A Brief History of *Strukturbericht* Symbols and Other Crystallographic Classification Schemes

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Abstract. In 1913, x-ray crystallography was first used to determine the crystal structure of diamond. Since that time hundreds of thousands, if not millions, of crystal structures have been determined. Published structures require critical review and indexing to make them easily available to other researchers. One of the first systems for doing this was *Strukturbericht* (Structure Reports), published in Germany from 1931-1943 and covering research from 1913-1939, and now best known for the *Strukturbericht* symbols which label common crystal structures. A comprehensive history of *Strukturbericht* has not been written. This brief report sketches the early history of *Strukturbericht*, as well as its post-World War II successor publications, handbooks, and online resources.

1. Introduction
In 1912, Max van Laue suggested that the diffraction of x-rays through crystals would produce a pattern which could be used to determine the crystal structure.[1] Within the year, this technique was used by Bragg and Bragg[2] to determine the structure of diamond. Later Hull[3] determined the structure of graphite, and the race was on to determine the structure of any compound that could be studied.¹

It quickly became obvious that nature frequently repeats itself. The metallic elements mostly take close-packed structures, either face-centered cubic or hexagonal close-packed, or the nearly close-packed body-centered cubic lattice. Of the remaining elements, the early row 14 elements all take on the diamond structure. We only see other patterns when we go to elements on the far right-hand side of the periodic table or in the actinides.²

A similar trend shows in compounds. Many AB type binaries take either the sodium chloride, cesium chloride or zincblende structures, and A₂B compounds can frequently have the positions found in fluorite (CaF₂).

All of this means that we can think (hope) that elements and most compounds exist in a limited number of structures, and that compounds having similar structures are somehow related to one another. This suggests that we can categorize them according to their atomic configuration. One possibility for doing this is to note that all periodic crystals must belong to one of the 230 three-dimensional space groups, and only occupy allowed positions within those space groups.[5] Of course this allows an infinite number of possible structures, and so is not

¹ Of interest is the work of Davey[4], who found that tungsten was too opaque for standard X-ray diffraction techniques, and so diluted his sample with ten parts wheat flour in order to get a diffraction pattern.

² The one exception being manganese, which takes on two unique atomic arrangements.
an optimal characterization scheme, although it can make a useful indexing scheme. A better scheme that this needs to be devised.

Scientists being human, and therefore fallible, it is also necessary to have the published structures reviewed for accuracy. Such a review is also useful for those who might have missed the original research in the literature.

In 1931 Ewald and Hermann[6] published the first such review, “Strukturbericht (Structure Reports) 1913-1928” which was introduced

... to provide a compilation and critical review of all previously published articles on X-ray structure determination. The arrangement was made according to the chemical formula, along with a summary by type [emphasis mine] which allows a survey of the known structural types and their representatives. Unlike other published structural compositions, the present one is characterized by the fact that the individual works are discussed. It is expected that this will improve the accuracy of the determinations, the exact nature of the material used, the corrections to be made to older reports based on newer work, and other similar points.³

From the date it can be seen that this was intended to cover the field of structure determination from the beginning.

As indicated, this volume was a critical review of x-ray crystallographic literature, but it also attempted to group crystal structures into types. This was the introduction of the Strukturbericht symbol: A₁ was given to close-packed face-centered cubic crystals, A₂ for body-centered cubic, A₃ for hexagonal close-packed, etc. For binary materials, B₁ represented the sodium chloride structure, B₂ cesium chloride, and B₃ zincblende. More complicated structures were given other alphabetic indices with other letters.

The publication of Strukturbericht continued through the middle of World War II, and included research through 1939. Its successor, “Structure Reports,” published by the International Union of Crystallography (IUCr), began immediately after the War and continues. Post-War it was realized that the number of Strukturbericht symbols was growing uncontrollably, and so the practice of giving new structures symbols was dropped, although Smithells[7] and Pearson[8] did add new symbols to cover structures of some of the transuranic elements and intermetallic compounds, as we will discuss below.

Even though the generation of new symbols ceased, the ones found in the Strukturbericht volumes, Smithells, and Pearson are still in use. Everyone interested in superconductivity knows what an A₁₅ (Cr₃Si or β-W) structure is, as compounds with this structure became known as the first “high temperature” (20K) superconductors[9] However, to our knowledge no complete history of Strukturbericht has been written. There is not even a complete index of all the symbols, the last one being published with volume II in 1937.[10] Smithells, Pearson, and Villers,[11] among others, have published partial lists, but these are weighted toward the intermetallics and essentially ignore silicates (Strukturbericht S) and other systems.

This brief paper is by no means a complete history of Strukturbericht and the associated symbols, but it is meant to give a description of the symbols, some of the historical development and changes through the years, and, finally, note that we are in the process of actually producing a definitive index of Strukturbericht symbols as an online resource.[12]

2. Strukturbericht Band (Volume) I 1913-1928
The first volume of Strukturbericht[6], edited by Peter Paul Ewald and Carl Hermann, was published as a supplement to Zeitschrift für Kristallographie in 1931 and covered research from 1913 (the crystallographic dawn of time) through 1928. This introduced the original form for Strukturbericht symbols: a letter, representing the compound type (element, binary, ternary,

³ All translations from the original German were done by the author with the assistance of Google Translate.
etc.), followed by a number, representing the order of compounds in the list. The original list of Strukturbericht letters were

- **Type A**, elements. As noted above, the first elements were
  - $A_1$, copper, representing close-packed face-centered cubic structures
  - $A_2$, tungsten, representing body-centered cubic structures
  - $A_3$, magnesium, representing hexagonal close-packed structures
  - $A_4$, diamond
- **Type B**, binary compounds with stoichiometry $AB$, including
  - $B_1$, NaCl (rock salt)
  - $B_2$, CsCl
  - $B_3$, Znblende, the cubic ZnS phase analogous to diamond
- **Type C**, binary compounds with stoichiometry $A_2B$, including
  - $C_1$, fluorite, CaF$_2$
  - $C_2$, pyrite, FeS$_2$
  - $C_3$, cuprite, Cu$_2$O
- **Type D**, binary compounds with stoichiometry $A_mB_n$. These were divided into several ranges:
  - $D_1$ – $D_{10}$: $AB_3$ compounds, including $D_1$, ammonia (NH$_3$)
  - $D_{11}$ – $D_{20}$: $AB_n$ with $n > 3$, starting with $D_{11}$, SnI$_4$
  - $D_{31}$ – $D_{50}$: $(AB_n)_2$, including $D_{31}$, (HgCl)$_2$ and $D_{41}$, (BH$_3$)$_2$
  - $D_{51}$ and up: more general $A_mB_n$ compounds, including $D_{51}$, corundum (Al$_2$O$_3$) and $D_{61}$ La$_2$O$_3$

  This scheme proved to be limiting and was modified in volume II.
- **Type E**, compounds with more than two atom types but without radicals. No E type symbols were defined in the first volume.
- **Type F**, compounds with two- and three-atom radicals. This was again divided into two parts,
  - $F_1$ – $F_{50}$, compounds of the form $A_m(BC)_n$, such as $F_1$, CoAsS, and
  - $F_{50}$ – $F_{100}$, compounds with form $A_m(BC_2)_n$ and $A_m(BCD)_n$. Examples included $F_{51}$, NaHF$_2$, and $F_{61}$, chalcopyrite, CuFeS$_2$.

  This division would also prove to be limiting.
- **Type G**, compounds with four-atom radicals. This was divided into several categories, ending with $G_{31}$ – $G_{40}$, “complex formula.” Examples included $G_1$, calcite CaCO$_2$, and $G_{31}$, beryl, Be$_3$Al$_2$(SiO$_3$)$_6$.
- **Type H**, which was divided in to $H_1$ – $H_{50}$, compounds with five-atom radicals, and $H_{51}$ – $H_{100}$, containing all of the higher-order radicals. (One might imagine Ewald and Hermann throwing up their hands at this point, as they realized what they had gotten into.)

  The range $H_{41}$ – $H_{50}$ was set aside for hydrated materials, e.g. $H_{41}$, K$_2$CuCl$_4$·2H$_2$O.
- **Type L**, “alloys,” (Legierungen in German) which included
  - $L_1$ – $L_{19}$, ordered alloys based on the fcc lattice, including $L_{10}$, CuAu, and $L_{12}$, Cu$_3$Au, and
  - $L_{20}$ – $L_{39}$, ordered alloys based on the bcc lattice, ($L_{21}$, Heusler alloy, prototype Cu$_2$AlMn).
- **Type M**, “miscellaneous,” a category so nebulous that it was never used, and
- **Type O**, organic systems, a subject all its own which is beyond the scope of this article.
Each section of Strukturbericht was divided into a listing of the elements and prototype compounds indexed by Strukturbericht symbols, including the space group, occupied Wyckoff positions, lattice constants, and atomic positions, as well as drawings of the crystal.

At the end of each alphabetic Strukturbericht section the editors placed a long review of the literature for each type.

3. Strukturbericht Band II, 1928-1932

The second volume of Strukturbericht[10] was published in 1937 and covered the years 1928 through 1932. In 1937 Ewald emigrated to England, having resigned his post at the University of Munich in protest over the firing of all Jewish professors,[13] and so the volume was edited by Hermann, Otto Lohrmann, and Hans Philipp.

The new publication included the only index of Strukturbericht symbols ever published in the original volumes. It also made some changes in the format of the labels: as an example, by this time the editors had identified thirteen compounds with composition $AB_3$ which were impossible to fit in the limited range $D1 - D10$ of volume I, so the format “letter-number-subscript” was introduced. Ammonia, $\text{NH}_3$, formerly $D1$, became $D01$, and skutterudite, formerly $D2$, became $D02$. (Eventually the D0 range would extend to $D024$, Ni$_3$Ti.) This practice was extended to all the other types.

The second volume also introduced the first fourteen entries in the rather general $E$ category, including $E01$, PbFCl. Other $E$ entries included chalcopyrite ($\text{CuFeS}_2$), cubic perovskite ($\text{CaTiO}_3$), and ilmenite ($\text{FeTiO}_3$), which were reclassified from the original $F61$, $G05$, and $G04$ designations, respectively, to $E11$, $E21$, and $E22$.

Other new labels were added:

- Type I, compounds with $BX_6$ radicals. These were mostly renamed from type $H$, e.g. $\text{K}_2\text{PtCl}_6$, which was originally $H61$ and now became $I11$.
- Type K, “complex radicals,” including $K11$, $K2S2O5$, $K11$, $K2S2O6$, and $K12$, Cs$_2$S$_2$O$_6$.
- Type S, the silicates. Several of these had been previously listed in other categories, such as kyanite, Al$_2$SO$_5$, which originally was labeled $H51$ and now became $S01$. In all, thirty-two compounds were identified, all but six of these new to this volume.

4. Strukturbericht Band III, 1933-1935

Volume III was the last multi-year volume of the series, published in 1937.[14] Edited by Carl Gottfried and F. Schlossberger, it covered papers from 1933 through 1935.

This volume did not include any new Strukturbericht types, but, perhaps reflecting the confusion between the letters in all Latin alphabets, it renamed class I as class J.

5. The War Years: Strukturbericht Band IV-VII

The remaining volumes each covered a single year. Remarkably, most were published while World War II was in progress, and despite the fact that many German scientists, following Ewald, had fled the country, or like Hermann, had been imprisoned by the Nazi regime.[15]

- Band IV (covering 1936),[16] edited by Gottfried, published in 1938.
- Band V (1937),[17] again edited by Gottfried, was published in 1940.
- Band VI (1938),[18] was edited by K. Herrmann, was published in 1941, and the last volume,
- Band VII (1939),[19] was again edited by Herrmann and published in 1943, while the Eastern Front with the Soviet Union was collapsing, the allies were invading Italy, and preparations for D-Day were underway.

Much of the final volume concerns updating the list of compounds belonging to a previously defined Strukturbericht symbol. It opens by noting that scandium takes on the face-centered
cubic A1 structure, and ends with an entry for cronstedtite, Fe$_4^{II}$Fe$_2^{III}$[(OH)$_8$—Fe$_2^{III}$Si$_2$O$_{10}$], assigning it to the S5$_1$ type along with the prototype, muskovite (KH$_2$Al$_3$Si$_3$O$_{12}$).

In spite of the War, these later volumes were distributed throughout the world. In the United States, Edwards Brothers (Ann Arbor) published all seven volumes in 1943, “in the Public Interest by Authority of the Alien Property Custodian,” an office created by Presidential order to manage enemy alien property.[20]

6. Post-War: Continuation and Extension of Strukturbericht

With the end of the War, the task of collecting structure reports was transferred to the newly-created International Union of Crystallography (IUCr),[15] which began publishing yearly Structure Reports in English. These volumes emphasize the connection with Strukturbericht by starting with Volume 8, published in 1956 but covering research from 1940-1941,[21] and Volume 9 (1942-1944, published in 1955.[22] Volumes 8 & 9 were actually preceded by Volume 10, published in 1953 and covering the years 1945-1946.[23] Since then the Reports have been published more-or-less regularly.[24]

Structure Reports did not continue the use of Strukturbericht symbols to designate structure types, but this did not end the generation of new labels. In 1949 Colin J. Smithells published his first Metals Reference Book,[25] which included a partial index of Strukturbericht symbols and compounds assigned to each symbol. This list concentrated on metallic systems, and so left out some elements and compounds. In addition, Smithells listed two new compounds, ThSi$_2$, and TeCu$_2$, provisionally giving them the Strukturbericht designation C$_x$. In the second edition of Metals Reference,[7] Smithells extended this, adding many new Strukturbericht. While still following the letter-number-subscript scheme started in Strukturbericht II, the subscripts for the new entries were alphabetic rather than numeric. Thus ThSi$_2$ became Strukturbericht type C$_c$ and TeCu$_2$ became C$_g$. Reflecting the advances in physics in the war and postwar era, the list included the unique structures for uranium and the transuranic elements: A$_a$ (Pa), A$_b$ (β-U), A$_c$ (α-Np), A$_d$ (β-Np), etc. Altogether, Smithells added seventy-five new structures to the list.

In 1958 W. B. Pearson published the first edition of his influential Handbook of Lattice Spacings and Structures of Metals and Alloys.[8] The Handbook included most of Smithells’ Strukturbericht index and added new structures, using the letter-number-alphabetic subscript format, with subscripts chosen to avoid overlap with Smithells. Pearson soon realized the further extensions would become unwieldy, and in the next edition of his Handbook[26] he dropped the Strukturbericht index and listed structures by their Pearson symbols, which have the advantage of making the crystal type and number of atoms readily apparent, at the cost of having numerous structures of wildly different types using the same symbol.

7. Modern indices of compounds

Despite the demise of the Strukturbericht labeling system, it is still useful to have lists of possible crystal structures.

- Trotter and Bree[27] published an index to the original seven volumes of Strukturbericht, but regrettably did not include an index by Strukturbericht type.
- Modern versions of Smithells Metals Reference Book[28] and Pearson’s Handbook[11] include indices of metallic structures by Strukturbericht, Pearson symbol, and space group.
- The Gmelin Handbook of Inorganic and Organometallic Chemistry[29] also includes a Strukturbericht symbols, including the Pearson symbol, space group, and occupied Wyckoff positions for each structure. Unlike the Pearson and Smithells Handbooks, this list includes many non-metallic systems, and shows duplicate structures, which frequently show up in the original Strukturbericht.
Electronic databases are also available:

- The *The American Mineralogist Crystal Structure Database*\(^4\)[30] gives structural information for a large number of minerals, including mineral names, but does not include the *Strukturbericht* designation. When possible, it also links to PDF versions of the original publications.

- *Springer Materials*\(^5\)[31] maintains a constantly updated list of crystal structures. Edited by P. Villars, this is essentially an electronic form of *Pearson’s Handbook*, but it includes non-metallic systems as well.

None of these lists gives a comprehensive list of *Strukturbericht* symbols, which one would think should at least have been included in the 1976 index. In 1995, work was begun to collect the common *Strukturbericht* structures into a web page, eventually called *Crystal Lattice Structures*. The web page was eventually expanded to nearly three hundred structures, both in and out of *Strukturbericht*, but eventually went off line. Recently, the database has been revised and updated as part of a collaboration between the United States Naval Academy and the Curtarolo Research Group at *Duke University*. The resulting page, now known as the Library of Crystallographic Prototypes,\(^6\)[12] is integrated with the AFLOW system for materials discovery.\(^7\)

The site\(^6\) currently includes 590 unique crystal structures, and we are constantly adding to it. We index structures by *Strukturbericht*, Pearson symbol, space group and prototype material. Each entry includes

- The *Strukturbericht* designation of the structure, if one has been given,
- the Pearson symbol
- the space group,
- occupied Wyckoff positions,
- primitive vectors for the lattice,
- basis vectors for each atom in the primitive unit cell,
- a rotatable view of the primitive or conventional unit cell, which can be expanded to show multiple unit cells,
- a standardized Crystallographic Information File (CIF), and
- a structure file which can be used as input for a variety of electronic structure codes.

We will continue to update the database. Our next goal is to include all of the inorganic structures found in the original *Strukturbericht*, Smithells, and Pearson, though we will as always include other systems of interest. We invite suggestions for structures that should be listed.

8. Summary

This has been a very brief review of the history of *Strukturbericht* symbols. This will be expanded in the future, including more historical data. In particular, research is needed to determine how publication of *Strukturbericht* was continued during the Second World War, and to find out why Colin Smithells decided to expand the system when the crystallographic community, as represented by the IUCr, decided not to continue it.

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\(^4\) [http://rruff.geo.arizona.edu/AMS/amcsd.php](http://rruff.geo.arizona.edu/AMS/amcsd.php)

\(^5\) [https://materials.springer.com/](https://materials.springer.com/)

\(^6\) [http://www.aflowlib.org/CrystalDatabase/](http://www.aflowlib.org/CrystalDatabase/)
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