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Research Article

The temperature and solvent effect on the structural, thermodynamic and electronic properties of Auxin: A computational study

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ABSTRACT

Indol-3-acetic acid (IAA) is the major and naturally synthesized auxin that can regulate plant growth and many physiological processes involving the response to directional light. Computational analysis of the impacts of solvents on different polarity and temperature (100K–1000K) on the structural, thermodynamic, and electrical properties of IAA is done using the density functional theory (DFT) approach. The optimized structure of the IAA molecule shows four (4) stable conformers depending on their energies. The increasing intensities of molecular vibration were seen to generate a rise in enthalpy (H), entropy (S), and specific heat capacity (Cv) with temperature. Conversely, it was found that Gibbs's free energy (G) decreased when temperature increased. Our computations demonstrate that when solvation lowers excitation energies, the UV-light absorption maxima (λ_{max}) are red-shifted in the presence of polar protic, aprotic, and non-polar solvents. Conversely, exothermic and spontaneous behavior is seen in the interactions between IAA and solvents with varying polarity.

Introduction

Growth is essential to all multicellular or living things, including plants and animals. In plants, growth results from an increase in the quantity and size of cells. Although there is a distinction between growth in plants and animals, in both cases, the growth is regulated by hormones (Liu et al., 2014). Several types of hormones can regulate plant growth, like auxin, gibberellins (GA), cytokinins, abscisic acid (ABA), and ethylene. Auxin is the most significant of them all for plant growth and development in a variety of areas, including the form of the plant, stimulated cell division, and cell elongation (Fendrych et al., 2018; Frim, 2003; Zivanovic et al., 2018; Sorefan et al., 2009). Furthermore, it contributes to flowering and postpones senescence (McSteen et al., 2007). It also promotes the normal growth of plant stem cells toward the light (Fuente and Leopold, 1968). It is essential for numerous physiological processes in plant life cycles that result in plant development and growth. The major and most naturally cell-synthesized auxin is indole-3-acetic acid (IAA), which is found in plants to a greater extent (Masuda and Kamisaka, 2000). Because it has a carboxylic acid group and an aromatic ring, IAA is significant (Fig. 1) (Simon and Petrasek, 2011).

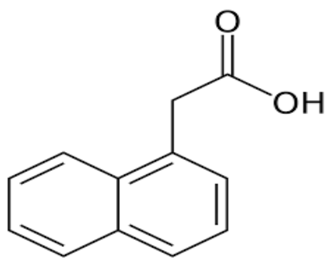

Fig. 1. Structure of indole-3-acetic acid (IAA).

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The structural motifs and the properties of the phytohormone IAA have been studied experimentally and theoretically to reveal its physicochemical behaviors (Ilbeigi et al., 2022; Ung et al., 2023; Bogaert et al., 2022). Nigivic et al. studied some of the alkylated derivatives of IAA and revealed that these derivatives had exhibited their growth-promoting activity in plants and they also exhibited their physicochemical properties in plants (Nigović et al., 2000; Schmit et al., 2011; Förner and Badawi, 2014). Flasinski and Hac-Wydro (2014) studied and emphasized the discrepancies in the interaction of natural IAA and synthetic 1-naphthalene acetic acid (NAA) (Fig. 2) phytohormones with phospholipids in the plasma membranes of both plants and animals.

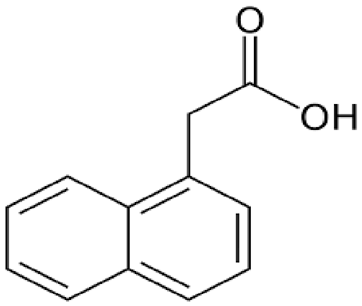

Fig. 2. Structure of 1-naphthalinic acetic acid (NAA).

They reported that the naturally occurring IAA interacts with biological membranes or lipids more strongly than the synthetic auxin, NAA, due to its capability of forming an H-bond by its NH donor group of indoles ring (Flasiński and Hac-Wydro, 2014).

The plant hormone auxin can rapidly degrade the AUX/IAA protein family of transcription. This auxin-induced degron (AID) system can be transplanted into non-plant cells to control the stability of proteins (Nishimura et al., 2009; Luo et al., 2018). Addressing particular protein activities within a given time frame is not viable. Having conditional and reversible control over particular proteins is ideal for better understanding how the brain works. Auxin-induced protein degradation systems can be applied in neuroscience to control the specific protein functions in the brain (Nakano et al., 2019). Nowadays, chemical herbicides have been used to accommodate crop production with the increasing global population. Such kinds of herbicides are unsafe for agricultural products and also for the environment. A higher amount of IAA can degrade the plant growth activity. So, IAA-producing microbes have been used recently to reduce the use of chemical herbicides in crop production and to save agricultural products and the environment. These microbes can evaluate and enhance the inhibitory effect of IAA.

However, an optimum process for commercial-scale IAA production will be needed, and this process can replace the toxic elements in the agricultural sectors (Bunsangiam et al., 2021).

IAA is a weak polar molecule. Therefore, organic solvents close to IAA's polarity are the most effective for extracting IAA from plant tissues (Su et al., 2017). Moreover, all auxins are always stored in the refrigerator at 5-10℃ because of the effect of light. Therefore, in this work, indole-3-acetic acid (IAA) has been investigated to examine its structural and conformational landscape and the temperature and solvent impacts on its electronic and thermodynamic properties. All of these analyses have been done with the aid of computational analysis. The thermodynamic and electronic properties have been analyzed only for the most stable conformer of IAA.

Computational Methodology

IAA, the most abundant plant hormone among the natural and synthetic auxins, has been studied computationally. All the calculations have been performed with the *Gaussian* 16 software packages (Frisch et al., 2016). *GaussView* 6.0 has also been used for all the visual presentations. The possible conformers of IAA have been optimized in the gas phase using density functional theory (DFT) without any imaginary frequency. The DFT computations were implemented and presented with the help of Origin Pro 2018 software (OriginPro, 2018).

Temperature effects on the most stableconformer of IAA have been analyzed by varying the temperature from 100K to 1000K. The solvent effect has been observed using the Integral Equation Formalism Variant Polarizable Continuum Model (IEF-PCM) model at the DFT/ωB97XD/cc-pVTZ level of theory. Nineteen (19) solvents of different polarities have been used in this calculation and optimized without any imaginary frequency. TD-DFT calculations of these solvent-IAA interactions have been also carried out at the same level of theory.

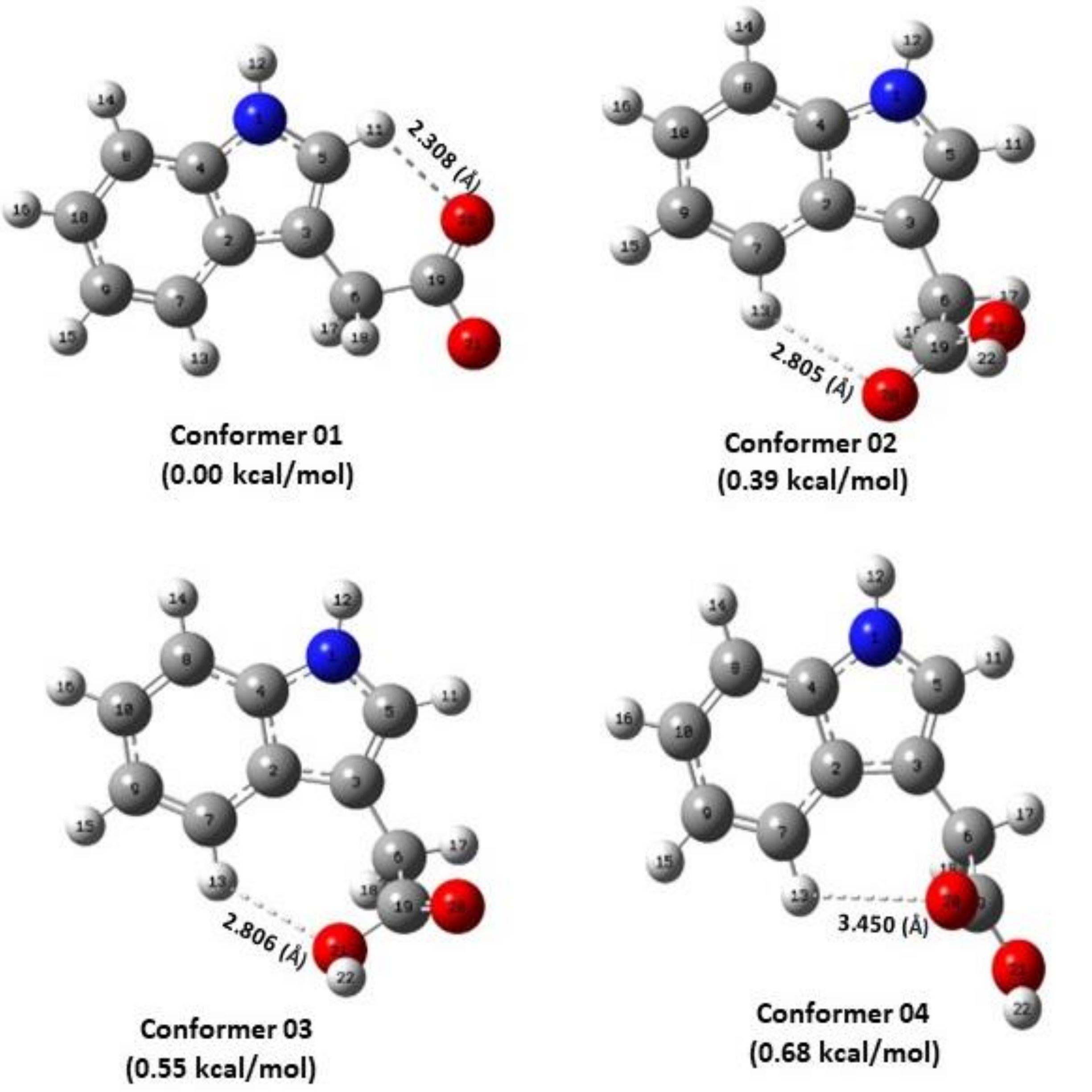

Fig. 3. The optimized structures of the four (4) conformers of the indole-3-acetic acid (IAA)

Results and Discussion

Optimization of Molecular Geometry

The possible structures of the IAA molecule have been optimized using DFT with hybrid functional of ωB97XD and basis set of cc-pVTZ. Through the optimization of the IAA molecule without any imaginary frequency, four (4) stable conformershavebeen found. They are shown in Fig. 3, along with their atom number, stability order, and relative energies. The most stable conformer is assigned as conformer 01. The second lowest energy conformer is conformer 02, which is only 0.39 kcal/mol higher than conformer 01. Conformers 03 and 04 are 0.55 and 0.68 kcal/mol higher than conformers 01.

Temperature effect on the thermodynamic properties

The most significant thermodynamic parameters, H, G, S, and C_v, of the most stable conformer of IAA have been computed and presented in Table 1. The calculations were done in the region of 100K to 1000K at 1 atmospheric pressure. To understand the effect oftemperature on these parameters, the graphical representation of thermodynamic properties vs temperature plots for conformer 01 are presented in Fig. 4, and data are tabulated in Table 2. Using quadratic formulae, the correlation fitting equation between changes in H, G, S, and Cv with temperatures was fitted. Origin Pro 2018 software was then used to produce the fitting equations using regression factors (R^2). Equations for fitting thermodynamic correlations are

$$H = 107.98146 + 0.01781T + 4.5177 \times E^{-5}T^2 \; (R^2 = 0.99944)$$

$$G = 111.12551 - 0.06641T - 6.44468 \times E^{-5}T^2 \; (R^2 = 0.99997)$$

$$S = 17.16729 + 0.04975T - 1.03511 \times E^{-5}T^2 \; (R^2 = 0.99999)$$

$$C_v = -0.34162 + 0.04899T - 2.03210 \times E^{-5}T^2 \; (R^2 = 0.99908)$$

Table 1. Calculated thermodynamic parameters of the conformers of indole-3-acetic acid (IAA) at the DFT/*w*B97XD/cc-pVTZ level of theory in the gas phase.

Conformers	Enthalpy, H (kcal/mol)	Free energy, G (kcal/mol)	Entropy, S (kcal/mol)	Heat capacity, Cv (kcal/mol)	Dipole moment, μ (Debye)	Polarizability, α (a.u.)
01	116.84	85.78	31.030	12.203	0.619	120.831
02	117.09	86.35	30.732	12.134	3.679	120.136
03	117.08	86.23	30.828	12.136	1.929	120.637
04	116.82	85.52	31.295	12.223	2.410	120.522

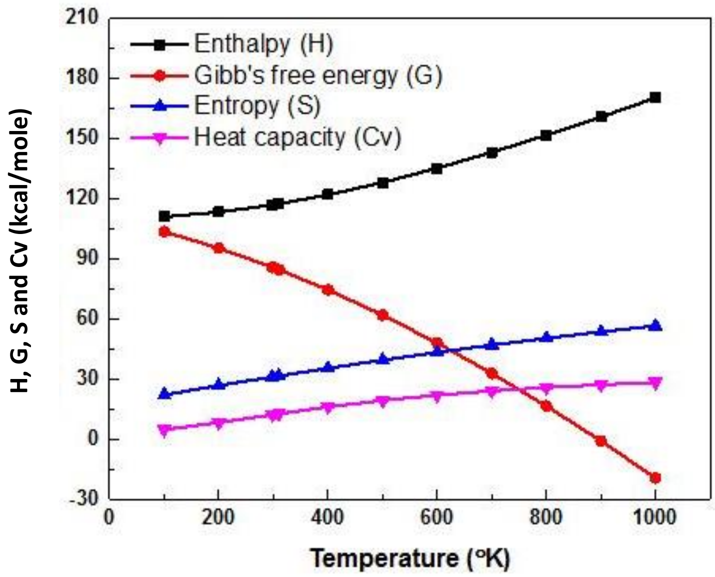

Fig. 4. The dependency of Gibbs free energy, enthalpy, entropy, and specific heat capacity at different temperatures (100k-1000k) for the most stable confirmer (01) of indole-3-acetic acid (IAA).

Following the related Figure and Table, the H rises slowly at lower temperatures but increases steeply at higher temperatures. This is because, at a lower temperature, the translational and rotational motion are the major contributions to the thermodynamic functions in a molecule. In contrast, the vibrational motion also contributes to the molecule at a higher temperature. Because thermal energy is distributed among translational, rotational, and vibrational motions, the S value rises as temperature rises. It also can be seen that the value of G decreases steeply as the temperature increases due to the dependency of G on the -TΔS, and the relation between them is the free energy change, $\Delta G = \Delta H - T\Delta S$. That means the G decreases with the increase of entropy along with the increase of temperature. Another thermodynamic parameter, C_v, rises slowly and gradually with increased temperatures. At very high temperatures, the molecule will be fragmented into atoms, and the molecular motion is not increased, resulting in the constant value of specific heat capacity (Alauddin, 2021).

Solvent effect on the thermodynamic properties

The effect of various solvent types (polar protic, aprotic, and non-polar) on the thermodynamic characteristics has been performed using the IEFPCM model at the *ω*B97XD/cc-pVTZ method. Nineteen (19) solvents of different polarities have been applied to quantify the solvent effect on the thermodynamic parameters of the conformer 01. Among the solvents, the polar protic solvents are (H_2O), methanol (CH_3OH), ethanol (C_2H_5OH), and aniline (C_6H_5-NH_2).

The polar aprotic solvents are dimethyl sulfoxide (DMSO), nitromethane (CH_3NO_2), acetonitrile (CH_3CN), acetone (C_2H_6CO), dichloro-ethane($C_2H_4Cl_2$), dichloromethane (CH_2Cl_2), tetrahydrofuran (THF), chlorobenzene (C_6H_5-Cl). And the chosen non-polar solvents are diethyl ether ($(C_2H_5)_2O$), toluene (C_6H_5-CH_3), benzene (C_6H_6), carbon tetra chloride (CCl_4), cyclohexane (C_6H_{12}), heptane (C_7H_{16}).

The thermodynamic parameters H, G, S, and Cv and ΔH, ΔG, and ΔS values have been calculated at room temperature (298.15 K) and 1 atmospheric pressure and presented in Tables 3 and 4, respectively.

According to the calculated data, the values of H, G, and Cv of the conformer 01 in the solvent phase are less than in the gas phase.

The values also increase with the decrease of polarity. This means the molecules are stabilized in the presence of solvents (Srivastava and Khan, 2020).

On the other hand, the value of S in the solvent phase is larger than in the gas phase and decreases with the decrease of the polarity. Strong hydrogen bonding forms between the carboxylic (-COOH) group of IAA and polar solvents, releasing energy to the system.

Due to these hydrogen bonding interactions, entropy increases with the increase in polarity of the solvents (Crane-Robinson and Privalov, 2022). The results obtained from our calculation show that the studied molecule is highly stabilized in polar solvents compared to the non-polar solvents.

On the other hand, in all types of solvents, the values of ΔH are negative, which means the reactions are exothermic. Consequently, ΔH becomes more negative as the polarity of the solvent increases. The values of ΔG are also negative in all the solvent cases, which indicates that the reactions are spontaneous. The ΔG becomes more negative with the increase of the polarity of the solvent. Calculations also show that the values of ΔS become more positive as the polarity increases. That means the solvents' polarity increases the system's randomness or disorder.

Table 2. Temperature affects the thermodynamic parameters of the most stable conformer (01) indole-3-acetic acid (IAA) calculated by the DFT/*w*B97XD/cc-pVTZ method.

Temperature (Kelvin)	Energy E (kcal/mol)	Enthalpy H (kcal/mol)	Gibbs free energy G (kcal/mol)	Entropy S (kcal/mol)	Heat capacity Cv (kcal/mol)
100	110.73	110.92	103.53	22.04	4.78
200	112.89	113.29	95.31	26.78	8.25
298.15	116.25	116.84	85.79	31.04	12.20
310	116.75	117.36	84.54	31.55	12.68
400	121.10	121.89	74.43	35.36	16.10
500	127.07	128.06	61.88	39.45	19.33
600	134.01	135.20	47.98	43.32	21.94
700	141.74	143.13	32.83	46.96	24.04
800	150.10	151.69	16.49	50.36	25.75
900	158.99	160.78	-0.94	53.55	27.17
1000	168.31	170.29	-19.42	56.54	28.35

Table 3. Solvent effect on thermodynamic properties for the most stable conformer (01) of indole-3-acetic acid (IAA) calculated by DFT/*w*B97XD/cc-pVTZ method.

Types of solvent	Name of Solvent	H (kcal/mol)	G (kcal/mol)	S (kcal/mol)	C v(kcal/mol)	μ (Debye)	α (a.u)
Polar protic	Gas phase	116.840		31.040	12.203	0.619	120.831
	Water	116.805	84.737	32.052	12.173	0.752	163.935
	Methanol	116.809	85.051	31.742	12.174	0.748	162.368
	Ethanol	116.812	85.132	31.664	12.174	0.746	161.557
	Aniline	116.828	85.422	31.391	12.178	0.727	153.699
Polar aprotic	DMSO	116.807	84.934	31.857	12.174	0.750	163.174
	Nitromethane	116.808	85.015	31.777	12.174	0.749	162.653
	Acetonitrile	116.808	85.059	31.733	12.174	0.749	162.598
	Acetone	116.813	85.185	31.613	12.174	0.745	160.847
	Dichloroethane	116.823	85.351	31.455	12.176	0.735	156.961
	Dichloromethane	116.825	85.376	31.432	12.177	0.733	156.001
	THF	116.827	85.409	31.402	12.178	0.729	154.411
	Chlorobenzene	116.832	85.451	31.365	12.180	0.721	151.719
	Chloroform	116.834	85.477	31.342	12.181	0.715	149.467
Non-polar	Diethylether	116.834	85.489	31.331	12.183	0.711	148.095
	Toluene	116.837	85.550	31.271	12.191	0.683	138.932
	Benzene	116.837	85.556	31.265	12.191	0.680	138.117
	Carbon tetrachloride	116.836	85.558	31.262	12.192	0.679	137.765
	Cyclohexane	116.837	85.570	31.251	12.193	0.672	135.872
	Heptane	116.837	85.578	31.242	12.194	0.669	134.825

Electronic properties

Frontier molecular orbital (FMO) analysis

The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are known as frontier molecular orbitals (FMO). Whereas LUMO is an electron acceptor, HOMO is an electron donor. These molecular orbitals play a significant role in determining how molecular interactions with other species occur. TD-DFT has calculated the energies of HOMO and LUMO with ωB97XD/cc-pVTZ in the ground state. The energy of HOMO denotes the ability of electron-donating, and the energy of LUMO denotes the ability of electron-accepting. The data obtained show that the HOMO-LUMO gap of conformer 01 is 8.96 eV.

Solvent effect on the electronic excitation

The type of solvent has a great impact on the FMOs and the electronic excitation of any molecule. Another important property for exploring the solvent effect is the dipole moment of a molecule. To observe the solvent effect on the absorption spectra, the TD-DFT calculations have been carried out on the optimized structure of the most stable conformer in the nineteen (19) solvents of different polarity using the IEFPCM model at ωB97XD/cc-pVTZ method.

Table 4. Solvent effect on the ΔH, ΔG, and ΔS of conformer 01 calculated at the DFT/*w*B97XD/cc-pVTZ level of method.

Types of solvent	Name of Solvent	ΔH (kcal/mol)	ΔG (kcal/mol)	ΔS (kcal/mol)
Polar protic	Water	-0.035	-1.048	1.008
	Methanol	-0.030	-0.733	0.698
	Ethanol	-0.028	-0.653	0.620
	Aniline	-0.011	-0.362	0.347
Polar aprotic	DMSO	-0.032	-0.851	0.813
	Nitromethane	-0.031	-0.769	0.733
	Acetonitrile	-0.032	-0.726	0.689
	Acetone	-0.026	-0.599	0.569
	Dichloro ethane	-0.017	-0.433	0.412
	Dichloro methane	-0.015	-0.408	0.389
	THF	-0.013	-0.375	0.358
	Chloro benzene	-0.008	-0.334	0.321
	Chloroform	-0.006	-0.308	0.298
Non-polar	Diethylether	-0.006	-0.296	0.287
	Toluene	-0.003	-0.234	0.227
	Benzene	-0.003	-0.229	0.221
	Carbon tetrachloride	-0.004	-0.226	0.218
	Cyclohexane	-0.003	-0.215	0.207
	Heptane	-0.003	-0.206	0.198

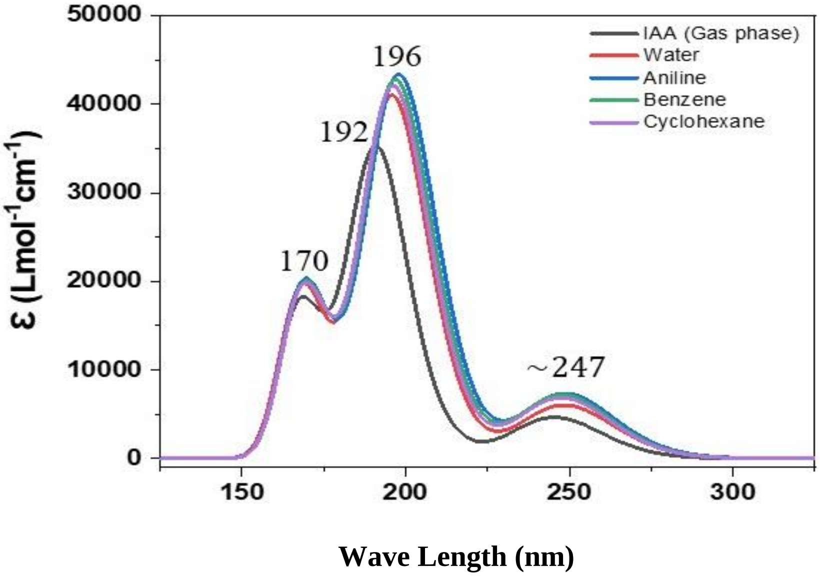

Fig. 5. Solvent effects on the UV/Visible spectrum of the most stable conformer (01) of indole-3-acetic acid (IAA)

The solvent effect on the absorption maxima of UV/Vis spectra has been presented in Table 5, and the absorption spectra for conformer 01 in the gas and solvent phases are presented in Figure 5. To avoid complexity, two polar solvents (water and aniline) and two non-polar solvents (benzene and cyclohexane) along with the gas phase are chosen to present UV/Vis spectral data of solvents. Following Table 5 and Figure 5, the UV/Visible absorption maxima (λ_{max}) in solvents of various polarity shift towardsthe longer wavelength, which is known as redshift or bathochromic shift, compared to the gas phase. This is because the dipole moment is expected to be larger in the solvent than in the gas phase.

It has been found that the dipole moment of the conformer 01 is less in the gas phase than in polar or non-polar solvents. That means the presence of solvation reduces the gas phase's excitation energies and induces the electronic absorption spectrum's redshift (Alauddin, 2021).

Table 5. Solvent effect on the UV/Visible spectrum of the most stable conformer (01) of indole-3-acetic acid (IAA) calculated by TD-DFT/*w*B97XD/cc-pVTZ method.

Types of solvent	Name of solvents	λ_{max1}/ nm	λ_{max2}/nm	λ_{max3}/nm
Polar protic	Gas phase	192.49	169.84	247.23
	Water	195.89	169.88	251.02
	Methanol	195.87	169.89	250.94
	Ethanol	196.09	169.97	251.02
	Aniline	197.33	170.5	251.38
Polar aprotic	DMSO	196.42	170.07	251.29
	Nitro methane	196.21	170.17	251.14
	Acetonitrile	195.97	169.92	251.01
	Acetone	196.08	169.98	250.98
	Dichloro methane	196.49	170.18	250.98
	Dichloro ethane	196.61	170.21	251.1
	THF	196.38	170.16	250.84
	Chloro benzene	197.04	171.33	251.09
	Chloroform	196.63	170.32	250.73
Non-polar	Diethyle ether	196.04	170.15	250.34
	Toluene	196.86	170.57	250.32
	Benzene	196.89	170.59	250.29
	Carbon tetrachloride	196.65	170.53	250.14
	Cyclohexane	196.43	170.5	249.91
	Heptane	196.18	170.44	249.72

*Experimental value obtained in ethanol solutions (Kamnev et at., 2001)

Solvent effect on the global reactivity descriptors

Since the solvent has an important effect on the frontier molecular orbitals (FMO), it also affects the global chemical reactivity descriptors (GCRD) parameters. Ionization potential (I), electron affinity (A), chemical potential (μ), absolute electronegativity (χ), hardness (η), softness (S), and electrophilicity index (ω) are the key GCRD metrics. For closed-shell molecules, all of these values are calculated using the HOMO and LUMO energies, formulating Koopman's theorem (Koopmans, 1934).

$$\chi = \left(\frac{I+A}{2}\right),\ \eta = \left(\frac{I-A}{2}\right),\ \mu = -\left(\frac{I+A}{2}\right),$$

$$S = \frac{1}{2\eta}\ , \omega = \frac{\mu^2}{2\eta}$$

where the energy of LUMO is represented by A (electron affinity) and the energy of HOMO by I (ionization potential). The calculated GCRD parameters are presented in Table 6.

The chemical potential energy becomes lower with the increase of polarity. No significant effect of the polarity of solvents on the global hardness and softness has been observed. Compared to the gas phase, the electrophilicity increases with solvent polarity, confirming that conformer 01 would be energetically preferred for electrophilic attack. The effect of solvent on the FMO and global chemical reactivity descriptors (GCRD) of the conformer 01 are listed and tabulated in Table 7.

Table 6. Global chemical reactivity descriptors (GCRD) of the most stable conformer of IAA at DFT/*w*B97XD/cc-pVTZ method.

Molecular properties	Mathematical descriptors	Energy (eV)
E_{HOMO}	Energy of HOMO	-7.57
E_{LUMO}	Energy of LUMO	1.39
Energy gap	$\Delta E_g = E_{LUMO} - E_{HOMO}$	8.96
Ionization Potential (IP)	$IP = - E_{HOMO}$	7.57
Electron Affinity (EA)	$EA = - E_{LUMO}$	-1.39
Electronegativity (χ)	$\chi = - ½ (E_{LUMO} + E_{HOMO})$	3.09
Chemical Potential (μ)	$\mu = ½ (E_{LUMO} + E_{HOMO})$	-3.09
Global hardness (η)	$\eta = ½ (E_{LUMO} - E_{HOMO})$	4.48
Global softness (S)	$S = \frac{1}{2\eta}$	0.11
Electrophilicity index (ω)	$\omega = \frac{\mu^2}{2\eta}$	1.07

Table 7. Solvent effect on the FMO and Global chemical reactivity descriptors (GCRD) of the indole-3-acetic acid (IAA).

Types of solvent	Name of solvents	E_{HOMO} (eV)	E_{LUMO} (eV)	(H-L) gap	μ	η	S	ω
Polar protic	Gas phase	-7.57	1.39	8.96	-3.09	4.48	0.1116	1.065
	Water	-7.70	1.23	8.93	-3.24	4.47	0.1119	1.172
	Methanol	-7.69	1.23	8.92	-3.23	4.46	0.1121	1.169
	Ethanol	-7.69	1.24	8.93	-3.23	4.47	0.1119	1.165
	Aniline	-7.66	1.27	8.93	-3.20	4.47	0.1119	1.143
Polar aprotic	DMSO	-7.69	1.23	8.92	-3.23	4.46	0.1121	1.169
	Nitromethane	-7.69	1.23	8.92	-3.23	4.46	0.1121	1.169
	Acetonitrile	-7.69	1.23	8.92	-3.23	4.46	0.1121	1.169
	Acetone	-7.69	1.24	8.93	-3.23	4.47	0.1119	1.165
	Dichloro methane	-7.67	1.26	8.93	-3.21	4.47	0.1119	1.150
	Dichloro ethane	-7.67	1.26	8.93	-3.21	4.47	0.1119	1.150
	THF	-7.66	1.27	8.93	-3.20	4.47	0.1119	1.143
	Chlorobenzene	-7.65	1.28	8.93	-3.19	4.47	0.1119	1.136
	Chloroform	-7.64	1.29	8.93	-3.18	4.47	0.1119	1.129
Non-polar	Diethyl ether	-7.64	1.29	8.93	-3.18	4.47	0.1119	1.129
	Toluene	-7.61	1.33	8.94	-3.14	4.47	0.1118	1.103
	Benzene	-7.61	1.33	8.94	-3.14	4.47	0.1118	1.103
	Carbon tetrachloride	-7.61	1.33	8.94	-3.14	4.47	0.1118	1.103
	Cyclohexane	-7.60	1.34	8.94	-3.13	4.47	0.1118	1.096
	Heptane	-7.60	1.34	8.94	-3.13	4.47	0.1118	1.096

Conclusion

The present study examines the effects of temperature (100K–1000K) and solvents (polar protic, aprotic, and non-polar) on the electronic, thermodynamic, and structural characteristics of the indole-3-acetic acid (IAA) molecule using the DFT/ωB97XD/cc-pVTZ computational technique. The four (4) lowest energy conformers have been obtained and assigned as conformers 01, 02, 03, and 04 depending on their relative energies. To simplify, the most stable conformer (01) is considered for studying the effect of solvent and temperature. The temperature effect on the thermodynamic properties has been observed, and it is seen that the calculated values of H and S increase. At the same time, G decreases steeply with the increase in temperature. The Cv rises slowly and gradually as the temperature increases. According to the calculations, the solvent-IAA interactions are found to be spontaneous and exothermic. The UV/Visible absorption spectra have been calculated and occurred $\pi\rightarrow\pi^*$ transition at the maximum absorption wavelength (λ_{max}) ~192 nm with two weak absorption bands at 167 & 247 nm. The polarity of solvents has no significant effect on the GCRD parameters. The solvent effect on the UV/Visible spectra of the most stable conformer has been analyzed, and significant bathochromic or redshifts, as well as hyperchromic effects, have been observed due to the decrease of HOMO-LUMO gap for the presence of the solvent of different (polar protic, aprotic and non-polar) polarities.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Authors contribution

Manuscript prepared by Md. Alauddin, all the computational tasks have been completed by Nasima Tabassum Barna and Md. Masud Parvez, Gazi Jahirul Islam, and Mohammad Abdul Matin played a role in the final version of the manuscript.

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