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DFT Based Study of Charge Transfer and Interaction Energy Between Tin(IV) Halides and Derivatives of Pyridine

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ABSTRACT

Interaction of tin(IV) halides (chloride, bromide and iodide) have been discussed with eleven ortho, meta and para derivatives of pyridine i.e. total number of interactions are 33 x 3 = 99. Tin(IV) halides form most stable complexes with ortho, meta and para derivatives of phenylacetatopyridine and least stable complexes with ortho, meta and para derivatives of nitropyridine. The order is ortho > meta > para. Best interaction is shown by $SnBr_4$ with phenylacetatopyridine-m.

Key words: Donor, acceptor, DFT, interaction energy, charge transfer, energy lowering.

INTRODUCTION

The behavior of pyridinium ion with respect to nucleophilic addition and the behavior of pyridine oxide with respect to electrophilic substitution were first studied with the help of interaction energy [1-5]. The application of the concept was extended to organic chemistry by Pearson [6-8]. Recently, the interaction energy has been used for evaluation of metal-ligand bond strength [1-3]. With the help of this the acceptor strength of a series of metal halides and donor strength of organic bases have been studied. The organic bases that were classified were quinoline derivatives and derivatives of toluene. In this paper we have calculated the interaction energy of reactions of ortho, meta and para derivatives of eleven pyridine derivatives with tin(IV) halides. On the basis of the results, their relative acceptor and donor strength have been evaluated and are presented in this paper.

According to density functional theory, the interaction energy of molecules A and B is given by

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

Interaction energy [1] is also given by

$$\Delta E_{int} = \Delta E_{v} + \Delta E_{\mu} \qquad (2)$$

where

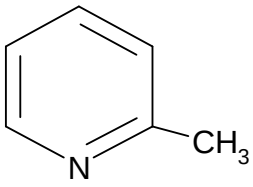
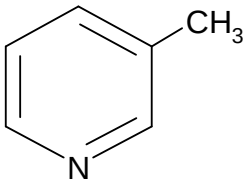
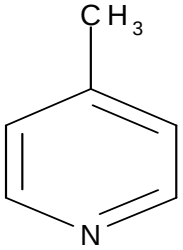
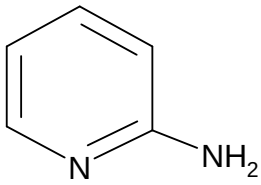
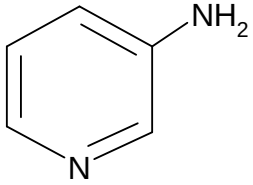
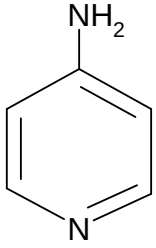
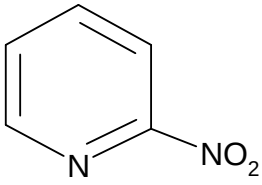
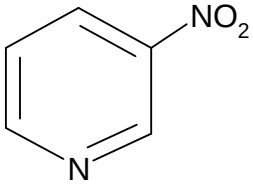
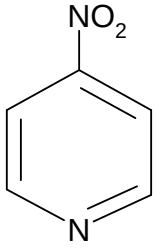
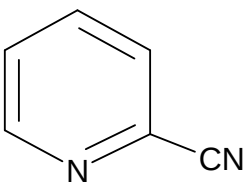
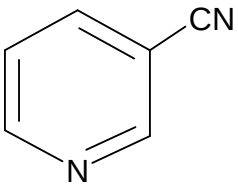
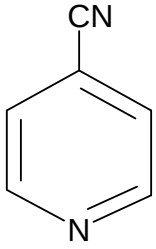
$$\Delta E_{v} \approx - \frac{1}{2} \frac{(\mu_A - \mu_B)^2}{S_A + S_B} S_A S_B \qquad (3)$$

and

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

where μ_A and μ_B are the chemical potential of A and B, S_A and S_B are their global softness, and λ is a constant related to an "effective number of valence electrons N_A and N_B" [10-13] and is proportional to $(N_A+N_B)^2$.

Table-1: Derivatives of pyridine (B) as donor molecules

Compound	Ortho Derivatives	Meta Derivatives	Para Derivatives
1 Methylpyridine			
2 Aminopyridine			
3 Nitropyridine			
4 Cyanopyridine			

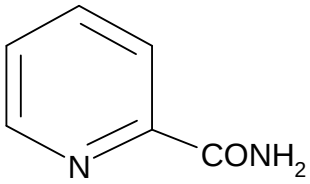
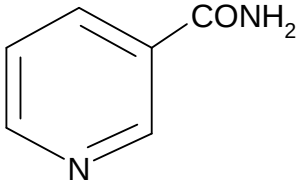
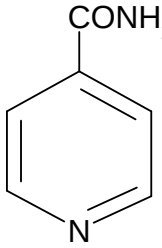
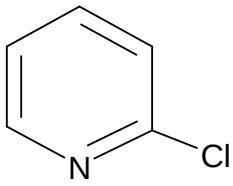
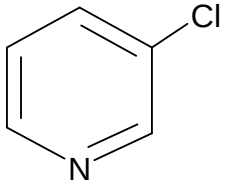
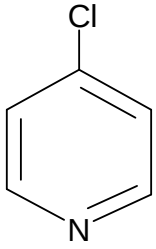
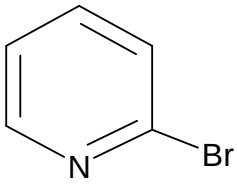
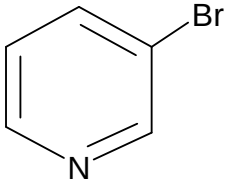
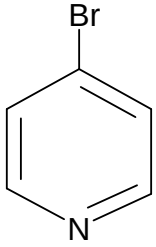
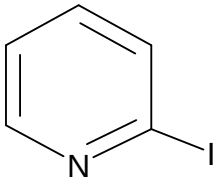
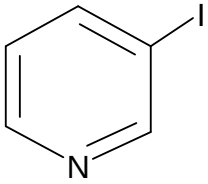
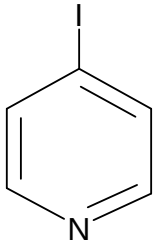
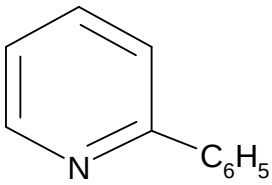
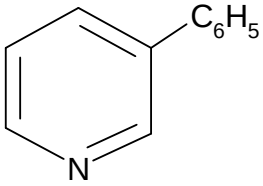
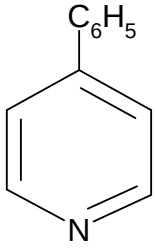
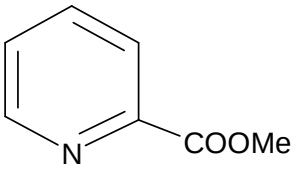
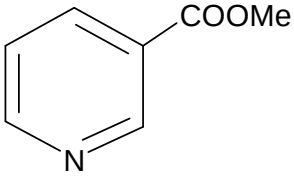
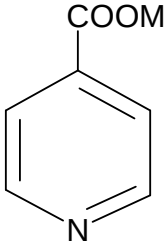
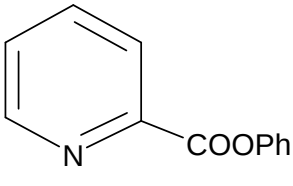
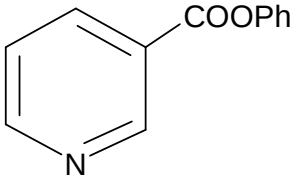
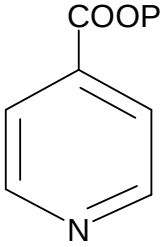
Compound	Ortho Derivatives	Meta Derivatives	Para Derivatives
5 Amidopyridine			
6 Chloropyridine			
7 Bromopyridine			
8 Iodopyridine			
9 Phenylpyridine			
10 Methylacetatopyridine			
11 Phenylacetatopyridine			

Table-2: List of Acceptor Molecules (A)

Name of acceptor(A)	Molecular formula of acceptor(A)
Tin(IV) Chloride	$SnCl_4$
Tin(IV) Bromide	$SnBr_4$
Tin(IV) Iodide	SnI_4

In this paper, we have taken eleven pyridine derivatives listed in Table-1 as donor molecules and tin(IV) halides listed in Table-2 as acceptor molecules. The structures of all the above compounds have been drawn and their geometries have been optimized with the help of Cache software by DFT PW91. HOMO and LUMO energies, chemical potential and number of free electrons calculated by DFT PW91 method of donors and acceptors are given in Table-3.

Table-3: Values of HOMO and LUMO energies alongwith number of valence electrons donors and acceptors

Compound	HOMO Energy (eV)	LUMO Energy (eV)	No. of valence electrons	Chemical Potential
Methylpyridine-o	-5.827	-1.621	36	-3.724
Methylpyridine-m	-5.83	-1.638	36	-3.734
Methylpyridine-p	-5.865	-1.638	36	-3.752
Aminopyridine-o	-5.042	-1.336	36	-3.189
Aminopyridine-m	-5.009	-1.388	36	-3.199
Aminopyridine-p	-5.374	-1.046	36	-3.210
Nitropyridine-o	-6.114	-4.646	46	-5.380
Nitropyridine-m	-6.299	-4.756	46	-5.528
Nitropyridine-p	-6.52	-5.004	46	-5.762
Cyanopyridine-o	-6.79	-2.939	38	-4.865
Cyanopyridine-m	-6.685	-2.933	38	-4.809
Cyanopyridine-p	-6.661	-3.177	38	-4.919
Amidopyridine-o	-5.702	-2.42	46	-4.061
Amidopyridine-m	-5.883	-2.459	46	-4.171
Amidopyridine-p	-6.101	-2.668	46	-4.385
Chloropyridine-o	-6.524	-2.129	36	-4.327
Chloropyridine-m	-6.303	-2.137	36	-4.220
Chloropyridine-p	-6.298	-2.086	36	-4.192
Bromopyridine-o	-6.358	-2.132	36	-4.245
Bromopyridine-m	-6.289	-2.131	36	-4.210
Bromopyridine-p	-6.276	-2.093	36	-4.185
Iodopyridine-o	-6.069	-2.14	36	-4.105
Iodopyridine-m	-6.177	-2.134	36	-4.156

Compound	HOMO Energy (eV)	LUMO Energy (eV)	No. of valence electrons	Chemical Potential
Iodopyridine-p	-6.251	-2.135	36	-4.193
Phenylpyridine-o	-5.746	-2.202	58	-3.974
Phenylpyridine-m	-5.841	-2.263	58	-4.052
Phenylpyridine-p	-5.986	-2.46	58	-4.223
Methylacetatopyridine-o	-6.067	-2.606	52	-4.337
Methylacetatopyridine-m	-6.151	-2.639	52	-4.395
Methylacetatopyridine-p	-6.216	-2.862	52	-4.539
Phenylacetatopyridine-o	-5.921	-2.784	74	-4.353
Phenylacetatopyridine-m	-6.111	-2.831	74	-4.471
Phenylacetatopyridine-p	-6.186	-3.037	74	-4.612
$SnCl_4$	-8.313	-4.411	32	-6.362
$SnBr_4$	-7.48	-4.229	32	-5.855
SnI_4	-6.707	-4.265	32	-5.486

The method of evaluation has been developed within the framework of density functional theory [1-11] and is based on hard and soft acids and bases principle of Pearson. The basis for the focus on electronegativity [12-13] and hardness [14-15] is provided by density functional theory (DFT), which guarantees that the ground state energy of many electron systems is a unique function of its density. For the change from one ground state to another of an electronic system, the change of electronic energy E(ρ) is given by the formula [16].

$$dE(\rho) = \mu\, dN + \int \rho(r)\, dv(r)\, dr \qquad (5)$$

where v(r) is the external electronic potential an electron at "r" experiences due to the nuclei, N is the number of electrons, and μ the chemical potential is defined as [17]

$$\mu = (\delta E / \delta N)v_{(r)} \qquad (6)$$

and the electron density $\rho_{(r)}$ is defined as [18]

$$\rho_{(r)} = [(\delta E / \delta v(r)]_N \qquad (7)$$

Parr et al [17] have shown that the electronegativity of any chemical species is equal to the negative value of chemical potential indeed it follows rigorously [18-19] that

$$\chi = -\mu = (I + A)/2 \qquad (8)$$

where I and A are ionization potential and electron affinity of atomic or molecular system. Eqn-8 may be written as:

$$A = 2\chi - I \qquad (9)$$

Density functional theory provides a quantum mechanical justification for electronegativity. A concept use intuitively for a long time and validates Sanderson's postulates [20] that when two

and more atoms combine to form a molecule, their electronegativity gets equalized and unique electronegativity exists everywhere in a molecule. [21]

According to Koopman's theorem the I and A are simply the eigen value of HOMO and LUMO respectively with change in sign [22]. Therefore, from equation-9 we get

$A = -(\varepsilon HOMO + \varepsilon LUMO) - I$ (10)

The chemical potential itself depend on N and v i.e. $\mu = \mu(N,v)$. Parr and Pearson[23] have defined hardness with respect to N as

$$\eta = \tfrac{1}{2}. (\delta\mu/\delta N)_{v(r)}$$

$$= \tfrac{1}{2}. (\delta^2 E/ \delta N^2)_{v(r)}$$

$$= (I - A)/2 \qquad (11)$$

When Lewis acid (electrophile) reacts with Lewis base (nucleophile) or when there is metal ligand interaction, there is a shift of electron from the Lewis base to Lewis acid, until the chemical potentials of both become equal [7]. The condition of equilibrium is that the chemical potential, μ_A and μ_B, become equal. This leads to shift in charge, ΔN, from less electronegative base (B) to more electronegative acid (A).

$$\Delta N = (\chi^o_A - \chi^o_B) / 2(\eta_A + \eta_B) \qquad (12)$$

Electron transfer leads to an energy lowering given by equation-13.

$$\Delta E = -(\chi^o_A - \chi^o_B)^2 / 4(\eta_A + \eta_B) \qquad (13)$$

In equations 5 and 6 the electronegativity difference derive the electron transfer, and the sum of hardness parameters inhibits it [24].

With the help of the values of interaction energy E_{int}, charge transfer ΔN and energy lowering ΔE the following have been evaluated-

1. The comparative acceptor strength of a set of metal halides.
2. The comparative donor ability of each donor molecule.
3. The magnitude of metal-ligand bond strength formed between organic ligand and metal halides.
4. The effect of ortho, meta and para substitution on donor ability.
5. Chemical potential and global softness values of donor and acceptor molecules.
6. The metal-ligand bond strength evaluated by E_{int}, ΔN and ΔE.
7.

RESULTS AND DISCUSSION

Metal-ligand bond strength

(a) with acceptor $SnCl_4$

Metal-ligand bond strength depends on the value of interaction energy (E_{int}). the bond strength increases as the value of interaction energy decreases. Values of interaction energy of ortho derivatives of donors with the acceptor $SnCl_4$ is shown in Table-4 which indicates that most stable complexes are formed by phenylacetatopyridine-o and least stable by nitropyridine-o with the acceptor $SnCl_4$. Exact order of complex formation is as under-

Phenylacetatopyridine-o> Phenylpyridine-o> Aminopyridine-o> Methylacetatopyridine-o> Amidopyridine-o> Methylpyridine-o> Iodopyridine-o> Bromopyridine-o> Chloropyridine-o > Cyanopyridine-o> Nitropyridine-o

Values of interaction energy of meta derivatives of donors with the acceptor $SnCl_4$ is shown in Table-5 which indicates that most stable complexes are formed by phenylacetatopyridine-m and least stable by nitropyridine-m with the acceptor $SnCl_4$. Exact order of complex formation is as under-

Phenylacetatopyridine-m> Phenylpyridine-m> Aminopyridine-m> Methylacetatopyridine-m > Amidopyridine-m> Methylpyridine-m> Iodopyridine-m> Bromopyridine-m> Chloropyridine-m> Cyanopyridine-m> Nitropyridine-m

Values of interaction energy of para derivatives of donors with the acceptor $SnCl_4$ is shown in Table-6 which indicates that most stable complexes are formed by phenylacetatopyridine-p and least stable by nitropyridine-p with the acceptor $SnCl_4$. Exact order of complex formation is as under-

Phenylacetatopyridine-p> Phenylpyridine-p> Aminopyridine-p> Methylacetatopyridine-p> Methylpyridine-p> Amidopyridine-p> Bromopyridine-p> Chloropyridine-p> Iodopyridine-p > Cyanopyridine-p> Nitropyridine-p

Table-4: Values of interaction energy of ortho derivatives of donors with the acceptor $SnCl_4$

Compound	μ_A	S_A	λ	Ev	Eμ	E_{int}
Methylpyridine-o	-3.724	0.476	2.312	-0.858	-1.170	-2.028
Aminopyridine-o	-3.189	0.540	2.312	-1.323	-1.099	-2.422
Nitropyridine-o	-5.380	1.362	3.042	-0.180	-0.811	-0.991
Cyanopyridine-o	-4.865	0.519	2.450	-0.289	-1.187	-1.476
Amidopyridine-o	-4.061	0.609	3.042	-0.737	-1.356	-2.093
Chloropyridine-o	-4.327	0.455	2.312	-0.499	-1.195	-1.694
Bromopyridine-o	-4.245	0.473	2.312	-0.551	-1.173	-1.724
Iodopyridine-o	-4.105	0.509	2.312	-0.651	-1.132	-1.782
Phenylpyridine-o	-3.974	0.564	4.050	-0.766	-1.880	-2.646
Methylacetatopyridine-o	-4.337	0.578	3.528	-0.557	-1.618	-2.175
Phenylacetatopyridine-o	-4.353	0.638	5.618	-0.574	-2.442	-3.016

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B =-6.362, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B = 0.513, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{\square}$,= 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 from the Tables 4-6 that the order of stable complex formation for ortho, meta and para derivatives of donors are almost in same order.

Further, metal-ligand bond strength increases with the increase in the value of charge transfer and decrease in the energy lowering. Tables 7-9 indicate that the least stable complex is formed

by nitropyridine-o with $SnCl_4$ and most stable with aminopyridine-o. Same order is for meta and para derivatives.

Table-5: Values of interaction energy of meta derivatives of donors with the acceptor $SnCl_4$

Compound	μ_A	S_A	λ	Ev	Eμ	E_{int}
Methylpyridine-m	-3.734	0.477	2.312	-0.853	-1.168	-2.021
Aminopyridine-m	-3.199	0.552	2.312	-1.330	-1.086	-2.416
Nitropyridine-m	-5.528	1.296	3.042	-0.128	-0.841	-0.969
Cyanopyridine-m	-4.809	0.533	2.450	-0.315	-1.172	-1.487
Amidopyridine-m	-4.171	0.584	3.042	-0.655	-1.387	-2.042
Chloropyridine-m	-4.220	0.480	2.312	-0.569	-1.165	-1.733
Bromopyridine-m	-4.210	0.481	2.312	-0.575	-1.163	-1.738
Iodopyridine-m	-4.156	0.495	2.312	-0.613	-1.148	-1.760
Phenylpyridine-m	-4.052	0.559	4.050	-0.713	-1.890	-2.603
Methylacetatopyridine-m	-4.395	0.569	3.528	-0.522	-1.630	-2.152
Phenylacetatopyridine-m	-4.471	0.610	5.618	-0.498	-2.503	-3.001

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B =-6.362, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B = 0.513, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{□}$,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

Table-6: Values of interaction energy of para derivatives of donors with the acceptor $SnCl_4$

Compound	μ_A	S_A	λ	Ev	Eμ	E_{int}
Methylpyridine-p	-3.752	0.473	2.312	-0.838	-1.173	-2.011
Aminopyridine-p	-3.210	0.462	2.312	-1.207	-1.186	-2.393
Nitropyridine-p	-5.762	1.319	3.042	-0.066	-0.830	-0.897
Cyanopyridine-p	-4.919	0.574	2.450	-0.282	-1.127	-1.409
Amidopyridine-p	-4.385	0.583	3.042	-0.533	-1.389	-1.922
Chloropyridine-p	-4.192	0.475	2.312	-0.580	-1.171	-1.751
Bromopyridine-p	-4.185	0.478	2.312	-0.586	-1.167	-1.753
Iodopyridine-p	-4.193	0.486	2.312	-0.587	-1.158	-1.745
Phenylpyridine-p	-4.223	0.567	4.050	-0.616	-1.875	-2.491
Methylacetatopyridine-p	-4.539	0.596	3.528	-0.458	-1.591	-2.049
Phenylacetatopyridine-p	-4.612	0.635	5.618	-0.435	-2.448	-2.882

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B = -6.362, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B = 0.513, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{□}$,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

Table-7: Values of ΔN and ΔE for the interaction of ortho derivatives of donors with the acceptor $SnCl_4$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-o	6.362	3.724	1.951	2.103	0.325	-0.429
Aminopyridine-o	6.362	3.189	1.951	1.853	0.417	-0.662
Nitropyridine-o	6.362	5.380	1.951	0.734	0.183	-0.090
Cyanopyridine-o	6.362	4.865	1.951	1.926	0.193	-0.145
Amidopyridine-o	6.362	4.061	1.951	1.641	0.320	-0.368
Chloropyridine-o	6.362	4.327	1.951	2.198	0.245	-0.250
Bromopyridine-o	6.362	4.245	1.951	2.113	0.260	-0.276
Iodopyridine-o	6.362	4.105	1.951	1.965	0.288	-0.325
Phenylpyridine-o	6.362	3.974	1.951	1.772	0.321	-0.383
Methylacetatopyridine-o	6.362	4.337	1.951	1.731	0.275	-0.279
Phenylacetatopyridine-o	6.362	4.353	1.951	1.569	0.285	-0.287

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

Table-8: Values of ΔN and ΔE for the interaction of meta derivatives of donors with the acceptor $SnCl_4$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-m	6.362	3.734	1.951	2.096	0.325	-0.427
Aminopyridine-m	6.362	3.199	1.951	1.811	0.421	-0.665
Nitropyridine-m	6.362	5.528	1.951	0.772	0.153	-0.064
Cyanopyridine-m	6.362	4.809	1.951	1.876	0.203	-0.158
Amidopyridine-m	6.362	4.171	1.951	1.712	0.299	-0.328
Chloropyridine-m	6.362	4.220	1.951	2.083	0.265	-0.284
Bromopyridine-m	6.362	4.210	1.951	2.079	0.267	-0.287
Iodopyridine-m	6.362	4.156	1.951	2.022	0.278	-0.306
Phenylpyridine-m	6.362	4.052	1.951	1.789	0.309	-0.357
Methylacetatopyridine-m	6.362	4.395	1.951	1.756	0.265	-0.261
Phenylacetatopyridine-m	6.362	4.471	1.951	1.640	0.263	-0.249

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

(b) with acceptor $SnBr_4$

Values of interaction energy of ortho derivatives of donors with the acceptor $SnBr_4$ is shown in Table-10 which indicates that most stable complexes are formed by phenylacetatopyridine-o and least stable by nitropyridine-o with the acceptor $SnBr_4$. Exact order of complex formation is as under-

Phenylacetatopyridine-o > Phenylpyridine-o > Aminopyridine-o > Methylacetatopyridine-o > Amidopyridine-o > Methylpyridine-o > Iodopyridine-o > Bromopyridine-o > Chloropyridine-o > Cyanopyridine-o > Nitropyridine-o

Table-9: Values of ΔN and ΔE for the interaction of para derivatives of donors with the acceptor $SnCl_4$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-p	6.362	3.752	1.951	2.114	0.321	-0.419
Aminopyridine-p	6.362	3.210	1.951	2.164	0.383	-0.604
Nitropyridine-p	6.362	5.762	1.951	0.758	0.111	-0.033
Cyanopyridine-p	6.362	4.919	1.951	1.742	0.195	-0.141
Amidopyridine-p	6.362	4.385	1.951	1.717	0.270	-0.267
Chloropyridine-p	6.362	4.192	1.951	2.106	0.267	-0.290
Bromopyridine-p	6.362	4.185	1.951	2.092	0.269	-0.293
Iodopyridine-p	6.362	4.193	1.951	2.058	0.271	-0.293
Phenylpyridine-p	6.362	4.223	1.951	1.763	0.288	-0.308
Methylacetatopyridine-p	6.362	4.539	1.951	1.677	0.251	-0.229
Phenylacetatopyridine-p	6.362	4.612	1.951	1.575	0.248	-0.217

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

Values of interaction energy of meta derivatives of donors with the acceptor $SnBr_4$ is shown in Table-11 which indicates that most stable complexes are formed by phenylacetatopyridine-m and least stable by nitropyridine-m with the acceptor $SnBr_4$. Exact order of complex formation is as under-

Phenylacetatopyridine-m > Phenylpyridine-m > Aminopyridine-m > Methylacetatopyridine-m > Amidopyridine-m > Methylpyridine-m > Iodopyridine-m > Bromopyridine-m > Chloropyridine-m > Cyanopyridine-m > Nitropyridine-m

Values of interaction energy of para derivatives of donors with the acceptor $SnBr_4$ is shown in Table-12 which indicates that most stable complexes are formed by phenylacetatopyridine-p and least stable by nitropyridine-p with the acceptor $SnBr_4$. Exact order of complex formation is as under-

Phenylacetatopyridine-p > Phenylpyridine-p > Aminopyridine-p > Methylacetatopyridine-p > Methylpyridine-p > Amidopyridine-p > Bromopyridine-p > Chloropyridine-p > Iodopyridine-p > Cyanopyridine-p > Nitropyridine-p

It is evident from the Tables 10-12 that the order of stable complex formation for ortho, meta and para derivatives of donors are almost in same order.

Values of ΔN and ΔE are given in Tables 13-15 which indicate that the least stable complex is formed by nitropyridine-o with $SnBr_4$ and most stable with aminopyridine-o. Same order is for meta and para derivatives.

Table-10: Values of interaction energy of ortho derivatives of donors with the acceptor $SnBr_4$

Compound	μ_A	S_A	λ	Eν	Eμ	E_{int}
Methylpyridine-o	-3.724	0.476	2.312	-0.609	-1.060	-1.669
Aminopyridine-o	-3.189	0.540	2.312	-1.021	-1.001	-2.022
Nitropyridine-o	-5.380	1.362	3.042	-0.048	-0.769	-0.817
Cyanopyridine-o	-4.865	0.519	2.450	-0.138	-1.080	-1.218
Amidopyridine-o	-4.061	0.609	3.042	-0.492	-1.242	-1.734
Chloropyridine-o	-4.327	0.455	2.312	-0.305	-1.080	-1.385
Bromopyridine-o	-4.245	0.473	2.312	-0.346	-1.062	-1.409
Iodopyridine-o	-4.105	0.509	2.312	-0.427	-1.028	-1.455
Phenylpyridine-o	-3.974	0.564	4.050	-0.520	-1.717	-2.237
Methylacetatopyridine-o	-4.337	0.578	3.528	-0.343	-1.479	-1.822
Phenylacetatopyridine-o	-4.353	0.638	5.618	-0.353	-2.242	-2.595

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B=-5.855, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B =0.615, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{□}$,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

Table-11: Values of interaction energy of meta derivatives of donors with the acceptor $SnBr_4$

Compound	μ_A	S_A	λ	Eν	Eμ	E_{int}
Methylpyridine-m	-3.734	0.477	2.312	-0.604	-1.058	-1.662
Aminopyridine-m	-3.199	0.552	2.312	-1.027	-0.990	-2.017
Nitropyridine-m	-5.528	1.296	3.042	-0.022	-0.796	-0.818
Cyanopyridine-m	-4.809	0.533	2.450	-0.156	-1.067	-1.223
Amidopyridine-m	-4.171	0.584	3.042	-0.425	-1.268	-1.693
Chloropyridine-m	-4.220	0.480	2.312	-0.360	-1.055	-1.416
Bromopyridine-m	-4.210	0.481	2.312	-0.365	-1.055	-1.420
Iodopyridine-m	-4.156	0.495	2.312	-0.396	-1.042	-1.437
Phenylpyridine-m	-4.052	0.559	4.050	-0.476	-1.725	-2.200
Methylacetatopyridine-m	-4.395	0.569	3.528	-0.315	-1.489	-1.804
Phenylacetatopyridine-m	-4.471	0.610	5.618	-0.293	-2.293	-2.586

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B=-5.855, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B =0.615, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{□}$,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

Table-12: Values of interaction energy of para derivatives of donors with the acceptor $SnBr_4$

Compound	μ_A	S_A	λ	Eν	Eμ	E_{int}
Methylpyridine-p	-3.752	0.473	2.312	-0.591	-1.062	-1.654
Aminopyridine-p	-3.210	0.462	2.312	-0.923	-1.073	-1.996
Nitropyridine-p	-5.762	1.319	3.042	-0.002	-0.786	-0.788
Cyanopyridine-p	-4.919	0.574	2.450	-0.130	-1.030	-1.160
Amidopyridine-p	-4.385	0.583	3.042	-0.323	-1.270	-1.593
Chloropyridine-p	-4.192	0.475	2.312	-0.370	-1.061	-1.431
Bromopyridine-p	-4.185	0.478	2.312	-0.375	-1.057	-1.432
Iodopyridine-p	-4.193	0.486	2.312	-0.375	-1.050	-1.425
Phenylpyridine-p	-4.223	0.567	4.050	-0.393	-1.713	-2.105
Methylacetatopyridine-p	-4.539	0.596	3.528	-0.262	-1.456	-1.718
Phenylacetatopyridine-p	-4.612	0.635	5.618	-0.241	-2.247	-2.488

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B=-5.855, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B =0.615, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{□}$,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

Table-13: Values of ΔN and ΔE for the interaction of ortho derivatives of donors with the acceptor $SnBr_4$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-o	5.855	3.724	1.626	2.103	0.286	-0.304
Aminopyridine-o	5.855	3.189	1.626	1.853	0.383	-0.511
Nitropyridine-o	5.855	5.380	1.626	0.734	0.101	-0.024
Cyanopyridine-o	5.855	4.865	1.626	1.926	0.139	-0.069
Amidopyridine-o	5.855	4.061	1.626	1.641	0.275	-0.246
Chloropyridine-o	5.855	4.327	1.626	2.198	0.200	-0.153
Bromopyridine-o	5.855	4.245	1.626	2.113	0.215	-0.173
Iodopyridine-o	5.855	4.105	1.626	1.965	0.244	-0.213
Phenylpyridine-o	5.855	3.974	1.626	1.772	0.277	-0.260
Methylacetatopyridine-o	5.855	4.337	1.626	1.731	0.226	-0.172
Phenylacetatopyridine-o	5.855	4.353	1.626	1.569	0.235	-0.177

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

Table-14: Values of ΔN and ΔE for the interaction of meta derivatives of donors with the acceptor $SnBr_4$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-m	5.855	3.734	1.626	2.096	0.285	-0.302
Aminopyridine-m	5.855	3.199	1.626	1.811	0.386	-0.513
Nitropyridine-m	5.855	5.528	1.626	0.772	0.068	-0.011
Cyanopyridine-m	5.855	4.809	1.626	1.876	0.149	-0.078
Amidopyridine-m	5.855	4.171	1.626	1.712	0.252	-0.212
Chloropyridine-m	5.855	4.220	1.626	2.083	0.220	-0.180
Bromopyridine-m	5.855	4.210	1.626	2.079	0.222	-0.183
Iodopyridine-m	5.855	4.156	1.626	2.022	0.233	-0.198
Phenylpyridine-m	5.855	4.052	1.626	1.789	0.264	-0.238
Methylacetatopyridine-m	5.855	4.395	1.626	1.756	0.216	-0.157
Phenylacetatopyridine-m	5.855	4.471	1.626	1.640	0.212	-0.147

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

Table-15: Values of ΔN and ΔE for the interaction of para derivatives of donors with the acceptor $SnBr_4$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-p	5.855	3.752	1.626	2.114	0.281	-0.296
Aminopyridine-p	5.855	3.210	1.626	2.164	0.349	-0.461
Nitropyridine-p	5.855	5.762	1.626	0.758	0.019	-0.001
Cyanopyridine-p	5.855	4.919	1.626	1.742	0.139	-0.065
Amidopyridine-p	5.855	4.385	1.626	1.717	0.220	-0.162
Chloropyridine-p	5.855	4.192	1.626	2.106	0.223	-0.185
Bromopyridine-p	5.855	4.185	1.626	2.092	0.225	-0.188
Iodopyridine-p	5.855	4.193	1.626	2.058	0.226	-0.187
Phenylpyridine-p	5.855	4.223	1.626	1.763	0.241	-0.196
Methylacetatopyridine-p	5.855	4.539	1.626	1.677	0.199	-0.131
Phenylacetatopyridine-p	5.855	4.612	1.626	1.575	0.194	-0.121

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

(c) with acceptor SnI_4

Values of interaction energy of ortho derivatives of donors with the acceptor SnI_4 is shown in Table-16 which indicates that most stable complexes are formed by phenylacetatopyridine-o and least stable by nitropyridine-o with the acceptor SnI_4. Exact order of complex formation is as under-

Phenylacetatopyridine-o > Phenylpyridine-o > Aminopyridine-o > Methylacetatopyridine-o > Amidopyridine-o > Methylpyridine-o > Iodopyridine-o > Bromopyridine-o > Chloropyridine-o > Cyanopyridine-o > Nitropyridine-o

Values of interaction energy of meta derivatives of donors with the acceptor SnI_4 is shown in Table-17 which indicates that most stable complexes are formed by phenylacetatopyridine-m and least stable by nitropyridine-m with the acceptor SnI_4. Exact order of complex formation is as under-

Phenylacetatopyridine-m> Phenylpyridine-m > Aminopyridine-m > Methylacetatopyridine-m > Amidopyridine-m > Methylpyridine-m > Iodopyridine-m > Bromopyridine-m > Chloropyridine-m > Cyanopyridine-m > Nitropyridine-m

Values of interaction energy of para derivatives of donors with the acceptor SnI_4 is shown in Table-18 which indicates that most stable complexes are formed by phenylacetatopyridine-p and least stable by nitropyridine-p with the acceptor SnI_4. Exact order of complex formation is as under-

Phenylacetatopyridine-p > Phenylpyridine-p > Aminopyridine-p > Methylacetatopyridine-p > Methylpyridine-p > Amidopyridine-p > Bromopyridine-p > Chloropyridine-p > Iodopyridine-p > Cyanopyridine-p > Nitropyridine-p

It is evident from the Tables 16-18 that the order of stable complex formation for ortho, meta and para derivatives of donors are almost in same order.

Values of ΔN and ΔE are given in Tables 19-21 which indicate that the least stable complex is formed by nitropyridine-o with $SnBr_4$ and most stable with aminopyridine-o. Same order is for meta and para derivatives.

Table-22 includes donors and acceptors arranged in decreasing order of interaction energy. A close look to Table-22 indicates that $SnCl_4$ forms most stable complexes with ortho, meta and para derivatives of phenylacetatopyridine and the order is ortho > meta > para.

It is also clear from the Table-22 that the least stable complexes are formed by nitropyridine-o with SnI_4.

Global Softness (S_A and S_B)

Best interaction is shown in the case in which S_A and S_B are approximately equal. This situation occurs in the case of interaction of donor phenylacetatopyridine-m with the acceptor $SnBr_4$ in which case S_A= 0.610 and S_B=0.615

CONCLUSION

- All metal halides form most stable complexes with the ortho, meta and para derivatives of the donor phenylacetatopyridine.
- All metal halides form least stable complexes with the ortho, meta and para derivatives of the donor nitropyridine.
- Order of stable complex formation for ortho, meta and para derivatives of donors with tin (IV) halides are almost in same order.
- Best interaction of $SnBr_4$ is shown with phenylacetatopyridine-m. In this case $S_A \approx S_B$.

Table-16: Values of interaction energy of ortho derivatives of donors with the acceptor SnI_4

Compound	μ_A	S_A	λ	Eν	Eμ	E_{int}
Methylpyridine-o	-3.724	0.476	2.312	-0.467	-0.893	-1.360
Aminopyridine-o	-3.189	0.540	2.312	-0.858	-0.851	-1.709
Nitropyridine-o	-5.380	1.362	3.042	-0.003	-0.697	-0.700
Cyanopyridine-o	-4.865	0.519	2.450	-0.061	-0.915	-0.977
Amidopyridine-o	-4.061	0.609	3.042	-0.355	-1.065	-1.420
Chloropyridine-o	-4.327	0.455	2.312	-0.197	-0.907	-1.104
Bromopyridine-o	-4.245	0.473	2.312	-0.231	-0.895	-1.126
Iodopyridine-o	-4.105	0.509	2.312	-0.300	-0.870	-1.170
Phenylpyridine-o	-3.974	0.564	4.050	-0.382	-1.464	-1.846
Methylacetatopyridine-o	-4.337	0.578	3.528	-0.224	-1.263	-1.487
Phenylacetatopyridine-o	-4.353	0.638	5.618	-0.230	-1.929	-2.159

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B=-5.486, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B =0.819, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{□}$,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

Table-17: Values of interaction energy of meta derivatives of donors with the acceptor SnI_4

Compound	μ_A	S_A	λ	Eν	Eμ	E_{int}
Methylpyridine-m	-3.734	0.477	2.312	-0.463	-0.892	-1.355
Aminopyridine-m	-3.199	0.552	2.312	-0.863	-0.843	-1.706
Nitropyridine-m	-5.528	1.296	3.042	0.000	-0.719	-0.720
Cyanopyridine-m	-4.809	0.533	2.450	-0.074	-0.906	-0.980
Amidopyridine-m	-4.171	0.584	3.042	-0.295	-1.084	-1.379
Chloropyridine-m	-4.220	0.480	2.312	-0.243	-0.890	-1.132
Bromopyridine-m	-4.210	0.481	2.312	-0.247	-0.889	-1.136
Iodopyridine-m	-4.156	0.495	2.312	-0.273	-0.880	-1.153
Phenylpyridine-m	-4.052	0.559	4.050	-0.342	-1.470	-1.811
Methylacetatopyridine-m	-4.395	0.569	3.528	-0.200	-1.270	-1.470
Phenylacetatopyridine-m	-4.471	0.610	5.618	-0.180	-1.966	-2.146

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B=-5.486, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B =0.819, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{□}$,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

Table-18: Values of interaction energy of para derivatives of donors with the acceptor SnI_4

Compound	μ_A	S_A	λ	Eν	Eμ	E_{int}
Methylpyridine-p	-3.752	0.473	2.312	-0.838	-1.173	-2.011
Aminopyridine-p	-3.210	0.462	2.312	-1.207	-1.186	-2.393
Nitropyridine-p	-5.762	1.319	3.042	-0.066	-0.830	-0.897
Cyanopyridine-p	-4.919	0.574	2.450	-0.282	-1.127	-1.409
Amidopyridine-p	-4.385	0.583	3.042	-0.533	-1.389	-1.922
Chloropyridine-p	-4.192	0.475	2.312	-0.580	-1.171	-1.751

Bromopyridine-p	-4.185	0.478	2.312	-0.586	-1.167	-1.753
Iodopyridine-p	-4.193	0.486	2.312	-0.587	-1.158	-1.745
Phenylpyridine-p	-4.223	0.567	4.050	-0.616	-1.875	-2.491
Methylacetatopyridine-p	-4.539	0.596	3.528	-0.458	-1.591	-2.049
Phenylacetatopyridine-p	-4.612	0.635	5.618	-0.435	-2.448	-2.882

μA=Chemical potential of donor molecule A, μB=Chemical potential of acceptor molecule B=-5.486, S_A=Global Softness of donor molecule A, S_B=Global Softness of acceptor molecule B =0.819, N_A = total number of electrons in donor molecule A, N_B = total number of electrons in acceptor molecule B, $\lambda = (N_A + N_B)^2 / 2000$, $E_{\square}$,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

Table-19: Values of ΔN and ΔE for the interaction of ortho derivatives of donors with the acceptor SnI_4

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-o	5.486	3.724	1.221	2.103	0.265	-0.234
Aminopyridine-o	5.486	3.189	1.221	1.853	0.374	-0.429
Nitropyridine-o	5.486	5.380	1.221	0.734	0.027	-0.001
Cyanopyridine-o	5.486	4.865	1.221	1.926	0.099	-0.031
Amidopyridine-o	5.486	4.061	1.221	1.641	0.249	-0.177
Chloropyridine-o	5.486	4.327	1.221	2.198	0.170	-0.098
Bromopyridine-o	5.486	4.245	1.221	2.113	0.186	-0.115
Iodopyridine-o	5.486	4.105	1.221	1.965	0.217	-0.150
Phenylpyridine-o	5.486	3.974	1.221	1.772	0.253	-0.191
Methylacetatopyridine-o	5.486	4.337	1.221	1.731	0.195	-0.112
Phenylacetatopyridine-o	5.486	4.353	1.221	1.569	0.203	-0.115

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

Table-20: Values of ΔN and ΔE for the interaction of meta derivatives of donors with the acceptor SnI_4

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-m	5.486	3.734	1.221	2.096	0.264	-0.231
Aminopyridine-m	5.486	3.199	1.221	1.811	0.377	-0.432
Nitropyridine-m	5.486	5.528	1.221	0.772	-0.010	0.000
Cyanopyridine-m	5.486	4.809	1.221	1.876	0.109	-0.037
Amidopyridine-m	5.486	4.171	1.221	1.712	0.224	-0.147
Chloropyridine-m	5.486	4.220	1.221	2.083	0.192	-0.121
Bromopyridine-m	5.486	4.210	1.221	2.079	0.193	-0.123
Iodopyridine-m	5.486	4.156	1.221	2.022	0.205	-0.136
Phenylpyridine-m	5.486	4.052	1.221	1.789	0.238	-0.171
Methylacetatopyridine-m	5.486	4.395	1.221	1.756	0.183	-0.100
Phenylacetatopyridine-m	5.486	4.471	1.221	1.640	0.177	-0.090

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

Table-21: Values of ΔN and ΔE for the interaction of para derivatives of donors with the acceptor SnI_4

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Methylpyridine-p	5.486	3.752	1.221	2.114	0.260	-0.226
Aminopyridine-p	5.486	3.210	1.221	2.164	0.336	-0.383
Nitropyridine-p	5.486	5.762	1.221	0.758	-0.070	-0.010
Cyanopyridine-p	5.486	4.919	1.221	1.742	0.096	-0.027
Amidopyridine-p	5.486	4.385	1.221	1.717	0.187	-0.103
Chloropyridine-p	5.486	4.192	1.221	2.106	0.194	-0.126
Bromopyridine-p	5.486	4.185	1.221	2.092	0.196	-0.128
Iodopyridine-p	5.486	4.193	1.221	2.058	0.197	-0.127
Phenylpyridine-p	5.486	4.223	1.221	1.763	0.212	-0.134
Methylacetatopyridine-p	5.486	4.539	1.221	1.677	0.163	-0.077
Phenylacetatopyridine-p	5.486	4.612	1.221	1.575	0.156	-0.068

χ^o_A = Electronegativity of acceptor, χ^o_B = Electronegativity of donor, η_A = absolute hardness of acceptor, η_B = absolute hardness of donor, ΔN = Charge transfer, ΔE = Energy lowering

Table-22: Metal-ligand bond strength arranged in decreasing order

Donor	Acceptor	μ_A	S_A	λ	Eν	Eμ	E_{int}
Phenylacetatopyridine-o	$SnCl_4$	-4.353	0.638	5.618	-0.574	-2.442	-3.016
Phenylacetatopyridine-m	$SnCl_4$	-4.471	0.61	5.618	-0.498	-2.503	-3.001
Phenylacetatopyridine-p	$SnCl_4$	-4.612	0.635	5.618	-0.435	-2.448	-2.882
Phenylacetatopyridine-p	SnI_4	-4.612	0.635	5.618	-0.435	-2.448	-2.882
Phenylpyridine-o	$SnCl_4$	-3.974	0.564	4.05	-0.766	-1.88	-2.646
Phenylpyridine-m	$SnCl_4$	-4.052	0.559	4.05	-0.713	-1.89	-2.603
Phenylacetatopyridine-o	$SnBr_4$	-4.353	0.638	5.618	-0.353	-2.242	-2.595
Phenylacetatopyridine-m	$SnBr_4$	-4.471	0.61	5.618	-0.293	-2.293	-2.586
Phenylpyridine-p	$SnCl_4$	-4.223	0.567	4.05	-0.616	-1.875	-2.491
Phenylpyridine-p	SnI_4	-4.223	0.567	4.05	-0.616	-1.875	-2.491
Phenylacetatopyridine-p	$SnBr_4$	-4.612	0.635	5.618	-0.241	-2.247	-2.488
Aminopyridine-o	$SnCl_4$	-3.189	0.54	2.312	-1.323	-1.099	-2.422
Aminopyridine-m	$SnCl_4$	-3.199	0.552	2.312	-1.33	-1.086	-2.416
Aminopyridine-p	$SnCl_4$	-3.21	0.462	2.312	-1.207	-1.186	-2.393
Aminopyridine-p	SnI_4	-3.21	0.462	2.312	-1.207	-1.186	-2.393
Phenylpyridine-o	$SnBr_4$	-3.974	0.564	4.05	-0.52	-1.717	-2.237
Phenylpyridine-m	$SnBr_4$	-4.052	0.559	4.05	-0.476	-1.725	-2.2
Methylacetatopyridine-o	$SnCl_4$	-4.337	0.578	3.528	-0.557	-1.618	-2.175
Phenylacetatopyridine-o	SnI_4	-4.353	0.638	5.618	-0.23	-1.929	-2.159
Methylacetatopyridine-m	$SnCl_4$	-4.395	0.569	3.528	-0.522	-1.63	-2.152
Phenylacetatopyridine-m	SnI_4	-4.471	0.61	5.618	-0.18	-1.966	-2.146
Phenylpyridine-p	$SnBr_4$	-4.223	0.567	4.05	-0.393	-1.713	-2.105
Amidopyridine-o	$SnCl_4$	-4.061	0.609	3.042	-0.737	-1.356	-2.093

Donor	Acceptor	μ_A	S_A	λ	Eν	Eμ	E_{int}
Methylacetatopyridine-p	$SnCl_4$	-4.539	0.596	3.528	-0.458	-1.591	-2.049
Methylacetatopyridine-p	SnI_4	-4.539	0.596	3.528	-0.458	-1.591	-2.049
Amidopyridine-m	$SnCl_4$	-4.171	0.584	3.042	-0.655	-1.387	-2.042
Methylpyridine-o	$SnCl_4$	-3.724	0.476	2.312	-0.858	-1.17	-2.028
Aminopyridine-o	$SnBr_4$	-3.189	0.54	2.312	-1.021	-1.001	-2.022
Methylpyridine-m	$SnCl_4$	-3.734	0.477	2.312	-0.853	-1.168	-2.021
Aminopyridine-m	$SnBr_4$	-3.199	0.552	2.312	-1.027	-0.99	-2.017
Methylpyridine-p	$SnCl_4$	-3.752	0.473	2.312	-0.838	-1.173	-2.011
Methylpyridine-p	SnI_4	-3.752	0.473	2.312	-0.838	-1.173	-2.011
Aminopyridine-p	$SnBr_4$	-3.21	0.462	2.312	-0.923	-1.073	-1.996
Amidopyridine-p	$SnCl_4$	-4.385	0.583	3.042	-0.533	-1.389	-1.922
Amidopyridine-p	SnI_4	-4.385	0.583	3.042	-0.533	-1.389	-1.922
Phenylpyridine-o	SnI_4	-3.974	0.564	4.05	-0.382	-1.464	-1.846
Methylacetatopyridine-o	$SnBr_4$	-4.337	0.578	3.528	-0.343	-1.479	-1.822
Phenylpyridine-m	SnI_4	-4.052	0.559	4.05	-0.342	-1.47	-1.811
Methylacetatopyridine-m	$SnBr_4$	-4.395	0.569	3.528	-0.315	-1.489	-1.804
Iodopyridine-o	$SnCl_4$	-4.105	0.509	2.312	-0.651	-1.132	-1.782
Iodopyridine-m	$SnCl_4$	-4.156	0.495	2.312	-0.613	-1.148	-1.76
Bromopyridine-p	$SnCl_4$	-4.185	0.478	2.312	-0.586	-1.167	-1.753
Bromopyridine-p	SnI_4	-4.185	0.478	2.312	-0.586	-1.167	-1.753
Chloropyridine-p	$SnCl_4$	-4.192	0.475	2.312	-0.58	-1.171	-1.751
Chloropyridine-p	SnI_4	-4.192	0.475	2.312	-0.58	-1.171	-1.751
Iodopyridine-p	$SnCl_4$	-4.193	0.486	2.312	-0.587	-1.158	-1.745
Iodopyridine-p	SnI_4	-4.193	0.486	2.312	-0.587	-1.158	-1.745
Bromopyridine-m	$SnCl_4$	-4.21	0.481	2.312	-0.575	-1.163	-1.738
Amidopyridine-o	$SnBr_4$	-4.061	0.609	3.042	-0.492	-1.242	-1.734
Chloropyridine-m	$SnCl_4$	-4.22	0.48	2.312	-0.569	-1.165	-1.733
Bromopyridine-o	$SnCl_4$	-4.245	0.473	2.312	-0.551	-1.173	-1.724
Methylacetatopyridine-p	$SnBr_4$	-4.539	0.596	3.528	-0.262	-1.456	-1.718
Aminopyridine-o	SnI_4	-3.189	0.54	2.312	-0.858	-0.851	-1.709
Aminopyridine-m	SnI_4	-3.199	0.552	2.312	-0.863	-0.843	-1.706
Chloropyridine-o	$SnCl_4$	-4.327	0.455	2.312	-0.499	-1.195	-1.694
Amidopyridine-m	$SnBr_4$	-4.171	0.584	3.042	-0.425	-1.268	-1.693
Methylpyridine-o	$SnBr_4$	-3.724	0.476	2.312	-0.609	-1.06	-1.669
Methylpyridine-m	$SnBr_4$	-3.734	0.477	2.312	-0.604	-1.058	-1.662
Methylpyridine-p	$SnBr_4$	-3.752	0.473	2.312	-0.591	-1.062	-1.654
Amidopyridine-p	$SnBr_4$	-4.385	0.583	3.042	-0.323	-1.27	-1.593
Cyanopyridine-m	$SnCl_4$	-4.809	0.533	2.45	-0.315	-1.172	-1.487
Methylacetatopyridine-o	SnI_4	-4.337	0.578	3.528	-0.224	-1.263	-1.487
Cyanopyridine-o	$SnCl_4$	-4.865	0.519	2.45	-0.289	-1.187	-1.476
Methylacetatopyridine-m	SnI_4	-4.395	0.569	3.528	-0.2	-1.27	-1.47

Donor	Acceptor	μ_A	S_A	λ	Ev	Eμ	E_{int}
Iodopyridine-o	$SnBr_4$	-4.105	0.509	2.312	-0.427	-1.028	-1.455
Iodopyridine-m	$SnBr_4$	-4.156	0.495	2.312	-0.396	-1.042	-1.437
Bromopyridine-p	$SnBr_4$	-4.185	0.478	2.312	-0.375	-1.057	-1.432
Chloropyridine-p	$SnBr_4$	-4.192	0.475	2.312	-0.37	-1.061	-1.431
Iodopyridine-p	$SnBr_4$	-4.193	0.486	2.312	-0.375	-1.05	-1.425
Bromopyridine-m	$SnBr_4$	-4.21	0.481	2.312	-0.365	-1.055	-1.42
Amidopyridine-o	SnI_4	-4.061	0.609	3.042	-0.355	-1.065	-1.42
Chloropyridine-m	$SnBr_4$	-4.22	0.48	2.312	-0.36	-1.055	-1.416
Cyanopyridine-p	$SnCl_4$	-4.919	0.574	2.45	-0.282	-1.127	-1.409
Bromopyridine-o	$SnBr_4$	-4.245	0.473	2.312	-0.346	-1.062	-1.409
Cyanopyridine-p	SnI_4	-4.919	0.574	2.45	-0.282	-1.127	-1.409
Chloropyridine-o	$SnBr_4$	-4.327	0.455	2.312	-0.305	-1.08	-1.385
Amidopyridine-m	SnI_4	-4.171	0.584	3.042	-0.295	-1.084	-1.379
Methylpyridine-o	SnI_4	-3.724	0.476	2.312	-0.467	-0.893	-1.36
Methylpyridine-m	SnI_4	-3.734	0.477	2.312	-0.463	-0.892	-1.355
Cyanopyridine-m	$SnBr_4$	-4.809	0.533	2.45	-0.156	-1.067	-1.223
Cyanopyridine-o	$SnBr_4$	-4.865	0.519	2.45	-0.138	-1.08	-1.218
Iodopyridine-o	SnI_4	-4.105	0.509	2.312	-0.3	-0.87	-1.17
Cyanopyridine-p	$SnBr_4$	-4.919	0.574	2.45	-0.13	-1.03	-1.16
Iodopyridine-m	SnI_4	-4.156	0.495	2.312	-0.273	-0.88	-1.153
Bromopyridine-m	SnI_4	-4.21	0.481	2.312	-0.247	-0.889	-1.136
Chloropyridine-m	SnI_4	-4.22	0.48	2.312	-0.243	-0.89	-1.132
Bromopyridine-o	SnI_4	-4.245	0.473	2.312	-0.231	-0.895	-1.126
Chloropyridine-o	SnI_4	-4.327	0.455	2.312	-0.197	-0.907	-1.104
Nitropyridine-o	$SnCl_4$	-5.38	1.362	3.042	-0.18	-0.811	-0.991
Cyanopyridine-m	SnI_4	-4.809	0.533	2.45	-0.074	-0.906	-0.98
Cyanopyridine-o	SnI_4	-4.865	0.519	2.45	-0.061	-0.915	-0.977
Nitropyridine-m	$SnCl_4$	-5.528	1.296	3.042	-0.128	-0.841	-0.969
Nitropyridine-p	$SnCl_4$	-5.762	1.319	3.042	-0.066	-0.83	-0.897
Nitropyridine-p	SnI_4	-5.762	1.319	3.042	-0.066	-0.83	-0.897
Nitropyridine-m	$SnBr_4$	-5.528	1.296	3.042	-0.022	-0.796	-0.818
Nitropyridine-o	$SnBr_4$	-5.38	1.362	3.042	-0.048	-0.769	-0.817
Nitropyridine-p	$SnBr_4$	-5.762	1.319	3.042	-0.002	-0.786	-0.788
Nitropyridine-m	SnI_4	-5.528	1.296	3.042	0	-0.719	-0.72
Nitropyridine-o	SnI_4	-5.38	1.362	3.042	-0.003	-0.697	-0.7

REFERENCES

[1] D Singh; S Ahmad; PP Singh, *Journal of Molecular Structure: THEOCHEM*. **2009**, 905, 13.
[2] PP Singh; PP Agrawal; MK Pandey. *Organic Chemistry: An Indian Journal*, **2010**, 5(2), 8.
[3] PP Singh; P Kumar ; AK Srivastava. *Organic Chemistry: An Indian Journal*, **2010**, 6(2), 12.
[4] F Mendez; JL Gazquez. *Proc. Indian Acad. Sci.*, **1994**, 106, 183.

[5] JL Gázquez; F. Méndez. *J. Phys. Chem*., **1993**, 98, 4591.
[6] RG Parr; RG Pearson. *J. Am. Chem. Soc*., **1983**, 105, 7512.
[7] RG Pearson. *J. Am. Chem. Soc*., **1988**, 110, 2092.
[8] RG Pearson. *J. Chem. Educ*., **1987**, 64, 561.
[9] JL Gazquez; KD Sen. Chemical hardness: Structure and Bonding 80 (ed.) (Berlin: Springer – Verlag), **1993.**
[10] RG Parr; JL Gazquez. *J. Phys. Chem*., **1993**, 97, 3939.
[11] RG Parr; PK Chattaraj. *J. Am. Chem. Soc*., **1991**, 113, 1855.
[12] RG Parr; W Yang. Density functional theory of atoms and molecules, New York: Oxford University Press, **1989.**
[13] W Yang; RG Parr. *Proc. Natl. Acad. Sci. USA*, **1985**, 82, 6723.
[14] RG Parr; PK Chattaraj. *J. Am. Chem. Soc*., **1991**, 113, 1854.
[15] CJ Umrigar; MP Nightingale; KJ Runge. *J. Chem. Phys*., **1993**, 99, 2865.
[16] A Mushinski; MP Nightingale. *J. Chem. Phys*., **1994**, 101, 883.
[17] RG Parr; Z Zhou. *Acc. Chem. Res*., **1993**, 26, 256.
[18] FD Proft; P Geerlings. *J. Chem. Phys*., **1997**, 106, 3270.
[19] S Shankar. *Proc Natl. Acad. Sci. USA*, **1985**, 82, 264.
[20] RT Sanderson. Academic Press, New York, **1976.**
[21] MJS Dewar; TF Morita. *J. Am. Chem. Soc*., **1969**, 91, 796.
[22] G Klopman. *J. Am. Chem. Soc*., **1968**, 90, 223.
[23] PP Singh; FA Pasha; HK Srivastava. *QSAR & Combi. Sci*., **2003**, 22, 84.