Ethiopian International Journal of Multidisciplinary Research

pISSN:2349-5707 Volume:12,Issue 12,December-2025 eISSN:2349-5715

STUDY OF MOLECULAR ORBITALS AND PHYSICAL AND CHEMICAL PROPERTIES OF INDENE BY CALCULATION

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Abstract: The aim of this article is to conduct an in-depth study of the structure and physicochemical properties of the indene molecule. Modern computational chemistry methods were used in the study. Indene is an aromatic compound, a dicyclic conjugated system with a complex electron cloud. Therefore, determining its electron density, molecular orbitals, partial charge distribution, and reactivity centers is crucial for a complete understanding of its chemical nature. The obtained computational results serve as an important scientific resource for the theoretical evaluation of the physicochemical properties of indene, the scientific substantiation of the synthesis processes for its derivatives, and the expansion of the application of this compound in organic chemistry, materials science, and the chemistry of natural compounds.

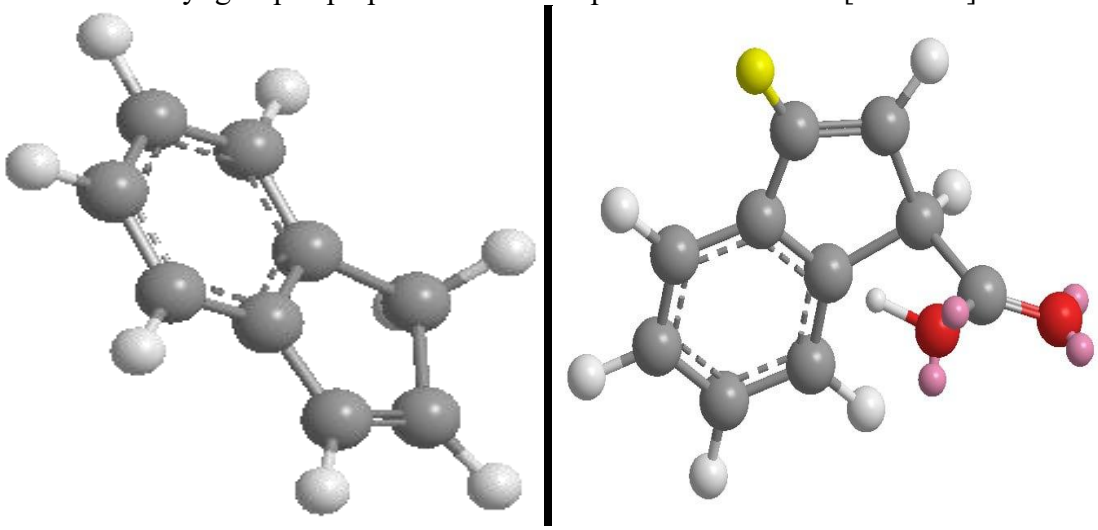
Key words: Indene, molecular orbitals, electron density, computational chemistry, energy parameters, dipole moment, computer modeling.

Introduction. Currently, the rapid development of the chemical industry is considered a key component of the global economy, on which the lifestyle and well-being of the population largely depend [1]. In this regard, the efficient production of a wide range of biologically active substances, drugs, protective agents and chemical intermediates with high added value is of particular importance in the development of a range of products formed during the synthesis of organic chemistry [2]. Indene and its derivatives, due to the polycyclic aromatic system, have high reactivity to various oxidation reactions, combinations and the introduction of functional groups. In particular, the process of obtaining carboxylic acids and their derivatives as a result of the interaction of indene with strong oxidizing agents, including potassium permanganate ($KMnO_4$), is considered one of the promising areas of modern organic synthesis. The oxidation reaction with potassium permanganate allows not only to study the processes of redistribution of the indene molecule in the aromatic system, but also provides a convenient method for the synthesis of compounds rich in carboxyl groups, which are of practical importance in industrial and laboratory conditions. The resulting indene carboxylic acids can then be converted into more complex organic compounds through reactions such as esterification, amidation, and salt formation. This process plays an important role in the creation of substances used in a number of fields, such as pharmaceuticals, inorganic inhibitors, polymer chemistry, and agrochemistry [3].
Indene is an aromatic hydrocarbon whose molecule consists of one benzene ring and one cyclopentadiene ring. These two rings are joined together to form two carbon rings. Thus, it is a polycyclic aromatic compound. It occurs naturally in coal tar and crude oil, and is also released during the incomplete combustion of coal tar and similar substances. Indene was isolated from coal tar in 1890 by the Kroemer method. Indene is a colorless or pale yellow liquid; in its pure form, it is colorless, but may become slightly colored during storage. Odor: strong, characteristic aromatic. Molecular formula: C_9H_8. Molecular weight: 116.16 g/mol, melting point: -50°C,

pISSN:2349-5707 Volume:12,Issue 12,December-2025 eISSN:2349-5715

boiling point: 181-182°C (at normal pressure), density (at 250°C): about 0.996 g/cm³, solubility in water: very low (practically insoluble in water), solubility in organic solvents: readily soluble in ether, ethanol, benzene and other organic solvents. Chemical properties of indene: Indene molecules contain highly reactive olefin compounds and are prone to polymerization or addition reactions. Indene can be polymerized at room temperature with heating or in the presence of an acid catalyst, which significantly increases the polymerization rate. Indene polymerizes at room temperature and in the dark, easily forming polymer compounds depending on the conditions. The physicochemical properties of indene are of scientific and practical importance in research. Therefore, it is important to correctly analyze the composition and physicochemical properties of indene. Computer-aided research methods are also becoming increasingly important in chemistry. They make it easier for students and researchers to understand the properties of molecules. This is not only theoretical chemistry, but also the most advanced field of science and technology. They shorten experimental time, reduce risks, make results more accurate, and pave the way for new scientific discoveries [4,5]. The indene molecule is used to theoretically substantiate the mechanisms of chemical reactions, view electron density, orbitals, and molecular geometry in three dimensions, find the minimum energy using a program, determine the charge distribution and reaction centers, use safe methods that replace experiments, predict experimental results, assist in the creation of new substances, integrate interdisciplinary research, evaluate the reactivity of compounds, reduce experimental work and reduce errors, and also make it easier for students and researchers to understand the properties of molecules when studying their geometric electronic structure [6].

Results and discussion. A three-dimensional model of the indene molecule, obtained as a result of a semi-empirical quantum chemical calculation (Figure-1), is presented, demonstrating an ordered arrangement of atoms [7.8.9]. The figure shows that steric changes occur in the molecule, and the carboxyl group is perpendicular to the plane of the indene [10.11.12].



1.-Fig. Molecular three-dimensional structure of indene and the bonding of carboxyl groups

This structure of the molecule facilitates the movement of electrons in the carboxyl group along the carbon and oxygen atoms, which we can see from the overall charge density (Figure 2) and the electrostatic potential.

Figure 2. **Figure 3.**

pISSN:2349-5707 Volume:12,Issue 12,December-2025 eISSN:2349-5715

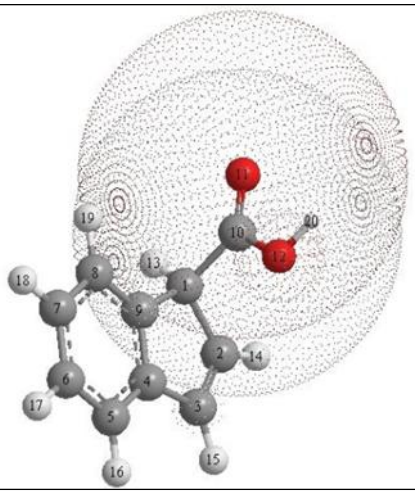


Figure 2. Diagram of the distribution of the total charge density.

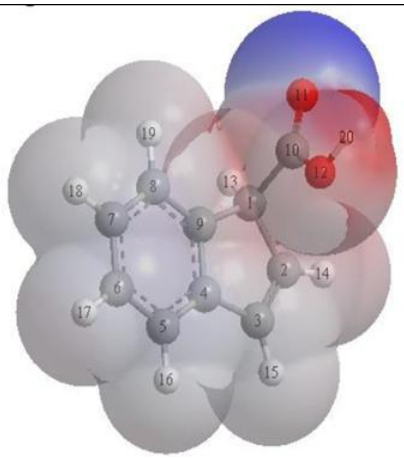


Figure 3. Schematic diagram of the distribution of electrostatic potential in a molecule: positive values are shown in blue, negative values in red.

This allows us to calculate the overall charge density of the molecule (Fig. 3) and the distribution of electrostatic potential within this group. The calculation results describe the geometric parameters of the molecule, such as bond lengths and bond angles.

Table 1.

Calculated bond lengths and bond angles in the indene molecule

Atoms		Cord length, A^0	Atom	Garden angle, degree	Atom	Double angle, degree
4C						
9C	C(4)	1.3941				
1C	C(9)	1.5227	C(4)	109.1543		
8C	C(9)	1.3737	C(1)	129.8258	C(4)	120.9903
3C	C(4)	1.4784	C(9)	108.1452	C(1)	0.8818
5C	C(4)	1.3782	C(3)	131.2942	C(9)	120.5585
6C	C(5)	1.3888	C(4)	118.5612	C(3)	-179.4707
7C	C(8)	1.3914	C(9)	118.5459	C(1)	178.5070
2C	C(1)	1.5258	C(9)	101.6839	C(4)	-1.3584
10C	C(1)	1.5044	C(2)	111.8187	C(9)	111.3844
12O	C(10)	1.3506	C(1)	112.2719	C(2)	-55.9773
11O	C(10)	1.2038	C(1)	125.3525	O(12)	122.3755
14H	C(2)	1.06833	C(1)	122.1697	C(3)	126.6719
15H	C(3)	1.0692	C(2)	126.1202	C(4)	124.0304
16H	C(5)	1.0727	C(4)	120.9862	C(6)	120.4525
17H	C(6)	1.0721	C(5)	119.5943	C(7)	119.5988
18H	C(7)	1.0711	C(6)	119.8061	C(8)	119.6596
19H	C(8)	1.0724	C(7)	120.2932	C(9)	121.1607
13H	C(1)	1.0810	C(2)	112.2702	C(9)	112.2132
20H	O(12)	0.9689	C(10)	111.7573	C(1)	-178.1882

The energy values of atoms in a molecule are calculated in charge units and are presented in Table 2.

pISSN:2349-5707 Volume:12,Issue 12,December-2025 eISSN:2349-5715

Table 2.

Calculated values of charges on atoms in the indene molecule.

Atom	The value of the charge in atomic units	Atom	The value of the charge in atomic units
[C(1)]	-0.048	[O(11)]	-0.630
[C(2)]	0.006	[O(12)]	-0.178
[C(3)]	-0.099	[H(13)]	0.067
[C(4)]	0.027	[H(14)]	0.026
[C(5)]	-0.062	[H(15)]	0.029
[C(6)]	-0.054	[H(16)]	0.029
[C(7)]	-0.050	[H(17)]	0.029
[C(8)]	-0.069	[H(18)]	0.029
[C(9)]	0.084	[H(19)]	0.029
[C(10)]	0.628	[H(20)]	0.205

Conclusion. In this study, a comprehensive analysis of the electronic structure, molecular orbitals, and physicochemical properties of the indene molecule was performed using computational chemistry methods. This energy difference is also important when analyzing the role of the molecule in oxidation and reduction reactions. Summarizing the study, the following conclusions can be drawn. A correct analysis of the composition, physicochemical properties, and quantum chemical analysis of the indene molecule allow us to predict its reactivity, create stable modifications, and use it in the synthesis of new materials. Using quantum chemical methods, the structure of the indene-1-carboxylic acid molecule was studied. It was found that the molecular core is characterized by a single plane, and steric distortion is observed in the carboxyl group. As a result, different distributions

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