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DFT based study of interaction of ortho, meta and para derivatives of pyridine and phenol derivatives with halides of titanium and silicon

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ABSTRACT

Interaction of 27 ortho, meta and para derivatives of pyridine and phenol have been studied with the halides (chloride, bromide and iodide) of titanium and silicon. It has been found that the donor organic base $C_6H_4OHNO_2-m$ forms least stable complex with the acceptor metal halide TiI_4 and donor organic base $C_6H_4OHCONH_2-p$ forms most stable complex with the acceptor metal halide $SiCl_4$.

Key words: Donors, Acceptors, DFT, HOMO energy, LUMO energy, Interaction.

INTRODUCTION

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.

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

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 [2-5] is given by

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

where

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

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

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 related to an “effective number of valence electrons” that participate in the interaction between A and B.

We in this paper present a study based on interaction energy between ortho, meta and para derivatives of pyridine and phenol with tetrahalides of titanium and silicon.

EXPERIMENTAL SECTION

The study materials of this paper are derivatives of pyridine and phenol listed in Table-B, which have been used as a donor molecule. Metal halides (TiX_4 and SiX_4), listed in Table-A, 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 B88LYP method using the basis DZVP. [6-12]

The essential values of chemical potential, softness, numbers of electron, and lambda have been obtained by solving the equation described elsewhere.[13-26] DFT calculations are also very useful in the development of QSAR models to predict the activity of any compound. [27-32]

RESULTS AND DISCUSSION

Interaction of donors with acceptor metal halide $TiCl_4$

Interaction energy of donors (B) with acceptor $TiCl_4$ (A) is shown in Table-1. Lowest value of interaction energy of interaction of organic base $C_6H_4OHCONH_2$ -p with acceptor $TiCl_4$ has been observed and its value is -17.003 eV, which indicates formation of most stable complex of organic base $C_6H_4OHCONH_2$ -p with acceptor $TiCl_4$.

The value of interaction energy of organic base $C_6H_4OHNO_2$ -m with metal halide $TiCl_4$ is highest and is equal to -10.566 eV, which indicates that the organic base $C_6H_4OHNO_2$ -m forms least stable complex with $TiCl_4$. The values of interaction energy indicate that the order of the stability of complexes formed by donors with $TiCl_4$ is in the following order-

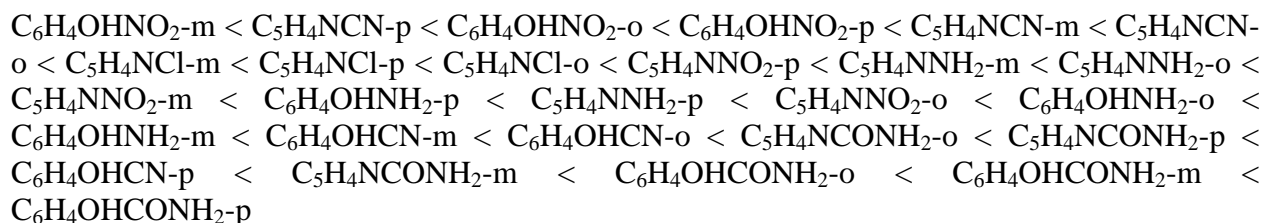
$C_6H_4OHNO_2$ -m < C_5H_4NCN -p < $C_6H_4OHNO_2$ -o < $C_6H_4OHNO_2$ -p < C_5H_4NCN -m < $C_5H_4NNO_2$ -p < C_5H_4NCN -o < C_5H_4NCl -m < C_5H_4NCl -p < C_5H_4NCl -o < $C_5H_4NNH_2$ -m < $C_5H_4NNO_2$ -m < $C_5H_4NNH_2$ -o < $C_6H_4OHNH_2$ -p < $C_5H_4NNO_2$ -o < $C_5H_4NNH_2$ -p < $C_6H_4OHNH_2$ -o < $C_6H_4OHNH_2$ -m < C_6H_4OHCN -m < C_6H_4OHCN -o < $C_5H_4NCONH_2$ -p < $C_5H_4NCONH_2$ -o < C_6H_4OHCN -p < $C_5H_4NCONH_2$ -m < $C_6H_4OHCONH_2$ -o < $C_6H_4OHCONH_2$ -m < $C_6H_4OHCONH_2$ -p

Graph between interaction energy of donors with the acceptor metal halide $TiCl_4$ is shown in Graph-1.

Interaction of donors with acceptor metal halide TiBr₄

Interaction energy of donors (B) with acceptor TiBr₄ (A) is shown in Table-2. Lowest value of interaction energy of interaction of organic base C₆H₄OHCONH₂-p with acceptor TiBr₄ has been observed and its value is -15.143 eV, which indicates formation of most stable complex of organic base C₆H₄OHCONH₂-p with acceptor TiBr₄.

The value of interaction energy of organic base C₆H₄OHNO₂-m with metal halide TiBr₄ is highest and is equal to -9.511 eV, which indicates that the organic base C₆H₄OHNO₂-m forms least stable complex with TiBr₄. The values of interaction energy indicate that the order of the stability of complexes formed by donors with TiBr₄ is in the following order-

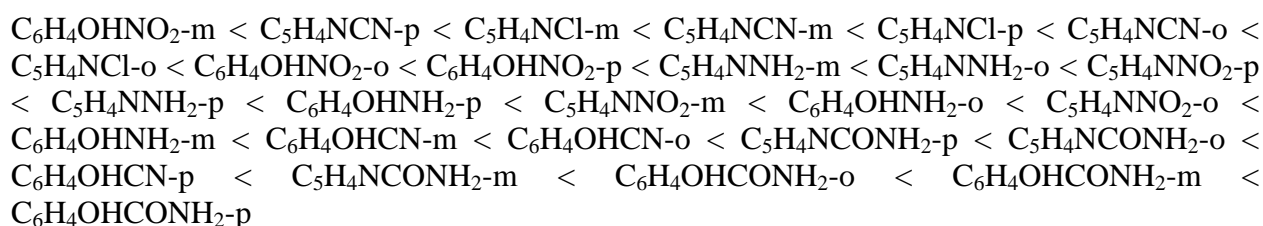


Graph between interaction energy of donors with the acceptor metal halide TiBr₄ is shown in Graph-2.

Interaction of donors with acceptor metal halide TiI₄

Interaction energy of donors (B) with acceptor TiI₄ (A) is shown in Table-3. Lowest value of interaction energy of interaction of organic base C₆H₄OHCONH₂-p with acceptor TiI₄ has been observed and its value is -12.763 eV, which indicates formation of most stable complex of organic base C₆H₄OHCONH₂-p with acceptor TiI₄.

The value of interaction energy of organic base C₆H₄OHNO₂-m with metal halide TiI₄ is highest and is equal to -8.188 eV, which indicates that the organic base C₆H₄OHNO₂-m forms least stable complex with TiI₄. The values of interaction energy indicate that the order of the stability of complexes formed by donors with TiI₄ is in the following order-



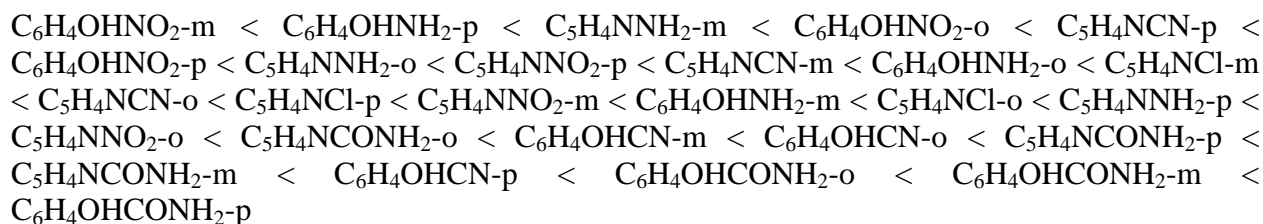
Graph between interaction energy of donors with the acceptor metal halide TiI₄ is shown in Graph-3.

Interaction of donors with acceptor metal halide SiCl₄

Interaction energy of donors (B) with acceptor SiCl₄ (A) is shown in Table-4. Lowest value of interaction energy of interaction of organic base C₆H₄OHCONH₂-p with acceptor SiCl₄ has been observed and its value is -20.566 eV, which indicates formation of most stable complex of organic base C₆H₄OHCONH₂-p with acceptor SiCl₄.

The value of interaction energy of organic base C₆H₄OHNO₂-m with metal halide SiCl₄ is highest and is equal to -12.291 eV, which indicates that the organic base C₆H₄OHNO₂-m forms

least stable complex with SiCl_4 . The values of interaction energy indicate that the order of the stability of complexes formed by donors with TiBr_4 is in the following order-

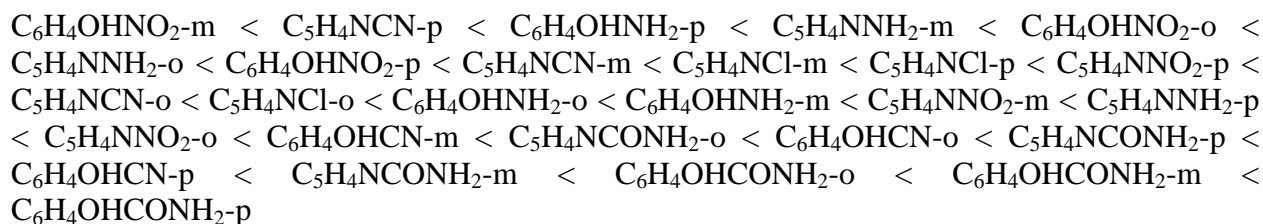


Graph between interaction energy of donors with the acceptor metal halide SiCl_4 is shown in Graph-4.

Interaction of donors with acceptor metal halide SiBr_4

Interaction energy of donors (B) with acceptor SiBr_4 (A) is shown in Table-5. Lowest value of interaction energy of interaction of organic base $\text{C}_6\text{H}_4\text{OHCONH}_2\text{-p}$ with acceptor SiBr_4 has been observed and its value is -17.779 eV, which indicates formation of most stable complex of organic base $\text{C}_6\text{H}_4\text{OHCONH}_2\text{-p}$ with acceptor SiBr_4 .

The value of interaction energy of organic base $\text{C}_6\text{H}_4\text{OHNO}_2\text{-m}$ with metal halide SiBr_4 is highest and is equal to -10.922 eV, which indicates that the organic base $\text{C}_6\text{H}_4\text{OHNO}_2\text{-m}$ forms least stable complex with SiBr_4 . The values of interaction energy indicate that the order of the stability of complexes formed by donors with TiBr_4 is in the following order-

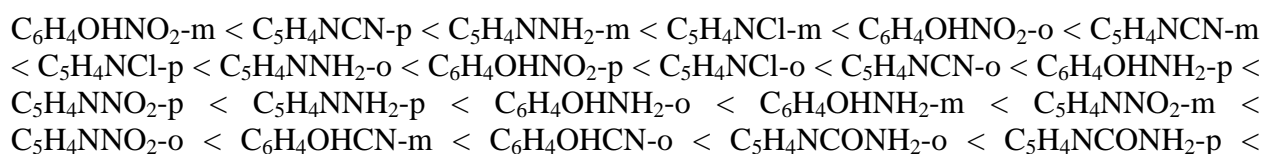


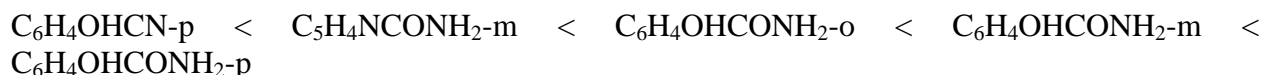
Graph between interaction energy of donors with the acceptor metal halide SiBr_4 is shown in Graph-5.

Interaction of donors with acceptor metal halide SiI_4

Interaction energy of donors (B) with acceptor SiI_4 (A) is shown in Table-6. Lowest value of interaction energy of interaction of organic base $\text{C}_6\text{H}_4\text{OHCONH}_2\text{-p}$ with acceptor SiI_4 has been observed and its value is -13.976 eV, which indicates formation of most stable complex of organic base $\text{C}_6\text{H}_4\text{OHCONH}_2\text{-p}$ with acceptor SiI_4 .

The value of interaction energy of organic base $\text{C}_6\text{H}_4\text{OHNO}_2\text{-m}$ with metal halide SiI_4 is highest and is equal to -8.906 eV, which indicates that the organic base $\text{C}_6\text{H}_4\text{OHNO}_2\text{-m}$ forms least stable complex with SiI_4 . The values of interaction energy indicate that the order of the stability of complexes formed by donors with TiI_4 is in the following order-





Graph between interaction energy of donors with the acceptor metal halide SiI_4 is shown in Graph-6.

Ortho, meta and para effect

Sequence of stable complex formation of ortho derivatives of pyridine and phenol with halides of titanium and silicon is as under-

C_5H_4NCN-o with $TiI_4 < C_5H_4NCl-o$ with $TiI_4 < C_6H_4OHNO_2-o$ with $TiI_4 < C_5H_4NNH_2-o$ with $TiI_4 < C_6H_4OHNH_2-o$ with $TiI_4 < C_6H_4OHNO_2-o$ with $SiI_4 < C_5H_4NNH_2-o$ with $SiI_4 < C_5H_4NCl-o$ with $SiI_4 < C_5H_4NNO_2-o$ with $TiI_4 < C_5H_4NCN-o$ with $SiI_4 < C_6H_4OHNH_2-o$ with $SiI_4 < C_6H_4OHNO_2-o$ with $TiBr_4 < C_6H_4OHCN-o$ with $TiI_4 < C_5H_4NCN-o$ with $TiBr_4 < C_5H_4NCl-o$ with $TiBr_4 < C_5H_4NCONH_2-o$ with $TiI_4 < C_5H_4NNO_2-o$ with $SiI_4 < C_5H_4NNH_2-o$ with $TiBr_4 < C_5H_4NNO_2-o$ with $TiBr_4 < C_6H_4OHNH_2-o$ with $TiBr_4 < C_6H_4OHCN-o$ with $SiI_4 < C_6H_4OHNO_2-o$ with $TiCl_4 < C_5H_4NCONH_2-o$ with $SiI_4 < C_5H_4NCN-o$ with $TiCl_4 < C_6H_4OHNO_2-o$ with $SiBr_4 < C_5H_4NCl-o$ with $TiCl_4 < C_5H_4NNH_2-o$ with $SiBr_4 < C_5H_4NNH_2-o$ with $TiCl_4 < C_6H_4OHCN-o$ with $TiBr_4 < C_5H_4NCN-o$ with $SiBr_4 < C_5H_4NNO_2-o$ with $TiCl_4 < C_5H_4NCONH_2-o$ with $TiBr_4 < C_5H_4NCl-o$ with $SiBr_4 < C_6H_4OHNH_2-o$ with $SiBr_4 < C_6H_4OHCONH_2-o$ with $TiI_4 < C_6H_4OHNH_2-o$ with $TiCl_4 < C_5H_4NNO_2-o$ with $SiBr_4 < C_6H_4OHNO_2-o$ with $SiCl_4 < C_6H_4OHCONH_2-o$ with $SiI_4 < C_5H_4NNH_2-o$ with $SiCl_4 < C_6H_4OHCN-o$ with $TiCl_4 < C_5H_4NCONH_2-o$ with $TiCl_4 < C_6H_4OHNH_2-o$ with $SiCl_4 < C_5H_4NCONH_2-o$ with $SiBr_4 < C_5H_4NCN-o$ with $SiCl_4 < C_6H_4OHCN-o$ with $SiBr_4 < C_5H_4NCl-o$ with $SiCl_4 < C_6H_4OHCONH_2-o$ with $TiBr_4 < C_5H_4NNO_2-o$ with $SiCl_4 < C_5H_4NCONH_2-o$ with $SiCl_4 < C_6H_4OHCONH_2-o$ with $TiCl_4 < C_6H_4OHCN-o$ with $SiCl_4 < C_6H_4OHCONH_2-o$ with $SiBr_4 < C_6H_4OHCONH_2-o$ with $SiCl_4$

Similarly, sequence of stable complex formation of meta and para derivatives of pyridine and phenol with halides of titanium and silicon can easily be developed with the help of the Tables-1-6.

Table-A: List of acceptor-A

Ti(IV) chloride	$TiCl_4$
Ti(IV) bromide	$TiBr_4$
Ti(IV) iodide	TiI_4
Si(IV) chloride	$SiCl_4$
Si(IV) bromide	$SiBr_4$
Si(IV) iodide	SiI_4

Table-B: Organic bases (B) as donor molecules

Disubstituted ortho	Disubstituted meta	Disubstituted para
C_5H_4NCl-o	C_5H_4NCl-m	C_5H_4NCl-p
$C_5H_4NNH_2-o$	$C_5H_4NNH_2-m$	$C_5H_4NNH_2-p$
$C_6H_4OH NH_2-o$	$C_6H_4OHNH_2-m$	$C_6H_4OHNH_2-p$
$C_5H_4NCONH_2-o$	$C_5H_4NCONH_2-m$	$C_5H_4NCONH_2-p$
$C_6H_4OHCONH_2-o$	$C_6H_4OHCONH_2-m$	$C_6H_4OHCONH_2-p$
$C_5H_4NNO_2-o$	$C_5H_4NNO_2-m$	$C_5H_4NNO_2-p$
$C_6H_4OHNO_2-o$	$C_6H_4OHNO_2-m$	$C_6H_4OHNO_2-p$
C_5H_4NCN-o	C_5H_4NCN-m	C_5H_4NCN-p
$C_6H_4OHCN-o$	$C_6H_4OHCN-m$	$C_6H_4OHCN-p$

Table-1: Interaction energy of organic bases for interaction with TiCl₄

Donor	ϵ HOMO	ϵ LUMO	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
C ₅ H ₄ NCl-o	-6.337	-2.011	-4.174	0.462	36	23.120	-0.729	-10.938	-11.667
C ₅ H ₄ NCl-m	-6.174	-2.020	-4.097	0.481	36	23.120	-0.795	-10.744	-11.539
C ₅ H ₄ NCl-p	-6.170	-1.962	-4.066	0.475	36	23.120	-0.810	-10.806	-11.615
C ₅ H ₄ NNH ₂ -o	-4.865	-1.223	-3.044	0.549	36	23.120	-1.747	-10.108	-11.854
C ₅ H ₄ NNH ₂ -m	-4.830	-1.268	-3.049	0.561	36	23.120	-1.762	-10.000	-11.762
C ₅ H ₄ NNH ₂ -p	-5.186	-0.938	-3.062	0.471	36	23.120	-1.591	-10.851	-12.442
C ₆ H ₄ OHNH ₂ -o	-4.469	-0.630	-2.550	0.521	36	23.120	-2.213	-10.363	-12.576
C ₆ H ₄ OHNH ₂ -m	-4.436	-0.514	-2.475	0.510	36	23.120	-2.270	-10.467	-12.737
C ₆ H ₄ OHNH ₂ -p	-4.076	-0.776	-2.426	0.606	36	23.120	-2.542	-9.629	-12.171
C ₅ H ₄ NCONH ₂ -o	-5.590	-2.286	-3.938	0.605	46	30.420	-1.017	-12.677	-13.693
C ₅ H ₄ NCONH ₂ -m	-5.815	-2.294	-4.055	0.568	46	30.420	-0.899	-13.083	-13.982
C ₅ H ₄ NCONH ₂ -p	-5.967	-2.535	-4.251	0.583	46	30.420	-0.772	-12.920	-13.692
C ₆ H ₄ OHCONH ₂ -o	-5.278	-1.864	-3.571	0.586	52	35.280	-1.302	-14.945	-16.247
C ₆ H ₄ OHCONH ₂ -m	-5.530	-1.946	-3.738	0.558	52	35.280	-1.132	-15.305	-16.437
C ₆ H ₄ OHCONH ₂ -p	-5.553	-1.707	-3.630	0.520	52	35.280	-1.176	-15.827	-17.003
C ₅ H ₄ NNO ₂ -o	-6.543	-3.630	-5.087	0.687	46	30.420	-0.337	-11.873	-12.210
C ₅ H ₄ NNO ₂ -m	-6.611	-3.840	-5.226	0.722	46	30.420	-0.283	-11.555	-11.838
C ₅ H ₄ NNO ₂ -p	-6.644	-4.025	-5.335	0.764	46	30.420	-0.244	-11.199	-11.443
C ₆ H ₄ OHNO ₂ -o	-6.165	-3.258	-4.712	0.688	42	27.380	-0.534	-10.674	-11.209
C ₆ H ₄ OHNO ₂ -m	-6.100	-3.492	-4.796	0.767	42	27.380	-0.510	-10.056	-10.566
C ₆ H ₄ OHNO ₂ -p	-6.269	-3.315	-4.792	0.677	42	27.380	-0.485	-10.766	-11.251
C ₅ H ₄ NCN-o	-6.646	-2.795	-4.721	0.519	38	24.500	-0.460	-10.998	-11.457
C ₅ H ₄ NCN-m	-6.540	-2.790	-4.665	0.533	38	24.500	-0.495	-10.861	-11.356
C ₅ H ₄ NCN-p	-6.513	-3.024	-4.769	0.573	38	24.500	-0.459	-10.490	-10.949
C ₆ H ₄ OHCN-o	-5.950	-2.261	-4.106	0.542	44	28.880	-0.842	-12.704	-13.545
C ₆ H ₄ OHCN-m	-5.982	-2.341	-4.162	0.549	44	28.880	-0.809	-12.624	-13.433
C ₆ H ₄ OHCN-p	-5.926	-2.070	-3.998	0.519	44	28.880	-0.896	-12.972	-13.868

HOMO of TiCl ₄	LUMO of TiCl ₄	μ_A of TiCl ₄	N_A of TiCl ₄	S_A of TiCl ₄
-8.224	-4.86	-6.542	32	0.595

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

Table-2: Interaction energy of organic bases for interaction with TiBr₄

Donor	ϵ HOMO	ϵ LUMO	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
C ₅ H ₄ NCl-o	-6.337	-2.011	-4.174	0.462	36	23.120	-0.435	-9.863	-10.298
C ₅ H ₄ NCl-m	-6.174	-2.020	-4.097	0.481	36	23.120	-0.486	-9.705	-10.190
C ₅ H ₄ NCl-p	-6.170	-1.962	-4.066	0.475	36	23.120	-0.498	-9.755	-10.253
C ₅ H ₄ NNH ₂ -o	-4.865	-1.223	-3.044	0.549	36	23.120	-1.296	-9.183	-10.478
C ₅ H ₄ NNH ₂ -m	-4.830	-1.268	-3.049	0.561	36	23.120	-1.307	-9.094	-10.401
C ₅ H ₄ NNH ₂ -p	-5.186	-0.938	-3.062	0.471	36	23.120	-1.170	-9.792	-10.962
C ₆ H ₄ OHNH ₂ -o	-4.469	-0.630	-2.550	0.521	36	23.120	-1.724	-9.393	-11.117
C ₆ H ₄ OHNH ₂ -m	-4.436	-0.514	-2.475	0.510	36	23.120	-1.778	-9.478	-11.256
C ₆ H ₄ OHNH ₂ -p	-4.076	-0.776	-2.426	0.606	36	23.120	-2.015	-8.786	-10.801
C ₅ H ₄ NCONH ₂ -o	-5.590	-2.286	-3.938	0.605	46	30.420	-0.653	-11.566	-12.219
C ₅ H ₄ NCONH ₂ -m	-5.815	-2.294	-4.055	0.568	46	30.420	-0.559	-11.904	-12.463
C ₅ H ₄ NCONH ₂ -p	-5.967	-2.535	-4.251	0.583	46	30.420	-0.455	-11.768	-12.223
C ₆ H ₄ OHCONH ₂ -o	-5.278	-1.864	-3.571	0.586	52	35.280	-0.898	-13.616	-14.514
C ₆ H ₄ OHCONH ₂ -m	-5.530	-1.946	-3.738	0.558	52	35.280	-0.755	-13.914	-14.670
C ₆ H ₄ OHCONH ₂ -p	-5.553	-1.707	-3.630	0.520	52	35.280	-0.799	-14.344	-15.143
C ₅ H ₄ NNO ₂ -o	-6.543	-3.630	-5.087	0.687	46	30.420	-0.126	-10.893	-11.019
C ₅ H ₄ NNO ₂ -m	-6.611	-3.840	-5.226	0.722	46	30.420	-0.091	-10.625	-10.716
C ₅ H ₄ NNO ₂ -p	-6.644	-4.025	-5.335	0.764	46	30.420	-0.067	-10.323	-10.390
C ₆ H ₄ OHNO ₂ -o	-6.165	-3.258	-4.712	0.688	42	27.380	-0.262	-9.795	-10.057
C ₆ H ₄ OHNO ₂ -m	-6.100	-3.492	-4.796	0.767	42	27.380	-0.240	-9.271	-9.511
C ₆ H ₄ OHNO ₂ -p	-6.269	-3.315	-4.792	0.677	42	27.380	-0.227	-9.872	-10.099
C ₅ H ₄ NCN-o	-6.646	-2.795	-4.721	0.519	38	24.500	-0.222	-9.967	-10.189
C ₅ H ₄ NCN-m	-6.540	-2.790	-4.665	0.533	38	24.500	-0.246	-9.855	-10.101
C ₅ H ₄ NCN-p	-6.513	-3.024	-4.769	0.573	38	24.500	-0.216	-9.548	-9.765
C ₆ H ₄ OHCN-o	-5.950	-2.261	-4.106	0.542	44	28.880	-0.516	-11.535	-12.050
C ₆ H ₄ OHCN-m	-5.982	-2.341	-4.162	0.549	44	28.880	-0.488	-11.469	-11.957
C ₆ H ₄ OHCN-p	-5.926	-2.070	-3.998	0.519	44	28.880	-0.563	-11.755	-12.319

HOMO of TiBr ₄	LUMO of TiBr ₄	μ_A of TiBr ₄	N_A of TiBr ₄	S_A of TiBr ₄
-7.346	-4.528	-5.937	32	0.710

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

Table-3: Interaction energy of organic bases for interaction with TiI₄

Donor	ϵ HOMO	ϵ LUMO	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
C ₅ H ₄ NCl-o	-6.337	-2.011	-4.174	0.462	36	23.120	-0.231	-8.358	-8.589
C ₅ H ₄ NCl-m	-6.174	-2.020	-4.097	0.481	36	23.120	-0.268	-8.244	-8.512
C ₅ H ₄ NCl-p	-6.170	-1.962	-4.066	0.475	36	23.120	-0.279	-8.280	-8.559
C ₅ H ₄ NNH ₂ -o	-4.865	-1.223	-3.044	0.549	36	23.120	-0.954	-7.864	-8.818
C ₅ H ₄ NNH ₂ -m	-4.830	-1.268	-3.049	0.561	36	23.120	-0.963	-7.799	-8.762
C ₅ H ₄ NNH ₂ -p	-5.186	-0.938	-3.062	0.471	36	23.120	-0.851	-8.307	-9.158
C ₆ H ₄ OHNH ₂ -o	-4.469	-0.630	-2.550	0.521	36	23.120	-1.351	-8.018	-9.369
C ₆ H ₄ OHNH ₂ -m	-4.436	-0.514	-2.475	0.510	36	23.120	-1.403	-8.080	-9.483
C ₆ H ₄ OHNH ₂ -p	-4.076	-0.776	-2.426	0.606	36	23.120	-1.615	-7.571	-9.186
C ₅ H ₄ NCONH ₂ -o	-5.590	-2.286	-3.938	0.605	46	30.420	-0.390	-9.966	-10.356
C ₅ H ₄ NCONH ₂ -m	-5.815	-2.294	-4.055	0.568	46	30.420	-0.318	-10.216	-10.534
C ₅ H ₄ NCONH ₂ -p	-5.967	-2.535	-4.251	0.583	46	30.420	-0.235	-10.116	-10.351
C ₆ H ₄ OHCONH ₂ -o	-5.278	-1.864	-3.571	0.586	52	35.280	-0.598	-11.708	-12.306
C ₆ H ₄ OHCONH ₂ -m	-5.530	-1.946	-3.738	0.558	52	35.280	-0.479	-11.928	-12.408
C ₆ H ₄ OHCONH ₂ -p	-5.553	-1.707	-3.630	0.520	52	35.280	-0.520	-12.243	-12.763
C ₅ H ₄ NNO ₂ -o	-6.543	-3.630	-5.087	0.687	46	30.420	-0.019	-9.463	-9.482
C ₅ H ₄ NNO ₂ -m	-6.611	-3.840	-5.226	0.722	46	30.420	-0.006	-9.260	-9.266
C ₅ H ₄ NNO ₂ -p	-6.644	-4.025	-5.335	0.764	46	30.420	-0.001	-9.030	-9.030
C ₆ H ₄ OHNO ₂ -o	-6.165	-3.258	-4.712	0.688	42	27.380	-0.093	-8.509	-8.602
C ₆ H ₄ OHNO ₂ -m	-6.100	-3.492	-4.796	0.767	42	27.380	-0.076	-8.112	-8.188
C ₆ H ₄ OHNO ₂ -p	-6.269	-3.315	-4.792	0.677	42	27.380	-0.072	-8.568	-8.640
C ₅ H ₄ NCN-o	-6.646	-2.795	-4.721	0.519	38	24.500	-0.076	-8.506	-8.582
C ₅ H ₄ NCN-m	-6.540	-2.790	-4.665	0.533	38	24.500	-0.091	-8.424	-8.515
C ₅ H ₄ NCN-p	-6.513	-3.024	-4.769	0.573	38	24.500	-0.070	-8.199	-8.269
C ₆ H ₄ OHCN-o	-5.950	-2.261	-4.106	0.542	44	28.880	-0.285	-9.870	-10.156
C ₆ H ₄ OHCN-m	-5.982	-2.341	-4.162	0.549	44	28.880	-0.263	-9.822	-10.086
C ₆ H ₄ OHCN-p	-5.926	-2.070	-3.998	0.519	44	28.880	-0.326	-10.031	-10.357

HOMO of TiI ₄	LUMO of TiI ₄	μ_A of TiI ₄	N_A of TiI ₄	S_A of TiI ₄
-6.485	-4.313	-5.399	32	0.921

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

Table-4: Interaction energy of organic bases for interaction with SiCl₄

Donor	ϵ HOMO	ϵ LUMO	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
C ₅ H ₄ NCl-o	-6.337	-2.011	-4.174	0.462	36	23.120	-0.112	-14.248	-14.359
C ₅ H ₄ NCl-m	-6.174	-2.020	-4.097	0.481	36	23.120	-0.131	-13.919	-14.050
C ₅ H ₄ NCl-p	-6.170	-1.962	-4.066	0.475	36	23.120	-0.137	-14.024	-14.161
C ₅ H ₄ NNH ₂ -o	-4.865	-1.223	-3.044	0.549	36	23.120	-0.512	-12.870	-13.382
C ₅ H ₄ NNH ₂ -m	-4.830	-1.268	-3.049	0.561	36	23.120	-0.514	-12.696	-13.210
C ₅ H ₄ NNH ₂ -p	-5.186	-0.938	-3.062	0.471	36	23.120	-0.473	-14.100	-14.573
C ₆ H ₄ OHNH ₂ -o	-4.469	-0.630	-2.550	0.521	36	23.120	-0.753	-13.287	-14.040
C ₆ H ₄ OHNH ₂ -m	-4.436	-0.514	-2.475	0.510	36	23.120	-0.789	-13.458	-14.246
C ₆ H ₄ OHNH ₂ -p	-4.076	-0.776	-2.426	0.606	36	23.120	-0.873	-12.103	-12.977
C ₅ H ₄ NCONH ₂ -o	-5.590	-2.286	-3.938	0.605	46	30.420	-0.186	-15.937	-16.123
C ₅ H ₄ NCONH ₂ -m	-5.815	-2.294	-4.055	0.568	46	30.420	-0.150	-16.586	-16.736
C ₅ H ₄ NCONH ₂ -p	-5.967	-2.535	-4.251	0.583	46	30.420	-0.105	-16.323	-16.429
C ₆ H ₄ OHCONH ₂ -o	-5.278	-1.864	-3.571	0.586	52	35.280	-0.302	-18.869	-19.172
C ₆ H ₄ OHCONH ₂ -m	-5.530	-1.946	-3.738	0.558	52	35.280	-0.240	-19.447	-19.687
C ₆ H ₄ OHCONH ₂ -p	-5.553	-1.707	-3.630	0.520	52	35.280	-0.269	-20.298	-20.566
C ₅ H ₄ NNO ₂ -o	-6.543	-3.630	-5.087	0.687	46	30.420	-0.003	-14.687	-14.689
C ₅ H ₄ NNO ₂ -m	-6.611	-3.840	-5.226	0.722	46	30.420	0.000	-14.204	-14.204
C ₅ H ₄ NNO ₂ -p	-6.644	-4.025	-5.335	0.764	46	30.420	-0.001	-13.670	-13.671
C ₆ H ₄ OHNO ₂ -o	-6.165	-3.258	-4.712	0.688	42	27.380	-0.032	-13.201	-13.233
C ₆ H ₄ OHNO ₂ -m	-6.100	-3.492	-4.796	0.767	42	27.380	-0.023	-12.268	-12.291
C ₆ H ₄ OHNO ₂ -p	-6.269	-3.315	-4.792	0.677	42	27.380	-0.022	-13.342	-13.364
C ₅ H ₄ NCN-o	-6.646	-2.795	-4.721	0.519	38	24.500	-0.028	-14.107	-14.134
C ₅ H ₄ NCN-m	-6.540	-2.790	-4.665	0.533	38	24.500	-0.034	-13.883	-13.917
C ₅ H ₄ NCN-p	-6.513	-3.024	-4.769	0.573	38	24.500	-0.024	-13.282	-13.306
C ₆ H ₄ OHCN-o	-5.950	-2.261	-4.106	0.542	44	28.880	-0.135	-16.203	-16.338
C ₆ H ₄ OHCN-m	-5.982	-2.341	-4.162	0.549	44	28.880	-0.123	-16.074	-16.197
C ₆ H ₄ OHCN-p	-5.926	-2.070	-3.998	0.519	44	28.880	-0.159	-16.641	-16.801

HOMO of SiCl ₄	LUMO of SiCl ₄	μ_A of SiCl ₄	N_A of SiCl ₄	S_A of SiCl ₄
-8.099	-2.369	-5.234	32	0.349

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

Table-5: Interaction energy of organic bases for interaction with SiBr₄

Donor	ϵ HOMO	ϵ LUMO	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
C ₅ H ₄ NCl-o	-6.337	-2.011	-4.174	0.462	36	23.120	-0.113	-12.156	-12.269
C ₅ H ₄ NCl-m	-6.174	-2.020	-4.097	0.481	36	23.120	-0.134	-11.916	-12.050
C ₅ H ₄ NCl-p	-6.170	-1.962	-4.066	0.475	36	23.120	-0.141	-11.993	-12.134
C ₅ H ₄ NNH ₂ -o	-4.865	-1.223	-3.044	0.549	36	23.120	-0.573	-11.139	-11.712
C ₅ H ₄ NNH ₂ -m	-4.830	-1.268	-3.049	0.561	36	23.120	-0.576	-11.008	-11.584
C ₅ H ₄ NNH ₂ -p	-5.186	-0.938	-3.062	0.471	36	23.120	-0.522	-12.049	-12.571
C ₆ H ₄ OHNH ₂ -o	-4.469	-0.630	-2.550	0.521	36	23.120	-0.852	-11.450	-12.302
C ₆ H ₄ OHNH ₂ -m	-4.436	-0.514	-2.475	0.510	36	23.120	-0.892	-11.576	-12.468
C ₆ H ₄ OHNH ₂ -p	-4.076	-0.776	-2.426	0.606	36	23.120	-1.003	-10.560	-11.563
C ₅ H ₄ NCONH ₂ -o	-5.590	-2.286	-3.938	0.605	46	30.420	-0.198	-13.904	-14.102
C ₅ H ₄ NCONH ₂ -m	-5.815	-2.294	-4.055	0.568	46	30.420	-0.157	-14.394	-14.552
C ₅ H ₄ NCONH ₂ -p	-5.967	-2.535	-4.251	0.583	46	30.420	-0.107	-14.197	-14.304
C ₆ H ₄ OHCONH ₂ -o	-5.278	-1.864	-3.571	0.586	52	35.280	-0.331	-16.418	-16.749
C ₆ H ₄ OHCONH ₂ -m	-5.530	-1.946	-3.738	0.558	52	35.280	-0.259	-16.853	-17.113
C ₆ H ₄ OHCONH ₂ -p	-5.553	-1.707	-3.630	0.520	52	35.280	-0.290	-17.489	-17.779
C ₅ H ₄ NNO ₂ -o	-6.543	-3.630	-5.087	0.687	46	30.420	-0.001	-12.942	-12.943
C ₅ H ₄ NNO ₂ -m	-6.611	-3.840	-5.226	0.722	46	30.420	-0.001	-12.566	-12.567
C ₅ H ₄ NNO ₂ -p	-6.644	-4.025	-5.335	0.764	46	30.420	-0.005	-12.146	-12.151
C ₆ H ₄ OHNO ₂ -o	-6.165	-3.258	-4.712	0.688	42	27.380	-0.027	-11.635	-11.662
C ₆ H ₄ OHNO ₂ -m	-6.100	-3.492	-4.796	0.767	42	27.380	-0.019	-10.904	-10.922
C ₆ H ₄ OHNO ₂ -p	-6.269	-3.315	-4.792	0.677	42	27.380	-0.018	-11.744	-11.762
C ₅ H ₄ NCN-o	-6.646	-2.795	-4.721	0.519	38	24.500	-0.023	-12.153	-12.176
C ₅ H ₄ NCN-m	-6.540	-2.790	-4.665	0.533	38	24.500	-0.030	-11.987	-12.016
C ₅ H ₄ NCN-p	-6.513	-3.024	-4.769	0.573	38	24.500	-0.019	-11.536	-11.555
C ₆ H ₄ OHCN-o	-5.950	-2.261	-4.106	0.542	44	28.880	-0.140	-14.009	-14.148
C ₆ H ₄ OHCN-m	-5.982	-2.341	-4.162	0.549	44	28.880	-0.126	-13.912	-14.038
C ₆ H ₄ OHCN-p	-5.926	-2.070	-3.998	0.519	44	28.880	-0.167	-14.335	-14.502

HOMO of SiBr ₄	LUMO of SiBr ₄	μ_A of SiBr ₄	N_A of SiBr ₄	S_A of SiBr ₄
-7.195	-3.102	-5.149	32	0.489

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

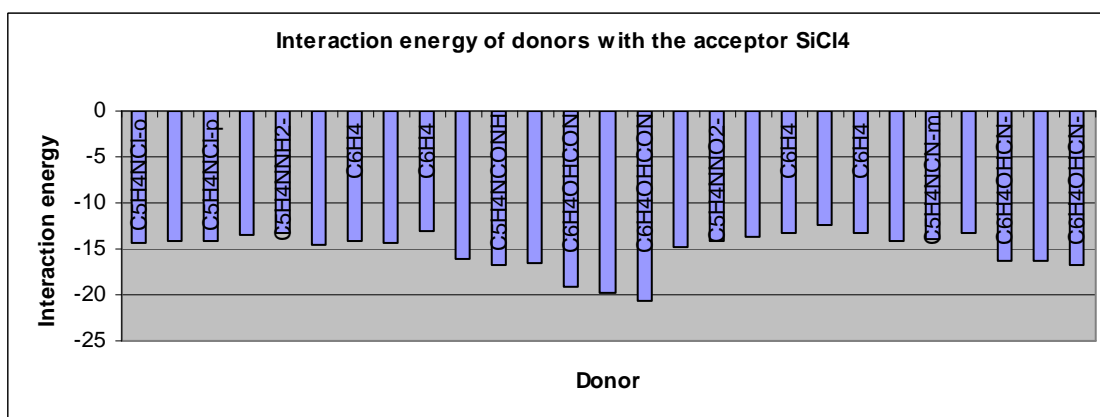
Table-6: Interaction energy of organic bases for interaction with SiI₄

Donor	ϵ HOMO	ϵ LUMO	μ_B	S_B	N_B	λ	E_v	E_μ	E_{int}
C ₅ H ₄ NCl-o	-6.337	-2.011	-4.174	0.462	36	23.120	-0.127	-9.353	-9.480
C ₅ H ₄ NCl-m	-6.174	-2.020	-4.097	0.481	36	23.120	-0.153	-9.210	-9.363
C ₅ H ₄ NCl-p	-6.170	-1.962	-4.066	0.475	36	23.120	-0.161	-9.256	-9.416
C ₅ H ₄ NNH ₂ -o	-4.865	-1.223	-3.044	0.549	36	23.120	-0.686	-8.739	-9.425
C ₅ H ₄ NNH ₂ -m	-4.830	-1.268	-3.049	0.561	36	23.120	-0.692	-8.658	-9.350
C ₅ H ₄ NNH ₂ -p	-5.186	-0.938	-3.062	0.471	36	23.120	-0.615	-9.289	-9.904
C ₆ H ₄ OHNH ₂ -o	-4.469	-0.630	-2.550	0.521	36	23.120	-1.022	-8.929	-9.951
C ₆ H ₄ OHNH ₂ -m	-4.436	-0.514	-2.475	0.510	36	23.120	-1.068	-9.006	-10.074
C ₆ H ₄ OHNH ₂ -p	-4.076	-0.776	-2.426	0.606	36	23.120	-1.225	-8.378	-9.604
C ₅ H ₄ NCONH ₂ -o	-5.590	-2.286	-3.938	0.605	46	30.420	-0.234	-11.030	-11.263
C ₅ H ₄ NCONH ₂ -m	-5.815	-2.294	-4.055	0.568	46	30.420	-0.183	-11.336	-11.519
C ₅ H ₄ NCONH ₂ -p	-5.967	-2.535	-4.251	0.583	46	30.420	-0.123	-11.213	-11.336
C ₆ H ₄ OHCONH ₂ -o	-5.278	-1.864	-3.571	0.586	52	35.280	-0.396	-12.975	-13.371
C ₆ H ₄ OHCONH ₂ -m	-5.530	-1.946	-3.738	0.558	52	35.280	-0.306	-13.246	-13.552
C ₆ H ₄ OHCONH ₂ -p	-5.553	-1.707	-3.630	0.520	52	35.280	-0.341	-13.635	-13.976
C ₅ H ₄ NNO ₂ -o	-6.543	-3.630	-5.087	0.687	46	30.420	0.000	-10.416	-10.416
C ₅ H ₄ NNO ₂ -m	-6.611	-3.840	-5.226	0.722	46	30.420	-0.002	-10.171	-10.173
C ₅ H ₄ NNO ₂ -p	-6.644	-4.025	-5.335	0.764	46	30.420	-0.010	-9.894	-9.903
C ₆ H ₄ OHNO ₂ -o	-6.165	-3.258	-4.712	0.688	42	27.380	-0.029	-9.366	-9.395
C ₆ H ₄ OHNO ₂ -m	-6.100	-3.492	-4.796	0.767	42	27.380	-0.019	-8.886	-8.906
C ₆ H ₄ OHNO ₂ -p	-6.269	-3.315	-4.792	0.677	42	27.380	-0.018	-9.437	-9.455
C ₅ H ₄ NCN-o	-6.646	-2.795	-4.721	0.519	38	24.500	-0.024	-9.474	-9.498
C ₅ H ₄ NCN-m	-6.540	-2.790	-4.665	0.533	38	24.500	-0.031	-9.372	-9.404
C ₅ H ₄ NCN-p	-6.513	-3.024	-4.769	0.573	38	24.500	-0.019	-9.095	-9.114
C ₆ H ₄ OHCN-o	-5.950	-2.261	-4.106	0.542	44	28.880	-0.161	-10.974	-11.135
C ₆ H ₄ OHCN-m	-5.982	-2.341	-4.162	0.549	44	28.880	-0.145	-10.915	-11.060
C ₆ H ₄ OHCN-p	-5.926	-2.070	-3.998	0.519	44	28.880	-0.192	-11.173	-11.366

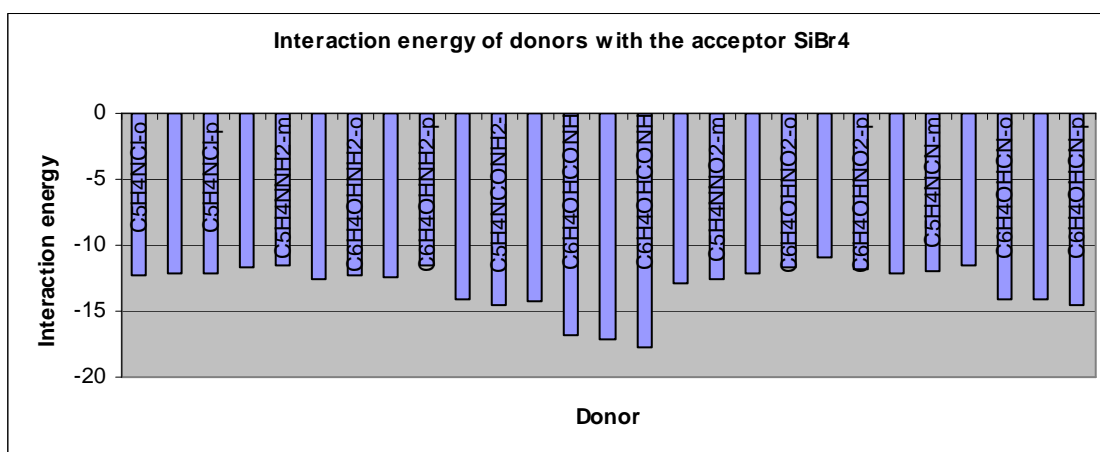
HOMO of SiI ₄	LUMO of SiI ₄	μ_A of SiI ₄	N_A of SiI ₄	S_A of SiI ₄
-6.404	-3.819	-5.112	32	0.774

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

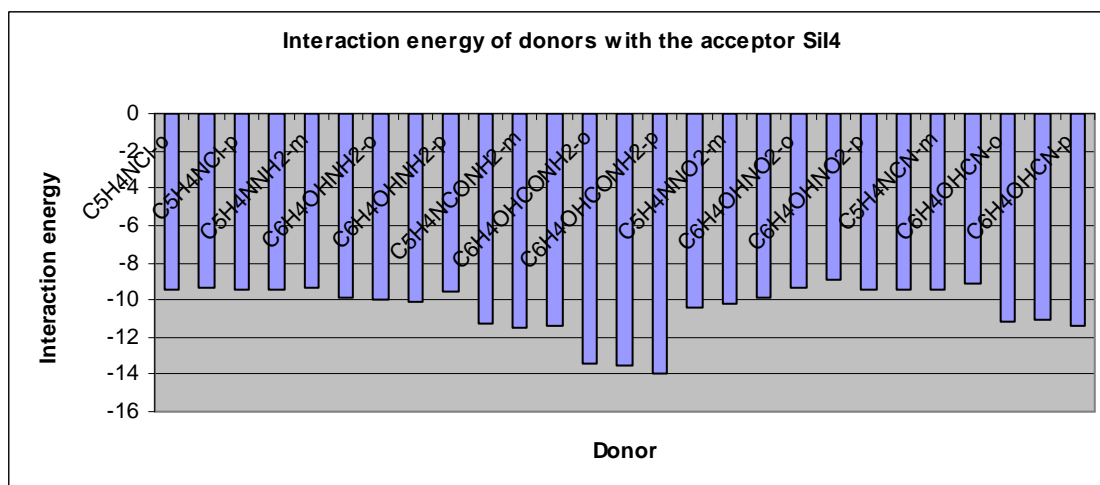
Graph-4: Interaction energy of organic bases with SiCl₄



Graph-5: Interaction energy of organic bases with SiBr₄



Graph-6: Interaction energy of organic bases with SiI₄



CONCLUSION

Interaction energy of organic base C₆H₄OHCNO₂-m for interaction with the acceptor TiI₄ is highest (-8.188 eV) among all the interaction of organic bases with the acceptors. It indicates that

the donor organic base C₆H₄OHNO₂-m forms least stable complex with the acceptor metal halide TiI₄. Interaction energy of organic base C₆H₄OHCONH₂-p for interaction with the acceptor SiCl₄ is lowest (-20.566 eV) among all the interaction of organic bases with the acceptors. It indicates that the donor organic base C₆H₄OHCONH₂-p forms most stable complex with the acceptor metal halide SiCl₄.

Among ortho derivatives of donors, C₆H₄OHCONH₂-o forms most stable complexes with SiCl₄ and C₅H₄NCN-o forms least stable complexes with TiI₄.

Among meta derivatives of donors, C₆H₄OHCONH₂-m forms most stable complexes with SiCl₄ and C₆H₄OHNO₂-m forms least stable complexes with TiI₄.

Among para derivatives of donors, C₆H₄OHCONH₂-p forms most stable complexes with SiCl₄ and C₅H₄NCN-p forms least stable complexes with TiI₄.

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