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DFT Based Study of Interaction Energy, Charge Transfer and Energy Lowering Between Halides of Chromium and Organic Bases

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Abstract: *Calculations of interaction energy (Eint), charge transfer (ÄN) and lowering of energy (ΔE) between acceptor Chromium halides (Fluride,chloride,bromide and iodide)and donor organic bases (Quinoline,8-nitroquinoline,5-nitroquinoline,8-quinolinesulphonic acid,2-aminoquinoline,2-phenylquinolne,quinolinic acid,isoquinoline) have been done by DFTB88PW91method using CAChe software. The results indicate that acceptor strength of chromium halides with organic basis is in order* CrF_2> $CrCl_2$ > $CrBr_2$ >CrI_2 *form stable complexes in most of the cases and the base strength show that the 5-nitroquinoline is the weakest base and 2-phenylquinoline is the strongest base against least of the acceptors. The result obtained by interaction energy,charge transfer and lowering of energy give almost the same result.The value of energy transfer showed that the complex formation capability is in the sequence flouride> chloride> bromide> iodide.*

Key Words: *DFT method; Interaction energy; Charge transfer; Lowering of energy; Donor; Acceptor.*

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I. 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. The ability of interaction with a ligand has been noticed to have relation with the number of electron in d-orbital. No precise calculations have even been made to give any quantitative nature to this interaction.

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.

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

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

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

where

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

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" that participate in the interaction between A and B.

The first term ΔE_v, corresponds to the charge transfer process between A and B arising from the chemical potential equalization principle at constant external potential. The second term, ΔE_μ, corresponds to a reshuffling of the charge distribution, and it is basically a manifestation of the minimum 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]. If two values are equal the best interaction is shown between them. This observation is in conformity with the observation of Chattaraj[5, 11]. The application of this concept has recently been made to metal-ligand interaction by Singh[24] in respect of non transition metal and organic bases.

The application of the concept has been extended to organic chemistry by Pearson [6]. We in this paper present the application of interaction energy to metal ligand interaction chemistry.

II. Material And Method

The study materials of this paper are Four metal halides listed in Table-1 have been used as Lewis acids (A) and 8 derivatives of quinoline as Lewis bases(B) listed in Table-2, which have been used as a donor 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.

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]

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

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

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

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

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

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 [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

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

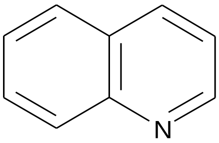
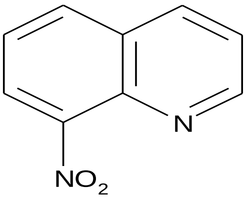
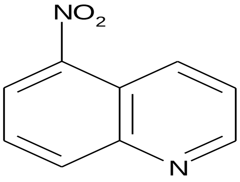
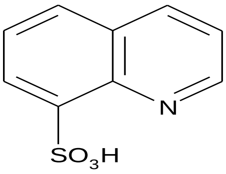
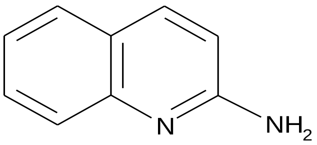
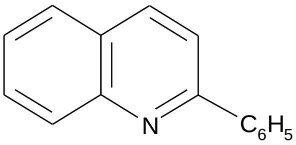
The chemical potential itself depend on N and v i.e. $\mu = \mu(N,v)$. Parr and Pearson [23] have defined hardness with respect to N as

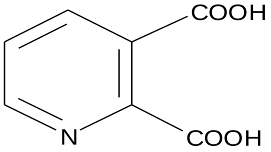
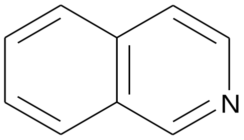
$$\begin{aligned}\eta &= ½.\,(\delta\mu/\delta N)_{v(r)} \\ &= ½.\,(\delta^2 E/\ \delta N^2)_{\ v(r)} \\ &= (I - A)/2 \qquad (11)\end{aligned}$$

Table-1: A series of chromium halides as a Lewis Acids (A)

S. No.	**Lewis Acids (A)**
1	**CrF2**
2	**CrCl2**
3	**CrBr2**
4	**CrI2**

Table-2: A series of eight quinoline derivatives as Lewis bases (:B)

S. No.	**Lewis bases (:B)**	**Structure**
1	Quinoline	
2	8-Nitroquinoline	
3	5-Nitroquinoline	
4	8-Quinolinesulphonic acid	
5	2-Aminoquinoline	
6	2-Phenylquinoline	

S. No.	**Lewis bases (:B)**	**Structure**
7	Quinolinic acid	
8	Isoquinoline	

III. Result And Discussion:

Donor Acceptor Interaction:

The donor acceptor interaction between 4 donor molecules listed in Table-1 and 8 acceptor molecules listed in Table-2 has been studied in terms of metal ligand interaction energy (E_{int}) In total there are 32 (8x4) interactions. The interaction energy of disubstituted donors and chromium halides are presented in Tables 3 to 6

A reference to TABLE 3-6 where the interaction energy between organic bases-B and metal halides-A are presented very clearly indicates that the order of stable complex formation with acceptor molecules is different with all the halides of chromium; chromium fluoride and chromium chloride form least stable complexes with the organic base 2-Phenylquinoline; chromium bromide and chromium iodide form least stable complexes with the organic base 8-Nitroquinoline. Formation of most stable complexes of halides of chromium with organic bases is entirely different viz. CrF_2 forms most stable complex with 8-Nitroquinoline, $CrCl_2$ with Quinoline, $CrBr_2$ and CrI_2 with 8-Quinolinesulphonic acid. Order of formation of stable complexes of chromium halides with organic bases is as follows-

$$CrF_2 > CrCl_2 > CrBr_2 > CrI_2$$

in most of the cases. The acceptor strength of different metal halides is in the following order: $CrF_2 > CrI_2 > CrCl_2 > CrBr_2$

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 7. Metal halides in decreasing order of electronegativity are arranged as below- $CrF_2 > CrI_2 > CrCl_2 > CrBr_2$

This provides the different order of acceptor molecules as predicted by the TABLES 3-6 as higher will be the value of electronegativity; the greater will be the acceptor strength.

Table-3: Interaction of acceptor molecule CrF_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	46.240	-20.295	78.390	58.095
8-Nitroquinoline	-10.816	-0.405	64	70.560	18.335	27.553	45.888
5-Nitroquinoline	-11.647	-1.012	64	70.560	35.740	18.693	54.433
8-Quinolinesulphonic acid	-4.695	0.606	72	84.640	-28.584	156.976	128.392
2-Aminoquinoline	-3.497	0.656	54	54.760	-23.015	124.867	101.852
2-Phenylquinoline	-4.099	0.657	76	92.160	-30.307	211.188	180.880
Quinolinic acid	-11.197	-1.040	62	67.240	33.602	17.555	51.156
Isoquinoline	-4.121	0.590	48	46.240	-20.939	80.879	59.940

Values of μ_A, S_A and N_A for acceptor molecule CrF_2 (A)		
μ_A	**S_A**	**N_A**
0.694	-0.876	20

Table-4: Interaction of acceptor molecule $CrCl_2$ (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	46.240	-21.917	43.692	21.775
8-Nitroquinoline	-10.816	-0.405	64	70.560	23.756	23.292	47.048
5-Nitroquinoline	-11.647	-1.012	64	70.560	48.138	16.630	64.767
8-Quinolinesulphonic acid	-4.695	0.606	72	84.640	-28.518	83.999	55.481
2-Aminoquinoline	-3.497	0.656	54	54.760	-22.883	60.376	37.493
2-Phenylquinoline	-4.099	0.657	76	92.160	-28.455	101.853	73.399
Quinolinic acid	-11.197	-1.040	62	67.240	45.623	15.642	61.264
Isoquinoline	-4.121	0.590	48	46.240	-22.366	44.455	22.089

Values of μ_A, S_A and N_A for acceptor molecule $CrCl_2$ (A)		
μ_A	S_A	N_A
1.841	-1.110	20

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-5: Interaction of acceptor molecule $CrBr_2$ (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	46.240	28.381	-140.043	-111.662
8-Nitroquinoline	-10.816	-0.405	64	70.560	17.032	43.003	60.035
5-Nitroquinoline	-11.647	-1.012	64	70.560	27.725	24.719	52.444
8-Quinolinesulphonic acid	-4.695	0.606	72	84.640	30.295	-222.230	-191.936
2-Aminoquinoline	-3.497	0.656	54	54.760	17.575	-113.725	-96.151
2-Phenylquinoline	-4.099	0.657	76	92.160	21.522	-190.543	-169.022
Quinolinic acid	-11.197	-1.040	62	67.240	26.142	23.104	49.247
Isoquinoline	-4.121	0.590	48	46.240	26.995	-132.745	-105.750

Values of μ_A, S_A and N_A for acceptor molecule $CrBr_2$ (A)		
μ_A	S_A	N_A
2.073	-0.416	20

Table-6: Interaction of acceptor molecule CrI_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	46.240	16.299	-127.933	-111.634
8-Nitroquinoline	-10.816	-0.405	64	70.560	13.755	43.838	57.593
5-Nitroquinoline	-11.647	-1.012	64	70.560	22.483	24.992	47.475
8-Quinolinesulphonic acid	-4.695	0.606	72	84.640	18.270	-205.376	-187.107
2-Aminoquinoline	-3.497	0.656	54	54.760	9.798	-106.793	-96.995
2-Phenylquinoline	-4.099	0.657	76	92.160	12.651	-178.978	-166.327

Quinolinic acid	-11.197	-1.040	62	67.240	21.058	23.355	44.413
Isoquinoline	-4.121	0.590	48	46.240	15.528	-121.815	-106.286

Values of μ_A, S_A and N_A for acceptor molecule CrI_2 (A)		
μ_A	**S_A**	**N_A**
0.878	-0.400	20

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-7: Values of HOMO Energy, LUMO Energy, Chemical Potential, Ionization Potemtial, Electron Affinity, Absolute Hardness and Global Softness Potential of acceptor molecules

Metal Halide	HOMO Energy (eV)	LUMO Energy (eV)	Chemical Potential	Electron-egativity	Ionization Potential	Electron Affinity	Absolute Hardness	Global Softness
CrF_2	**1.836**	**-0.448**	**0.694**	**-0.694**	**-1.836**	**0.448**	**-1.142**	**-0.876**
CrCl2	**2.742**	**0.94**	**1.841**	**-1.841**	**-2.742**	**-0.940**	**-0.901**	**-1.110**
CrBr2	**4.479**	**-0.333**	**2.073**	**-2.073**	**-4.479**	**0.333**	**-2.406**	**-0.416**
CrI2	**3.378**	**-1.622**	**0.878**	**-0.878**	**-3.378**	**1.622**	**-2.500**	**-0.400**

Table-8: 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
5-Nitroquinoline	-10.658	-12.635	-11.647	-1.012
Quinolinic acid	-10.235	-12.159	-11.197	-1.04
8-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-9: 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
CrF2	1.836	-0.448	0.694	-0.876
CrCl2	2.742	0.94	1.841	-1.110
CrBr2	4.479	-0.333	2.073	-0.416
CrI2	3.378	-1.622	0.878	-0.400

CHEMICAL POTENTIAL OF DONOR AND ACCEPTOR MOLECULES (μ_A, μ_B) E_μ:

The chemical potential (μ_A, μ_B) and global softness (S_A, S_B) of donor (B) and acceptor (A) are included in Table-8 and Table-9 respectively. We conclude the following from these two Tables-

1. The chemical potential (μ_B) value of 5-Nitroquinoline is lowest hence it is best donor out of them. The next is Quinolinic acid and the last is 2-Aminoquinoline.
2. The values of chemical potential (μ_B) of organic bases in increasing order are tabulated in Table-8. On the basis of values of chemical potential (μ_B) the compounds can be arranged in the following order of their donor ability.
3. 5-Nitroquinoline < Quinolinic acid < 8-Nitroquinoline < 8-Quinolinesulphonic acid < Quinoline < Isoquinoline < 2-Phenylquinoline < 2-Aminoquinoline
4. The acceptor molecules that have been studied for donor-acceptors interaction are listed in Table-9 alongwith their values of chemical potential (μ_A), global softness, HOMO energy and LUMO energy.

The higher is the value of chemical potential (μ_A) better will be the acceptor property. Among all the halides the $CrBr_2$ has the highest value2.073 eV for chemical potential; hence, $CrBr_2$ is the best acceptor & CrF_2 has the lowest value0.694 ev hence it is week acceptor. The Acceptor strength can be arranged in the following order:

$CrBr_2 > CrCl_2 > CrI_2 > CrF_2$

Energy transfer ($\Delta E\mu$)

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. The term $\Delta E\mu$ is the energy transfer on account of this reshuffling and is given by-

$$\Delta E\mu = (\mu_A \sim \mu_B)/2$$

The $\Delta E\mu$ shows that fluorides have higher value than chloride, bromide and iodide in least of the interactions between metal halides and organic bases. The sequence is fluoride > iodide > bromide > chloride. These values do not demonstrate the order of acceptor 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-9.

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 $CrCl_2$ is -1.110 and S_B value of Quinolinic acid is -1.040. Since the two values are almost equal the best interaction is shown between them. This observation is in conformity with the global HSAB principle

TRANSFER OF CHARGE (ΔN) 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].

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

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

where χ^o_A, χ^o_B = Electronegativity of metal halide A and B
η_A, η_B = Absolute hardness of metal halide A and B

Table-10: Charge Transfer and Energy Change with acceptor molecule CrF_2

Organic Bases (B)	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	-0.6940	4.1580	-1.1420	1.7220	-4.18276	-10.1473
8-Nitroquinoline	-0.6940	10.8155	-1.1420	-2.4705	1.59301	9.16738
5-Nitroquinoline	-0.6940	11.6465	-1.1420	-0.9885	2.89615	17.86998
8-Quinolinesulphonic acid	-0.6940	4.6950	-1.1420	1.6500	-5.30413	-14.2919
2-Aminoquinoline	-0.6940	3.4965	-1.1420	1.5235	-5.49214	-11.5074
2-Phenylquinoline	-0.6940	4.0990	-1.1420	1.5210	-6.32322	-15.1535
Quinolinic acid	-0.6940	11.1970	-1.1420	-0.9620	2.82581	16.80084
Isoquinoline	-0.6940	4.1205	-1.1420	1.6955	-4.34914	-10.4694

Table-11: Charge Transfer and Energy Change with acceptor molecule $CrCl_2$

Organic Bases (B)	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	-1.841	4.1580	-0.9010	1.7220	-3.65347	-10.95859
8-Nitroquinoline	-1.841	10.8155	-0.9010	-2.4705	1.87698	11.87802
5-Nitroquinoline	-1.841	11.6465	-0.9010	-0.9885	3.56907	24.06889
8-Quinolinesulphonic acid	-1.841	4.6950	-0.9010	1.6500	-4.36315	-14.25878
2-Aminoquinoline	-1.841	3.4965	-0.9010	1.5235	-4.28715	-11.44133
2-Phenylquinoline	-1.841	4.0990	-0.9010	1.5210	-4.79032	-14.22726
Quinolinic acid	-1.841	11.1970	-0.9010	-0.9620	3.49919	22.81125
Isoquinoline	-1.841	4.1205	-0.9010	1.6955	-3.75173	-11.18297

Table-12: Charge Transfer and Energy Change with acceptor molecule $CrBr_2$

Organic Bases (B)	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	-2.073	4.1580	-2.406	1.7220	4.55482	14.19056
8-Nitroquinoline	-2.073	10.8155	-2.406	-2.470	1.32149	8.51602
5-Nitroquinoline	-2.073	11.6465	-2.406	-0.988	2.02084	13.86247
8-Quinolinesulphonic acid	-2.073	4.6950	-2.406	1.6500	4.47619	15.14743
2-Aminoquinoline	-2.073	3.4965	-2.406	1.5235	3.15552	8.78735
2-Phenylquinoline	-2.073	4.0990	-2.406	1.5210	3.48701	10.76090
Quinolinic acid	-2.073	11.1970	-2.406	-0.962	1.97001	13.07103
Isoquinoline	-2.073	4.1205	-2.406	1.6955	4.35855	13.49734

Table-13: Charge Transfer and Energy Change with acceptor molecule CrI_2

Organic Bases (B)	χ^o_A	χ^o_B	η_A	η_B	ΔN	ΔE
Quinoline	-0.878	4.1580	-2.5000	1.7220	3.23650	8.14952
8-Nitroquinoline	-0.878	10.8155	-2.5000	-2.470	1.17629	6.87747
5-Nitroquinoline	-0.878	11.6465	-2.5000	-0.988	1.79511	11.24144
8-Quinolinesulphonic acid	-0.878	4.6950	-2.5000	1.6500	3.27824	9.13480
2-Aminoquinoline	-0.878	3.4965	-2.5000	1.5235	2.23989	4.89919
2-Phenylquinoline	-0.878	4.0990	-2.5000	1.5210	2.54188	6.32547
Quinolinic acid	-0.878	11.1970	-2.5000	-0.962	1.74393	10.52900
Isoquinoline	-0.878	4.1205	-2.5000	1.6955	3.10659	7.76414

Metal ligand bond strength of organic bases (B) with the acceptor CrF_2 (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule CrF_2 are included in Table-10. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor CrF_2 is in the following order as predicted by the values of ΔN.

2-Phenylquinoline > 2-Aminoquinoline>8-Quinolinesulphonic acid >Isoquinoline > Quinoline > 8-Nitroquinoline > Quinolinic acid > 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 CrF_2 (A) as predicted by the value of lowering in energy ΔE is as follows-

2-Phenylquinoline >8-Quinolinesulphonic acid > 2-Aminoquinoline > Isoquinoline >Quinoline > 8-Nitroquinoline>Quinolinic 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 2-Phenylquinoline and The Minimum strength is in 5-Nitroquinoline as predicted by both ΔN and ΔE.

Metal ligand bond strength of organic bases (B) with the acceptor $CrCl_2$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule $CrCl_2$ are included in Table-11. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $CrCl_2$ is in the following order as predicted by the values of ΔN.

2-Phenylquinoline > 8-Quinolinesulphonic acid >2-Aminoquinoline > Isoquinoline > Quinoline > 8-Nitroquinoline >Quinolinic acid >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 $CrCl_2$ (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Quinolinesulphonic acid > 2-Phenylquinoline > 2-Aminoquinoline > Isoquinoline > Quinoline > 8-Nitroquinoline > Quinolinic 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 2-Phenylquinoline as predicted by ΔN and is in 8-Quinolinesulphonic acid as predicted by and ΔE and The minimum strength is in 5-Nitroquinoline as predicted by ΔN and ΔE.

Metal ligand bond strength of organic bases (B) with the acceptor $CrBr_2$ (A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule $CrBr_2$ are included in Table-12. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor $CrBr_2$ is in the following order as predicted by the values of ΔN.

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

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 $CrBr_2$ (A) as predicted by the value of lowering in energy ΔE is as follows-

8-Nitroquinoline > 2-Aminoquinoline > 2-Phenylquinoline > Quinolinic acid>Isoquinoline>5-Nitroquinoline>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 8-Nitroquinoline as predicted by both ΔN and ΔE; and the minimum strength is in Quinoline as predicted by ΔN and is in 8-Quinolinesulphonic acid as predicted by ΔE.

Metal ligand bond strength of organic bases (B) with the acceptor CrI_2(A) as predicted by the values of ΔN and ΔE

The values of ΔN, ΔE (calculated in eV) with the acceptor molecule CrI_2 are included in Table-13. As the value of ΔN increases, the metal ligand bond strength decreases. Metal ligand bond strength with the acceptor CrI_2 is in the following order as predicted by the values of ΔN.

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

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 CrI_2 (A) as predicted by the value of lowering in energy ΔE is as follows-

2-Aminoquinoline > 2-Phenylquinoline > 8-Nitroquinoline > Isoquinoline >Quinoline >8-Quinolinesulphonic acid > Quinolinic 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 ΔN and is in 2-Aminoquinoline as predicted by ΔE. The Minimum strength is in 8-Quinolinesulphonic acid and is in 5-Nitroquinoline as predicted by ΔN and ΔE respectively.

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.

IV. Conclusions

1) The acceptor strength is in the order
2) The chemical potential (μ_B) values of organic bases indicate the same order of base strength as is indicated by interaction energy.
3) The organic bases show that the 5-Nitroquinoline is the weakest base and 2-phenylquinoline is the strongest base against least of the acceptors.
4) $E\mu$ is the energy transfer on account of flow of electrons from lower μ to high μ. The $E\mu$ does not demonstrate the order of acid or base strength.
5) The best interaction is when global softness values of acid and base are approximately equal i.e. $S_A \approx S_{B.}$
6) Higher interaction energy (E_{int}) indicates strong metal ligand interaction.
7) All the results of interaction energy are in consonance with the results of ΔN and ΔE.

References

[1]. Francisco Mendez, Jose L Gazquez, Proc. Indian Acad. Sci. 106 (**1994**) 183
[2]. J. L. Gázquez, F. Méndez, J. Phys. Chem. 98 (**1993**) 4591
[3]. J. L.Gazquez, K.D. Sen, Chemical hardness: Structure and Bonding 80 (ed.) (Berlin : Springer – Verlag) , **1993**
[4]. R. G. Parr, J. L. Gazquez, J. Phys. Chem. 97 (**1993**) 3939
[5]. R. G. Parr, P. K. Chattaraj, J. Am. Chem. Soc. 113 (**1991**) 1855
[6]. R. G. Parr, W. Yang, Density functional theory of atoms and molecules, New York: Oxford University Press, **1989**
[7]. R. G. Pearson, Hard and soft acids and bases, Stroudsville, PA: Dowden, Hutchinson and Ross, **1973**

[8]. R. G. Pearson, J. Am. Chem. Soc. 110 (**1988**) 2092
[9]. R. G. Pearson, J. Chem. Educ. 64 (**1987**) 561
[10]. W. Yang, R. G. Parr, Proc. Natl. Acad. Sci. USA 82 (**1985**) 6723
[11]. R. G. Parr, P. K. Chattaraj, J. Am. Chem. Soc. 113 (**1991**) 1854
[12]. C. J. Umrigar, M. P. Nightingale, K. J. Runge, J. Chem. Phys. 99 (**1993**) 2865
[13]. A. Mushinski, M. P. Nightingale, J. Chem. Phys. 101 (**1994**) 883
[14]. R. G. Parr, Z. Zhou, Acc. Chem. Res. 26 (**1993**) 256
[15]. F. De Proft, , P. Geerlings, J. Chem. Phys. 106 (**1997**) 3270
[16]. S. Shankar, Proc Natl. Acad. Sci. USA 82 (**1985**) 264
[17]. R. A. Donnelly, W. E. Palke, M. Levy, J. Chem. Phys. 69 (**1978**) 3801
[18]. Y. Li, N. S. Evans, J. Am. Chem. Soc. 117 (**1995**) 7756
[19]. J. P. Perdew, R. G. Parr, M. Levy, J. L. Balduz, Phys. Rev. Lett. 49 (**1982**) 1691
[20]. R. T. Sanderson, Academic Press, New York **1976**
[21]. M. J. S. Dewar, T. F. Morita, J. Am. Chem. Soc. 91 (**1969**) 796
[22]. G. Klopman, J. Am. Chem. Soc. 90 (**1968**) 223
[23]. R. G. Parr, R. G. Pearson, J. Am. Chem. Soc. 105 (**1983**) 7512
[24]. Divya Singh, Shahin Ahmad, P.P. Singh, Journal of Molecular Structure: THEOCHEM 905 (**2009**) 13

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