TOPOLOGICAL PROPERTIES OF SODIUM CHLORIDE

Ali AHMAD[1]

Sodium chloride $NaCl$, commonly known as salt, is one of the most abundant minerals on Earth and an essential nutrient for many animals and plants. It is naturally found in seawater and in underground rock formations. A representation of unit cell of sodium chloride $NaCl$ is the same as the cartesian product of three paths of length 3. We present a formula, which can be used to obtain any degree-based topological index for sodium chloride. This result generalizes other known results in the area. We also give exact values of the most well-known degree-based topological indices for sodium chloride.

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1. Introduction

Sodium chloride has many uses beyond seasoning and preserving foods. Hospitals use an intravenous sodium chloride solution to supply water and salt to patients to alleviate dehydration. Icy sidewalks and roadways are often deiced by rock salt, the same type of salt that is used on your dinner table, before it is ground down to finer crystals. Large quantities of sodium chloride are also used in industrial manufacturing settings to help make a range of products, from plastic, paper, rubber and glass, to chlorine, polyester, household bleach, soaps, detergents and dyes. Graph representation of molecular structures is widely used in computational chemistry. Trinajstic noted that the roots of chemical graph theory may be found in the works by chemists of 18-19th centuries such as Higgins, Kopp, Crum Brown. First chemical graphs for representing molecules were used by them [5].

A graph G consists of a set of non-empty vertices $V(G)$ and a set of edges $E(G)$. Two vertices u and v in an undirected graph G are called adjacent (or neighbors) in G if u and v are endpoints of an edge e of G. Such an edge e is called incident with the vertices u and v and e is said to connect u and v. The number of vertices adjacent to a vertex u is called the degree of vertex u, it is denoted as d_u. In chemical structures, the vertices represent the atoms of the molecule, and the edges represent the chemical bonds between them. The

[1]College of Computer Science & Information Technology, Jazan University, Jazan, KSA, e-mail: `ahmadsms@gmail.com`

order $V(G)$ and size $E(G)$ are known as the number of vertices and edges in a graph, respectively.

To identify molecular structures of chemical compound, the molecular graph invariants, called topological indices could be used. Topological indices are designed basically by transforming a molecular graph into a number. The first use of a topological index was made in 1947 by the chemist Harold Wiener. Wiener originally defined his index (W) on trees and studied its use for correlations of physico-chemical properties of alkanes, alcohols, amines and their analogous compounds [21].

Depending on the importance of Topological indices on a graph, these indices are categorized in "topological indices based on degrees" [1–3, 16], "topological indices based on distances" [6, 9, 13, 15] and "topological indices based on eccentricities" of graphs [10, 12, 19]. Some well-known topological indices based on the degrees of a graph are Randi connectivity index, Zagreb indices, Harmonic index, atom bond connectivity, geometric arithmetic index etc. and Wiener index, Hosaya index, Estrada index are distance based topological indices [20]. Similarly eccentric based topological indices are Zagreb eccentric index , geometric-arithmetic eccentric index, connectivity of atomic bond eccentric index and fourth type of eccentric harmonic index [7,8,11]. Topological indices guide us that how the chemical structure can further grow and what mathematical operations on the graphs with the relieve of topological indices can extend multidisciplinary research.

We present results, which can be used to compute any degree-based topological index (defined as the summation over all edges) for sodium chloride (NaCl). Our results generalize known results in the area. We give exact values of the most well-known degree-based indices for sodium chloride. Vetrík [18] introduced a new method to calculate the topological indices, we follow the same technique in this paper.

We study general topological invariant $T(G)$ based on the degree of vertices in graph G.

$$T(G) = \sum_{uv\in E(G)} \phi(d_u, d_v), \tag{1}$$

- If $\phi(d_u, d_v) = (d_u d_v)^\alpha$, where $\alpha \neq 0$ is a real number, then $T(G)$ is the general Randić index R_α of G. Moreover, $T(G)$ is the Randić index if $\alpha = \frac{-1}{2}$, the second Zagreb index if $\alpha = 1$ and the second modified Zagreb index if $\alpha = -1$.
- If $\phi(d_u, d_v) = (d_u + d_v)^\alpha$, where $\alpha \neq 0$ is a real number, then $T(G)$ is the general sum-connectivity index of G. Moreover, $T(G)$ is the sum-connectivity index if $\alpha = \frac{-1}{2}$, the first Zagreb index if $\alpha = 1$ and the hyper-Zagreb index if $\alpha = 2$.
- If $\phi(d_u, d_v) = d_u^\alpha d_v^\beta + d_v^\alpha d_u^\beta$, we obtain the generalized Zagreb index of G.
- If $\phi(d_u, d_v) = \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, we obtain the geometric-arithmetic index $GA(G)$.

- If $\phi(d_u, d_v) = \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$,we obtain the atom-bond connectivity index $ABC(G)$.
- If $\phi(d_u, d_v) = \frac{2}{d_u+d_v}$, we get the harmonic index $H(G)$.
- If $\phi(d_u, d_v) = \frac{d_u^2+d_v^2}{d_u d_v}$, we get the symmetric division degree index $SDD(G)$.
- If $\phi(d_u, d_v) = \frac{d_u+d_v}{d_u d_v}$, then $T(G)$ is the first redefined Zagreb index of G.
- If $\phi(d_u, d_v) = \frac{d_u d_v}{d_u+d_v}$, then $T(G)$ is the second redefined Zagreb index of G.
- If $\phi(d_u, d_v) = d_u d_v\,(d_u + d_v)$, then $T(G)$ is the third redefined Zagreb index of G.
- If $\phi(d_u, d_v) = \left(\frac{d_u\ d_v}{d_u+d_v-2}\right)^3$, we obtain the augmented Zagreb index $AZI(G)$.
- If $\phi(d_u, d_v) = \frac{1}{\max\{d_u,d_v\}}$, we obtain the variation of the Randić index $R'(G)$.
- If $\phi(d_u, d_v) = |d_u - d_v|$, we obtain the Albertson index $A(G)$ [4].

2. Sodium chloride

In our day-to-day life, the common salt $NaCl$ is used as an important preservative because it retards the growth of microorganism. It also improves the flavour of food items. Chlorine products are used in metal cleaners, paper bleach, plastics and water treatment [5]. They are also used in medicines. Sodium chloride is a white crystalline solid with a density of 2.16 g/mL, and a melting point of 801 C. It is also available as aqueous solutions of different concentrations, called saline solutions. sodium chloride is readily soluble in water and other polar solvents. It is a stable solid. It only decomposes at high temperatures to give toxic fumes of hydrochloric acid (HCl) and disodium oxide (Na_2O). A three dimensional mesh $M(l, w, h)$ is defined as the cartesian product $P_l \times P_w \times P_h$. In a three dimensional mesh there are lwh number of vertices and $(2lw-l-w)h+(h-1)lw$ number of edges. We find that the unit cell representation of sodium chloride $NaCl$ is the same as the three dimensional mesh $M(3, 3, 3)$. The three dimensional mesh $M(3, 3, 3)$ is shown in Figure 1. In fact in Figure 1 the hollow circles represent Na^+ and solid circles represent Cl^- ions. For more detail see [5]. Let the vertex set of $M(l, w, h)$ be the set $V(M) = \{v_1v_2v_3 : 0 \le v_1 \le l-1, 0 \le v_2 \le w-1, 0 \le v_3 \le h-1\}$ and two vertices $v = v_1v_2v_3$ and $v' = v'_1v'_2v'_3$ are linked by an edge if $\sum_{i=1}^{3} |v_i - v'_i| = 1$.

3. Main results

Let us give a formula, which can be used to obtain any degree-based topological index for sodium chloride (NaCl).

Lemma 3.1. *Let $M(l, w, h)$ be a sodium chloride* (NaCl). *Then* $T(M(l, w, h)) = 3lwh\phi(6, 6) + 4\Big\{\phi(4, 4) + 2\phi(4, 5) - 5\phi(5, 5) - 2\phi(5, 6) + 4\phi(6, 6)\Big\}(l + w + h) +$

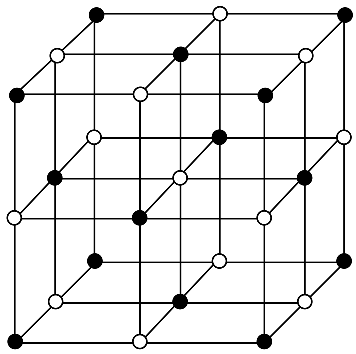

FIGURE 1. The three dimensional mesh $M(3,3,3)$

$\Big\{4\phi(5,5)+2\phi(5,6)-7\phi(6,6)\Big\}(lw+wh+hl)+12\Big\{2\phi(3,4)-3\phi(4,4)-4\phi(4,5)+ 6\phi(5,5)+2\phi(5,6)-3\phi(6,6)\Big\}.$

Proof. The graph $M(l,w,h)$ contains lwh vertices and $3lwh-lw-wh-hl$ edges. Let us divide the edges of $M(l,w,h)$ into partition sets according to the degree of its end vertices.

$$\Xi_{r,s}=\{uv\in E(M(l,w,h)): d_u=r, d_v=s\}.$$

This means that the set $\Xi_{r,s}$ contains the edges incident with one vertex of degree r and the other vertex of degree s. We have $|\Xi_{3,4}|=24$, $|\Xi_{4,4}|=4(l+w+h-9)$, $|\Xi_{4,5}|=8(l+w+h-6)$, $|\Xi_{5,5}|=4(lw+wh+hl)-20(l+w+h)+72$, $|\Xi_{5,6}|=2(lw+wh+hl)-8(l+w+h)+24$, $|\Xi_{6,6}|=3lwh-7(lw+wh+hl)+16(l+w+h)-36$ and $E(M(l,w,h))=\Xi_{3,4}\cup\Xi_{4,4}\cup\Xi_{4,5}\cup\Xi_{5,5}\cup\Xi_{5,6}\cup\Xi_{6,6}$. Then

$$\begin{aligned}
T(M(l,w,h)) &= \sum_{uv\in E(M(l,w,h))}\phi(d_u,d_v)\\
&= \sum_{uv\in\Xi_{3,4}}\phi(3,4)+\sum_{uv\in\Xi_{4,4}}\phi(4,4)+\sum_{uv\in\Xi_{4,5}}\phi(4,5)\\
&+\sum_{uv\in\Xi_{5,5}}\phi(5,5)+\sum_{uv\in\Xi_{5,6}}\phi(5,6)+\sum_{uv\in\Xi_{6,6}}\phi(6,6)\\
&=24\phi(3,4)+4(l+w+h-9)\phi(4,4)+8(l+w+h-6)\phi(4,5)\\
&+\{4(lw+wh+hl)-20(l+w+h)+72\}\phi(5,5)\\
&+\{2(lw+wh+hl)-8(l+w+h)+24\}\phi(5,6)\\
&+\{3lwh-7(lw+wh+hl)+16(l+w+h)-36\}\phi(6,6).
\end{aligned}$$

After simplification, we get

$T(M(l,w,h)) = 3lwh\phi(6,6) + 4\Big\{\phi(4,4) + 2\phi(4,5) - 5\phi(5,5) - 2\phi(5,6) + 4\phi(6,6)\Big\}(l+w+h) + \Big\{4\phi(5,5) + 2\phi(5,6) - 7\phi(6,6)\Big\}(lw+wh+hl) + 12\Big\{2\phi(3,4) - 3\phi(4,4) - 4\phi(4,5) + 6\phi(5,5) + 2\phi(5,6) - 3\phi(6,6)\Big\}.$ □

Now we present values of the best-known degree-based topological indices of sodium chloride (NaCl).

Theorem 3.1. *Let $M(l,w,h)$ be a sodium chloride* (NaCl). *Then the general Randić index R_α of $M(l,w,h)$ is;*

$R_\alpha(M(l,w,h)) = 3lwh(36)^\alpha + 4\Big\{(16)^\alpha + 2(20)^\alpha - 5(25)^\alpha - 2(30)^\alpha + 4(36)^\alpha\Big\}(l+w+h) + \Big\{4(25)^\alpha + 2(30)^\alpha - 7(36)^\alpha\Big\}(lw+wh+hl) + 12\Big\{2(12)^\alpha - 3(16)^\alpha - 4(20)^\alpha + 6(25)^\alpha + 2(30)^\alpha - 3(36)^\alpha\Big\},$

Randić index is

$R_{-\frac{1}{2}}(M(l,w,h)) = \frac{1}{2}lwh - 4(\sqrt{\frac{1}{5}} - \sqrt{\frac{2}{15}} - \frac{1}{12})(l+w+h) + (\sqrt{\frac{2}{15}} - \frac{11}{30})(lw+wh+hl) + 12(\sqrt{\frac{1}{3}} - \sqrt{\frac{4}{5}} + \sqrt{\frac{2}{15}} - \frac{1}{20}),$

the second Zagreb index is

$$R_1(M(l,w,h)) = 108lwh + 60(l+w+h) - 92(lw+wh+hl) - 24,$$

the second modified Zagreb index is

$$R_{-1}(M(l,w,h)) = lwh + \frac{1}{36}(l+w+h) + \frac{29}{900}(lw+wh+hl) + \frac{3}{100},$$

the general sum-connectivity index χ_α of $M(l,w,h)$ is

$\chi_\alpha(M(l,w,h)) = 3lwh(12)^\alpha + 4\Big\{(8)^\alpha + 2(9)^\alpha - 5(10)^\alpha - 2(11)^\alpha + 4(12)^\alpha\Big\}(l+w+h) + \Big\{4(10)^\alpha + 2(11)^\alpha - 7(12)^\alpha\Big\}(lw+wh+hl) + 12\Big\{2(7)^\alpha - 3(8)^\alpha - 4(9)^\alpha + 6(10)^\alpha + 2(11)^\alpha - 3(12)^\alpha\Big\},$

the sum-connectivity index

$\chi_{-\frac{1}{2}}(M(l,w,h)) = \frac{\sqrt{3}}{2}lwh - 4(\sqrt{\frac{1}{8}} - \sqrt{\frac{5}{2}} - \sqrt{\frac{4}{11}} + \sqrt{\frac{4}{3}} + \frac{2}{3})(l+w+h) + (\sqrt{\frac{8}{5}} + \sqrt{\frac{4}{11}} - \sqrt{\frac{49}{12}})(lw+wh+hl) + 12(\sqrt{\frac{4}{7}} - \sqrt{\frac{9}{8}} + \sqrt{\frac{12}{5}} + \sqrt{\frac{4}{11}} - \frac{2}{3} - \frac{\sqrt{3}}{2})$,

the first Zagreb index

$$\chi_1(M(l,w,h)) = 36lwh + 8(l+w+h) - 22(lw+wh+hl),$$

the hyper-Zagreb index

$$\chi_2(M(l,w,h)) = 432lwh + 240(l+w+h) - 366(lw+wh+hl) - 96,$$

the geometric-arithmetic index GA of $M(l,w,h)$ is

$GA(M(l,w,h)) = 3lwh + 16\left\{\frac{2\sqrt{5}}{9} - \frac{\sqrt{30}}{11}\right\}(l+w+h) + \left\{\frac{4\sqrt{30}}{11} - 3\right\}(lw+wh+hl) + 48\left\{\frac{2\sqrt{3}}{7} - \frac{4\sqrt{5}}{9} + \frac{\sqrt{30}}{11}\right\}$,

the symmetric division degree index SDD of $M(l,w,h)$ is

$$SDD(M(l,w,h)) = 6lwh + \frac{2}{15}(l+w+h) - \frac{29}{15}(lw+wh+hl) + \frac{2}{5},$$

the atom-bond connectivity index ABC of $M(l,w,h)$ is

$ABC(M(l,w,h)) = \frac{\sqrt{10}}{2}lwh + 4\left\{\sqrt{\frac{3}{8}} + \sqrt{\frac{7}{5}} - 2\sqrt{2} - \sqrt{\frac{6}{5}} + \frac{2\sqrt{10}}{3})\right\}(l+w+h) + \left\{\frac{8\sqrt{2}}{5} + \sqrt{\frac{6}{5}} - \frac{7\sqrt{10}}{6}\right\}(lw+wh+hl) + 12\left\{\sqrt{\frac{5}{3}} - \sqrt{\frac{27}{8}} - \sqrt{\frac{28}{5}} + \frac{12\sqrt{2}}{5} + \sqrt{\frac{6}{5}} - \frac{\sqrt{10}}{2}\right\}$,

the augmented Zagreb index AZI of $M(l,w,h)$ is

$AZI(M(l,w,h)) = \frac{17496}{125}lwh + \frac{5052254057}{49392000}(l+w+h) - \frac{56353369}{432000}(lw+wh+hl) - \frac{315544153}{4939200}$,

the Albertson index A of $M(l,w,h)$ is

$$A(M(l,w,h)) = 2(lw+wh+hl),$$

the harmonic index H of $M(l,w,h)$ is

$$H(M(l,w,h)) = \frac{1}{2}lwh - \frac{1}{99}(l+w+h) - \frac{1}{330}(lw+wh+hl) - \frac{53}{1155},$$

the first redefined Zagreb index $ReZG_1$ of $M(l,w,h)$ is

$$ReZG_1(M(l,w,h)) = lwh,$$

the second redefined Zagreb index $ReZG_2$ of $M(l,w,h)$ is

$$ReZG_2(M(l,w,h)) = 9lwh + \frac{194}{99}(l+w+h) - \frac{61}{11}(lw+wh+hl) - \frac{16}{231},$$

the third redefined Zagreb index $ReZG_3$ of $M(l,w,h)$ is

$$ReZG_3(M(l,w,h)) = 1296lwh - 1656(l+w+h) - 1364(lw+wh+hl) - 864,$$

the variation of the Randić index R' of $M(l,w,h)$ is

$$R'(M(l,w,h)) = \frac{1}{2}lwh - \frac{1}{15}(l+w+h) - \frac{1}{30}(lw+wh+hl) - \frac{1}{5},$$

Proof. For the general Randić index R_α of $M(l,w,h)$, we obtain $\phi(d_u,d_v) = (d_ud_v)^\alpha$. So $\phi(3,4) = (12)^\alpha, \phi(4,4) = (16)^\alpha, \phi(4,5) = (20)^\alpha, \phi(5,5) = (25)^\alpha, \phi(5,6) = (30)^\alpha$ and $\phi(6,6) = (36)^\alpha$. Thus by Lemma 3.1,

$$R_\alpha(M(l,w,h)) = 3lwh(36)^\alpha + 4\Big\{(16)^\alpha + 2(20)^\alpha - 5(25)^\alpha - 2(30)^\alpha + 4(36)^\alpha\Big\}(l+w+h) + \Big\{4(25)^\alpha + 2(30)^\alpha - 7(36)^\alpha\Big\}(lw+wh+hl) + 12\Big\{2(12)^\alpha - 3(16)^\alpha - 4(20)^\alpha + 6(25)^\alpha + 2(30)^\alpha - 3(36)^\alpha\Big\},$$

If $\alpha = -\frac{1}{2}$, then we get Randić index

$$R_{-\frac{1}{2}}(M(l,w,h)) = 3lwh(\tfrac{1}{6}) + 4\Big\{\tfrac{1}{4} + 2(\tfrac{1}{\sqrt{20}}) - 1 - 2(\tfrac{1}{\sqrt{30}}) + \tfrac{2}{3}\Big\}(l+w+h) + \Big\{4(\tfrac{1}{5}) + 2(\tfrac{1}{\sqrt{30}}) - 7(\tfrac{1}{6})\Big\}(lw+wh+hl) + 12\Big\{2(\tfrac{1}{\sqrt{12}}) - 3(\tfrac{1}{\sqrt{16}}) - 4(\tfrac{1}{\sqrt{20}}) + 6(\tfrac{1}{\sqrt{25}}) + 2(\tfrac{1}{\sqrt{30}}) - 3(\tfrac{1}{\sqrt{36}})\Big\}$$

$$= \tfrac{1}{2}lwh - 4(\sqrt{\tfrac{1}{5}} - \sqrt{\tfrac{2}{15}} - \tfrac{1}{12})(l+w+h) + (\sqrt{\tfrac{2}{15}} - \tfrac{11}{30})(lw+wh+hl) + 12(\sqrt{\tfrac{1}{3}} - \sqrt{\tfrac{4}{5}} + \sqrt{\tfrac{2}{15}} - \tfrac{1}{20}).$$

If $\alpha = 1$, then we obtain the second Zagreb index

$$R_1(M(l,w,h)) = 3lwh(36) + 4\Big\{16 + 2(20) - 5(25) - 2(30) + 4(36)\Big\}(l+w+h) + \Big\{4(25) + 2(30) - 7(36)\Big\}(lw+wh+hl) + 12\Big\{2(12) - 3(16) - 4(20) + 6(25) + 2(30) - 3(36)\Big\}$$

$$= 108lwh + 60(l+w+h) - 92(lw+wh+hl) - 24.$$

If $\alpha = -1$, then we obtain the second modified Zagreb index

$R_{-1}(M(l,w,h)) = 3lwh(\frac{1}{36}) + 4\left\{\frac{1}{16} + \frac{2}{20} - \frac{5}{25} - \frac{2}{30} + \frac{4}{36}\right\}(l+w+h) + \left\{\frac{4}{25} + \frac{2}{30} - \frac{7}{36})\right\}(lw+wh+hl) + 12\left\{\frac{2}{12} - \frac{3}{16} - \frac{4}{20} + \frac{6}{25} + \frac{2}{30} - \frac{3}{36}\right\}$
$= lwh + \frac{1}{36}(l+w+h) + \frac{29}{900}(lw+wh+hl) + \frac{3}{100}$.

For the general sum-connectivity index χ_α of $M(l,w,h)$, we obtain $\phi(d_u,d_v) = (d_u+d_v)^\alpha$. So $\phi(3,4) = (7)^\alpha, \phi(4,4) = (8)^\alpha, \phi(4,5) = (9)^\alpha, \phi(5,5) = (10)^\alpha, \phi(5,6) = (11)^\alpha$ and $\phi(6,6) = (12)^\alpha$. Thus by Lemma 3.1,

$\chi_\alpha(M(l,w,h)) = 3lwh(12)^\alpha + 4\left\{(8)^\alpha + 2(9)^\alpha - 5(10)^\alpha - 2(11)^\alpha + 4(12)^\alpha\right\}(l+w+h) + \left\{4(10)^\alpha + 2(11)^\alpha - 7(12)^\alpha\right\}(lw+wh+hl) + 12\left\{2(7)^\alpha - 3(8)^\alpha - 4(9)^\alpha + 6(10)^\alpha + 2(11)^\alpha - 3(12)^\alpha\right\}$,

If $\alpha = -\frac{1}{2}$, then we get sum-connectivity index

$\chi_{-\frac{1}{2}}(M(l,w,h)) = 3lwh(12)^{-\frac{1}{2}} + 4\left\{(8)^{-\frac{1}{2}} + 2(9)^{-\frac{1}{2}} - 5(10)^{-\frac{1}{2}} - 2(11)^{-\frac{1}{2}} + 4(12)^{-\frac{1}{2}}\right\}(l+w+h) + \left\{4(10)^{-\frac{1}{2}} + 2(11)^{-\frac{1}{2}} - 7(12)^{-\frac{1}{2}}\right\}(lw+wh+hl) + 12\left\{2(7)^{-\frac{1}{2}} - 3(8)^{-\frac{1}{2}} - 4(9)^{-\frac{1}{2}} + 6(10)^{-\frac{1}{2}} + 2(11)^{-\frac{1}{2}} - 3(12)^{-\frac{1}{2}}\right\}$
$= \frac{\sqrt{3}}{2}lwh - 4(\sqrt{\frac{1}{8}} - \sqrt{\frac{5}{2}} - \sqrt{\frac{4}{11}} + \sqrt{\frac{4}{3}} + \frac{2}{3})(l+w+h) + (\sqrt{\frac{8}{5}} + \sqrt{\frac{4}{11}} - \sqrt{\frac{49}{12}})(lw+wh+hl) + 12(\sqrt{\frac{4}{7}} - \sqrt{\frac{9}{8}} + \sqrt{\frac{12}{5}} + \sqrt{\frac{4}{11}} - \frac{2}{3} - \frac{\sqrt{3}}{2})$.

If $\alpha = 1$, then we get the first Zagreb index $\chi_1(M(l,w,h))$

$\chi_1(M(l,w,h)) = 3lwh(12) + 4\left\{(8) + 2(9) - 5(10) - 2(11) + 4(12)\right\}(l+w+h) + \left\{4(10) + 2(11) - 7(12)\right\}(lw+wh+hl) + 12\left\{2(7) - 3(8) - 4(9) + 6(10) + 2(11) - 3(12)\right\}$
$= 36lwh + 8(l+w+h) - 22(lw+wh+hl)$.

If $\alpha = -\frac{1}{2}$, then we get hyper-Zagreb index $\chi_2(M(l,w,h))$

$\chi_2(M(l,w,h)) = 3lwh((12)^2) + 4\left\{(8)^2 + 2((9)^2) - 5((10)^2) - 2((11)^2)) + 4((12)^2)\right\}(l+w+h) + \left\{4((10)^2) + 2((11)^2) - 7((12)^2)\right\}(lw+wh+hl) + 12\left\{2((7)^2) - 3((8)^2) - 4((9)^2) + 6((10)^2) + 2((11)^2)) - 3((12)^2)\right\}$
$= 432lwh + 240(l+w+h) - 366(lw+wh+hl) - 96$.

For the geometric-arithmetic index GA of $M(l,w,h)$ we obtain $\phi(d_u,d_v) = \frac{2\sqrt{d_u d_v}}{d_u+d_v}$. So $\phi(3,4) = \frac{4\sqrt{3}}{7}, \phi(4,4) = 1, \phi(4,5) = \frac{4\sqrt{5}}{9}, \phi(5,5) = 1, \phi(5,6) = \frac{2\sqrt{30}}{11}$ and $\phi(6,6) = 1$. Thus by Lemma 3.1,

$$GA(M(l,w,h)) = 3lwh(1) + 4\Big\{1 + 2(\tfrac{4\sqrt{5}}{9}) - 5(1) - 2(\tfrac{2\sqrt{30}}{11}) + 4(1)\Big\}(l + w + h) + \Big\{4(1) + 2(\tfrac{2\sqrt{30}}{11}) - 7(1)\Big\}(lw + wh + hl) + 12\Big\{2(\tfrac{4\sqrt{3}}{7}) - 3(1) - 4(\tfrac{4\sqrt{5}}{9}) + 6(1) + 2(\tfrac{2\sqrt{30}}{11}) - 3(1)\Big\}$$

$$= 3lwh + 16\Big\{\tfrac{2\sqrt{5}}{9} - \tfrac{\sqrt{30}}{11}\Big\}(l + w + h) + \Big\{\tfrac{4\sqrt{30}}{11} - 3\Big\}(lw + wh + hl) + 48\Big\{\tfrac{2\sqrt{3}}{7} - \tfrac{4\sqrt{5}}{9} + \tfrac{\sqrt{30}}{11}\Big\}.$$

For the symmetric division degree index SDD of $M(l,w,h)$ we obtain $\phi(d_u,d_v) = \frac{d_u^2+d_v^2}{d_u d_v}$. So $\phi(3,4) = \frac{25}{12}, \phi(4,4) = 2, \phi(4,5) = \frac{41}{20}, \phi(5,5) = 2, \phi(5,6) = \frac{61}{30}$ and $\phi(6,6) = 2$. Thus by Lemma 3.1,

$$SDD(M(l,w,h)) = 3lwh(2) + 4\Big\{2 + 2(\tfrac{41}{20}) - 5(2) - 2(\tfrac{61}{30}) + 4(2)\Big\}(l + w + h) + \Big\{4(2) + 2(\tfrac{61}{30}) - 7(2)\Big\}(lw + wh + hl) + 12\Big\{2(\tfrac{25}{12}) - 3(2) - 4(\tfrac{41}{20}) + 6(2) + 2(\tfrac{61}{30}) - 3(2)\Big\} = 6lwh + \tfrac{2}{15}(l + w + h) - \tfrac{29}{15}(lw + wh + hl) + \tfrac{2}{5}.$$

For the atom-bond connectivity index ABC of $M(l,w,h)$, we obtain $\phi(d_u,d_v) = \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$. So $\phi(3,4) = \sqrt{\frac{5}{12}}, \phi(4,4) = \sqrt{\frac{3}{8}}, \phi(4,5) = \sqrt{\frac{7}{20}}, \phi(5,5) = \frac{2\sqrt{2}}{5}, \phi(5,6) = \sqrt{\frac{3}{10}}$ and $\phi(6,6) = \frac{\sqrt{10}}{6}$. Thus by Lemma 3.1,

$$ABC(M(l,w,h)) = 3lwh(\tfrac{\sqrt{10}}{6}) + 4\Big\{\sqrt{\tfrac{3}{8}} + 2(\sqrt{\tfrac{7}{20}}) - 5(\tfrac{2\sqrt{2}}{5}) - 2(\sqrt{\tfrac{3}{10}}) + 4(\tfrac{\sqrt{10}}{6})\Big\}(l+w+h) + \Big\{4(\tfrac{2\sqrt{2}}{5}) + 2(\sqrt{\tfrac{3}{10}}) - 7(\tfrac{\sqrt{10}}{6})\Big\}(lw+wh+hl) + 12\Big\{2(\sqrt{\tfrac{5}{12}}) - 3(\sqrt{\tfrac{3}{8}}) - 4(\sqrt{\tfrac{7}{20}}) + 6(\tfrac{2\sqrt{2}}{5}) + 2(\sqrt{\tfrac{3}{10}}) - 3(\tfrac{\sqrt{10}}{6})\Big\}$$

$$= \tfrac{\sqrt{10}}{2}lwh + 4\Big\{\sqrt{\tfrac{3}{8}} + \sqrt{\tfrac{7}{5}} - 2\sqrt{2} - \sqrt{\tfrac{6}{5}} + \tfrac{2\sqrt{10}}{3})\Big\}(l + w + h) + \Big\{\tfrac{8\sqrt{2}}{5} + \sqrt{\tfrac{6}{5}} - \tfrac{7\sqrt{10}}{6}\Big\}(lw + wh + hl) + 12\Big\{\sqrt{\tfrac{5}{3}} - \sqrt{\tfrac{27}{8}} - \sqrt{\tfrac{28}{5}} + \tfrac{12\sqrt{2}}{5} + \sqrt{\tfrac{6}{5}} - \tfrac{\sqrt{10}}{2}\Big\}.$$

For the augmented Zagreb index AZI of $M(l,w,h)$, we obtain $\phi(d_u,d_v) = \left(\frac{d_u\ d_v}{d_u+d_v-2}\right)^3$. So $\phi(3,4) = \frac{1728}{125}, \phi(4,4) = \frac{512}{27}, \phi(4,5) = \frac{8000}{343}, \phi(5,5) = \frac{15625}{512}, \phi(5,6) = \frac{1000}{27}$ and $\phi(6,6) = \frac{5832}{125}$. Thus by Lemma 3.1,

$AZI(M(l,w,h)) = 3lwh(\frac{5832}{125}) + 4\Big\{\frac{512}{27} + 2(\frac{8000}{343}) - 5(\frac{15625}{512}) - 2(\frac{1000}{27}) + 4(\frac{5832}{125})\Big\}(l+w+h) + \Big\{4(\frac{15625}{512}) + 2(\frac{1000}{27}) - 7(\frac{5832}{125})\Big\}(lw+wh+hl) + 12\Big\{2(\frac{1728}{125}) - 3(\frac{512}{27}) - 4(\frac{8000}{343}) + 6(\frac{15625}{512}) + 2(\frac{1000}{27}) - 3(\frac{5832}{125})\Big\}$
$= \frac{17496}{125}lwh + \frac{5052254057}{49392000}(l+w+h) - \frac{56353369}{432000}(lw+wh+hl) - \frac{315544153}{4939200}$.

For the Albertson index A of $M(l,w,h)$, we obtain $\phi(d_u,d_v) = |d_u - d_v|$. So $\phi(3,4) = 1, \phi(4,4) = 0, \phi(4,5) = 1, \phi(5,5) = 0, \phi(5,6) = 1$ and $\phi(6,6) = 0$. Thus by Lemma 3.1,

$A(M(l,w,h)) = 3lwh(0) + 4\Big\{(0) + 2(1) - 5(0) - 2(1) + 4(0)\Big\}(l+w+h) + \Big\{4(0) + 2(1) - 7(0)\Big\}(lw+wh+hl) + 12\Big\{2(1) - 3(0) - 4(1) + 6(0) + 2(1) - 3(0)\Big\}$
$= 2(lw+wh+hl)$.

For the harmonic index H of $M(l,w,h)$, we obtain $\phi(d_u,d_v) = \frac{2}{d_u+d_v}$. So $\phi(3,4) = \frac{2}{7}, \phi(4,4) = \frac{1}{4}, \phi(4,5) = \frac{2}{9}, \phi(5,5) = \frac{1}{5}, \phi(5,6) = \frac{2}{11}$ and $\phi(6,6) = \frac{1}{6}$. Thus by Lemma 3.1,

$H(M(l,w,h)) = 3lwh(\frac{1}{6}) + 4\Big\{\frac{1}{4} + 2(\frac{2}{9}) - 5(\frac{1}{5}) - 2(\frac{2}{11}) + 4(\frac{1}{6})\Big\}(l+w+h) + \Big\{4(\frac{1}{5}) + 2(\frac{2}{11}) - 7(\frac{1}{6})\Big\}(lw+wh+hl) + 12\Big\{2(\frac{2}{7}) - 3(\frac{1}{4}) - 4(\frac{2}{9}) + 6(\frac{1}{5}) + 2(\frac{2}{11}) - 3(\frac{1}{6})\Big\}$
$= \frac{1}{2}lwh - \frac{1}{99}(l+w+h) - \frac{1}{330}(lw+wh+hl) - \frac{53}{1155}$.

For the first redefined Zagreb index $ReZG_1$ of $M(l,w,h)$, we obtain $\phi(d_u,d_v) = \frac{d_u+d_v}{d_ud_v}$. So $\phi(3,4) = \frac{7}{12}, \phi(4,4) = \frac{1}{2}, \phi(4,5) = \frac{9}{20}, \phi(5,5) = \frac{2}{5}, \phi(5,6) = \frac{11}{30}$ and $\phi(6,6) = \frac{1}{3}$. Thus by Lemma 3.1,

$ReZG_1(M(l,w,h)) = 3lwh(\frac{1}{3}) + 4\Big\{\frac{1}{2} + 2(\frac{9}{20}) - 5(\frac{2}{5}) - 2(\frac{11}{30}) + 4(\frac{1}{3})\Big\}(l+w+h) + \Big\{4(\frac{2}{5}) + 2(\frac{11}{30}) - 7(\frac{1}{3})\Big\}(lw+wh+hl) + 12\Big\{2(\frac{7}{12}) - 3(\frac{1}{2}) - 4(\frac{9}{20}) + 6(\frac{2}{5}) + 2(\frac{11}{30}) - 3(\frac{1}{3})\Big\}$
$= lwh$.

For the second redefined Zagreb index $ReZG_2$ of $M(l,w,h)$, we obtain $\phi(d_u,d_v) = \frac{d_ud_v}{d_u+d_v}$. So $\phi(3,4) = \frac{12}{7}, \phi(4,4) = 2, \phi(4,5) = \frac{20}{9}, \phi(5,5) = \frac{5}{2}, \phi(5,6) = \frac{30}{11}$ and $\phi(6,6) = 3$. Thus by Lemma 3.1,

$ReZG_2(M(l,w,h)) = 3lwh(3) + 4\Big\{2 + 2(\frac{20}{9}) - 5(\frac{5}{2}) - 2(\frac{30}{11}) + 4(3)\Big\}(l+w+h) + \Big\{4(\frac{5}{2}) + 2(\frac{30}{11}) - 7(3)\Big\}(lw+wh+hl) + 12\Big\{2(\frac{12}{7}) - 3(2) - 4(\frac{20}{9}) +$

$6(\frac{5}{2}) + 2(\frac{30}{11}) - 3(3)\Big\}$
$= 9lwh + \frac{194}{99}(l + w + h) - \frac{61}{11}(lw + wh + hl) - \frac{16}{231}.$

For the third redefined Zagreb index $ReZG_3$ of $M(l, w, h)$, we obtain $\phi(d_u, d_v) = d_u d_v\,(d_u + d_v)$. So $\phi(3, 4) = 84, \phi(4, 4) = 128, \phi(4, 5) = 180, \phi(5, 5) = 250, \phi(5, 6) = 330$ and $\phi(6, 6) = 432$. Thus by Lemma 3.1,

$ReZG_3(M(l, w, h)) = 3lwh(432) + 4\Big\{128 + 2(180) - 5(250) - 2(330) + 4(432)\Big\}(l+w+h) + \Big\{4(250) + 2(330) - 7(432))\Big\}(lw+wh+hl) + 12\Big\{2(84) - 3(128) - 4(180) + 6(250) + 2(330) - 3(432)\Big\}$
$= 1296lwh - 1656(l + w + h) - 1364(lw + wh + hl) - 864.$

For the variation of the Randić index R' of $M(l, w, h)$, we obtain $\phi(d_u, d_v) = \frac{1}{\max\{d_u,d_v\}}$. So $\phi(3, 4) = \frac{1}{4}, \phi(4, 4) = \frac{1}{4}, \phi(4, 5) = \frac{1}{5}, \phi(5, 5) = \frac{1}{5}, \phi(5, 6) = \frac{1}{6}$ and $\phi(6, 6) = \frac{1}{6}$. Thus by Lemma 3.1,

$R'(M(l, w, h)) = 3lwh(\frac{1}{6}) + 4\Big\{(\frac{1}{4}) + 2(\frac{1}{5}) - 5(\frac{1}{5}) - 2(\frac{1}{6}) + 4(\frac{1}{6})\Big\}(l+w+h) + \Big\{4(\frac{1}{5}) + 2(\frac{1}{6}) - 7(\frac{1}{6})\Big\}(lw+wh+hl) + 12\Big\{2(\frac{1}{4}) - 3(\frac{1}{4}) - 4(\frac{1}{5}) + 6(\frac{1}{5}) + 2(\frac{1}{6}) - 3(\frac{1}{6})\Big\}$
$= \frac{1}{2}lwh - \frac{1}{15}(l + w + h) - \frac{1}{30}(lw + wh + hl) - \frac{1}{5}.$

□

4. **Conclusion**

This article is devoted on the computation of Zagreb indices, geometric-arithmetic index, atom-bond connectivity index harmonic index etc. for sodium chloride $NaCl$. This study is useful for further comprehension the attributes of various physical structures like carbohydrates, silicone structures, polymers, hexagonal chains, cylindrical fullerenes. They can likewise be useful in creating productive physical structure in mechanics as well as for different computer network problems.

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