purpose. In hardly any other field of science are the capabilities and limitations of natural language on the one hand and indexing language on the other so clearly revealed as in chemistry. The key to the understanding of the pecularities of both kinds of language is representational predictability and, hence, the differentiation between individual and general concepts. The answer to the everlasting question of whether to prefer natural or indexing language is found to be not one of "either/or" but rather one of "both/and". Chemistry, in several respects, has thus been a pioneer in information science. Through a consistent continuation of the analytico-synthetic approach the accessibility of the chemical literature can further be improved. This would also exert a beneficial influence on the documentation of the literature of other fields.

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Searching the Literature To Learn How the Term "Ligand" Became a Part of the Chemical Language

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An examination is made of the origins, dissemination, and eventual general adoption of the term "ligand", which is used by chemists to refer to atoms or groups attached to a central atom in coordination compounds or organometallic compounds. The term, first proposed by the German chemist Alfred Stock in 1916, was not readily accepted into other languages, particularly English. The first influential use of ligand in English did not occur until 1941 in Jannik Bjerrum's doctoral dissertation "Metal Ammine Formation in Aqueous Solution". Suggestions are made as to criteria and factors facilitating the adoption and acceptance of neologisms into scientific language and literature.

INTRODUCTION

In the course of editing an encyclopedia article by Kauffman on "Coordination Chemistry",[1] in which the word ligand[2] appeared, Brock became interested in the origin of the term. Letters by Kauffman and Jensen directed to authorities who were active in the field of coordination chemistry during the period from the 1930s to the 1950s elicited varying replies based on memory as well as documentation. Jørgensen located a reference to the origin in Fritz Ephraim's "Anorganische Chemie".[3] Ephraim attributed the word to Alfred Stock (1876–1946), the inventor of the well-known oxidation number system of inorganic nomenclature. Although Stock proposed the term ligand in 1916,[4] it did not come into extensive usage among English-speaking chemists until the 1940s and 1950s. Jensen has used his long-term expertise in matters of nomenclature to follow the progress of the term from Stock's original proposal to its almost universal use today in English and other languages. This article, then, is a brief account of our joint efforts to trace the origin and dissemination of a common chemical term and to offer some speculations on the factors governing the acceptance of such a term into scientific nomenclature.[5]

ORIGIN

During his pioneering experimental work on the boron hydrides during his World War I sojourn at the Kaiser-Wilhelm-Institut für Chemie in Berlin, Alfred Stock directed his attention to the analogous hydrides of silicon, thinking that their highly reactive and volatile character might have military applications. At a K-W-I meeting on Nov 27, 1916, he discussed the similarities between carbon and silicon chemistry first noticed as early as 1857 by Wöhler and Buff. For Stock, these analogies were made more evident and interesting by the deeper knowledge of atomic structure that was then becoming available to chemists:

> The surprisingly rapid development of our knowledge of the nature of atoms promises that in the not too distant future, it will be possible to develop an atomic–

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> structural chemistry in which fundamental chemical properties of atoms, such as their affinities and valencies, will be explicable from their atomic structure.[4]

In the published version of the paper the phrase "affinities and valencies" was accompanied by a footnote:

> To prevent misunderstandings the meaning of several words used here must be explained. Affinity is the expression for the firmness with which one element binds other elements or radicals (generally: "Ligands" (*ligare* [Latin], to bind); the introduction of a word hitherto lacking simplifies the manner of expression for this immediately clear concept). Valence (*Valenz*) means the unit of force which can bind a univalent ligand; positive valencies bind negative ligands; negative valencies bind positive ligands. Atomicity (*Wertigkeit*) is the number of valencies which an atom manifests; the highest atomicity is the highest number of valencies observed for an element.[4]

Thus Stock first coined "ligand" (Latin gerundive ligandum, "that should be bound") to fill the gap caused by the absence of a general term for the concept of elements and radicals bound to another element.

EARLY DISSEMINATION

Having made this clarification in the context of silicon chemistry—not, it should be stressed, in the context of Werner's coordination theory or in a discussion of inorganic complexes, the context usually employed today—Stock made no further use of the term ligand in the paper, nor did he use it frequently in later experimental papers. Although Stock's 1917 paper[4] was reviewed for the British Chemical Society in 1919,[6] the reviewer drew no attention to the footnote, for he was far more interested in Stock's preparation of, and proposed nomenclature for, the silanes.

The classical textbooks of coordination chemistry by Werner, Urbain and Sênêchal, and Weinland[7] had no term corresponding to ligand (although Werner occasionally used "Addend"), probably because Werner's distinction between primary and secondary valencies made it difficult to consider all coordinated atoms or groups as equivalent. Furthermore, Stock's proposal was not followed in the second edition of Weinland's book (1924) or in the fifth and final edition of Werner's "Neuere Anschauungen", edited by Paul Pfeiffer (1923).

In the 1920s in Germany a commission on inorganic chemical nomenclature of the Deutsche Chemische Gesellschaft (R. Lorenz, R. J. Meyer, S. Meyer, P. Pfeiffer, A. Rosenheim, and A. Stock) recommended[8] the use of a Roman numeral (the Stock number) to designate the oxidation state of an element. The complete German proposal, which was not published in German but is known from a French translation,[9] probably contained the term ligand to designate atoms, groups, or molecules attached to a central atom, although it is absent in the preliminary version.[8] The proposal was submitted by Stock at the Hauptversammlung des Vereins deutscher Chemiker at Nürnberg in 1925, and one can deduce from the appearance of the term ligand in the German literature since 1927 that the term was included in his report. As mentioned earlier, the fourth (1929) edition of Ephraim's textbook "Anorganische Chemie" adopted the word in introducing the elements of periodic group 4 and referred to Stock explicitly as its originator.[3] By 1930, therefore, the word ligand had become widely used in German publications, including the monographs on stereochemistry by Goldschmidt and Freudenberg,[10] and it was adopted by the Japanese coordination chemist Ryūtarō Tsuchida when writing in English on the spectrochemical series in a Japanese journal.[11] Because of the demonstration by Werner's former student and colleague Paul Pfeiffer that there was a close relationship between Werner's coordination theory and the structure of crystals as revealed by the then new experimental technique of X-ray diffraction,[12] one might have expected that geochemists and crystallographers would have used the term ligand at an early date. However, to take one example, the crystallographer V. M. Goldschmidt used instead the phrase "nächste Nachbarn" (nearest neighbors).[13]

In 1926 the Commission on the Nomenclature of Inorganic Chemistry (W. P. Jorissen, Chairman), appointed in 1921 by the Union Internationale de Chimie Pure et Appliquêe (UIC), discussed and rejected Werner's proposal to use the endings a, o, i, e, an, on, in, and en to designate valencies 1+ through 8+ but adopted the use of Stock numbers.[14] Following a further conference at Washington in 1926, a definitive proposal containing detailed rules for naming coordination compounds by the use of Stock numbers was drawn up;[15] the term ligand, however, was not used.

After 1930, when Germany had been readmitted to the UIC, a collaboration between the International and German commissions on nomenclature was initiated, and Delêpine's French translation of the German proposal was published.[9] This contains the expression "ordre des constituants liês à l'atome central" as a rendering of the original "Reihenfolge der Liganden". Clearly, the term ligand was not acceptable as a French term.

In 1936 the International Commission (Remy, Jorissen, Delêpine, and Fichter; the English member, Clarence Smith, was absent) drafted a proposal adopted at the Tenth UIC Congress held at Rome in 1938. (Here A. Damiens and H. Bassett had replaced Delêpine and Smith.) The German version was published in 1940 by Remy, who mentioned that Stock had been active in the German chemists' deliberations.[16] However, in translating this German report, Bassett, of the University of Reading, rendered ligands as "attached atoms or groups",[17] just as the French had done in 1937.[9] Although Bassett was not a coordination chemist, it is astonishing that he did not adopt ligand, the derivation of which from the Latin ligare seems obvious. No doubt he was affected by the outbreak of World War II and the absence of the word in English textbooks,[18] Patterson's "German–English Dictionary for Chemists",[19] and *Chemical Abstracts*.[20] Since Bassett's translation was used in the American version[21] with only minor amendments of spelling and footnotes, not surprisingly the word was omitted in Scott's 1943 review of inorganic nomenclature.[22] Similarly, the French version of the 1938 rules avoided the term by rendering ligands as "radicaux".[23] The reluctance of English chemists to employ ligand is underscored by the use of the word groups in the English translation of Hückel's important text "Anorganische Strukturchemie".[24]

Indeed, the word ligand seems to have been totally ignored by English-language chemists until the 1940s. In view of the widely used English words ligature and ligament as well as the more obscure words ligate and ligation, all sharing a common origin with ligand, this reluctance to accept ligand is surprising. Furthermore, its adoption by coordination chemists in the 1950s evidently suggested to some of them that it was a term of recent vintage.[25]

On the other hand, there seems to have been less reluctance to take ligand into other languages either directly from German usage or from the German version of the 1938 rules.[16] For example, around 1935 Jensen introduced ligand into Danish, having learned the term from Pfeiffer's chapter on coordination chemistry in Freudenberg's "Stereochemie".[10] After first using it in a paper on platinum complexes,[26] which he published in German, Jensen subsequently used it in his dissertation[27] and other Danish papers. On Jensen's suggestion, J. Bjerrum adopted the word in 1941 in the context of discussion of

stepwise equilibria, e.g., a "step system consisting of a central group M and *n* ligands A" and "ligand effect".[28] Although the two chemists used ligand freely in Danish and German conversations on coordination chemistry, Bjerrum was initially in doubt as to whether he could use ligand in English. However, Jensen assured him that because Stock's term was of Latin origin it could be used in any language. In this way, together with Tsuchida, Bjerrum became the first to use ligand in an English publication. His use of the term was also immediately accepted by Swedish chemists working in the same field.

Although in Brazil Rheinboldt introduced ligante as a translation of ligand into Portuguese,[29] there seems to be no other language into which ligand has been taken from the German. The German version of the 1938 rules[16] was not translated into Russian. The word addend, which was in use in Russian chemistry around 1950, was obviously derived from Werner's "Neuere Anschauungen".[7] A little later the expression "addends or ligands" was used, for example, in a book on coordination chemistry by Golovnya and Fedorov.[30] (The Russian term "teoriya polya ligandov" has been used for "ligand field theory" since at least 1962.)[31] Similarly, ligand did not appear in the huge Czechoslovakian and Polish six-language dictionaries published in the 1950s.[32] The former cites the German version of the 1938 rules[16] but uses the term "koordinovaně molekuly" for ligands. However, after 1960 ligand is used in Czechoslovakian, Polish, and Croatian. Clearly, its introduction into Slavic languages was due to the impact of the huge quantity of papers on coordination chemistry which were published in English during the early post-World War II years.[33]

DISSEMINATION IN ENGLISH

How then did ligand suddenly become so widespread in English? A decisive factor was undoubtedly the first post-war meeting in London in 1947 of the revived UIC, which was renamed the International Union of Pure and Applied Chemistry (IUPAC). Once again, nomenclature discussions were reopened by a Commission on the Nomenclature of Inorganic Chemistry, using the 1938 rules[16,17] as a starting point. Although Bassett, who had replaced Jorissen as chairman, was not very happy with the proposal to adopt the continental nomenclature for coordination compounds, Niels Bjerrum and K. A. Jensen, seconded by Bassett's secretary, E. V. G. Ewens, argued vigorously that the primary work of the Commission had to be an expansion of, and a more precise formulation of, the 1938 rules.[16,17] It followed that ligand should be used instead of expressions such as "attached groups and molecules". On the basis of this discussion, Bassett and Ewens published a review paper[34] in 1949 in which ligand was used.

Following further meetings of the Commission, a considerably extended set of rules for the nomenclature of inorganic chemistry was prepared and presented as "Tentative Rules" at a conference in Stockholm[35] in 1953. The contents of the new rules were therefore known 4 years before they were finally adopted by the IUPAC Council at the Paris conference in 1957 and published as "Nomenclature of Inorganic Chemistry 1957".

The adoption of ligand into English by the IUPAC commission became immediately known to many chemists from Ewens and Bassett's review paper[34] and from oral communication. However, the word ligand was already familiar to some English chemists who worked on equilibria in solution (from Bjerrum's thesis[36]) or on the preparation of coordination compounds of platinum and other transition metals (from the German literature[37]). The effect of the IUPAC decision was primarily to reassure chemists that ligand would be an acceptable word in an English text, but chemists using English as their mother tongue accepted it only around 1949.[38]

The explosive dissemination of ligand during the 1950s can be explained as the result of a sort of branched chain reaction, the traces of which are impossible to map out. It is reasonable to assume that the initiators were those to whom the term was already familiar and who used it in their lectures and discussions. The foci for the dissemination of ligand in English were apparently University College, London, The Butterwick Research Laboratories, Welwyn, and the laboratory for inorganic chemistry at Oxford University. By communication between supervisor and student and between authors, referees, and editors, the term was used in a great number of English and American papers, in what Nyholm described as "The Renaissance of Inorganic Chemistry", and from these it spread into other languages. The first two coordination chemistry conferences, at Welwyn in September 1950[39] and at Copenhagen in August 1953,[40a] undoubtedly did much to make the term familiar. In an ACS lecture in 1951, Fernelius stated, "The coordinated ions or molecules have been referred to as ligands or ligates, addenda, and adducts", but his preference is evident from the text that follows where he employs ligand (together with "coordinated group").[41] Thus the term ligand was in widespread use even before the Copenhagen conference in 1953. At this time too, ligand became frequently used in the context of "ligand field theory", an expression first appearing in print in 1954 in the published version of a paper delivered by Orgel and Sutton at the Copenhagen meeting.[40b]

After Jannik Bjerrum had been appointed full Professor in Copenhagen in 1948, he had a great number of American and Danish chemists working with him on coordination chemistry. Several important publications in English by Bjerrum and his students combined to make the term ligand known, and his American students brought it to the U.S.A. R. S. Nyholm, who attended the Welwyn Conference as an ICI Fellow, probably brought the term ligand to Australia on his return there the same year. At a meeting on coordination chemistry in Sydney[42] in 1953, Nyholm read a paper entitled "Nature of the Metal–Ligand Bond in Complex Compounds", leading his countryman, the late D. P. Mellor, to comment that "The use of the anything but euphonious term 'ligand' to designate the atom, group of atoms, or molecule attached to the central metal atom has now become so widespread that it is not likely to be abandoned". Recent textbook writers are either content to define ligands as molecules coordinated to a central metal atom or to use the term without any explanation.

CONCLUSIONS

As Crosland has noted in connection with organic nomenclature, "The establishment of any system of nomenclature presupposes the authority of an individual or group to impose such a system".[43] Partly because the phenomenon of isomerism forced attention on the problems of indexing compounds very early, organic chemists seem to have found international cooperation comparatively straightforward. (The Geneva Rules of 1892 were revised at Liège in 1930.) Conversely, as Fernelius has noted, since inorganic chemistry lacked "the barrier to mutual understanding" which the large numbers of compounds raised for organic chemistry, the inorganic nomenclature commission set up in 1919 "had to pioneer for such cooperative effort",[44] its communications and authority being hampered by the aftermath of World War I and the disruption caused by World War II, when agreement might otherwise have been reached.[45]

By expressing in a noncommittal way that something is "bound" to a central atom, the term ligand could be used in abstract papers without implying adherence to misleading metaphorical images. Its strength lay in its ready extension

into combinations such as "ligand field" and "ligand effect" or transformations such as "ligancy". Moreover, the term's Latin origin[46] meant that it could be used in most Indo-European languages with no, or only minor, changes. Hence its adoption in influential post-World War II papers (i.e., ones which attracted multiple citation), its acceptance by the IUPAC Nomenclature Commission in 1947, and its use in *Chemical Abstracts* and other journals were probably momentous in its acceptance by languages other than German. In principle, a term can be introduced in English, German, French, the Scandinavian languages, or any other language, but the acceptance of a new chemical term may be seriously delayed until it is adopted in English-language publications. Since few chemists would now agree with Mellor that the term ligand is "anything but euphonious",[42] we may conclude that euphony is not one of the more important conditions for a chemical term to be accepted.

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(38) E.g., from the Inorganic Chemistry Laboratory at Oxford University: Irving, H.; Williams, R. J. P. "On the Order of Stability of Metal Complexes"; *Nature (London)* **1948**, *162*, 746. This is the first use of ligand in a British paper known to us. According to Professor R. J. P. Williams, Professor Irving adopted the term from Bjerrum's thesis. In the United States Linus Pauling did not use the terms ligand or ligancy in print before 1945. John C. Bailar, Jr. used terms like "donor molecule" (e.g., *J. Am. Chem. Soc.* **1953**, *75*, 4574-5) and "coordinating agent" (e.g., *Ibid.* **1952**, *74*, 3131-4, 3535-8), adopting ligand only in 1954 (*Ibid.* **1954**, *76*, 4051-2).
(39) Imperial Chemical Industries. "A Discussion on Herts, Chemistry"; Report No. BRL/146; Butterwick Research Laboratories: "The Frythe", Welwyn, Herts, 1951. Ligand was used in 6 of the 11 lectures, as well as in the discussion. N. V. Sidgwick's remarks in the discussion, in which ligand is used, were probably the subject of editing.
(40) (a) "Proceedings of the Symposium on Co-ordination Chemistry, Copenhagen, 1953"; Danish Chemical Society: Copenhagen, 1954. The word ligand was used in 17 of the 34 papers presented at this meeting: Danish, 3; German, 3; Swedish, 3; Dutch, 1; Austrian, 1; English, 5; American, 1. (b) Orgel, L. E.; Sutton, L. E. "Factors Determining the Stability of Complexes". *Ibid.*, pp 17-24.
(41) Fernelius, W. C. In "Chemical Nomenclature"; American Chemical Society: Washington, DC, 1953; Adv. Chem. Ser. No. 8, p 9.
(42) "A Conference on Coordination Chemistry, Sydney, May 1953". *Rev. Pure Appl. Chem.* **1954**, *4*, 1-110 (see R. S. Nyholm, pp 15-40, and D. P. Mellor, p 47).
(43) Crosland, M. P. "Historical Studies in the Language of Chemistry"; Harvard University Press: Cambridge, 1962; p 338.
(44) See also: Fernelius, W. C. In Kauffman, G. B., Ed. "Werner Centennial"; American Chemical Society: Washington, DC, 1967; pp 147-60.
(45) Jensen, K. A. In "Chemical Nomenclature"; American Chemical Society: Washington, DC, 1953; Adv. Chem. Ser. No. 8, pp 38-48.
(46) By adopting metaphorical English terms such as "charm" and "strangeness" rather than terms of Latin or Greek origin, theoretical physicists have caused difficulties for non-English languages. See: Mermin, N. D. "E Pluribus Boojum: the Physicist as Neologist". *Phys. Today* **1981**, *34*, 46-53.

Cambridge Crystallographic Data Centre. 6. Preparation and Computer Typesetting of "Molecular Structures and Dimensions" Bibliographic Volumes

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Current accessions to the computer-based bibliographic file of the Cambridge Crystallographic Data Centre are disseminated annually via the reference book series *Molecular Structures and Dimensions*. Each volume contains a bibliographic listing ordered in 86 chemical classes and includes cross-references. A set of five indexes, based on compound names, molecular formulas, and authors' names, is also included. Twelve volumes (containing over 30 000 references) have been prepared since 1970 by use of computer typesetting techniques. The present production system is based on an FR80 microfilm recorder which employs special circuitry to display proportionally spaced text at high speed using a serifed font. Programs have been developed for cross-referencing, indexing, and typesetting (including complete page makeup) which enable casebound books to be produced from the master bibliographic file in under 3 months.

INTRODUCTION

The Cambridge Crystallographic Data Centre (CCDC)[1] is concerned with X-ray- and neutron-diffraction studies of organics, organometallics, and metal complexes. The CCDC maintains computer-based files of bibliographic (BIB),[2] chemical connectivity (CONN),[1,3] and numeric structural data (DATA)[3,4] on a current basis. The CCDC is also responsible for worldwide dissemination of the database: in machine-readable form (together with software for search, retrieval, numeric analysis, and visual display),[3] via traditional printed publications in the reference book series *Molecular Structures and Dimensions* (MSD),[5-8] and via a current awareness service.

At its inception in 1965 the CCDC was faced with problems of file definition, system organization, and software development, while simultaneously assimilating both current and backlog input. The first priority was the establishment of a bibliographic file, fully retrospective to 1935 and updated on a current basis. This was achieved by 1970, whereas currency of DATA (1973) and CONN (1977) came much later. The BIB file, which also contains chemical text (Table I), therefore became the master file for the system and the first file available for dissemination.

The first two bibliographic volumes[5] in the MSD series were published in 1970 and covered the literature for 1935-1969. Ten annual updates have now been added with vol. 12 appearing in 1981. Each volume contains a bibliographic listing of recent accessions (3000-4000 per year) ordered in 86 chemical classes, with cross-referencing between classes. Volumes 1-7 included indexes based on authors' names, molecular formulas, and rarer elements; this system was extended from vol. 8 to include indexing on compound names[9] and improvements in other indexes.[10]

Volumes 1-7 were produced from the card-image BIB file[2] by computer typesetting methods via a software package de-

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