International Journal of ChemTech Research
CODEN(USA): IJCRGG ISSN : 0974-4290
Vol.3, No.1, pp 253-266, Jan-Mar 2011

PM3 Based Calculation of Interaction Energy between Metal Halides and Organic Bases and its Comparison with DFT

Divya Singh*, Shahin Ahmad

Department of Chemistry Bareilly College, Bareilly, U.P.,India

Corres. Author: dr_ppsingh@sify.com

Abstract: Interactions between 24 organic bases and 12 metal halides have been studied with the help of interaction energy, charge transfer and energy lowering using PM3 method. The sequences of base strength against metal halides obtained by PM3 calculations are different from the order obtained by DFT calculations. The DFT based results show that the order of acceptor strength in tin (IV) halides is $SnCl_4$ > $SnBr_4$ > SnI_4 but PM3 based results show that $snBr_4$ is the strongest acceptor. The ΔN and ΔE values evaluated by PM3 method provide the same order for base strength as evaluated by DFT method.

Key words: - Interaction energy, charge transfer, energy lowering, chemical potential, PM3, metal halides, organic bases.

INTRODUCTION:

The interaction energy calculated for interaction between two chemical species A and B has recently been used for measuring magnitude of interaction in metal-ligand chemistry.[1-5] Singh et. al. applied the concept for interaction of metal halide with number of nitrogen and sulphur donors and evaluated the magnitude of donor and acceptor strengths.[1, 2, 4] All calculations were DT based. The interaction energy concept was also applied in medicinal chemistry in the study of interaction of hydroxamate inhibitor and metalloproteinases but the calculations were PM3 based.[3] Very recently bicyclam complexes have also been studied with the help of interaction energy.[5] The DFT based calculations are very reliable but they are time consuming and expensive. PM3 based calculations of interaction energy[4] has also provided dependable results. In this paper we present PM3 based calculation of interaction energy between metal halide and organic bases and have compared the results with DFT calculation.

MATERIALS AND METHODS:

The study materials of this paper are 24 organic and twelve metal halides listed in Table-A and Table-B. The structures of all the above compounds have been drawn and their geometries have been optimized with the help of Cache software by PM3 method.

According to density functional theory, interaction between a stable molecule A and a stable molecule B in terms of interaction energy [6] is given by-

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

The HSAB principle indicates that the interaction energy[7] is given by

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

where

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

and

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

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.

Parr et al [8-11] have shown that the electronegativity of any chemical species is equal to the negative value of chemical potential indeed it follows rigorously [12] that

$$\chi = -\mu = (I + A)/2 \quad (5)$$

where I and A are ionization potential and electron affinity of atomic or molecular system.

The physical meaning of chemical potential in DFT is the measure of the escaping tendency of an electron cloud from one system to another. It is constant in three-dimensional space for the ground state of an atom, molecule or solid.

Eqn-5 may be written as:

$$A = 2\chi - I \quad (6)$$

A concept use intuitively for a long time and validates Sanderson's postulates[13] that when two and more atoms combine to form a molecule, their electronegativity gets equalized and unique electronegativity exists everywhere in a molecule.[14]

According to Koopman's theorem the I and A are simply the eigen value of HOMO and LUMO respectively with change in sign [15]. Therefore, from equation-9 we get

$$A = -(\varepsilon HOMO + \varepsilon LUMO) - I \quad (7)$$

The chemical potential itself depend on N and v i.e. $\mu = \mu(N,v)$. Parr and Pearson [16] have defined hardness with respect to N as

$$\eta = \tfrac{1}{2}. (\delta\mu/\delta N)_{v(r)}$$
$$= \tfrac{1}{2}. (\delta^2 E/ \delta N^2)_{v(r)}$$
$$= (I - A)/2 \quad (8)$$

The inverse of the hardness is expressed as the global softness,

$$S = 1/2\eta \quad (9)$$

RESULT AND DISCUSSION:

Donor Acceptor Interaction:

The result of DFT based calculation as reported earlier by us[1] indicate that in case of SnX_4 [X =Cl, Br] the most stable complexes are formed by amino toluene in all the halides. The sequence of stability of complexes formed by organic bases is as below.

amino toluene > amino benzoic acid > amido toluene > amido benzoic acid > cyano benzoic acid > cyano toluene > nitro benzoic acid > nitro toluene.

The sequence of stability in case of SnI_4 is slightly changed; the weakest ligand in this case is nitro benzoic acid, whereas in $SnCl_4$ and $SnBr_4$ complexes the weakest is nitro toluene.

In case of results obtained by PM3 calculations presented in Table-1(c)-3, a different sequence is obtained. The strongest donor against $SnCl_4$ is amino benzoic acid in ortho substituent, amido benzoic acid in meta and para substituent. The sequence of stability of complexes formed by organic bases is a below:-

1. $SnCl_4$

Ortho - amino benzoic acid > amido benzoic acid > amido toluene > amino toluene >nitro benzoic acid > nitro toluene> cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > amino benzoic acid > amido toluene > nitro benzoic acid > cyano benzoic acid > amino toluene > nitro toluene > cyano toluene.

Para- amido benzoic acid > nitro benzoic acid > amino benzoic acid > amido toluene > cyano benzoic acid > amino toluene > nitro toluene > cyano toluene.

2. $SnBr_4$

Ortho - amino benzoic acid > amido benzoic acid > amido toluene > amino toluene > nitro benzoic acid > nitro toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > amino benzoic acid > nitro benzoic acid > amido toluene > amino toluene > cyano benzoic acid > nitro toluene > cyano toluene.

Para- amido benzoic acid > Amino benzoic acid > nitro benzoic acid > amido toluene > amino toluene > cyano benzoic acid > nitro toluene > cyano toluene.

3. SnI_4

Ortho - amino benzoic acid >amido benzoic acid >amido toluene > amino toluene > nitro benzoic acid >nitro toluene >cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid >nitro benzoic acid >amino benzoic acid > amido toluene > cyano benzoic acid > amino toluene >nitro toluene >cyano toluene.

Para- amido benzoic acid > nitro benzoic acid >amino benzoic acid >amido toluene > cyano benzoic acid >amino toluene >nitro toluene >cyano toluene.

The sequence of base strength in DFT based calculation of Zn (II) halides indicated the following order of base strength:-

Amino benzoic acid > amido toluene > amino toluene > Amido benzoic acid > cyano benzoic acid > cyano toluene > nitro benzoic acid > nitro toluene.

DFT based calculations where cadmium halides are acceptor-A indicates that amino toluene and the least stable complex form most stable complexes by nitro toluene. The sequence of base strength towards cadmium halide is as below.

Amino toluene > amino benzoic acid > amido toluene > amido benzoic acid > cyano benzoic acid > cyano toluene > nitro benzoic acid > nitro toluene.

DFT based calculations where mercury halides are acceptor A indicates that most stable complexes are formed by amino toluene and least stable by nitro toluene or nitro benzoic acid. The order of base strength is amino toluene > amino benzoic acid > amido toluene > amido benzoic acid > cyano toluene > cyano benzoic acid > nitro benzoic acid > nitro toluene. In case of PM3 based calculations presented in Table-4-12 the base strength for interaction with halides of Zn(II), Cd(II), Hg(II) are as below:-

4. $ZnCl_2$

Ortho - amido benzoic acid > amino benzoic acid > amido toluene > nitro benzoic acid > nitro toluene > amino toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene > amino toluene > cyano toluene.

Para- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene > amino toluene > cyano toluene.

5. $ZnBr_2$

Ortho - amido benzoic acid > amino benzoic acid > amido toluene > nitro benzoic acid > amino toluene > nitro toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > amido toluene > cyano benzoic acid > amino benzoic acid > nitro toluene >amino toluene > cyano toluene.

Para- amido benzoic acid > nitro benzoic acid > amido toluene > amino benzoic acid > cyano benzoic acid > amino toluene > nitro toluene >cyano toluene.

6.ZnI_2

Ortho - amino benzoic acid > amido benzoic acid > amido toluene > nitro benzoic acid > nitro toluene > amino toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amino benzoic acid > amido toluene > nitro toluene > amino toluene > cyano toluene.

Para- amido benzoic acid > nitro benzoic acid > amino benzoic acid > amido toluene > cyano benzoic acid > amino toluene > nitro toluene > cyano toluene.

7. $CdCl_2$

Ortho - amido benzoic acid > amino benzoic acid > amido toluene > nitro benzoic acid > nitro toluene >amino toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene >cyano toluene > amino toluene.

Para- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene >cyano toluene > amino toluene.

8. $CdBr_2$

Ortho - amido benzoic acid > amino benzoic acid > amido toluene > nitro benzoic acid > nitro toluene >amino toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene > cyano toluene > amino toluene.

Para- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene >cyano toluene > amino toluene.

9. CdI_2

Ortho - amido benzoic acid > amino benzoic acid > amido toluene > nitro benzoic acid > nitro toluene >amino toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene > amino toluene > cyano toluene.

Para- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene > amino toluene > cyano toluene.

10. $HgCl_2$

Ortho - amido benzoic acid > amino benzoic acid > amido toluene > nitro benzoic acid > nitro toluene >amino toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene >amino toluene > cyano toluene.

Para- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene > amino toluene > cyano toluene.

11.$HgBr_2$

Ortho - amido benzoic acid > amino benzoic acid > amido toluene > nitro benzoic acid > nitro toluene > amino toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > cyano benzoic acid > amido toluene > amino benzoic acid > nitro toluene >amino toluene > cyano toluene.

Para- amido benzoic acid > nitro benzoic acid > amido toluene > cyano benzoic acid > amino benzoic acid > nitro toluene >amino toluene > cyano toluene.

12. HgI_2

Ortho - amino benzoic acid > amido benzoic acid > amido toluene > nitro benzoic acid > nitro toluene > amino toluene > cyano benzoic acid > cyano toluene.

Meta- amido benzoic acid > nitro benzoic acid > amino benzoic acid > cyano benzoic acid > amido toluene > nitro toluene > amino toluene > cyano toluene.

Para- amido benzoic acid > nitro benzoic acid > amino benzoic acid > amido toluene > cyano benzoic acid > amino toluene > nitro toluene >cyano toluene.

The interaction energy evaluated by PM3 methods indicates that:- (a) the strongest donor is either amido benzoic acid or amino benzoic acid, the weakest donor is mostly cyano toluene or amino toluene (b) the interaction energy values of complexes of $SnBr_4$ are higher than $SnCl_4$. Similarly in case of zinc halide complexes the interaction energy of complexes of bromide are higher. The chemical potential values as discussed later also show that trends shown by PM3 calculation are against the established trends. It can be inferred that results obtained by PM3 calculation are inconsistent, and are also different from established trend, hence are not reliable inrespect of evaluating acceptor strength of metal halides or for deciding the base strength of organic bases.

CHEMICAL POTENTIAL (μ_A, μ_B):

The chemical potential provides a measure of acceptor strength of metal halides, and base strength of donor molecules. Higher is the value of chemical potential better is the acceptor strength. The lower is the chemical potential better is the base strength. The chemical potential values evaluated by DFT and PM3 method are included in Table-S-2 for acceptor halides and Table-S-1 for donor molecules.

A reference to Table-S-1 indicates that DFT and PM3 based chemical potential provide similar order for base strength. Both the methods indicate that amino toluene is the strongest donor and nitro benzoic acid is the weakest base. The only difference is in second and third position.

The chemical potential values **(μ_A)** of acceptor halides evaluated by DFT and PM3 methods and included in Table- S-2.

The orders of acceptor strength shown by DFT and PM3 based calculations are entirely different. The DFT based results show that the order of acceptor strength in tin (IV) halides is $SnCl_4$ > $SnBr_4$ > SnI_4, the PM3 based results show that $snBr_4$ is the strongest acceptor which is not in conformity with experimental results. It is strongly indicated that in respect of metal halides only the DFT based calculations be treated is reliable.

Shift in charge ΔN and lowering of energy ΔE:

Metal ligand bond strength has also been evaluated by calculating the shift in charge ΔN and loweing of energy ΔE . the relevant equation are given below:-

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

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

The values of ΔN, and ΔE have been evaluated by PM3 method which are presented in Table- 13-15 for reaction with Sn(IV) halides. The ΔN and ΔE values evaluated by PM3, DFT and Ab inito methods for interaction of $SnCl_4$ and ortho derivatives of organic bases are presented in Table-S-3.

Table-S-1. Chemical potential values of organic bases (B)

Compd.	DFT	PM3
amino toluene	2.62	3.705
amido toluene	3.55	4.309
amino benzoic acid	3.64	4.888
amido benzoic acid	4.14	5.217
cyano toluene	4.48	5.378
cyano benzoic acid	5.05	5.714
nitro toluene	5.12	5.744
nitro benzoic acid	5.39	5.997

Table-S-2. Chemical potential (μ_A) and global softness (S_A) values of acceptor (A).

	$SnCl_4$	$SnBr_4$	SnI_4	$ZnCl_2$	$ZnBr_2$	ZnI_2	$CdCl_2$	$CdBr_2$	CdI_2	$HgCl_2$	$HgBr_2$	HgI_2
DFT												
Base	-6.362	-5.855	-5.846	-5.214	-5.007	-4.773	-5.352	-5.057	-4.793	-6.083	-5.667	-5.326
PM3												
Base	-9.208	-7.842	7.772	-7.662	0.7449	6.839	6.837	-6.614	-6.528	-6.357	-6.181	6.013

Table-S-3. ΔN and ΔE for interaction of organic bases with $SnCl_4$

Organic Base	PM3		DFT		Ab inito	
	ΔN	ΔE	ΔN	ΔE	ΔN	ΔE
$C_6H_4CH_3NO_2$	0.137	0.146	0.225	-0.139	0.329	-0.390
$C_6H_4CH_3CONH_2$	0.169	0.250	0.346	-0.486	0.455	-0.684
$C_6H_4CH_3N\ H_2$	0.253	0.523	0.481	-0.902	0.619	-1.311
$C_6H_4CH_3CN$	0.153	0.201	0.234	-0.220	0.311	-0.343
$C_6H_4COOH\ CN$	0.124	0.130	0.171	-0.111	0.242	-0.187
$C_6H_4COOHNO_2$	0.119	0.110	0.177	-0.086	0.232	-0.147
$C_6H_4COOHCONH_2$	0.142	0.175	0.313	-0.347	0.386	-0.395
$C_6H_4COOHNH_2$	0.224	0.396	0.395	-0.536	0.531	-0.799

ΔN and ΔE values evaluated by PM3 methods show the following order of base strength against $SnCl_4$.

amino toluene > amino benzoic acid > nitro toluene > cyano benzoic acid > nitro benzoic acid.

ΔN and ΔE values evaluated by DFT and Ab inito methods show the same order of base strength. The graphs drawn for ΔN and ΔE values, for all the three methods demonstrate the quality of relationship between three methods in respect of ΔE and ΔN.

Table-A. Metal Halides

S. No.	Metal Halide
1	$SnCl_4$
2	$SnBr_4$
3	SnI_4
4	$ZnCl_2$
5	$ZnBr_2$
6	ZnI_2
7	$CdCl_2$
8	$CdBr_2$
9	CdI_2
10	$HgCl_2$
11	$HgBr_2$
12	HgI_2

Table-B. Organic bases

S. No.	Organic Base (B)
	Ortho
1	$C_6H_4CH_3NO_2$-o
2	$C_6H_4CH_3CONH_2$-o
3	$C_6H_4CH_3NH_2$-o
4	$C_6H_4CH_3CN$-o
5	$C_6H_4COOHCN$-o
6	$C_6H_4COOHNO_2$-o
7	$C_6H_4COOHCONH_2$-o
8	$C_6H_4COOHNH_2$-o
	Meta
9	$C_6H_4CH_3NO_2$-m
10	$C_6H_4CH_3CONH_2$-m
11	$C_6H_4CH_3NH_2$-m
12	$C_6H_4CH_3CN$-m
13	$C_6H_4COOHCN$-m
14	$C_6H_4COOHNO_2$-m
15	$C_6H_4COOHCONH_2$-m
16	$C_6H_4COOHNH_2$-m
	Para
17	$C_6H_4CH_3NO_2$-p
18	$C_6H_4CH_3CONH_2$-p
19	$C_6H_4CH_3NH_2$-p
20	$C_6H_4CH_3CN$-p
21	$C_6H_4COOHCN$-p
22	$C_6H_4COOHNO_2$-p
23	$C_6H_4COOHCONH_2$-p
24	$C_6H_4COOHNH_2$-p

. Table-1. Interaction energy evaluated by PM3 method for interaction of organic bases with $SnCl_4$ (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-7.842	0.258	3.528	-0.292	-3.415	-3.707
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-7.842	0.258	3.528	-0.501	-3.797	-4.298
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-7.842	0.258	2.738	-1.047	-2.791	-3.838
$C_6H_4CH_3CN$-o	-5.217	0.214	-7.842	0.258	2.450	-0.403	-2.597	-3.000
$C_6H_4COOHCN$-o	-5.744	0.217	-7.842	0.258	2.888	-0.259	-3.044	-3.303
$C_6H_4COOHNO_2$-o	-5.997	0.257	-7.842	0.258	3.698	-0.219	-3.592	-3.811
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-7.842	0.258	4.418	-0.351	-4.731	-5.081
$C_6H_4COOHNH_2$-o	-4.309	0.249	-7.842	0.258	4.418	-0.791	-4.356	-5.147
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-7.842	0.258	3.528	-0.283	-3.431	-3.714
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-7.842	0.258	3.528	-0.474	-3.743	-4.216
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-7.842	0.258	2.738	-1.036	-2.797	-3.833
$C_6H_4CH_3CN$-m	-5.219	0.213	-7.842	0.258	2.888	-0.401	-3.067	-3.468
$C_6H_4COOHCN$-m	-5.750	0.214	-7.842	0.258	3.698	-0.256	-3.918	-4.174
$C_6H_4COOHNO_2$-m	-6.016	0.254	-7.842	0.258	4.418	-0.214	-4.313	-4.527
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-7.842	0.258	4.418	-0.367	-4.606	-4.973
$C_6H_4COOHNH_2$-m	-4.344	0.248	-7.842	0.258	3.528	-0.774	-3.486	-4.260
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-7.842	0.258	3.528	-0.301	-3.407	-3.708
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-7.842	0.258	3.528	-0.474	-3.730	-4.204
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-7.842	0.258	2.738	-1.075	-2.791	-3.865
$C_6H_4CH_3CN$-p	-5.186	0.216	-7.842	0.258	2.888	-0.415	-3.045	-3.460
$C_6H_4COOHCN$-p	-5.871	0.218	-7.842	0.258	3.698	-0.229	-3.889	-4.118
$C_6H_4COOHNO_2$-p	-6.147	0.258	-7.842	0.258	4.418	-0.185	-4.283	-4.468
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-7.842	0.258	4.418	-0.327	-4.572	-4.899
$C_6H_4COOHNH_2$-p	-4.309	0.249	-7.842	0.258	3.528	-0.791	-3.479	-4.270

Table-2. Interaction energy evaluated by PM3 method for interaction of organic bases with $SnBr_4$ (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-9.208	0.262	3.528	-0.795	-3.386	-4.181
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-9.208	0.262	3.528	-1.079	-3.761	-4.840
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-9.208	0.262	2.738	-1.867	-2.767	-4.633
$C_6H_4CH_3CN$-o	-5.217	0.214	-9.208	0.262	2.450	-0.938	-2.573	-3.511
$C_6H_4COOHCN$-o	-5.744	0.217	-9.208	0.262	2.888	-0.712	-3.016	-3.728
$C_6H_4COOHNO_2$-o	-5.997	0.257	-9.208	0.262	3.698	-0.669	-3.561	-4.230
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-9.208	0.262	4.418	-0.854	-4.687	-5.540
$C_6H_4COOHNH_2$-o	-4.309	0.249	-9.208	0.262	4.418	-1.534	-4.319	-5.852
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-9.208	0.262	3.528	-0.779	-3.401	-4.180
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-9.208	0.262	3.528	-1.045	-3.708	-4.753
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-9.208	0.262	2.738	-1.852	-2.772	-4.624
$C_6H_4CH_3CN$-m	-5.219	0.213	-9.208	0.262	2.888	-0.935	-3.038	-3.974
$C_6H_4COOHCN$-m	-5.750	0.214	-9.208	0.262	3.698	-0.705	-3.882	-4.587
$C_6H_4COOHNO_2$-m	-6.016	0.254	-9.208	0.262	4.418	-0.658	-4.277	-4.934
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-9.208	0.262	4.418	-0.889	-4.564	-5.453
$C_6H_4COOHNH_2$-m	-4.344	0.248	-9.208	0.262	3.528	-1.509	-3.456	-4.964
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-9.208	0.262	3.528	-0.810	-3.378	-4.189
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-9.208	0.262	3.528	-1.047	-3.695	-4.742
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-9.208	0.262	2.738	-1.904	-2.766	-4.670
$C_6H_4CH_3CN$-p	-5.186	0.216	-9.208	0.262	2.888	-0.959	-3.017	-3.977
$C_6H_4COOHCN$-p	-5.871	0.218	-9.208	0.262	3.698	-0.662	-3.853	-4.516
$C_6H_4COOHNO_2$-p	-6.147	0.258	-9.208	0.262	4.418	-0.609	-4.247	-4.856
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-9.208	0.262	4.418	-0.829	-4.531	-5.360
$C_6H_4COOHNH_2$-p	-4.309	0.249	-9.208	0.262	3.528	-1.534	-3.449	-4.982

Table-3. Interaction energy evaluated by PM3 method for interaction of organic bases with SnI_4 (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-7.449	0.348	3.528	-0.223	-2.908	-3.131
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-7.449	0.348	3.528	-0.425	-3.180	-3.605
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-7.449	0.348	2.738	-0.977	-2.358	-3.335
$C_6H_4CH_3CN$-o	-5.217	0.214	-7.449	0.348	2.450	-0.330	-2.180	-2.510
$C_6H_4COOHCN$-o	-5.744	0.217	-7.449	0.348	2.888	-0.194	-2.558	-2.752
$C_6H_4COOHNO_2$-o	-5.997	0.257	-7.449	0.348	3.698	-0.156	-3.056	-3.212
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-7.449	0.348	4.418	-0.280	-3.965	-4.245
$C_6H_4COOHNH_2$-o	-4.309	0.249	-7.449	0.348	4.418	-0.716	-3.699	-4.414
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-7.449	0.348	3.528	-0.215	-2.919	-3.134
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-7.449	0.348	3.528	-0.398	-3.142	-3.540
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-7.449	0.348	2.738	-0.967	-2.362	-3.328
$C_6H_4CH_3CN$-m	-5.219	0.213	-7.449	0.348	2.888	-0.328	-2.574	-2.902
$C_6H_4COOHCN$-m	-5.750	0.214	-7.449	0.348	3.698	-0.191	-3.290	-3.481
$C_6H_4COOHNO_2$-m	-6.016	0.254	-7.449	0.348	4.418	-0.151	-3.668	-3.818
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-7.449	0.348	4.418	-0.295	-3.877	-4.172
$C_6H_4COOHNH_2$-m	-4.344	0.248	-7.449	0.348	3.528	-0.699	-2.959	-3.657
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-7.449	0.348	3.528	-0.232	-2.902	-3.133
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-7.449	0.348	3.528	-0.399	-3.133	-3.531
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-7.449	0.348	2.738	-1.006	-2.357	-3.363
$C_6H_4CH_3CN$-p	-5.186	0.216	-7.449	0.348	2.888	-0.342	-2.559	-2.901
$C_6H_4COOHCN$-p	-5.871	0.218	-7.449	0.348	3.698	-0.167	-3.269	-3.436
$C_6H_4COOHNO_2$-p	-6.147	0.258	-7.449	0.348	4.418	-0.125	-3.646	-3.771
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-7.449	0.348	4.418	-0.257	-3.853	-4.110
$C_6H_4COOHNH_2$-p	-4.309	0.249	-7.449	0.348	3.528	-0.716	-2.953	-3.669

Table-4. Interaction energy evaluated by PM3 method for interaction of organic bases with $ZnCl_2$ (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-6.357	0.218	3.042	-0.024	-3.190	-3.215
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-6.357	0.218	3.042	-0.114	-3.580	-3.695
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-6.357	0.218	2.312	-0.396	-2.565	-2.961
$C_6H_4CH_3CN$-o	-5.217	0.214	-6.357	0.218	2.048	-0.070	-2.371	-2.441
$C_6H_4COOHCN$-o	-5.744	0.217	-6.357	0.218	2.450	-0.020	-2.819	-2.839
$C_6H_4COOHNO_2$-o	-5.997	0.257	-6.357	0.218	3.200	-0.008	-3.368	-3.376
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-6.357	0.218	3.872	-0.051	-4.532	-4.583
$C_6H_4COOHNH_2$-o	-4.309	0.249	-6.357	0.218	3.872	-0.244	-4.143	-4.387
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-6.357	0.218	3.042	-0.022	-3.206	-3.228
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-6.357	0.218	3.042	-0.100	-3.525	-3.625
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-6.357	0.218	2.312	-0.390	-2.571	-2.961
$C_6H_4CH_3CN$-m	-5.219	0.213	-6.357	0.218	2.450	-0.070	-2.842	-2.912
$C_6H_4COOHCN$-m	-5.750	0.214	-6.357	0.218	3.200	-0.020	-3.703	-3.722
$C_6H_4COOHNO_2$-m	-6.016	0.254	-6.357	0.218	3.872	-0.007	-4.099	-4.105
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-6.357	0.218	3.872	-0.054	-4.402	-4.457
$C_6H_4COOHNH_2$-m	-4.344	0.248	-6.357	0.218	3.042	-0.235	-3.262	-3.497
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-6.357	0.218	3.042	-0.027	-3.182	-3.209
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-6.357	0.218	3.042	-0.100	-3.511	-3.611
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-6.357	0.218	2.312	-0.412	-2.564	-2.977
$C_6H_4CH_3CN$-p	-5.186	0.216	-6.357	0.218	2.450	-0.074	-2.820	-2.895
$C_6H_4COOHCN$-p	-5.871	0.218	-6.357	0.218	3.200	-0.013	-3.672	-3.685
$C_6H_4COOHNO_2$-p	-6.147	0.258	-6.357	0.218	3.872	-0.003	-4.067	-4.070
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-6.357	0.218	3.872	-0.040	-4.367	-4.407
$C_6H_4COOHNH_2$-p	-4.309	0.249	-6.357	0.218	3.042	-0.244	-3.255	-3.499

Table-5. Interaction energy evaluated by PM3 method for interaction of organic bases with $ZnBr_2$ (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-7.727	0.204	3.042	-0.231	-3.283	-3.515
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-7.727	0.204	3.042	-0.414	-3.698	-4.112
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-7.727	0.204	2.312	-0.880	-2.644	-3.525
$C_6H_4CH_3CN$-o	-5.217	0.214	-7.727	0.204	2.048	-0.329	-2.447	-2.776
$C_6H_4COOHCN$-o	-5.744	0.217	-7.727	0.204	2.450	-0.207	-2.909	-3.116
$C_6H_4COOHNO_2$-o	-5.997	0.257	-7.727	0.204	3.200	-0.170	-3.467	-3.637
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-7.727	0.204	3.872	-0.285	-4.680	-4.965
$C_6H_4COOHNH_2$-o	-4.309	0.249	-7.727	0.204	3.872	-0.656	-4.266	-4.922
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-7.727	0.204	3.042	-0.224	-3.300	-3.524
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-7.727	0.204	3.042	-0.390	-3.638	-4.028
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-7.727	0.204	2.312	-0.872	-2.650	-3.522
$C_6H_4CH_3CN$-m	-5.219	0.213	-7.727	0.204	2.450	-0.328	-2.934	-3.262
$C_6H_4COOHCN$-m	-5.750	0.214	-7.727	0.204	3.200	-0.205	-3.822	-4.026
$C_6H_4COOHNO_2$-m	-6.016	0.254	-7.727	0.204	3.872	-0.166	-4.219	-4.385
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-7.727	0.204	3.872	-0.298	-4.541	-4.839
$C_6H_4COOHNH_2$-m	-4.344	0.248	-7.727	0.204	3.042	-0.642	-3.359	-4.001
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-7.727	0.204	3.042	-0.239	-3.274	-3.513
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-7.727	0.204	3.042	-0.390	-3.624	-4.014
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-7.727	0.204	2.312	-0.905	-2.643	-3.548
$C_6H_4CH_3CN$-p	-5.186	0.216	-7.727	0.204	2.450	-0.340	-2.911	-3.250
$C_6H_4COOHCN$-p	-5.871	0.218	-7.727	0.204	3.200	-0.182	-3.790	-3.971
$C_6H_4COOHNO_2$-p	-6.147	0.258	-7.727	0.204	3.872	-0.142	-4.186	-4.328
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-7.727	0.204	3.872	-0.263	-4.504	-4.768
$C_6H_4COOHNH_2$-p	-4.309	0.249	-7.727	0.204	3.042	-0.656	-3.351	-4.008

Table-6. Interaction energy evaluated by PM3 method for interaction of organic bases with ZnI_2 (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-6.839	0.293	3.042	-0.087	-2.758	-2.845
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-6.839	0.293	3.042	-0.231	-3.044	-3.275
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-6.839	0.293	2.312	-0.637	-2.200	-2.837
$C_6H_4CH_3CN$-o	-5.217	0.214	-6.839	0.293	2.048	-0.163	-2.021	-2.183
$C_6H_4COOHCN$-o	-5.744	0.217	-6.839	0.293	2.450	-0.075	-2.405	-2.479
$C_6H_4COOHNO_2$-o	-5.997	0.257	-6.839	0.293	3.200	-0.049	-2.910	-2.959
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-6.839	0.293	3.872	-0.130	-3.857	-3.987
$C_6H_4COOHNH_2$-o	-4.309	0.249	-6.839	0.293	3.872	-0.431	-3.571	-4.002
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-6.839	0.293	3.042	-0.082	-2.769	-2.852
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-6.839	0.293	3.042	-0.210	-3.004	-3.214
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-6.839	0.293	2.312	-0.629	-2.204	-2.833
$C_6H_4CH_3CN$-m	-5.219	0.213	-6.839	0.293	2.450	-0.162	-2.422	-2.583
$C_6H_4COOHCN$-m	-5.750	0.214	-6.839	0.293	3.200	-0.073	-3.156	-3.230
$C_6H_4COOHNO_2$-m	-6.016	0.254	-6.839	0.293	3.872	-0.046	-3.538	-3.584
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-6.839	0.293	3.872	-0.138	-3.762	-3.900
$C_6H_4COOHNH_2$-m	-4.344	0.248	-6.839	0.293	3.042	-0.418	-2.811	-3.229
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-6.839	0.293	3.042	-0.092	-2.752	-2.843
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-6.839	0.293	3.042	-0.210	-2.994	-3.204
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-6.839	0.293	2.312	-0.659	-2.199	-2.859
$C_6H_4CH_3CN$-p	-5.186	0.216	-6.839	0.293	2.450	-0.170	-2.406	-2.576
$C_6H_4COOHCN$-p	-5.871	0.218	-6.839	0.293	3.200	-0.059	-3.134	-3.193
$C_6H_4COOHNO_2$-p	-6.147	0.258	-6.839	0.293	3.872	-0.033	-3.515	-3.548
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-6.839	0.293	3.872	-0.112	-3.737	-3.849
$C_6H_4COOHNH_2$-p	-4.309	0.249	-6.839	0.293	3.042	-0.431	-2.806	-3.237

Table-7. Interaction energy evaluated by PM3 method for interaction of organic bases with $CdCl_2$ (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-6.090	0.192	3.042	-0.008	-3.374	-3.382
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-6.090	0.192	3.042	-0.072	-3.813	-3.885
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-6.090	0.192	2.312	-0.299	-2.722	-3.021
$C_6H_4CH_3CN$-o	-5.217	0.214	-6.090	0.192	2.048	-0.039	-2.522	-2.561
$C_6H_4COOHCN$-o	-5.744	0.217	-6.090	0.192	2.450	-0.006	-2.998	-3.004
$C_6H_4COOHNO_2$-o	-5.997	0.257	-6.090	0.192	3.200	0.000	-3.563	-3.563
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-6.090	0.192	3.872	-0.025	-4.825	-4.850
$C_6H_4COOHNH_2$-o	-4.309	0.249	-6.090	0.192	3.872	-0.172	-4.386	-4.558
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-6.090	0.192	3.042	-0.007	-3.391	-3.398
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-6.090	0.192	3.042	-0.061	-3.750	-3.811
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-6.090	0.192	2.312	-0.295	-2.728	-3.023
$C_6H_4CH_3CN$-m	-5.219	0.213	-6.090	0.192	2.450	-0.038	-3.024	-3.062
$C_6H_4COOHCN$-m	-5.750	0.214	-6.090	0.192	3.200	-0.006	-3.939	-3.945
$C_6H_4COOHNO_2$-m	-6.016	0.254	-6.090	0.192	3.872	0.000	-4.337	-4.337
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-6.090	0.192	3.872	-0.027	-4.678	-4.705
$C_6H_4COOHNH_2$-m	-4.344	0.248	-6.090	0.192	3.042	-0.165	-3.454	-3.619
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-6.090	0.192	3.042	-0.009	-3.365	-3.374
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-6.090	0.192	3.042	-0.060	-3.735	-3.795
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-6.090	0.192	2.312	-0.313	-2.721	-3.034
$C_6H_4CH_3CN$-p	-5.186	0.216	-6.090	0.192	2.450	-0.042	-2.999	-3.041
$C_6H_4COOHCN$-p	-5.871	0.218	-6.090	0.192	3.200	-0.002	-3.905	-3.907
$C_6H_4COOHNO_2$-p	-6.147	0.258	-6.090	0.192	3.872	0.000	-4.301	-4.302
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-6.090	0.192	3.872	-0.017	-4.638	-4.656
$C_6H_4COOHNH_2$-p	-4.309	0.249	-6.090	0.192	3.042	-0.172	-3.446	-3.618

Table-8. Interaction energy evaluated by PM3 method for interaction of organic bases with $CdBr_2$ (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-6.614	0.190	3.042	-0.044	-3.393	-3.437
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-6.614	0.190	3.042	-0.147	-3.837	-3.984
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-6.614	0.190	2.312	-0.442	-2.738	-3.180
$C_6H_4CH_3CN$-o	-5.217	0.214	-6.614	0.190	2.048	-0.098	-2.538	-2.636
$C_6H_4COOHCN$-o	-5.744	0.217	-6.614	0.190	2.450	-0.038	-3.016	-3.054
$C_6H_4COOHNO_2$-o	-5.997	0.257	-6.614	0.190	3.200	-0.021	-3.583	-3.603
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-6.614	0.190	3.872	-0.076	-4.855	-4.931
$C_6H_4COOHNH_2$-o	-4.309	0.249	-6.614	0.190	3.872	-0.286	-4.411	-4.697
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-6.614	0.190	3.042	-0.041	-3.410	-3.452
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-6.614	0.190	3.042	-0.132	-3.773	-3.905
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-6.614	0.190	2.312	-0.436	-2.744	-3.180
$C_6H_4CH_3CN$-m	-5.219	0.213	-6.614	0.190	2.450	-0.098	-3.042	-3.140
$C_6H_4COOHCN$-m	-5.750	0.214	-6.614	0.190	3.200	-0.038	-3.963	-4.001
$C_6H_4COOHNO_2$-m	-6.016	0.254	-6.614	0.190	3.872	-0.019	-4.361	-4.380
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-6.614	0.190	3.872	-0.080	-4.706	-4.786
$C_6H_4COOHNH_2$-m	-4.344	0.248	-6.614	0.190	3.042	-0.277	-3.473	-3.751
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-6.614	0.190	3.042	-0.047	-3.383	-3.431
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-6.614	0.190	3.042	-0.131	-3.758	-3.889
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-6.614	0.190	2.312	-0.459	-2.737	-3.196
$C_6H_4CH_3CN$-p	-5.186	0.216	-6.614	0.190	2.450	-0.103	-3.018	-3.121
$C_6H_4COOHCN$-p	-5.871	0.218	-6.614	0.190	3.200	-0.028	-3.928	-3.956
$C_6H_4COOHNO_2$-p	-6.147	0.258	-6.614	0.190	3.872	-0.012	-4.325	-4.337
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-6.614	0.190	3.872	-0.063	-4.666	-4.729
$C_6H_4COOHNH_2$-p	-4.309	0.249	-6.614	0.190	3.042	-0.286	-3.465	-3.751

Table-9. Interaction energy evaluated by PM3 method for interaction of organic bases with CdI_2 (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-6.181	0.272	3.042	-0.014	-2.867	-2.882
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-6.181	0.272	3.042	-0.098	-3.178	-3.277
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-6.181	0.272	2.312	-0.384	-2.292	-2.676
$C_6H_4CH_3CN$-o	-5.217	0.214	-6.181	0.272	2.048	-0.056	-2.108	-2.164
$C_6H_4COOHCN$-o	-5.744	0.217	-6.181	0.272	2.450	-0.012	-2.509	-2.520
$C_6H_4COOHNO_2$-o	-5.997	0.257	-6.181	0.272	3.200	-0.002	-3.026	-3.028
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-6.181	0.272	3.872	-0.038	-4.026	-4.064
$C_6H_4COOHNH_2$-o	-4.309	0.249	-6.181	0.272	3.872	-0.228	-3.716	-3.943
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-6.181	0.272	3.042	-0.013	-2.880	-2.893
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-6.181	0.272	3.042	-0.084	-3.134	-3.218
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-6.181	0.272	2.312	-0.379	-2.296	-2.675
$C_6H_4CH_3CN$-m	-5.219	0.213	-6.181	0.272	2.450	-0.055	-2.527	-2.582
$C_6H_4COOHCN$-m	-5.750	0.214	-6.181	0.272	3.200	-0.011	-3.293	-3.304
$C_6H_4COOHNO_2$-m	-6.016	0.254	-6.181	0.272	3.872	-0.002	-3.680	-3.682
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-6.181	0.272	3.872	-0.041	-3.923	-3.964
$C_6H_4COOHNH_2$-m	-4.344	0.248	-6.181	0.272	3.042	-0.219	-2.925	-3.144
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-6.181	0.272	3.042	-0.016	-2.861	-2.877
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-6.181	0.272	3.042	-0.084	-3.124	-3.208
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-6.181	0.272	2.312	-0.401	-2.291	-2.693
$C_6H_4CH_3CN$-p	-5.186	0.216	-6.181	0.272	2.450	-0.060	-2.510	-2.569
$C_6H_4COOHCN$-p	-5.871	0.218	-6.181	0.272	3.200	-0.006	-3.269	-3.275
$C_6H_4COOHNO_2$-p	-6.147	0.258	-6.181	0.272	3.872	0.000	-3.655	-3.655
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-6.181	0.272	3.872	-0.028	-3.895	-3.923
$C_6H_4COOHNH_2$-p	-4.309	0.249	-6.181	0.272	3.042	-0.228	-2.919	-3.147

Table-10. Interaction energy evaluated by PM3 method for interaction of organic bases with $HgCl_2$ (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-6.528	0.235	3.042	-0.041	-3.078	-3.118
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-6.528	0.235	3.042	-0.148	-3.439	-3.587
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-6.528	0.235	2.312	-0.466	-2.469	-2.935
$C_6H_4CH_3CN$-o	-5.217	0.214	-6.528	0.235	2.048	-0.096	-2.278	-2.375
$C_6H_4COOHCN$-o	-5.744	0.217	-6.528	0.235	2.450	-0.035	-2.710	-2.744
$C_6H_4COOHNO_2$-o	-5.997	0.257	-6.528	0.235	3.200	-0.017	-3.249	-3.266
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-6.528	0.235	3.872	-0.073	-4.354	-4.427
$C_6H_4COOHNH_2$-o	-4.309	0.249	-6.528	0.235	3.872	-0.298	-3.993	-4.291
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-6.528	0.235	3.042	-0.038	-3.092	-3.130
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-6.528	0.235	3.042	-0.132	-3.387	-3.519
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-6.528	0.235	2.312	-0.460	-2.474	-2.934
$C_6H_4CH_3CN$-m	-5.219	0.213	-6.528	0.235	2.450	-0.096	-2.731	-2.827
$C_6H_4COOHCN$-m	-5.750	0.214	-6.528	0.235	3.200	-0.034	-3.558	-3.592
$C_6H_4COOHNO_2$-m	-6.016	0.254	-6.528	0.235	3.872	-0.016	-3.952	-3.968
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-6.528	0.235	3.872	-0.078	-4.234	-4.311
$C_6H_4COOHNH_2$-m	-4.344	0.248	-6.528	0.235	3.042	-0.288	-3.144	-3.432
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-6.528	0.235	3.042	-0.044	-3.070	-3.114
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-6.528	0.235	3.042	-0.131	-3.375	-3.506
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-6.528	0.235	2.312	-0.484	-2.469	-2.953
$C_6H_4CH_3CN$-p	-5.186	0.216	-6.528	0.235	2.450	-0.102	-2.711	-2.813
$C_6H_4COOHCN$-p	-5.871	0.218	-6.528	0.235	3.200	-0.024	-3.531	-3.555
$C_6H_4COOHNO_2$-p	-6.147	0.258	-6.528	0.235	3.872	-0.009	-3.923	-3.932
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-6.528	0.235	3.872	-0.060	-4.201	-4.261
$C_6H_4COOHNH_2$-p	-4.309	0.249	-6.528	0.235	3.042	-0.298	-3.137	-3.435

Table-11. Interaction energy evaluated by PM3 method for interaction of organic bases with $HgBr_2$ (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-7.662	0.191	3.042	-0.208	-3.385	-3.593
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-7.662	0.191	3.042	-0.382	-3.827	-4.209
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-7.662	0.191	2.312	-0.820	-2.731	-3.551
$C_6H_4CH_3CN$-o	-5.217	0.214	-7.662	0.191	2.048	-0.301	-2.531	-2.832
$C_6H_4COOHCN$-o	-5.744	0.217	-7.662	0.191	2.450	-0.186	-3.008	-3.195
$C_6H_4COOHNO_2$-o	-5.997	0.257	-7.662	0.191	3.200	-0.152	-3.574	-3.726
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-7.662	0.191	3.872	-0.260	-4.842	-5.103
$C_6H_4COOHNH_2$-o	-4.309	0.249	-7.662	0.191	3.872	-0.607	-4.401	-5.008
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-7.662	0.191	3.042	-0.201	-3.402	-3.604
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-7.662	0.191	3.042	-0.358	-3.763	-4.121
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-7.662	0.191	2.312	-0.812	-2.737	-3.549
$C_6H_4CH_3CN$-m	-5.219	0.213	-7.662	0.191	2.450	-0.300	-3.034	-3.335
$C_6H_4COOHCN$-m	-5.750	0.214	-7.662	0.191	3.200	-0.184	-3.953	-4.137
$C_6H_4COOHNO_2$-m	-6.016	0.254	-7.662	0.191	3.872	-0.148	-4.351	-4.498
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-7.662	0.191	3.872	-0.271	-4.694	-4.965
$C_6H_4COOHNH_2$-m	-4.344	0.248	-7.662	0.191	3.042	-0.594	-3.465	-4.059
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-7.662	0.191	3.042	-0.215	-3.375	-3.590
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-7.662	0.191	3.042	-0.358	-3.748	-4.106
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-7.662	0.191	2.312	-0.843	-2.730	-3.573
$C_6H_4CH_3CN$-p	-5.186	0.216	-7.662	0.191	2.450	-0.311	-3.010	-3.321
$C_6H_4COOHCN$-p	-5.871	0.218	-7.662	0.191	3.200	-0.163	-3.919	-4.082
$C_6H_4COOHNO_2$-p	-6.147	0.258	-7.662	0.191	3.872	-0.126	-4.315	-4.441
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-7.662	0.191	3.872	-0.239	-4.654	-4.893
$C_6H_4COOHNH_2$-p	-4.309	0.249	-7.662	0.191	3.042	-0.607	-3.457	-4.064

Table-12. Interaction energy evaluated by PM3 method for interaction of organic bases with HgI_2 (Acid A)

Organic Base (B)	μ_B	S_B	uA	μ_A	λ	E_v	E_μ	E_{int}
$C_6H_4CH_3NO_2$-o	-5.714	0.259	-6.837	0.295	3.042	-0.087	-2.747	-2.833
$C_6H_4CH_3CONH_2$-o	-4.888	0.207	-6.837	0.295	3.042	-0.231	-3.031	-3.262
$C_6H_4CH_3NH_2$-o	-3.705	0.233	-6.837	0.295	2.312	-0.638	-2.191	-2.829
$C_6H_4CH_3CN$-o	-5.217	0.214	-6.837	0.295	2.048	-0.163	-2.012	-2.175
$C_6H_4COOHCN$-o	-5.744	0.217	-6.837	0.295	2.450	-0.075	-2.394	-2.469
$C_6H_4COOHNO_2$-o	-5.997	0.257	-6.837	0.295	3.200	-0.048	-2.898	-2.947
$C_6H_4COOHCONH_2$-o	-5.378	0.209	-6.837	0.295	3.872	-0.130	-3.840	-3.970
$C_6H_4COOHNH_2$-o	-4.309	0.249	-6.837	0.295	3.872	-0.432	-3.556	-3.988
$C_6H_4CH_3NO_2$-m	-5.742	0.256	-6.837	0.295	3.042	-0.082	-2.758	-2.840
$C_6H_4CH_3CONH_2$-m	-4.995	0.214	-6.837	0.295	3.042	-0.210	-2.991	-3.201
$C_6H_4CH_3NH_2$-m	-3.721	0.232	-6.837	0.295	2.312	-0.630	-2.195	-2.825
$C_6H_4CH_3CN$-m	-5.219	0.213	-6.837	0.295	2.450	-0.162	-2.411	-2.573
$C_6H_4COOHCN$-m	-5.750	0.214	-6.837	0.295	3.200	-0.073	-3.142	-3.216
$C_6H_4COOHNO_2$-m	-6.016	0.254	-6.837	0.295	3.872	-0.046	-3.524	-3.570
$C_6H_4COOHCONH_2$-m	-5.362	0.222	-6.837	0.295	3.872	-0.138	-3.746	-3.884
$C_6H_4COOHNH_2$-m	-4.344	0.248	-6.837	0.295	3.042	-0.419	-2.799	-3.219
$C_6H_4CH_3NO_2$-p	-5.685	0.260	-6.837	0.295	3.042	-0.092	-2.740	-2.832
$C_6H_4CH_3CONH_2$-p	-5.000	0.215	-6.837	0.295	3.042	-0.210	-2.981	-3.191
$C_6H_4CH_3NH_2$-p	-3.651	0.233	-6.837	0.295	2.312	-0.661	-2.190	-2.851
$C_6H_4CH_3CN$-p	-5.186	0.216	-6.837	0.295	2.450	-0.170	-2.395	-2.566
$C_6H_4COOHCN$-p	-5.871	0.218	-6.837	0.295	3.200	-0.059	-3.121	-3.179
$C_6H_4COOHNO_2$-p	-6.147	0.258	-6.837	0.295	3.872	-0.033	-3.501	-3.533
$C_6H_4COOHCONH_2$-p	-5.510	0.225	-6.837	0.295	3.872	-0.112	-3.720	-3.833
$C_6H_4COOHNH_2$-p	-4.309	0.249	-6.837	0.295	3.042	-0.432	-2.794	-3.226

Table-13. Values of ΔN and ΔE evaluated by PM3 method for interaction of organic bases with $SnCl_4$

Organic Base (B)	χA	χB	η_A	η_B	ΔN	ΔE
$C_6H_4CH_3NO_2$-o	7.842	5.714	3.880	3.864	0.137	-0.146
$C_6H_4CH_3CONH_2$-o	7.842	4.888	3.880	4.834	0.169	-0.250
$C_6H_4CH_3NH_2$-o	7.842	3.705	3.880	4.297	0.253	-0.523
$C_6H_4CH_3CN$-o	7.842	5.217	3.880	4.673	0.153	-0.201
$C_6H_4COOHCN$-o	7.842	5.744	3.880	4.616	0.124	-0.130
$C_6H_4COOHNO_2$-o	7.842	5.997	3.880	3.890	0.119	-0.110
$C_6H_4COOHCONH_2$-o	7.842	5.378	3.880	4.780	0.142	-0.175
$C_6H_4COOHNH_2$-o	7.842	4.309	3.880	4.010	0.224	-0.396

Table-14. Values of ΔN and ΔE evaluated by PM3 method for interaction of organic bases with $SnBr_4$

Organic Base (B)	χA	χB	η_A	η_B	ΔN	ΔE
$C_6H_4CH_3NO_2$-o	9.208	5.714	3.815	3.864	0.228	-0.397
$C_6H_4CH_3CONH_2$-o	9.208	4.888	3.815	4.834	0.250	-0.539
$C_6H_4CH_3NH_2$-o	9.208	3.705	3.815	4.297	0.339	-0.933
$C_6H_4CH_3CN$-o	9.208	5.217	3.815	4.673	0.235	-0.469
$C_6H_4COOHCN$-o	9.208	5.744	3.815	4.616	0.205	-0.356
$C_6H_4COOHNO_2$-o	9.208	5.997	3.815	3.890	0.208	-0.335
$C_6H_4COOHCONH_2$-o	9.208	5.378	3.815	4.780	0.223	-0.427
$C_6H_4COOHNH_2$-o	9.208	4.309	3.815	4.010	0.313	-0.767

Table-15. Values of ΔN and ΔE evaluated by PM3 method for interaction of organic bases with SnI_4

Organic Base (B)	χA	χB	η_A	η_B	ΔN	ΔE
$C_6H_4CH_3NO_2$-o	7.449	5.714	2.875	3.864	0.129	-0.112
$C_6H_4CH_3CONH_2$-o	7.449	4.888	2.875	4.834	0.166	-0.213
$C_6H_4CH_3NH_2$-o	7.449	3.705	2.875	4.297	0.261	-0.489
$C_6H_4CH_3CN$-o	7.449	5.217	2.875	4.673	0.148	-0.165
$C_6H_4COOHCN$-o	7.449	5.744	2.875	4.616	0.114	-0.097
$C_6H_4COOHNO_2$-o	7.449	5.997	2.875	3.890	0.107	-0.078
$C_6H_4COOHCONH_2$-o	7.449	5.378	2.875	4.780	0.135	-0.140
$C_6H_4COOHNH_2$-o	7.449	4.309	2.875	4.010	0.228	-0.358

CONCLUSION:-

The interaction energy indicates:-

1. That the sequences of base strength against metal halides obtained by PM3 calculations are different from the order obtained by DFT calculations and are also against the established trend.
2. The orders of acceptor strength shown by DFT and PM3 based calculations are entirely different. The DFT based results show that the order of acceptor strength in tin (IV) halides is $SnCl_4$ > $SnBr_4$ > SnI_4, the PM3 based results show that $snBr_4$ is the strongest acceptor which is not in conformity with experimental results. It is strongly indicated that in respect of metal halides only the DFT based calculations be treated is reliable.
3. The ΔN and ΔE values evaluated by PM3, Ab inito and DFT provide the same order for base strength.

REFERENCES:

1. Singh P. P., Singh D., Ahmad S., Journal of Molecular Structure:THEOCHEM, 2009, 905, 13.
2. Singh P. P., Mittal S., Sharma U., Inorganic Chemistry:AIJ, 2009, 4, 45.
3. Singh R. K., Rai S., Singh P. P., Organic Chemistry:AIJ, 2009, 5, 296.
4. Singh P. P., Kumar P., Srivastava A. K., Organic Chemistry:AIJ, 2010, 6, 190.
5. Singh R. K., Khan A., Int. J. Quan. Chem., 2010, In Press
6. Francisco Mendez, Jose L Gazquez, Proc. Indian Acad. Sci., 1994, 106, 183.
7. J. L. Gázquez, F. Méndez, J. Phys. Chem., 1993, 98, 4591.
8. J. L.Gazquez, K.D. Sen, Chemical hardness: Structure and Bonding 80 (ed.) (Berlin : Springer – Verlag) , 1993.
9. Parr R. G., Pearson R. G., J. Am. Chem. Soc., 1983, 105, 7512.
10. Parr R. G., Gazquez J. L., J. Phys. Chem., 1993, 97, 3939.
11. Parr R. G., . Chattaraj P. K, J. Am. Chem. Soc., 1991, 113, 1855 .
12. Perdew J. P., Parr R. G., Levy M., Balduz J. L., Phys. Rev. Lett., 1982, 49, 1691.
13. Sanderson R. T., Academic Press, New York, 1976.
14. Dewar M. J. S., Morita T. F., J. Am. Chem. Soc., 1969, 91, 796.
15. Klopman G., J. Am. Chem. Soc., 1968, 90, 223 .
16. Parr R. G., Pearson R. G., J. Am. Chem. Soc., 1983, 105, 7512.

*****