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BRIEF COMMUNICATION

Structural chemistry and the transcendental numbers φ, e and π

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Abstract Certain number theory relations that emerge from considerations of the topological character of several patterns taken from structural chemistry are reviewed. These relations define the products $e \cdot \pi$ and $\phi \cdot e$ from topological considerations of the respective structural-types. We further present here an approximate number theory formula for the quotient π / ϕ and for the product $\phi \cdot e \cdot\ e \cdot \pi$ that are derived from the earlier formulas based in structural chemistry.

The transcendental numbers are here defined as those numbers that can be expressed as infinitely non-repeating continued fractions. Earlier work by us has drawn connections between the transcendental numbers φ, e and π and the strict topological indexes, n, the weighted average polygon size, and p, the weighted average connectivity, within the unit of pattern of several structures. These topological indexes, n and p, of the polyhedra and patterns, have been defined and described earlier by us [1]. In this communication, we survey the results for the Waserite structural-type (MPt_3O_4) and the Moravia structural-type (A_3B_8), and derive further number theory relations.

Thus from the Waserite structural-type (Wells point symbol $(8^4)_3(8^3)_4$), shown in Fig. 1, the weighted average connectivity, p, given as Eq. (1a), admits a number theory relation for the product $e \cdot \pi$ shown as Eq. (1b) below [1]:

$$p = (3 \cdot 4 + 4 \cdot 3)/7 \tag{1a}$$

$$(1) \cdot (2.33333\ldots\ldots) \cdot (e) \cdot (\pi) \quad \approx (4) \cdot (5) \tag{1b}$$

This manuscript on the transcendence and its connection to structural chemistry is dedicated to the memory of my (MJB) mother Barbara A. Bucknum.

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Fig. 1 Catalan Waserite (MPt_3O_4) pattern in space group Pm-3n

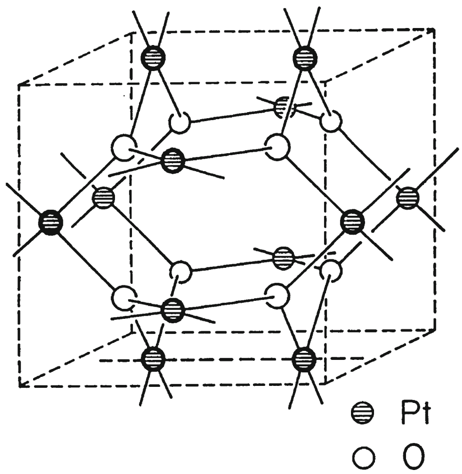
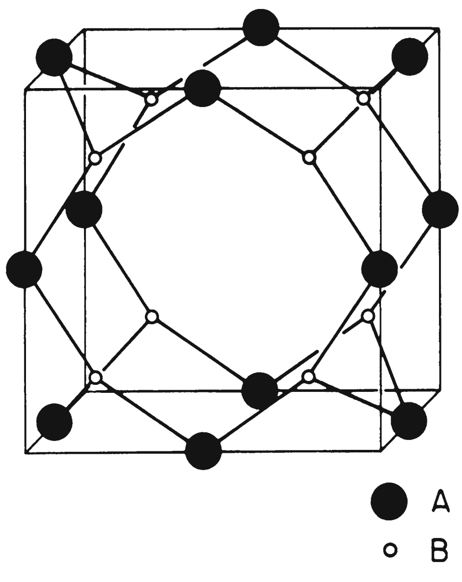


Fig. 2 Wellsean Moravia (A_3B_8) pattern in space group Pm-3m



And here Eq. (1b) is known as the "Timaeus" relation, and this relation is true to better than 99 parts in 100 [1].

From the Moravia structural-type (Wells point symbol $(4^4 6^8 8^{12})_3(4^3)_8$) shown in Fig. 2, the weighted average connectivity, p, given as Eq. (2a), admits a number theory relation for the product $\phi \cdot e$ given as Eq. (2b) below. [1]

$$p = (3 \cdot 8 + 8 \cdot 3)/11 \tag{2a}$$

$$(1) \cdot (1) \cdot (2) \cdot (3) \cdot (5) \cdot (8) \approx (\phi) \cdot (e) \cdot (55) \tag{2b}$$

And here Eq. (2b) is known as the “Golden” relation, and this relation is true to better than 99 parts in 100 [1].

Further, by combining Eq. (1b) with Eq. (2b) into a quotient form, one can derive a rational approximation to the quotient π / ϕ, given as Eq. (3) below:

$$\pi / \phi \quad \approx 5 \cdot 11/4 \cdot 7 \tag{3}$$

And there is one final number theory relation that can be gotten from yet another combination of Eq. (1b) with Eq. (2b), this relation is formed as a product of these equations. It describes a rational approximation of the product $\phi \cdot e \cdot\ e \cdot \pi$ as given by Eq. (4):

$$\phi \cdot e \cdot e \cdot \pi \quad \approx 6! \cdot 4/7 \cdot 11 \tag{4}$$

In conclusion one can see the mathematical richness that is present in various patterns and the structural chemistry they are based upon in reality. Equations (1b), (2b), (3) and (4) are very interesting number theory results as various rational approximations to certain transcendental mathematical constants and their products and quotients.

References

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