A Note on the Use of Rhombus Silicate Networks and Rhombus Oxide Networks

Wolfgang Quapp*

Mathematisches Institut, Universität Leipzig, PF 100920, D-04009 Leipzig, Germany

E-mail: quapp@math.uni-leipzig.de

submitted: Nov. 4, 2022 revised: Nov. 22, 2022 for Canadian Journal of Chemistry

Abstract

We question the use of Rhombus Silicate Networks and Rhombus Oxide Networks in some papers by the count of the included oxygen atoms and oxygen ions.

Keywords: Rhombus Silicate Network, Rhombus Oxide Network

Comment

The combination of chemistry, mathematics and information sciences leads to a new subject called cheminformatics. Important papers on this field are refs.[1,2] They treat a molecular graph (V, E) with the vertex set V and the edge set E. A graph whose vertices denote atoms and edges denote valence bonds or nearest neighbors between the atoms of an underlying chemical structure is often used. We will observed this chemical case here. This note concerns the most interesting class of minerals, the silicates. All silicates contain SiO_4 tetrahedra as it is a basic unit, compare Figure 1. Note that four O-atoms form the outer tetrahedron of an SiO_4, but the Si-atom sits in the center.

*To whom correspondence should be addressed

Three oxygens and the Si also form a tetrahedron. This fact is the source of the commented error, see below.

Leafs of silicates, or sheets (phyllosilicate), form different structures.[3] Interesting here are the rhombus silicate and the so-called rhombus oxide networks. In ref.[1] layers are studied where the upper oxygen ions are missing. In Figure 1, the rhombus silicate network (1) is presented in a 3-

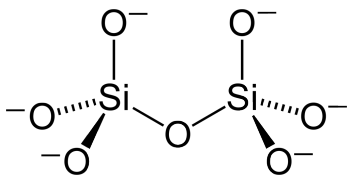


Figure 1: Molecular representation of the Rhombus Silicate Network (1) by Benjah-bmm27.

dimensional picture. Two tetrahedra are combined by one common O-atom. Of course, the upper oxygens belong to the structure. The networks of Ref. [1] are 2-dimensional, orthogonal projections of the structures of interest. There every Si-atom overlaps one O-ion which is then missing in the study.

In Figure 2, the rhombus silicate network (3) is shown.[4] In the representation one can overlook the upper oxygens. Notice that the structure is of importance. If we simplify some minerals then all the tetrahedra point upward in a mineral muskovite, but in a mineral sepiolite one half points upward, but the other one downward.[3] The artifical mineral hexacelsian forms a non-bifurcated double sheet[5,6] where the tetrahedra of the lower sheet point upward but the tetrahedra of the upper sheet point downward.

Because the upper layer of O-ions is missing, the claimed rhombus oxide networks[1] are incorrect, at least in a chemical meaning.

The order and size of a graph is $|V|$ and $|E|$ respectively. These numbers of the vertices and the edges in a rhombus silicate network with all O-atoms and O-ions, of 'dimension (n)' (see Ref.[1]) are given by $|V| = 7n^2 + 2n$ and $|E| = 20n^2$. If the upper O-ions are missing, then the vertices and the edges in a rhombus silicate of dimension n are (falsely[1]) counted by $|V| = 5n^2 + 2n$ and $|E| = 12n^2$. If one deletes all the silicon atoms from the rhombus silicate network, then one obtains

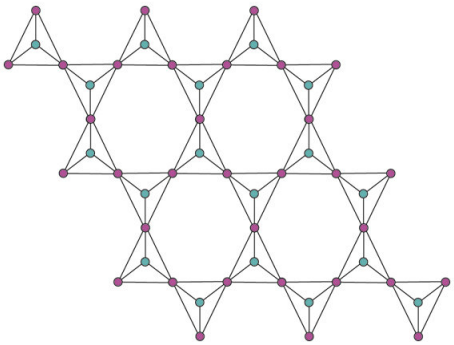


Figure 2: Rhombus Silicate Network (3) in a projection on a plane. Si-atoms are green, O-atoms and O-ions are dark red. The projection is from below, thus every Si-atom superimposes one oxygen. Copy of ref.[4]

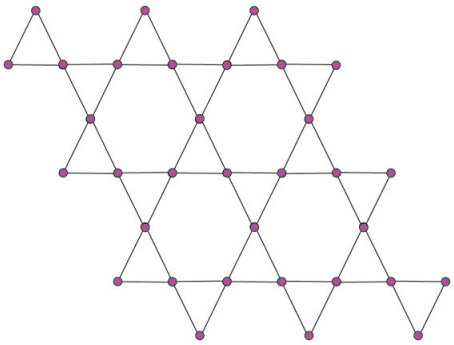


Figure 3: Incorrect Rhombus Oxide Network (3). The former superimposed O-atoms are missing. Copy of ref.[4]

no new projection of the network because now the place of the Si-atoms is occupied by the upper oxygens This correct rhombus oxide network now has the former nodes and edges $|V| = 5n^2 + 2n$ and $|E| = 12n^2$.

Discussion

This comment does not only concern Ref.[1] but a row of following works.[4,7–11] One could guess that a row of indices change which are studied in the further cited references for the networks of interest.

Competing interests: The author declares there are no competing interests.

References

(1) Javaid, M.; Rehman, M. U.; Cao, J. Topological indices of rhombus type silicate and oxide networks. *Canad. J. Chem.* **2017**, *95*, 134–143.

(2) Alghazzawi, D.; Raza, A.; Munir, U.; Ali, M. S. Chemical Applicability of Newly Introduced Topological Invariants and Their Relation with Polycyclic Compounds. *Hindawi J. Math.* **2022**, 867040.

(3) Strunz, H.; Nickel, E. *Strunz Mineralogical Tables. Ninth Edition*; Schweizerbart Science Publishers: Stuttgart, Germany, 2001.

(4) Qi, R.; Ali, H.; Babar, U.; Liu, J.-B.; ; Ali, P. On the Sum of Degree-Based Topological Indices of Rhombus-Type Silicate and Oxide Structures. *Hindawi J. Math.* **2021**, 100024.

(5) Withers, R.; Tabira, Y.; Valgoma, A.; Aroyo, M.; Dove, M. T. The inherent displacive flexibility of the hexacelsian tetrahedral framework and its relationship to polymorphism in Ba-hexacelsian. *Phys. Chem. Minerals* **2000**, *27*, 747–756.

(6) Kremenovic, A.; Colomban, P.; Piriou, B.; Massiot, D.; Florian, P. Structural and spectroscopic characterization of the quenched hexacelsian. *J. Phys. Chem. Solids* **2003**, *64*, 2253–2268.

(7) Kulli, V. R. Some Gourava indices and inverse sum indeg index of certain networks. *Int. Res. J. Pure Alg.* **2017**, *7*, 787–798.

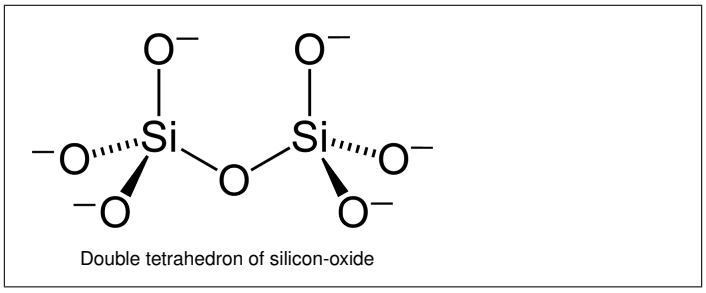
(8) Dayan, F.; Javaid, M.; Ali, U.; Ahmad, B.; Zulqarnain, M. On Some Banhatti Indices of Triangular Silicate, Triangular Oxide, Rhombus Silicate and Rhombus Oxide Networks. *Am. J. Inform. Sci. Technol.* **2018**, *2*, 42–49.

(9) Mondal, S.; De, N.; Pal, A. On Some New Neighborhood Degree-Based Indices for Some Oxide and Silicate Networks. *Multidisciplinary Sci. J.* **2019**, *2*, 384–409.

(10) Ibraheem, M.; Riaz, A.; Kashif, A. Computing Analysis of Irregularity Indices for Rhombus type Silicate and Oxide Networks. *Comp. J. Combin. Math.* **2021**, *3*, 23–41.

(11) Jayanna, G. K.; Swamy, N. N. Multiplicative Reverse Geometric-Arithmetic Indices and Arithmetic-Geometric of Silicate Network. *Biointerface Res. Appl. Chem.* **2022**, *12*, 4192–4199.

Graphical TOC Entry



Double tetrahedron of silicon-oxide