

BOOK REVIEW

SEYMOUR B. ELK

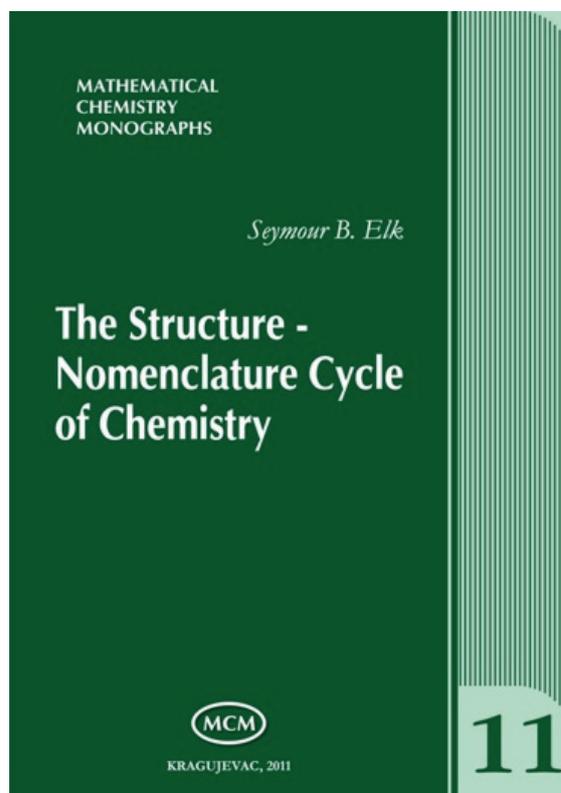
The Structure - Nomenclature Cycle of Chemistry

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There are three great symbolic systems: language, arithmetics and geometry. Language rests on letters, arithmetics on numbers, and geometry on geometrical figures and bodies. All the three systems are in use in chemistry; the molecule can be defined by name (language), by molecular or rational formula (arithmetics) or by constitutional or 3-D structural formula (geometry).

But the things are not at all so simple as this simple scheme suggests. Names of chemical compounds have either a weak resemblance to ordinary words (IUPAC names) or convey little structural information (trivial names). On the other hand, it is hard if not impossible to translate all chemical structures into line formulas.

All this problems are solved in the new chemical nomenclature proposed by Seymour B. Elk, and have been recently presented in the book *The Structure - Nomenclature Cycle of Chemistry*, published as the 11th book in the series *Mathematical Chemistry Monographs* edited by Ivan Gutman. The basis of Elk's endeavour is 3-D simplex, *i.e.* tetrahedron. As the tetrahedron is the the simplest body in the 3-D space (3-D simplex!), any chemical structure, and in principle any 3-D object, can be reduced to tetrahedron or the set of interconnected tetrahedra. The atoms are placed either on the four vertices or six edges of tetrahedron; Elk's formulas therefore have the form V_4E_6 . If additional atoms are bonded to vertices, the formula is written as $V_4E_6F_4$. Atom positions are denoted by numbers, and the numbers in superscript define the bonds. Therefore, P_4 is written as $(P1)_4^{(1-5,3-7)}(1)$, P_4O_6 as $(P1O1)_4^{(1-9,5-13)}(1O1)$, and P_4O_{10} as $(P1O1)_4^{(1-9,5-13)}(1O1);^{(1,5,9,13)}(2O)$.



The numbers 1 and 2 written near the symbols denote bond order, n ; 1 for single and 2 for double bond. As a special feature of his nomenclature Seymour B. Elk introduced "alpha bond" ($n < 1$), "beta bond" ($1 < n < 2$) and "gamma bond" ($n > 2$). Therefore the formula of naphthalene is $(C\beta)_{10}^{(1-11)}(\beta);^{(3,5,7,9,13,15,17,19)}(1H)$.

The Elk's nomenclature can be used in all fields of chemistry in a systematic and simple way. This is stressed in the preface of this book; and in the next chapters the author tries to persuade the reader in it. He gave the example of phosphorous, sulphur, and boron compounds (especially boron hydrides), aromatic and sandwich compounds, cubane and its analogs, covalently bonded lithium compounds and alkali metals

complexes with crown ethers. In the separate section of the book he also put the names to macromolecules and polymers, giving even the formula of graphite, $[(^{1/2}C^{1/2})^{(2)}(^{1/2})]_{\infty}$, and diamond, $[(^{1/2}C^{1/2})^{(2,2)}(^{1/2})]_{\infty}$. Any molecular structure, no matter how complicated, can be written in the new way. The examples from all the fields of chemistry corroborate this assumption.

But the problem is not the nomenclature itself, but its application. The Elk's system is not aimed so much to humans as to computers: written in the new way any structure can be easily stored in computer memory and possibly automatically converted to structural formula. But I am not very sure the opposite is possible. This means it is needed to teach thousands if not millions of

chemists the new chemical language. Besides, over 50 million names in CA registry have to be translated, along with a few million new compounds synthesized every year.

As it is not based on language (names) but formulas (numbers), the traditional chemical (IUPAC) nomenclature cannot be abandoned. This means that chemists would be forced to learn another, "artificial" language, besides traditional ones. What is simple and easy to learn is not always practical. The case of Esperanto speaks for itself.

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