DFT based study of acceptor strength and stability of complexes formed by metal-ligand interaction

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ABSTRACT

Interaction energy of 190 interactions between Tin (IV) chloride and their organometallic derivatives as acceptors (A) and derivatives of pyridine, bipyridine and phenanthroline as donors (B) have been calculated. Various calculations indicate that the order of acidic strength of acceptors based on the values of chemical potential is Triethyl tin (IV) chloride < Trimethyl tin (IV) chloride < Triphenyl tin (IV) chloride < Diphenyl tin (IV) chloride < Diethyl tin (IV) chloride < Dimethyl tin (IV) chloride < Phenyl tin (IV) chloride < Ethyl tin (IV) chloride < Methyl tin (IV) chloride < Tin (IV) chloride. Interaction energy for the interaction of dimethyl tin (IV) chloride with 2-nitropyridine is lowest and is equal to -1823.15eV which indicates that the least stable complex is formed by dimethyl tin (IV) chloride with 2-nitropyridine. Most stable complex is formed by triethyl tin (IV) chloride with 2-nitropyridine and in this case the value of interaction energy is 1082.43eV. The values of charge transfer (ΔN) and lowering of energy (ΔE) also indicate almost the same sequence of the stability of complexes formed by the donors with the acceptors. © 2010 Trade Science Inc. - INDIA

INTRODUCTION

Tin (IV) halides are well known Lewis acids. Their complexes have been extensively studied[1-6]. The study has mainly been based on physicochemical and infrared spectral studies. The comparative donor strength of ligands has been based on the magnitude of shift in infrared frequency of the donor group. The application of density functional theory (DFT)[7] has given a new concept to chemical system. The concept focuses on the electron density function instead of wave function[8]. For every chemical system there is a quantity μ called the electronic chemical potential. A chemical system is an atom, molecule, ion or radical or several such unit in a state of interaction.

THEORY

This concept has been applied for theoretical determination of comparative donor strength of various derivatives of pyridine, bipyridine and phenanthroline against acceptor tin (IV) chloride and their organometallic derivatives. Recent work based on density functional theory has developed the concept of absolute electronegativity (χ) and absolute hardness (η)[9,10]. The definitions are,

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TABLE 1 : List of acceptors

S.No.	Name of acceptor (A)	Formula of Acceptor (A)
1	Tin (IV) chloride	$SnCl_4$
2	Methyl tin (IV) chloride	CH_3SnCl_3
3	Dimethyl tin (IV) chloride	$(CH_3)_2SnCl_2$
4	Trimethyl tin (IV) chloride	$(CH_3)_3SnCl$
5	Ethyl tin (IV) chloride	$C_2H_5SnCl_3$
6	Diethyl tin (IV) chloride	$(C_2H_5)_2SnCl_2$
7	Triethyl tin (IV) chloride	$(C_2H_5)_3SnCl$
8	Phenyl tin (IV) chloride	$C_6H_5SnCl_3$
9	Diphenyl tin (IV) chloride	$(C_6H_5)_2SnCl_2$
10	Triphenyl tin (IV) chloride	$(C_6H_5)_3SnCl$

$$\chi = -E / N_z = - \mu \tag{1}$$
$$\eta = \tfrac{1}{2}. E / N_z^2 \tag{2}$$

where E is the electronic energy of a molecule, atom, or ion, N is the number of electrons, and Z is a fixed set of nuclear charges. The absolute electro negativity is also equal to the electronic chemical potential with change in sign. The operational definitions are,

$$\chi = (I + A)/2 \tag{3}$$
$$\eta = (I - A)/2 \tag{4}$$

where I is the ionization potential and A is the electron affinity. The absolute electro negativity is the same as the Mulliken value.

There has been DFT based calculations of metal-ligand interaction which have provided reliable information about the magnitude of metal-ligand interaction. The present work of the paper is based upon such calculations on the complex of tin (IV) halides and their organometallic derivatives as Lewis acids and derivatives of pyridine, bipyridine and phenanthroline as Lewis bases.

DFT provided a quantitative measure for a qualitative concept that was so successfully used in a description of lewis acids and bases[13]. Parr and Pearson also derived simple expressions for the amount of charge transfer ΔN and energy change ΔE which accompany the formation of A:B complex from acid A and base B. These expressions are,

$$\Delta N = (\chi^{\circ}_A - \chi^{\circ}_B) / 2 (\eta_A + \eta_B) \tag{3}$$
$$\Delta E = - (\chi^{\circ}_A - \chi^{\circ}_B)^2 / 4(\eta_A + \eta_B) \tag{4}$$

Although equations (3) and (4) are incomplete, they have a great value in trying to predict a global change during the reaction with a minimum number of param-

eters. The shortcomings of equations (3) and (4) are known and were pointed out in original derivation. Thus the dependence of the chemical potential on the changing external field was neglected. Also, stereo selectivity of the reaction is not manifested through these expressions.

The process involving electron transfer reaction, was also described by interaction energy[14,15] (ΔE_{int}), which is described as follows:

Consider a stable molecule A formed by the bonding of K atoms with a total number of electrons N_A, and a stable molecule B formed by the binding of L atoms with a total number of electrons N_B. The interaction energy between these two chemical species, according to DFT, is given by,

$$\Delta E_{int} = E [\rho_{AB}] - [\rho_A] - [\rho_B] \tag{5}$$

It has been shown by Gazquez[13], that if the interaction energy is divided into two steps and one makes use of the properties of hardness and softness functions, then equation (5) can be written in the following form,
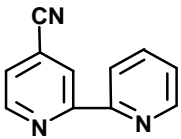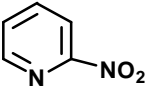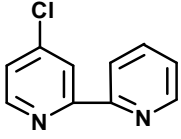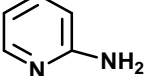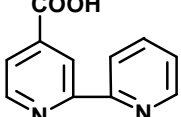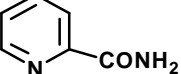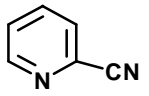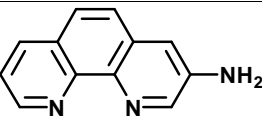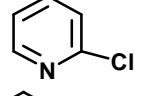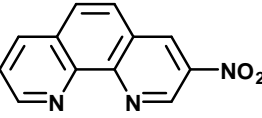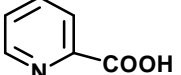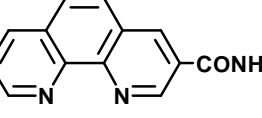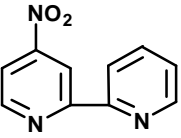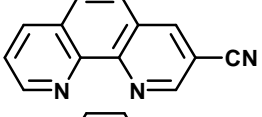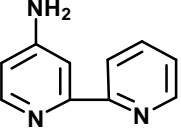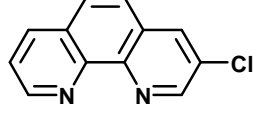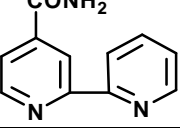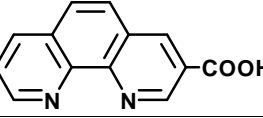
$$\Delta E_{int} = \Delta E_v + \Delta E\mu \tag{6}$$
$$\text{where, } \Delta E_v \approx - (\mu_A - \mu_B)^2 . S_A S_B /\{2(S_A + S_B)\} \tag{7}$$
$$\Delta E_\mu \tilde{} - \tfrac{1}{2} . \lambda / (S_A + S_B) \tag{8}$$

μ = Chemical potential, $S = 1 / \eta$, $\lambda = (N_A + N_B)^2 / 200$, N_A = total number of electrons in molecule A, N_B = total number of electrons in molecule B.

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. The second term, ΔE_μ corresponds to a reshuffling of the charge distribution, and it is basically a manifestation of the maximum hardness principle. In the original derivation of Gazquez[13] of equation (8), the proportionality factor was given by the product of a constant times the square of the total number of electrons ($N_A + N_B$). However, using the hardness functional, and the properties of the hardness and softness kernels, it was shown by Parr and Gazquez[16a] at the correct proportionality factor is given by the product of a constant times the square of an "effective number of valence electrons". Thus, in equation (8), we have replaced this product by another constant λ. Recently we have published a paper in which interaction energy (Eint)

TABLE 2 : List of donors

S. No.	Molecular formula of donor(B)	Name of donor(B)	Structure of donor (B)
	Derivatives of pyridine		
1	C_5H_5N	Pyridine	(pyridine)
2	$C_5H_4N_2O_2$	2-nitropyridine	(pyridine–NO_2)
3	$C_5H_6N_2$	2-aminopyridine	(pyridine–NH_2)
4	$C_6H_6N_2O$	Pyridine-2-carboxamide	(pyridine–$CONH_2$)
5	$C_6H_4N_2$	2-cyanopyridine	(pyridine–CN)
6	C_5H_4NCl	2-chloropyridine	(pyridine–Cl)
7	C_6H_5NO2	Pyridine-2-carboxylic acid	(pyridine–COOH)
	Derivatives of bipyridine		
8	$C_{10}H_7N_3O_2$	4-nitro-2,2'-bipyridine	(NO_2–bipyridine)
9	$C_{10}H_9N_3$	4-amino-2,2'-bipyridine	(NH_2–bipyridine)
10	$C_{11}H_9N_3O$	2,2'-bipyridine-4-carboxamide	($CONH_2$–bipyridine)
11	$C_{11}H_7N_3$	4-cyano-2,2'-bipyridine	(CN–bipyridine)
12	$C_{10}H_7N_2Cl$	4-chloro-2,2'-bipyridine	(Cl–bipyridine)
13	$C_{11}H_8N_2O_2$	2,2'-bipyridine-4-carboxylic acid	(COOH–bipyridine)
	Derivatives of phenanthroline		
14	$C_{12}H_9N_3$	3-amino-1,10-phenanthroline	(phenanthroline–NH_2)
15	$C_{12}H_7N_3O_2$	3-nitro-1,10-phenanthroline	(phenanthroline–NO_2)
16	$C_{13}H_9N_3O$	1,10-phenanthroline-3-carboxamide	(phenanthroline–$CONH_2$)
17	$C_{13}H_7N_3$	3-cyano-1,10-phenanthroline	(phenanthroline–CN)
18	$C_{12}H_7N_2Cl$	3-chloro-1,10-phenanthroline	(phenanthroline–Cl)
19	$C_{13}H_8N_2O_2$	1,10-phenanthroline-3-carboxylic acid	(phenanthroline–COOH)
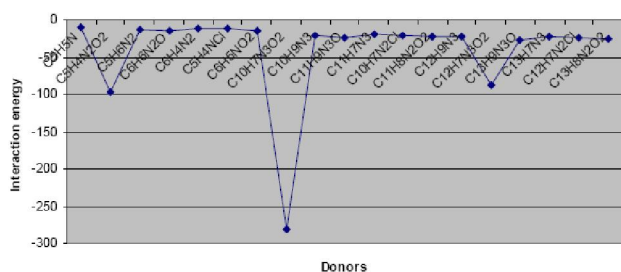
Graph 1 : Interaction energy of organic bases with tin (IV) chloride

Graph 2 : Interaction energy of organic bases with methyl tin (IV) chloride

for 324 interactions between 12 metal halides (A), and 27 organic bases (B) have been evaluated with the help of Cache software using DFT-B88-PW91 method[16b]. Interaction energy (E_{int}), charge transfer (ΔN) and

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lowering of energy (ΔE) for 72 interactions between 12 metal halides (A) and 6 sulphur donors (B) have also been evaluated by us with the help of Cache software using DFT B88-LYP method[16c].

MATERIALS AND METHOD

The DFT based study of metal-ligand interaction is mainly based on the following quantum chemical descriptors:

1. Electronegativity (χ)
2. Ionization potential (I)
3. Absolute hardness (η)
4. Chemical potential (μ)
5. Global softness (S)
6. Electron affinity (A)

The above parameters have been evaluated for acceptor (A) and donor (B) molecules, and the magnitude of interaction will be evaluated by solving the following equations. The input of the equation will be the values of quantum chemical descriptors described above.

$$\Delta N = (\chi^{\circ}_A - \chi^{\circ}_B) / 2\,(\eta_A + \eta_B)$$
$$\Delta E = - (\chi^{\circ}_A - \chi^{\circ}_B)^2 / 4(\eta_A + \eta_B)$$
$$\Delta E_{int} = \Delta E_v + \Delta E_\mu$$

The values of descriptors have been evaluated with the help of computational chemistry by using the Cache software. The compounds chosen for study as acceptor (A) are listed in TABLE 1 and donor (B) are listed in TABLE 2.

The 3D modeling and geometry optimization[17-19] of all the compounds listed in TABLE 1 and 2 have

been first done by Cache software using DFT B88-VWN method. The values of various quantum chemical parameters such as χI, A, ηS, ϵHOMO, ϵHOMO and Lambda (λ) have also been evaluated with the same software using same method.

RESULT AND DISCUSSION

Comparison of accepter strength of tin (IV) chloride and its derivatives

The lower is the value of chemical potential (μ_A) better will be the acceptor property. Thus the acceptor having lowest value of chemical potential possesses highest acidic strength. The values of chemical potential, absolute hardness, global softness, ionization potential and electron affinity of tin (IV) chloride and its derivatives are shown in TABLE 3. The value of chemical potential of triethyl tin (IV) chloride is highest and is equal to -3.478eV which indicates that the acidic strength of triethyl tin (IV) chloride is lowest among all the chloride derivatives of tin. The value of chemical potential of tin (IV) chloride is lowest and is equal to -6.296eV which indicates that the acidic strength of tin (IV) chloride is highest among all the chloride derivatives of tin. Order of acidic strength based on the values of chemical potential can be arranged as given below;

Triethyl tin (IV) chloride < Trimethyl tin (IV) chloride < Triphenyl tin (IV) chloride < Diphenyl tin (IV) chloride < Diethyl tin (IV) chloride < Dimethyl tin (IV) chloride < Phenyl tin (IV) chloride < Ethyl tin (IV) chloride < Methyl tin (IV) chloride < Tin (IV) chloride.

The lower is the value of absolute hardness (η_A) better will be the acceptor property. Thus the acceptor having lowest value of absolute hardness possesses highest acidic strength. The value of absolute hardness of triethyl tin (IV) chloride is highest and is equal to 2.735eV which indicates that the acidic strength of tri-

TABLE 3 : Values of chemical potential, absolute hardness, global softness, ionization potential and electron affinity of tin (IV) chloride and its derivatives

Acceptor	Chemical potential (μ_A)	Absolute hardness (η_A)	Global softness (S_A)	Ionization potential (I_A)	Electron affinity (A_A)
Tin (IV) chloride	-6.296	1.791	0.279	8.086	4.505
Methyl tin (IV) chloride	-5.411	2.113	0.237	7.524	3.298
Dimethyl tin (IV) chloride	-4.469	2.404	0.208	6.873	2.065
Trimethyl tin (IV) chloride	-3.669	2.735	0.183	6.403	0.934
Ethyl tin (IV) chloride	-5.323	2.061	0.243	7.384	3.262
Diethyl tin (IV) chloride	-4.286	2.261	0.221	6.546	2.025
Triethyl tin (IV) chloride	-3.478	2.571	0.195	6.048	0.907
Phenyl tin (IV) chloride	-5.011	1.751	0.286	6.762	3.260
Diphenyl tin (IV) chloride	-4.281	2.153	0.232	6.434	2.128
Triphenyl tin (IV) chloride	-3.987	2.094	0.239	6.080	1.893

Graph 3 : Interaction energy of organic bases with dimethyl tin (IV) chloride

ethyl tin (IV) chloride is lowest among all the chloride derivatives of tin. The value of absolute hardness of tin (IV) chloride is lowest and is equal to 1.791eV which indicates that the acidic strength of tin (IV) chloride is highest among all the chloride derivatives of tin. Order of acidic strength based on the values of absolute hardness can be arranged as given below;
Triethyl tin (IV) chloride < Trimethyl tin (IV) chloride < Triphenyl tin (IV) chloride < Diphenyl tin (IV) chloride < Diethyl tin (IV) chloride < Dimethyl tin (IV) chloride < Phenyl tin (IV) chloride < Ethyl tin (IV) chloride < Methyl tin (IV) chloride < Tin (IV) chloride.

Order of acidic strength of tin (IV) chloride and its derivatives shown by the values of chemical potential and absolute hardness is same.

Acidic strength of acceptors depends on the value of ionization potential (I_A). As the value of ionization potential increases, the acidic strength increases. Thus the acceptor having highest value of ionization potential possesses highest acidic strength. The value of ionization potential of triethyl tin (IV) chloride is lowest and is equal to 6.048eV which indicates that the acidic strength of triethyl tin (IV) chloride is lowest among all the chloride derivatives of tin. The value of ionization potential of tin (IV) chloride is highest and is equal to 8.086eV which indicates that the acidic strength of tin (IV) chloride is highest among all the chloride derivatives of tin. Order of acidic strength based on the values of ionization potential can be arranged as given below;
Triethyl tin (IV) chloride < Triphenyl tin (IV) chloride < Trimethyl tin (IV) chloride < Diphenyl tin (IV) chloride < Diethyl tin (IV) chloride < Phenyl tin (IV) chloride < Dimethyl tin (IV) chloride < Ethyl tin (IV) chloride < Methyl tin (IV) chloride < Tin (IV) chloride.

Acidic strength of acceptors depends on the value of electron affinity (A_A). As the value of electron affinity increases, the acidic strength increases. Thus the acceptor having highest value of electron affinity possesses highest acidic strength. The value of electron affinity of triethyl tin (IV) chloride is lowest and is equal to 0.907eV which indicates that the acidic strength of triethyl tin (IV) chloride is lowest among all the chloride derivatives of tin. The value of electron affinity of tin (IV) chloride is highest and is equal to 4.505eV which indicates that the acidic strength of tin (IV) chloride is highest among all the chloride derivatives of tin. Order

of acidic strength based on the values of electron affinity can be arranged as given below;
Triethyl tin (IV) chloride < Trimethyl tin (IV) chloride < Triphenyl tin (IV) chloride < Diethyl tin (IV) chloride < Dimethyl tin (IV) chloride < Diphenyl tin (IV) chloride < Phenyl tin (IV) chloride < Ethyl tin (IV) chloride < Methyl tin (IV) chloride < Tin (IV) chloride.

Above discussion indicates that the acceptor triethyl tin (IV) chloride have the lowest acidic strength and tin (IV) chloride has highest acidic strength among all the derivatives of tin (IV) chloride. Exact order of acidic strength of the derivatives of tin (IV) chloride based on the values of chemical potential is given below;
Triethyl tin (IV) chloride < Trimethyl tin (IV) chloride < Triphenyl tin (IV) chloride < Diphenyl tin (IV) chloride < Diethyl tin (IV) chloride < Dimethyl tin (IV) chloride < Phenyl tin (IV) chloride < Ethyl tin (IV) chloride < Methyl tin (IV) chloride < Tin (IV) chloride.

Interaction of donors with acceptor metal halide SnCl₄

The donors are divided in three sets. The first set of donors are pyridine derivatives, the second set and third set are derivatives of bipyridine and phenanthroline respectively. They are included in TABLE 2 under three sets.

The interaction energy between all the three sets of donors (B) and acceptor (A) have been evaluated and included in the TABLE 4-13. With the decrease of interaction energy the stability of complexes formed by organic bases and acceptors decrease. Interaction energy of donors (B) with acceptor metal halide $SnCl_4$ (A) is shown in TABLE 4. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

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TABLE 4 : Interaction of donors (B) with the acceptor tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_ν	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-6.296	0.559	-3.734	0.482	32	30	19.220	-0.849	-9.234	-10.083
2-nitropyridine	-6.296	0.559	-8.568	-0.408	32	46	30.420	3.922	-101.339	-97.417
2-aminopyridine	-6.296	0.559	-3.041	0.549	32	36	23.120	-1.466	-10.439	-11.905
pyridine-2-carboxamide	-6.296	0.559	-3.929	0.606	32	46	30.420	-0.814	-13.059	-13.873
2-cyanopyridine	-6.296	0.559	-4.725	0.518	32	38	24.500	-0.331	-11.381	-11.712
2-chloropyridine	-6.296	0.559	-4.173	0.462	32	36	23.120	-0.570	-11.325	-11.895
pyridine-2-carboxylic acid	-6.296	0.559	-4.384	0.568	32	46	30.420	-0.514	-13.504	-14.018
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-6.296	0.559	-30.352	-1.082	32	74	56.180	-334.117	53.693	-280.425
4-amino-2,2'-bipyridine	-6.296	0.559	-3.531	0.632	32	64	46.080	-1.133	-19.361	-20.494
2,2'-bipyridine-4-carboxamide	-6.296	0.559	-4.053	0.694	32	74	56.180	-0.779	-22.423	-23.202
4-cyano-2,2'-bipyridine	-6.296	0.559	-4.424	0.711	32	66	48.020	-0.548	-18.913	-19.461
4-chloro-2,2'-bipyridine	-6.296	0.559	-4.026	0.642	32	64	46.080	-0.770	-19.191	-19.961
2,2'-bipyridine-4-carboxylic acid	-6.296	0.559	-4.233	0.743	32	74	56.180	-0.678	-21.588	-22.267
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-6.296	0.559	-3.575	0.678	32	72	54.080	-1.133	-21.873	-23.006
3-nitro-1,10-phenanthroline	-6.296	0.559	-22.641	-1.299	32	82	64.980	-130.904	43.894	-87.010
1,10-phenanthroline-3-carboxamide	-6.296	0.559	-4.088	0.709	32	82	64.980	-0.762	-25.624	-26.385
3-cyano-1,10-phenanthroline	-6.296	0.559	-4.456	0.695	32	74	56.180	-0.524	-22.402	-22.926
3-chloro-1,10-phenanthroline	-6.296	0.559	-4.080	0.637	32	72	54.080	-0.731	-22.611	-23.342
1,10-phenanthroline-3-carboxylic acid	-6.296	0.559	-4.260	0.724	32	82	64.980	-0.653	-25.341	-25.994

μ_A = Chemical potential of molecule A, μ_B = Chemical potential of molecule B, S_A = Global Softness of molecule A, S_B = Global Softness of molecule B, N_A = total number of electrons in molecule A, N_B = total number of electrons in molecule B, $\lambda = (N_A + N_B)^2 / 200$, E_μ, = Energy corresponds to a reshuffling of the charge distribution, E_ν = Energy corresponds to the charge transfer process, E_{int} = Interaction energy

2-nitropyridine < pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-aminopyridine < 2-chloropyridine < 2-cyanopyridine < pyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.

3-nitro-1,10-phenanthroline < 1,10-phenanthroline-3-carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-amino-1,10-phenanthroline < 3-cyano-1,10-phenanthroline.

It is evident that the nitro derivatives of pyridine, bipyridine and phenanthroline form least stable complexes with the tin (IV) chloride. Graph between interaction energy of donors with the acceptor $SnCl_4$ is shown in graph 1.

Interaction of donors with the acceptor methyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal halide $SnCl_4$ (A) is shown in TABLE 5. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

2-nitropyridine < pyridine-2-carboxylic acid < pyridine-

TABLE 5 : Interaction of donors (B) with the acceptor methyl tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_v	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-5.411	0.473	-3.734	0.482	30	32	19.220	-0.336	-10.058	-10.394
2-nitropyridine	-5.411	0.473	-8.568	-0.408	46	32	30.420	14.849	-234.550	-219.702
2-aminopyridine	-5.411	0.473	-3.041	0.549	36	32	23.120	-0.714	-11.310	-12.024
pyridine-2-carboxamide	-5.411	0.473	-3.929	0.606	46	32	30.420	-0.292	-14.090	-14.382
2-cyanopyridine	-5.411	0.473	-4.725	0.518	38	32	24.500	-0.058	-12.360	-12.418
2-chloropyridine	-5.411	0.473	-4.173	0.462	36	32	23.120	-0.179	-12.357	-12.537
pyridine-2-carboxylic acid	-5.411	0.473	-4.384	0.568	46	32	30.420	-0.136	-14.609	-14.745
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-5.411	0.473	-30.352	-1.082	74	32	56.180	-261.686	46.170	-215.516
4-amino-2,2'-bipyridine	-5.411	0.473	-3.531	0.632	64	32	46.080	-0.478	-20.855	-21.333
2,2'-bipyridine-4-carboxamide	-5.411	0.473	-4.053	0.694	74	32	56.180	-0.260	-24.061	-24.320
4-cyano-2,2'-bipyridine	-5.411	0.473	-4.424	0.711	66	32	48.020	-0.139	-20.275	-20.413
4-chloro-2,2'-bipyridine	-5.411	0.473	-4.026	0.642	64	32	46.080	-0.261	-20.658	-20.919
2,2'-bipyridine-4-carboxylic acid	-5.411	0.473	-4.233	0.743	74	32	56.180	-0.201	-23.102	-23.302
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-5.411	0.473	-3.575	0.678	72	32	54.080	-0.470	-23.493	-23.963
3-nitro-1,10-phenanthroline	-5.411	0.473	-22.641	-1.299	82	32	64.980	-110.526	39.361	-71.165
1,10-phenanthroline-3-carboxamide	-5.411	0.473	-4.088	0.709	82	32	64.980	-0.249	-27.470	-27.719
3-cyano-1,10-phenanthroline	-5.411	0.473	-4.456	0.695	74	32	56.180	-0.128	-24.036	-24.164
3-chloro-1,10-phenanthroline	-5.411	0.473	-4.080	0.637	72	32	54.080	-0.241	-24.347	-24.588
1,10-phenanthroline-3-carboxylic acid	-5.411	0.473	-4.260	0.724	82	32	64.980	-0.190	-27.146	-27.336

μ_A = Chemical potential of molecule A, μ_B = Chemical potential of molecule B, S_A = Global Softness of molecule A, S_B = Global Softness of molecule B, N_A = total number of electrons in molecule A, N_B = total number of electrons in molecule B, $\lambda = (N_A + N_B)^2$ / 200, E_μ, = Energy corresponds to a reshuffling of the charge distribution, E_v = Energy corresponds to the charge transfer process, E_{int} = Interaction energy

2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.

3-nitro-1,10-phenanthroline < 1,10-phenanthroline-3-carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline.

It is evident that the nitro derivatives of pyridine, bipyridine and phenanthroline form least stable complexes with the methyl tin (IV) chloride. Line graph between interaction energy of donors with the acceptor $SnCl_4$ is shown in graph 2.

Interaction of donors with acceptor dimethyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal halide $SnCl_4$ (A) is shown in TABLE 6. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

2-nitropyridine < pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-

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TABLE 6 : Interaction of donors (B) with the acceptor dimethyl tin (IV) chloride (A)

</div>

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_v	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-4.469	0.416	-3.734	0.482	30	32	19.220	-0.060	-10.700	-10.760
2-nitropyridine	-4.469	0.416	-8.568	-0.408	46	32	30.420	188.738	-2011.888	-1823.150
2-aminopyridine	-4.469	0.416	-3.041	0.549	36	32	23.120	-0.241	-11.981	-12.223
pyridine-2-carboxamide	-4.469	0.416	-3.929	0.606	46	32	30.420	-0.036	-14.879	-14.915
2-cyanopyridine	-4.469	0.416	-4.725	0.518	38	32	24.500	-0.008	-13.118	-13.125
2-chloropyridine	-4.469	0.416	-4.173	0.462	36	32	23.120	-0.010	-13.163	-13.173
pyridine-2-carboxylic acid	-4.469	0.416	-4.384	0.568	46	32	30.420	-0.001	-15.460	-15.461
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-4.469	0.416	-30.352	-1.082	74	32	56.180	-226.395	42.197	-184.199
4-amino-2,2'-bipyridine	-4.469	0.416	-3.531	0.632	64	32	46.080	-0.110	-21.996	-22.106
2,2'-bipyridine-4-carboxamide	-4.469	0.416	-4.053	0.694	74	32	56.180	-0.023	-25.302	-25.325
4-cyano-2,2'-bipyridine	-4.469	0.416	-4.424	0.711	66	32	48.020	0.000	-21.305	-21.305
4-chloro-2,2'-bipyridine	-4.469	0.416	-4.026	0.642	64	32	46.080	-0.025	-21.776	-21.801
2,2'-bipyridine-4-carboxylic acid	-4.469	0.416	-4.233	0.743	74	32	56.180	-0.007	-24.244	-24.251
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-4.469	0.416	-3.575	0.678	72	32	54.080	-0.103	-24.723	-24.826
3-nitro-1,10-phenanthroline	-4.469	0.416	-22.641	-1.299	82	32	64.980	-101.047	36.806	-64.241
1,10-phenanthroline-3-carboxamide	-4.469	0.416	-4.088	0.709	82	32	64.980	-0.019	-28.869	-28.888
3-cyano-1,10-phenanthroline	-4.469	0.416	-4.456	0.695	74	32	56.180	0.000	-25.275	-25.275
3-chloro-1,10-phenanthroline	-4.469	0.416	-4.080	0.637	72	32	54.080	-0.019	-25.671	-25.690
1,10-phenanthroline-3-carboxylic acid	-4.469	0.416	-4.260	0.724	82	32	64.980	-0.006	-28.511	-28.517

μ_A = **Chemical potential of molecule A**, μ_B = **Chemical potential of molecule B**, S_A = **Global Softness of molecule A**, S_B = **Global Softness of molecule B**, N_A = **total number of electrons in molecule A**, N_B = **total number of electrons in molecule B**, $\lambda = (N_A + N_B)^2 / 200$, E_μ, = **Energy corresponds to a reshuffling of the charge distribution**, E_v = **Energy corresponds to the charge transfer process**, E_{int} = **Interaction energy**

amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.
3-nitro-1,10-phenanthroline < 1,10-phenanthroline-3-carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline.

It is evident that the nitro derivatives of pyridine, bipyridine and phenanthroline form least stable complexes with the dimethyl tin (IV) chloride. Line graph between interaction energy of donors with the acceptor SnCl$_4$ is shown in graph 3.

Interaction of donors with acceptor trimethyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal halide SnCl$_4$ (A) is shown in TABLE 7. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor SnCl$_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor SnCl$_4$.

The value of interaction energy of organic base pyridine with metal halide SnCl$_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with SnCl$_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with SnCl$_4$ is in the following order;
pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine < 2-nitropyridine.
4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.
3-nitro-1,10-phenanthroline < 1,10-phenanthroline-3-

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TABLE 7 : Interaction of donors (B) with the acceptor trimethyl tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_v	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-3.669	0.366	-3.734	0.482	30	32	19.220	0.000	-11.334	-11.335
2-nitropyridine	-3.669	0.366	-8.568	-0.408	46	32	30.420	-41.958	356.075	314.116
2-aminopyridine	-3.669	0.366	-3.041	0.549	36	32	23.120	-0.043	-12.640	-12.683
pyridine-2-carboxamide	-3.669	0.366	-3.929	0.606	46	32	30.420	-0.008	-15.649	-15.657
2-cyanopyridine	-3.669	0.366	-4.725	0.518	38	32	24.500	-0.120	-13.864	-13.984
2-chloropyridine	-3.669	0.366	-4.173	0.462	36	32	23.120	-0.026	-13.963	-13.989
pyridine-2-carboxylic acid	-3.669	0.366	-4.384	0.568	46	32	30.420	-0.057	-16.293	-16.349
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-3.669	0.366	-30.352	-1.082	74	32	56.180	-196.680	39.234	-157.447
4-amino-2,2'-bipyridine	-3.669	0.366	-3.531	0.632	64	32	46.080	-0.002	-23.104	-23.107
2,2'-bipyridine-4-carboxamide	-3.669	0.366	-4.053	0.694	74	32	56.180	-0.018	-26.502	-26.520
4-cyano-2,2'-bipyridine	-3.669	0.366	-4.424	0.711	66	32	48.020	-0.069	-22.300	-22.369
4-chloro-2,2'-bipyridine	-3.669	0.366	-4.026	0.642	64	32	46.080	-0.015	-22.863	-22.878
2,2'-bipyridine-4-carboxylic acid	-3.669	0.366	-4.233	0.743	74	32	56.180	-0.039	-25.344	-25.383
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-3.669	0.366	-3.575	0.678	72	32	54.080	-0.001	-25.914	-25.915
3-nitro-1,10-phenanthroline	-3.669	0.366	-22.641	-1.299	82	32	64.980	-91.615	34.823	-56.792
1,10-phenanthroline-3-carboxamide	-3.669	0.366	-4.088	0.709	82	32	64.980	-0.021	-30.219	-30.240
3-cyano-1,10-phenanthroline	-3.669	0.366	-4.456	0.695	74	32	56.180	-0.074	-26.472	-26.547
3-chloro-1,10-phenanthroline	-3.669	0.366	-4.080	0.637	72	32	54.080	-0.020	-26.958	-26.978
1,10-phenanthroline-3-carboxylic acid	-3.669	0.366	-4.260	0.724	82	32	64.980	-0.042	-29.827	-29.869

μ_A = Chemical potential of molecule A, μ_B = Chemical potential of molecule B, S_A = Global Softness of molecule A, S_B = Global Softness of molecule B, N_A = total number of electrons in molecule A, N_B = total number of electrons in molecule B, $\lambda = (N_A + N_B)^2 / 200$, E_μ = Energy corresponds to a reshuffling of the charge distribution, E_v = Energy corresponds to the charge transfer process, E_{int} = Interaction energy

carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline.

It is evident that the nitro derivatives of bipyridine and phenanthroline form least stable complexes with the trimethyl tin (IV) chloride; but carboxylic derivative of pyridine forms most stable complex. Line graph between interaction energy of donors with the acceptor $SnCl_4$ is shown in graph 4.

Interaction of donors with acceptor ethyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal halide $SnCl_4$ (A) is shown in TABLE 8. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates

formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

2-nitropyridine < pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.

3-nitro-1,10-phenanthroline < 1,10-phenanthroline-3-

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TABLE 8 : Interaction of donors (B) with the acceptor ethyl tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_v	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-5.323	0.485	-3.734	0.482	30	38	23.120	-0.305	-11.950	-12.255
2-nitropyridine	-5.323	0.485	-8.568	-0.408	46	38	35.280	13.583	-229.723	-216.140
2-aminopyridine	-5.323	0.485	-3.041	0.549	36	38	27.380	-0.671	-13.239	-13.910
pyridine-2-carboxamide	-5.323	0.485	-3.929	0.606	46	38	35.280	-0.262	-16.162	-16.424
2-cyanopyridine	-5.323	0.485	-4.725	0.518	38	38	28.880	-0.045	-14.396	-14.441
2-chloropyridine	-5.323	0.485	-4.173	0.462	36	38	27.380	-0.157	-14.450	-14.607
pyridine-2-carboxylic acid	-5.323	0.485	-4.384	0.568	46	38	35.280	-0.115	-16.751	-16.867
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-5.323	0.485	-30.352	-1.082	74	38	62.720	-275.594	52.576	-223.018
4-amino-2,2'-bipyridine	-5.323	0.485	-3.531	0.632	64	38	52.020	-0.441	-23.292	-23.732
2,2'-bipyridine-4-carboxamide	-5.323	0.485	-4.053	0.694	74	38	62.720	-0.230	-26.590	-26.820
4-cyano-2,2'-bipyridine	-5.323	0.485	-4.424	0.711	66	38	54.080	-0.117	-22.605	-22.722
4-chloro-2,2'-bipyridine	-5.323	0.485	-4.026	0.642	64	38	52.020	-0.233	-23.074	-23.306
2,2'-bipyridine-4-carboxylic acid	-5.323	0.485	-4.233	0.743	74	38	62.720	-0.174	-25.540	-25.715
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-5.323	0.485	-3.575	0.678	72	38	60.500	-0.432	-26.012	-26.444
3-nitro-1,10-phenanthroline	-5.323	0.485	-22.641	-1.299	82	38	72.000	-116.155	44.253	-71.902
1,10-phenanthroline-3-carboxamide	-5.323	0.485	-4.088	0.709	82	38	72.000	-0.220	-30.134	-30.354
3-cyano-1,10-phenanthroline	-5.323	0.485	-4.456	0.695	74	38	62.720	-0.107	-26.563	-26.670
3-chloro-1,10-phenanthroline	-5.323	0.485	-4.080	0.637	72	38	60.500	-0.213	-26.948	-27.160
1,10-phenanthroline-3-carboxylic acid	-5.323	0.485	-4.260	0.724	82	38	72.000	-0.164	-29.782	-29.946

μ_A = **Chemical potential of molecule A,** μ_B = **Chemical potential of molecule B,** S_A = **Global Softness of molecule A,** S_B = **Global Softness of molecule B,** N_A = **total number of electrons in molecule A,** N_B = **total number of electrons in molecule B,** $\lambda = (N_A + N_B)^2 / 200$, E_μ = **Energy corresponds to a reshuffling of the charge distribution,** E_v = **Energy corresponds to the charge transfer process,** E_{int} = **Interaction energy**

carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline.

It is evident that the nitro derivatives of pyridine, bipyridine and phenanthroline form least stable complexes with the ethyl tin (IV) chloride.

Interaction of donors with acceptor diethyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal halide $SnCl_4$ (A) is shown in TABLE 9. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

2-nitropyridine < pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.

3-nitro-1,10-phenanthroline < 1,10-phenanthroline-3-carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline.

TABLE 9 : Interaction of donors (B) with the acceptor diethyl tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_v	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-3.734	0.482	-4.286	0.442	30	44	27.380	-0.035	-14.807	-14.842
2-nitropyridine	-8.568	-0.408	-4.286	0.442	46	44	40.500	48.765	-596.172	-547.408
2-aminopyridine	-3.041	0.549	-4.286	0.442	36	44	32.000	-0.190	-16.142	-16.331
pyridine-2-carboxamide	-3.929	0.606	-4.286	0.442	46	44	40.500	-0.016	-19.311	-19.327
2-cyanopyridine	-4.725	0.518	-4.286	0.442	38	44	33.620	-0.023	-17.506	-17.529
2-chloropyridine	-4.173	0.462	-4.286	0.442	36	44	32.000	-0.001	-17.687	-17.689
pyridine-2-carboxylic acid	-4.384	0.568	-4.286	0.442	46	44	40.500	-0.001	-20.045	-20.046
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-30.352	-1.082	-4.286	0.442	74	44	69.620	-254.280	54.451	-199.829
4-amino-2,2'-bipyridine	-3.531	0.632	-4.286	0.442	64	44	58.320	-0.074	-27.154	-27.228
2,2'-bipyridine-4-carboxamide	-4.053	0.694	-4.286	0.442	74	44	69.620	-0.007	-30.627	-30.634
4-cyano-2,2'-bipyridine	-4.424	0.711	-4.286	0.442	66	44	60.500	-0.003	-26.228	-26.230
4-chloro-2,2'-bipyridine	-4.026	0.642	-4.286	0.442	64	44	58.320	-0.009	-26.890	-26.898
2,2'-bipyridine-4-carboxylic acid	-4.233	0.743	-4.286	0.442	74	44	69.620	0.000	-29.374	-29.375
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-3.575	0.678	-4.286	0.442	72	44	67.280	-0.068	-30.033	-30.100
3-nitro-1,10-phenanthroline	-22.641	-1.299	-4.286	0.442	82	44	79.380	-113.024	46.349	-66.675
1,10-phenanthroline-3-carboxamide	-4.088	0.709	-4.286	0.442	82	44	79.380	-0.005	-34.458	-34.463
3-cyano-1,10-phenanthroline	-4.456	0.695	-4.286	0.442	74	44	69.620	-0.004	-30.594	-30.598
3-chloro-1,10-phenanthroline	-4.080	0.637	-4.286	0.442	72	44	67.280	-0.006	-31.156	-31.161
1,10-phenanthroline-3-carboxylic acid	-4.260	0.724	-4.286	0.442	82	44	79.380	0.000	-34.040	-34.040

μ_A = **Chemical potential of molecule A,** μ_B = **Chemical potential of molecule B,** S_A = **Global Softness of molecule A,** S_B = **Global Softness of molecule B,** N_A = **total number of electrons in molecule A,** N_B = **total number of electrons in molecule B,** $\lambda = (N_A + N_B)^2 / 200$, E_μ = **Energy corresponds to a reshuffling of the charge distribution,** E_v = **Energy corresponds to the charge transfer process,** E_{int} = **Interaction energy**

It is evident that the nitro derivatives of pyridine, bipyridine and phenanthroline form least stable complexes with the diethyl tin (IV) chloride.

Interaction of donors with acceptor triethyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal halide $SnCl_4$ (A) is shown in TABLE 10. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values

of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine < 2-nitropyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.

3-nitro-1,10-phenanthroline < 1,10-phenanthroline-3-carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline.

It is evident that the nitro derivatives of bipyridine and phenanthroline form most stable complexes with the triethyl tin (IV) chloride. In the case of pyridine de-

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TABLE 10 : Interaction of donors (B) with the acceptor triethyl tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_v	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-3.478	0.389	-3.734	0.482	30	50	32.000	-0.007	-18.366	-18.373
2-nitropyridine	-3.478	0.389	-8.568	-0.408	46	50	46.080	-106.181	1188.613	1082.432
2-aminopyridine	-3.478	0.389	-3.041	0.549	36	50	36.980	-0.022	-19.715	-19.736
pyridine-2-carboxamide	-3.478	0.389	-3.929	0.606	46	50	46.080	-0.024	-23.149	-23.174
2-cyanopyridine	-3.478	0.389	-4.725	0.518	38	50	38.720	-0.173	-21.348	-21.520
2-chloropyridine	-3.478	0.389	-4.173	0.462	36	50	36.980	-0.051	-21.721	-21.772
pyridine-2-carboxylic acid	-3.478	0.389	-4.384	0.568	46	50	46.080	-0.095	-24.078	-24.173
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-3.478	0.389	-30.352	-1.082	74	50	76.880	-219.384	55.498	-163.886
4-amino-2,2'-bipyridine	-3.478	0.389	-3.531	0.632	64	50	64.980	0.000	-31.836	-31.836
2,2'-bipyridine-4-carboxamide	-3.478	0.389	-4.053	0.694	74	50	76.880	-0.041	-35.486	-35.528
4-cyano-2,2'-bipyridine	-3.478	0.389	-4.424	0.711	66	50	67.280	-0.113	-30.581	-30.694
4-chloro-2,2'-bipyridine	-3.478	0.389	-4.026	0.642	64	50	64.980	-0.036	-31.511	-31.547
2,2'-bipyridine-4-carboxylic acid	-3.478	0.389	-4.233	0.743	74	50	76.880	-0.073	-33.967	-34.039
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-3.478	0.389	-3.575	0.678	72	50	74.420	-0.001	-34.881	-34.882
3-nitro-1,10-phenanthroline	-3.478	0.389	-22.641	-1.299	82	50	87.120	-101.983	47.885	-54.097
1,10-phenanthroline-3-carboxamide	-3.478	0.389	-4.088	0.709	82	50	87.120	-0.047	-39.654	-39.701
3-cyano-1,10-phenanthroline	-3.478	0.389	-4.456	0.695	74	50	76.880	-0.119	-35.447	-35.566
3-chloro-1,10-phenanthroline	-3.478	0.389	-4.080	0.637	72	50	74.420	-0.044	-36.254	-36.298
1,10-phenanthroline-3-carboxylic acid	-3.478	0.389	-4.260	0.724	82	50	87.120	-0.077	-39.151	-39.228

μ_A = **Chemical potential of molecule A**, μ_B = **Chemical potential of molecule B**, S_A = **Global Softness of molecule A**, S_B = **Global Softness of molecule B**, N_A = **total number of electrons in molecule A**, N_B = **total number of electrons in molecule B**, $\lambda = (N_A + N_B)^2 / 200$, E_μ = **Energy corresponds to a reshuffling of the charge distribution**, E_v = **Energy corresponds to the charge transfer process,** E_{int} = **Interaction energy**

rivatives, the least stable complex is formed with the donor pyridine-2-carboxylic acid.

Interaction of donors with acceptor phenyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal halide $SnCl_4$ (A) is shown in TABLE 11. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

2-nitropyridine < pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.

3-nitro-1,10-phenanthroline < 1,10-phenanthroline-3-carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline.

It is evident that the nitro derivatives of pyridine, bipyridine and phenanthroline form least stable complexes with the phenyl tin (IV) chloride.

Interaction of donors with acceptor diphenyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal

TABLE 11 : Interaction of donors (B) with the acceptor phenyl tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_v	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-3.734	0.482	-5.011	0.571	30	54	35.280	-0.213	-16.748	-16.961
2-nitropyridine	-8.568	-0.408	-5.011	0.571	46	54	50.000	9.067	-153.668	-144.600
2-aminopyridine	-3.041	0.549	-5.011	0.571	36	54	40.500	-0.543	-18.081	-18.624
pyridine-2-carboxamide	-3.929	0.606	-5.011	0.571	46	54	50.000	-0.172	-21.234	-21.406
2-cyanopyridine	-4.725	0.518	-5.011	0.571	38	54	42.320	-0.011	-19.431	-19.442
2-chloropyridine	-4.173	0.462	-5.011	0.571	36	54	40.500	-0.090	-19.597	-19.687
pyridine-2-carboxylic acid	-4.384	0.568	-5.011	0.571	46	54	50.000	-0.056	-21.950	-22.006
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-30.352	-1.082	-5.011	0.571	74	54	81.920	-388.470	80.225	-308.245
4-amino-2,2'-bipyridine	-3.531	0.632	-5.011	0.571	64	54	69.620	-0.329	-28.945	-29.274
2,2'-bipyridine-4-carboxamide	-4.053	0.694	-5.011	0.571	74	54	81.920	-0.144	-32.372	-32.516
4-cyano-2,2'-bipyridine	-4.424	0.711	-5.011	0.571	66	54	72.000	-0.055	-28.079	-28.134
4-chloro-2,2'-bipyridine	-4.026	0.642	-5.011	0.571	64	54	69.620	-0.147	-28.694	-28.841
2,2'-bipyridine-4-carboxylic acid	-4.233	0.743	-5.011	0.571	74	54	81.920	-0.098	-31.177	-31.275
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-3.575	0.678	-5.011	0.571	72	54	79.380	-0.320	-31.782	-32.101
3-nitro-1,10-phenanthroline	-22.641	-1.299	-5.011	0.571	82	54	92.480	-158.418	63.551	-94.867
1,10-phenanthroline-3-carboxamide	-4.088	0.709	-5.011	0.571	82	54	92.480	-0.135	-36.109	-36.244
3-cyano-1,10-phenanthroline	-4.456	0.695	-5.011	0.571	74	54	81.920	-0.048	-32.341	-32.389
3-chloro-1,10-phenanthroline	-4.080	0.637	-5.011	0.571	72	54	79.380	-0.131	-32.844	-32.974
1,10-phenanthroline-3-carboxylic acid	-4.260	0.724	-5.011	0.571	82	54	92.480	-0.090	-35.715	-35.805

μ_A = **Chemical potential of molecule A,** μ_B = **Chemical potential of molecule B,** S_A = **Global Softness of molecule A,** S_B = **Global Softness of molecule B,** N_A = **total number of electrons in molecule A,** N_B = **total number of electrons in molecule B,** $\lambda = (N_A + N_B)^2 / 200$, E_μ = **Energy corresponds to a reshuffling of the charge distribution,** E_v = **Energy corresponds to the charge transfer process,** E_{int} = **Interaction energy**

halide $SnCl_4$ (A) is shown in TABLE 12. Lowest value of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

2-nitropyridine < pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.

1,10-phenanthroline-3-carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline < 3-nitro-1,10-phenanthroline.

It is evident that the nitro derivatives of pyridine and bipyridine form most stable complexes with the diphenyl tin (IV) chloride. In the case of phenanthroline derivatives, the least stable complex is formed with the donor 1,10-phenanthroline-3-carboxamide.

Interaction of donors with acceptor triphenyl tin (IV) chloride

Interaction energy of donors (B) with acceptor metal halide $SnCl_4$ (A) is shown in TABLE 13. Lowest value

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TABLE 12 : Interaction of donors (B) with the acceptor diphenyl tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_ν	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-4.281	0.464	-3.734	0.482	30	76	56.180	-0.035	-29.674	-29.709
2-nitropyridine	-4.281	0.464	-8.568	-0.408	46	76	74.420	31.090	-663.814	-632.724
2-aminopyridine	-4.281	0.464	-3.041	0.549	36	76	62.720	-0.193	-30.948	-31.141
pyridine-2-carboxamide	-4.281	0.464	-3.929	0.606	46	76	74.420	-0.016	-34.753	-34.769
2-cyanopyridine	-4.281	0.464	-4.725	0.518	38	76	64.980	-0.024	-33.074	-33.098
2-chloropyridine	-4.281	0.464	-4.173	0.462	36	76	62.720	-0.001	-33.841	-33.843
pyridine-2-carboxylic acid	-4.281	0.464	-4.384	0.568	46	76	74.420	-0.001	-36.045	-36.046
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-4.281	0.464	-30.352	-1.082	74	76	112.500	-276.626	91.138	-185.489
4-amino-2,2'-bipyridine	-4.281	0.464	-3.531	0.632	64	76	98.000	-0.075	-44.709	-44.784
2,2'-bipyridine-4-carboxamide	-4.281	0.464	-4.053	0.694	74	76	112.500	-0.007	-48.547	-48.554
4-cyano-2,2'-bipyridine	-4.281	0.464	-4.424	0.711	66	76	100.820	-0.003	-42.886	-42.888
4-chloro-2,2'-bipyridine	-4.281	0.464	-4.026	0.642	64	76	98.000	-0.009	-44.283	-44.292
2,2'-bipyridine-4-carboxylic acid	-4.281	0.464	-4.233	0.743	74	76	112.500	0.000	-46.598	-46.598
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-4.281	0.464	-3.575	0.678	72	76	109.520	-0.069	-47.942	-48.011
3-nitro-1,10-phenanthroline	-4.281	0.464	-22.641	-1.299	82	76	124.820	-121.869	74.811	-47.058
1,10-phenanthroline-3-carboxamide	-4.281	0.464	-4.088	0.709	82	76	124.820	-0.005	-53.163	-53.168
3-cyano-1,10-phenanthroline	-4.281	0.464	-4.456	0.695	74	76	112.500	-0.004	-48.496	-48.501
3-chloro-1,10-phenanthroline	-4.281	0.464	-4.080	0.637	72	76	109.520	-0.005	-49.700	-49.705
1,10-phenanthroline-3-carboxylic acid	-4.281	0.464	-4.260	0.724	82	76	124.820	0.000	-52.531	-52.531

μ_A = Chemical potential of molecule A, μ_B = Chemical potential of molecule B, S_A = Global Softness of molecule A, S_B = Global Softness of molecule B, N_A = total number of electrons in molecule A, N_B = total number of electrons in molecule B, $\lambda = (N_A + N_B)^2 / 200$, E_μ = Energy corresponds to a reshuffling of the charge distribution, E_ν = Energy corresponds to the charge transfer process, E_{int} = Interaction energy

of interaction energy of interaction of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$ has been observed and its value is -280.425eV, which indicates formation of least stable complex of organic base 4-nitro-2,2'-bipyridine with acceptor $SnCl_4$.

The value of interaction energy of organic base pyridine with metal halide $SnCl_4$ is highest and is equal to -10.083eV, which indicates that the organic base pyridine forms most stable complex with $SnCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $SnCl_4$ is in the following order;

2-nitropyridine < pyridine-2-carboxylic acid < pyridine-2-carboxamide < 2-chloropyridine < 2-cyanopyridine < 2-aminopyridine < pyridine.

4-nitro-2,2'-bipyridine < 2,2'-bipyridine-4-carboxamide < 2,2'-bipyridine-4-carboxylic acid < 4-amino-2,2'-bipyridine < 4-chloro-2,2'-bipyridine < 4-cyano-2,2'-bipyridine.

1,10-phenanthroline-3-carboxamide < 1,10-phenanthroline-3-carboxylic acid < 3-chloro-1,10-phenanthroline < 3-cyano-1,10-phenanthroline < 3-amino-1,10-phenanthroline < 3-nitro-1,10-phenanthroline.

It is evident that the nitro derivatives of pyridine and bipyridine form least stable complexes with the diphenyl tin (IV) chloride. In the case of phenanthroline derivatives, the most stable complex is formed with the donor 1,10-phenanthroline-3-carboxamide.

Charge transfer and lowering of energy

The values of ΔN, E (calculated in eV) are included in TABLE 14 to TABLE 23. Metal ligand bond strength between interaction of acceptor (A) and donor (B) in-

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TABLE 13 : Interaction of donors (B) with the acceptor triphenyl tin (IV) chloride (A)

Donor (B)	μ_A	S_A	μ_B	S_B	N_A	N_B	λ	E_ν	E_μ	E_{int}
Derivatives of pyridine										
pyridine	-3.987	0.478	-3.734	0.482	30	98	81.920	-0.008	-42.674	-42.682
2-nitropyridine	-3.987	0.478	-8.568	-0.408	46	98	103.680	29.557	-748.531	-718.974
2-aminopyridine	-3.987	0.478	-3.041	0.549	36	98	89.780	-0.114	-43.730	-43.845
pyridine-2-carboxamide	-3.987	0.478	-3.929	0.606	46	98	103.680	0.000	-47.827	-47.827
2-cyanopyridine	-3.987	0.478	-4.725	0.518	38	98	92.480	-0.068	-46.447	-46.515
2-chloropyridine	-3.987	0.478	-4.173	0.462	36	98	89.780	-0.004	-47.761	-47.765
pyridine-2-carboxylic acid	-3.987	0.478	-4.384	0.568	46	98	103.680	-0.020	-49.583	-49.603
Derivatives of bipyridine										
4-nitro-2,2'-bipyridine	-3.987	0.478	-30.352	-1.082	74	98	147.920	-297.311	122.451	-174.860
4-amino-2,2'-bipyridine	-3.987	0.478	-3.531	0.632	64	98	131.220	-0.028	-59.152	-59.180
2,2'-bipyridine-4-carboxamide	-3.987	0.478	-4.053	0.694	74	98	147.920	-0.001	-63.113	-63.113
4-cyano-2,2'-bipyridine	-3.987	0.478	-4.424	0.711	66	98	134.480	-0.027	-56.568	-56.595
4-chloro-2,2'-bipyridine	-3.987	0.478	-4.026	0.642	64	98	131.220	0.000	-58.595	-58.595
2,2'-bipyridine-4-carboxylic acid	-3.987	0.478	-4.233	0.743	74	98	147.920	-0.009	-60.606	-60.615
Derivatives of phenanthroline										
3-amino-1,10-phenanthroline	-3.987	0.478	-3.575	0.678	72	98	144.500	-0.024	-62.532	-62.556
3-nitro-1,10-phenanthroline	-3.987	0.478	-22.641	-1.299	82	98	162.000	-131.466	98.656	-32.810
1,10-phenanthroline-3-carboxamide	-3.987	0.478	-4.088	0.709	82	98	162.000	-0.001	-68.231	-68.233
3-cyano-1,10-phenanthroline	-3.987	0.478	-4.456	0.695	74	98	147.920	-0.031	-63.048	-63.079
3-chloro-1,10-phenanthroline	-3.987	0.478	-4.080	0.637	72	98	144.500	-0.001	-64.797	-64.798
1,10-phenanthroline-3-carboxylic acid	-3.987	0.478	-4.260	0.724	82	98	162.000	-0.011	-67.429	-67.440

μ_A = Chemical potential of molecule A, μ_B = Chemical potential of molecule B, S_A = Global Softness of molecule A, S_B = Global Softness of molecule B, N_A = total number of electrons in molecule A, N_B = total number of electrons in molecule B, $\lambda = (N_A + N_B)^2$ / 200, E_μ = Energy corresponds to a reshuffling of the charge distribution, E_ν = Energy corresponds to the charge transfer process, E_{int} = Interaction energy

TABLE 14 : Charge transfer and lowering of energy in the interaction of donors with the acceptor Tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	6.296	3.734	1.791	2.074	0.331	-0.424
2-nitropyridine	-6.119	-11.016	6.296	8.568	1.791	-2.449	1.726	1.961
2-aminopyridine	-4.863	-1.219	6.296	3.041	1.791	1.822	0.450	-0.733
pyridine-2-carboxamide	-5.578	-2.279	6.296	3.929	1.791	1.650	0.344	-0.407
2-cyanopyridine	-6.656	-2.794	6.296	4.725	1.791	1.931	0.211	-0.166
2-chloropyridine	-6.336	-2.009	6.296	4.173	1.791	2.164	0.268	-0.285
pyridine-2-carboxylic acid	-6.145	-2.623	6.296	4.384	1.791	1.761	0.269	-0.257
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	6.296	30.352	1.791	-0.925	-13.889	-167.059
4-amino-2,2'-bipyridine	-5.114	-1.947	6.296	3.531	1.791	1.584	0.410	-0.566
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	6.296	4.053	1.791	1.441	0.347	-0.389
4-cyano-2,2'-bipyridine	-5.830	-3.017	6.296	4.424	1.791	1.407	0.293	-0.274
4-chloro-2,2'-bipyridine	-5.583	-2.468	6.296	4.026	1.791	1.558	0.339	-0.385
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	6.296	4.233	1.791	1.347	0.329	-0.339

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Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	6.296	3.575	1.791	1.476	0.417	-0.567
3-nitro-1,10-phenanthroline	-21.871	-23.411	6.296	22.641	1.791	-0.770	-8.009	-65.452
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	6.296	4.088	1.791	1.410	0.345	-0.381
3-cyano-1,10-phenanthroline	-5.894	-3.018	6.296	4.456	1.791	1.438	0.285	-0.262
3-chloro-1,10-phenanthroline	-5.649	-2.511	6.296	4.080	1.791	1.569	0.330	-0.365
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	6.296	4.260	1.791	1.382	0.321	-0.326

χ_A = Electronegativity of acceptor, χ_B = Electronegativity of donor, η_A = Absolute hardness of acceptor, η_B = Absolute hardness of donor, ΔN = Charge transfer, ΔE = Lowering of energy, εHOMO = HOMO energy of donor, εLUMO = LUMO energy of donor

TABLE 15 : Charge transfer and lowering of energy in the interaction of donors with the acceptor methyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	5.411	3.734	2.113	2.074	0.200	-0.168
2-nitropyridine	-6.119	-11.016	5.411	8.568	2.113	-2.449	4.704	7.424
2-aminopyridine	-4.863	-1.219	5.411	3.041	2.113	1.822	0.301	-0.357
pyridine-2-carboxamide	-5.578	-2.279	5.411	3.929	2.113	1.650	0.197	-0.146
2-cyanopyridine	-6.656	-2.794	5.411	4.725	2.113	1.931	0.085	-0.029
2-chloropyridine	-6.336	-2.009	5.411	4.173	2.113	2.164	0.145	-0.090
pyridine-2-carboxylic acid	-6.145	-2.623	5.411	4.384	2.113	1.761	0.133	-0.068
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	5.411	30.352	2.113	-0.925	-10.492	-130.843
4-amino-2,2'-bipyridine	-5.114	-1.947	5.411	3.531	2.113	1.584	0.254	-0.239
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	5.411	4.053	2.113	1.441	0.191	-0.130
4-cyano-2,2'-bipyridine	-5.830	-3.017	5.411	4.424	2.113	1.407	0.140	-0.069
4-chloro-2,2'-bipyridine	-5.583	-2.468	5.411	4.026	2.113	1.558	0.189	-0.131
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	5.411	4.233	2.113	1.347	0.170	-0.100
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	5.411	3.575	2.113	1.476	0.256	-0.235
3-nitro-1,10-phenanthroline	-21.871	-23.411	5.411	22.641	2.113	-0.770	-6.415	-55.263
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	5.411	4.088	2.113	1.410	0.188	-0.124
3-cyano-1,10-phenanthroline	-5.894	-3.018	5.411	4.456	2.113	1.438	0.134	-0.064
3-chloro-1,10-phenanthroline	-5.649	-2.511	5.411	4.080	2.113	1.569	0.181	-0.120
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	5.411	4.260	2.113	1.382	0.165	-0.095

χ_A = Electronegativity of acceptor, χ_B = Electronegativity of donor, η_A = Absolute hardness of acceptor, η_B = Absolute hardness of donor, ΔN = Charge transfer, ΔE = Lowering of energy, εHOMO = HOMO energy of donor, εLUMO = LUMO energy of donor

creases as the lowering in energy (ΔE) decreases. The bond strength between 2-nitropyridine and dimethyl tin (IV) chloride is weakest as the value of ΔE is highest (94.369eV). Strongest bond strength has been observed between 4-nitro-2,2'-bipyridine and phenyl tin (IV) chloride in which case the value of E is lowest (-194.235eV).

Metal ligand bond strength between interaction of acceptor (A) and donor (B) increases as the charge transfer (ΔN) increases. The values of charge transfer indicate that the least stable complex formation is between 2-nitropyridine and triethyl tin (IV) chloride (ΔN = -20.861eV). The most stable complex is formed with 2-nitropyridine and dimethyl tin (IV) chloride (ΔN = 46.051eV). The values of charge transfer (ΔN) and lowering of energy (ΔE) also indicate almost the same sequence of the stability of complexes formed by the donors with the acceptors.

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TABLE 16 : Charge transfer and lowering of energy in the interaction of donors with the acceptor dimethyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	4.469	3.734	2.404	2.074	0.082	-0.030
2-nitropyridine	-6.119	-11.016	4.469	8.568	2.404	-2.449	46.051	94.369
2-aminopyridine	-4.863	-1.219	4.469	3.041	2.404	1.822	0.169	-0.121
pyridine-2-carboxamide	-5.578	-2.279	4.469	3.929	2.404	1.650	0.067	-0.018
2-cyanopyridine	-6.656	-2.794	4.469	4.725	2.404	1.931	-0.030	-0.004
2-chloropyridine	-6.336	-2.009	4.469	4.173	2.404	2.164	0.032	-0.005
pyridine-2-carboxylic acid	-6.145	-2.623	4.469	4.384	2.404	1.761	0.010	0.000
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	4.469	30.352	2.404	-0.925	-8.747	-113.198
4-amino-2,2'-bipyridine	-5.114	-1.947	4.469	3.531	2.404	1.584	0.118	-0.055
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	4.469	4.053	2.404	1.441	0.054	-0.011
4-cyano-2,2'-bipyridine	-5.830	-3.017	4.469	4.424	2.404	1.407	0.006	0.000
4-chloro-2,2'-bipyridine	-5.583	-2.468	4.469	4.026	2.404	1.558	0.056	-0.012
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	4.469	4.233	2.404	1.347	0.032	-0.004
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	4.469	3.575	2.404	1.476	0.115	-0.052
3-nitro-1,10-phenanthroline	-21.871	-23.411	4.469	22.641	2.404	-0.770	-5.561	-50.523
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	4.469	4.088	2.404	1.410	0.050	-0.010
3-cyano-1,10-phenanthroline	-5.894	-3.018	4.469	4.456	2.404	1.438	0.002	0.000
3-chloro-1,10-phenanthroline	-5.649	-2.511	4.469	4.080	2.404	1.569	0.049	-0.010
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	4.469	4.260	2.404	1.382	0.028	-0.003

χ_A = Electronegativity of acceptor, χ_B = Electronegativity of donor, η_A = Absolute hardness of acceptor, η_B = Absolute hardness of donor, ΔN = Charge transfer, ΔE = Lowering of energy, εHOMO = HOMO energy of donor, εLUMO = LUMO energy of donor

TABLE 17 : Charge transfer and lowering of energy in the interaction of donors with the acceptor trimethyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	3.669	3.734	2.735	2.074	-0.007	0.000
2-nitropyridine	-6.119	-11.016	3.669	8.568	2.735	-2.449	-8.565	-20.979
2-aminopyridine	-4.863	-1.219	3.669	3.041	2.735	1.822	0.069	-0.022
pyridine-2-carboxamide	-5.578	-2.279	3.669	3.929	2.735	1.650	-0.030	-0.004
2-cyanopyridine	-6.656	-2.794	3.669	4.725	2.735	1.931	-0.113	-0.060
2-chloropyridine	-6.336	-2.009	3.669	4.173	2.735	2.164	-0.051	-0.013
pyridine-2-carboxylic acid	-6.145	-2.623	3.669	4.384	2.735	1.761	-0.080	-0.028
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	3.669	30.352	2.735	-0.925	-7.371	-98.340
4-amino-2,2'-bipyridine	-5.114	-1.947	3.669	3.531	2.735	1.584	0.016	-0.001
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	3.669	4.053	2.735	1.441	-0.046	-0.009
4-cyano-2,2'-bipyridine	-5.830	-3.017	3.669	4.424	2.735	1.407	-0.091	-0.034
4-chloro-2,2'-bipyridine	-5.583	-2.468	3.669	4.026	2.735	1.558	-0.042	-0.007
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	3.669	4.233	2.735	1.347	-0.069	-0.019
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	3.669	3.575	2.735	1.476	0.011	-0.001

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Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
3-nitro-1,10-phenanthroline	-21.871	-23.411	3.669	22.641	2.735	-0.770	-4.829	-45.808
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	3.669	4.088	2.735	1.410	-0.051	-0.011
3-cyano-1,10-phenanthroline	-5.894	-3.018	3.669	4.456	2.735	1.438	-0.094	-0.037
3-chloro-1,10-phenanthroline	-5.649	-2.511	3.669	4.080	2.735	1.569	-0.048	-0.010
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	3.669	4.260	2.735	1.382	-0.072	-0.021

χ_A = **Electronegativity of acceptor,** χ_B = **Electronegativity of donor,** η_A = **Absolute hardness of acceptor,** η_B = **Absolute hardness of donor,** ΔN = **Charge transfer,** ΔE = **Lowering of energy,** εHOMO = **HOMO energy of donor,** εLUMO = **LUMO energy of donor**

TABLE 18 : Charge transfer and lowering of energy in the interaction of donors with the acceptor ethyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	5.323	3.734	2.061	2.074	0.192	-0.153
2-nitropyridine	-6.119	-11.016	5.323	8.568	2.061	-2.449	4.186	6.791
2-aminopyridine	-4.863	-1.219	5.323	3.041	2.061	1.822	0.294	-0.335
pyridine-2-carboxamide	-5.578	-2.279	5.323	3.929	2.061	1.650	0.188	-0.131
2-cyanopyridine	-6.656	-2.794	5.323	4.725	2.061	1.931	0.075	-0.022
2-chloropyridine	-6.336	-2.009	5.323	4.173	2.061	2.164	0.136	-0.078
pyridine-2-carboxylic acid	-6.145	-2.623	5.323	4.384	2.061	1.761	0.123	-0.058
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	5.323	30.352	2.061	-0.925	-11.011	-137.797
4-amino-2,2'-bipyridine	-5.114	-1.947	5.323	3.531	2.061	1.584	0.246	-0.220
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	5.323	4.053	2.061	1.441	0.181	-0.115
4-cyano-2,2'-bipyridine	-5.830	-3.017	5.323	4.424	2.061	1.407	0.130	-0.058
4-chloro-2,2'-bipyridine	-5.583	-2.468	5.323	4.026	2.061	1.558	0.179	-0.116
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	5.323	4.233	2.061	1.347	0.160	-0.087
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	5.323	3.575	2.061	1.476	0.247	-0.216
3-nitro-1,10-phenanthroline	-21.871	-23.411	5.323	22.641	2.061	-0.770	-6.707	-58.078
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	5.323	4.088	2.061	1.410	0.178	-0.110
3-cyano-1,10-phenanthroline	-5.894	-3.018	5.323	4.456	2.061	1.438	0.124	-0.054
3-chloro-1,10-phenanthroline	-5.649	-2.511	5.323	4.080	2.061	1.569	0.171	-0.106
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	5.323	4.260	2.061	1.382	0.154	-0.082

χ_A = **Electronegativity of acceptor,** χ_B = **Electronegativity of donor,** η_A = **Absolute hardness of acceptor,** η_B = **Absolute hardness of donor,** ΔN = **Charge transfer,** ΔE = **Lowering of energy,** εHOMO = **HOMO energy of donor,** εLUMO = **LUMO energy of donor**

CONCLUSION

Order of acidic strength of acceptors based on the values of chemical potential has been observerd to be in the following order;
Triethyl tin (IV) chloride < Trimethyl tin (IV) chloride < Triphenyl tin (IV) chloride < Diphenyl tin (IV) chloride < Diethyl tin (IV) chloride < Dimethyl tin (IV) chloride < Phenyl tin (IV) chloride < Ethyl tin (IV) chloride < Methyl tin (IV) chloride < Tin (IV) chloride.

Lowest value of interaction energy has been found for the interaction of dimethyl tin (IV) chloride with 2-nitropyridine and is equal to -1823.15eV which indicates that the least stable complex is formed by dimethyl tin (IV) chloride with 2-nitropyridine. This is in accordance with the established fact that the nitro-derivatives are the weakest. Also the value of ΔE is highest (94.369eV) in this case which also suggests that the bond strength between 2-nitropyridine and dimethyl tin (IV) chloride is weakest i.e. least stable complex is formed in this case.

TABLE 19 : Charge transfer and lowering of energy in the interaction of donors with the acceptor diethyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	4.286	3.734	2.261	2.074	0.064	-0.018
2-nitropyridine	-6.119	-11.016	4.286	8.568	2.261	-2.449	11.388	24.382
2-aminopyridine	-4.863	-1.219	4.286	3.041	2.261	1.822	0.152	-0.095
pyridine-2-carboxamide	-5.578	-2.279	4.286	3.929	2.261	1.650	0.046	-0.008
2-cyanopyridine	-6.656	-2.794	4.286	4.725	2.261	1.931	-0.052	-0.012
2-chloropyridine	-6.336	-2.009	4.286	4.173	2.261	2.164	0.013	-0.001
pyridine-2-carboxylic acid	-6.145	-2.623	4.286	4.384	2.261	1.761	-0.012	-0.001
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	4.286	30.352	2.261	-0.925	-9.755	-127.140
4-amino-2,2'-bipyridine	-5.114	-1.947	4.286	3.531	2.261	1.584	0.098	-0.037
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	4.286	4.053	2.261	1.441	0.031	-0.004
4-cyano-2,2'-bipyridine	-5.830	-3.017	4.286	4.424	2.261	1.407	-0.019	-0.001
4-chloro-2,2'-bipyridine	-5.583	-2.468	4.286	4.026	2.261	1.558	0.034	-0.004
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	4.286	4.233	2.261	1.347	0.007	0.000
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	4.286	3.575	2.261	1.476	0.095	-0.034
3-nitro-1,10-phenanthroline	-21.871	-23.411	4.286	22.641	2.261	-0.770	-6.157	-56.512
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	4.286	4.088	2.261	1.410	0.027	-0.003
3-cyano-1,10-phenanthroline	-5.894	-3.018	4.286	4.456	2.261	1.438	-0.023	-0.002
3-chloro-1,10-phenanthroline	-5.649	-2.511	4.286	4.080	2.261	1.569	0.027	-0.003
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	4.286	4.260	2.261	1.382	0.004	0.000

χ_A = Electronegativity of acceptor, χ_B = Electronegativity of donor, η_A = Absolute hardness of acceptor, η_B = Absolute hardness of donor, ΔN = Charge transfer, ΔE = Lowering of energy, εHOMO = HOMO energy of donor, εLUMO = LUMO energy of donor

TABLE 20 : Charge transfer and lowering of energy in the interaction of donors with the acceptor triethyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	3.478	3.734	2.571	2.074	-0.028	-0.004
2-nitropyridine	-6.119	-11.016	3.478	8.568	2.571	-2.449	-20.861	-53.090
2-aminopyridine	-4.863	-1.219	3.478	3.041	2.571	1.822	0.050	-0.011
pyridine-2-carboxamide	-5.578	-2.279	3.478	3.929	2.571	1.650	-0.053	-0.012
2-cyanopyridine	-6.656	-2.794	3.478	4.725	2.571	1.931	-0.139	-0.086
2-chloropyridine	-6.336	-2.009	3.478	4.173	2.571	2.164	-0.073	-0.026
pyridine-2-carboxylic acid	-6.145	-2.623	3.478	4.384	2.571	1.761	-0.105	-0.047
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	3.478	30.352	2.571	-0.925	-8.163	-109.692
4-amino-2,2'-bipyridine	-5.114	-1.947	3.478	3.531	2.571	1.584	-0.006	0.000
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	3.478	4.053	2.571	1.441	-0.072	-0.021
4-cyano-2,2'-bipyridine	-5.830	-3.017	3.478	4.424	2.571	1.407	-0.119	-0.056
4-chloro-2,2'-bipyridine	-5.583	-2.468	3.478	4.026	2.571	1.558	-0.066	-0.018
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	3.478	4.233	2.571	1.347	-0.096	-0.036
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	3.478	3.575	2.571	1.476	-0.012	-0.001

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Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
3-nitro-1,10-phenanthroline	-21.871	-23.411	3.478	22.641	2.571	-0.770	-5.322	-50.991
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	3.478	4.088	2.571	1.410	-0.077	-0.023
3-cyano-1,10-phenanthroline	-5.894	-3.018	3.478	4.456	2.571	1.438	-0.122	-0.060
3-chloro-1,10-phenanthroline	-5.649	-2.511	3.478	4.080	2.571	1.569	-0.073	-0.022
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	3.478	4.260	2.571	1.382	-0.099	-0.039

χ_A = Electronegativity of acceptor, χ_B = Electronegativity of donor, η_A = Absolute hardness of acceptor, η_B = Absolute hardness of donor, ΔN = Charge transfer, ΔE = Lowering of energy, εHOMO = HOMO energy of donor, εLUMO = LUMO energy of donor

TABLE 21 : Charge transfer and lowering of energy in the interaction of donors with the acceptor phenyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	5.011	3.734	1.751	2.074	0.167	-0.107
2-nitropyridine	-6.119	-11.016	5.011	8.568	1.751	-2.449	2.549	4.534
2-aminopyridine	-4.863	-1.219	5.011	3.041	1.751	1.822	0.276	-0.272
pyridine-2-carboxamide	-5.578	-2.279	5.011	3.929	1.751	1.650	0.159	-0.086
2-cyanopyridine	-6.656	-2.794	5.011	4.725	1.751	1.931	0.039	-0.006
2-chloropyridine	-6.336	-2.009	5.011	4.173	1.751	2.164	0.107	-0.045
pyridine-2-carboxylic acid	-6.145	-2.623	5.011	4.384	1.751	1.761	0.089	-0.028
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	5.011	30.352	1.751	-0.925	-15.330	-194.235
4-amino-2,2'-bipyridine	-5.114	-1.947	5.011	3.531	1.751	1.584	0.222	-0.164
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	5.011	4.053	1.751	1.441	0.150	-0.072
4-cyano-2,2'-bipyridine	-5.830	-3.017	5.011	4.424	1.751	1.407	0.093	-0.027
4-chloro-2,2'-bipyridine	-5.583	-2.468	5.011	4.026	1.751	1.558	0.149	-0.073
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	5.011	4.233	1.751	1.347	0.126	-0.049
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	5.011	3.575	1.751	1.476	0.223	-0.160
3-nitro-1,10-phenanthroline	-21.871	-23.411	5.011	22.641	1.751	-0.770	-8.986	-79.209
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	5.011	4.088	1.751	1.410	0.146	-0.067
3-cyano-1,10-phenanthroline	-5.894	-3.018	5.011	4.456	1.751	1.438	0.087	-0.024
3-chloro-1,10-phenanthroline	-5.649	-2.511	5.011	4.080	1.751	1.569	0.140	-0.065
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	5.011	4.260	1.751	1.382	0.120	-0.045

χ_A = Electronegativity of acceptor, χ_B = Electronegativity of donor, η_A = Absolute hardness of acceptor, η_B = Absolute hardness of donor, ΔN = Charge transfer, ΔE = Lowering of energy, εHOMO = HOMO energy of donor, εLUMO = LUMO energy of donor

TABLE 22 : Charge transfer and lowering of energy in the interaction of donors with the acceptor diphenyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	4.281	3.734	2.153	2.074	0.065	-0.018
2-nitropyridine	-6.119	-11.016	4.281	8.568	2.153	-2.449	7.253	15.545
2-aminopyridine	-4.863	-1.219	4.281	3.041	2.153	1.822	0.156	-0.097
pyridine-2-carboxamide	-5.578	-2.279	4.281	3.929	2.153	1.650	0.046	-0.008
2-cyanopyridine	-6.656	-2.794	4.281	4.725	2.153	1.931	-0.054	-0.012
2-chloropyridine	-6.336	-2.009	4.281	4.173	2.153	2.164	0.013	-0.001
pyridine-2-carboxylic acid	-6.145	-2.623	4.281	4.384	2.153	1.761	-0.013	-0.001
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	4.281	30.352	2.153	-0.925	-10.611	-138.313

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
4-amino-2,2'-bipyridine	-5.114	-1.947	4.281	3.531	2.153	1.584	0.100	-0.038
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	4.281	4.053	2.153	1.441	0.032	-0.004
4-cyano-2,2'-bipyridine	-5.830	-3.017	4.281	4.424	2.153	1.407	-0.020	-0.001
4-chloro-2,2'-bipyridine	-5.583	-2.468	4.281	4.026	2.153	1.558	0.034	-0.004
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	4.281	4.233	2.153	1.347	0.007	0.000
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	4.281	3.575	2.153	1.476	0.097	-0.034
3-nitro-1,10-phenanthroline	-21.871	-23.411	4.281	22.641	2.153	-0.770	-6.638	-60.934
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	4.281	4.088	2.153	1.410	0.027	-0.003
3-cyano-1,10-phenanthroline	-5.894	-3.018	4.281	4.456	2.153	1.438	-0.024	-0.002
3-chloro-1,10-phenanthroline	-5.649	-2.511	4.281	4.080	2.153	1.569	0.027	-0.003
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	4.281	4.260	2.153	1.382	0.003	0.000

χ_A = **Electronegativity of acceptor**, χ_B = **Electronegativity of donor**, η_A = **Absolute hardness of acceptor**, η_B = **Absolute hardness of donor**, ΔN = **Charge transfer**, ΔE = **Lowering of energy**, εHOMO = **HOMO energy of donor**, εLUMO = **LUMO energy of donor**

TABLE 23 : Charge transfer and lowering of energy in the interaction of donors with the acceptor triphenyl tin (IV) chloride

Donor (B)	εHOMO	εLUMO	χ_A	χ_B	η_A	η_B	ΔN	ΔE
Derivatives of pyridine								
pyridine	-5.808	-1.660	3.987	3.734	2.094	2.074	0.030	-0.004
2-nitropyridine	-6.119	-11.016	3.987	8.568	2.094	-2.449	6.452	14.779
2-aminopyridine	-4.863	-1.219	3.987	3.041	2.094	1.822	0.121	-0.057
pyridine-2-carboxamide	-5.578	-2.279	3.987	3.929	2.094	1.650	0.008	0.000
2-cyanopyridine	-6.656	-2.794	3.987	4.725	2.094	1.931	-0.092	-0.034
2-chloropyridine	-6.336	-2.009	3.987	4.173	2.094	2.164	-0.022	-0.002
pyridine-2-carboxylic acid	-6.145	-2.623	3.987	4.384	2.094	1.761	-0.052	-0.010
Derivatives of bipyridine								
4-nitro-2,2'-bipyridine	-29.427	-31.276	3.987	30.352	2.094	-0.925	-11.277	-148.656
4-amino-2,2'-bipyridine	-5.114	-1.947	3.987	3.531	2.094	1.584	0.062	-0.014
2,2'-bipyridine-4-carboxamide	-5.493	-2.612	3.987	4.053	2.094	1.441	-0.009	0.000
4-cyano-2,2'-bipyridine	-5.830	-3.017	3.987	4.424	2.094	1.407	-0.062	-0.014
4-chloro-2,2'-bipyridine	-5.583	-2.468	3.987	4.026	2.094	1.558	-0.005	0.000
2,2'-bipyridine-4-carboxylic acid	-5.579	-2.886	3.987	4.233	2.094	1.347	-0.036	-0.004
Derivatives of phenanthroline								
3-amino-1,10-phenanthroline	-5.050	-2.099	3.987	3.575	2.094	1.476	0.058	-0.012
3-nitro-1,10-phenanthroline	-21.871	-23.411	3.987	22.641	2.094	-0.770	-7.047	-65.733
1,10-phenanthroline-3-carboxamide	-5.497	-2.678	3.987	4.088	2.094	1.410	-0.014	-0.001
3-cyano-1,10-phenanthroline	-5.894	-3.018	3.987	4.456	2.094	1.438	-0.066	-0.016
3-chloro-1,10-phenanthroline	-5.649	-2.511	3.987	4.080	2.094	1.569	-0.013	-0.001
1,10-phenanthroline-3-carboxylic acid	-5.642	-2.878	3.987	4.260	2.094	1.382	-0.039	-0.005

χ_A = **Electronegativity of acceptor**, χ_B = **Electronegativity of donor**, η_A = **Absolute hardness of acceptor**, η_B = **Absolute hardness of donor**, ΔN = **Charge transfer**, ΔE = **Lowering of energy**, εHOMO = **HOMO energy of donor**, εLUMO = **LUMO energy of donor**

Most stable complex is formed by triethyl tin (IV) chloride with 2-nitropyridine and in this case the value of interaction energy is highest (1082.43eV). The values of charge transfer (ΔN) and lowering of energy (ΔE) also indicate almost the same sequence of the stability of complexes formed by the donors with the acceptors.

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REFERENCES

[1] R.C.Aggarwal, P.P.Singh; J.Inorg.Nucl.Chem., **26**, 2185 **(1964)**.

[2] R.C.Aggarwal, P.P.Singh; J.Inorg.Nucl.Chem., **27**, 2597 **(1965)**.

[3] R.C.Aggarwal, P.P.Singh; J.Inorg.Nucl.Chem., **27**, 2593 **(1965)**.

[4] R.C.Aggarwal, P.P.Singh; J.Inorg.Nucl.Chem., **28**, 1655 **(1966)**.

[5] R.C.Aggarwal, P.P.Singh; J.Inorg.Nucl.Chem., **28**, 1651 **(1966)**.

[6] P.P.Singh; J.Sc.Ind.Res., **42**, 140 **(1983)**.

[7] R.G.Parr, R.A.Donnelly, M.Levy; J.Am.Chem.Soc., **69**, 3801 **(1978)**.

[8] R.G.Parr, R.A.Donnelly, M.Levy; J.Am.Chem.Soc., **105**, 1503 **(1983)**.

[9] R.G.Parr, W.Yand; J.Am.Chem.Soc., **106**, 4049 **(1984)**.

[10] R.G.Parr; J.Am.Chem.Soc., **105**, 7512 **(1983)**.

[11] R.G.Parr, R.G.Pearson; J.Am.Chem.Soc., **105**, 7512 **(1983)**.

[12] K.D.Jordon, P.D.Burrow; Am.Chem.Res., **11**, 341 **(1978)**.

[13] J.L.Gazquez; In: Chemical Hardness, Structure and Bonding, 80 (Ed.,) K.D.Sen; Berlin: Spinger-Verlag, **(1993)**.

[14] R.G.Parr, J.L.Gazaquez; J.Phys.Chem., **97**, 3931 **(1993)**.

[15] F.Mendez, J.L.Gazquez; Proc.Indian Acad.Sci. (Chem.Sci.), **106(2)**, 183 **(1994)**.

[16] (a) R.G.Parr, P.K.Chattaraj; J.Am.Chem.Soc., **113**, 1854 **(1991)**; **(b)** P.P.Singh, Singh Divya, S.Ahmad; Journal of Molecular Structure, **905**, 13 **(2009)**; **(c)** P.P.Singh, P.Kumar, A.K.Srivastava; Organic Chemistry: An Indian Journal, (in press), **(2010)**.

[17] M.C.lanigan, A.Komornicki, J.W.Mclver; Modern Theoritical Chemistry, Plenum Press, New York, **8**, **(1977)**.

[18] M.J.S.Dewar, H.S.Rzepy, R.G.Parr, R.A.Donnelly, M.Levy; J.Am.Chem.Soc., **100**, 777 **(1978)**.

[19] J.J.P.Stewart; J.Comp.Chem., **10**, 209 **(1989)**.

[20] M.J.S.Dewar, T.F.Martia; J.Am.Chem.Soc., **91**, 796 **(1968)**.

[21] R.G.Parr, R.A.Donnely, M.Levy, W.E.Palke; J.Chem.Phys., **68**, 3801 **(1978)**.

[22] L.Pauling; 'The Nature of the Chemical Bond', Cornell University Press Ithaca, New York, **(1960)**.

[23] R.G.Pearson; Acc.Chem.Res., **26**, 250 **(1993)**.

[24] P.P.Singh, F.A.Pasha, H.K.Srivastava; QSAR & Combi.Sci., **22**, 843 **(2003)**.

[25] R.G.Parr, R.A.Donnelly, M.Levy, Palke; J.Chem. Phys., **68**, 380 **(1978)**.

[26] R.T.Sanderson; Chemical Bonds and Bond Energy, Academic, New York, **(1976)**.

[27] A.Cartier, J.L.Rivail; Chemom.Intell.Lab.Sys., **1**, 335 **(1987)**.

[28] J.Sotomatsu, Y.Murata, T.Fujita; J.Comput.Chem., **10**, 94 **(1989)**.

[29] R.Franke; 'Theoretical Drug Design Methods', Elsevier: Amster-dam, 115-123 **(1984)**.

[30] K.Fukui; 'Theory of Orientation and Stereoselection', Springer Verlag: New York, 34-39 **(1975)**.