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A STUDY OF ENERGIES AND THERMODYNAMIC ASPECTS OF POLYCYCLIC AROMATIC COMPOUNDS IN QUANTITATIVE STRUCTURE-PROPERTY RELATIONSHIP

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Abstract. Polycyclic refers to a molecule that contains more than one cyclic component, usually two or more fused rings. Naphthalene, anthracene, pyrene, and benzo(a)pyrene are examples of polycyclic organic compounds. A number of polycyclic hydrocarbons are hazardous to human health, including the carcinogen benzo(a)pyrene found in automobile exhaust and tobacco smoke. The natural world has a wide range of polycyclic aromatic compounds, including pigments from plants and animals, that are notably beautiful and have unusually high chemical stability. In this study, polycyclic aromatic compounds are modeled as molecular graphs using their molecular structures, and various energies are computed for them. There is also statistical modeling for the physicochemical properties of energies. For these substances, the QSPR analysis is performed, and conclusions are based on the results.

Keywords: polycyclic aromatic compounds; QSPR analysis; correlation coefficients; physicochemical properties.
2020 AMS Subject Classification: 05C92.

1. INTRODUCTION

Polycyclic aromatic compounds (PACs) are prevalent environmental pollutants. PACs can exist as complex mixtures or as single chemicals. PACs occur naturally in fossil fuels (petroleum and coal). Burning organic material, including fuel, trash, and wood, results in its creation

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and release into the environment. Some PACs are difficult to degrade and persist in the environment for extended periods of time. Natural occurrences like volcanic eruptions and forest fires can emit PACs. Polycyclic aromatic compounds (PACs) are compounds that contain aromatic elements like nitrogen, oxygen, or sulfur together with substituent moieties like alkyl, amino, chloro, cyano, hydroxyl, or thiol groups. These compounds share a fundamental polycyclic aromatic hydrocarbon (PAH) structure. In addition to carbon and hydrogen, heterocyclic PACs also contain other atoms like nitrogen, oxygen, or sulfur in their ring structure [1, 2, 3]. The cooking methods and processes that could decrease the development and contamination of these compounds in food are unknown. Meanwhile, it is expected that advances in analytical approaches (water extraction and sediment extraction) will focus on developing processes that are more efficient, less expensive, and less harmful to the environment. There are numerous ways that people can be exposed to PACs, including by consuming particular meals such as grilled meat or smoked seafood, taking in tainted air, consuming tainted water, absorbing PACs from contaminated soil through the skin, being exposed at jobs that use coal or petroleum, and also being exposed in the workplace by those who make tar or asphalt or who utilize these materials in paving and roofing. The carcinogenic potential of naphthalene, a white, crystalline powder used in manufacturing and as a moth repellent, was investigated in this inhalation study. In one experiment, 5-nitroacenaphthene was fed to animals in order to test for carcinogenicity. The Polycyclic Aromatic Compounds Mixtures Assessment Programme (PAC-MAP) is one of NTP's (National Toxicology Program) research initiatives. NTP will conduct a variety of studies in cells and animals as part of this initiative to evaluate the toxicity of individual PACs and PAC combinations and to find any possible health risks. Since most PACs have not been studied for possible health consequences, it is required to study the combined effects of several PACs. Polycyclic aromatic compounds that act as cytostatic antibiotics and have the primary antitumor effect of intercalating into DNA and preventing tumor cell DNA and RNA synthesis[4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15].

1.1. Impact of Polycyclic Aromatic Compounds.

Polycyclic aromatic compounds (PACs) encompass a wide range of organic chemicals composed of multiple fused aromatic rings. These compounds are ubiquitous in the environment and can be found in various forms,including naturally occurring substances (e.g., in fossil fuels, tar, and coal) as well as synthetic compounds (e.g., from incomplete combustion of organic matter, industrial processes, and vehicle emissions). The impact of polycyclic aromatic compounds can be both beneficial and harmful, depending on their specific properties and concentrations. Here are some key aspects of their impact:

- **Toxicology and Environmental Impact Assessment**: PACs are frequently contaminants and cause substantial worry due to their potential toxicity and environmental persistence. PACs have a tendency to accumulate in living organisms through processes such as bio-accumulation (the gradual accumulation of substances in an organism) and biomagnification (the increase in concentration of substances at higher trophic levels in food chains). This can result in high concentrations of PACs in creatures at the top of the food chain, posing threats to predators and human consumers. QSPR models can forecast the toxicity, bioaccumulation, and environmental destiny of PACs, which can help with risk assessment and regulatory decisions.
- **Health and Ecological Effects**: Many PACs are known or suspected to be carcinogens and mutagens. For example, benzo[a]pyrene, a well-studied polycyclic aromatic hydrocarbon (PAH), is classified as a Group 1 carcinogen by the International Agency for Research on Cancer (IARC). PACs can have detrimental effects on ecosystems by disrupting biological processes and impairing the health of organisms. For example, they can interfere with hormone systems, cause genetic damage, reduce reproductive success, and alter behavior in various species. In aquatic ecosystems, PACs can accumulate in sediments, affecting benthic organisms and disrupting food webs. Exposure to PACs through inhalation, ingestion, or dermal contact can lead to adverse health effects, including cancer, respiratory ailments, cardiovascular diseases, and developmental abnormalities. QSPR models can provide beneficial information on PACs' chemical characteristics and toxicity, allowing for risk assessment and regulatory compliance. Understanding the structure-activity connections of PACs is critical for determining their possible health hazards.

- **Drug Design and Pharmacology**: Some PACs exhibit pharmaceutical properties and are potential candidates for drug development. QSPR models can assist in predicting various pharmacokinetics and pharmacodynamics properties, such as drug solubility, permeability, and biological activity, thereby accelerating the drug discovery process.
- **Material Science and Engineering Applications**: PACs have diverse applications in materials science, including in electronic devices, coatings, and pharmaceuticals. QSPR models can predict various properties, such as solubility, melting point, and thermal stability, which are crucial for designing new materials with specific properties.

A molecular graph is a graph-theoretic representation of a chemical compound's structural formula, where the edges stand in for bonds and the vertices for atoms. A polynomial, matrix, integer sequence, or numerical value can all be used to depict a graph. Information science, chemistry, and mathematics are combined in the relatively new area of cheminformatics. Specifically, we look at correlations between quantitative structure-activity (QSAR) and structure-property (QSPR), which are used to measure the biological activity and properties of different chemicals. A graphical energy is a graph-related numerical quantity that is invariant under graph automorphism and describes the energy of a graph. The concept of energies was introduced by Ivan Gutman [16] in the study of organic compounds. Upon getting inspiration from this work, numerous kinds and applications of energies come into being. In this paper, we selected a set of molecular descriptors for each property of the molecular structure. We conduct a statistical analysis of polycyclic aromatic compounds to verify the calculated values, compare them with the experimental values, and show how they correlate with the physicochemical properties of these compounds. Our study provides valuable insights into the thermodynamic properties of polycyclic aromatic compounds and their correlation with the various molecular descriptors.

2. FUNDAMENTAL DEFINITIONS

A graph G (V, E) is a collection of sets of nodes and a collection of lines that define a connection between nodes. All the graphs under consideration in this article are undirected, planar, and finite graphs. The concept of degree at a vertex is connected with the concept of bonding in chemistry. The total number of edges connected to a vertex defines the degree of that vertex in a graph. The vertices of the graphs under consideration have a maximum degree of four, and the minimum degree of the vertex here is one.

(1) **First Zagreb Energy**

The first Zagreb energy in 2018 was presented by Jafari, Gutman, and Jahanbani [17]. The energy can be calculated by adding up all of the absolute values of the first Zagreb matrix's polynomial root. In mathematics, the first Zagreb matrix has the following definition in order to get the first Zagreb energy:

$$Z_1(M) = \begin{cases} d_i + d_j; & if i, j \varepsilon E(G) \\ 0, & otherwise. \end{cases}$$

(2) **Sum Connectivity Energy**

Sum connection energy was first introduced by Zhou in 2010 [18]. The sum connectivity energy can be computed by applying the following mathematical formula to the sum connectivity matrix:

$$SC(M) = \begin{cases} 1/\sqrt{d_i + d_j}; & if i, j \varepsilon E(G) \\ 0, & otherwise. \end{cases}$$

(3) **Second Zagreb Energy**

Ivan Gutman also presented the idea of second Zagreb energy in 2018 [17]. The matrix formation for determining the second Zagreb energy is as follows, in compliance with the rule:

$$Z_2(M) = \begin{cases} d_i . d_j; & if i, j \varepsilon E(G) \\ 0, & otherwise. \end{cases}$$

(4) **Randic Energy**

The idea of randic energy was defined in 2010 by Ivan Gutman, Sinan Cevik, Bozkurt, and Gungor [19]. This is the definition of the randic matrix:

$$R(M) = \begin{cases} 1/\sqrt{d_i . d_j}; & if i, j \varepsilon E(G) \\ 0, & otherwise. \end{cases}$$

3. METHODS AND STRATEGIES

There are numerous methods that are used for the determination of energy in molecular structure. In order to calculate the energy of the chemical molecular structure, we apply linear algebraic and graphical theoretical approaches. We selected a set of polycyclic aromatic compounds that differ in the number of rings in the molecule, the position of the rings, and the type of functional groups attached to the rings. ChemSketch is a tool for drawing chemical structures in two dimensions. Microsoft Excel is used to construct correlation and line graphs. We used the calculators to calculate the values of the chemical energies listed in Table 3, and we used Matlab and Mathematica to confirm the results. The best program available is SPSS, which is used for statistical calculations.

4. GRAPHICAL ANALYSIS OF POLYCYCLIC AROMATIC COMPOUNDS

The five most well-known molecular descriptors are used in this article to assess the 25 two-dimensional structures of polycyclic aromatic compounds. The molecular structures are 3D in nature, but for computing the graphical energies, we are discussing the 2D graphs for these medicines. There are many polycyclic aromatic compounds, but only 25 of them are under discussion here. These are Acenaphthylene, Acephenanthrylene, Acridine, Anthanthrene, Benzanthrene, Biphenylene, Benzanthracene, Chrysene, Dibenzothiophene, Fluoranthene, Isoquinoline, Naphthacene, Naphthalene, Pentaphene, Perylene, Phenanthraqinone, Phenanthrene, Phenanthridine, Phenazine, Phenazone, Picene, Pyrene, Quinoline, Triphenylene, and 9H-Xanthen. These compounds' structures are displayed in Figure 1.

These graphical energies are significantly associated with the physical properties of the chemical compounds, as the QSPR analysis for the graphical energies describes and amply illustrates. Tables 1, 2 display the experimental values of the twelve physicochemical parameters of polycyclic aromatic compounds, including molecular mass, boiling point, density, enthalpy of vaporization, flash point, and refractive index, which are represented in Table 1. The other six properties, which are molecular refraction, vapor pressure, logP, polarization, surface tension, and molecular volume, are represented below in Table 2.

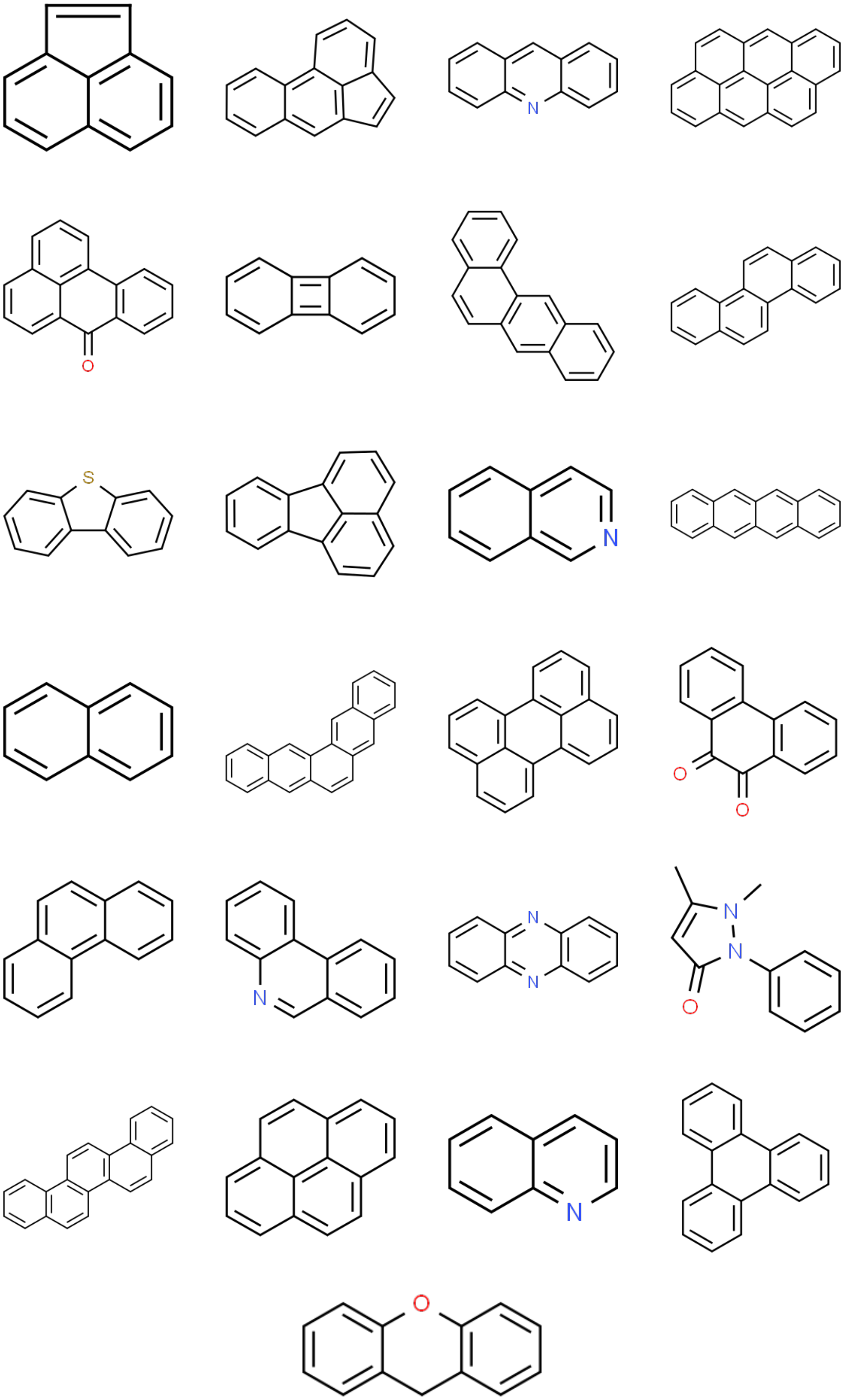

FIGURE 1. Structures of Polycyclic Aromatic Compounds

Compound Name	MM	BP	Dens	EV	FP	IR
Acenaphthylene	152.192	298.9±7.0	1.2±0.1	51.7±0.8	137.2±8.9	1.732
Acephenanthrylene	202.251	405.7±12.0	1.2±0.1	63.2±0.8	188.6±3.7	1.796
Acridine	179.217	346.7±11.0	1.2±0.1	56.8±3.0	153.8±11.9	1.727
Anthanthrene	276.331	497.1±12.0	1.4±0.1	73.6±70.8	247.2±13.7	2.009
Benzanthrone	230.261	436.2±12.0	1.3±0.1	69.3±3.0	196.1±14.5	1.735
Biphenylene	152.192	469.9±12.0	1.2±0.1	70.4±0.8	187.2±14.4	1.697
Benzanthracene	228.288	436.7±12.0	1.2±0.1	66.7±0.8	209.1±13.7	1.771
Chrysene	228.288	448.0±0.0	1.2±0.1	67.9±0.8	209.1±13.7	1.771
Dibenzothiophene	184.257	332.5±11.0	1.3±0.1	55.2±3.0	114.8±5.5	1.756
Fluoranthene	184.257	375.0±0.0	1.2±0.1	59.8±0.8	168.4±12.8	1.852
Isoquinoline	129.159	243.2±0.0	1.1±0.1	46.1±3.0	107.2±0.0	1.642
Naphthacene	228.288	436.7±12.0	1.2±0.1	66.7±0.8	209.1±13.7	1.771
Naphthalene	128.171	221.5±7.0	1.0±0.1	43.9±0.8	78.9±0.0	1.632
Pentaphene	278.347	524.7±17.0	1.2±0.1	76.9±0.8	264.5±15.1	1.812
Perylene	252.309	467.5±12.0	1.3±0.1	70.2±0.8	228.6±13.7	1.887
Phenanthraqinone	208.21	360.0±0.0	1.3±0.1	60.0±3.0	163.1±14.4	1.659
Phenanthrene	178.229	337.4±9.0	1.1±0.1	55.8±0.8	146.6±12.8	1.715
Phenanthridine	179.217	350.4±11.0	1.2±0.1	57.2±3.0	155.9±11.9	1.727
Phenazine	180.205	357.2±15.0	1.3±0.1	57.9±3.0	160.3±11.7	1.740
Phenazone	188.226	319.0±0.0	1.2±0.1	56.1±3.0	114.8±15.0	1.585
Picene	278.347	519.0±0.0	1.2±0.1	76.2±0.8	264.5±15.1	1.812
Pyrene	202.251	404.0±0.0	1.2±0.1	63.0±0.8	168.8±12.8	1.852
Quinoline	129.159	234.1±9.0	1.1±0.1	45.2±3.0	101.1±0.0	1.642
Triphenylene	228.288	425.0±0.0	1.2±0.1	65.3±0.8	209.1±13.7	1.771
9H-Xanthene	182.218	311.0±17.0	1.2±0.1	137.5±16.7	1.623	–

TABLE 1. Type 1 Physicochemical Characteristics of Polycyclic Aromatic Compounds

Compound Name	MR	VP	logP	Pol	ST	MV
Acenaphthylene	51.3±0.3	0.0±0.3	4.26	20.3±0.5	54.7±3.0	128.2±3.0
Acephenanthrylene	69.1±0.3	0.0±0.4	5.50	27.4±0.5	60.4±3.0	162.3±3.0
Acridine	60.0±0.3	0.0±0.7	3.40	23.8±0.5	54.0±3.0	150.9±3.0
Anthanthrene	100.8±0.3	0.0±0.6	6.89	40.0±0.5	74.2±3.0	200.4±3.0
Benzanthrone	71.8±0.3	0.0±1.0	4.81	28.5±0.5	58.3±3.0	178.9±3.0
Biphenylene	50.0±0.4	0.0±0.6	2.57	19.8±0.5	43.2±5.0	129.9±5.0
Benzanthracene	79.8±0.3	0.0±0.5	5.91	31.6±0.5	53.5±3.0	191.8±3.0
Chrysene	79.8±0.3	0.0±0.5	5.91	31.6±0.5	53.5±3.0	191.8±3.0
Dibenzothiophene	60.3±0.3	0.0±0.7	4.38	23.9±0.5	53.6±3.0	147.1±3.0
Fluoranthene	72.5±0.3	0.0±0.4	5.17	28.7±0.5	59.4±3.0	162.0±3.0
Isoquinoline	42.2±0.3	0.1±0.4	1.96	16.7±0.5	46.7±3.0	116.8±3.0
Naphthacene	79.8±0.3	0.0±0.5	5.91	31.6±0.5	53.5±3.0	191.8±3.0
Naphthalene	44.1±0.3	0.2±0.2	3.45	17.5±0.5	40.2±3.0	123.5±3.0
Pentaphene	97.6±0.3	0.0±0.7	7.14	38.7±0.5	57.7±3.0	225.9±3.0
Perylene	90.3±0.3	0.0±0.6	6.40	35.8±0.5	63.5±3.0	196.1±3.0
Phenanthraqinone	58.7±0.3	0.0±0.8	3.13	23.3±0.5	55.8±3.0	159.1±3.0
Phenanthrene	61.9±0.3	0.0±0.3	4.68	24.6±0.5	48.0±3.0	157.7±3.0
Phenanthridine	60.0±0.3	0.0±0.7	3.32	23.8±0.5	54.0±3.0	150.9±3.0
Phenazine	58.1±0.3	0.0±0.8	2.84	23.0±0.5	61.3±3.0	144.1±3.0
Phenazone	54.6±0.3	0.0±0.6	0.27	21.6±0.5	42.7±3.0	162.8±3.0
Picene	97.6±0.3	0.0±0.6	7.14	38.7±0.5	57.7±3.0	225.9±3.0
Pyrene	72.5±0.3	0.0±0.4	5.17	28.7±0.5	59.4±3.0	162.0±3.0
Quinoline	42.2±0.3	0.1±0.4	2.08	16.7±0.5	46.7±3.0	116.8±3.0
Triphenylene	79.8±0.3	0.0±0.5	5.9173	1.6±0.5	53.5±3.0	191.8±3.0
9H-Xanthene	55.4±0.3	0.0±0.6	3.93	22.0±0.5	47.0±3.0	157.1±3.0

TABLE 2. Type 2 Physicochemical Characteristics of Polycyclic Aromatic Compounds

All the graphical energies are computed by utilizing their corresponding matrices. The number of edges in all the chemical structures is considered the degree of vertex. Since all the graphs under examination are connected, the highest degree of a vertex in these structures is four, while the minimum degree of vertices in these structures is one. The computed values for all the graphical energies are given below in Table 3.

5. REGRESSION MODELS

Using linear regression, the observed data are fitted to a linear equation to model the connection between two variables. The first variable is thought to be an explanatory variable, whereas the second variable is seen as a dependent variable. The linear regression values for each of the graphical energies can be determined using the regression model, as indicated below:

$$P = a + bX$$

P is the dependent variable, and X is the independent parameter in this case. The estimated values of the attributes or graphical energies are represented by parameter X, whereas the physical or chemical properties of the polycyclic aromatic compounds are represented by parameter P. The constant, also referred to as the intercept parameter a, specifies the expected response when x_i=0. For every unit change in x_i, the expected change in response is indicated by the slope parameter b.

(1) **Energy E(G)**

$$MM = 21.8393 + 8.1802[E(G)]$$

$$BP = 68.59536 + 14.4418[E(G)]$$

$$Dens = 1.02891 + 0.00824[E(G)]$$

$$VP = 0.31978 + 0.01069[E(G)]$$

$$EV = 27.0563 + 1.56948[E(G)]$$

$$FP = -21.32429 + 8.93964[E(G)]$$

$$IR = 1.4449 + 0.01398[E(G)]$$

Compound Names	E(G)	EZ_1(G)	EZ_2(G)	E_{SC}(G)	E_R(G)
Acenaphthylene	16.6188	79.3260	95.4279	7.4089	10.2512
Acephenanthrylene	22.3820	108.7643	133.4210	9.5245	10.2512
Acridine	19.3136	90.3386	105.7300	8.5000	9.6732
Anthanthrene	30.3676	157.1953	201.0184	12.8450	4.0626
Benzanthrene	24.9606	120.8142	148.3020	10.8510	11.4840
Biphenylene	16.5054	78.2146	93.5190	6.7840	7.6070
Benzanthracene	25.1012	119.3506	143.8000	10.8480	11.6100
Chrysene	25.1920	120.0698	144.8832	10.9254	11.6548
Dibenzothiophene	17.9146	84.4312	100.6063	7.8385	8.3201
Fluoranthene	22.5002	109.7122	136.2285	9.5570	10.306
Isoquinoline	13.6832	61.2720	68.9768	5.6730	6.5126
Naphthacene	24.9308	116.3466	142.4164	10.7320	11.4780
Naphthalene	13.6832	61.2720	67.8712	6.2632	6.5126
Pentaphene	30.7628	149.0508	180.6366	13.0966	14.0315
Perylene	28.2454	138.6322	174.4084	11.8700	12.8860
Phenanthraqinone	21.6790	24.2568	106.1668	9.7938	10.0886
Phenanthrene	19.4484	90.7148	106.9666	8.3156	9.0888
Phenanthridine	19.4484	90.7148	106.9666	8.3156	9.0888
Phenazine	19.3136	90.3386	105.7300	8.5000	9.6732
Phenazone	16.5821	82.7915	96.7775	8.2616	8.2942
Picene	30.9420	149.4560	185.6000	13.1396	14.2240
Pyrene	25.1950	120.0720	144.8820	10.9254	11.6543
Quinoline	13.6832	61.2720	68.9768	5.6730	6.5126
Triphenylene	25.2760	120.8860	145.9740	10.9904	11.6882
9H-Xanthene	19.3136	90.3386	105.7300	8.5000	9.6732

TABLE 3. Graphical energies of Polycyclic Aromatic Compounds

$$MR = -2.19775 + 3.21364[E(G)]$$

$$LogP = -1.90766 + 0.29431[E(G)]$$

$$Pol = -0.89803 + 1.27495[E(G)]$$

$$ST = 31.65864 + 1.03313[E(G)]$$

$$MV = 44.14324 + 5.56497[E(G)]$$

(2) **First Zagreb Energy** $EZ_1(G)$

$$MM = 83.6053 + 1.152[EZ_1(G)]$$

$$BP = 165.62501 + 2.15325[EZ_1(G)]$$

$$Dens = 1.11004 + 0.00097[EZ_1(G)]$$

$$VP = 0.47705 + 0.00074[EZ_1(G)]$$

$$EV = 38.16493 + 0.2284[EZ_1(G)]$$

$$FP = 40.82907 + 1.31211[EZ_1(G)]$$

$$IR = 1.5112 + 0.00236[EZ_1(G)]$$

$$MR = 18.05621 + 0.49244[EZ_1(G)]$$

$$LogP = -0.13946 + 0.04596[EZ_1(G)]$$

$$Pol = 7.1491 + 0.19525[EZ_1(G)]$$

$$ST = 39.18193 + 0.14825[EZ_1(G)]$$

$$MV = 83.19691 + 0.81319[EZ_1(G)$$

(3) **Second Zagreb Energy** $EZ_2(G)$

$$MM = 55.3863 + 1.1583[EZ_2(G)]$$

$$BP = 130.39031 + 2.03488[EZ_2(G)]$$

$$Dens = 1.06304 + 0.00117[EZ_2(G)]$$

$$VP = 0.39717 + 0.00125[EZ_2(G)]$$

$$EV = 33.80803 + 0.22085[EZ_2(G)]$$

$$FP = 16.72328 + 1.26127[EZ_2(G)]$$

$$IR = 1.49124 + 0.00208[EZ_2(G)]$$

$$MR = 11.53291 + 0.45297[EZ_2(G)]$$

$$LogP = -0.55233 + 0.04069[EZ_2(G)]$$

$$Pol = 4.55101 + 0.17969[EZ_2(G)]$$

$$ST = 35.46128 + 0.15056[EZ_2(G)]$$

$$MV = 70.34343 + 0.76483[EZ_2(G)]$$

(4) **Sum Connectivity Energy E_{SC}(G)**

$$MM = 12.8868 + 19.8441[E_{SC}(G)]$$

$$BP = 187.3851 + 19.75768[E_{SC}(G)]$$

$$Dens = 1.16854 + 0.004[E_{SC}(G)]$$

$$VP = 0.3862 + 0.01681[E_{SC}(G)]$$

$$EV = 40.00648 + 2.14307[E_{SC}(G)]$$

$$FP = 51.16634 + 12.33582[E_{SC}(G)]$$

$$IR = 1.65566 + 0.00942[E_{SC}(G)]$$

$$MR = 28.66474 + 3.94759[E_{SC}(G)]$$

$$LogP = 0.40979 + 0.41312[E_{SC}(G)]$$

$$Pol = 11.37378 + 1.56332[E_{SC}(G)]$$

$$ST = 46.89114 + 0.73075[E_{SC}(G)]$$

$$MV = 82.65428 + 8.34964[E_{SC}(G)]$$

(5) **Randic Energy E_R(G)**

$$MM = 94.3372 + 10.6628[E_R(G)]$$

$$BP = 63.32954 + 33.91354[E_R(G)]$$

$$Dens = 1.01696 + 0.02031[E_R(G)]$$

$$VP = 0.29092 + 0.02776[E_R(G)]$$

$$EV = 26.2496 + 3.71051[E_R(G)]$$

$$FP = -23.34291 + 20.86092[E_R(G)]$$

$$IR = 1.45083 + 0.03166[E_R(G)]$$

$$MR = -4.2001 + 7.63487[E_R(G)]$$

$$LogP = -1.87812 + 0.67657[E_R(G)]$$

$$Pol = -1.69108 + 3.02884[E_R(G)]$$

$$ST = 31.48495 + 2.4045[E_R(G)]$$

$$MV = 37.72418 + 13.53493[E_R(G)]$$

5.1. Calculations of Statistical Parameters. Various statistical parameters are employed in this context, as shown in Table 4,5,6,7,8. A parameter connects the characteristics that are utilized to categorize a certain population. It can be used to show the population as a whole a certain attribute. The number of members in a sample is represented by the letter ”N”. There are twenty-five samples in all. ”b” denotes the slope value, while ”a” denotes the constant term. The correlation coefficient (r) indicates how well one variable’s value predicts changes in another. The correlation coefficient ”r” may be positive or negative. An inverse relationship is shown by a negative value, while a direct relationship is indicated by a positive number. Each correlation coefficient has a value that is positive. The strong, direct correlation between the two things is indicated by these positive results. The range of the correlation coefficient is $-1 \leq r \leq 1$. A p-value is used to calculate the probability of obtaining the observed results in the case that the null hypothesis is true. As the p-value decreases, so does the significance level of the observed difference. Generally speaking, a p-value of 0.05 or less is considered statistically significant.

Physical property	N	a	b	r	r^2	p	Indicator
MM	25	21.8393	8.1802	0.9716	0.9441	0.0000	Significance
BP	25	68.59536	14.4418	0.8954	0.8017	0.00001	Significance
VP	25	0.31978	0.01069	0.3089	0.0954	0.1329	Not Significance
Dens	25	1.02891	0.00824	0.5361	0.2874	0.0057	Significance
EV	25	27.0563	1.56948	0.8936	0.7985	0.00001	Significance
FP	25	-21.32429	8.93964	0.9378	0.8795	0.00001	Significance
IR	25	1.4449	0.01398	0.7844	0.6153	0.00001	Significance
MR	25	-2.19775	3.21364	0.981	0.9624	0.00001	Significance
LogP	25	-1.90766	0.29431	0.8743	0.7644	0.00001	Significance
Pol	25	-0.89803	1.27495	0.9812	0.9628	0.00001	Significance
ST	25	31.65864	1.03313	0.7338	0.5385	0.00003	Significance
MV	25	44.14324	5.56497	0.9498	0.9021	0.00001	Significance

TABLE 4. Statistical analysis for Energy

Physical property	N	a	b	r	r^2	p	Indicator
MM	25	83.6053	1.152	0.8229	0.6771	0.0040	Significance
BP	25	165.62501	2.15325	0.8029	0.6446	0.00001	Significance
VP	25	0.47705	0.00074	0.1294	0.0167	0.53758	Not Significance
Dens	25	1.11004	0.00097	0.3807	0.14497	0.60456	Not Significance
EV	25	38.16493	0.2284	0.782	0.6115	0.00001	Significance
FP	25	40.82907	1.31211	0.8278	0.6853	0.00001	Significance
IR	25	1.5112	0.00236	0.796	0.6336	0.00001	Significance
MR	25	18.05621	0.49244	0.904	0.8172	0.00001	Significance
LogP	25	-0.13946	0.04596	0.8211	0.6742	0.00001	Significance
Pol	25	7.1491	0.195257	0.9036	0.8165	0.00001	Significance
ST	25	39.18193	0.14825	0.6332	0.4009	0.00068	Significance
MV	25	83.19691	0.81319	0.8346	0.6966	0.00001	Significance

TABLE 5. Statistical analysis for First Zagreb Energy

Physical property	N	a	b	r	r^2	p	Indicator
MM	25	55.3863	1.1583	0.9587	0.9191	0.0000	Significance
BP	25	7130.39031	2.03488	0.8929	0.7973	0.00001	Significance
VP	25	0.39717	0.00125	0.2557	0.0654	0.217322	Not Significance
Dens	25	1.06304	0.00117	0.5389	0.2904	0.00544	Significance
EV	25	33.80803	0.22085	0.8898	0.7917	0.00001	Significance
FP	25	16.72328	1.26127	0.9364	0.8768	0.00001	Significance
IR	25	1.49124	0.00208	0.8255	0.6815	0.00001	Significance
MR	25	11.53291	0.45297	0.9786	0.9577	0.00001	Significance
LogP	25	-0.55233	0.04069	0.8555	0.7319	0.00001	Significance
Pol	25	4.551017	0.17969	0.9787	0.9579	0.00001	Significance
ST	25	35.46128	0.15056	0.7568	0.5727	0.00001	Significance
MV	25	70.34343	0.76483	0.9238	0.8534	0.00001	Significance

TABLE 6. Statistical analysis for Second Zagreb Energy

Physical property	N	a	b	r	r^2	p	Indicator
MM	25	12.8868	19.8441	0.9806	0.9615	0	Significance
BP	25	187.3851	19.75768	0.5654	0.3197	0.00322	Significance
VP	25	0.3862	0.01681	0.2241	0.0502	0.28152	Not Significance
Dens	25	1.16854	0.004	0.1201	0.0144	0.56743	Not Significance
EV	25	40.00648	2.14307	0.5631	0.3171	0.00338	Significance
FP	25	51.16634	12.33582	0.5973	0.3568	0.00161	Significance
IR	25	1.65566	0.00942	0.244	0.0595	0.23983	Not Significance
MR	25	28.66474	3.94759	0.5562	0.3094	0.00388	Significance
LogP	25	0.40979	0.41312	0.5664	0.3208	0.00316	Significance
Pol	25	11.37378	1.56332	0.5553	0.3084	0.003958	Significance
ST	25	46.89114	0.73075	0.2395	0.0574	0.248881	Not Significance
MV	25	82.65428	8.34964	0.6577	0.4326	0.00035	Significance

TABLE 7. Statistical analysis for Sum Connectivity Energy

Physical property	N	a	b	r	r^2	p	Indicator
MM	25	94.3372	10.6628	0.5845	0.3417	0.002151	Significance
BP	25	63.32954	33.91354	0.8747	0.7651	0.00001	Significance
VP	25	0.29092	0.02776	0.3336	0.1113	0.10316	Not Significance
Dens	25	1.01696	0.02031	0.5495	0.302	0.0044	Significance
EV	25	26.2496	3.71051	0.8788	0.7723	0.00001	Significance
FP	25	-23.34291	20.86092	0.9104	0.8288	0.00001	Significance
IR	25	1.45083	0.03166	0.7389	0.546	0.00002	Significance
MR	25	-4.2001	7.63487	0.9696	0.9401	0.00001	Significance
LogP	25	-1.87812	0.67657	0.8361	0.6991	0.00001	Significance
Pol	25	-1.69108	3.02884	0.9697	0.9403	0.00001	Significance
ST	25	31.48495	2.4045	0.7105	0.5048	0.00006	Significance
MV	25	37.72418	13.53493	0.961	0.9235	0.00001	Significance

TABLE 8. Statistical analysis for Randic Energy

Energies	MM	BP	VP	Dens	EV	FP	IR	MR	LogP	Pol	ST	MV
E(G)	0.9716	0.8954	0.3089	0.5361	0.8936	0.9378	0.7844	0.981	0.8743	0.9812	0.7338	0.9498
$EZ_1(G)$	0.8229	0.8029	0.1294	0.3807	0.782	0.8278	0.796	0.904	0.8211	0.9036	0.6332	0.8346
$EZ_2(G)$	0.9587	0.8929	0.2557	0.5389	0.8898	0.9364	0.8255	0.9786	0.8555	0.9787	0.7568	0.9238
$E_{SC}(G)$	0.9806	0.5654	0.2241	0.1201	0.5631	0.5973	0.244	0.5562	0.5664	0.5553	0.2395	0.6577
$E_R(G)$	0.5845	0.8747	0.3336	0.5495	0.8788	0.9104	0.7389	0.9696	0.8361	0.9697	0.7105	0.961

TABLE 9. Comparison of Correlation Coefficients for Graphical Energies

6. GRAPHICAL ANALYSIS OF CORRELATION COEFFICIENTS

A graph is a representation of the data that shows the frequency distribution and correlation of the relationships between the data points based on the number of vertices and edges. There are many different types of graphs, including bubble charts, area graphs, pie charts, line graphs, scatter plots, and pictographs. The association between the physicochemical qualities and graphical energies shown in Figure 2 & 3 is represented here using line graphs.

Microsoft Excel was used to create each of these line graphs. Correlation coefficient analysis is another application for the scatter plot. Table 9 lists the correlation coefficient values for each. Table 9 provides numerical numbers that illustrate the fluctuation in the correlation coefficient values. Excellent relationships exist between almost all of the characteristics and the molecular energies of chemical structures. Properties like density, enthalpy, and boiling point can be easily calculated using the energies listed above because of the almost 0.9 correlation between all of these characteristics. 2D graphs can be created with the numerical data table. Graphs offer a clear and easy method for comprehending comparisons and variances in data.

FIGURE 2. Correlation between Energies and all physicochemical properties

FIGURE 3. Correlation between Energies and all physicochemical properties

7. APPLICATIONS OF GRAPH ENERGIES IN VARIOUS FIELDS OF SCIENCE

The energies have been used in a variety of engineering and science sectors.

- Graph energies have uses in macromolecule theory, protein sequence analysis, and comparison. Based on the codons that code for the amino acids, a novel two-dimensional graphical representation of proteins is developed using the graph energy and Laplacian energy of twenty amino acids. Based on the Laplacian energies of 20 amino acids and the graph energy, proteins have a unique 2-D graph. It facilitates the organized analysis of protein data and can be used to extract information from the fundamental sequence of proteins [20].

- The graph energy is used as a general segmentation measure in the hierarchical segmentation approach. A new hierarchical image analysis method that applies graph energy as a generic measure for segmentation [21].
- It is also not unusual to apply graph energies to the network analysis of problems in biology, satellite communication, and aviation. Research has indicated that energy and robustness in networks are closely related. Graph energy is also frequently used as a statistic for classification jobs [22].

They also have uses in crystallography. Two unanticipated applications are object identification and pattern recognition. These techniques might be helpful for achieving military goals. On the other side, face recognition might be useful to police enforcement.

8. RESULTS AND ITS SIGNIFICANCE

We used five types of invariants for the analysis of various chemical structures. The QSPR analysis of the adjacency energy depicts that it is a powerful technique for determining the physical features of the compounds, as the correlation values for this energy with the properties MM, BP, EV, FP, MR, Logp, Pol, and MV are all almost nearly equal to one. Similarly, the QSPR analysis of first zagreb energy and second zagreb energy also demonstrates that these are powerful techniques for determining the characteristics of the compounds. The randic energy also exhibits a strong positive correlation with the seven properties, and the correlation range for this is nearly equal to one that describes the importance of this descriptor. However, the sum connectivity energy represents a strong positive relationship with only one molecular mass. The positive range of sum connectivity energy with molecular mass represents that this descriptor cannot be neglected. It can also be used in the future for determining some properties of the compounds, and it may show a strong relationship with the characteristics of some other compounds. As these invariants have a very strong correlation with the properties of compounds, they may also have a good correlation with other structures.

The line graphs in Figure 2 & 3 are the graphical representations of the correlation coefficients. There are various twelve graphs for the representation of various twelve physical properties of the chemical compounds. The values of the calculated correlation coefficients are displayed on the y-axis, whereas the names of the molecular descriptors are shown on the x-axis. The values of all the computed correlation coefficients are positive, so the range we set for these graphs is from 0 to 1. The results show that these invariants are a theoretical tool for approximating the properties of chemicals and medication structures, eliminating the need for time-consuming trials. This article assists chemists, pharmacists, and chemical researchers in their professional endeavors. These invariants are quite valuable. However, they are sufficient for investigating many complex chemical compounds. This effort benefits society by motivating researchers and chemical students to pursue mathematical studies. This paper provides a theoretical foundation for researchers studying various chemical substances. So, this work has a good future scope for the researchers.

9. CONCLUSION AND DISCUSSION

The polycyclic aromatic compounds are studied in the current work, and numerous energies are used for each compound. There are a total of 25 polycyclic compounds that are studied with graphical energies. Tables 4 to 9 and Figure 2 & 3 represent the computed values for the graphical energies and their correlation with the physicochemical properties. The initial zagreb energy, r = 0.904, exhibits a strong association with molar refractivity, while the second zagreb energy depicts a high correlation with polarizability, as estimated r = 0.9787, with flash point (0.9364), with molar refractivity (0.9786), and with molar volume (0.9238). The randic energy also depicts a high correlation coefficient with molar refractivity (0.9696) and polarizability (0.9697) and also shows a high relation coefficient with flash point (0.9104). The second Zagreb energy has the highest correlation with the four physicochemical characteristics of polycyclic aromatic molecules, making it the most efficient energy. We examine the physicochemical characteristics of polycyclic aromatic compounds to evaluate the prediction capacity of these energies. The findings demonstrate a robust positive linear correlation and the high significance of every result with regard to the molecular volume, enthalpy, flash point, boiling point, and molar refractivity. This study aims to extract structure-related information from the graphic energies in a cheap and efficient manner.

9.1. Limitations.

Although the numerous energies presented in this article are meant for the study of the physicochemical aspects of polycyclic compounds, they are insufficient to cover all chemical compound properties.

CONFLICT OF INTERESTS

The author declares that there is no conflict of interests.

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