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Comparative study of interaction of benzene sulfonamides with Zn-metal, Zn^{2+}-ion and carbonic anhydrase (Zn^{2+}-CA)

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ABSTRACT

Interaction of benzene sulfonamies has been discussed with Zn-metal, Zn^{2+}-ion and carbonic anhydrase (Zn^{2+}-CA) in terms of metal ligand interaction energy (E_{int}), shift in charge (ΔN) and lowering in energy (ΔE). The structure of all the above compounds has been drawn and their geometries have been optimized with the help of CAChe software by applying semiempirical PM3 method. Interaction energy shows that the interactions between sulfonamides and carbonic anhydrase are dominant over Zn-metal and Zn^{2+}-ion. Charge transfer phenomenon shows that the interactions between sulfonamides and Zn^{2+}-ion are dominant over Zn-metal and Zn^{2+}-CA. Energy lowering show that the interactions between sulfonamides and Zn^{2+}-ion are dominant over Zn-metal and Zn^{2+}-CA.

Keywords: Benzene sulfonamides, interaction energy, Zn-metal, Zn^{2+}-ion and carbonic anhydrase

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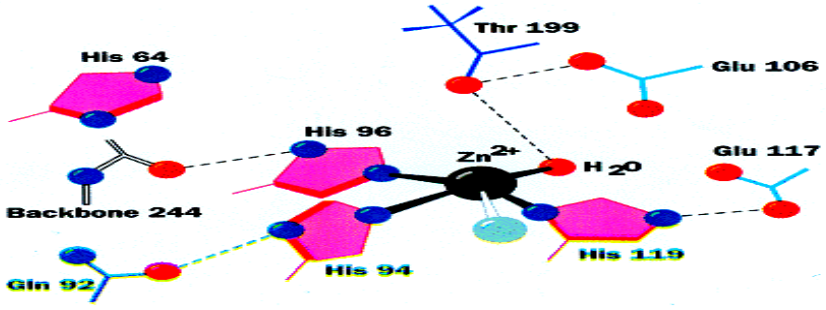
INTRODUCTION

The primary function of the enzyme carbonic anhydrase (CA) is to inter convert carbon dioxide and dioxide and bicarbonate to maintain acid-base balance in blood and other tissues and to help transport carbon dioxide out of tissues.[1,2] CAs are a family of structurally related zinc containing enzyme.[3] CAs, as shown in figure-1, have a single zinc ion tetrahedrally coordinated in the active site by three histidine residues (His94, 96, and 119) and a bound water molecule, which serves as the fourth ligand.



His –Histidine
Thr-Threonine
Gln-glutamine
Glu-glutamic acid

Figure 1. Structure of carbonic anhydrase

The zinc ion is very rigidly coordinated and has an estimated dissociation constant of 1.4×10^{-6} s^{-1} for hCA II corresponding to a half-life of about five days.[4] Excess production of CA may disturb the normal physiological function of the body. In such an event synthetic inhibitors are required to prevent the over functioning of the enzyme. Inorganic and organic anions have been useful in studying the properties of the metal center in carbonic anhydrase. Most monovalent anions inhibit CA with varying affinities. These inhibitors bind to the metal ion and disrupt the coordination of the zinc-OH^- group that disrupts the catalytic activity of the enzyme.[5] Spectrophotometric

analysis of Co^{2+}-substituted CA suggests that some anions have the ability to replace the zinc-OH^- group, while others displace this group forming a pentacoordinated metal-binding sphere.[6] The objective of the paper is to study the donor-acceptor interaction between donor molecules (derivatives of sulfonamide listed in Table-1) and acceptor molecules (Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA) in terms of metal ligand interaction energy (ΔE_{int}).[7-9] And the measurement of bond strength (formed between metal and ligand after interaction) by shift in charge (ΔN) from donor to accepter and lowering in energy (ΔE) of the system.[7]

EXPERIMENTAL SECTION

The study material of this work is derivatives of benzene sulfonamide listed in Table-1, which have been used as a donor molecule. And Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA have been used as acceptor molecule. The structure of all the above compounds has been drawn and their geometries have been optimized with the help of CAChe software[10] by applying semiempirical PM3 method.[11,12] The donor acceptor interaction between molecules listed in Table-1 and Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA have been studied in terms of metal ligand interaction energy (E_{int}), shift in charge (ΔN) and lowering in energy (ΔE).

$\Delta E_{int.}$, ΔN and ΔE and have been evaluated by solving the respective equations given below. The ΔE_{int} between two chemical species A and B, is given by

$$\Delta E_{\text{int}} = E[\rho_{AB}] - E[\rho_A] - E[\rho_B] \qquad \text{Eq.1}$$

It has been shown by Gazquez[7] that if the interaction energy is divided into two steps and one makes the properties of the hardness and softness functions then the above equation can be written as

$$\Delta E_{\text{int}} = \Delta E_v + \Delta E_\mu \qquad \text{Eq.2}$$

Here the first term ΔE_v corresponds to the charge transfer process between A and B arising from the chemical potential equalization principle at constant external potential

$$\Delta E_v \approx -\frac{1}{2}\frac{(\mu_A - \mu_B)^2}{(S_A + S_B)} S_A S_B \qquad \text{Eq.3}$$

where μ_A and μ_B are the chemical potential of A and B, S_A and S_B are their global softness. The second term ΔE_μ, corresponds to a reshuffling of the charge distribution, and is basically a manifestation of the maximum hardness principle.[7]

$$\Delta E_\mu \approx -\frac{1}{2}\frac{\lambda}{(S_A + S_B)} \qquad \text{Eq.4}$$

where λ is a constant related to an "effective number of valence electrons" that participates in the interaction between A and B, and S_A and S_B are their global softness.

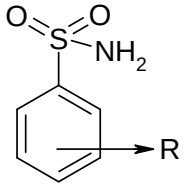
If two systems, A and B (acceptor and donor), are brought together, electrons will flow from that of lower χ to that of higher χ, until the chemical potentials (μ) become equal.[7] The shift in charge ΔN and lowering energy ΔE have been defined as

$$\Delta N = \frac{\chi_A - \chi_B}{2(\eta_A + \eta_B)} \qquad \text{Eq.5}$$

$$\Delta E = \frac{-(\chi_A - \chi_B)}{4(\eta_A + \eta_B)} \qquad \text{Eq.6}$$

where χ_A and χ_B are the electronegativity of A and B, while η_A and η_B are their global hardness.

Table 1. Derivatives of benzene sulfonamides



No.	Substituents (R)	log K
1	H	6.69
2	4-CH_3	7.09
3	4-C_2H_5	7.53
4	4-C_3H_7	7.77
5	4-C_4H_9	8.30
6	4-C_5H_{11}	8.86
7	4-CO_2CH_3	7.99
8	4-$CO_2C_2H_5$	8.50
9	4-$CO_2C_3H_7$	8.77
10	4-$CO_2C_4H_9$	9.11
11	4-$CO_2C_5H_{11}$	9.39
12	4-$CO_2C_6H_{13}$	9.39
13	4-$CONHCH_3$	7.08
14	4-$CONHC_2H_5$	7.53
15	4-$CONHC_3H_7$	8.08
16	4-$CONHC_4H_9$	8.49
17	4-$CONHC_5H_{11}$	8.75
18	4-$CONHC_6H_{13}$	8.88
19	4-$CONHC_7H_{15}$	8.93
20	3-CO_2CH_3	5.87
21	3-$CO_2C_2H_5$	6.21
22	3-$CO_2C_3H_7$	6.44
23	3-$CO_2C_4H_9$	6.95
24	3-$CO_2C_5H_{11}$	6.86
25	2-CO_2CH_3	4.41
26	2-$CO_2C_2H_5$	4.80
27	2-$CO_2C_3H_7$	5.28
28	2-$CO_2C_4H_9$	5.76
29	2-$CO_2C_5H_{11}$	6.18

Where log K is binding constants of benzene sulfonamides to CA

The essential values of electronegativity, absolute hardness, softness, chemical potential, numbers of electron and lambda have been obtained by solving the equation described below and have been listed in Table 2 and 3.

According to Koopman's theorem electronegativity[13,14] is defined as

$$\chi = -\frac{1}{2} \cdot (\varepsilon LUMO + \varepsilon HOMO) \qquad \text{Eq.7}$$

Parr et al. have shown that the electro negativity of any chemical species is equal tp the negative value of chemical potential. Thus,

$$-\mu = \chi = -\frac{1}{2} \cdot (\varepsilon LUMO + \varepsilon HOMO) \qquad \text{Eq.8}$$

The absolute hardness,[13,14] η, is defined as

$$\eta = \frac{1}{2} \cdot (\varepsilon LUMO - \varepsilon HOMO) \qquad \text{Eq.9}$$

where εLUMO and εHOMO are the frontier orbital energies.
The corresponding global softness[9] is defined as

$$S = \frac{1}{(\varepsilon LUMO - \varepsilon HOMO)} \qquad \text{Eq.10}$$

The value of lambda,[8] λ, is defined as

$$\lambda = (N_A + N_B)^2 / 1000 \qquad \text{Eq.11}$$

where NA and NB are number of effective electrons of acid (accepter) and base (donor).

Table 2. Values of HOMO and LUMO energies, electronegativity and chemical potential of donors and acceptors

	C.No.	HOMO Energy	LUMO Energy	χ	μ
Base(B)	1	-9.552	-1.883	5.718	-5.718
	2	-9.493	-1.843	5.668	-5.668
	3	-9.488	-1.837	5.663	-5.663
	4	-9.504	-1.849	5.677	-5.677
	5	-9.512	-1.848	5.680	-5.680
	6	-9.510	-1.849	5.680	-5.680
	7	-9.596	-2.289	5.943	-5.943
	8	-9.491	-2.330	5.911	-5.911
	9	-9.647	-2.261	5.954	-5.954
	10	-9.648	-2.260	5.954	-5.954
	11	-9.648	-2.261	5.955	-5.955
	12	-9.650	-2.260	5.955	-5.955
	13	-9.663	-2.097	5.880	-5.880
	14	-9.657	-2.088	5.873	-5.873
	15	-9.657	-2.089	5.873	-5.873
	16	-9.655	-2.089	5.872	-5.872
	17	-9.654	-2.089	5.872	-5.872
	18	-9.653	-2.089	5.871	-5.871
	19	-9.656	-2.089	5.873	-5.873
	20	-9.656	-2.189	5.923	-5.923
	21	-9.691	-2.201	5.946	-5.946
	22	-9.555	-2.186	5.871	-5.871
	23	-9.688	-2.198	5.943	-5.943
	24	-9.689	-2.198	5.944	-5.944
	25	-9.775	-2.200	5.988	-5.988
	26	-9.792	-2.189	5.991	-5.991
	27	-9.788	-2.186	5.987	-5.987
	28	-9.788	-2.187	5.988	-5.988
	29	-9.789	-2.187	5.988	-5.988
Acid (A)	Zn-metal	-8.855	3.825	2.515	-2.515
	Zn^{2+}-ion	-30.371	-22.317	26.344	-26.344
	Zn^{2+}-CA	-14.533	-6.998	10.766	-10.766

Table 3. Values of absolute hardness, global softness and effective number of valence electrons of donors and acceptors

	C.No.	η	S	N
Base(B)	1	3.835	0.261	54
	2	3.825	0.261	60
	3	3.826	0.261	66
	4	3.828	0.261	72
	5	3.832	0.261	78
	6	3.831	0.261	84
	7	3.654	0.274	76
	8	3.581	0.279	82
	9	3.693	0.271	88
	10	3.694	0.271	94
	11	3.694	0.271	100
	12	3.695	0.271	106
	13	3.783	0.264	76
	14	3.785	0.264	82
	15	3.784	0.264	88
	16	3.783	0.264	94
	17	3.783	0.264	100
	18	3.782	0.264	106
	19	3.784	0.264	112
	20	3.734	0.268	76
	21	3.745	0.267	82
	22	3.685	0.271	88
	23	3.745	0.267	94
	24	3.746	0.267	100
	25	3.788	0.264	76
	26	3.802	0.263	82
	27	3.801	0.263	88
	28	3.801	0.263	94
	29	3.801	0.263	100
Acid (A)	Zn-metal	6.340	0.158	2
	Zn^{2+}-ion	4.027	0.248	0
	Zn^{2+}-CA	3.768	0.265	180

Table 4. Values of interaction energy, shift in charge and lowering energy for interaction of donors with acceptors

C.No.	Zn-metal			Zn^{2+}-ion			Zn^{2+}-CA		
	E_{int}	ΔN	ΔE	E_{int}	ΔN	ΔE	E_{int}	ΔN	ΔE
1	-4.251	-0.157	-0.252	-29.923	1.312	-13.530	-53.704	0.332	-0.838
2	-5.074	-0.155	-0.245	-30.753	1.317	-13.611	-56.374	0.336	-0.856
3	-6.003	-0.155	-0.244	-31.508	1.317	-13.617	-59.149	0.336	-0.857
4	-7.026	-0.155	-0.246	-32.278	1.316	-13.596	-61.990	0.335	-0.852
5	-8.135	-0.156	-0.246	-33.139	1.315	-13.583	-64.929	0.335	-0.851
6	-9.322	-0.156	-0.246	-34.099	1.315	-13.586	-67.891	0.335	-0.851
7	-7.639	-0.171	-0.294	-32.628	1.328	-13.548	-62.346	0.325	-0.784
8	-8.654	-0.171	-0.291	-33.814	1.343	-13.721	-64.613	0.330	-0.802
9	-10.041	-0.171	-0.295	-34.386	1.321	-13.463	-68.525	0.322	-0.776
10	-11.345	-0.171	-0.295	-35.435	1.320	-13.462	-71.567	0.322	-0.776
11	-12.730	-0.171	-0.295	-36.557	1.320	-13.462	-74.662	0.322	-0.776
12	-14.204	-0.171	-0.295	-37.743	1.320	-13.459	-77.844	0.322	-0.775
13	-7.767	-0.166	-0.280	-32.444	1.310	-13.405	-63.434	0.324	-0.790
14	-8.918	-0.166	-0.278	-33.384	1.310	-13.412	-66.385	0.324	-0.793
15	-10.154	-0.166	-0.278	-34.379	1.310	-13.413	-69.382	0.324	-0.792
16	-11.474	-0.166	-0.278	-35.449	1.311	-13.416	-72.443	0.324	-0.793
17	-12.880	-0.166	-0.278	-36.586	1.311	-13.417	-75.576	0.324	-0.793
18	-14.372	-0.166	-0.278	-37.794	1.311	-13.419	-78.776	0.324	-0.793
19	-15.954	-0.166	-0.278	-39.063	1.311	-13.414	-82.064	0.324	-0.793
20	-7.724	-0.169	-0.288	-32.464	1.316	-13.435	-63.010	0.323	-0.782
21	-8.890	-0.170	-0.292	-33.292	1.312	-13.384	-66.006	0.321	-0.773
22	-9.999	-0.167	-0.281	-34.628	1.327	-13.589	-68.503	0.328	-0.804
23	-11.431	-0.170	-0.291	-35.349	1.312	-13.388	-72.048	0.321	-0.774
24	-12.831	-0.170	-0.291	-36.476	1.312	-13.386	-75.174	0.321	-0.774
25	-7.808	-0.171	-0.298	-32.151	1.302	-13.257	-63.401	0.316	-0.755
26	-8.980	-0.171	-0.298	-33.033	1.300	-13.229	-66.451	0.315	-0.753
27	-10.218	-0.171	-0.297	-34.041	1.300	-13.235	-69.457	0.316	-0.754
28	-11.544	-0.171	-0.297	-35.108	1.300	-13.235	-72.529	0.316	-0.754
29	-12.956	-0.171	-0.297	-36.244	1.300	-13.233	-75.678	0.316	-0.754

RESULTS AND DISCUSSION

A. Interaction with Zn-metal: The interaction energy between all the donor (derivatives of benzene sulfonamide) and acceptor (Zn metal) have been evaluated and included in Table-4. The higher the negative value of ΔE_{int}, higher the energy lost by the system and thus greater will be the stability of complexes formed by donor and acceptor.[7,8] Lowest value of interaction energy of interaction of benzene sulfonamide derivative C1 with acceptor has been observed and its value is -4.251 eV, which indicates formation of least stable complex of benzene sulfonamide derivatives C1 and acceptor CA. The value of interaction energy of benzene sulfonamide derivative C19 with Zn metal is highest and is equal to -15.954 eV, which indicates that benzene sulfonamide C19 forms most stable complex with Zn metal. The value of interaction energy indicates that the order of the stability of complexes formed by donors with acceptor Zn metal is in the order: C19 > C18 > C12 > C29 > C17 > C24 > C11 > C28 > C16 > C23 > C10 > C27 > C15 > C9 > C22 > C6 > C26 > C14 > C21> C8 > C5 > C25 > C13 > C20 > C7 > C4 > C3 > C2 > C1.

When donor and acceptor come close to each other, electrons will flow from that of lower χ (B) to that of higher χ (A), until the chemical potentials become equal. Stability of complex formed between the interactions of benzene sulfonamide derivative with Zn metal has also been measured in term of shift in charge (ΔN from Eq.5.2) and lowering of energy (ΔE from Eq.5.3). Higher the value of ΔN, higher the values of charge transfer from B to A and thus greater will be the stability of complex. And higher the negative value of ΔE, higher the energy lowering of the system and thus greater will be the stability of complex.[7,8] The values of ΔN are presented in Table-4. The value of charge transfer indicate that the least stable complex formation is between benzene sulfonamide derivative C7 and Zn metal (ΔN = -0.171eV). The benzene sulfonamide derivatives (C8 to C12 and C25 to C29) also have the same value of ΔN (i.e., -0.171eV). The most stable complex is formed with benzene sulfonamide derivative C2 to C4 and Zn metal (ΔN = -0.155 eV). Graph between charge transfers (ΔN) for interaction of derivatives of benzene sulfonamide with Zn metal is given in Graph-2. Order of stable complex formation is C2 = C3 = C4 > C5 = C6 > C1 > C13 = C14 = C15 = C16 = C17 = C18 = C19 > C22 > C20 > C21 = C23 = C24 > C7 = C8 = C9 = C10 = C11 = C12 = C25 = C26 = C27 = C28 = C29.

The values of ΔE are also presented in Table-4. Higher the negative value of ΔE, higher the energy lowering of the system and thus greater will be the stability of complex.[7,8] The bond strength between benzene sulfonamide derivatives C3 and Zn metal is weakest as the value of ΔE is lowest (-0.244eV). Strongest bond strength has been observed between benzene sulfonamide derivatives C25 and C26, and Zn metal in which case the value if ΔE is highest (-0.298eV). Value of energy lowering indicate the following order of complex formation of derivatives of benzene sulfonamide with Zn metal, C25 = C26 > C27 = C28 = C29 > C9 = C10 = C11 = C12 > C7 > C21 > C8 = C23 = C24 > C20 > C22 > C13 > C14 = C15 = C16 = C17 = C18 = C19 > C1 > C4 = C5 = C6 > C2 > C3.

B. Interaction with Zn^{2+}-ion: The interaction energy between all the donor (derivatives of benzene sulfonamide) and acceptor (Zn^{2+}-ion) have also been evaluated and included in Table-4. The higher the negative value of ΔE_{int}, higher the energy lost by the system and thus greater will be the stability of complexes formed by donor and acceptor.[1,2] Lowest value of interaction energy of interaction of benzene sulfonamide derivative C1 with acceptor has been observed and its value is -29.923 eV, which indicates formation of least stable complex of benzene sulfonamide derivatives C1 and acceptor Zn^{2+}-ion. The value of interaction energy of benzene sulfonamide derivative C29 with Zn^{2+}-ion is highest and is equal to -39.063 eV, which indicates that benzene sulfonamide C19 forms most stable complex with Zn^{2+}-ion. The value of interaction energy indicate that the order of the stability of complexes formed by donors with acceptor Zn^{2+}-ion is in the order: C19 > C18 > C12 > 17 > C11 > C24 > C29 > C16 > C10 > C23 > C28 > C22 > C9 > C15 > C6 > C27 > C8 > C14 > C21 > C5 > C26 > C7 > C20 > 13 > C4 > C25 > C3 > C2 > C1.

When donor and acceptor come close to each other, electrons will flow from that of lower χ (B) to that of higher χ (A), until the chemical potentials become equal. Stability of complex formed between the interactions of benzene sulfonamide derivative with Zn^{2+}-ion has also been measured in term of shift in charge (ΔN from Eq.5) and lowering of energy (ΔE from Eq.5.3). Higher the value of ΔN, higher the values of charge transfer from B to A and thus greater will be the stability of complex. The values of ΔN are presented in Table-4. The value of charge transfer indicate that the least stable complex formation is between benzene sulfonamide derivative C26 and Zn^{2+}-ion (ΔN = 1.30 eV). The benzene sulfonamide derivatives (C27 to C29) also have the same value of ΔN (i.e., 1.30 eV). The most stable complex is formed with benzene sulfonamide derivative C8 and Zn^{2+}-ion (ΔN = 1.343 eV). Order of stable complex formation is C8 > C7 > C22 > C9 > C10 = C11 = C12 > C2 = C3 > C4 = C20 > C5 = C6 > C1 = C21 = C23 = C24 > C16 = C17 = C18 = C19 > C13 = C14 = C15 > C25 > C26 = C27 = C28 = C29.

The values of ΔE are also presented in Table-4. Higher the negative value of ΔE, higher the energy lowering of the system and thus greater will be the stability of complex.[1,2] The bond strength between benzene sulfonamide derivatives C26 and Zn^{2+}-ion is weakest as the value of ΔE is lowest -13.229 eV). Strongest bond strength has been observed between benzene sulfonamide derivatives C8 and Zn^{2+}-ion in which case the value if ΔE is highest (-13.721 eV). Value of energy lowering indicate the following order of complex formation of derivatives of benzene sulfonamide with Zn^{2+}-ion, C8 > C3 > C2 > C4 > C22 > C6 > C5 > C7 > C1 > C9 > C10 = C11 > C12 > C20 > C18 > C17 > C16 > C19 > C15 > C14 > C13 > C23 > C24 > C21 > C25 > C27 = C28 = C29 > C26.

C. Interaction with Zn^{2+}-CA: The interaction energy between all the donor, derivatives of benzene sulfonamide, and acceptor, Zn^{2+}-CA, have been evaluated and included in Table-4. The higher the negative value of ΔE_{int}, higher the energy lost by the system and thus greater will be the stability of complexes formed by donor and acceptor.[7,8] Lowest value of interaction energy of interaction of benzene sulfonamide derivative C1 with acceptor has been observed and its value is -53.704 eV, which indicates formation of least stable complex of benzene sulfonamide derivatives C1 and acceptor Zn^{2+}-CA. The value of interaction energy of benzene sulfonamide derivative C19 with CA is highest and is equal to -82.064 eV, which indicates that benzene sulfonamide C19 forms most stable complex with Zn^{2+}-CA. The value of interaction energy indicates that the order of the stability of complexes formed by donors with acceptor CA is in the order: C19 > C18 > C12 > C29 > C17 > C24 > C11 > C28 > C16 > C23 > C10 > C27 > C15 > C9 > C22 > C6 > C26 > C14 > C21 > C5 > C8 > C13 > C25 > C20 > C7 > C4 > C3 > C2 > C1.

When donor and acceptor come close to each other, electrons will flow from that of lower χ (B) to that of higher χ (A), until the chemical potentials become equal. Stability of complex formed between the interactions of benzene sulfonamide derivative with Zn^{2+}-CA has also been measured in term of shift in charge (ΔN from Eq.5) and lowering of energy (ΔE from Eq.6). Higher the value of ΔN, higher the values of charge transfer from B to A and thus greater will be the stability of complex. And higher the negative value of ΔE, higher the energy lowering of the system and thus greater will be the stability of complex.[7,8] The values of ΔN are presented in Table-4. The value of charge transfer indicate that the least stable complex formation is between benzene sulfonamide derivative C26 and Zn^{2+}-CA (ΔN = 0.315 eV). The most stable complex is formed with benzene sulfonamide derivative C2 and C3, and CA (ΔN = 0.336 eV). Order of stable complex formation is C2 = C3 > C4 = C5 = C6 > C1 > C7 = C8 = C22 > C13 = C14 = C15 = C16 = C17 = C18 = C19 > C20 > C9 = C10 = C11= C12 > C21 = C23 = C24 > C25 = C27 = C28 = C29 > C26.

The values of ΔE are also presented in Table-4. Higher the negative value of ΔE, higher the energy lowering of the system and thus greater will be the stability of complex.[7,8] The bond strength between benzene sulfonamide derivatives C26 and Zn^{2+}-CA is weakest as the value of ΔE is lowest (-0.753 eV). Strongest bond strength has been observed between benzene sulfonamide derivatives C3 and Zn^{2+}-CA in which case the value if ΔE is highest (-0.857 eV). Value of energy lowering indicate the following order of complex formation of derivatives of benzene sulfonamide with Zn metal, C3 > C2 > C4 > C5 = C6 > C1 > C22 > C8 > C14 = C16 = C17 = C18 = C19 > C15 > C13 > C7 > C20 > C9 = C10 = C11 > C12 > C23 = C24 > C21 > C25 > C27 = C28 = C29 > C26.

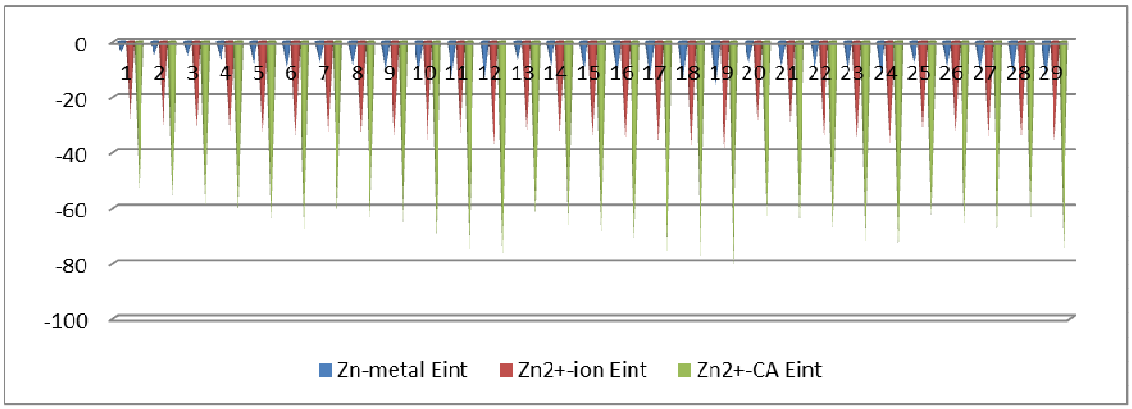


Figure 2. Graph between interaction energy (ΔE_{int}) of derivatives of benzene sulfonamide for interaction with Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA

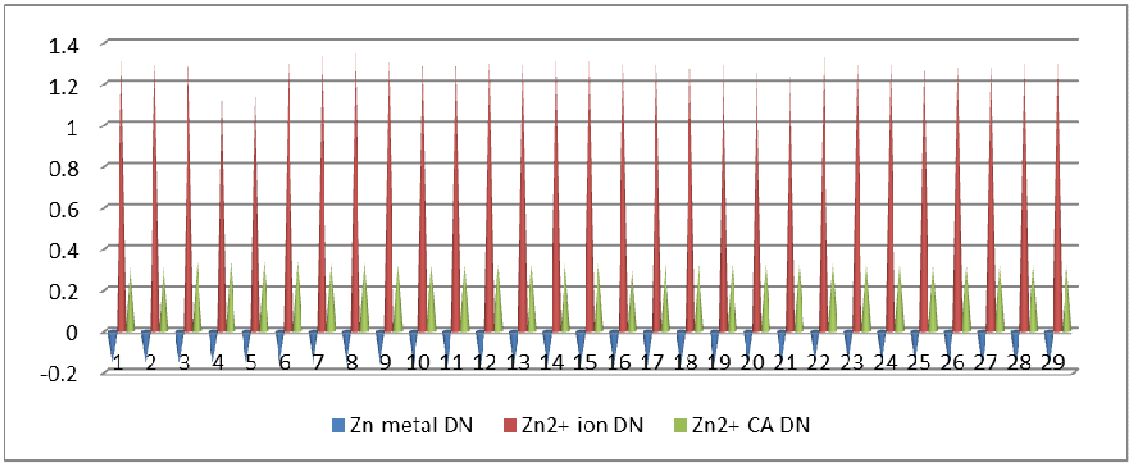


Figure 3. Graph between charge transfers (ΔN) for interaction of derivatives of benzene sulfonamide with Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA

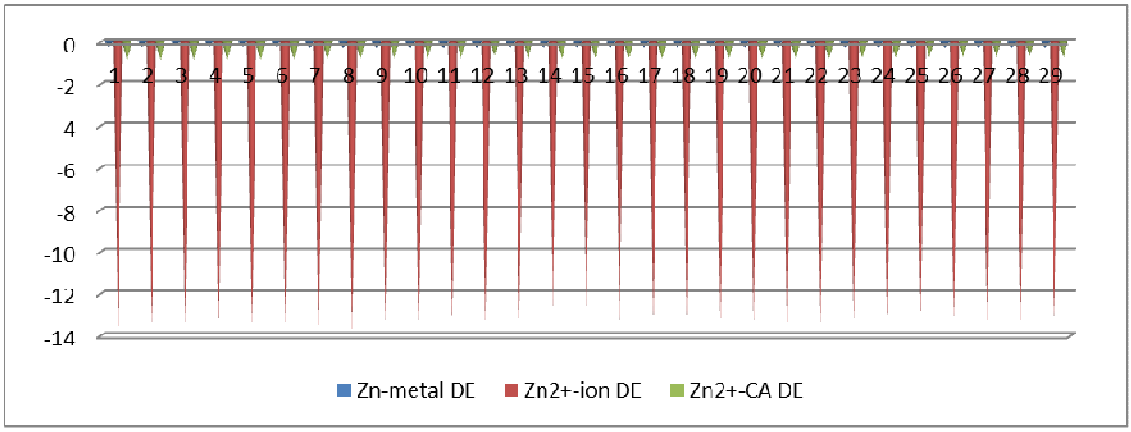


Figure 4. Graph between energy lowering (ΔE) for interaction of derivatives of benzene sulfonamide with Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA

A comparative study of these interactions shows that:

1. Interaction energy of benzene sulfonamides show that C19 (ΔE_{int} =-15.954 eV), C29 (ΔE_{int} =-39.063 eV) and C19 (ΔE_{int} =-82.064 eV) form most stable complex with Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA, respectively. Further, the interactions between sulfonamides and carbonic anhydrase are dominant over Zn-metal and Zn^{2+}-ion. It is also demonstrated by the figure-2.
2. Charge transfer show that C2 (ΔN = -0.155eV), C8 (ΔN = 1.343 eV) and C2 (ΔN = 0.336 eV) form most stable complex with Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA, respectively. Further, the interactions between sulfonamides and Zn^{2+}-ion are dominant over Zn-metal and Zn^{2+}-CA. It is also demonstrated by the figure-3.
3. Energy lowering show that C25 (ΔE = -0.298eV), C8 (ΔE = -13.721 eV) and C3 (ΔE = -0.857 eV) form most stable complex with Zn-metal, Zn^{2+}-ion and Zn^{2+}-CA, respectively. Further, the interactions between sulfonamides and Zn^{2+}-ion are dominant over Zn-metal and Zn^{2+}-CA. It is also demonstrated by the figure-4.

CONCLUSION

The higher the negative value of ΔE_{int}, higher the energy lost by the system and thus greater will be the stability of complexes formed by donor and acceptor. The value of interaction energy of benzene sulfonamide derivative C19 with Zn^{2+}-CA is highest and is equal to -82.064 eV, which indicates that benzene sulfonamide C19 forms most stable complex with Zn^{2+}-CA. Higher the value of ΔN, higher the values of charge transfer from B to A and thus greater will be the stability of complex. Study of charge transfer phenomenon indicate that the most stable complex is formed with benzene sulfonamide derivative C2 and C3, and Zn^{2+}-CA (ΔN = 0.336 eV). Higher the negative value of ΔE, higher the energy lowering of the system and thus greater will be the stability of complex. Strongest bond strength has been observed between benzene sulfonamide derivatives C3 and Zn^{2+}-CA in which case the value if ΔE is highest (-0.857 eV).

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