PART VIII

The Consolidation of the New Crystallography

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Before the First World War the number of scientists who were engaged in X-ray diffraction and crystal structure analysis was small: perhaps ten in Germany, ten in England, five in France, four in Japan, five in USA, two in Russia and five in the Netherlands and the Scandinavian countries. In the years of the war, these numbers did not materially increase, although the field itself expanded by the invention of the powder method, improved apparatus design by closer attention to the X-ray geometrical optics, and by the dynamical theory.

After the war, from about 1920 onwards, the number of research workers increased, at first mainly in England, but soon also in USA and the Scandinavian countries. The determining feature for this increase was the presence of scientific leadership, such as that offered by W. H. and W. L. Bragg in England, Siegbahn and Westgren, later Phragmén, in Sweden, Wyckoff, Pauling and A. H. Compton in USA. In all these instances 'schools' developed quite naturally, and the advance, both with respect to subject matter and to numbers of workers, was rapid once a nucleus was formed. The interest in the particular crystal, which was most pronounced in W. L. Bragg's large series of structure determinations, soon brought the subject close to the border between physics and chemistry, and wherever this was the case, it flourished. It is interesting to remark how few structure determinations came from Germany, where X-ray diffraction belonged to physics, and the great majority of chemists, proud of the achievements gained by their traditional methods, for a long time did not tolerate the intrusion of a physical method in their research or their teaching. This lack of structural results contrasts sharply with the important extension of physical methods originating in Germany: powder diagrams, layer-line rotation and oscillation diagrams, the Weissenberg and Schiebold-Sauter goniometer method, wide-angle diagrams and micro cameras; Niggli's adaptation of the theory of space groups from

the form in which Schoenflies had left it to a more suitable shape for practical work also belongs here. These methods, now widely used everywhere, found a very slow acceptance in England, where the merits of the Bragg spectrometer were exploited to the full; conversely, except for early work of Mark, the spectrometer was little used during the twenties in Germany.

Much of the personal contact between the workers in the new field was gained by visits to other laboratories for shorter or longer periods. The two British schools at the Royal Institution and in Manchester were the focal points to which especially American, Canadian, French and Dutch adepts converged. In Germany, Mark and Polanyi's laboratories in Dahlem, Rinne-Schiebold's institute in Leipzig and also Glocker's and Ewald's schools in Stuttgart attracted foreign students, and the same holds for Mauguin's laboratory in Paris – but all this on a very much smaller scale than what the British laboratories had to offer. Later on, the seedlings of the two main schools, such as J. M. Robertson's school in Glasgow, G. E. Cox' in Leeds, Bernal's and Lonsdale's in London, joined with the older ones in the dissemination of the experimental and theoretical methods of crystal analysis. An important part in making possible the international exchange of young scientists was played by several Foundations, in particular in the 1920's by the International Education Board (Rockefeller Foundation).

It was a fortunate circumstance that many of the workers in the new field were of a rather homogeneous age group, and so found it easy to get to know one another and to discuss their problems. Sir William Bragg (*1862), Charles Mauguin (*1878) and Max v. Laue (*1879) were the elders; there followed an intermediate group – born 1888–90 – with Andrade, W. L. Bragg, Darwin, Brentano, Glocker, Ewald and Westgren among them, and this led over, via James and Bijvoet, to a large group born between 1895 and 1905 whose main training took place after the end of the war. This last group contains the principal pupils of Sir William at the Royal Institution and of W. L. Bragg in Manchester, besides the veterans in USA like Wyckoff, Pauling, Patterson, Warren, Buerger, Donnay and others, and leading early figures in other countries, such as Mark in Germany, Mathieu and Wyart in France, Hägg in Sweden, Nitta in Japan.

Whether the reason be the humane and friendly example set by the elders, the similarity of age and interests, or the immense field of exploration open to everyone – the fact is that the crystallographers soon became a very friendly crowd, from laboratory to laboratory and from country to country.

A first step towards the international consolidation within the new crystallography was taken by Ewald in 1927 when he proposed to the other editors and the publisher of the *Zeitschrift für Kristallographie* at a meeting held in Romanshorn on Lake Constance to 'internationalize' the journal by allowing papers in English and French besides in German. The ready acceptance of this proposal by the editor-in-chief, Niggli, the co-editors Laue and Fajans, and the publisher, K. Jacoby, was followed by a similar reaction on the part of the authors whose papers had up to then been translated for publication. The unique role which the *Zs.f. Krist.* had gained in the pre-X-ray days under Groth as *the* specialized journal of crystallography was preserved by this step. In later years, when many renowned German scientific journals had to bow to the racist decrees of the Nazi 'Chamber of Culture' the *Zs.f. Krist.* could refuse to recognize their applicability to a journal of international character and having a Swiss editor-in-chief.

The further history of the *Zs.f.Krist.* need be mentioned only briefly. Like all other scientific journals in Germany the *Zeitschrift* had to close down towards the end of the war; the last issue was number 1 of Vol. 106, dated February 1945. Thus it came that the second number of Vol. 106 appeared in October 1954, after a break of nearly ten years, just in time for Laue's 75th birthday. From then on the *Zeitschrift*, under the editorship of G. Menzer, M. Buerger, F. Laves and I. N. Stranski, has developed very well, continuing the tradition of an international authorship. The *Strukturbericht*, which in the pre-war days of the *Zeitschrift* had been a supplement to its volumes, as a service to the consolidation of the new crystallography, had meanwhile become an independent undertaking under the title *Structure Reports* which was not connected with any journal.

As a second step in the international consolidation, the *International Tables* (*Internationale Tabellen zur Bestimmung von Kristallstrukturen*) should be mentioned. The following situation led to their planning. By the late 1920's a number of books had appeared on X-ray diffraction. There was the Bragg classic *X-rays and Crystal Structure* (1st ed. 1915, 4th ed. 1924), which was in the main a summary of the work of the Braggs in classic simplicity but without any attempt at being comprehensive of the whole field of work. The second book to appear was Ewald's *Kristalle und Röntgenstrahlen* (Springer 1923), followed but little later by Ch. Mauguin's *La Structure des Cristaux* (Paris 1924). Wyckoff published *The Structure of Crystals* in 1924; Mark in 1926 *Die Verwendung der Röntgenstrahlen in Chemie und Technik*; G. L. Clark

in 1927 *Applied X-rays*, and in the same year R. Glocker's *Materialprüfung mit Röntgenstrahlen* appeared. A. Scheede and E. Schneider were preparing two volumes *Röntgenspektroskopie und Kristallstrukturanalyse* which came out in 1929. Besides, there were comprehensive Handbook articles, by Ewald (*Hndb. d. Physik*, Springer 1927, Bd. 24) and by H. Ott (*Hndb. d. Experimentalphysik*, Lpz. 1928, Bd. 7). A number of these books aimed at including all the material that would be needed for practical work, and this led not only to the repetition of lengthy wave-length and space-group tabulations, but, worse, to confusion caused by different numerical values and designations. This was worst in the case of space groups. Niggli, in his *Geometrische Kristallographie des Diskontinuums* (Bornträger 1919) had taken over the Schoenflies nomenclature. There existed, among the mineralogists, a wide variety of designations of the 32 crystal classes, and this meant that there were tendencies in diverging directions for the closer attachment of space-group symbolism and terminology to those of the point groups (e.g. Rinne and Schiebold). Soon after Niggli's mode of representing the space groups there appeared Wyckoff's much used tables *The Analytical Expression of the Results of the Theory of Space Groups* (Carnegie Institute of Washington, 1922; 2nd ed. 1930), and in 1924 Astbury-Yardley (Lonsdale)'s *Tabulated Data for the Examination of the 230 Space Groups by Homogeneous X-rays* (*Phil. Trans. Royal Soc.* A 224) which used a pictorial representation of space groups very different from Niggli's. One of the perplexing features for the user was that neither the axial directions nor the position of the origins were always the same in these descriptions.

The prospect that textbooks, in order to be useful in the laboratory, would have each to present the *complete* tabulations, each one very likely in its own form and with its own faults and misprints, weighed so heavily on Ewald that after a meeting of the Faraday Society in London (March 1929) which had brought many crystallographers together, he laid the matter before a representative group of crystallographers whom Sir William Bragg had invited to the Royal Institution. It was decided to form three committees: one for the nomenclature of space groups, one for the abstracting of crystallographic papers, and a third one for the simplified and standardized publication of structural work. These commissions were to report to Sir William Bragg. In the course of their work the first and last of these commissions merged into a *Tables* Committee with Astbury, Bernal, Hermann, Mauguin, Niggli and Wyckoff as members. The commission on abstracting, consisting of Bernal and Ewald, worked out

rules for abstracting crystallographic papers on one-page set forms, and delivered a report, but it turned out that the tabular form of abstracting was not adaptable enough for general use, and nothing came of this work.

Ewald and Bernal, however, prepared a detailed agenda for a conference on standard crystallographic tables, and when Wyckoff announced that he would be coming to Europe in the summer, Bernal, as chairman of the *Tables* Committee, called a working conference to Zürich in July 1930 on the invitation of Niggli to hold the conference in his institute.

In three or four days of intensive work the members of the Committee, reinforced by Kolkmeijer, James and Mrs. Lonsdale, Mark, Schneider, Schiebold and Brandenberger, discussed the material prepared by Bernal and Ewald under the latter's chairmanship and agreed on point after point. A tight-lipped Niggli watched the proceedings without taking much part, until on the third day he exclaimed: 'Gentlemen, you are stealing my book. I will not agree to any such publication unless it is given to my publisher, Gebr. Bornträger in Berlin, in lieu of a new edition of my book'. Neither this surprising accusation, nor the curious condition was allowed to stand in the way of materializing the *Tables*. Ewald, feeling that his further participation in the work on the *Tables* was likely to jeopardize the good understanding between him and the chief editor of the *Zeitschrift*, withdrew officially from the *Tables* and took part in their growth only indirectly, through their editor, C. Hermann. Sir William Bragg and M. von Laue accepted the Honorary Editorship and through their efforts, as well as those of Mauguin, Kolkmeijer and Wyckoff, substantial subsidies for the preparation and publication of the *Tables* were obtained from academies and other learned societies. The Rockefeller Foundation enabled Hermann to go to USA for a month in connection with the sections prepared by Wyckoff and by Pauling. The two volumes appeared in 1935, and their consolidating influence on the field of crystal analysis is undeniable. It includes the general acceptance of the more meaningful designation of the space groups which was worked out between Hermann and Mauguin.

A third step towards the international consolidation of the new crystallography occurred at the end of the war. By 1943 the British crystallographers had formed an 'X-ray Analysis Group' (XRAG) within the Institute of Physics, and two similar groups existed in USA, the 'American Society for X-ray and Electron Diffraction' (ASXRED),

founded in 1941, which was biased towards physics, and a mineralogically inclined 'Crystallographic Society of America' (CSA), founded in 1945. In 1944 the yearly meeting of XRAG was held in Oxford, and Ewald, who then taught in Belfast, was invited to give the evening lecture. In it he gave a historical survey of some stages of X-ray crystallography and ended with a strong plea for the formation of an international society or union which would represent the new crystallography. This idea was followed up by the British crystallographers, and in particular by Sir Lawrence Bragg, the chairman of XRAG. In June 1946, within a year of the termination of the fighting, he arranged for an international meeting of crystallographers in London which was attended by some 120 crystallographers from most of the allied countries. In spite of the general travel restrictions still imposed on Germans at the time, it was possible to have Laue there. The Russian delegation arrived at the end of the meetings and could take part in various committee meetings following the plenary sessions. It was a wonderful re-union of old friends who had been separated during the years of the war, and a first meeting of many colleagues known to one another only as authors of important papers. The result was the decision to form an *International Union*, if possible an independent Union of Crystallography, and until this be consolidated, to form an *interim* representative committee; – to prepare national committees for crystallography in the participating countries; – to charge R. C. Evans and Ewald to explore and prepare the necessary steps with the International Council of Scientific Unions (ICSU) for the recognition of this Union by drafting statutes and by preparing the constitutive First General Assembly as soon as possible which, on the invitation of the USA delegation, was to be held at Harvard University. Furthermore it was decided to prepare the publication, by the Union, of

(i) a special journal for the new crystallography, belonging to the Union and under the editorship of Ewald and R. C. Evans, I. Fankuchen, J. Wyart and A. V. Shubnikov as national co-editors;

(ii) *Structure Reports*, under the Editorship of A. J. C. Wilson, as a continuation of *Strukturbericht*; and

(iii) *International Tables for X-ray Crystallography* under the editorship of Mrs. Lonsdale. (The German *Internationale Tabellen* had been reprinted during the war in USA but were no longer to be had; besides, a revision of the first *Tables* seemed desirable.)

Of these projects the quickest to materialize was the journal. It received its name, *Acta Crystallographica*, on the proposal of Shubnikov,

at a meeting of the journal commission in Cambridge a few days after the London meeting where all attempts at finding a suitable name had led to nothing. Shubnikov withdrew as co-editor after the first few issues had appeared as there was no probability of his transmitting papers in Russian in the near future. The publication of a new journal of unknown appeal was a somewhat risky affair in the early post-war period, with shortages of paper and labour and instability of prices. Sir Lawrence Bragg appealed to British industrialists for a subsidy over the first five-year period, and obtained it, and USA sources matched this, while smaller guarantees came from other countries; in addition substantial subventions to the journal and the other publications launched by the Union were received from UNESCO. Specifications for the production of *Acta Crystallographica* were prepared and sent to firms in seven different countries, and tenders received. Finally, the production was entrusted to the Cambridge University Press, with whom Evans, who undertook to act also as the technical editor, had the easiest contact. When in 1951 the Cambridge Press found it impossible to accomodate the growing volume of *Acta* with their other obligations, the publication was transferred to the Danish firm of Ejnar Munksgaard, in whose hands it still is. The first number of the new journal appeared in March 1948, and at the time of the Harvard meeting (28 July to 3 August 1948) the third issue had appeared.

Since then *Acta* has been growing steadily, the first twelve volumes under Ewald's editorship, with Evans (later Asmussen), Fankuchen, Wyart and later also Hughes, Lipson and Nitta as co-editors; and from 1960 onwards under A. J. C. Wilson's editorship with the same co-editors and Jagodzinski. Vol. 1 of 1948 had 348 pages, the latest complete volume, 14 (1961) has 1318 pages. The number of subscribers has been growing steadily year by year reflecting the still increasing interest in crystal structure, and so has the demand for back volumes which contain many essential papers.

The formal establishment of the *International Union of Crystallography* (IUCr) was greatly facilitated by the very helpful interest the then Secretary General of ICSU took in it, the Cambridge astronomer F. J. M. Stratton, an old personal friend of both Ewald and Evans. During the war, most of the international unions lay dormant, and they slowly emerged again to activity in the period 1945–50. Stratton, who had devoted many years to these Unions, was much in favour of small unions which he considered closer-knit and quicker of action

than those which covered enormous and in some respects heterogeneous parts of science. The application of the provisional representation of crystallography for the recognition of an International Union of Crystallography was granted in 1947, pending acceptance of the provisional statutes by the constitutive assembly. This First General Assembly was called for Cambridge (Mass.) where the University of Harvard had offered to be host to the meeting (28 July to 3 August 1948).

Here again, the joy of finding old friends and new, in even greater numbers than two years previously in London, the pleasure of discussing with expert colleagues after a long pause, and the progress reported on crystal structures and methods – all this made the meeting to those participating a truly memorable one. Added to this was the satisfaction that the business meetings decided on statutes and thereby changed the *interim* representation of crystallographers into the first formal Executive Committee of the International Union of Crystallography, with R. C. Evans as General Secretary, elected Sir Lawrence Bragg as its first President, and M. von Laue as its first and only Honorary President. The establishment of the Union meant the scientific, and to a certain extent also professional organization of the large number of workers in the ever expanding field that had been opened up 36 years earlier by the genius of M. von Laue, W. H. and W. L. Bragg.

From that day on the Union has steadily developed. The following Table giving details of the five General Assemblies and International Congresses shows this:

IUCr General Assemblies and International Congresses

	Year	Place	Country	President	Papers	Participants
1	1948	Harvard	U.S.A.		86	310
2	1951	Stockholm	Sweden	Sir L. Bragg	225	340
3	1954	Paris	France	M. J. Bijvoet	420	630
4	1957	Montreal	Canada	R. W. G. Wyckoff	325	600
5	1960	Cambridge	U.K.	J. Wyart	600	1250
6	1963	Roma	Italy	P. P. Ewald	?	?

The number of countries which adhere to the Union through their national academies or other learned societies has grown to 26. R. C. Evans, to whom the Union owes so much for its establishment, served

as secretary to the Union from 1948 to 1954; he was succeeded by D. W. Smits, the present secretary.

In the years between the triennial congresses a number of other meetings were arranged. Thus there was a symposium on 'Structures on a scale between the atomic and microscopic dimensions' in Madrid (2–6 April 1956) and a conference on 'Precision determination of lattice parameters' in Stockholm in 1959. IUCr further participated in the Fedorov Commemoration meetings in Leningrad in 1959, and also co-sponsored an international symposium on 'Electron diffraction' in Kyoto in September 1961. Generous financial contributions from UNESCO facilitated the attendance of many participants in the congresses and other meetings.

These meetings mean a great deal to all crystallographers, by acquainting them with their colleagues abroad and their work. This is particularly true for those who still are in a pioneer position in their countries and ordinarily have little chance of regional contact with other crystallographers.

The most important work of the Union lies, however, with its various Commissions. The editing of the journal by the *Acta Crystallographica Commission* (chairman A. J. C. Wilson) has been mentioned above. Before taking over *Acta Cryst.*, Wilson was chairman of the *Structure Reports Commission*, and under his editorship and with the splendid cooperation of a large number of section editors and abstractors, ten volumes of *Structure Reports* were prepared, covering the years 1940–1954. Now Wilson has been succeeded by W. B. Pearson in Ottawa who, with the help of an increased board of section editors and abstractors, is attempting to halve the present six-year gap between the publication of a paper and of its review in *Structure Reports*. With the ever increasing rate at which crystal structures are being determined, their uniform and complete registration in *Structure Reports* becomes the longer the more indispensable.

The *International Tables Commission*, still under the chairmanship of Dame Kathleen Lonsdale, has revised and enlarged the former *Internationale Tabellen* to a three-volume, not yet completed work which assembles all the geometrical, analytical and physical data required for crystal structure analysis by X-ray diffraction. Again, the existence of this standard work is a real service to the community of crystallographers in all countries.

Besides these publishing commissions of IUCr there are others for which publication is only incidental. Only a few examples of their work will be mentioned:

In the *Commission on Crystallographic Apparatus* (present chairman W. Parrish) questions of standardization have been discussed – matters that were investigated also by special national commissions, for instance of XRAG, but should be agreed upon internationally. The commission also conducted an international testing of the accuracy of high-precision lattice parameter determination and held a conference in Stockholm (1959) on this topic, and on counter methods for crystal structure analysis. Its latest activity is a second experimental comparison of the properties of commercially available X-ray films; a first comparison had been carried out under the auspices of the commission some five years earlier. Besides an *Index of Crystallographic Supplies* has been compiled by the commission, of which the third edition is being prepared for the Rome Congress.

One of the most effective contributions to the international consolidation of crystallographers comes from the initiative of the chairman of this commission: the compilation of a *World Directory of Crystallographers*, the first edition of which appeared in 1957. In the second edition, which was edited by the General Secretary of IUCr, D. W. Smits, more than 3500 scientists from 54 countries are listed who employ crystallographic methods. A new edition will be prepared soon after the Rome Congress in 1963.

The increasing use of electronic computers led in 1960 to the formation of a *Commission on Crystallographic Computing*, with G. A. Jeffrey as chairman. The best utilization of computers, the standardization and exchange of programs, and problems of publication were among the topics discussed at a meeting of this commission near Frankfurt, in preparation of a full-scale symposium in connection with the Rome Congress in 1963.

The *Commissions on Crystallographic Data, on Crystallographic Nomenclature, on Electron Diffraction*, and *on Crystallographic Teaching* are further commissions of IUCr which show the type of important international work to be done. IUCr is also represented on some Commissions of the International Unions of Pure and Applied Physics (IUPAP) and of Pure and Applied Chemistry (IUPAC), and on the ICSU Abstracting Board.

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Bearing in mind the picture of world-wide activity and cooperation, of which this Commemoration Volume presents another example, it is in a mood of pride and gratitude for the past and of serene confidence in the future of their science that crystallographers convene in Munich, the birth place of their particular branch of science, for celebrating the fiftieth anniversary of M. von Laue's, W. H. Bragg's and W. L. Bragg's pioneer work which started the development of

THE NEW CRYSTALLOGRAPHY.