kostorz (1999–2007) and A. R. Pyzalla (from October 2007).

In-house typesetting. The impact of the production costs of the journals on the finances of the Union was a constant worry and, at the Eleventh General Assembly, held in 1978 in Warsaw, Poland, the Commission on Journals suggested that the most efficient method of production was to undertake in-house composition. In order to examine that possibility in detail, the Executive Committee appointed a subcommittee comprising S. E. Rasmussen (Chairman), S. C. Abrahams, J. N. King and D. W. Penfold. In 1980 the subcommittee presented a report to the Executive Committee concluding that satisfactory typesetting systems were available and that in-house typesetting would both be cost efficient and reduce production time. The financial situation of the Union in 1981 was, however, not good enough to make the necessary investments [see *Acta Cryst.* (1983), **A39**, 425–480]. The first Union Office computer was bought thanks to a generous donation by the Japanese crystallographic community and was placed in service on 1 January 1984. It enabled one to monitor the progress of papers throughout the whole production process and to generate the subject and author indexes. In 1989, a desktop publishing system was introduced in the Editorial Office for onward transmission of articles to the printer as camera-ready copy, with the effect of reducing the publication time from receipt of a paper from a Co-editor until it appeared in print to about three months. This enabled the accommodation of the new *Fast Communications* section that was approved by the Commission on Journals in 1988.

10. 1983: Creation of *Section C*

By 1978, the total number of pages published per year in *Section B* of *Acta* had nearly reached 4000 (Fig. 10) and, for the first time, the combined number of short structural papers and short communications exceeded the number of regular articles. This led the Commission on Journals to consider the possibility of splitting *Section B* into two sections, one of them devoted to biological, chemical, mineralogical and metallurgical crystallography and the other one, *Section C*, devoted to crystal structure papers. This proposal was agreed at the meetings of the European and American crystallographers in London in June 1979 and in Boston in August 1979, respectively. The idea was that *Section C* would absorb the *Crystal Structure Communications*, which had been launched in 1972 and were edited by L. Cavalca and M. Nardelli and supported by the University of Parma, Italy. The split took effect from 1 January 1983, the names of the three sections of *Acta* being *Section A: Foundations of Crystallography*, *Section B: Struc-*

tural Science and *Section C: Crystal Structure Communications*. The criteria for deciding which papers should go to *Section B* and which ones should go to *Section C* were given in *Acta Cryst.* (1983), **A39**, 174–186 and *Acta Cryst.* (1990), **A46**, 152: papers would be considered for *Section B* if they contained a major structural element, if they presented an experimental and/or theoretical original contribution and if they combined these two types of contribution to provide new structural insight. A special format was developed for *Section C* papers as detailed in *Acta Cryst.* (1982), **B38**, 699–700. A new category of papers, ‘short-format papers’, was introduced in 1984.

The number of papers published per year in *Section C* was very large from the start, as shown in Fig. 11. This resulted rapidly in an increasing backlog of *Section C* papers. To solve this problem, a number of changes took place in the Editorial Office: checking procedures were instigated, additional staff were hired and new computer equipment was installed. Further changes in the procedures for handling structural papers were introduced at the Fifteenth General Assembly held in Bordeaux in 1990. From that time on, the handling of papers was centralized in the Editorial Office, with manuscripts being sent to the Technical Editor for checking before being transferred to the Co-editors. Furthermore, authors of *Section C* papers were invited to submit them in machine-readable format, either by e-mail or by diskettes mailed to the Editorial Office, a possibility first considered during the Fourteenth General Assembly held in Perth, Australia, in 1987.

New procedures for the submission, validation and publication of *Section C* papers and structure papers in *Section B*

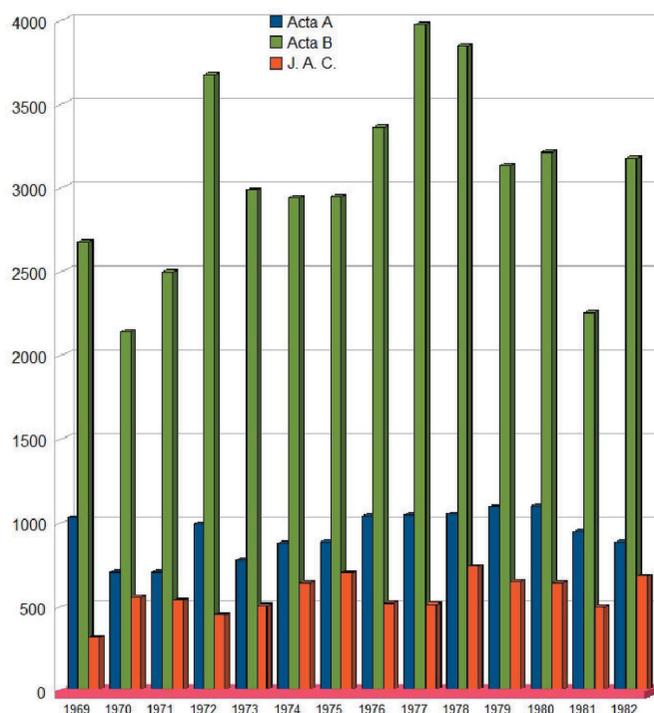


Figure 10
No. of pages published per year in *Acta A*, *Acta B* and *JAC*, 1969–1982.

were introduced in 1991 in order to facilitate the direct transfer of text and numerical data from authors' computers to the typesetting programs in the Technical Editor's office, by use of the Crystallographic Information File (CIF), developed by Hall *et al.* (1991) and derived from the STAR File system (see §13). The CIF had already been adopted in 1990 by the International Union of Crystallography as a file structure for the archiving and distribution of crystallographic information [for details, see Brown & McMahon (2002)]. These procedures became effective on 1 January 1992 and since that date all structural papers published in *Sections B* and *C* have had their numerical content checked in the Editorial Office and an archived CIF has been associated with each paper. Submission became fully electronic in May 1996, but this did not come easily. In the early 1990s, most people were not ready for the use of electronic communication. For instance, at the Bordeaux IUCr Congress in 1990, only about a quarter of the abstracts were submitted electronically, a new procedure introduced by the Chair of the Program Committee, A. Authier.

When Syd Hall, of the University of Western Australia in Perth, Australia, was asked in 1993 by Charlie Bugg to take on the *Section C* Editorship, it was with the specific objective of moving *Section C* into a fully electronic regime of submission and publication. He remembers that at that time *'there was not a great deal of enthusiasm within the C Editorial Board for electronic submissions or for electronic editorial communications. Many referees and most authors viewed the changes as disruptive and complicated, and initially there was considerable negative feedback to the C Editorial Board both by e-mail and*

when attending crystallographic meetings'. It was estimated that the average hard-copy submission involved up to four times the editorial effort required for an electronic submission and it was therefore necessary to keep up the pressure, despite the difficulties encountered with some authors. Electronic submission and validation meant more accurate published results, a faster publication time and a smaller load for the editorial staff in Chester. The efforts of the Editor, the Co-editors, the editorial staff, especially the Research and Development Officer Brian McMahon and his assistant Mike Hoyland, and the Managing Editor Peter Strickland, were however eventually rewarded, and by 1999 few could remember what it was like to process a non-prevalidated hard-copy submission. As evidence of the rapidity of the editorial changes in *Section C*, Syd Hall recalls that *"a prominent author, who, when CIF auto-checking and validation was introduced, claimed that this step would 'destroy all of the well established approaches for reviewing scientific papers that had taken 100's of years to evolve', at the Fifteenth Congress in Glasgow in 1999 inquired at an open editorial meeting whether it was possible to implement in Section D validation and review processes similar to Section C, which work so well?"*.

11. 1993: Creation of *Section D* and separate Editors for *Sections A, B, C* and *D*

In his Editorial for the first issue of *Acta Crystallographica*, in March 1948, P. P. Ewald mentioned as one of the major developments of crystallography the *'extension of X-ray analysis to the extremely complex molecules of biological substances'*. Indeed, in 1937, Perutz had started work on haemoglobin with Bernal, in Cambridge, UK, and, in 1938, W. T. Astbury had taken the first diffraction diagrams of DNA fibres in Leeds, UK. After the war, work on biological substances developed very rapidly with the determination of the structures of penicillin (1949) and vitamin B₁₂ (1955) by Dorothy Crowfoot Hodgkin, the structures of DNA by Rosalind Franklin, Francis Crick, Jim Watson and Maurice Wilkins in 1953 and of the globular proteins by John Kendrew (myoglobin, 1958–1960) and Max Perutz (haemoglobin, 1960–1962). In 1971, the Protein Data Bank was established at the Brookhaven National Laboratories to store the data related to protein structures. By 1981, it contained 86 entries and the biological macromolecule community was becoming large and important, but was under-represented at IUCr Congresses. At the suggestion of the US National Committee for Crystallography, the Executive Committee considered it desirable to bring the members of that community more closely into the general activities of the Union and the Twelfth General Assembly, held in 1981, in Ottawa, Canada, decided to establish a Commission on Biological Macromolecular Crystallography, of which M. G. Rossmann was the first Chairman. During the discussion, R. Diamond asked that the Commission be requested to make use of *Acta* for publications in that field, since most publications were sent to other journals.

The field continued its rapid expansion and, by 1990, there were 500 entries in the Protein Data Bank. At the time, most

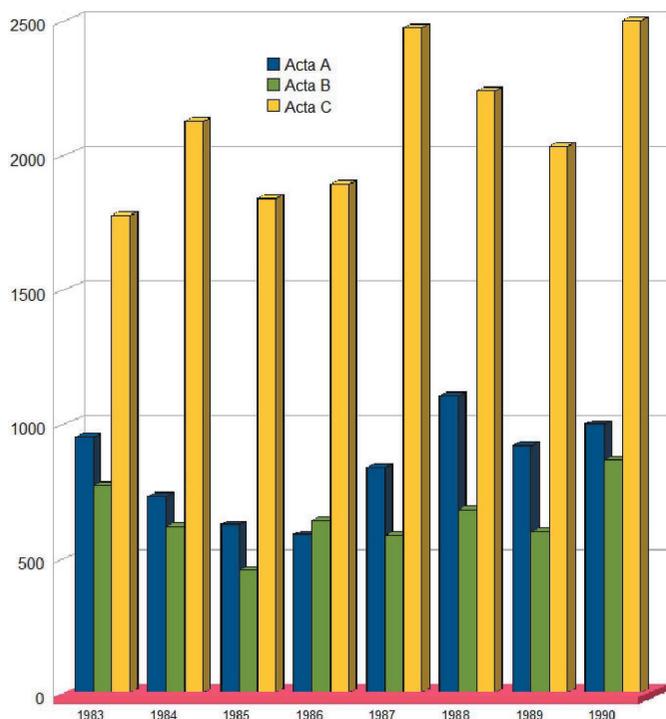


Figure 11
No. of pages published per year in *Acta A*, *Acta B* and *Acta C*, 1983–1990.

of the protein-crystallography papers still went to other journals: the *Journal of Molecular Biology*, which was receiving the main stream of the full papers, *Science* and *Nature*. The Protein Data Bank needed reorganization, in particular with regard to file structure and software for evaluating structures. Charlie Bugg recalls: ‘we felt that there was a large area of protein crystallography that was of limited interest to biologists, but of considerable importance for the development of this important field, including theoretical aspects of protein crystallography, forefront structure determining methods, protein crystal growth, and detailed descriptions of structures that might be of limited immediate interest to biologists. We also felt that the developments of standards in this new field should be a major responsibility of the IUCr, with *Acta* playing a lead role’. At the Fifteenth General Assembly, held in Bordeaux in 1990, the Commission on Biological Macromolecular Crystallography considered that it was time to investigate the feasibility of initiating a new journal or a new *Acta* section covering biological crystallography. The first task of the newly elected President of the IUCr (A. Authier) was, together with Charlie Bugg, the Editor of *Acta*, and Wayne Hendrickson, to initiate discussions to this end and a questionnaire was circulated to more than 400 crystallographers in October 1990. There was quite some resistance from other journals and it took a lot of determination and many meetings – I remember one of them in between planes at Paris Charles de Gaulle airport, of all places! A Working Party, chaired by Charlie Bugg, was established to make further recommendations regarding this new initiative. The Working Party met in

Chester in March 1991 and, following its recommendations, the Executive Committee approved in August 1991 the establishment of the new *Section D* of *Acta Crystallographica*, entitled *Biological Crystallography*. The aim of this new section was to provide a publishing home for details of crystal structure determinations of molecules of biological interest. Jenny P. Glusker of The Fox Chase Cancer Center in Philadelphia was appointed the first Editor of *Section D*. The first issue, in January 1993, contained a set of papers presented at a conference on direct methods of phasing in macromolecular crystallography, held in Florida, USA, in April 1992. The journal was published bimonthly until 1998 and has been published monthly since 1999. Fig. 12 shows the number of published pages per year in *Section D* for the period 1993–2005.

At the Sixteenth General Assembly, held in Beijing in 1993, it was decided that the other sections of *Acta* would also have their own Editors: A. Authier for *Section A*, F. Allen for *Section B* and S. R. Hall for *Section C*, with C. Bugg remaining as General Editor. Their successors have been: for *Section A*, D. Schwarzenbach (since 2002); for *Section B*, C. Brock (since 2002); for *Section C*, G. Ferguson (1999–2008) and A. Linden (since 2008); for *Section D*, E. N. Baker and Z. Dauter (since 2003).

12. 1994: Creation of the *Journal of Synchrotron Radiation*

The decision to establish an IUCr journal on synchrotron radiation was not an easy one to take. The difficulties arose partly because its topic was lying somewhat outside the range of fields covered by the journals already published by the Union, and partly because of the financial risks involved and the additional strain on the Editorial Office staff, particularly at the time *Section D* was being launched.

The advent of synchrotron radiation, first at storage rings (first generation) around 1965 and then at dedicated sources (second generation) in the 1970s, brought about a major revolution in methods for X-ray diffraction. Soon many papers were devoted to the various uses of synchrotron radiation and this prompted the launch of a new magazine, *Synchrotron Radiation News*, published by Gordon and Breach from 1988. Plans were being made in Europe, the United States and Japan for the high-brilliance third-generation sources which were to become operational in the mid-1990s. The importance of synchrotron radiation for crystallography was recognized at the Fifteenth General Assembly held in Bordeaux in 1990 by the establishment of a Commission on Synchrotron Radiation, with John Helliwell as its Chairman.

Samar Hasnain, of the SERC Daresbury Laboratory, UK, was the first to suggest the establishment of a journal of synchrotron radiation. He drafted a list of motivations, pointing out the dramatic increase of the community of synchrotron-radiation users over the preceding years and the diversity of the journals where research papers on synchrotron-radiation instrumentation and methods were being published; none of them reached the entire community

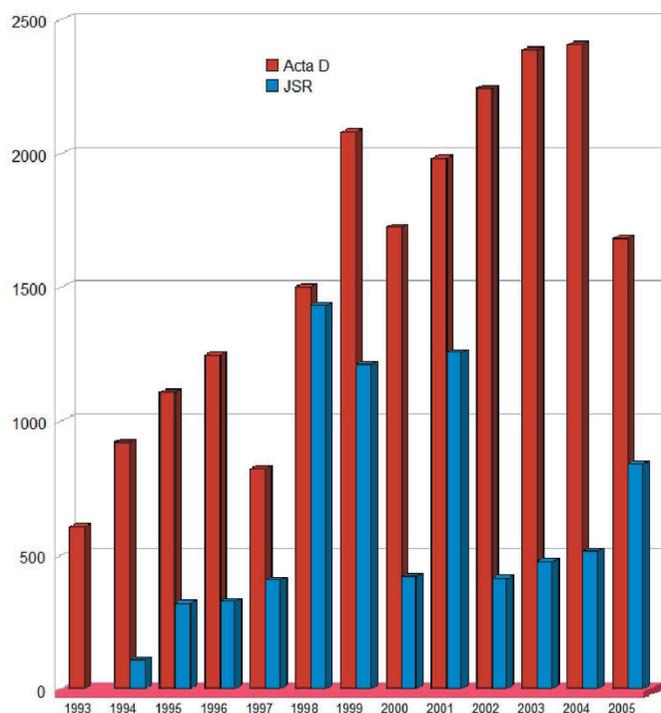


Figure 12

No. of pages published per year in *Acta D* and *JSR*, 1993–2005. The fluctuations in the number of pages published per year for *JSR* are due to the publication of conference proceedings in some issues.

because of the variety of fields concerned: life sciences, physics, chemistry, crystallography; furthermore, many papers were going to *Nuclear Instruments and Methods*, a privately owned publication. There was therefore an urgent need for a primary research journal dedicated to that topic and a potential market for it. S. Hasnain asked a number of colleagues to be part of a tentative Editorial Board and approached various potential publishers. I remember very vividly his first visit to Chester on the evening of 20 August 1991 to meet the IUCr Finance Committee, where he tried to sell us the idea! The initial reaction of the IUCr and its President was positive; John Helliwell, Chairman of the new Commission on Synchrotron Radiation, supported the initiative and accepted an offer to be Joint Editor. Other publishers also showed their interest. The reactions from the community at large were mixed, however; some were very supportive but others objected that ‘*synchrotron radiation was only a tool and that they preferred their research to be compared to other techniques in journals specialized in the topic of their research*’. There was an obvious advantage for a journal of synchrotron radiation to be a publication of the International Union of Crystallography, since this new source of X-rays had become a major one for crystallographers, but there was a difficulty in that there were also many applications of synchrotron radiation lying outside crystallography. Another problem noted by many was the large number of publications that already existed. The potential editors, S. Hasnain and J. R. Helliwell, were asked to finalize their proposal before the March 1992 meeting of the Finance Committee. The Finance Committee’s response was favourable, but launching a new journal was a major operation for the IUCr involving serious risks, in particular financially, considering that *Section D* was due to start publication in January 1993. Such a step could not be taken without serious consideration and a Working Group, chaired by P. Coppens, was set up to report on the proposal. The report was discussed at the meeting of the Executive Committee in August 1992 in Pittsburgh. Some concerns emerged about the financial viability of the journal, the additional burden on the Editorial Office and the impact on the other journals of the Union, in particular *Journal of Applied Crystallography*. On the other hand, there was a general feeling that a journal of synchrotron radiation was bound to be launched in any case and that there was more danger for the IUCr in not being involved than in taking the risks just mentioned, a view that I shared strongly throughout the whole decision-making process. Besides, the community preferred a journal run by a non-profit organization rather than by a private publisher. After discussion, the Executive Committee took the decision in principle to publish this new journal, but considered that it would also be necessary to expand the Editorial Office staff to meet the commitments created by the additional journal. The Executive Committee also wished to have the support of the scientific societies representing the synchrotron-radiation communities in Europe, the United States and Japan. The response here was also mixed, some being enthusiastic, like the Organization of Structural Biology Synchrotron Users; others, such as the

European Synchrotron Radiation Research Society, were distinctly negative. The IUCr Commission on Journals was also not very supportive, mainly because of the fear of the impact on the *Journal of Applied Crystallography*. It also appeared that the launch of the journal would create a new situation in relation to the tax situation of the IUCr in the UK and this needed careful consideration. On the other hand, Gordon and Breach was on the verge of starting a journal of synchrotron radiation research of its own. Finally, the Finance Committee, at its March 1993 meeting, taking every aspect into consideration, decided to recommend to the Executive Committee that the *Journal of Synchrotron Radiation (JSR)* be published by the IUCr, with January 1995 as a possible starting date. The Executive Committee accepted the proposal by postal ballot in May 1993 and the decision was taken by the Sixteenth General Assembly held in Beijing, China, in August 1993, with S. S. Hasnain (1994–2002), J. R. Helliwell (1994–2000) and H. Kamitsubo (1994–2002) as Editors. The first issue was published in October 1994 as a pilot one. The journal was then published bimonthly from 1 January 1995. Fig. 12 shows the number of published pages per year in the *Journal of Synchrotron Radiation* for the period 1994–2005. The successive Editors have been D. R. Mills (2000–2008), Å. Kvik (since 2002), T. Ohta (since 2002) and G. E. Ice (since 2008).

13. 1999: *Crystallography Journals Online*

The most important event in the history of the IUCr journals was the launch, at the Eighteenth General Assembly held in Glasgow, Scotland, in August 1999, of ‘*Crystallography Journals Online*’. It was the result of many years of planning and painstaking preparations, especially by the staff of the Editorial Office.

Very early on, the IUCr rose to the challenge of the coming age of electronic information and it took a little over a decade for the transition from the paper world to the electronic one to take place. These were most exciting times to be associated with the operations of the IUCr! The transition was not an easy one; it took place in two stages. The first stage concerned the storage of information, the automatic checking of CIFs and the electronic submission of manuscripts, and was achieved relatively rapidly. Uncertainties about the second stage, namely the dissemination of information electronically and electronic publishing, remained until almost the end of the 1990s. They were both technical and financial: what could be made available electronically and what should be made available, for what price? Would electronic publishing kill printing on paper? Would electronic publishing be profit making? Those were the nagging questions of the day and the topics of endless discussions. A timeline of the events leading up to the transition from print (and beyond) is given below.

1987. At the Fourteenth General Assembly, held in Perth, Australia, a proposal for establishing a ‘Commission on Crystallographic Information’ to replace the existing Commissions on Journals, Structure Reports and Crystallographic Data was discussed. The objection was raised that such a commission would involve too many persons; instead, a

Working Party on Crystallographic Information, chaired by E. N. Maslen (Fig. 13), of the University of Western Australia, Perth, Australia, was set up to consider the relations between the existing commissions, with the mandate to report in three years' time. The Working Party worked in conjunction with the Commission on Crystallographic Data on the development of the Crystallographic Information File, and collaborated with the Commission on Journals to finalize proposals for machine-readable submission of manuscripts.

1988. The Working Party met in Vienna during the European Crystallography Meeting and decided that the STAR File electronic universal exchange approach would be tested for its possible adaptation to crystallographic applications (Hall, 1991). This task was given to a working party composed of I. D. Brown, F. Allen and S. R. Hall as Chair. The CIF approach did in fact evolve directly from the STAR File syntax.

1990. The Working Party reported to the Fifteenth General Assembly, held in Bordeaux, France, and made a list of recommendations.

June 1991. E. N. Maslen was appointed Director of Archiving and Crystallographic Information.

1993. The position of Director of Archiving was replaced by a Subcommittee on Electronic Publishing, Dissemination and Storage of Information, with E. N. Maslen as its Chairman until his untimely death in January 1997. He was then replaced by H. D. Flack, from Geneva, Switzerland. Brian McMahon, who had joined the Editorial Office staff as Editorial Assistant in 1986, was appointed Research and Development Officer, with M. Hoyland as his assistant.

1996. All-electronic CIF-access papers were introduced in *Section C*.

February: Four members of the Electronic Publishing Subcommittee (Y. Epelboin, H. D. Flack, S. R. Hall and B. McMahon) attended an ICSU Press/UNESCO Conference on

Electronic Publishing in Science in Paris, for which A. Authier was one of the co-organizers.

The IUCr worldwide web information server was developed by in-house staff, following on experience gained from experiments by H. D. Flack using the pre-worldwide web European information server CONCISE.

1998. Negotiations were under way with Munksgaard to provide an online version of *Section D* of *Acta Crystallographica*.

March 1999. The negotiations with Munksgaard having been unsuccessful, it was decided to explore the possibility of providing online access to the IUCr journals through the Editorial Office. Thanks to the strenuous efforts of the Editorial and Research and Development staff, it was possible to launch the new service for all six journals under the brand *Crystallography Journals Online* in 1999.

2000. *Section C* papers formerly known as 'CIF-access papers' were renamed 'electronic papers' (for inorganic, metal-organic and organic compounds).

2001. An entirely electronic journal, *Acta Crystallographica Section E: Structure Reports Online*, was established, with W. Clegg (2001–2008) and D. G. Watson (2001–2008) as Joint Editors. They were succeeded by W. T. A. Harrison, J. Simpson and M. Weil from 2008.

2005. Another entirely electronic journal, *Acta Crystallographica Section F: Structural Biology and Crystallization Communications*, was established, with H. Einspahr and M. Guss (2005–2008) as Joint Editors. M. S. Weiss replaced M. Guss as Joint Editor in 2008.

2008. *Acta Crystallographica Section E: Structure Reports Online* was newly defined as an 'open access' journal with modest fees to be paid by the authors.

14. Conclusion

The IUCr journals have been very successful and are *the* widely recognized source for articles on crystallography and its many applications; they are also the only international scientific journals in the field published by an international non-profit organization. Over the years they have also become a financial success, providing the necessary resources for launching new journals and for the many activities of the Union. They are unique in that they have all been developed by the Union's Editorial Office. These developments and the success of the journals would not have been possible without the high level of professionalism and the devotion of its Editorial and Research and Development staff, who were awarded the highly competitive ALPSP Award for Publishing Innovation in 2006 for their work on CIF and *checkCIF*, showing that the IUCr journals continue to lead the way in innovation.

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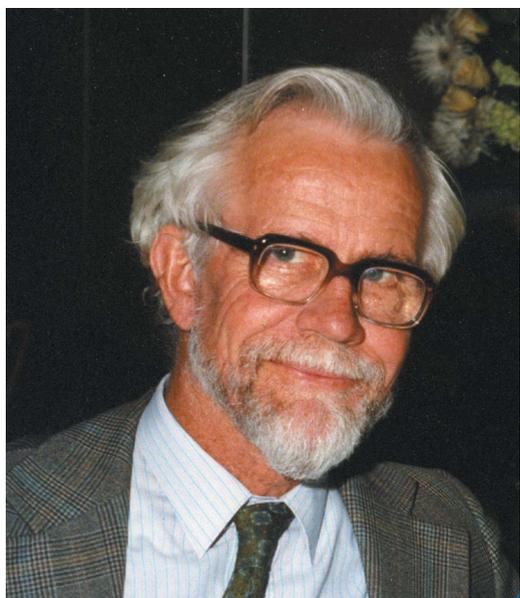


Figure 13
E. N. Maslen (1935–1997), courtesy of S. R. Hall.

birth of *Section D* and the *Journal of Synchrotron Radiation*, and to Helmut Klapper for photocopies of early issues of the *Zeitschrift für Kristallographie*.

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