June 2009 *Volume 4 Issue 2*

Trade Science Inc.

Inorganic CHEMISTRY

An Indian Journal

Full Paper

ICAIJ, 4(2), 2009 [45-58]

Interaction energy, charge transfer and energy lowering in metal-ligand interaction

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Received: 29th April, 2009 ; Accepted: 4th May, 2009

ABSTRACT

Calculations of interaction energy (E_{int}), charge transfer (ΔN) and lowering of energy (ΔE) between acceptor metal halides (chloride, bromide and iodide) of tin, zinc, mercury, cadmium and donor organic bases (8-nitroquinoline> quinolinic acid> isoquinoline>quinoline>2-aminoquinoline>8-quinoline sulphonicacid> 2-phenylquinoline>5-nitroquinoline) have been done by DFT-B88PW91 method using CAChe software. The results indicate that acceptor strength is in the order $SnCl_4$>$HgCl_2$>$SnBr_4$>$HgBr_2$>SnI_4>$CdCl_2$> HgI_2>$ZnCl_2$> $CdBr_2$>$ZnBr_2$>CdI_2>ZnI_2 and the base strength is in the order 8-nitroquinoline> quinolinic acid>isoquinoline>quinoline>2-aminoquinoline>8-quinolinesulphonic acid>2-phenylquinoline>5-nitroquinoline in most of the cases. The results obtained by interaction energy, charge transfer and lowering of energy give almost the same result. The values of energy transfer ($\Delta E\mu$) showed that the complex formation capability is in the sequence chloride>bromide>iodide.

KEYWORDS

DFT method;
Interaction energy;
Charge transfer;
Lowering of energy;
Donor;
Acceptor.

INTRODUCTION

Very recently a new method for evaluating the magnitude of metal-ligand interaction has been described ("DFT based calculation of interaction energy between metal halides and organic bases", DOI=10.1016/j. theochem. 2009.03.002). The evaluation is based on calculation of interaction energy for interaction between metal halide and organic bases.

Interaction between 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 in terms of interaction energy[1] is given by equation-1 according to density functional theory.

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

The HSAB principle has been interpreted as the result of two opposing tendencies, one related to the charge transfer process, and the other one related to the reshuffling of the electronic density. This interpretation is the result of making the assumption that the interaction energy between two chemical species A and B, may be divided into two steps which can be taken as happening in succession, that is the interaction energy[2] is given by

$$\Delta E_{int} = \Delta E\nu + \Delta E\mu \quad (2)$$

where

$$\Delta E\nu \approx -1/2((\mu_A - \mu_B)^2 / S_A + S_B)S_A S_B \quad (3)$$

and

$$\Delta E\mu \approx -1/2\ (\lambda/S\ S_A + S_B) \quad (4)$$

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" that participate in the

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interaction between A and B.

The first term $\Delta E\nu$, corresponds to the charge transfer process between A and B arising from the chemical potential equalization principle at constant external potential. The second term, $\Delta E\mu$, corresponds to a reshuffling of the charge distribution, and it is basically a manifestation of the maximum hardness principle. In the original derivation[3] of Eqn.-4, the proportionality factor was given by the product of constant times the square of the total number of the electrons (N_A+N_B). However, using the hardness functional and the properties of the hardness and softness kernels, it was shown[4] that the correct proportionality factor is given by the product of a constant times the square of an "effective number of valence electron". Thus in equation-4, we have replaced this product by another constant λ.

Analysis of the equation-3 indicates that for a given value of S_A the larger the value of S_B the better, while equation-4 indicates that for the same value of S_A, the smaller the value of S_B the better. Since the total energy is given by the summation of these two terms, it seems that the best situation corresponds to the average between the two extreme situations, that is $S_A \approx S_B$, which is precisely the global HSAB principle. A similar analysis, based on the two opposing tendencies was first given by Chattaraj et al[5]. The S_A value of $SnCl_4$ if two values are equal the best interaction is shown between them. This observation is in conformity with the observation of Chattaraj[5]. The application of the concept has been extended to organic chemistry by Pearson[6]. We in this paper present the application of interaction energy for interaction between metal halides ($SnCl_4$, $SnBr_4$, SnI_4, $ZnCl_2$, $ZnBr_2$, ZnI_2, $CdCl_2$, $CdBr_2$, CdI_2, $HgCl_2$, $HgBr_2$ and HgI_2) and derivatives of quinolines.

MATERIAL AND METHOD

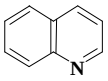
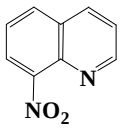
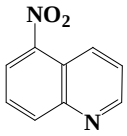
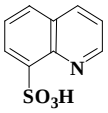
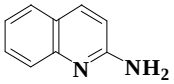
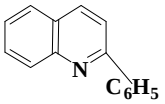
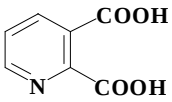
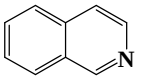
The study materials of this paper are 8 organic bases listed in TABLE 1, which have been used as a donor molecule. Twelve metal halides listed in TABLE 2 have been used as acceptor molecule. The structures of all the above compounds have been drawn and their geometries have been optimized with the help of Cache software by DFT method using the basis DZVP.

The essential values of chemical potential, softness, numbers of electron, and lambda have been obtained by solving the equation described below.

TABLE 1: A series of twelve lewis acids (A)

S. no.	Lewis acids (A)	S. no.	Lewis acids (A)
1	$SnCl_4$	7	$CdCl_2$
2	$SnBr_4$	8	$CdBr_2$
3	SnI_4	9	CdI_2
4	$ZnCl_2$	10	$HgCl_2$
5	$ZnBr_2$	11	$HgBr_2$
6	ZnI_2	12	HgI_2

TABLE 2: A series of eight quinoline derivatives as organic bases (B)

S. no.	Organic bases (:B)	Structure
1	Quinoline	
2	5-Nitroqinoline	
3	8-Nitroquinoline	
4	8-Quinolinesulphonic acid	
5	2-Aminoquinoline	
6	2-Phenylquinoline	
7	Quinolinic acid	
8	Isoquinoline	

The method of evaluation has been developed within the framework of density functional theory[7-12] and is based on hard and soft acids and bases principle of Pearson. The basis for the focus on electronegativity [13-14] and hardness[15-16] 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 $E(\rho)$ is given by the formula[17].

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

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[18]

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

and the electron density $\rho_{(r)}$ is defined as[19].

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

Parr et al.[18] have shown that the electronegativity of any chemical species is equal to the negative value of chemical potential indeed it follows rigorously[20] that

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

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

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

Density functional theory provides a quantum mechanical justification for electronegativity. A concept use intuitively for a long time and validates Sanderson's postulates[21] that when two and more atoms combine to form a molecule, their electronegativity gets equalized and unique electronegativity exists everywhere in a molecule[22].

According to Koopman's theorem the I and A are simply the eigen value of HOMO and LUMO respectively with change in sign[23]. Therefore, from equation-9 we get

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

The chemical potential itself depend on N and v i.e. $\mu = \mu(N,v)$. Parr and Pearson[24] have defined hardness with respect to N as

$$\eta = \tfrac{1}{2}.(\delta\mu/\delta N)_{v(r)} = \tfrac{1}{2}.(\delta^2 E/\delta N^2)_{v(r)} = (I - A)/2 \quad (11)$$

RESULT AND DISCUSSION

Donor acceptor interaction

The donor acceptor interaction between 8 donor molecules listed in TABLE 1 and twelve acceptor molecules listed in TABLE 2 has been studied in terms of metal ligand interaction energy (E_{int}) In total there are 96 (8×12) interactions. The interaction energy of disubstituted donors and metal halides are presented in TABLES 3 to 14.

A reference to TABLE 3-14 where the interaction

TABLE 3: Interaction of acceptor molecule $SnCl_4$ (A) with organic bases (B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	64.00	-0.661	-29.270	-29.931
5-Nitroquinoline	-10.816	-0.405	64	92.16	19.089	-427.532	-408.443
8-Nitroquinoline	-11.647	-1.012	64	92.16	-14.507	92.331	77.824
8-Quinolinesulphonic acid	-4.695	0.606	72	108.16	-0.386	-48.345	-48.731
2-Aminoquinoline	-3.497	0.656	54	73.96	-1.182	-31.635	-32.817
2-Phenylquinoline	-4.099	0.657	76	116.64	-0.737	-49.845	-50.583
Quinolinic acid	-11.197	-1.040	62	88.36	-11.819	83.842	72.023
Isoquinoline	-4.121	0.590	48	64.000	-0.689	-29.029	-29.718

Values of μ_A, S_A and N_A for acceptor molecule $SnCl_4$ (A)

μ_A	S_A	N_A
-6.362	0.513	32

TABLE 4: Interaction of acceptor molecule $SnBr_4$ (A) with organic bases (B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	64.000	-0.430	-26.758	-27.188
5-Nitroquinoline	-10.816	-0.405	64	92.160	14.563	-218.992	-204.429
8-Nitroquinoline	-11.647	-1.012	64	92.160	-26.332	116.235	89.903
8-Quinolinesulphonic acid	-4.695	0.606	72	108.160	-0.205	-44.282	-44.488
2-Aminoquinoline	-3.497	0.656	54	73.960	-0.883	-29.082	-29.965
2-Phenylquinoline	-4.099	0.657	76	116.640	-0.490	-45.825	-46.315
Quinolinic acid	-11.197	-1.040	62	88.360	-21.509	104.123	82.614
Isoquinoline	-4.121	0.590	48	64.000	-0.453	-26.556	-27.009

Values of μ_A, S_A and N_A for acceptor molecule $SnBr_4$ (A)

μ_A	S_A	N_A
-5.855	0.615	32

μA=Chemical potential of molecule A, μB=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, $\lambda = (N_A + N_B)^2 / 100$, Eμ,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

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TABLE 5: Interaction of acceptor molecule SnI_4 (A) with organic bases (B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	64.000	-0.300	-22.862	-23.161
5-Nitroquinoline	-10.816	-0.405	64	92.160	11.366	-111.244	-99.878
8-Nitroquinoline	-11.647	-1.012	64	92.160	-81.617	239.211	157.595
8-Quinolinesulphonic acid	-4.695	0.606	72	108.160	-0.109	-37.949	-38.058
2-Aminoquinoline	-3.497	0.656	54	73.960	-0.721	-25.065	-25.786
2-Phenylquinoline	-4.099	0.657	76	116.640	-0.351	-39.500	-39.851
Quinolinic acid	-11.197	-1.040	62	88.360	-62.964	200.363	137.398
Isoquinoline	-4.121	0.590	48	64.000	-0.320	-22.714	-23.034

Values of μ_A, S_A and N_A for acceptor molecule SnI_4 (A)

μ_A	S_A	N_A
-5.486	0.819	32

TABLE 6: Interaction of acceptor molecule $ZnCl_2$(A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	40.960	-0.132	-20.848	-20.981
5-Nitroquinoline	-10.816	-0.405	64	64.000	-804.533	10094.843	9290.310
8-Nitroquinoline	-11.647	-1.012	64	64.000	-13.779	52.457	38.678
8-Quinolinesulphonic acid	-4.695	0.606	72	77.440	-0.033	-38.425	-38.458
2-Aminoquinoline	-3.497	0.656	54	49.000	-0.367	-23.157	-23.525
2-Phenylquinoline	-4.099	0.657	76	84.640	-0.155	-39.960	-40.115
Quinolinic acid	-11.197	-1.040	62	60.840	-11.713	47.688	35.975
Isoquinoline	-4.121	0.590	48	40.960	-0.143	-20.658	-20.800

Values of μ_A, S_A and N_A for acceptor molecule $ZnCl_2$ (A)

μ_A	S_A	N_A
-5.214	0.402	16

TABLE 7: Interaction of acceptor molecule $ZnBr_2$(A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	40.960	-0.091	-19.839	-19.931
5-Nitroquinoline	-10.816	-0.405	64	64.000	65.907	-683.865	-617.958
8-Nitroquinoline	-11.647	-1.012	64	64.000	-17.981	57.136	39.155
8-Quinolinesulphonic acid	-4.695	0.606	72	77.440	-0.013	-36.610	-36.623
2-Aminoquinoline	-3.497	0.656	54	49.000	-0.305	-22.113	-22.418
2-Phenylquinoline	-4.099	0.657	76	84.640	-0.110	-38.159	-38.270
Quinolinic acid	-11.197	-1.040	62	60.840	-15.298	51.741	36.442
Isoquinoline	-4.121	0.590	48	40.960	-0.100	-19.666	-19.767

Values of μ_A, S_A and N_A for acceptor molecule $ZnBr_2$ (A)

μ_A	S_A	N_A
-5.007	0.452	16

TABLE 8: Interaction of acceptor molecule ZnI_2 (A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	40.960	-0.052	-18.681	-18.732
5-Nitroquinoline	-10.816	-0.405	64	64.000	34.386	-288.755	-254.369
8-Nitroquinoline	-11.647	-1.012	64	64.000	-24.843	64.511	39.668
8-Quinolinesulphonic acid	-4.695	0.606	72	77.440	-0.001	-34.520	-34.521
2-Aminoquinoline	-3.497	0.656	54	49.000	-0.235	-20.905	-21.140
2-Phenylquinoline	-4.099	0.657	76	84.640	-0.066	-36.077	-36.142
Quinolinic acid	-11.197	-1.040	62	60.840	-21.112	58.064	36.952
Isoquinoline	-4.121	0.590	48	40.960	-0.058	-18.527	-18.586

Values of μ_A, S_A and N_A for acceptor molecule ZnI_2 (A)

μ_A	S_A	N_A
-4.773	0.516	16

μA=Chemical potential of molecule A, μB=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, $\lambda = (N_A + N_B)^2 / 100$, E_μ= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

TABLE 9: Interaction of acceptor molecule $CdCl_2$(A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	40.960	-0.186	-19.425	-19.611
5-Nitroquinoline	-10.816	-0.405	64	64.000	41.551	-464.977	-423.426
8-Nitroquinoline	-11.647	-1.012	64	64.000	-17.632	59.475	41.843
8-Quinolinesulphonic acid	-4.695	0.606	72	77.440	-0.058	-35.863	-35.921
2-Aminoquinoline	-3.497	0.656	54	49.000	-0.474	-21.682	-22.156
2-Phenylquinoline	-4.099	0.657	76	84.640	-0.217	-37.416	-37.633
Quinolinic acid	-11.197	-1.040	62	60.840	-14.853	53.755	38.902
Isoquinoline	-4.121	0.590	48	40.960	-0.200	-19.259	-19.459

Values of μ_A, S_A and N_A for acceptor molecule ZnI_2 (A)

μ_A	S_A	N_A
-5.354	0.474	16

TABLE 10: Interaction of acceptor molecule $CdBr_2$(A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	40.96	-0.110	-18.739	-18.850
5-Nitroquinoline	-10.816	-0.405	64	64.00	31.991	-297.986	-265.995
8-Nitroquinoline	-11.647	-1.012	64	64.00	-22.511	64.068	41.557
8-Quinolinesulphonic acid	-4.695	0.606	72	77.44	-0.018	-34.626	-34.645
2-Aminoquinoline	-3.497	0.656	54	49.00	-0.351	-20.966	-21.317
2-Phenylquinoline	-4.099	0.657	76	84.64	-0.133	-36.183	-36.315
Quinolinic acid	-11.197	-1.040	62	60.84	-19.021	57.686	38.665
Isoquinoline	-4.121	0.590	48	40.96	-0.121	-18.585	-18.706

Values of μ_A, S_A and N_A for acceptor molecule $CdBr_2$ (A)

μ_A	S_A	N_A
-5.059	0.512	16

μA=Chemical potential of molecule A, μB=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, $\lambda = (N_A + N_B)^2 / 100$, E_μ,= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

TABLE 11: Interaction of acceptor molecule CdI_2 (A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
5-Nitroquinoline	-10.816	-0.405	64	64.000	24.792	-187.940	-163.149
8-Nitroquinoline	-11.647	-1.012	64	64.000	-31.293	73.295	42.002
8-Quinolinesulphonic acid	-4.695	0.606	72	77.440	-0.001	-32.783	-32.784
2-Aminoquinoline	-3.497	0.656	54	49.000	-0.258	-19.896	-20.153
2-Phenylquinoline	-4.099	0.657	76	84.640	-0.074	-34.337	-34.410
Quinolinic acid	-11.197	-1.040	62	60.840	-26.391	65.496	39.105
Isoquinoline	-4.121	0.590	48	40.960	-0.066	-17.582	-17.648
5-Nitroquinoline	-10.816	-0.405	64	64.000	24.792	-187.940	-163.149

Values of μ_A, S_A and N_A for acceptor molecule CdI_2 (A)

μ_A	S_A	N_A
-4.793	0.575	16

TABLE 12: Interaction of acceptor molecule $HgCl_2$(A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	54.760	-0.535	-23.690	-24.225
5-Nitroquinoline	-10.816	-0.405	64	81.000	15.309	-237.86	-222.55
8-Nitroquinoline	-11.647	-1.012	64	81.000	-20.621	92.764	72.143
8-Quinolinesulphonic acid	-4.695	0.606	72	96.040	-0.284	-40.657	-40.941
2-Aminoquinoline	-3.497	0.656	54	64.000	-1.025	-25.986	-27.011
2-Phenylquinoline	-4.099	0.657	76	104.040	-0.604	-42.207	-42.810
Quinolinic acid	-11.197	-1.040	62	77.440	-16.829	83.366	66.537
Isoquinoline	-4.121	0.590	48	54.760	-0.561	-23.505	-24.066

Values of μ_A, S_A and N_A for acceptor molecule $HgCl_2$(A)

μ_A	S_A	N_A
-6.083	0.575	26

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TABLE 13: Interaction of acceptor molecule $HgBr_2$(A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	54.760	-0.341	-22.785	-23.127
5-Nitroquinoline	-10.816	-0.405	64	81.000	15.414	-187.371	-171.957
8-Nitroquinoline	-11.647	-1.012	64	81.000	-28.746	103.658	74.912
8-Quinolinesulphonic acid	-4.695	0.606	72	96.040	-0.145	-39.137	-39.281
2-Aminoquinoline	-3.497	0.656	54	64.000	-0.751	-25.053	-25.804
2-Phenylquinoline	-4.099	0.657	76	104.040	-0.392	-40.692	-41.084
Quinolinic acid	-11.197	-1.040	62	77.440	-23.582	92.504	68.922
Isoquinoline	-4.121	0.590	48	54.760	-0.361	-22.615	-22.976

Values of μ_A, S_A and N_A for acceptor molecule $HgBr_2$ (A)

μ_A	S_A	N_A
-5.667	0.621	26

TABLE 14: Interaction of acceptor molecule HgI_2(A) with organic bases(B)

Compound	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
Quinoline	-4.158	0.581	48	54.760	-0.219	-21.030	-21.249
5-Nitroquinoline	-10.816	-0.405	64	81.000	13.902	-127.977	-114.074
8-Nitroquinoline	-11.647	-1.012	64	81.000	-50.195	139.466	89.271
8-Quinolinesulphonic acid	-4.695	0.606	72	96.040	-0.065	-36.179	-36.244
2-Aminoquinoline	-3.497	0.656	54	64.000	-0.575	-23.228	-23.803
2-Phenylquinoline	-4.099	0.657	76	104.040	-0.259	-37.731	-37.990
Quinolinic acid	-11.197	-1.040	62	77.440	-40.606	121.661	81.055
Isoquinoline	-4.121	0.590	48	54.760	-0.236	-20.884	-21.120

Values of μ_A, S_A and N_A for acceptor molecule HgI_2 (A)

μ_A	S_A	N_A
-5.326	0.721	26

μA=Chemical potential of molecule A, μB=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, $\lambda = (N_A + N_B)^2 / 100$, E_μ= Energy corresponds to a reshuffling of the charge distribution, E_v= Energy corresponds to the charge transfer process, E_{int}= Interaction energy

energy between organic bases-B and metal halides-A ($HgCl_2$>$SnBr_4$>$HgBr_2$>SnI_4>$CdCl_2$>HgI_2>$ZnCl_2$> $CdBr_2$>$ZnBr_2$>CdI_2>ZnI_2) are presented very clearly indicates that the acceptor strength of halides is in the order chloride>bromide>iodide; and the base strength is in the order 8-Nitroquinoline>Quinolinic acid> Isoquinoline> Quinoline> 2-Aminoquinoline>8-Quino linesulphonic acid>2-Phenylquinoline> 5-Nitroquinoline in most of the cases. The acceptor strength of different metal halides is in the following order:

$SnCl_4$>$HgCl_2$ >$SnBr_4$>$HgBr_2$>SnI_4>$CdCl_2$>HgI_2> $ZnCl_2$>$CdBr_2$>$ZnBr_2$>CdI_2>ZnI_2

Values of HOMO energy, LUMO energy, ionization potential, electron affinity, absolute hardness and global softness potential of acceptor molecules (metal halides) are given in the TABLE 15. Metal halides in decreasing order of electronegativity are arranged as below-

$SnCl_4$>$HgCl_2$>$SnBr_4$>$HgBr_2$>SnI_4>$CdCl_2$>HgI_2> $ZnCl_2$>$CdBr_2$>$ZnBr_2$>CdI_2>ZnI_2

This provides the same order of acceptor molecules as predicted by the TABLES 3-14 as higher will be the value of electronegativity; the greater will be the acceptor strength.

TABLE 15: Values of HOMO energy, LUMO energy, ionization potential, electron affinity, absolute hardness and global softness potential of acceptor molecules

Metal halide	HOMO energy (eV)	LUMO energy (eV)	Electronegativity	Ionization Potential	Electron Affinity	Absolute Hardness	Global softness
$SnCl_4$	-8.313	-4.411	6.362	8.313	4.411	1.951	0.513
$SnBr_4$	-7.480	-4.229	5.855	7.480	4.229	1.626	0.615
SnI_4	-6.707	-4.265	5.486	6.707	4.265	1.221	0.819
$ZnCl_2$	-7.704	-2.724	5.214	7.704	2.724	2.490	0.402
$ZnBr_2$	-7.221	-2.792	5.007	7.221	2.792	2.215	0.452
ZnI_2	-6.712	-2.833	4.773	6.712	2.833	1.940	0.516
$CdCl_2$	-7.465	-3.242	5.354	7.465	3.242	2.112	0.474
$CdBr_2$	-7.011	-3.106	5.059	7.011	3.106	1.953	0.512
CdI_2	-6.532	-3.054	4.793	6.532	3.054	1.739	0.575
$HgCl_2$	-7.822	-4.344	6.083	7.822	4.344	1.739	0.575
$HgBr_2$	-7.277	-4.056	5.667	7.277	4.056	1.611	0.621
HgI_2	-6.712	-3.939	5.326	6.712	3.939	1.387	0.721

TABLE 16: HOMO energy, LUMO energy, chemical potential and global softness values of organic bases (B)

Donor organic bases B	HOMO energy (eV)	LUMO energy (eV)	Chemical potential μ_B	Global softness S_B
8-Nitroquinoline	-10.658	-12.635	-11.647	-1.012
Quinolinic acid	-10.235	-12.159	-11.197	-1.04
5-Nitroquinoline	-8.345	-13.286	-10.816	-0.405
8-Quinolinesulphonic acid	-6.345	-3.045	-4.695	0.606
Quinoline	-5.88	-2.436	-4.158	0.581
Isoquinoline	-5.816	-2.425	-4.121	0.59
2-Phenylquinoline	-5.62	-2.578	-4.099	0.657
2-Aminoquinoline	-5.02	-1.973	-3.497	0.656

TABLE 17: Chemical potential (μ_A) and global softness (S_A) values of acceptor (A)

Metal halides	HOMO energy (eV)	LUMO energy (eV)	Chemical potential μ_A	Global softness S_A
$SnCl_4$	-8.313	-4.411	-6.362	0.513
$HgCl_2$	-7.822	-4.344	-6.083	0.575
$SnBr_4$	-7.48	-4.229	-5.855	0.615
$HgBr_2$	-7.277	-4.056	-5.667	0.621
SnI_4	-6.707	-4.265	-5.486	0.819
$CdCl_2$	-7.465	-3.242	-5.354	0.474
HgI_2	-6.712	-3.939	-5.326	0.721
$ZnCl_2$	-7.704	-2.724	-5.214	0.402
$CdBr_2$	-7.011	-3.106	-5.059	0.512
$ZnBr_2$	-7.221	-2.792	-5.007	0.452
CdI_2	-6.532	-3.054	-4.793	0.575
ZnI_2	-6.712	-2.833	-4.773	0.516

Chemical potential of donor and acceptor molecules

The chemical potential (μ_A, μ_B) and global softness (S_A, S_B) of donor (B) and acceptor (A) are included in TABLES 16 and 17 respectively which clearly indicate that-

- The chemical potential (μ_B) value of 8-Nitroquinoline is lowest hence it is best donor. The next is Quinolinic acid and the last is 2-aminoquinoline.
- The values of chemical potential (μ_B) of organic bases in increasing order are tabulated in TABLE 16. On the basis of values of chemical potential (μ_B) the compounds can be arranged in the following order of their donor ability.
  8-Nitroquinoline>Quinolinicacid>5-Nitroquinoline>8-Quinolinesulphonic acid>Quinoline>Isoquinoline>2-Phenylquinoline>2-Aminoquinoline
- The acceptor molecules that have been studied for donor-acceptors interaction are listed in TABLE 17, alongwith their values of chemical potential (μ_A) in ascending order, and global softness values.

The higher is the value of chemical potential (μ_A) better will be the acceptor property. Among tin (iv) halides the $SnCl_4$ has the highest value hence best acceptor. Among MCl_2 (M= Zn, Cd, Hg), the mercury chloride is the best acceptor as it has the highest value. The acceptor strength can be arranged in the following order:

$SnCl_4 > HgCl_2 > SnBr4 > HgBr_2 > SnI_4 > CdCl_2 > HgI_2 > ZnCl_2 > CdBr_2 > ZnBr_2 > CdI_2 > ZnI_2$

Energy transfer (ΔE)

For a molecule μ measures the ability to attract electrons to itself. If two molecules (A and B) are brought together electrons will flow from the one, which has lower value of μ to that which has higher value. At equilibrium a single value of μ will exist through out. ΔEμ is the energy transfer on account of this reshuffling.

The ΔEμ shows that chlorides have higher value than bromide and iodide. The sequence is chloride>bromide>iodide. The values do not demonstrate the order of acceptor or base strength.

Global softness of donor and acceptor molecules (S_A, S_B)

The global softness (S_A) values are lowest in chlorides and highest in iodides, in other words chlorides are harder acids as compared to their bromide and iodide counterparts in terms of HSAB principle. The scale of softness of various halides is as given in TABLE 17.

Analysis of the equation-3 indicates that for a given values of S_A the larger the value of S_B, the better, while equation-4 indicates that for the same values of S_A the smaller value of S_B the better. Since the total energy is given by the summation of these two terms, it seems that the best situation corresponds to the average between the two extreme situations, that is $S_A \approx S_B$, which is precisely the global HSAB principle. A similar analysis, based on the two opposing tendencies, was first given by Chattaraj et al.[5,11]. The S_A value of SnCl4 is 0.513 and S_B value of amino toluene is 0.513 (DOI=10.1016/j.theochem.2009.03.002). Since the two values are equal the best interaction is shown between them. This observation is in conformity with the global HSAB principle

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TABLE 18: Charge transfer and energy change with acceptor molecule $SnCl_4$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	6.362	4.158	1.951	1.722	0.300027	-0.33063
5-Nitroquinoline	6.362	10.8155	1.951	-2.4705	4.286333	9.544592
8-Nitroquinoline	6.362	11.6465	1.951	-0.9885	-2.74519	-7.25349
8-Quinolinesulphonic acid	6.362	4.695	1.951	1.65	0.231463	-0.19292
2-Aminoquinoline	6.362	3.4965	1.951	1.5235	0.412361	-0.59081
2-Phenylquinoline	6.362	4.099	1.951	1.521	0.325893	-0.36875
Quinolinic acid	6.362	11.197	1.951	-0.962	-2.44439	-5.90931
Isoquinoline	6.362	4.1205	1.951	1.6955	0.30735	-0.34446

TABLE 19: Charge transfer and energy change with acceptor molecule $SnBr_4$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	5.8545	4.158	1.6255	1.722	0.253398	-0.21494
5-Nitroquinoline	5.8545	10.8155	1.6255	-2.4705	2.935503	7.281515
8-Nitroquinoline	5.8545	11.6465	1.6255	-0.9885	-4.54631	-13.1661
8-Quinolinesulphonic acid	5.8545	4.695	1.6255	1.65	0.176996	-0.10261
2-Aminoquinoline	5.8545	3.4965	1.6255	1.5235	0.374405	-0.44142
2-Phenylquinoline	5.8545	4.099	1.6255	1.521	0.278961	-0.24486
Quinolinic acid	5.8545	11.197	1.6255	-0.962	-4.026	-10.7544
Isoquinoline	5.8545	4.1205	1.6255	1.6955	0.261066	-0.22634

Transfer of charge (N) and change in energy (ΔE)

Metal ligand bond strength between interaction of acceptor (A) and ligand (B) has also been calculated by solving the following equations for shift in charge (ΔN) and lowering energy (ΔE)[23].

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

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

Metal ligand bond strength of organic bases (B) with the acceptor $SnCl_4$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule $SnCl_4$ are included in TABLE 18. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $SnCl_4$ is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquino line>2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor $SnCl_4$ (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquino line>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor $SnBr_4$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule $SnBr_4$ are included in TABLE 19. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $SnBr_4$ is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquino line>2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor $SnBr_4$ (A) as predicted by the value of lowering in energy ΔE is as follows-

TABLE 20: Charge transfer and energy change with acceptor molecule SnI_4

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	5.486	4.158	1.221	1.722	0.22562	-0.14981
5-Nitroquinoline	5.486	10.8155	1.221	-2.4705	2.132653	5.682987
8-Nitroquinoline	5.486	11.6465	1.221	-0.9885	-13.2484	-40.8083
8-Quinolinesulphonic acid	5.486	4.695	1.221	1.65	0.137757	-0.05448
2-Aminoquinoline	5.486	3.4965	1.221	1.5235	0.362452	-0.36055
2-Phenylquinoline	5.486	4.099	1.221	1.521	0.252918	-0.1754
Quinolinic acid	5.486	11.197	1.221	-0.962	-11.0251	-31.4822
Isoquinoline	5.486	4.1205	1.221	1.6955	0.234099	-0.15983

TABLE 21: Charge transfer and energy change with acceptor molecule $ZnCl_2$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	5.214	4.158	2.49	1.722	0.125356	-0.06619
5-Nitroquinoline	5.214	10.8155	2.49	-2.4705	-143.628	-402.267
8-Nitroquinoline	5.214	11.6465	2.49	-0.9885	-2.14202	-6.88929
8-Quinolinesulphonic acid	5.214	4.695	2.49	1.65	0.062681	-0.01627
2-Aminoquinoline	5.214	3.4965	2.49	1.5235	0.213965	-0.18374
2-Phenylquinoline	5.214	4.099	2.49	1.521	0.138993	-0.07749
Quinolinic acid	5.214	11.197	2.49	-0.962	-1.95779	-5.85672
Isoquinoline	5.214	4.1205	2.49	1.6955	0.13063	-0.07142

8-Nitroquinoline>Quinolinic acid>2-Aminoquino line>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor SnI_4 (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 20. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor SnI_4 is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquino line >2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor SnI_4 (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquino line>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline and the minimum strength is in 5-Nitroquinoline.

The metal ligand bond strength of donor organic bases with all the halides of tin(iv) is exactly in the same order.

Metal ligand bond strength of organic bases (B) with the acceptor $ZnCl_2$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 21. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $ZnCl_2$ is in the following order as predicted by the values of ΔN.

5-Nitroquinoline>8-Nitroquinoline>Quinolinic acid> 8-Quinolinesulphonic acid>Quinoline> Isoquino line >2-Phenylquinoline>2-Aminoquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of

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TABLE 22: Charge transfer and energy change with acceptor molecule $ZnBr_2$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	5.0065	4.158	2.2145	1.722	0.107773	-0.04572
5-Nitroquinoline	5.0065	10.8155	2.2145	-2.4705	11.3457	32.95359
8-Nitroquinoline	5.0065	11.6465	2.2145	-0.9885	-2.70799	-8.99054
8-Quinolinesulphonic acid	5.0065	4.695	2.2145	1.65	0.040303	-0.00628
2-Aminoquinoline	5.0065	3.4965	2.2145	1.5235	0.20198	-0.15249
2-Phenylquinoline	5.0065	4.099	2.2145	1.521	0.12147	-0.05512
Quinolinic acid	5.0065	11.197	2.2145	-0.962	-2.47126	-7.64916
Isoquinoline	5.0065	4.1205	2.2145	1.6955	0.113299	-0.05019

TABLE 23: Charge transfer and energy change with acceptor molecule ZnI_2

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	4.7725	4.158	1.9395	1.722	0.083914	-0.02578
5-Nitroquinoline	4.7725	10.8155	1.9395	-2.4705	5.690207	17.19296
8-Nitroquinoline	4.7725	11.6465	1.9395	-0.9885	-3.61409	-12.4216
8-Quinolinesulphonic acid	4.7725	4.695	1.9395	1.65	0.010795	-0.00042
2-Aminoquinoline	4.7725	3.4965	1.9395	1.5235	0.184233	-0.11754
2-Phenylquinoline	4.7725	4.099	1.9395	1.521	0.097313	-0.03277
Quinolinic acid	4.7725	11.197	1.9395	-0.962	-3.28619	-10.5561
Isoquinoline	4.7725	4.1205	1.9395	1.6955	0.089684	-0.02924

donor organic bases (B) with the acceptor $ZnCl_2$ (A) as predicted by the value of lowering in energy ΔE is as follows-

5-Nitroquinoline>8-Nitroquinoline>Quinolinic acid>2-Aminoquinoline>2-Phenylquinoline> Isoquinoline> Quinoline>8-Quinolinesulphonic acid.

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 5-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 2-Aminoquinoline as predicted by ΔN and in 8-Quinolinesulphonic acid as predicted by ΔE.

Metal ligand bond strength of organic bases (B) with the acceptor $ZnBr_2$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 22. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $ZnBr_2$ is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinolinesulphonic acid>Quinoline>Isoquinoline>2-Phenylquinoline>2-Aminoquinoline>5-Nitroquinoline.

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor $ZnBr_2$ (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquinoline>2-Phenylquinoline> Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline.

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor ZnI_2 (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 23. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor ZnI_2 is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquinoline>2-Aminoquinoline>5-Nitroquinoline.

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond

TABLE 24: Charge transfer and energy change with acceptor molecule $CdCl_2$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	5.3535	4.158	2.1115	1.722	0.155928	-0.09321
5-Nitroquinoline	5.3535	10.8155	2.1115	-2.4705	7.607242	20.77538
8-Nitroquinoline	5.3535	11.6465	2.1115	-0.9885	-2.80187	-8.81608
8-Quinolinesulphonic acid	5.3535	4.695	2.1115	1.65	0.087532	-0.02882
2-Aminoquinoline	5.3535	3.4965	2.1115	1.5235	0.255433	-0.23717
2-Phenylquinoline	5.3535	4.099	2.1115	1.521	0.172677	-0.10831
Quinolinic acid	5.3535	11.197	2.1115	-0.962	-2.54176	-7.42638
Isoquinoline	5.3535	4.1205	2.1115	1.6955	0.161939	-0.09984

TABLE 25 : Charge transfer and energy change with acceptor molecule $CdBr_2$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	5.0585	4.158	1.9525	1.722	0.122534	-0.05517
5-Nitroquinoline	5.0585	10.8155	1.9525	-2.4705	5.55695	15.99568
8-Nitroquinoline	5.0585	11.6465	1.9525	-0.9885	-3.41701	-11.2556
8-Quinolinesulphonic acid	5.0585	4.695	1.9525	1.65	0.050451	-0.00917
2-Aminoquinoline	5.0585	3.4965	1.9525	1.5235	0.224684	-0.17548
2-Phenylquinoline	5.0585	4.099	1.9525	1.521	0.138117	-0.06626
Quinolinic acid	5.0585	11.197	1.9525	-0.962	-3.09869	-9.51065
Isoquinoline	5.0585	4.1205	1.9525	1.6955	0.128564	-0.0603

strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor ZnI_2 (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquino line>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor $CdCl_2$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 24. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $CdCl_2$ is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquino line>2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor $CdCl_2$ (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquin oline>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor $CdBr_2$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 25. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $CdBr_2$ is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquino line>2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond

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TABLE 26 : Charge transfer and energy change with acceptor molecule CdI_2

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	4.793	4.158	1.739	1.722	0.091736	-0.02913
5-Nitroquinoline	4.793	10.8155	1.739	-2.4705	4.116541	12.39594
8-Nitroquinoline	4.793	11.6465	1.739	-0.9885	-4.56596	-15.6464
8-Quinolinesulphonic acid	4.793	4.695	1.739	1.65	0.014459	-0.00071
2-Aminoquinoline	4.793	3.4965	1.739	1.5235	0.198697	-0.12881
2-Phenylquinoline	4.793	4.099	1.739	1.521	0.106442	-0.03694
Quinolinic acid	4.793	11.197	1.739	-0.962	-4.12098	-13.1954
Isoquinoline	4.793	4.1205	1.739	1.6955	0.097904	-0.03292

TABLE 27 : Charge transfer and energy change with acceptor molecule $HgCl_2$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	6.083	4.158	1.739	1.722	0.278099	-0.26767
5-Nitroquinoline	6.083	10.8155	1.739	-2.4705	3.234792	7.654325
8-Nitroquinoline	6.083	11.6465	1.739	-0.9885	-3.70653	-10.3106
8-Quinolinesulphonic acid	6.083	4.695	1.739	1.65	0.20478	-0.14212
2-Aminoquinoline	6.083	3.4965	1.739	1.5235	0.396398	-0.51264
2-Phenylquinoline	6.083	4.099	1.739	1.521	0.304294	-0.30186
Quinolinic acid	6.083	11.197	1.739	-0.962	-3.29086	-8.41473
Isoquinoline	6.083	4.1205	1.739	1.6955	0.285704	-0.28035

strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor $CdBr_2$ (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquinoline>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor CdI_2 (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 26. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor CdI_2 is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinolinesulphonic acid>Quinoline>Isoquinoline>2-Phenylquinoline>2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor CdI_2 (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquinoline>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor $HgCl_2$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 27. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $HgCl_2$ is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquinoline>2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond

TABLE 28 : Charge transfer and energy change with acceptor molecule $HgBr_2$

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	5.6665	4.158	1.6105	1.722	0.226332	-0.17071
5-Nitroquinoline	5.6665	10.8155	1.6105	-2.4705	2.993605	7.707035
8-Nitroquinoline	5.6665	11.6465	1.6105	-0.9885	-4.80707	-14.3732
8-Quinolinesulphonic acid	5.6665	4.695	1.6105	1.65	0.14898	-0.07237
2-Aminoquinoline	5.6665	3.4965	1.6105	1.5235	0.346203	-0.37563
2-Phenylquinoline	5.6665	4.099	1.6105	1.521	0.250279	-0.19616
Quinolinic acid	5.6665	11.197	1.6105	-0.962	-4.26407	-11.7912
Isoquinoline	5.6665	4.1205	1.6105	1.6955	0.233817	-0.18074

TABLE 29 : Charge transfer and energy change with acceptor molecule HgI_2

Compound	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	5.3255	4.158	1.3865	1.722	0.187792	-0.10962
5-Nitroquinoline	5.3255	10.8155	1.3865	-2.4705	2.532288	6.95113
8-Nitroquinoline	5.3255	11.6465	1.3865	-0.9885	-7.94095	-25.0974
8-Quinolinesulphonic acid	5.3255	4.695	1.3865	1.65	0.10382	-0.03273
2-Aminoquinoline	5.3255	3.4965	1.3865	1.5235	0.314261	-0.28739
2-Phenylquinoline	5.3255	4.099	1.3865	1.521	0.21092	-0.12935
Quinolinic acid	5.3255	11.197	1.3865	-0.962	-6.91578	-20.303
Isoquinoline	5.3255	4.1205	1.3865	1.6955	0.19549	-0.11778

strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor $HgCl_2$ (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquino line>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor $HgBr_2$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 28. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $HgBr_2$ is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquino line>2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor $HgBr_2$ (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquino line>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 5-Nitroquinoline.

Metal ligand bond strength of organic bases (B) with the acceptor HgI_2 (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule SnI_4 are included in TABLE 29. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor HgI_2 is in the following order as predicted by the values of ΔN.

8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenylquino line>2-Aminoquinoline>5-Nitroquinoline

The value of change in energy ΔE is also a measure of metal ligand bond strength. The metal ligand bond

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strength also decreases with the increase in the value of change in energy ΔE. Metal ligand bond strength of donor organic bases (B) with the acceptor HgI_2 (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline>Quinolinic acid>2-Aminoquino line>2-Phenylquinoline>Isoquinoline>Quinoline>8-Quinolinesulphonic acid>5-Nitroquinoline

It is clear that the values of ΔN and ΔE indicate almost the same trend of metal ligand bond strength as predicted by the values of interaction energy (E_{int}). Maximum strength of metal ligand bond is in 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in 5-Nitroquinoline.

A reference to the above Tables indicates that all the three methods viz interaction energy (E_{int}), shift in charge (ΔN), and lowering of energy (ΔE) provide results which are in consonance to each other, all of them have reliable predictive power.

CONCLUSIONS

1. The acceptor strength is in the order $SnCl_4$>$HgCl_2$>$SnBr_4$>$HgBr_2$>SnI_4>$CdCl_2$>HgI_2>$ZnCl_2$>$CdBr_2$>$ZnBr_2$>CdI_2>ZnI_2. The chemical potential (μ_B) values of organic bases indicate the same order of base strength as is indicated by interaction energy.
2. The organic bases show that the 8-nitroquinoline is the strongest base and 5-Nitroquinoline is the weakest base against all the acceptors. The order is 8-Nitroquinoline>Quinolinic acid>8-Quinoline sulphonic acid>Quinoline>Isoquinoline>2-Phenyl quinoline>2-Aminoquinoline>5-Nitroquinoline.
3. Eμ is the energy transfer on account of flow of electrons from lower μ to high μ. The Eμ does not demonstrate the order of acid or base strength.
4. The best interaction is when global softness values of acid and base are approximately equal i.e. $S_A \approx S_B$. For example, S_A = 0.615 for $SnBr_4$ and S_B = 0.606 for 8-Quinolinesulphonic acid.
5. Higher interaction energy (E_{int}) indicates strong metal ligand interaction.
6. All the results of interaction energy are in consonance with the results of ΔN and ΔE.

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