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X-ray diffraction studies on organic crystal structures in the second half of the 20th century and
Yu. T. Struchkov: A Cambridge Structural Database view

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Abstract

The Cambridge Structural Database (CSD) was used to evaluate Yury T. Struchkov's contribution to global X-ray diffraction research across different periods of his career and across several criteria. The first stage of the study was to search for different spellings of his last name and initials and combine the corresponding entries into a single group. Two periods were then examined: from Struchkov's first entry in the CSD (1952) to 1974 (before his team acquired an automatic diffractometer), and from 1975 to the last full year of his life (1994). It was found that in both periods, he ranked first or second in terms of the total number of entries, the number of entries with atomic coordinates, and the number of low-temperature studies. A comparison was made with the results of authors with the closest number of entries to him: James Trotter in 1952–1974, Allan H. White in 1975–1994, and John C. Huffman in the same period for research at low temperatures.

Keywords Comparative statistical analysis · History of science · R-factor · Low temperatures

The work of many scientists often includes various areas of activity: research itself, organizational, educational in the academic sphere, scientific popularization, editorial and publishing, etc. Yury Timofeevich Struchkov was very active in most of the areas listed [1–3], with the exception, perhaps, of academic teaching, which arose in his life only episodically, despite the fact that he spent a lot of time (especially in the middle of his career) training graduate students and new laboratory staff beginning to work under his supervision. Yu. T. Struchkov left behind no textbooks, scientific monographs, or books for the general public, but his persistence in expanding the instrumental horizons of chemists was crucially important for enhancing the role of X-ray structural analysis in the work of many scientific groups both at the Institute of Organoelement Compounds (INEOS) (where he worked from the moment of its creation) and in other scientific organizations not only in Moscow, but also in many cities of the Soviet Union.

Yury Struchkov's outstanding contribution to the development of structural research in the USSR is beyond doubt [1–3], but how does the level of work carried out directly by him or with his participation compare with the world level? His wife (a Doctor of Sciences, who worked at INEOS like Struchkov, but in a different department) recalled [1, p. 143] that in 1970, after returning from a two-month trip to major scientific centers in the UK, Yu. T. said: 'We're in the Stone Age! No one works like us anymore.' Meanwhile, in the 1980s, the staff of Struchkov's laboratory had no doubt, according to Yu. L. Slovokhotov (who was himself one of them in those years), that they were working 'at the maximum of the capabilities in the field of structural research for chemistry' [3], and according to his data [3], in certain years in the early 1990s the X-ray Structural Research Center, which Yu. T. directed, determined about 3% of the structures submitted to the Cambridge Crystallographic Database (CSD).

In my opinion, the use of the CSD [4] for the analysis of Yu. T. Struchkov's contribution to X-ray diffraction studies on organic crystal structures is particularly appropriate not only because this database is the most complete repository of this type of data, but also because access to it in the USSR became possible thanks to Yu. T.'s acquaintance [1–2] with the founder of the Cambridge Crystallographic Data Centre (CCDC) and the CSD, Olga Kennard [5].

The development of the CSD began in 1965 [4, 6], but the first papers devoted to diffraction studies of organic crystals began to appear in the early 1920s [7–9], so over the course of a number of years, the database was entered with results from both current publications and previously published works. There was no technical difference between entering old and new data, since both were received at that time only on paper; however, there was probably some difference in the methodology for selecting data and the completeness of their presentation for different time periods. This can be judged, in particular, by the fact that CSD version 6.00 (Apr 2025) + 1 update does not contain information from the above-mentioned papers [7–9] (and a number of other early publications), despite the fact that in [8–9] not only the unit cell parameters but also the coordinates of non-hydrogen atoms were determined. In addition, this version of the CSD contains ~400 records with results published before 1966 inclusive, in which the authors are listed without initials (e.g., 'Starovskii, Struchkov') and/or only the first author's last name is given (e.g., 'Struchkov +' or 'Okaya et al'). The largest number of such records pertain to publications from 1965–1966, and, in my observations, all records with incomplete author attribution correspond to structures for which atomic coordinates were not determined. However, at that time, obtaining even partial information on the crystal structure, which was usually given in articles in addition to the unit cell parameters, was time-consuming, i.e., when comparing the personal research activity of crystallographers before the early 1970s, such publications are also significant. Fig. 1 shows how the ratio between the number of the CSD

entries with and without atomic coordinates has changed over the 50 years since 1923 (the year in which the earliest entry in this database dates back).

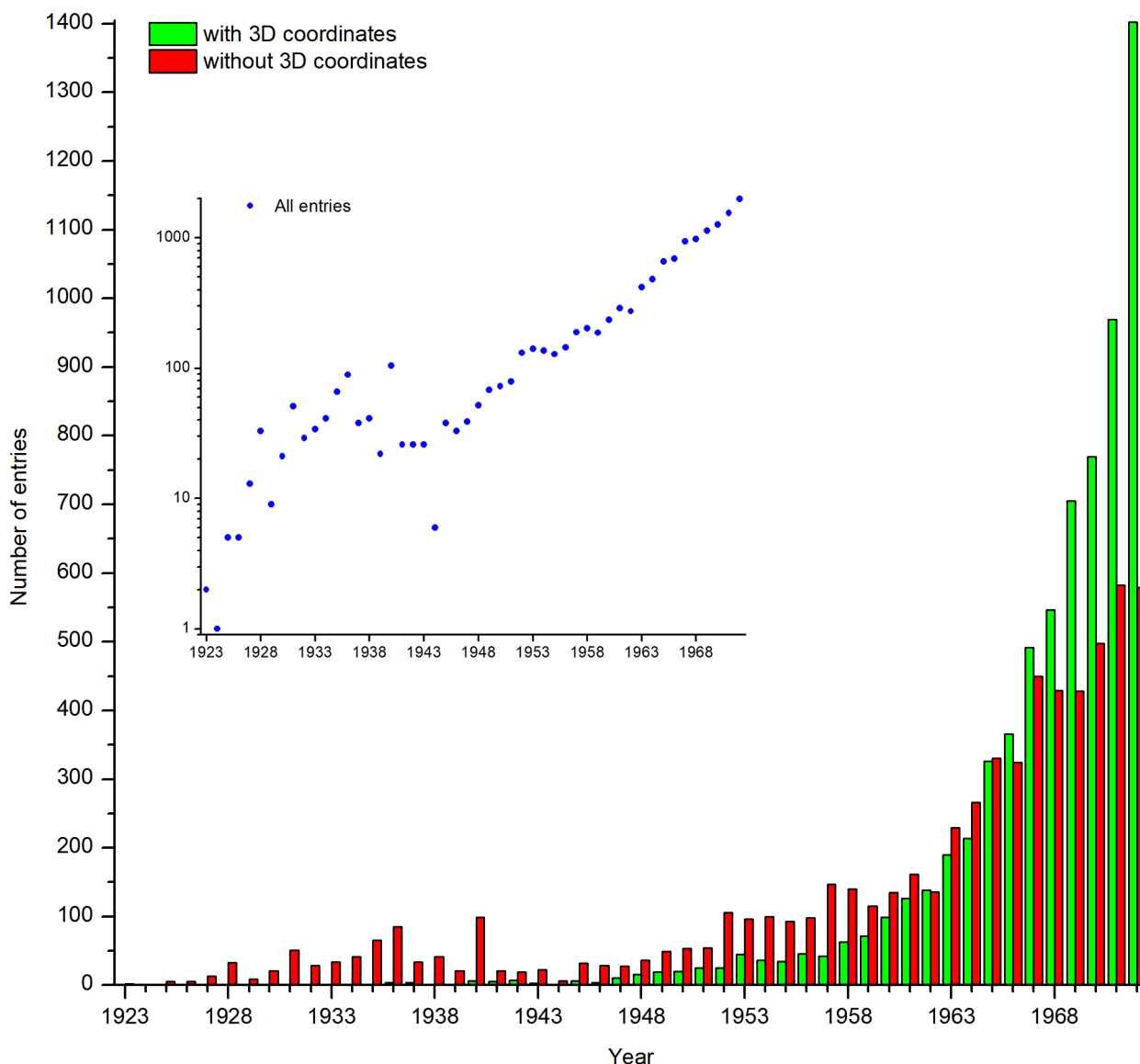


Fig. 1 Number of entries in the CSD (version 6.00 + 1 update) with and without atomic coordinates; the inset shows the change in the total number of entries on a semi-logarithmic scale

Despite the aforementioned incompleteness of the early research results in the CSD, one can expect that the general trends are accurately reflected in this figure. It can be seen that the first slight excess of entries with atomic coordinates over entries without coordinates occurs in 1962 (138/136). However, for several years afterward, entries without coordinates predominate in the CSD. Only since 1966 does a steady excess of entries with atomic coordinates over entries without coordinates begin, reaching ~ 2.4 times by 1972.

The change in the ratio between the number of entries with and without atomic coordinates reflects the qualitative changes in the methodology of X-ray diffraction experiments and the subsequent structural interpretation of their results that occurred in the late 1960s and

early 1970s thanks to the advent of mass-produced automatic diffractometers and computers. The latter were essential both for controlling the diffractometers and for solving structures, including by direct methods [10].

Before comparing Yu. T.'s results with global ones, it is necessary to examine in more detail the problem of identifying researchers in the CSD. In the annual information on authors [11] with a large number of records (in 2026, this meant 500 or more), one line (author) contains only one spelling variant of the initials and surname; for Yury Struchkov, this is 'Yu.T.Struchknov'. The incompleteness of the information on authors in some records up to and including 1966 has already been noted above. Moreover, in the publications themselves, even if they provide author's versions of the given and last names using letters of the Latin alphabet only, these versions may differ (for example, they may contain only one given name without other initials, and not always the exactly first one, or several initials without their decoding). Furthermore, typos in names/surnames are possible both directly in articles and as a result of data transfer to the CSD (in the past, publication in a journal was followed by data entry into the CSD, rather than the other way around, as is currently the case). Adapting names/surnames written with diacritics in the Latin alphabet, and especially those written in other alphabets or non-alphabetic scripts, to Latin letters is often ambiguous. Finally, different people may have the same surname, first name, and initials. Currently, there are several identifiers, such as ORCID [12], which, when specified by authors, allow to avoid the problems listed above, but their use only began in the 2010s.

In this paper, I have attempted to combine all records related to Yu. T. Struchkov as an individual. Some spelling variations of his initials and surname (e.g., 'Yu.Struchkov' or 'Y.T.Struchkov') are obviously possible, while others ('G.T.Struchkov') seem unexpected at first glance, although Yu. T. himself mentioned in his letters from the UK that he was called George there [1, p. 531]. It is possible that not all misspellings have been identified, but additional variations are unlikely to affect the statistical results. Thus, Table 1 lists five incorrect spellings, while the total number of records with them is 11, including 6 without atomic coordinates. The criteria for attributing erroneous spellings of the surname and initials in publications to Yury Struchkov were affiliation with INEOS, if indicated, or the presence of at least one of Yu. T.'s regular co-authors in the list of authors; in addition, in some cases, the spelling was correct in the original Russian-language articles.

Table 1 Variations of Yury T. Struchkov's designation in the CSD entries (version 6.00 + 1 update); incorrect spellings of the surname or initials are highlighted in italics

Variant	Years	Number of entries	
		with 3D coordinates	without 3D coordinates

G.T.Struchkov	1957	0	4
<i>G.T.Struckov</i>	1957	0	1
Struchkov	1960, 1964, 1966	0	4
Struchkov +	1952, 1965	0	13
Y.Struchkov	1999	1	0
Y.T.Struchkov	1975–2001	34	2
<i>Yu.P.Struchkov</i>	1987	1	0
Yu.Struchkov	1993, 1995, 1998	5	0
<i>Yu.T.Struchdov</i>	1988	1	0
Yu.T.Struchkov	1953–2004	2505	302
<i>Yu.T.Struchov</i>	1963, 1986	1	5
<i>Yu.T.Stuchkov</i>	1993, 1995	2	0
In total	1952–2004	2550	331

Thus, the total number of entries in the CSD (version 6.00 + 1 update) with Yury Struchkov is 2881, taking into account all spelling variations of his first name (initials) and last name. Their distribution by year is shown in Fig. 2. In the already mentioned list [11] of the most representative CSD authors for Yu.T.Struchkov as of January 1, 2026, there are 2807 records, which coincides with the results presented in Table 1. Taking into account the additional records, Yu. T.'s place in the ranked list may be slightly higher (in 2026, not 29, but 23), if the other authors do not have entries with alternative first names/last names or their number is less than that of Yu. T. (I did not conduct such a study as part of this work).

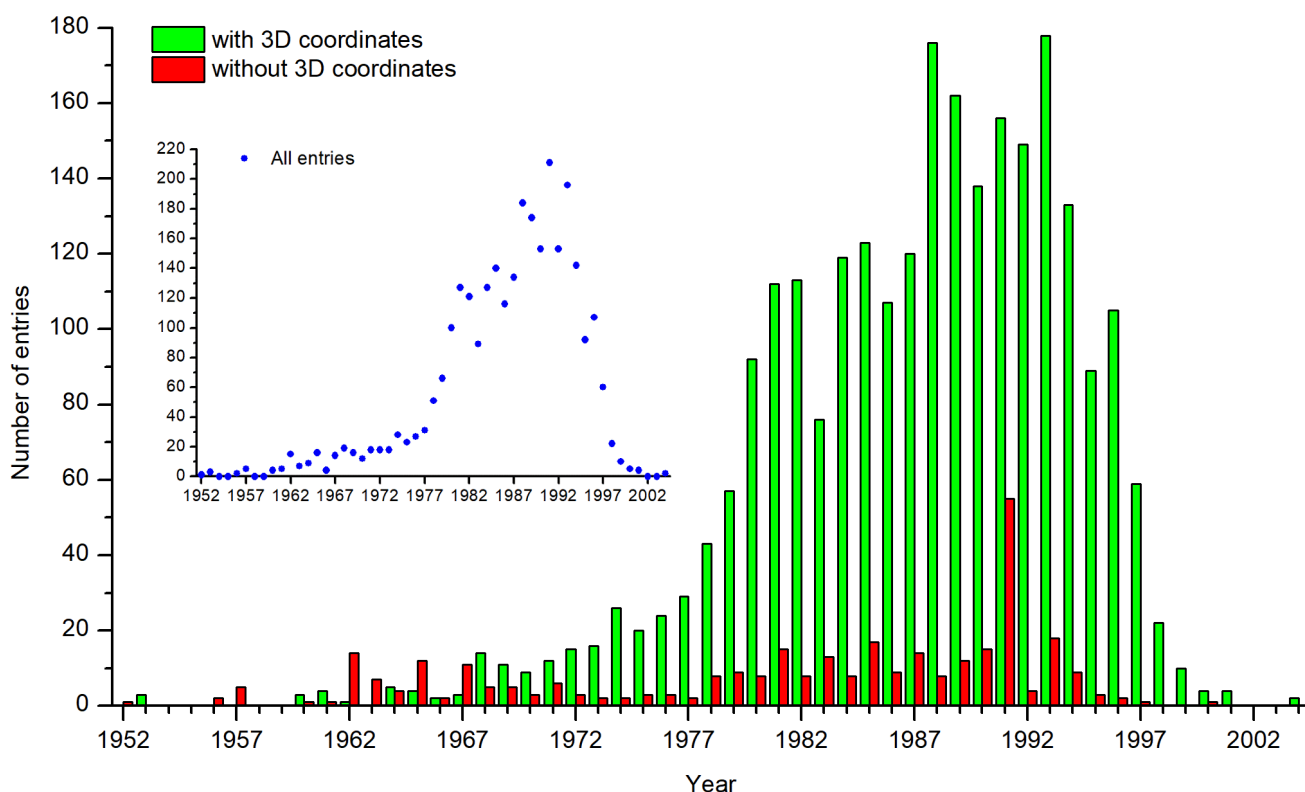


Fig. 2 Number of entries with Yury T. Struchkov (all spellings) in the CSD (version 6.00 + 1 update) with and without atomic coordinates; the inset shows the change in the total number of entries

The time interval of research with the participation of Yu. T., included in the CSD, covers 1952–2004, however, to assess his annual contribution to the CSD, it is appropriate, in my opinion, to take as the upper limit the last full year in which he directly participated in the work, i.e., 1994. Struchkov, who saw with his own eyes the capabilities of modern equipment in the UK, managed to convince the director of INEOS, Academician Alexander N. Nesmeyanov, to achieve the acquisition of the first foreign automatic diffractometer at the expense of three Moscow institutes (including INEOS) [1–2]. Four-circle diffractometer Hilger & Watts Y290 [13] was obtained by Yu. T.'s group in 1974, according to the majority of authors [1–2], although according to the recollections of L. A. Aslanov, the Hilger & Watts diffractometer was already working in 1972 [1, p. 247]. Fig. 2 likely indicates this date, as there is a noticeable increase in entries in 1974. That is, if we attribute this increase to the automation of the experiment, the device must have been obtained earlier, as time was needed to prepare papers, and the publication process at that time typically took at least several months. At the same time, there is a slight decrease in entries in 1975 and 1976, so it is possible that the 1974 surge is due to other factors, such as a change in work procedures due to the separation of the group into a separate administrative unit in 1973.

In any case, Yu.T.'s experimental career was divided into two almost equal parts: before and after his work on automatic diffractometers. Based on the more extensive evidence regarding the time of acquisition of the Hilger & Watts diffractometer in 1974, two periods of Yu.T.'s work will be discussed below: 1952–1974 and 1975–1994.

Finally, for a more accurate assessment of his contribution to the global diffraction studies of organic crystals, it is necessary, in my opinion, to exclude from the overall set of CSD entries those that relate to areas in which Yu. T. was not involved at all (in [1–3] it is described in detail what he was involved in). Yury T. Struchkov has no works using neutron or synchrotron radiation, studies at high pressures, and there is only one entry in the CSD, devoted to powder diffraction (without determining the coordinates of atoms). All these areas were just beginning during the first period of Yu. T.'s activity (1952–1974). Subsequently, the number of works in them increased (Table 2), although in comparison with the total number of studies (Fig. 1) it remained insignificant.

Table 2 Numbers of entries in the CSD (version 6.00 + 1 update) corresponding to the specified experimental conditions (numbers of compounds are given in brackets)

CSD queries/filters	1952–1974		1975–1994	
	with 3D coordinates	without 3D coordinates*	with 3D coordinates	without 3D coordinates*
Neutron radiation	130 (107)	34 (23)	599 (455)	129 (51)
Synchrotron	0	1	10 (9)	2 (2)
Powder	9 (9)	31 (28)	116 (86)	52 (27)
Pressure	4 (3)	3 (1)	23 (12)	23 (8)

The columns 'without 3D coordinates' indicate numbers of all entries, but when counting compounds, only those for which there are no entries with coordinates in the corresponding period for the corresponding query/filter are taken into account.

The following results refer to single-crystal X-ray diffraction studies at atmospheric pressure presented in the CSD (version 6.00 + 1 update) and hereinafter abbreviated as set I.

1952–1974

The author designations that appear most frequently in the entries of set I during 1952–1974 are given in Table 3.

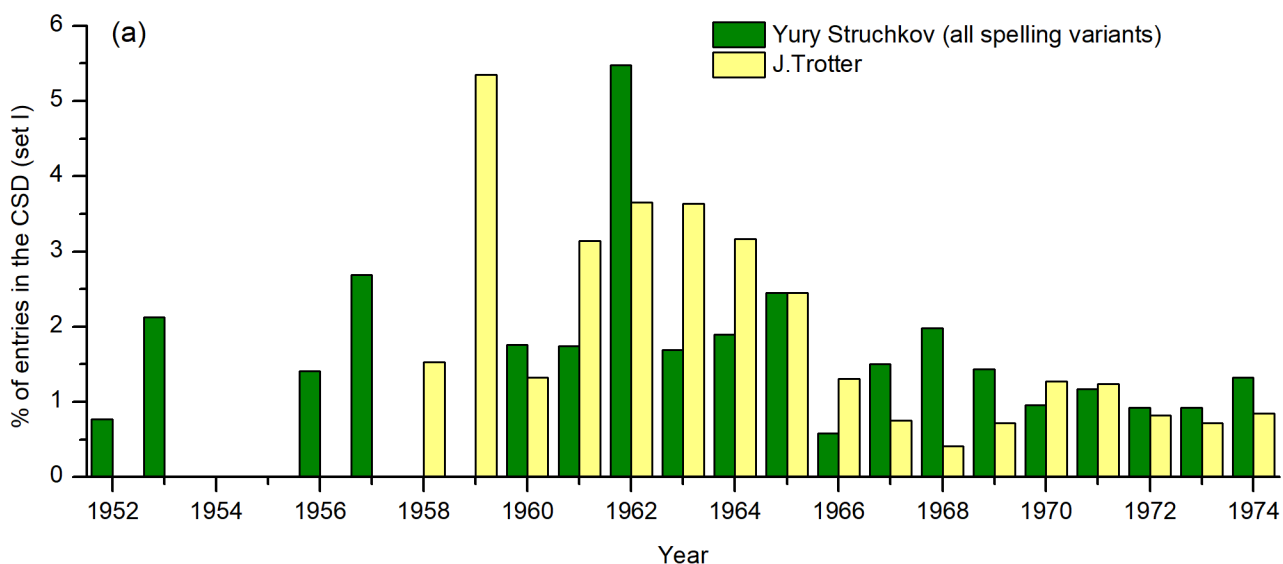
Table 3 Authors with the largest number of entries in the CSD (set I) in 1952–1974

Set I	Entries	Set I with 3D coordinates	Entries
Yury Struchkov (all spelling variants)	214	J.Trotter	163

J.Trotter	192	Yury Struchkov (all spelling variants)	128
G.M.J.Schmidt	183	G.A.Sim	108
G.A.Sim	142	F.A.Cotton	108
M.Nardelli	133	J.A.Ibers	103

During this period, Yu. T. ranks first in the total number of entries, but in terms of the number of entries with determined atomic coordinates, he yields this position to James (Jim) Trotter [14–15]. It is significant that Gerhard Schmidt [16], who ranks third in the total number of entries, is outside not only the top five, but also the top thirty in terms of the number of entries with coordinates (47 entries, 32–33 place). This once again illustrates how difficult it was to determine the structure of organic crystals before the 1970s.

Fig. 3 shows the values of the fractions that entries with Yury Struchkov and J. Trotter make up of the total number in set I in different years.



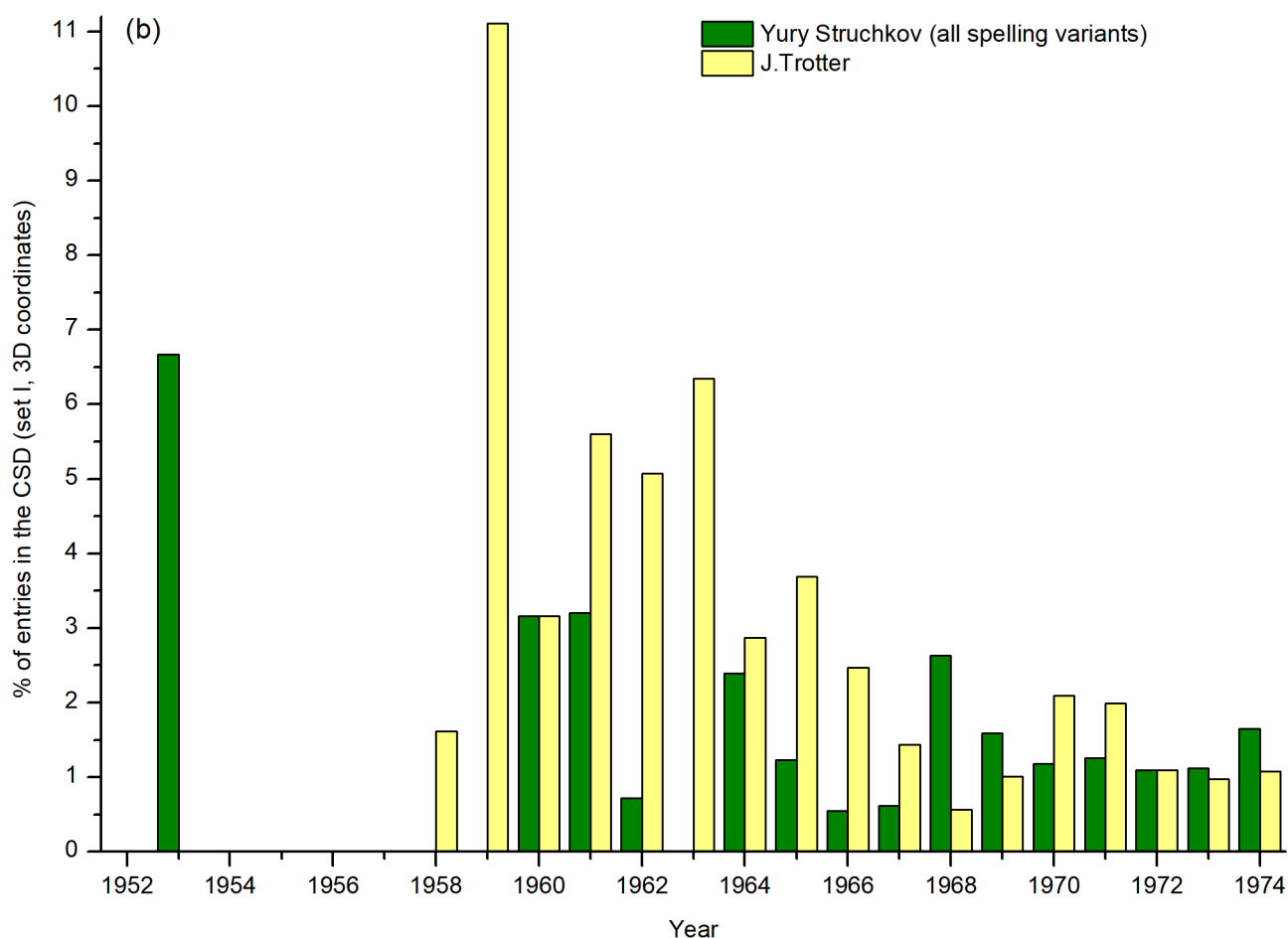


Fig. 3 Fractions of entries with Yury Struchkov and J. Trotter from the total number in set I (a) and in set I with 3D coordinates (b)

It is seen that each of them had a very high fraction of CSD entries in some years before 1965: >5% of the total number of entries and even more of the number of entries with atomic coordinates (up to 11% for J. Trotter). The main reason for this effect is the small total number of publications in 1952–1964, especially with atomic coordinates (Fig. 1), as a result of which the portion of each study was high. However, even after 1964, when the total number of annual entries began to exceed 600, reaching 2121 by 1974 (more than 300 and 1576, respectively, for entries with atomic coordinates), the fractions of studies with Struchkov or Trotter rarely fell below 1% for both the total number of entries and for structures with atomic coordinates (Fig. 3a, 3b).

In addition to the number of structures studied, it is of interest to compare their complexity and the quality of their determination. A detailed analysis of complexity requires taking into account the symmetry of the molecules and a discussion of what additional factors could have facilitated or hindered the interpretation of diffraction data at that time (e.g., the planarity or non-planarity of molecules). In this paper, I limited myself to a formal criterion (available when saving search results using the ConQuest program [17]) – the number of atoms

with certain coordinates (N_{at}). For many years, the main criterion for the quality of X-ray diffraction studies was the R -factor. Then, publications began to indicate several additional characteristics, but they are absent from the CSD. In statistical studies, to reduce the significance of individual anomalously high values in data sets, the median is used rather than the arithmetic mean. Figure 4 shows the median values of N_{at} and R -factor by year for sample I, as well as for entries with Yury Struchkov and J. Trotter. In their determination, in all cases, only entries were used for which the conditions $N_{\text{at}} > 0$ and $R > 0$ were simultaneously met.

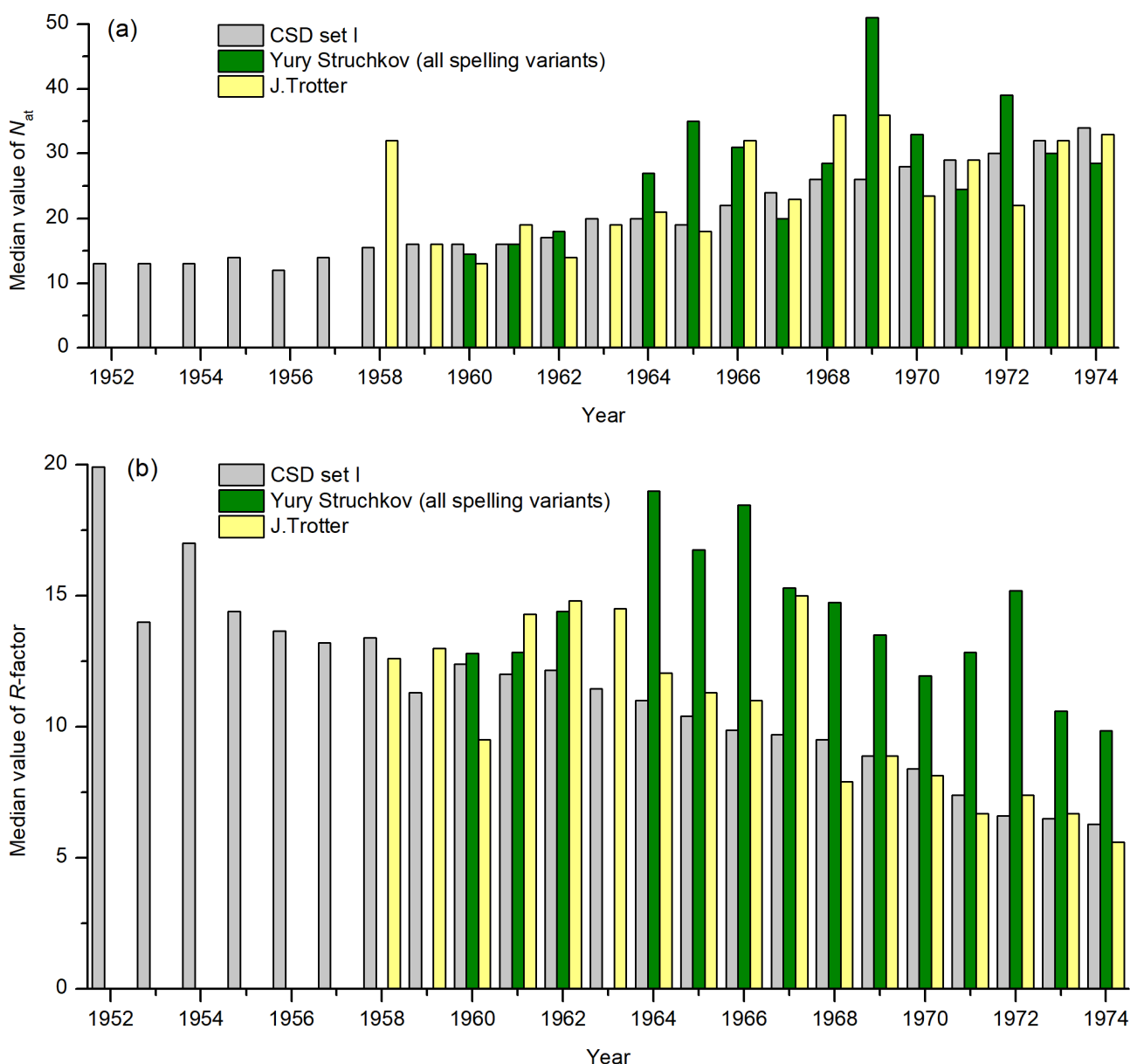


Fig. 4 Median values of N_{at} (a) and of R -factor (b) for set I and for entries with Yury Struchkov and J. Trotter

If we consider all the entries in set I, we see a gradual increase in median N_{at} values during the period under discussion, with minor deviations from this trend in individual years, and a gradual decrease in median R values, with fluctuations between 1952 and 1960 greater than

those for N_{at} , apparently explained by the aforementioned small number of studies. However, in sets of entries with Struchkov and Trotter, these trends are expressed to a significantly lesser extent, especially for N_{at} .

Thus, in Trotter's set, the median N_{at} value of 32 occurs in 1958 (with one entry per year), in 1966 (9 entries), and in 1973 (13 entries). It alternates with both higher and lower values in other years. For Yu. T.'s entries, one can note an increase in the median N_{at} values from less than 20 in 1960–1962 to higher ones in the period 1964–1974, but with fluctuations within it of up to ~2.5 times (20 in 1967 for 3 entries, 51 in 1969 for 11 entries, and 29 in 1974 for 26 entries). In 1959–1963, the median values of N_{at} for Yu. T.'s and Trotter's sets were close to the values for the whole set I. Subsequently, the values for Yu. T. often exceeded those for set I or were approximately equal to them, while for Trotter they were often approximately equal or slightly lower.

The trends in the median values of the R -factor for both authors were somewhat unexpected, especially for Struchkov. Trotter's median values of the R -factor increased slightly from 1958 to 1962 (from 12.6% to 14.8%), then began to gradually decline, initially remaining noticeably higher, then only slightly higher than the values for set I. In 1967, he had an outlier (from 11% in 1966 to 15% in 1967), but then his values got closer to the values of set I. For Struchkov, in 1960–1961, the median values of the R -factor only slightly exceeded the values for set I. In 1962, the difference increased, as did the median values of the R -factor themselves for Yu. T.'s entries. Then (in 1964), he experienced an even greater increase in the median value of the R -factor. Subsequently, his R -factor values began to decline, remaining significantly (at least 3.55%) higher than the values for set I until the end of the period under consideration. It is likely that this circumstance – a significant worst quality of the determined structures while maintaining a leading position in the number of studies – was one of the reasons for Yu. T.'s dissatisfaction with his work in the early 1970s, as mentioned above.

1975–1994

The author designations that appear most frequently in the entries of set I during 1975–1994 are given in Table 4.

Table 4 Authors with the largest number of entries in the CSD (set I) in 1975–1994

Set I	Entries	Set I with 3D coordinates	Entries
Yury Struchkov (all spelling variants)	2341	Yury Struchkov (all spelling variants)	2106
A.H.White	1783	A.H.White	1741
F.A.Cotton	1263	F.A.Cotton	1193
A.L.Rheingold	1042	A.L.Rheingold	1010

In this period, Yu. T. leads by a wide margin both in the total number of entries and in entries with atomic coordinates. The next five authors were also minimally affected by the inclusion of coordinates (unlike in the period 1952–1974): only a rearrangement of the authors in positions 5 and 6 occurred (M. B. Hursthouse and B. W. Skelton).

Figure 5 shows the percentages of entries with Yury Struchkov and Allan H. White [18–20] in the total number of entries in set I in different years.

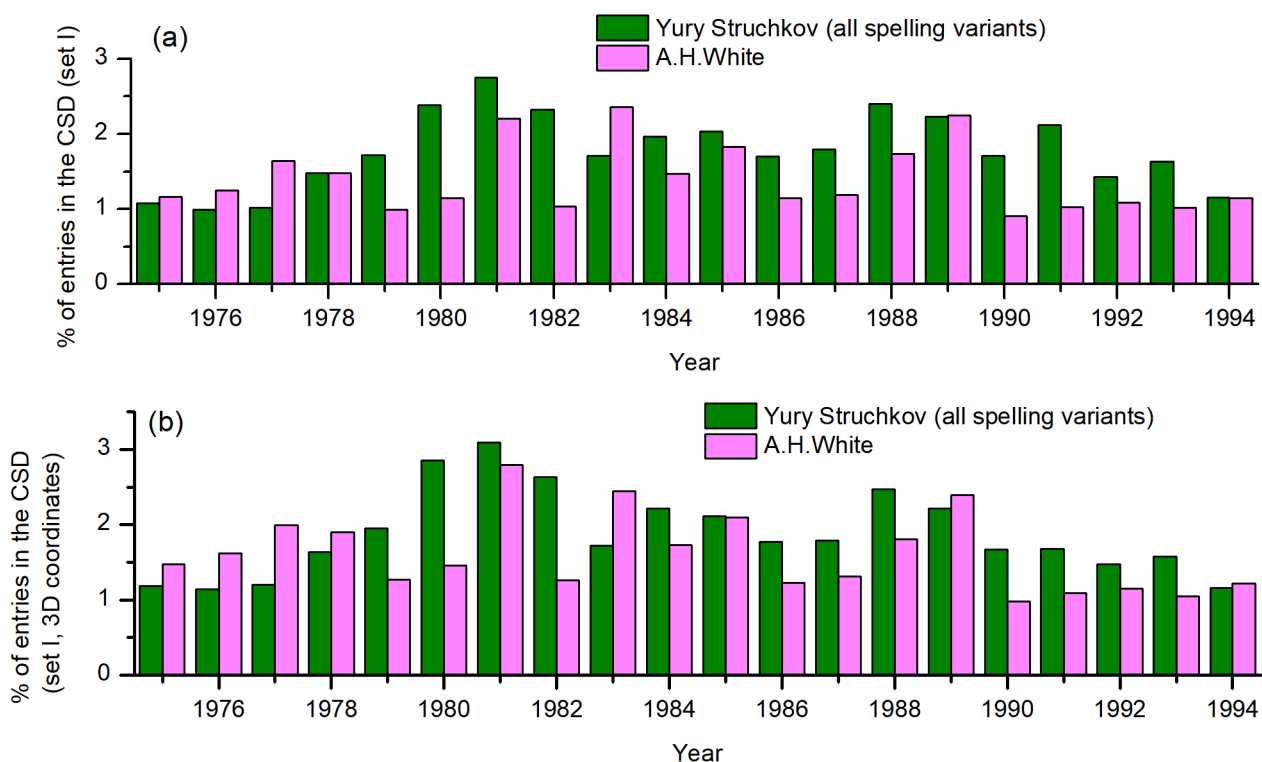


Fig. 5 Fractions of entries with Yury Struchkov and A.H. White from the total number in set I (a) and in set I with 3D coordinates (b)

During the period under consideration, the fractions of entries by both authors fluctuated, but the amplitude of these fluctuations was significantly smaller than that of Struchkov and J. Trotter in 1952–1974. Until 1978, Allan White had more entries, but then the lead passed to Yu. T. (with the exception of two years – 1983 and 1989). The fraction of Yu. T.'s entries did not fall below 1% (the minimum value for all entries was 0.99% in 1976, while for entries with atomic coordinates it was 1.14%), while A. H. White's minimum values correspond to 1990: 0.91% and 0.98% for all records and records with atomic coordinates, respectively. The maximum values of the fractions reach 2.75% (3.10% with atomic coordinates) for Yu. T. in 1981 and 2.36% for the total number of entries in 1983 and 2.79% for the number of entries with atomic coordinates in

1981 for A. H. White. It should be noted that Struchkov's most significant years in terms of contribution to the CSD were the early 1980s, and not the early 1990s, as was written in [3]. It was in 1980–1982 that the fraction of his entries with atomic coordinates was greater than 2.5%, reaching (as already written) 3.10%.

Figure 6 shows the median values of N_{at} and R -factor by year for set I, as well as entries with Yury Struchkov and A. H. White. As for the period 1952–1974, in all cases, only entries for which the conditions $N_{\text{at}} > 0$ and $R > 0$ were simultaneously met were used in determining these values.

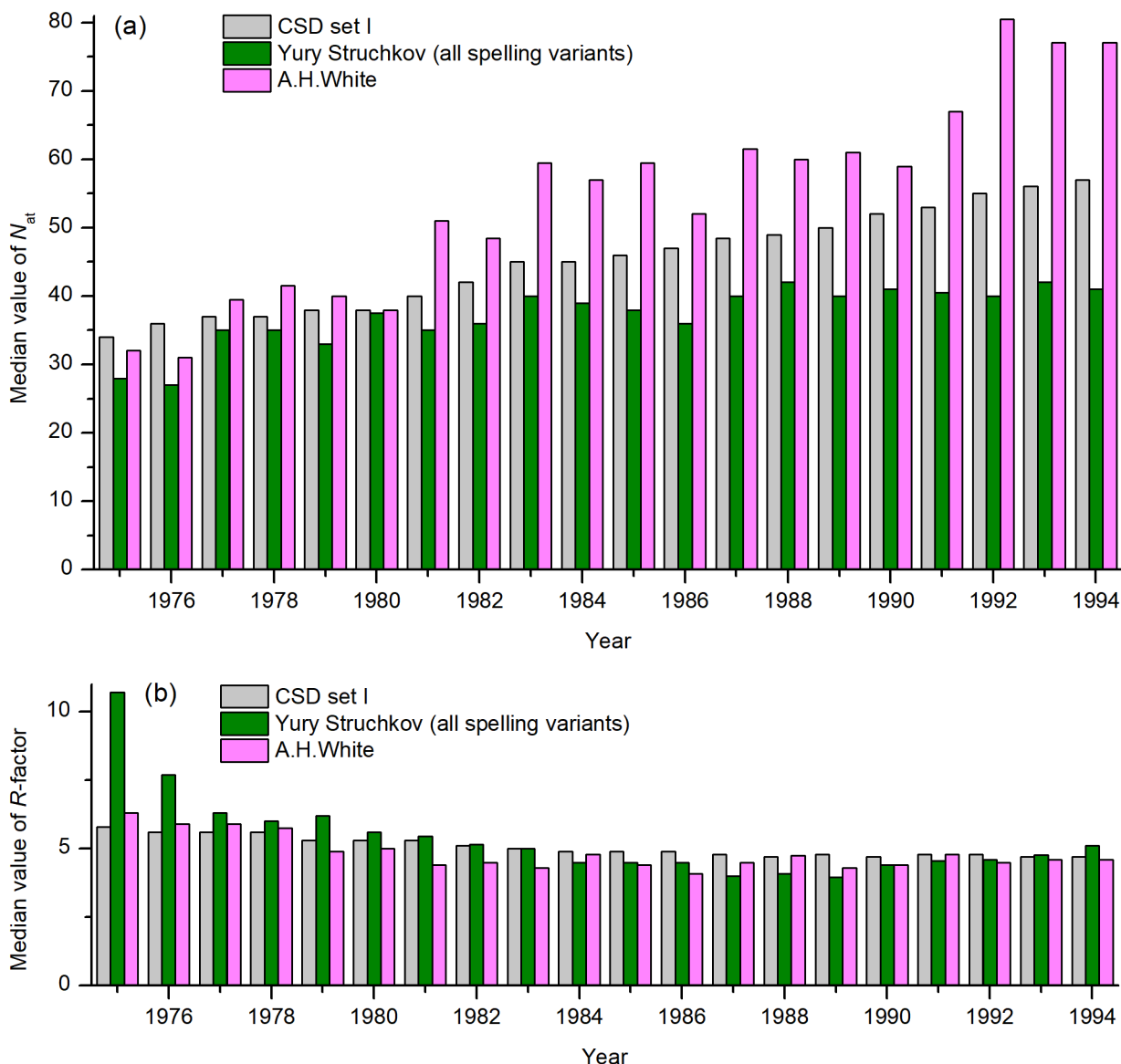


Fig. 6 Median values of N_{at} (a) and of R -factor (b) for set I and for entries with Yury Struchkov and A.H.White

The median N_{at} values for set I (Fig. 6a) continued to gradually increase in this period (from 34 in 1975 to 57 in 1994), with the trends for Struchkov and White differing both from

each other and from set I. For Yu. T., from 1975 to 1980, the median N_{at} values increased from 28 to 38 (slightly lagging behind set I), but subsequently they fluctuated in the range of 35–42 without an upward trend. For White, in 1975–1976, the values were also slightly lower than for set I, but then began to increase significantly faster than in set I (the maximum difference reached 26 in 1992). Thus, it can be stated that for Yu. T., the typical size of molecules forming crystals remained almost unchanged for most of the period under consideration, whereas Allan White took part in studies of crystals formed by significantly larger molecules.

The decrease in the median values of the R -factor for set I continued in 1975–1994 (from 5.8 to 4.7%) (Fig. 6b), but significantly slower than in 1952–1974 (from 19.9 to 6.3%, Fig. 4b), which is due to the physical limit of this parameter. For Struchkov, a sharp decrease in the median values of the R -factor occurred in 1975–1977 (from 10.7 to 6.3%), which, apparently, can be explained by the completion of the publication of the results obtained before the use of automatic diffractometers. Subsequently, the median values of the R -factor for Yu. T. were close to the values of set I, and in some years were noticeably lower than them (by 0.85% in 1989, by 0.8% in 1987). White's median R -factor values from 1975 to 1978 were slightly higher than those of set I, and then slightly lower or nearly equal to them. The difference between the lowest median R -factor values for White and those of set I was almost the same as for Struchkov: 0.9% in 1981 and 0.8% in 1986.

Low-temperature investigations

Nina G. Furmanova (nee Bokii) remembered about the process of writing an article together with Yu. T., devoted to the first low-temperature study of crystals in the Soviet Union, and the work itself [1, p. 210–212]. She did not indicate the bibliographic data of this publication, but it is not difficult to find it by the given name of the compound (1,1,4,4-tetramethyl-1,4-digermanacyclohexadiene) [21]. Meanwhile, if we search in the CSD (version 6.00 + 1 update), it turns out that the corresponding entry (TMGECH) has a temperature of 295 K, although the paper not only indicates the study temperature (-50 °C) in several places (Fig. 7), but also describes in detail the setup used for crystal growth in a capillary and the subsequent recording of diffraction patterns using liquid nitrogen.

CRYSTAL AND MOLECULAR STRUCTURE OF 1,1,4,4-
TETRAMETHYL-1, 4-DIGERMANIUM CYCLOHEXADIENE-2,5

N. G. Bokii, G. N. Zakharova,
and Yu. T. Struchkov

UDC 548.737

A complete x-ray structural investigation has been made of the compound $(\text{CH}_3)_2\text{Ge}(\text{CH})_2$ (m.p. about $+10^\circ\text{C}$). Photographs were taken on a Weissenberg x-ray goniometer at -50°C . It was found that the molecules of the substance are dimeric and contain practically flat six-membered heterocyclic rings, so that the compound must be named 1,1,4,4-tetramethyl-1,4-digermanium cyclohexadiene-2,5. As in previously investigated compounds of this class, the bond lengths found, $\text{Ge}-\text{C}$ ($1.97 \pm 0.02 \text{ \AA}$) and $\text{C}=\text{C}$ ($1.33 \pm 0.04 \text{ \AA}$), indicate that there is no appreciable $d-\pi$ -conjugation in the heterocyclic ring.

Fig. 7 The title, authors, and abstract of Yury Struchkov's paper, dedicated to a detailed description of the first low-temperature study of crystal structure in the Soviet Union

A brief report on the work being carried out, indicating the space group for crystals of this compound (among others) and preliminary values of the unit cell parameters, was published two years earlier [22] (in the English version, Nina Georgievna's middle initial was incorrectly indicated), but it was not included in the CSD. Thus, it can be regretfully noted once again that the data in this database on early (before the late 1960s) research is incomplete. However, their refinement and supplementation represent a very time-consuming and resource-intensive task, so the following discussion is based on the data available in the CSD.

From set I, entries were selected for which $0 < T < 283 \text{ K}$. Specifying the first inequality is necessary because the CSD contains entries in which the values 0 or -9999 are specified for T . Distributions of the selected entries (set I, low T) by year for the entire data set and separately (inset) for Yu. T. are shown in Fig. 8.

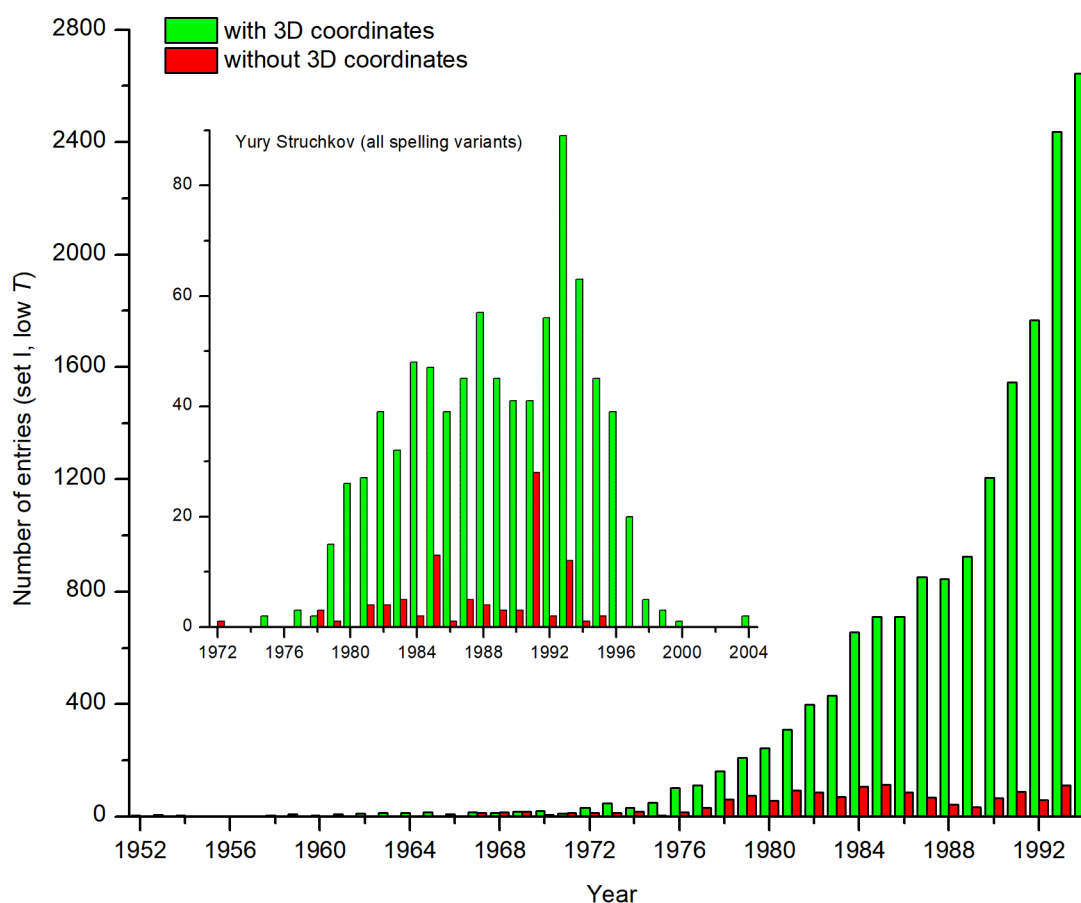


Fig. 8 The number of records in the CSD (set I) for which $0 < T < 283$ K; the inset shows the number of entries with Yury Struchkov

According to the CSD data, up until 1975, the total annual number of entries in the CSD (with and without atomic coordinates) describing the results of X-ray structural studies at temperatures below 283 K did not exceed 60 (58 in 1973, 54 in 1975). Only since 1976 has the number of entries, both total and with atomic coordinates, begun to increase rapidly. A similar situation is observed for entries with Yu. T., although I note once again that early studies are not fully presented in the CSD. Nevertheless, objectively low-temperature studies began to make up a significant part of the work in Struchkov's team only after the acquisition in 1976 of a Syntex 2₁ automatic diffractometer equipped with a low-temperature attachment [1, p. 576], which was further improved by the laboratory staff and an intern [23]. The advantages and possibilities of low-temperature diffraction studies are described in [24]. In the context of this work, I will mention the improvement in the quality of structural information compared to room temperature and the possibility of studying samples that are liquid (or gaseous) under normal conditions.

Undoubtedly, the advancement of mass-produced low-temperature devices contributed to an increase in the fraction of low-temperature experiments worldwide, but to what extent did this increase occur simultaneously at major X-ray centers? The authors most frequently encountered

in set I entries from 1975–1994, with the additional condition $0 < T < 283$ K, are listed in Table 5.

Table 5 Authors with the largest number of entries in the CSD (set I) relating to 1975–1994 with the additional condition $0 < T < 283$ K

Set I	Entries	Set I with 3D coordinates	Entries
J.C.Huffman	852	J.C.Huffman	807
Yury Struchkov (all spelling variants)	808	Yury Struchkov (all spelling variants)	717
M.M.Olmstead	449	M.M.Olmstead	441
P.G.Jones	398	P.G.Jones	391
M.H.Chisholm	387	M.H.Chisholm	366

It is noteworthy that, compared to Table 4, only Yury Struchkov remains in the top five! He occupies second place in both lists of Table 5 (by the total number of low-temperature entries and entries with atomic coordinates), rather than first place, but the difference in the number of entries between the second and third positions (Marilyn M. Olmstead [25]) is much greater than between the second and first (John C. Huffman [26]).

Figure 9 shows the values of the fractions of entries with Yury Struchkov and J.C. Huffman from the total number of low-temperature studies with atomic coordinates in set I in different years.

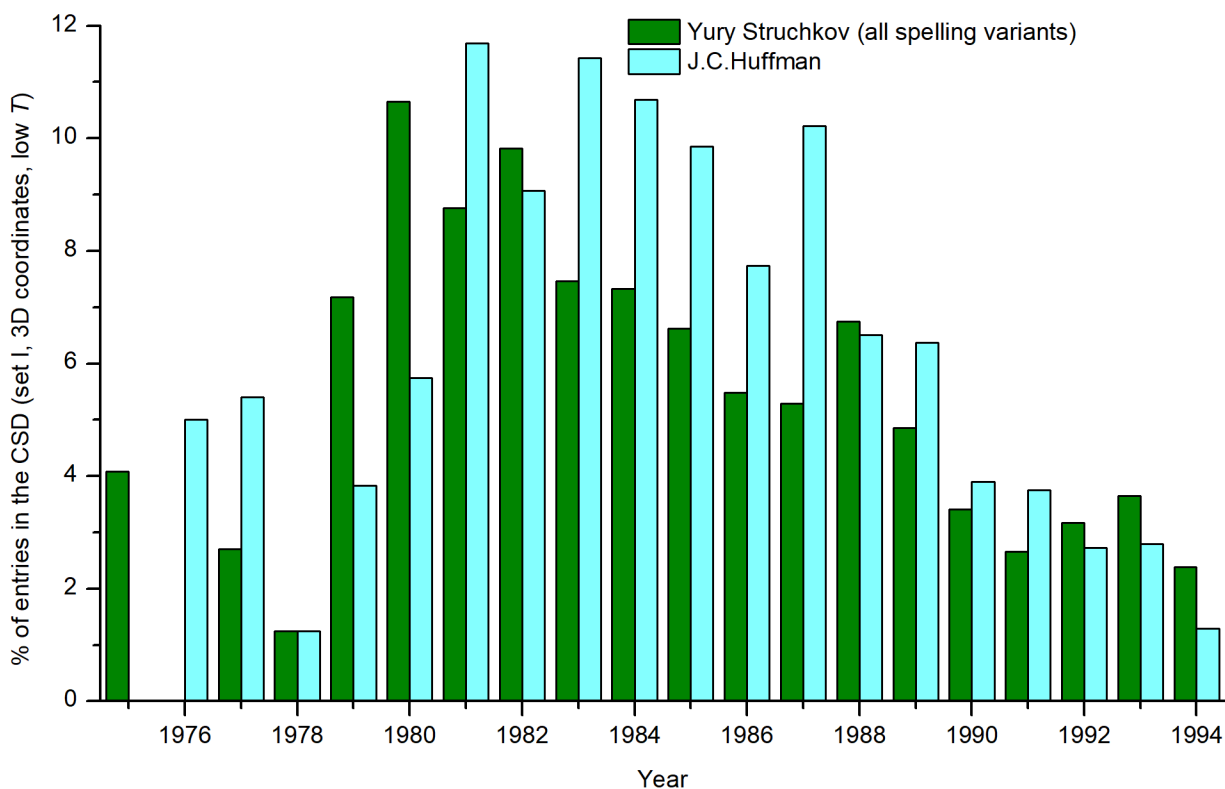


Fig. 9 The fractions of entries with Yury Struchkov and J.C. Huffman from the total number in set I, satisfying the condition $0 < T < 283$ K and containing the coordinates of atoms

Figure 9 clearly shows that these two teams have been the leaders in global low-temperature research for many years: from 1979 to 1989, their combined contribution was more than 10% (according to CSD data), including more than 16% in 1979–1989, exceeding 20% in 1981. The annual number of entries with John C. Huffman was generally significantly higher, but it was Yury Struchkov's team that first exceeded 10% (in 1980). The noticeable decrease in the fractions of entries after 1989 for both Yu. T. and J. C. Huffman is obviously due to the wider distribution of commercial low-temperature attachments to diffractometers, while the absolute number of entries for Yu. T. reached a maximum in these years (89 in 1993; the maximum for J. C. Huffman during 1975–1994 period was in 1987 – 87 records).

The fraction of low-temperature experiments with determination of atomic coordinates from the total number of studies with Yu. T. is shown in Fig. 10. The sum of the values of the two columns relating to one year is less than 100%, since some entries do not contain atomic coordinates, and a small part of works was carried out at temperatures higher than room temperature.

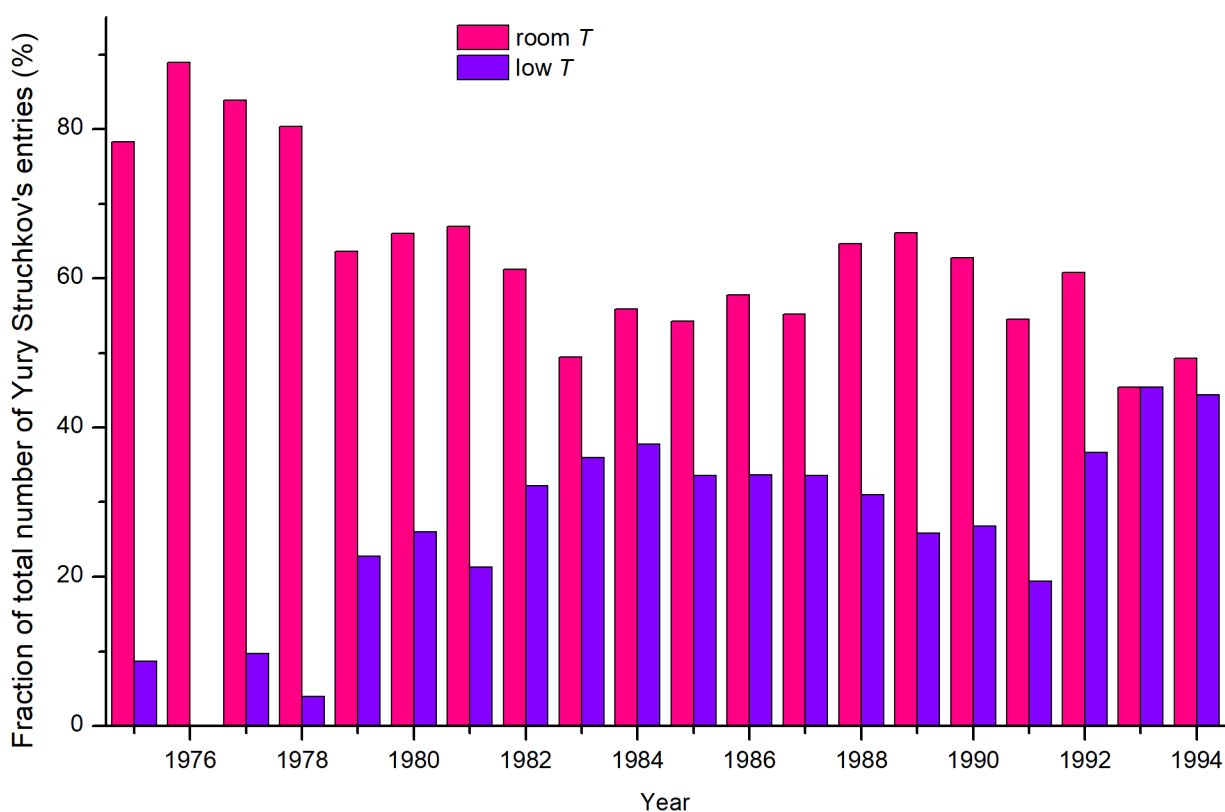


Fig. 10 Fractions of studies containing atomic coordinates and performed at room ($283 \leq T \leq 303$ K) or low ($0 < T < 283$ K) temperatures from the total number of Yury Struchkov's entries in set I

It is seen that the increase in the fraction of low-temperature studies in Struchkov's team was not monotonous. Two peaks are noticeable: in 1984 (37.8%) and in 1993 (45.4%), so in 1993–1994 the parts of determined structures corresponding to room and low temperatures became equal or close. This significantly outpaced the global average increase in the fraction of low-temperature studies: overall, in the CSD, the number of low-temperature structure determinations almost reached the number of room-temperature ones only in 2001 [24].

Conclusion

The Cambridge Crystallographic Database (CSD) currently contains the most comprehensive information on X-ray diffraction studies of organic and organometallic crystals. However, the results of a number of publications from before the early 1970s are either omitted or presented with errors. Nevertheless, the analysis of the available data presented in this paper convincingly demonstrates that Yu. T. Struchkov's crystallographic activity was extremely high throughout his career: from his early years, when his success depended primarily on his personal efforts, to his leadership of a large team (by the standards of X-ray diffraction centers of that time). This led to him having the largest number of entries among all authors in the CSD until the late 1990s (i.e., several years after his death) [27].

Struchkov's significant role in the development of low-temperature X-ray diffraction research both in the Soviet Union and internationally deserves special mention. On a global scale, his absolute leadership in this area did not cover such long periods of time as in terms of the total number of entries, but his team's maximum fractions of the annual number of entries in the CSD was achieved in it (10.7% in 1980).

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