International Journal of Scientific and Innovative Mathematical Research (IJSIMR)
Volume 1, Issue 2, October - 2013, PP 160-169
ISSN 2347-307X (Print) & ISSN 2347-3142 (Online)
www.arcjournals.org

Randic and Sh Indices of Pentachains in one Row

Srujana mellam

Assistant Professor
Department of Mathematics
Bapatla Engineering College, Bapatla, India
srujana.maths@gmail.com

Received: 31-08-2013 **Revised: 23-09-2013** **Accepted: 26-09-2013**

Abstract: *Pentachains are fused chains of pentagons (5-cycles). As an answer to Ivan Guttmann's open problem related to pentachains, Bo-Yin Yang computed Wiener indices in 1995, Ivan Guttmann presented formulas for Schultz and modified Schultz indices of pentachains in 2007 and A.Lakshmi Prasanna obtained formulas for PI and Szeged indices of pentachains in 2010. In this paper explicit formulas for Randic index of pentachains in one row are obtained. Also the eleven Sh indices of twenty structures of pentachains in one row are obtained using an algorithm in MATLAB version 6.5. Comparative study is also made among these topological indices.*

Keywords: Randic index, Sh index, correlation coefficient.

1. Introduction

A topological index is a numerical descriptor of the molecular structure based on certain topological features of the molecular graph. With the advent of application of topological indices ranging from correlations of physical to biological properties of chemical species, the study of various topological indices gained importance. Among the many topological indices available in the literature the most successful was the Randic molecular connectivity χ which is used much of QSAR/ QSPR studies. In 2004, Mojtaba Shamsipur introduced eleven Sh indices and observed that the boiling points of a wide range of alkanes can be well modeled (with $r^2 > 0.99$) by the Sh index.

2. Preliminaries

First we state the definitions of Randic and Sh indices.

Definition 2.1. The Randic index of a graph G is $\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)\, d(v)}}$, where E (G) is the edge set.

Definition 2.2. Sh indices of a graph G= (V, E), |V|= n are defined by

$$Sh1 = \log(\sum \frac{s_i s_j}{\delta_i \delta_j})$$

$$Sh2 = \log(\sum \frac{\delta_i \delta_j}{s_i s_j})$$

$$Sh3 = \log(\sum (s_i s_j \delta_i \delta_j)^{-0.5})$$

$$Sh4 = \log(\sum (\frac{\delta_i \delta_j}{s_i s_j})^{-0.5})$$

$$Sh5 = \sum (s_i s_j + \delta_i \delta_j)^{-0.5}$$

$$Sh6 = \log \sum ((s_i s_j) + (\delta_i \delta_j))$$

$$Sh7 = \sum (\delta_i \delta_j + \log(s_i s_j))$$

$$Sh8 = \log(S\delta^T)$$

$$Sh9 = \log(\sum_i \sum_j Sd_{ij})$$

$$SS = SVD(Sd)$$

$$Sh10 = \log(SS)$$

$$Sh = n + \sqrt{n}\ Sh1,$$

Where $S = [s_1, s_2, ..., s_n], s_i$ is the sum of elements in the i[th] row of distance matrix of G; $\delta = [\delta_1, \delta_2, ..., \delta_n], \delta_i$ is degree of the vertex i; $Sd = S^T \delta$ which has only one eigenvalue SS.

3. NOTATIONS

5-cycles which are ‘a’ in number can be concatenated in a single row as shown in figure (1) (we call this case as Straight chaining) or as in figure (2) (we call this case as Alternate chaining)

(i). Straight chaining:

The graph when a=6 is as shown below.

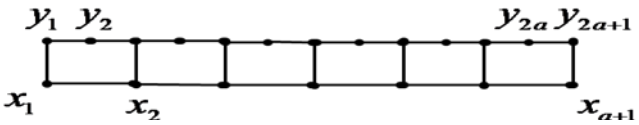

Figure 1

We denote the class of above graphs as G (a, S).

(ii). Alternate chaining:

The graph when a=6 is shown below:

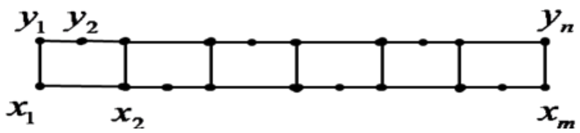

Figure 2

In G (a, A), if ‘a’ is even then m = n = (3a+2)/2 and if ‘a’ is odd then m= (3a+1)/2 and n= (3a+3)/2.

4. MAIN RESULTS

Theorem 4.1. $\chi(G(a,S)) = 2 + \frac{2a}{\sqrt{6}} + \frac{2a-3}{3}$**,** where a ≥ 2.

Proof: Partitioning the edge set based on the product of degrees of end points, we get three classes.

First one is the class of edges with 4 as the product of degrees of endpoints.

This class of is $\{(x_1, y_1), (x_{a+1}, y_{2a+1}), (y_1, y_2), (y_{2a}, y_{2a+1})\}$ with cardinality 4.

Second one is the class of edges with 6 as the product of degrees of endpoints.

This class of edges is $\{(x_1, x_2), (x_a, x_{a+1})\} \cup \{(y_i, y_{i+1}) / i = 2,3,...,a-1\}$ with cardinality 2a.

Third one is the class of edges with 9 as the product of degrees of end points.

This class of edges is $\{(x_i, x_{i+1}), (x_i, y_{2i-1}) / i = 2,3,...,a\}$ with cardinality 2a-3.

Hence the Randic index of the graph G(a, S) is

$$\chi(G(a,S)) = (4)\frac{1}{\sqrt{(2)(2)}} + (2a)\frac{1}{\sqrt{(2)(3)}} + (2a-3)\frac{1}{\sqrt{(3)(3)}}$$

$$= 2 + \frac{2a}{\sqrt{6}} + \frac{2a-3}{3}.$$

Theorem 4.2. $\chi(G(a,A)) = 2 + \frac{2a}{\sqrt{6}} + \frac{2a-3}{3}$**,** where a≥1 and 'a' is odd.

Proof: Here also we will get classes of edges same as in Theorem 4.1.

First class of edges is $\left\{(x_1,y_1),(y_1,y_2),(x_{\frac{3a+1}{2}},y_{\frac{3a+3}{2}}),(y_{\frac{3a+1}{2}},y_{\frac{3a+3}{2}})\right\}$ with cardinality 4. Second class of edges is $\left\{(x_i,x_{i+1})\,/\,i=2,5,8,...,\frac{3a-5}{2}\right\} \cup \left\{(x_i,x_{i+1})\,/\,i=3,6,9,...,\frac{3a-3}{2}\right\}$

$\cup \left\{(y_i,y_{i+1})\,/\,i=2,5,8,...,\frac{3a-3}{2}\right\} \cup \left\{(y_i,y_{i+1})\,/\,i=4,7,10,...,\frac{3a-1}{2}\right\}$ with cardinality 2a.

Third class of edges is $\left\{(x_i,x_{i+1})\,/\,i=4,7,10,...,\frac{3a-7}{2}\right\} \cup \left\{(y_i,y_{i+1})\,/\,i=3,6,9,...,\frac{3a-3}{2}\right\}$

$\cup \left\{(x_i,y_i)\,/\,i=4,7,10,...,\frac{3a-1}{2}\right\} \cup \left\{(x_i,y_{i+1})\,/\,i=2,5,8,...,\frac{3a-5}{2}\right\}$ with cardinality 2a-3.

Hence the Randic index of the graph G (a, A) is

$$\chi(G(a,A)) = (4)\frac{1}{\sqrt{(2)(2)}} + (2a)\frac{1}{\sqrt{(2)(3)}} + (2a-3)\frac{1}{\sqrt{(3)(3)}}$$

$$= 2 + \frac{2a}{\sqrt{6}} + \frac{2a-3}{3}.$$

Theorem 4.3. $\chi(G(a,A)) = 2 + \frac{2a}{\sqrt{6}} + \frac{2a-3}{3}$**,** where a≥2 and 'a' is even.

Proof: Here also we will get same classes of edges same as in Theorem 4.1.

First class of edges is $\left\{(x_1,y_1),(x_{\frac{3a}{2}},x_{\frac{3a+2}{2}}),(y_1,y_2),(x_{\frac{3a+2}{2}},y_{\frac{3a+2}{2}})\right\}$ with cardinality 4.

Second class of edges is $\left\{(x_1,x_2),(x_{\frac{3a}{2}},x_{\frac{3a+2}{2}})\right\} \cup \left\{(x_i,x_{i+1})\,/\,i=2,5,8,...,\frac{3a-2}{a}\right\}$

$\cup \left\{(x_i,x_{i+1})\,/\,i=3,6,9,...,\frac{3a-6}{2}\right\} \cup \left\{(y_i,y_{i+1})\,/\,i=2,5,8,...,\frac{3a-2}{2}\right\} \cup \left\{(y_i,y_{i+1})\,/\,i=4,7,10,...,\frac{3a-4}{2}\right\}$

with cardinality 2a.

Third class of edges is $\left\{(x_i,x_{i+1})\,/\,i=4,7,10,...,\frac{3a-4}{2}\right\} \cup \left\{(y_i,y_{i+1})\,/\,i=3,6,9,...,\frac{3a-6}{2}\right\}$

$\cup \left\{(x_i,y_i)\,/\,i=4,7,10,...,\frac{3a-4}{2}\right\} \cup \left\{(x_i,y_{i+1})\,/\,i=2,5,8,...,\frac{3a-2}{2}\right\}$ with cardinality 2a-3.

Hence the Randic index of the graph G (a, A) is

$$\chi(G(a,A)) = (4)\frac{1}{\sqrt{(2)(2)}} + (2a)\frac{1}{\sqrt{(2)(3)}} + (2a-3)\frac{1}{\sqrt{(3)(3)}}$$

$$= 2 + \frac{2a}{\sqrt{6}} + \frac{2a-3}{3}.$$

5. SH VALUES

By executing the programme in MATLAB version 6.5, the values of Sh indices for the first 20 graphs of G (a, S) (a= 1 to 20), are obtained and these are arranged in the following tables.

a	*Sh1*	*Sh2*	*Sh3*	*Sh4*
1	*1.65321251377534*	-0.25527250510331	-0.38021124171161	1.17609125905568
2	*2.53162082015801*	-0.52049250585998	-0.52940725789336	1.73130535775377
3	*3.14925333467044*	-0.78784451649328	-0.63393187429464	2.11489074278773
4	*3.61596757731093*	-1.01208755436221	-0.71296023674258	2.40474985887500
5	*3.99000321018233*	-1.20074850185018	-0.77602945539610	2.63714381318765
6	*4.30299674999158*	-1.36312319733281	-0.82870605155031	2.86407594160244
7	*4.57271674590292*	-1.50577608973413	-0.87416515370445	2.99860763306436
8	*4.81009094211038*	-1.63313628084957	-0.91431992465844	3.14552484559997
9	*5.02232020798878*	-1.74828201910157	-0.95039697183383	3.27668696183994
10	*5.21440580187547*	-1.85343397479787	-0.98322811090332	3.39523431426478
11	*5.38996736156706*	1.95024745379333	-1.01340419131583	3.50344193953017
12	*5.55171254205675*	-2.03999062084374	-1.04136107125736	3.60301235854376
13	*5.70172221998620*	-2.12365757090249	-1.06743039252122	3.69525400154591
14	*5.84163187941179*	-2.20204277771934	-1.09187105140521	3.78119497144365
15	*5.97275150737096*	-2.27579174114884	-1.11488953444583	3.86165838142175
16	*6.09614747563226*	-2.34543643461403	-1.13665353869376	3.93731387670451
17	*6.21270004772639*	-2.41142073401876	-1.15730138133015	4.00871385495657
18	*6.32314475691145*	-2.47411905704946	-1.17694867777638	4.07631954572785
19	*6.42810281494929*	-2.53385028709868	-1.19569319411239	4.14052018473018
20	*6.52810387939278*	-2.59088835069018	-1.21361844665698	4.20164737323124

a	*Sh5*	*Sh6*	*Sh7*
1	0.79056941504209	2.30102999566398	27.78151250383644

2	0.66884003936055	3.22582599146189	69.23386032699895
3	0.56113132843546	3.86723171451889	1.145163828459677e+002
4	0.48306646893205	4.35233690648196	1.616980449115941e+002
5	0.42570913894029	4.74032320638299	2.103029798471329e+002
6	0.38171637070579	5.06407594160244	2.600687732921139e+002
7	0.34670618117474	5.34235950612111	3.108230385921486e+002
8	0.31804254733525	5.58674254282644	3.624409790621145e+002
9	0.29405599396353	5.80483905756583	4.148269800139719e+002
10	0.27363378172924	5.80483905756583	4.679050267204233e+002
11	0.25600171611914	6.18181272908264	5.216130541088542e+002
12	0.24060184174813	6.34734406866382	5.758993404480355e+002
13	0.22702021243771	6.50070112990059	6.307200743770858e+002
14	0.21494221328088	6.64359537799830	6.860376439311891e+002
15	0.20412380182837	6.77739549985477	7.418193934759728e+002
16	0.19437235379926	6.90321406891279	7.980366964180499e+002
17	0.18553352609192	7.02196830335266	8.546642481149298e+002
18	0.17748201528665	7.13442371171314	9.116795165614758e+002
19	0.17011491118303	7.24122612009147	9.690623087517806e+002
20	0.16334682297107	7.34292561835530	1.026794423539818e+003

a	*Sh8*	*Sh9*	*Sh10*	*Sh*
1	1.77815125038364	2.47712125471966	1.77815125038364	8.69669556205498
2	2.38381536598043	3.29666519026153	2.40510281293166	15.16050499730711
3	2.78675142214556	3.83985498460189	2.81273031047818	21.44489168087739
4	3.08778141780954	4.24580867678749	3.11472470285442	27.52971179598050
5	3.32756326018728	4.56970155541097	3.35447273804737	33.45120468213530
6	3.52711411163981	4.83947804737420	3.55368097306110	39.24358647988370
7	3.69827457667437	5.07092403147615	3.72439964457819	44.92997911718119
8	3.84831230362728	5.27377883129013	3.87397450310785	50.52674757597674
9	3.98199971412988	5.45446678309675	4.00721045000337	56.04602203422164

10	4.10263948369130	5.61744908996761	4.12742363372672	61.49713361891697
11	4.21261369664506	5.76595153613552	4.23700096019171	66.88747693933370
12	4.31369852956031	5.90238368443247	4.33771935028161	72.22305453471310
13	4.40725490056078	6.02859402409084	4.43093856165869	77.50883574190308
14	4.49434942603846	6.14603248038075	4.51772322019442	82.74900221477512
15	4.57583418529854	6.25585792535972	4.59892312572555	87.94712134855999
16	4.65240107316205	6.35901162802524	4.67522787570533	93.10627219132823
17	4.72461989119966	6.45626883747443	4.74720508729910	98.22913905658645
18	4.79296569947070	6.54827588473660	4.81532780631247	1.033180825746773e+002
19	4.85783887799498	6.63557743172268	4.87999458719917	1.083751946039099e+002
20	4.91958011861277	6.7186368554823	4.94154448358844	1.134023413487058e+002

We have computed the values of Sh indices for the first 20 graphs of G (a, A) (a=1 to 20), alternate chaining case. The values obtained are tabulated below

a	*Sh1*	*Sh2*	*Sh3*	*Sh4*
1	1.65321251377534	-0.25527250510331	-0.38021124171161	1.17609125905568
2	2.67501414214221	-0.69377230780472	-0.58707851580199	1.76075510461276
3	3.14925333467044	-0.78784451649328	-0.63393187429464	2.11489074278773
4	3.70124408611097	-1.08657947149224	-0.74157214980175	2.41809944088342
5	4.02565625506470	-1.23649895681712	-0.79059886918582	2.65357121380907
6	4.40353802131897	-1.44961902921964	-0.86474986563447	2.85841843534685
7	4.64794015275333	-1.58094367368981	-0.90669081510432	3.03428506493577
8	4.93505821240092	-1.74490001776116	-0.96319118066963	3.18872181102849
9	5.13068249381119	-1.85647795841388	-0.99879575130567	3.32886500479080
10	5.36220718355005	-1.98925016433294	-1.04436678038210	3.45271383919679
11	5.52516391558988	-2.08512445271080	-1.07503060298893	3.56912430983155
12	5.71915519902672	-2.19652113210931	-1.11318038325117	3.67246199254138
13	5.85874907997805	-2.28020273800879	-1.14001202466424	3.77198326183708
14	6.02569559937911	-2.37608467935161	-1.17280105957767	3.86062121761742
15	6.14776619621150	-2.45017655150290	-1.19661067357053	3.94751842666864

16	6.29429693957398	-2.53430434199412	-1.22535005818634	4.02510906885770
17	6.40274343491847	-2.60070851766006	-1.24672921240281	4.10221667317693
18	6.53331456733763	-2.67563189285613	-1.27230363239618	4.17120366666213
19	6.63086760857397	-2.73575721922755	-1.29169166054704	4.24049971857041
20	6.74861876658666	-2.80328167666853	-1.31472563366928	4.30259774848725

a	*Sh5*	*Sh6*	*Sh7*
1	0.79056941504209	2.30102999566398	27.78151250383644
2	0.54736983031004	3.25261034056737	57.59994578105714
3	0.56113132843546	3.86723171451889	1.145163828459677e+002
4	0.43790289648124	4.36231279532651	1.491341591797098e+002
5	0.41093799529798	4.77529726448621	2.109723602559959e+002
6	0.34356993256363	5.10836203495517	2.478033413217608e+002
7	0.32061045446199	5.41809901549312	3.128567006875713e+002
8	0.27913677658357	5.66774985276854	3.512300496688114e+002
9	0.26194640860558	5.91496109761734	4.186434349196249e+002
10	0.23407132466865	6.11420952664717	4.582003130220948e+002
11	0.22112729762226	6.31968681309085	5.274730597175428e+002
12	0.20117448735842	6.48531376479941	5.679908713627488e+002
13	0.19118946516868	6.66102276273873	6.387963246250661e+002
14	0.17622802349428	6.80266934528811	6.801234608269539e+002
15	0.16833208470537	6.95610068678288	7.522321863900977e+002
16	0.15670861383839	7.07979924148146	7.942586550295657e+002
17	0.15032543047084	7.21594357637694	8.675008106409543e+002
18	0.14104039683104	7.32571287775934	9.101431135686610e+002
19	0.13578140751422	7.44805828968572	9.843879553491936e+002
20	0.12819645803814	7.54670740503534	1.027580511908115e+003

a	*Sh8*	*Sh9*	*Sh10*	*Sh*

1	1.77815125038364	2.47712125471966	1.77815125038364	8.69669556205498
2	2.37291200297011	3.30449052777349	2.43613642311210	15.56608255871470
3	2.78675142214556	3.83985498460189	2.81273031047818	21.44489168087739
4	3.07881918309885	4.24865974304834	3.13186063120934	27.84878727505047
5	3.34399906905716	4.58514476406575	3.37100730031865	33.59820595206018
6	3.53882498893790	4.85848907363121	3.58349304053277	39.69322071434827
7	3.73431968085901	5.10506032934099	3.76030139343138	45.29073790304537
8	3.88018455282643	5.31024285666258	3.91933872692904	51.16395812574861
9	4.03486899636113	5.50491648227820	4.05974738896615	56.62957080225309
10	4.15130854818202	5.66905641177766	4.18670173195867	62.33322449292368
11	4.27921051260140	5.82988244644349	4.30315851658172	67.68731053933280
12	4.37604745204147	5.96661849062543	4.40874644692176	73.25524039403315
13	4.48503964536526	6.10361765259977	4.50823186305750	78.51429823504488
14	4.56789643688516	6.22076896834693	4.59858228266489	83.96994280807238
15	4.66283335458967	6.34008542592565	4.68541090113547	89.14696160524738
16	4.73522351985725	6.44254749490841	4.76435274310542	94.50740048774496
17	4.81930698301336	6.54822082755589	4.84137915454463	99.61267579907585
18	4.88357059282062	6.63926011902964	4.91146241671444	1.048908494219933e+002
19	4.95902230203419	6.73408805943644	4.98067353876235	1.099326605362777e+002
20	5.01679524726309	6.81599192348420	5.04368092511717	1.151386773068073e+002

Using the above values of Sh indices and the values of Randic index obtained from formulas of section 3 for the first 20 graphs of G (a, S), G (a, A); correlation coefficients are obtained between these indices in Straight chaining and Alternate chaining cases separately. The values of ‘r’ rounded to three decimal places are tabulated in the following tables.

r	*Sh1*	*Sh2*	*Sh3*	*Sh4*	*Sh5*	*Sh6*	*Sh7*	*Sh8*	*Sh9*	*Sh10*	*sh*
χ	*0.952*	*-0.970*	*-0.954*	*0.951*	*-0.902*	*0.950*	*0.999*	*0.947*	*0.947*	*0.946*	*0.999*
Sh1		*-0.997*	*-0.999*	*0.999*	*-0.991*	*0.999*	*0.941*	*0.999*	*0.999*	*0.999*	*0.961*
Sh2			*0.997*	*-0.997*	*0.979*	*-0.997*	*-0.961*	*-0.996*	*-0.996*	*-0.995*	*-0.978*
Sh3				*-0.999*	*0.990*	*-0.999*	*-0.943*	*-0.999*	*-0.999*	*-0.999*	*-0.963*

Sh4					*-0.991*	*0.999*	*0.940*	*0.999*	*0.999*	*0.999*	*0.960*
Sh5						*-0.991*	*-0.887*	*-0.992*	*-0.992*	*-0.993*	*-0.915*
Sh6							*0.939*	*0.999*	*0.999*	*0.999*	*0.960*
Sh7								*0.936*	*0.936*	*0.934*	*0.998*
Sh8									*0.999*	*0.999*	*0.957*
Sh9										*0.999*	*0.957*
Sh10											*0.956*

r	*Sh1*	*Sh2*	*Sh3*	*Sh4*	*Sh5*	*Sh6*	*Sh7*	*Sh8*	*Sh9*	*Sh10*	*sh*
χ	*0.955*	*-0.974*	*-0.963*	*0.954*	*-0.896*	*0.954*	*0.999*	*0.951*	*0.950*	*0.949*	*0.999*
Sh1		*-0.996*	*-0.999*	*0.999*	*-0.985*	*0.999*	*0.943*	*0.999*	*0.999*	*0.999*	*0.964*
Sh2			*0.998*	*-0.996*	*0.972*	*-0.996*	*-0.964*	*-0.994*	*-0.994*	*-0.994*	*-0.981*
Sh3				*-0.999*	*0.982*	*-0.999*	*-0.952*	*-0.998*	*-0.998*	*-0.998*	*-0.971*
Sh4					*-0.984*	*0.999*	*0.941*	*0.999*	*0.999*	*0.999*	*0.963*
Sh5						*-0.984*	*-0.878*	*-0.985*	*-0.986*	*-0.987*	*-0.909*
Sh6							*0.942*	*0.999*	*0.999*	*0.999*	*0.963*
Sh7								*0.938*	*0.937*	*0.936*	*0.997*
Sh8									*0.999*	*0.999*	*0.960*
Sh9										*0.999*	*0.959*
Sh10											*0.958*

6. CONCLUSIONS

It may be noted that highest correlation is among Sh indices in both the cases. Also it may be noted that Randic index has highest correlation with Sh and Sh7 compared to other indices. In case of G (a, S), r (χ, Sh) = 0.99944295960141 and r (χ, Sh7) = 0.9994019717792, where as in case of G (a, A), r (χ, Sh)=0.99949424771335 and r(χ, Sh7)=0.99900751418763.

ACKNOWLEDGEMENT

I thank my research supervisor Prof. N. Prabhakara Rao for his encouragement and guidance in the preparation of this paper.

REFERENCES

[1] Mojtaba Shamsipur, Bahram Hemmateenejad, Morteza Akhond. : Highly correlating Distance/ Connectivity- Based Topological Indices, Bull.Korean Chem. Soc.,Vol-25,No. 2,P253-259, 2004.

[2] Randic M, Characterisation of molecular branching, journal of the American chemical society, 97[23], 6609-6615, 1975.

[3] Lavanya Lakshmi.K, Srujana.M. : A Comparision of Certain Topological indices of Pentachains, accepted for publication in International Journal of Computational Cognition.

AUTHOR'S BIOGRAPHY

She is working as Assistant Professor in the Department of Mathematics; Bapatla Engineering College. She has 6 years of teaching experience.She completed M.Sc(Mathematics) in Bapatla Engineering College. She has obtained M.Phil (Mathematics) from Acharya Nagarjuna University under the guidance of Prof.N.Prabhakara Rao. Her articles more than two were published in reputed international journals.