QSPR ANALYSIS OF CERTAIN DEGREE BASED TOPOLOGICAL INDICES OF BENZENOID HYDROCARBONS

V. LOKESHA, SUVARNA, AND K. ZEBA YASMEEN

Abstract. In this article, the $QSPR$ analysis of few Benzene derivatives with respect to some selected degree based topological indices is enciphered. In $QSPR$ studies, topological indices are extensively used in determining specific bioactivity of chemical compounds. Our study showcases some important results on the correlation between physico-chemical properties Molecular Weight, $XLogP3$, Exact Mass, Heavy Atom Count, Complexity of Benzene derivatives with the selected topological indices which further helps in characterizing the predicting power of these topological indices.

1. Introduction

Chemical graph theory is a engrossing branch of graph theory, provides umteen information on chemical compounds by victimisation an authoritative tool called the topological index [1, 3, 4]. Theoretical molecular descriptors alias topological indices are graph invariants that play an crucial role in chemistry, pharmaceutical sciences, materials science, engineering and so forth. Its role in $QSPR/QSAR$ analysis [5, 6, 8, 9],to model physical and chemical properties of molecules is also remarkable. Among several types of topological indices, vertex degree based topological indices are most investigated and widely used.

The following topological indices used in this article.

(1) $GO_1(G) = \sum_{uv \in E(G)} d_G(u) + d_G(v) + d_G(u)d_G(v)$.

(2) $GO_2(G) = \sum_{uv \in E(G)} d_G(u) + d_G(v) * (d_G(u)d_G(v))$.

(3) $HGO_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v) + d_G(u)d_G(v)]$

(4) $HGO_2(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v) * (d_G(u)d_G(v))]^2$

(5) $VL(G) = \frac{1}{2} \sum_{uv \in E(G)} d_G(e) + d_G(f) + 4$

where $d_G(e) = d_G(u) + d_G(v) - 2$ and $d_G(f) = (d_G(u) * d_G(v)) - 2$

Here GO_1, GO_2 and HGO_1, HGO_2 are Gourava and Hyper Gourava indices respectively introduced recently by V. R. Kulli [7, 8]. In [2] , T. Deepika introduced VL index.

Benzene C_6H_6 is a volatile, clear, colorless and flammable liquid aromatic hydrocarbon possessing a distinct, characteristic odur. Benzene is the simplest aromatic compound, with six carbon ring, a hydogen atom attached to each carbon atom, and alternating double bonds in the ring structure [10]. In the following main section, the $QSPR$ analysis of 30 Benzene derivatives with respect to some selected degree based topological indices are studied.

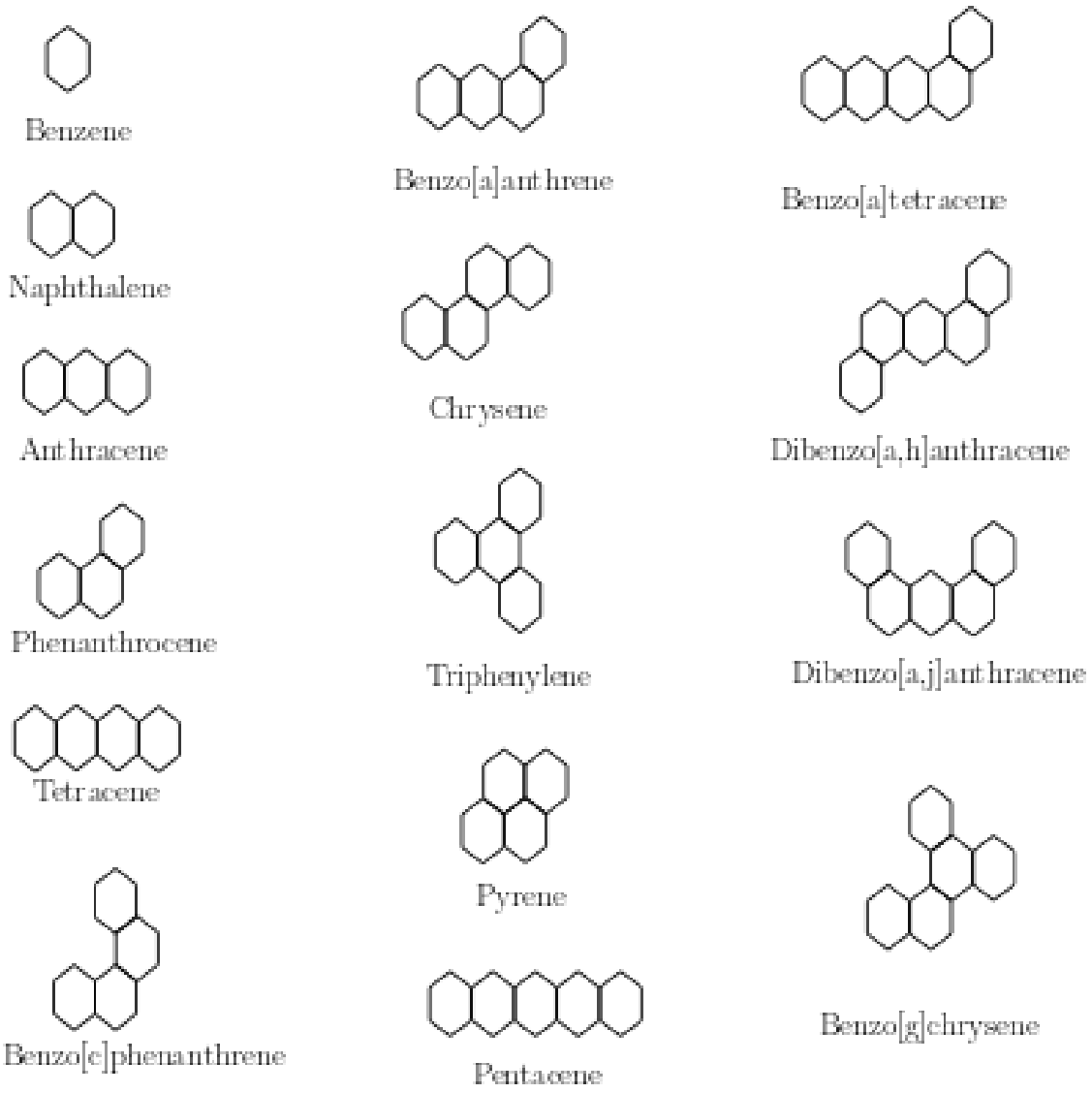

FIGURE 1. Some Molecular Graphs of Benzene derivatives

2. Some topological indices in QSPR analysis

In this section, the GO_1, GO_2, HGO_1, HGO_2 and VL indices to model physico-chemical properties [Molecular Weight, $XLogP3$, Exact Mass, Heavy Atom Count, Complexity] of the Benzene compound we consider the 30 lower benzenoid hydrocarbons, which are frequently used to access the performance of any topological descriptor in quantitative structure activity/property relationships.

Table 1: The physical and chemical properties (Molecular Weight, $XLogP3$, Exact mass, Heavy Atom Count, Complexity) of benzenoid hydrocarbons.

Name of the Compound	Molecular Weight	XLogP3	Exact Mass	Heavy Atom Count	Complexity
Benzene	78.11	2.1	78.04695	6	15.5
Naphthalene	128.17	3.3	128.0626	10	80.6
Anthracene	178.23	4.4	178.07825	14	154
Phenanthrene	178.23	4.5	178.07825	14	174
Tetracene	228.3	5.9	228.0909	18	236
Benzo[c]Phenanthrene	228.3	5.7	228.0909	18	266
Benz[a]anthracene	228.3	5.8	228.0909	18	294
Chrysene	228.3	5.7	228.0909	18	264
Triphenylene	228.3	4.9	228.0909	18	217
Pyrene	202.25	4.9	202.07825	16	217
Pentacene	278.3	6.7	278.10955	22	325
Benzo[a]tetracene	278.3	6.7	278.10955	22	399
Dibenzo[a, h]anthracene	278.3	6.5	278.10955	22	361
Dibenzo[a, j]anthracene	278.3	6.5	278.10955	22	363
Pentaphene	278.3	6.7	278.10955	22	361
Benzo[g]chrysene	278.3	7	278.10955	22	399
Pentahelicene	278.3	7	278.10955	22	361
Benzo[c]chrysene	278.3	7	278.10955	22	399
Picene	278.3	7	278.10955	22	361
Benzo[b]chrysene	278.3	6.5	278.10955	22	399
Dibenzo[a, c]anthracene	278.3	6.7	278.10955	22	361
Dibenzo[b, g]Phenanthrene	278.3	6.5	278.10955	22	399
Perylene	252.3	5.8	252.0939	20	304
Benzo[E]Pyrene	252.3	6.4	252.0939	20	336
Benzo[a]Pyrene	252.3	6	252.0939	20	372
Hexahelicene	328.4	7.9	328.125201	26	464
Benzo[ghi]perylene	276.3	6.6	276.0939	22	411
Hexacene	328.4	8.4	328.125201	26	418
Coronene	300.4	7.2	300.0939	24	376
Ovalene	398.5	10	398.10955	32	696

Table 2: Topological indices (GO_1, GO_2, HGO_1, HGO_2 and VL index) of benzenoid hydrocarbons.

Name of the Compound	GO_1	GO_2	HGO_1	HGO_2	VL
Benzene	48	96	384	1536	24
Naphthalene	107	270	1093	8052	53.5
Anthracene	166	444	1802	14568	83
Phenanthrene	167	454	1849	15940	83.5
Tetracene	225	618	2511	21084	112.5
Benzo[c]Phenanthrene	227	638	2605	17996	113.5
Benz[a]anthracene	226	628	2558	22456	113
Chrysene	227	638	2605	23828	113.5
Triphenylene	228	648	2652	25200	114
Pyrene	211	606	2477	23316	105.5
Pentacene	284	792	3220	27600	142
Benzo[a]tetracene	285	802	3269	28972	142.5
Dibenzo[a, h]anthracene	286	812	3314	30344	143
Dibenzo[a, j]anthracene	286	812	3314	30344	143
Pentaphene	285	802	2267	28972	142.5
Benzo[g]chrysene	288	832	3408	33088	144
Pentahelicene	287	822	3361	31716	143.5
Benzo[c]chrysene	287	822	3361	31716	143.5
Picene	287	822	3361	31716	143.5
Benzo[b]chrysene	286	812	3314	30344	143
Dibenzo[a, c]anthracene	287	822	3361	31716	143.5
Dibenzo[b, g]Phenanthrene	286	812	3314	30344	143
Perylene	272	800	3280	32576	136
Benzo[E]Pyrene	272	800	3280	32576	136
Benzo[a]Pyrene	271	790	3233	31204	135.5
Hexahelicene	360	1104	4536	47328	180
Benzo[ghi]perylene	316	952	3908	39952	158
Hexacene	343	966	3929	34116	171.5
Coronene	360	1104	4536	47328	180
Ovalene	509	1602	6595	71340	254.5

Table 3: Correlation of Topological indices with physico-chemical properties of benzene compounds

	Molecular weight	XLogP3	Exact Mass	Heavy Atom Count	Complexity
GO_1	0.98	0.97	0.98	0.98	0.97
GO_2	0.96	0.95	0.96	0.97	0.96
HGO_1	0.93	0.93	0.93	0.94	0.94
HGO_2	0.92	0.90	0.91	0.92	0.93
VL	0.98	0.97	0.98	0.98	0.97

2.1. **Regression model for Benzene compounds:**

In this section the following linear regression models are tested

$$P = m(TI) + c$$

where P is the physical property and TI is the topological index. Using the above formula, the following linear regression models for different degree based topological indices is as follows.

1. GO_1 **index:**
Molecular Weight $= 0.72601(GO_1) + 61.64756$.
$XLogP3 = 0.0175(GO_1) + 1.56204$.
Exact Mass $= 0.72538(GO_1) + 61.61324$.
Heavy Atom Count $= 0.05866(GO_1) + 4.55031$.
Complexity $= 1.49654(GO_1) - 71.42883$.

2. GO_2 **index:**
Molecular Weight $= 0.21932(GO_2) + 86.92693$.
$XLogP3 = 0.00529(GO_2) + 2.17131$.
Exact Mass $= 0.21912(GO_2) + 86.87537$.
Heavy Atom Count $= 0.01774(GO_2) + 6.5771$.
Complexity $= 0.45661(GO_2) - 22.78038$.

3. HGO_1 **index:**
Molecular Weight $= 0.05137(HGO_1) + 95.76593$.
$XLogP3 = 0.00124(HGO_1) + 2.37744$.
Exact Mass $= 0.05132(HGO_1) + 95.70963$.
Heavy Atom Count $= 0.00416(HGO_1) + 7.2856$.
Complexity $= 0.10749(HGO_1) - 6.04046$.

4. HGO_2 **index:**
Molecular Weight $= 0.00441(HGO_2) + 125.6334$.
$XLogP3 = 0.000119(HGO_2) + 3.11233$.
Exact Mass $= 0.0044(HGO_2) + 125.55166$.
Heavy Atom Count $= 0.00036(HGO_2) + 9.68773$.
Complexity $= 0.00935(HGO_2) + 52.57675$.

5. VL **index:**
Molecular Weight $= 1.45202(VL) + 61.64756$.
$XLogP3 = 0.035(VL) + 1.56204$.
Exact Mass $= 1.45076(VL) + 61.61324$.
Heavy Atom Count $= 0.11733(VL) + 4.55031$.
Complexity $= 2.99309(VL) - 71.42883$.

3. RESULTS AND DISCUSSION

By inspection of the data in Tables 1 to 3, many observations and conclusions can be made by evaluating the Pearson correlation coefficient of Benzene derivatives.

The QSPR study of GO_1, GO_2, HGO_1, HGO_2 and VL indices reveals that these indices can be useful in predicting the Molecular Weight, XLogP3, Exact Mass, Heavy Atom Count and Complexity of Benzene derivatives. Also from Table 3, one can easily verify that GO_1, GO_2, HGO_1, HGO_2 and VL indices shows good correlation with physico-chemical properties of Benzene derivatives. We can see that

- Correlation coefficient value of GO_1 with physico-chemical properties of Benzene derivatives lies between 0.97 to 0.98 and the correlation coefficient value of first Gourva index is very high for the Molecular Weight, Exact Mass and Heavy Atom Count of Benzene derivatives with $r = 0.98$.
- Correlation coefficient value of GO_2 with physico-chemical properties of Benzene derivatives lies between 0.95 to 0.97 and the correlation coefficient value of second Gourva index is very high for the Heavy Atom Count of Benzene derivatives with $r = 0.97$.
- Correlation coefficient value of HGO_1 with physico-chemical properties of Benzene derivatives lies between 0.93 to 0.94 and the correlation coefficient value of first hyper-Gourva index is very high for the Heavy Atom Count and Complexity of Benzene derivatives with $r = 0.98$.
- Correlation coefficient value of HGO_2 with physico-chemical properties of Benzene derivatives lies between 0.90 to 0.93 and the correlation coefficient value of second hyper-Gourva index is very high for the Complexity of Benzene derivatives with $r = 0.93$.
- Correlation coefficient value of VL with physico-chemical properties of Benzene derivatives lies between 0.97 to 0.98 and the correlation coefficient value of second hyper-Gourva index is very high for the Molecular weight, Exact mass and Heavy Atom Count of Benzene derivatives with $r = 0.98$.

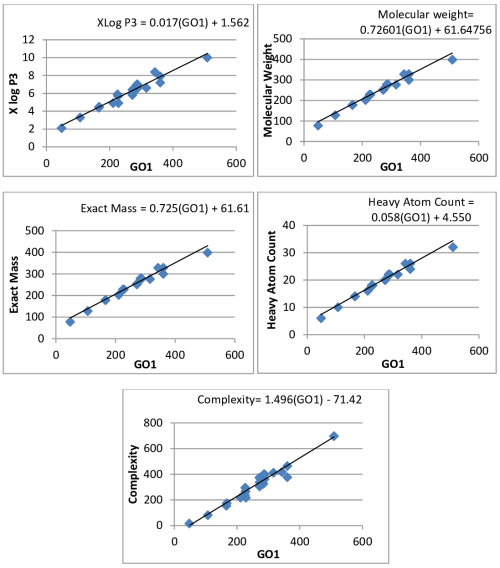

FIGURE 2. Correlation of GO_1 index with physico-chemical properties of Benzene derivatives

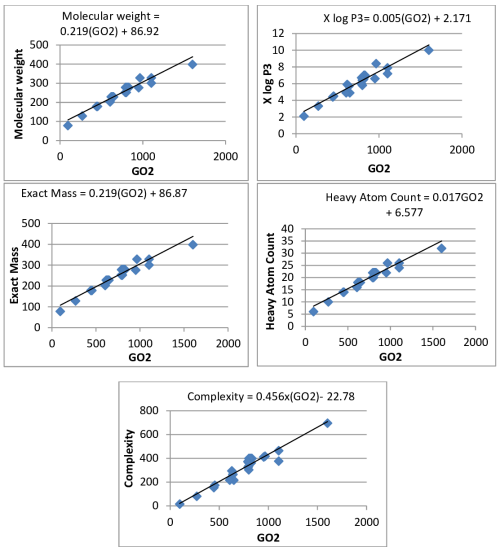

FIGURE 3. Correlation of GO_2 index with physico-chemical properties of Benzene derivatives

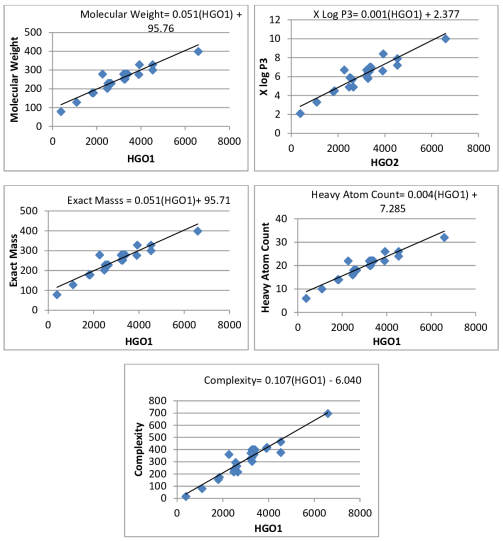

FIGURE 4. Correlation of HGO_1 index with physico-chemical properties of Benzene derivatives

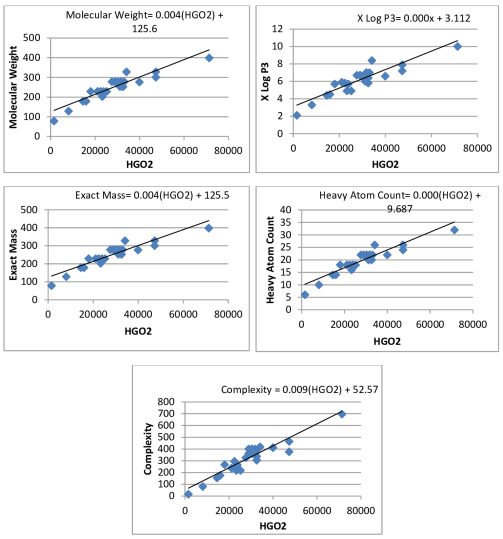

FIGURE 5. Correlation of HGO_2 index with physico-chemical properties of Benzene derivatives

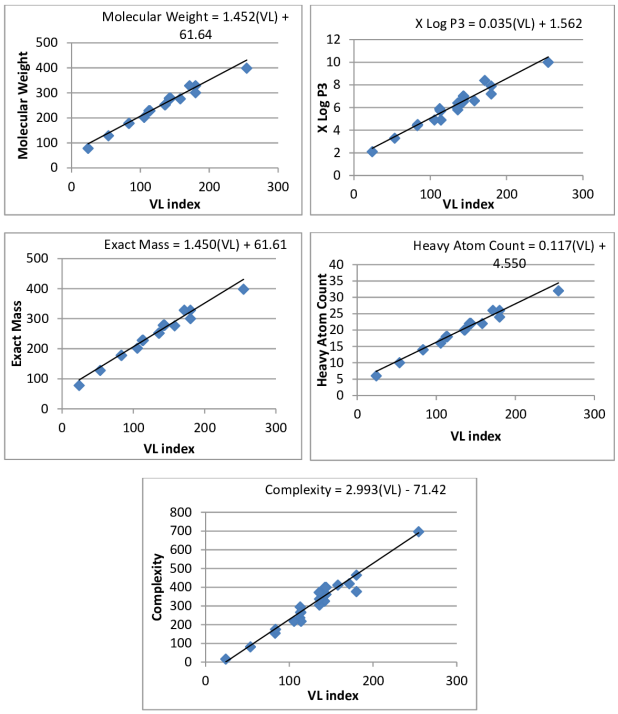

FIGURE 6. Correlation of VL index with physico-chemical properties of Benzene derivatives

4. ACKNOWLEDGEMENT

Third author is thankful to University Grant Commission UGC, New Delhi for providing Maulana Azad National Fellowship ($FileNo : F1-17.1/2017-18/MANF-2017-18-KAR-77292$) to carry out the present research work.

References

[1] J. Devillers and A. T. Balaban (Eds.), **Topological Indices and Related Descriptors in QSAR and QSPR**, Gordon and Breach, Amsterdam, 1999.

[2] T. Deepika, *VL Index and Bounds For The Tensor Products of F- Sum Graphs*, TWMS J. of Appl and Engineering Math., (2019) (Preprint).

[3] Gutman, I., Degree-Based Topological Indices, Croat. Chem. Acta., 86(4), 2013, pp. 351–361.

[4] R. Todeschini, V. Consonni, ***Handbook of Molecular Descriptors***, Wi-leyVCH, Weinheimk, Germany, 2000.

[5] M.Randic, *Quantitative Structure-Property Relationship: boiling points and planar benzenoids*, New. J. Chem.,20,(10), 1996, 1001-1009.

[6] M.Randic, *Comparative structure-property studies: Regressions using a single descriptor*, Croat. Chem. Acta,66, (1993), 289-312.

[7] V.R.Kulli, The Gourava indices and coindices of graphs, Annals of Pure and Applied Mathematics, 14(1), 2017 33-38.

[8] V.R.Kulli, On hyper-Gourava indices and coindices, International J. of Mathematical Archive-8(12), 2017, 116-120.

[9] M.Randic,*Comparative structure-propertystudies: Regressions using a single descriptor*, Croat. Chem. Acta,66, (1993), 289-312.

[10] V.S.Shigehalli, R. Kanabur, *QSPR Analysis of Degree-Based Topological Indices with physical properties of Benzenoid Hydrocarbons*, Journal of Mathematical Chemistry (preprint).

(V. Lokesha, Suvarna and K. Zeba Yasmeen) Department of Studies in Mathematics, Vijayanagara Sri krishnadevaraya University, Ballari, Karnataka, INDIA.

Email address: v.lokesha@gmail.com, suvarnasalimath17@gmail.com and zebasif44@gmail.com