On Molecular descriptors with python of 3D Lattice

S.Manimekalai
Assistant Professor
Dr.N.G.P.Arts and Science College
Coimbatore
manimekalai@drngpasc.ac.in
U.Mary
Nirmala College for Women
Coimbatore
marycbe@gmail.com
K.Rajam
Nirmala College for Women
Coimbatore

Abstract—Topological index of a graph G is a numerical value which reveals it's topological properties. A bravais lattice is an infinite arrangement of discrete molecules with orientation and arrangement appears exactly same.We give properties for the connectivity and neighbourhood degree based indices for frequently used three dimensional type lattice .
Keywords—bounds, connectivity, lattice,neighborhood, topological indices.

MSC (2010): 05C12.

I. INTRODUCTION

When the graph (*G)* represents the molecular structure of a chemical compound, it is called a molecular graph. This types of graphs are widely used in designing and create new things in all field of Science.First topological index was introduced by Wiener. We present various neighborhood degree based index of widely used chemical structures which will appear in mathematical chemistry and solid state physics. Solid state physics is study about solid through crystallography, metallurgy and others.

Molecular structure modeling is High priority in Proteins , Enzymes , Medical drugs,Virus, Bacteria, Field of Nano Science etc.There are so many 2D and 3D models to investigate the property and the activity of molecules.Simple 3D molecular formula is CH_4.

Lattices introduced by Augsut Bravais (1811-1863).bravais lattices include cubic , face centered cubic and body centered cubic. Another one is hexagonal close paced arrangements. In adding up to trasnslational symmetry the unit cell must have some symmetry to arrangement of the atoms with in the unit cell.

The precise combination of evenness elements in a crystal defines its space group which are 230 different space groups. Another main concept in lattices is reciprocal lattice. X-ray Crystallographers use a reciprocal lattice defined by 3 vectors. Just like real space lattice reciprocal lattice constructed from a series of primitive cells(Wigner Seitz cells) which entirely fill the space without overlapping and without gaps.Reciprocal Lattice’s Wigner Seitz cell is called as first Brillouin zone in electronic system.

Lattices investigated from eighteenth centuary by many mathematicians Gauss, Lagrange later Minkowski . Lattice points arranged like, each has one and the same background. To fill the space in efficient manner to maintain the surroundings. Its points denote the number of atoms in our basis.Recently it is active topic in research in the fields of Computer Science , Chemistry, Physics and Cryptography. Here we are found various descriptors for one type of face centered Lattice.

1.1 Definitions

Various indices were introduced in various periods of time,

Vertex level based topological index was introduced by M. Randic [9] in 1975,Connectivity index or Randic index.

$$R(A)=\sum_{uv\in E(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right)$$

The inverse Randic index [10] is

$$RR(A)=\sum_{uv\in E(A)}\sqrt{\deg(u)\deg(v)}$$

B. Zhou and N. Trinanjstic - sum connectivity index [13] given by

$$SCI(A)=\sum_{uv\in E(A)}\left(\frac{1}{\sqrt{\deg(u)+\deg(v)}}\right)$$

SDD index [14] is

SDD(A)= $\sum_{uv\in E(A)}\left[\frac{\deg(u)}{\deg(v)}+\frac{\deg(v)}{\deg(u)}\right]$

The 1st and 2nd Zagreb indices presented by Gutman and Trinajstic in [13,14].

M_1(A)= $\sum_{uv\in E(A)}(\deg(u)+\deg(v))$

M_2(A)= $\sum_{uv\in E(A)}(\deg(u)\deg(v))$

Furtula and Gutman [15] presented the forgotten topological index as:

F(A)= $\sum_{v\in V(A)}\deg(v)^3=\sum_{uv\in E(A)}(\deg(u)^2+\deg(v)^2)$

Ghorbani and Azimi [12] defined the two multiple Zagreb indices of a graph A are

PM_1(A)= $\prod_{uv\in E(A)}(\deg(u)+\deg(v))$

PM_2(A)= $\prod_{uv\in E(A)}\deg(u)\deg(v)$

Urtula [17] et al. have given an augmented Zagreb index as

AZI(A)= $\sum_{uv\in E(A)}\left(\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)-2}\right)^3$

The Balaban index [18,19]

J(A)= $\frac{m}{m-n+2}\sum_{uv\in E(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right)$

The new versions of the Zagreb indices introduced by Ranjini et al. [20]

ReZ_1(A)= $\sum_{uv\in E(A)}\frac{\deg(u)+\deg(v)}{\deg(u)\deg(v)}$

ReZ_2(A)= $\sum_{uv\in E(A)}\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)}$

ReZ_3(A)= $\sum_{uv\in E(A)}\deg(u)\deg(v)(\deg(u)+\deg(v))$

Fath-Tabar [21] introduced two Zagreb polynomials of a graph A

$$M_1(A,x)=\sum_{uv\in E(A)} x^{(\deg(u)+\deg(v))}$$

$$M_2(A,x)=\sum_{uv\in E(A)} x^{(\deg(u)\deg(v))}$$

Chaluvaraju et al. [22] redefined the two hyper-Zagreb polynomials as

$$HM_1(A,x)=\sum_{uv\in E(A)} x^{(\deg(u)+\deg(v))^2}$$

$$HM_2(A,x)=\sum_{uv\in E(A)} x^{(\deg(u)\deg(v))^2}$$

the geometric arithmetic index GA , introduced in [28]

$$GA_1(A) = \sum_{uv\in E(A)} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u)+\deg(v)}$$

The atom–bond connectivity index ABC

$$ABC(A) = \sum_{uv\in E(A)} \sqrt{\frac{\deg(u)+\deg(v)-2}{\deg(u)\deg(v)}}$$

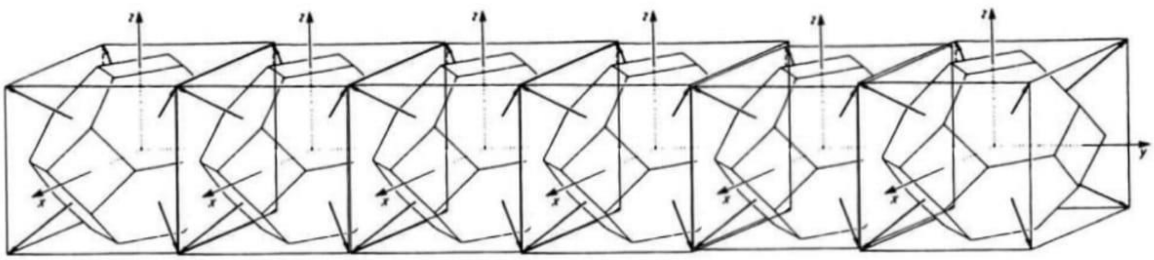
2. Face centered cubic Lattice

Face centered cubic lattice has gathering of cubes with atom at faces of each cube and also atoms at the edges. Solid state material have electronic, Physical and chemical properties. Wide variety of descriptors have developed to study the characteristic and properties through their structure. A crystalline system can be made by staking replica of some repeating unit in an organized manner in without break and without overlap. The structure specified by defining the shape and size of the cell and location of atoms within it. There are 14 distinct type basic unit cell these are bravais lattices. Materials with this structure include gold, aluminum, nickel silver, and copper. Lattice have some special properties of particular value for solid state electronic structure calculations.

Methodology for calculations:

The structure of graph A contains 20n+4 vertices and 32n+4 edges.To find the molecular descriptors we subdivide the Edge set into 3 partitions. The First edge set contains 4(n-1) edges where deg(u)=4 and deg(v)=4. The second edge set contains 4(n-1) edges where deg(u)=3 and deg(v)=4. The third edge set contains 24n+12 edges where deg(u)=3 and deg(v)=3. Table 1 shows the frequency as follows

Degree	*frequency*	*Edge set*
(4,4)	*4(n-1)*	E_1
(4,3)	*4(n-1)*	E_2
(3,3)	*24n+12*	E_3



. . .

2.1 THEOREM

LET A BE AN BRAVAIS LATTICE, FOR ALL N $\geqslant 2$. THEN THE RANDIC INDEX IS

$$R(A)=(n-1)+\frac{4(n-1)}{\sqrt{12}}+\frac{24n+12}{3}$$

Proof:

Let A be an bravais Lattice. Then

$$R(A)=\sum_{uv\in E(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right)$$

R(A)= $\sum_{uv\in E_1(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right) + \sum_{uv\in E_2(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right) + \sum_{uv\in E_3(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right)$

R(A)= $(n-1)+\frac{4(n-1)}{\sqrt{12}}+\frac{24n+12}{3}$

2.2 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the inverse Randic index is

RR(A)= $72n+4\sqrt{12}n+20-4\sqrt{12}$

Proof:

Let A be an bravais Lattice. Then

RR(A)= $\sum_{uv\in E(A)}\sqrt{\deg(u)\deg(v)}$

RR(A)= $\sum_{uv\in E_1(A)}\sqrt{\deg(u)\deg(v)} + \sum_{uv\in E2(A)}\sqrt{\deg(u)\deg(v)} + \sum_{uv\in E_3(A)}\sqrt{\deg(u)\deg(v)}$

RR(A)= $4(n-1)\sqrt{16} + 4(n-1)\sqrt{12} + (24n+12)\sqrt{9}$

RR(A)= $72n+4\sqrt{12}n+20-4\sqrt{12}$

2.3 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then sum connectivity index is

SCI(A)= $\frac{4(n-1)}{\sqrt{8}}+\frac{4(n-1)}{\sqrt{7}}+\frac{24n+12}{\sqrt{6}}$

Proof:

Let A be an bravais Lattice. Then

SCI(A)= $\sum_{uv\in E(A)}\left(\frac{1}{\sqrt{\deg(u)+\deg(v)}}\right)$

SCI(A)= $\sum_{uv\in E_1(A)}\left(\frac{1}{\sqrt{\deg(u)+\deg(v)}}\right) + \sum_{uv\in E_2(A)}\left(\frac{1}{\sqrt{\deg(u)+\deg(v)}}\right) + \sum_{uv\in E_3(A)}\left(\frac{1}{\sqrt{\deg(u)+\deg(v)}}\right)$

SCI(A)= $\frac{4(n-1)}{\sqrt{8}}+\frac{4(n-1)}{\sqrt{7}}+\frac{24n+12}{\sqrt{6}}$

2.4 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then SSD index is

SSD(A)= $\frac{193}{3}n+\frac{23}{3}$

Proof:

Let A be an bravais Lattice. Then the SDD index is

SDD(A)= $\sum_{uv\in E(A)}\left[\frac{\deg(u)}{\deg(v)}+\frac{\deg(v)}{\deg(u)}\right]$

SDD(A)= $\sum_{uv\in E_1(A)}\left[\frac{\deg(u)}{\deg(v)}+\frac{\deg(v)}{\deg(u)}\right]+\sum_{uv\in E_2(A)}\left[\frac{\deg(u)}{\deg(v)}+\frac{\deg(v)}{\deg(u)}\right]+\sum_{uv\in E_3(A)}\left[\frac{\deg(u)}{\deg(v)}+\frac{\deg(v)}{\deg(u)}\right]$

SDD(A)= $\left(\frac{4}{4}+\frac{4}{4}\right)4(n-1)+\left(\frac{4}{3}+\frac{3}{4}\right)4(n-1)+\left(\frac{3}{3}+\frac{3}{3}\right)(24n+12)$

SSD(A)= $\frac{193}{3}n+\frac{23}{3}$

2.5 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then Zagreb indices are

M_1(A)=244n-64

M_2(A)=328n-6

Proof:

Let A be an bravais Lattice. Then

M_1(A)= $\sum_{uv\in E(A)}(\deg(u)+\deg(v))$

M_1(A)= $\sum_{uv\in E_1(A)}(\deg(u)+\deg(v))+\sum_{uv\in E_2(A)}(\deg(u)+\deg(v))+\sum_{uv\in E_3(A)}(\deg(u)+\deg(v))$

M_1(A)= 424+(n-2)244

M_1(A)= 244n-64

$M_2(A)=\sum_{uv\in E(A)}(\deg(u)\deg(v))$

$M_2(A) = 652+(n-2)328$

$M_2(A) =328n-6$

2.6 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the Forgotton index is

$F(A)=796n-256$

Proof:

Let A be an bravais Lattice. Then

$F(A)=\sum_{v\in V(A)}\deg(v)^3 = \sum_{uv\in E(A)}(\deg(u)^2+\deg(v)^2)$

$F(A)= 1336+(n-2)796$

$F(A)=796n-256$

2.7 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the multiple Zagreb indices are

$PM_1(A)=8^{4(n-1)}\times 7^{4(n-1)}\times 6^{24n+12}$

$PM_2(A)= 16^{4(n-1)}\times 12^{4(n-1)}\times 9^{24n+12}$

Proof:

Consider a bravais Lattice A. Then

$PM_1(A)=\prod_{uv\in E(A)}\deg(u)+\deg(v)$

$PM_1(A)=\prod_{uv\in E_1(A)}\deg(u)+\deg(v)\times\prod_{uv\in E_2(A)}\deg(u)+\deg(v)\times\prod_{uv\in E_3(A)}\deg(u)+\deg(v)$

$PM_1(A)=8^{4(n-1)}\times 7^{4(n-1)}\times 6^{24n+12}$

$PM_2(A)=\prod_{uv\in E_1(A)}\deg(u)\deg(v)\times\prod_{uv\in E_2(A)}\deg(u)\deg(v)\times\prod_{uv\in E_3(A)}\deg(u)\deg(v)$

$PM_2(A)= 16^{4(n-1)}\times 12^{4(n-1)}\times 9^{24n+12}$

2.8 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the augmented Zagreb index is

$$AZI(A)=4\left(\frac{16}{6}\right)^3(n-1)+4\left(\frac{12}{5}\right)^3(n-1)+\left(\frac{9}{4}\right)^3(24n+12)$$

Proof:

Consider a bravais Lattice A. Then

$$AZI(A)=\sum_{uv\in E(A)}\left(\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)-2}\right)^3$$

AZI(A)=

$$\sum_{uv\in E_1(A)}\left(\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)-2}\right)^3+\sum_{uv\in E_2(A)}\left(\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)-2}\right)^3+\sum_{uv\in E_3(A)}\left(\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)-2}\right)^3$$

$$AZI(A)=4\left(\frac{16}{6}\right)^3(n-1)+4\left(\frac{12}{5}\right)^3(n-1)+\left(\frac{9}{4}\right)^3(24n+12)$$

2.9 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the redefined Zagreb indices are

$$ReZ_1(A)= 2(n-1)+\frac{7(n-1)}{3}+\frac{2}{3}(24n+12)$$

$$ReZ_2(A)= 8(n-1)+\frac{48(n-1)}{7}+\frac{3}{2}(24n+12)$$

$$ReZ_3(A)= 512(n-1)+336(n-1)+54(24n+12)$$

Proof:

Consider a bravais Lattice A. Then the redefined Zagreb indices are as follows

$$ReZ_1(A)=\sum_{uv\in E(A)}\frac{\deg(u)+\deg(v)}{\deg(u)\deg(v)}$$

$$ReZ_1(A)=\sum_{uv\in E_1(A)}\frac{\deg(u)+\deg(v)}{\deg(u)\deg(v)}+\sum_{uv\in E_2(A)}\frac{\deg(u)+\deg(v)}{\deg(u)\deg(v)}+\sum_{uv\in E_3(A)}\frac{\deg(u)+\deg(v)}{\deg(u)\deg(v)}$$

ReZ₁(A)= $2(n-1)+\frac{7(n-1)}{3}+\frac{2}{3}(24n+12)$

ReZ₂(A)= $\sum_{uv\in E_1(A)}\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)}+\sum_{uv\in E_2(A)}\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)}+\sum_{uv\in E_3(A)}\frac{\deg(u)\deg(v)}{\deg(u)+\deg(v)}$

ReZ₂(A)= $8(n-1)+\frac{48(n-1)}{7}+\frac{3}{2}(24n+12)$

ReZ₃(A)= $\sum_{uv\in E(A)}\deg(u)\deg(v)(\deg(u)+\deg(v))$

ReZ₃(A)=
$\sum_{uv\in E_1(A)}\deg(u)\deg(v)(\deg(u)+\deg(v))+\sum_{uv\in E_2(A)}\deg(u)\deg(v)(\deg(u)+\deg(v))+\sum_{uv\in E_3(A)}\deg(u)\deg(v)(\deg(u)+\deg(v))$

ReZ₃(A)= $512(n-1)+336(n-1)+54(24n+12)$

2.10. *THEOREM*

Let A be an bravais Lattice, for all n ≥ 2. Then the Balaban index is

J(A)= $\frac{32n+4}{12n+2}\left[4(n-1)\left(\frac{1}{\sqrt{16}}\right)+4(n-1)\left(\frac{1}{\sqrt{12}}\right)+24n+12\left(\frac{1}{\sqrt{9}}\right)\right]$

Proof:

Consider a bravais Lattice A. Then

J(A)= $\frac{m}{m-n+2}\sum_{uv\in E(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right)$

J(A)=
$\frac{m}{m-n+2}\left(\sum_{uv\in E_1(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right)+\sum_{uv\in E_2(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right)+\sum_{uv\in E_3(A)}\left(\frac{1}{\sqrt{\deg(u)\deg(v)}}\right)\right)$

J(A)= $\frac{32n+4}{12n+2}\left[4(n-1)\left(\frac{1}{\sqrt{16}}\right)+4(n-1)\left(\frac{1}{\sqrt{12}}\right)+24n+12\left(\frac{1}{\sqrt{9}}\right)\right]$

2.11 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the geometric arithmetic index is

$$GA_1(A)= \frac{8\sqrt{12}}{7}(n-1)+28n+8$$

Proof:

Consider a bravais Lattice A. Then

$$GA_1(A) = \sum_{uv\in E(A)} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u)+\deg(v)}$$

$$GA_1(A) = \frac{8(n-1)\sqrt{16}}{8}+\frac{8(n-1)\sqrt{12}}{7}+(24+12)\frac{2\sqrt{9}}{6}$$

$$GA_1(A)= \frac{8\sqrt{12}}{7}(n-1)+28n+8$$

2.12 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the atom-bond connectivity index is

$$ABC(A) = (n-1)4\sqrt{\frac{6}{16}}+4(n-1)\sqrt{\frac{5}{12}}+(24n+12)\sqrt{\frac{4}{9}}$$

Proof:

Consider a bravais Lattice A. Then atom-bond connectivity index is

$$ABC(A) = \sum_{uv\in E(A)} \sqrt{\frac{\deg(u)+\deg(v)-2}{\deg(u)\deg(v)}}$$

$$ABC(A) = \sum_{uv\in E_1(A)} \sqrt{\frac{\deg(u)+\deg(v)-2}{\deg(u)\deg(v)}}+\sum_{uv\in E_2(A)} \sqrt{\frac{\deg(u)+\deg(v)-2}{\deg(u)\deg(v)}}\sum_{uv\in E_3(A)} \sqrt{\frac{\deg(u)+\deg(v)-2}{\deg(u)\deg(v)}}$$

$$ABC(A) = (n-1)4\sqrt{\frac{6}{16}}+4(n-1)\sqrt{\frac{5}{12}}+(24n+12)\sqrt{\frac{4}{9}}$$

2.13 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the two Zagreb polynomials are

$$M_1(A,x)= 4(n-1)x^8+4(n-1)x^7+(24n+12)x^6$$

M2(A,x)= $4(n-1)x^{16}+4(n-1)x^{12}+(24n+12)x^{9}$

Proof:

Consider a bravais Lattice A. Then the two Zagreb polynomials are

M1(A,x)= $\sum_{uv\in E(A)} x^{(\deg(u)+\deg(v))}$

M1(A,x)= $\sum_{uv\in E_1(A)} x^{(\deg(u)+\deg(v))}+\sum_{uv\in E_2(A)} x^{(\deg(u)+\deg(v))}+\sum_{uv\in E_3(A)} x^{(\deg(u)+\deg(v))}$

M1(A,x)= $4(n-1)x^{8}+4(n-1)x^{7}+(24n+12)x^{6}$

M2(A,x)= $\sum_{uv\in E(A)} x^{(\deg(u)\deg(v))}$

M2(A,x)= $\sum_{uv\in E_1(A)} x^{(\deg(u)\deg(v))}+\sum_{uv\in E_2(A)} x^{(\deg(u)\deg(v))}+\sum_{uv\in E_3(A)} x^{(\deg(u)\deg(v))}$

M2(A,x)= $4(n-1)x^{16}+4(n-1)x^{12}+(24n+12)x^{9}$

2.14 THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the two hyper Zagreb polynomials are

HM1(A,x)= $4(n-1)x^{64}+4(n-1)x^{49}+(24n+12)x^{36}$

HM2(A,x)= $4(n-1)x^{156}+4(n-1)x^{144}+(24n+12)x^{82}$

Proof:

Consider a bravais Lattice A. Then the two hyper Zagreb polynomials are

HM1(A,x)= $\sum_{uv\in E(A)} x^{(\deg(u)+\deg(v))^2}$

HM1(A,x)= $\sum_{uv\in E_1(A)} x^{(\deg(u)+\deg(v))^2}+\sum_{uv\in E_2(A)} x^{(\deg(u)+\deg(v))^2}+\sum_{uv\in E_3(A)} x^{(\deg(u)+\deg(v))^2}$

HM1(A,x)= $4(n-1)x^{64}+4(n-1)x^{49}+(24n+12)x^{36}$

HM2(A,x)= $\sum_{uv\in E_1(A)} x^{(\deg(u)\deg(v))^2}+\sum_{uv\in E_2(A)} x^{(\deg(u)\deg(v))^2}+\sum_{uv\in E_3(A)} x^{(\deg(u)\deg(v))^2}$

HM2(A,x)= $4(n-1)x^{156}+4(n-1)x^{144}+(24n+12)x^{82}$

3. NEIGHBOURHOOD DEGREESUM BASED INDICES

Sourav Mondal, Nilanjan De, Anita pal introduced neighbourhood degree based indices to check the chemical applicability of indices.

Here we compute and given the relation between other topological indices of neighbourhood degree based indices. The indices are

$ND_1(A)= \sum_{uv\in E(A)} \sqrt{\delta_A(u)\delta_A(v)}$

$ND_2(A)= \sum_{uv\in E(A)} \left(\frac{1}{\sqrt{\delta_A(u)+\delta_A(v)}} \right)$

$ND_3(A)= \sum_{uv\in E(A)} \delta_A(u)\delta_A(v)(\delta_A(u)+\delta_A(v))$

$ND_4(A)= \sum_{uv\in E(A)} \left(\frac{1}{\sqrt{\delta_A(u)\delta_A(v)}} \right)$

$ND_5(A)= \sum_{uv\in E(A)} \left[\frac{\delta_A(u)}{\delta_A(v)} + \frac{\delta_A(v)}{\delta_A(u)} \right]$

$ND_6(A)= \sum_{uv\in E(A)} \delta_A(u)\deg(u)+\deg(v)+\delta_A(v)$

Where δ_A(u)= $\sum_{v\in N_A(u)} \deg(v)$

The fourth version of atom–bond connectivity index ABC_4 by Ghorbhani et al. [23]

$ABC_4= \sum_{uv\in E(A)} \sqrt{\frac{\delta_A(u)+\delta_A(v)-2}{\delta_A(u)\delta_A(v)}}$

Where δ_A(u)= $\sum_{v\in N_A(u)} \deg(v)$

The fifth version of the geometric arithmetic index GA_5 by Graovoc et al. [24]

$$GA_5(A) = \sum_{uv\in E(A)} \frac{2\sqrt{\delta_A(u)\delta_A(v)}}{\delta_A(u)+\delta_A(v)}$$

Where $\delta_A(u) = \sum_{v\in N_A(u)} \deg(v)$

3.1 . THEOREM

Let A be an bravais Lattice, for all n ≥ 2. Then the neighbourhood degree based indices

$$ND_1(A) = (32+4n)\sqrt{82} + 16(n-1)\sqrt{90} + 4(n-1)\sqrt{196} + 8(n-1)\sqrt{110}$$

$$ND_2(A) = \frac{32+4n}{\sqrt{18}} + \frac{16(n-1)}{\sqrt{19}} + \frac{4(n-1)}{\sqrt{28}} + \frac{8(n-1)}{\sqrt{21}}$$

$$ND_3(A) = (32+4n)(1458) + 16(n-1)1710 + 21952(n-1) + 18480(n-1)$$

$$ND_4(A) = \frac{32+4n}{\sqrt{82}} + \frac{16(n-1)}{\sqrt{90}} + \frac{4(n-1)}{\sqrt{196}} + \frac{8(n-1)}{\sqrt{110}}$$

$$ND_5(A) = 2(32+4n) + \left(\frac{9}{10}+\frac{10}{9}\right)16(n-1) + 8(n-1) + \left(\frac{10}{11}+\frac{11}{10}\right)8(n-1)$$

$$ABC_4 = \sqrt{\frac{16}{82}} \times (32+4n) + 16(n-1)\sqrt{\frac{17}{90}} + 4(n-1)\sqrt{\frac{26}{196}} + 8(n-1)\sqrt{\frac{19}{110}}$$

$$GA_5(A) = \frac{(32+4n)\sqrt{81}}{9} + \frac{32(n-1)\sqrt{90}}{19} + \frac{2(n-1)\sqrt{196}}{7} + \frac{16(n-1)\sqrt{110}}{21}$$

Proof:

$$ND_1(A) = \sum_{uv\in E(A)} \sqrt{\delta_A(u)\delta_A(v)}$$

$$ND_1(A) = \sum_{uv\in E_1(A)} \sqrt{\delta_A(u)\delta_A(v)} + \sum_{uv\in E_2(A)} \sqrt{\delta_A(u)\delta_A(v)} + \sum_{uv\in E_3(A)} \sqrt{\delta_A(u)\delta_A(v)} + \sum_{uv\in E_4(A)} \sqrt{\delta_A(u)\delta_A(v)}$$

$$ND_1(A) = (32+4n)\sqrt{82} + 16(n-1)\sqrt{90} + 4(n-1)\sqrt{196} + 8(n-1)\sqrt{110}$$

$$ND_2(A) = \sum_{uv\in E(A)} \left(\frac{1}{\sqrt{\delta_A(u)+\delta_A(v)}}\right)$$

ND2(A)= $\sum_{uv\in E_1(A)}\left(\frac{1}{\sqrt{\delta_A(u)+\delta_A(v)}}\right)+\sum_{uv\in E_2(A)}\left(\frac{1}{\sqrt{\delta_A(u)+\delta_A(v)}}\right)+\sum_{uv\in E_3(A)}\left(\frac{1}{\sqrt{\delta_A(u)+\delta_A(v)}}\right)+\sum_{uv\in E_4(A)}\left(\frac{1}{\sqrt{\delta_A(u)+\delta_A(v)}}\right)$

ND2(A)= $\frac{32+4n}{\sqrt{18}}+\frac{16(n-1)}{\sqrt{19}}+\frac{4(n-1)}{\sqrt{28}}+\frac{8(n-1)}{\sqrt{21}}$

ND3(A)= $\sum_{uv\in E_1(A)}\delta_A(u)\delta_A(v)(\delta_A(u)+\delta_A(v))+\sum_{uv\in E_2(A)}\delta_A(u)\delta_A(v)(\delta_A(u)+\delta_A(v)) + \sum_{uv\in E_3(A)}\delta_A(u)\delta_A(v)(\delta_A(u)+\delta_A(v))+\sum_{uv\in E_4(A)}\delta_A(u)\delta_A(v)(\delta_A(u)+\delta_A(v))$

ND3(A)= $(32+4n)(81\times 18)+16(n-1)(90\times 19)+21952(n-1)+18480(n-1)$

ND4(A)= $\sum_{uv\in E(A)}\left(\frac{1}{\sqrt{\delta_A(u)\delta_A(v)}}\right)$

ND4(A)=

$$\sum_{uv\in E_1(A)}\left(\frac{1}{\sqrt{\delta_A(u)\delta_A(v)}}\right)+\sum_{uv\in E_2(A)}\left(\frac{1}{\sqrt{\delta_A(u)\delta_A(v)}}\right)+\sum_{uv\in E_3(A)}\left(\frac{1}{\sqrt{\delta_A(u)\delta_A(v)}}\right)+\sum_{uv\in E_4(A)}\left(\frac{1}{\sqrt{\delta_A(u)\delta_A(v)}}\right)$$

ND4(A)= $\frac{32+4n}{\sqrt{82}}+\frac{16(n-1)}{\sqrt{90}}+\frac{4(n-1)}{\sqrt{196}}+\frac{8(n-1)}{\sqrt{110}}$

ND5(A)= $\sum_{uv\in E(A)}\left[\frac{\delta_A(u)}{\delta_A(v)}+\frac{\delta_A(v)}{\delta_A(u)}\right]$

ND5(A)= $\sum_{uv\in E_1(A)}\left[\frac{\delta_A(u)}{\delta_A(v)}+\frac{\delta_A(v)}{\delta_A(u)}\right]+\sum_{uv\in E_2(A)}\left[\frac{\delta_A(u)}{\delta_A(v)}+\frac{\delta_A(v)}{\delta_A(u)}\right]+\sum_{uv\in E_3(A)}\left[\frac{\delta_A(u)}{\delta_A(v)}+\frac{\delta_A(v)}{\delta_A(u)}\right]+$
$\sum_{uv\in E_4(A)}\left[\frac{\delta_A(u)}{\delta_A(v)}+\frac{\delta_A(v)}{\delta_A(u)}\right]$

ND5(A)= $2(32+4n)+\left(\frac{9}{10}+\frac{10}{9}\right)16(n-1)+8(n-1)+\left(\frac{10}{11}+\frac{11}{10}\right)8(n-1)$

ND6(A)= $\sum_{uv\in E(A)}\delta_A(u)\deg(u)+\deg(v)+\delta_A(v)$

The fourth version of atom–bond connectivity index ABC_4 by Ghorbhani et al. [23]

ABC_4= $\sum_{uv\in E(A)}\sqrt{\frac{\delta_A(u)+\delta_A(v)-2}{\delta_A(u)\delta_A(v)}}$

Where δ_A(u)= $\sum_{v\in N_A(u)} \deg(v)$

ABC_4=

$$\sum_{uv\in E_1(A)}\sqrt{\frac{\delta_A(u)+\delta_A(v)-2}{\delta_A(u)\delta_A(v)}}+\sum_{uv\in E_2(A)}\sqrt{\frac{\delta_A(u)+\delta_A(v)-2}{\delta_A(u)\delta_A(v)}}+\sum_{uv\in E_3(A)}\sqrt{\frac{\delta_A(u)+\delta_A(v)-2}{\delta_A(u)\delta_A(v)}}+\sum_{uv\in E_4(A)}\sqrt{\frac{\delta_A(u)+\delta_A(v)-2}{\delta_A(u)\delta_A(v)}}$$

$$ABC_4=\sqrt{\frac{16}{82}}\times(32+4n)+16(n-1)\sqrt{\frac{17}{90}}+4(n-1)\sqrt{\frac{26}{196}}+8(n-1)\sqrt{\frac{19}{110}}$$

Where δ_A(u)= $\sum_{v\in N_A(u)} \deg(v)$

The fifth version of the geometric arithmetic index GA_5 by Graovoc et al. [24]

$$GA_5(A) = \sum_{uv\in E(A)}\frac{2\sqrt{\delta_A(u)\delta_A(v)}}{\delta_A(u)+\delta_A(v)}$$

Where δ_A(u)= $\sum_{v\in N_A(u)} \deg(v)$

GA_5(A)=

$$\sum_{uv\in E_1(A)}\frac{2\sqrt{\delta_A(u)\delta_A(v)}}{\delta_A(u)+\delta_A(v)}+\sum_{uv\in E_2(A)}\frac{2\sqrt{\delta_A(u)\delta_A(v)}}{\delta_A(u)+\delta_A(v)}+\sum_{uv\in E_3(A)}\frac{2\sqrt{\delta_A(u)\delta_A(v)}}{\delta_A(u)+\delta_A(v)}+\sum_{uv\in E_4(A)}\frac{2\sqrt{\delta_A(u)\delta_A(v)}}{\delta_A(u)+\delta_A(v)}$$

$$GA_5(A)=\frac{(32+4n)\sqrt{81}}{9}+\frac{32(n-1)\sqrt{90}}{19}+\frac{2(n-1)\sqrt{196}}{7}+\frac{16(n-1)\sqrt{110}}{21}$$

Example Python Program for SSD index calculation of given lattice

```
n=int(input("Enter n value :"))

R=(193/3)*n+(23/3)

print(R)
```

Likewise we can use for trouble-free calculation.

Conclusion:

We find Topological indices namely Zagreb index,arithmetic geometric index, multiple Zagreb index, redefined Zagreb index for finding the total pi- electron energy of molecules of one type of Bravais Lattice using python program. More reference readers refer https://repl.it/@Manimekalai/eccentricity-based-index

.

References:

1. M. Randic,, On Characterization of molecular branching, ´ J. Am. Chem. Soc., 97, (1975), 6609-6615.
2. I. Gutman, B. Furtula, and C. Elphick, Three New/Old Vertex-Degree-Based Topological Indices, MATCH Commun. Math. Comput. Chem., 72, (2014), 617-632.
3. B. Zhou, N. Trinajstic, On a novel connectivity index, ´ J. Math. Chem., 46, (2009), 1252-1270.
4. D. Vukicevic, Bond additive modeling 2 mathematical properties of maxmin rodeg index, Croat. Chem. Acta, 54, (2010), 261-273.
5. Gutman, I.; Das, C.N. The first Zagreb index 30 years after. MATCH Commun. Math. Comput. Chem. 2004, 50, 83–92.
6. Gutman, I.; Trinajst, N. Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons. Chem. Phys. Lett. 1972, 17, 535–538. [CrossRef]
7. Furtula, B.; Gutman, I. A forgotten topological index. J. Math. Chem. 2015, 53, 1184–1190. [CrossRef]
8. Ghorbani, M.; Azimi, N. Note on multiple zagreb indices. Iran. J. Math. Chem. 2012, 3, 137–143
9. Furtula, B.; Graovac, A.; Vukicevic, D. Augmented zagreb index. J. Math. Chem. 2010, 48, 370–380. [CrossRef]
10. Balaban, A.T. Highly discriminating distance-based topological index. Chem. Phys. Lett. 1982, 89, 399–404. [CrossRef]
11. Balaban, A.T.; Quintas, L.V. The smallest graphs, trees, and 4-trees with degenerate topological index. J. Math. Chem. 1983, 14, 213–233.
12. Ranjini, P.S.; Lokesha, V.; Usha, A. Relation between phenylene and hexagonal squeez using harmonic index. Int. J. Graph. Theory 2013, 1, 116–121.
13. Fath-Tabar, G.H. Zagreb Polynomial and Pi Indices of some Nano Structures. Dig. J. Nanomater. Biostruct. 2009, 4, 189–191.
14. Chaluvaraju, B.; Boregowda, H.S.; Diwakar, S.A. Hyper-Zagreb indices and their polynomials of some special kinds of windmill graphs. Int. J. Adv. Math. 2017, 4, 21–32.
15. Graovac, A.; Ghorbani, M.; Hosseinzadeh, M.A. Computing fifth geometric–arithmetic index for nanostar dendrimers. J. Math. Nanosci. 2011, 1, 33–42.

16. D. Vukicevic, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end{vertex degrees of edges, J. Math. Chem. 46 (2009) 1369{1376.

17. Ghorbani, A.; Hosseinzadeh, M.A. Computing ABC4 index of nanostar dendrimers. Optoelectron. Adv. Mater. Rapid Commun. 2010, 4, 1419–1422.
18. Graovac, A.; Ghorbani, M.; Hosseinzadeh, M.A. Computing fifth geometric–arithmetic index for nanostar dendrimers. J. Math. Nanosci. 2011, 1, 33–42.
19. Sourav Mondala , Nilanjan Deb , Anita Pala, QSPR analysis of some novel neighborhood degree based topological descriptors