Density Functional Theory Based Study of The Interaction Energy Between Ethyl Tin (IV) Chloride and Derivatives of Pyridine

Section A-Research paper

Density Functional Theory Based Study of The Interaction Energy Between Ethyl Tin (IV) Chloride and Derivatives of Pyridine

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Abstract

Tin has one of the largest number of organometallic derivatives that are available for different commercial applications. In organic synthesis, organotin compounds participate as a precursor/catalyst in several organic transformations, and therefore it becomes imperative to study the interaction of these compounds with other co-precursor. This study explores the interaction of ethyl tin (IV) chloride ($C_2H_5SnCl_3$), an organotin compound, with pyridine derivative using density functional theory (DFT) calculations. Pyridine derivatives has been known for their multifaceted role as solvent, base, ligand, catalyst, functional group and molecular scaffold in several organic reactions. In particular, here, we have considered pyridine as a base/donor molecule. In this study, we have considered a total of 11 compounds with their ortho, meta, and para derivatives, enumerating 33 (11×3) interactions among donor and acceptor compounds. Among ortho-derivative donors, the interaction of o-Phenylacetatopyridine (o-PhAcPy) with $C_2H_5SnCl_3$ acceptor is thermodynamically most favorable. Similarly, in the case of meta and para

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derivatives, the phenylacetatopyridine shows thermodynamically most favorable interaction with $C_2H_5SnCl_3$. In addition, the Nitropyridine (NPy) derivative shows thermodynamically least favorable interaction with the $C_2H_5SnCl_3$ acceptor. The PhAcPy derivative complex shows good resolution of thermodynamic stability on ortho, meta, and para substitution. The study serves the basis of further exploration of PhAcPy derivative complexes in organic synthesis.

Keywords: DFT, electron donor, electron acceptor, interaction energy.

1. Introduction

Tin has one of the largest numbers of organotin derivatives compounds used in different commercial applications. Due to their broad application in various fields, especially stabilizing polyvinyl chloride (PVC) against thermal degradation and long-term photodegradation, they have been produced industrially on a large scale.[1-4] Tin-based compounds have been extensively used as a catalyst in many organic transformations.[5-12] Tin (IV) chloride is a Lewis acid and has been known for good chelation properties.[13-17] The derivative compounds of tin (IV) species can form (a) Lewis acid-base adduct and (b) metal-ligand bond formation.

With the development of powerful computer hardware, computational simulation has become a powerful tool for investigating complex problems. DFT is one of the most potent theories employed in several scientific domains to understand the chemistry and physics of a system.[18-28] The interaction energy between two species, for example, A and B, can be computed using the principle of HSAB combined with DFT.[29-34] It has the advantage of being an orbital-dependent theory. The interaction of tin (IV) halides with donor compounds has been studied extensively

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through their physicochemical and infrared spectral studies.[35-38] Computationally, Singh et al. studied the interaction of several metal halides (SnX_2, ZnX_2, CdX_2, HgX_2; X= Cl, Br, I) with different organic bases.[39] Similarly, Singh et al. investigated metal halide interaction with several organic bases.[40] These studies utilize the HSAB principle as a descriptor in defining favorable electrophile-nucleophile adduct formation, an essential step in designing novel synthesis protocols. This study explores the interaction of ethyl tin (IV) chloride ($C_2H_5SnCl_3$) with different donor molecules using the HSAB principle combined with DFT. As mentioned earlier, organotin compounds serve as a precursor in several organic transformations; we have studied the interaction between $C_2H_5SnCl_3$, an organotin compound, and pyridine derivatives, a multifaceted reagent. Among ortho-, meta-, and para-derivative donors, the interaction between Phenylacetatopyridine (PhAcPy) and $C_2H_5SnCl_3$ is thermodynamically most favorable, i.e., serving as the strongest base. The Nitropyridine (NPy) derivative shows thermodynamically the least favorable interaction with the $C_2H_5SnCl_3$ acceptor, thus serving as the weakest base. Similar observations have been made by Singh et al., where they showed Nitro toluene as the weakest base against all the acceptors.[39]

2. Computational methodology

DFT has been successful in studying chemical reactivity problems especially when combined with different concepts of chemical bonding, for example, hard and soft acids and bases (HSAB) principle, and electronegativity principle.[29-31, 41-43] According to DFT, the interaction energy between two chemical species A and B is given as

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

where ρ_A, ρ_A, and ρ_{AB} are the ground-state charge density of reactant A, B, and product AB respectively. In 1993, Gázquez has shown that if the interaction energy is divided into two parts and one apply the properties of hardness and softness function, the eq (1) can be written as[41]

$$\Delta E_{int} = \Delta E_v + \Delta E_\mu \tag{2}$$

where ΔE_v, and ΔE_μ are the change in energy at constant external potential and constant chemical potential respectively. The term ΔE_v (in eq. 2) correspond to charge transfer process between A and B resulting due to the chemical potential equalization principle at constant external potential and shown as

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

where μ_A and μ_B involved in eq (3) correspond to the chemical potential of species A and B respectively. S_A and S_B (in eq. 3) defines the global softness of A and B respectively. For computation, we have considered $S_A \approx S_B$ based on the literature.[39, 44] The chemical potential μ_A and global softness S_A in a natural way appears as response function of the change in electronic energy of a molecule A with the change in number of electron N_A and external potential (due to the nuclei), respectively. That is, chemical potential (μ_A) can be expressed as $\mu_A = (\partial E_A/\partial N_A)$, the global softness parameter (S_A) is the inverse of global hardness (η_A), that is $S_A = 1/(2\eta_A)$, where the global harness (η_A) is the change is chemical potential with respect the change in number of electrons, $\eta_A = 1/2(\partial^2 E/\partial^2 N_A)$, which was identified as a negative of electronegativity. The term ΔE_μ which correspond to change in energy at constant chemical potential is shown as

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

where λ is related to an "effective number of valence electrons" that participate in the interaction between A and B. For a nondegenerate system, the ground-state energy is obtained by minimizing energy functional $[v,]$, which has the dependence on electron density and external potential. Within DFT framework, the ground-state energy is defined as [42]

$$E[\rho] = T_s[\rho] + J[\rho] + E_{XC}[\rho] + \int v(r)\rho(r)dr \tag{5}$$

where $T_s[\rho]$ is the kinetic energy of the corresponding noninteracting reference system, $J[\rho]$ is the classical coulomb energy term, $E_{XC}[\rho]$ is called the exchange-correlation energy and the last term correspond to the effect of external potential of density. We have employed B88LYP exchange-correlation energy functional and double-zeta valence polarized (DZVP) basis set.[45, 46] The functional form of B88 exchange-correlation, in a spin-restricted case, is expressed as

$$E_X^{B88}[\rho] = C_x \int dr \, \rho^{4/3}(r) F_X^{B88}(s) \tag{6}$$

where $\rho(r)$ is the electron number density, $C_x = \frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3}$ and $F_X^{B88}(s)$ is the enhancement factor.
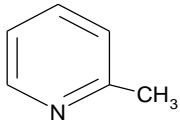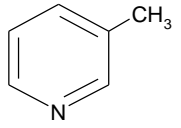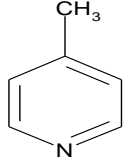
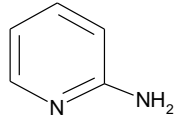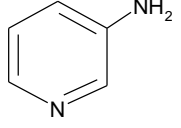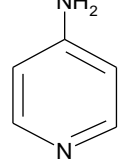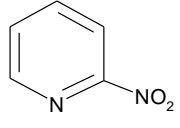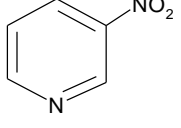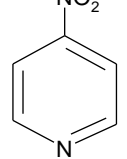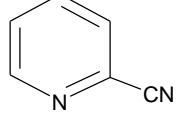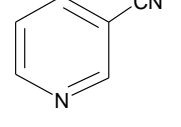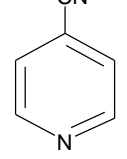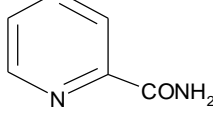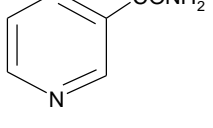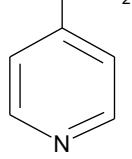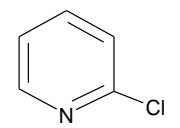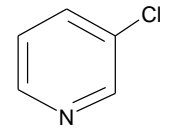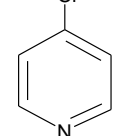$$F_X^{B88}(s) = 1 + \frac{\gamma C_2 C_1^2 S^2}{1 + 6\gamma C_1 s Sinh^{-1}(C_1 s)} \tag{7}$$
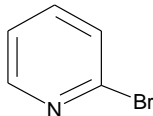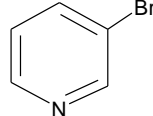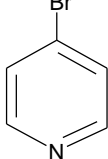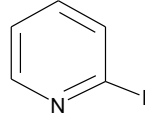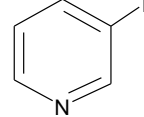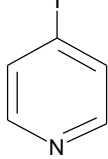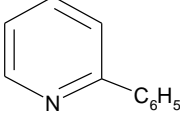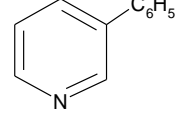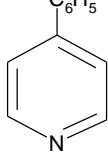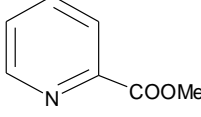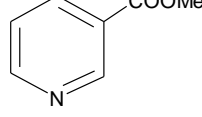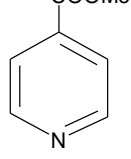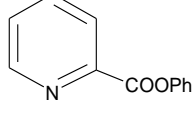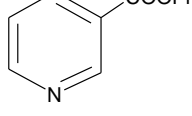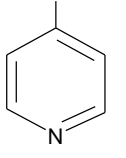
where, $C_1 = 2(6\pi^2)^{1/3}$, $C_2 = \left(2^{1/3}C_x\right)^{-1}$ and γ is a constant. All the computations are done using CAChe WorkSystems (Fujitsu Co. Ltd., Tokyo, Japan).

The derivatives of pyridine which have been used as a donor are shown in Table 1 along with their name, molecular formula and molecular structure. All the donor molecules along with their

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ortho-, meta-, and para-derivatives are listed in Table 1.

Table 1: Derivatives of pyridine as donor molecules along with their name, molecular formula and molecular structure. Ethyl tin (IV) chloride ($C_2H_5SnCl_3$) has been used as an acceptor.

SN	Molecular formula of donor (B)	Name of donor	Molecular structure of donor (B)		
			Ortho	Meta	Para
1	C_6H_7N	o-Methylpyridine (o-MePy)			
2	$C_5H_6N_2$	o-Aminopyridine (o-APy)			
3	$C_5H_4N_2O_2$	o-Nitropyridine (o-NPy)			
4	$C_6H_4N_2$	o-Cyanopyridine (o-CNPy)			
5	$C_6H_6N_2O$	o-Amidopyridine (o-AmPy)			
6	C_5H_4NCl	o-Chloropyridine (o-ClPy)			

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7	C$_5$H$_4$NBr	o-Bromopyridine (o-BrPy)			
8	C$_5$H$_4$NI	o-Iodopyridine (o-IPy)			
9	C$_{11}$H$_9$N	o-Phenylpyridine (o-PhPy)			
10	C$_7$H$_7$NO$_2$	o-Methylacetatopyridine (o-MeAcPy)			
11	C$_{12}$H$_9$NO$_2$	o-Phenylacetatopyridine (o-PhAcPy)			

3. Results and discussion

The donor-acceptor interaction between 11 donor molecules and their ortho-, meta-, and para-derivatives with acceptor are listed in Table 1. We have computed total 33 (11 x 3) interactions between donor and acceptor and the corresponding metal-ligand interaction energy (E_{int}) is computed along with other essential parameters which are specified at the figure captions. The metal-ligand bond strength depends on the value of interaction energy (E_{int}) as the bond strength increases the value of interaction energy decreases.

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3.1 Interaction of ortho-derivatives of donors with acceptor ethyl tin (IV) chloride

The interaction energy (E_{int}) of ortho derivatives of donors with acceptor ethyl tin (IV) chloride is shown in Figure 1. The complex of o-PhAcPy with acceptor shows the lowest value of interaction energy, that is, its forms a most stable complex compared to all other donor molecules. Conversely, o-NPy has the highest interaction energy with donor resulting in a formation of least stable donor-acceptor complex.

Figure 1: Variation of interaction energy (E_{int}) of ethyl tin (IV) chloride with ortho-derivatives of pyridine.

Based on the interaction energy (E_{int}) value shown in the Figure 1, the donor molecules can be arranged in their decreasing order of stable complex formation as follows

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

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Chemical potential (μ_B) Effective number of valence electron (λ)
Change in energy at constant external potential (E_ν) Global softness (S_B)
Change in energy at constant chemical potential (E_μ)

Figure 2: All the essential parameters, chemical potential (μ_B), effective number of valence electron (λ), change in energy at constant external potential (E_ν), global softness (S_B), and change in energy at constant chemical potential (E_μ), used to compute the (E_{int}). The value of chemical potential of acceptor is set as 5.366. The global softness parameter (S_A) of acceptor molecule is set as 0.452, N_A, N_B are the total number of electrons in acceptor and donor molecules respectively; $\lambda = (N_A + N_B)^2/2000$, E_μ is the energy corresponds to a reshuffling of the charge distribution; E_ν correspond to the energy of charge transfer process, and E_{int}, interaction energy; all the energy values are in eV.

The complexes of pyridine which consist of electron withdrawing groups form less stable complexes with acceptor molecule. Among halide derivatives, the o-ClPy forms most stable complex, followed by oBrPy and o-IPy. Figure 2 shows all the essential parameters used to compute the interaction energy (E_{int}) of ortho-derivative complex with C$_2$H$_5$SnCl$_3$ acceptor. As can be seen from Figure 2 that the global softness parameter (S_B) of all the donor molecule is

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similar except for case of o-NPy derivative which has higher S_B value compared to others. The higher S_B value of o-NPy derivative indicate it's harder basic nature compared to the other derivatives. The higher chemical potential o-NPy derivative reinforce the argument presented above about its hard nature. Singh et al. also studied the interaction between metal halides and organic bases.[39] They also observed that the nitro-derivative complex, for example, nitro-toluene, forms the least stable complex with metal halides. The observation holds for all ortho-, meta-, and para-derivatives where nitro-group is present in the organic bases. A similar observation has been made by Singh et al., where they showed that cyno- and nitro-derivative organic bases form the least stable complexes with metal halides.[40] All these studies corroborate our observations about the stability of metal halide complexes where the pyridine derivatives with a strong electron-withdrawing group form less stable complexes.

3.2 Interaction of meta-derivatives of donors with ethyl tin (IV) chloride:

The interaction energy of meta derivatives of donors with acceptor $C_2H_5SnCl_3$ is shown in Figure 3. The value of interaction energy of m-PhAcPy with acceptor $C_2H_5SnCl_3$ is the lowest, as in the case of ortho-derivatives, indicating that m-PhAcPy forms the most stable complex with acceptor molecule. Similarly, again, as in case of ortho-derivatives, the value of interaction energy of m-NPy with acceptor $C_2H_5SnCl_3$ is the highest, and therefore forming least stable complex with acceptor $C_2H_5SnCl_3$.

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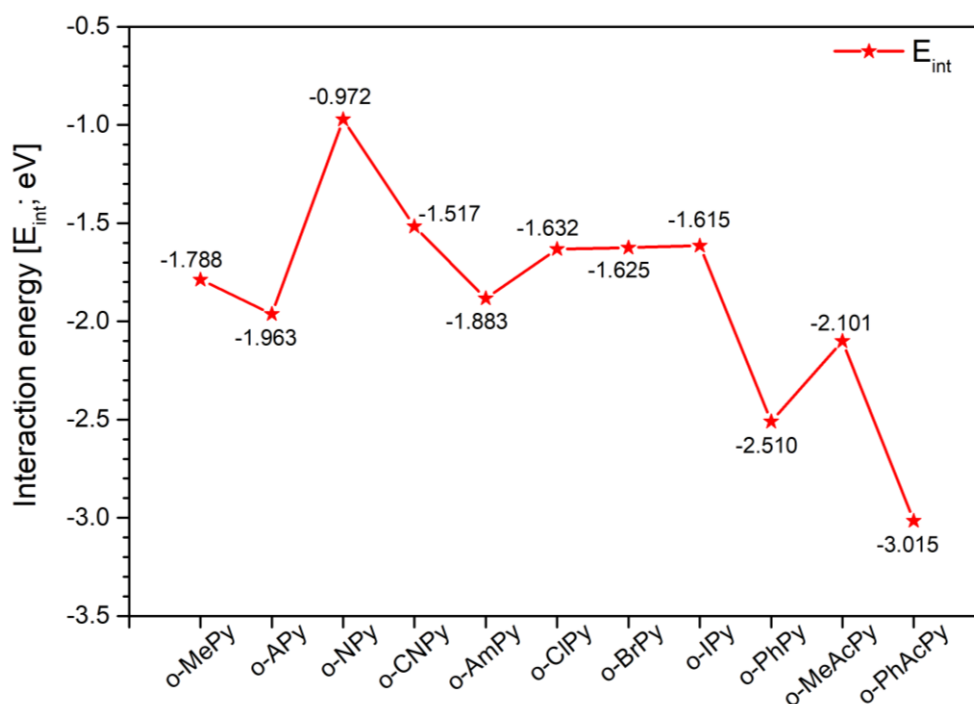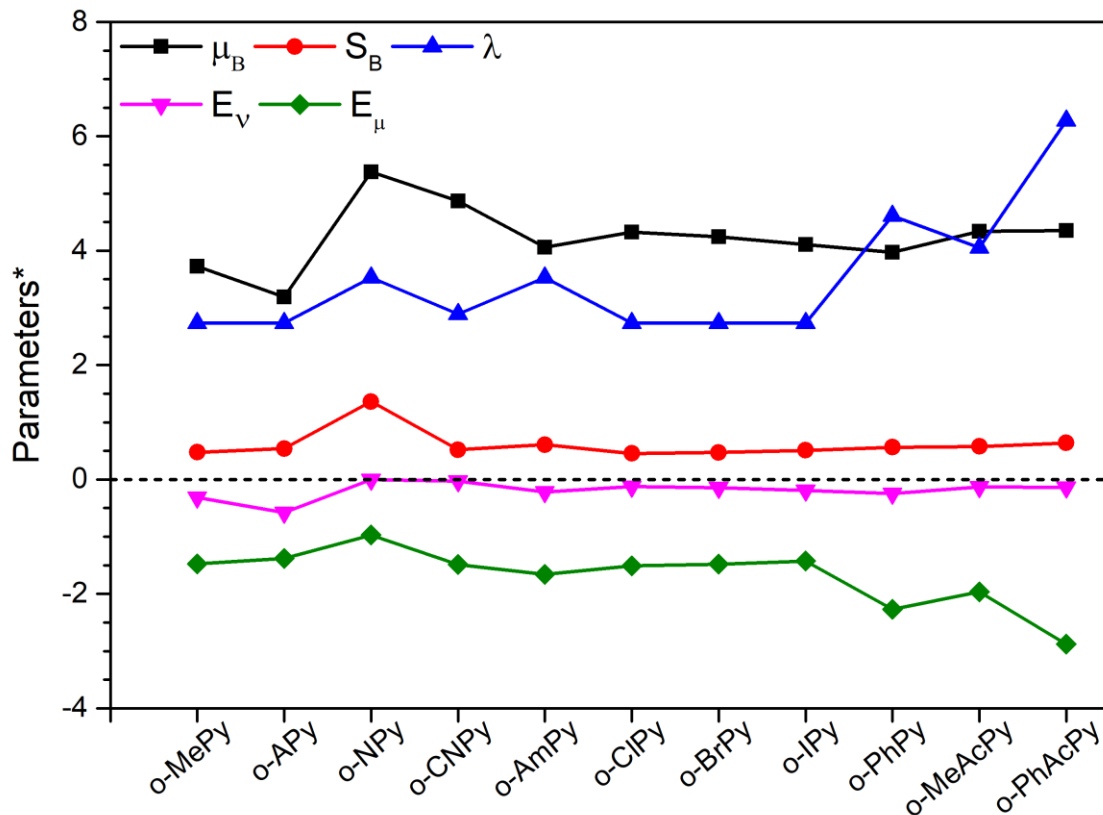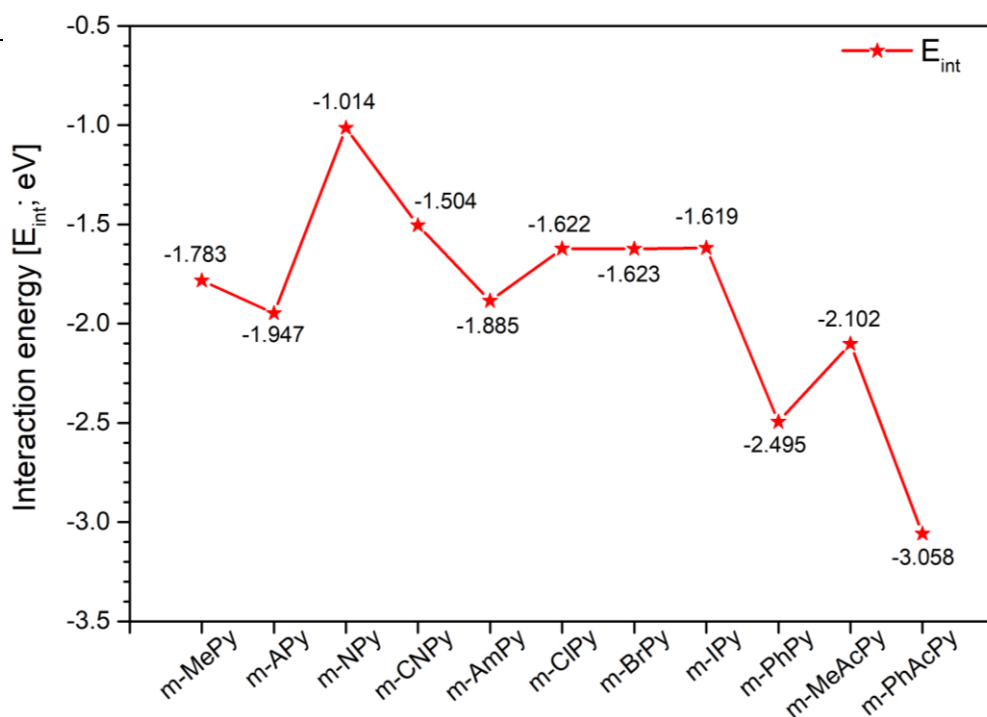**Figure 3:** Variation of interaction energy (E_{int}) of ethyl tin (IV) chloride with meta-derivatives of pyridine.

The exact order of the stability of the donor-acceptor complex is as follows

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

The order of stability of meta-derivative complexes is same as in case of ortho-derivative, except for halide derivative. In case of meta-derivative, the m-BrPy and m-ClPy are almost energetically degenerate; however for ortho-derivative case, the o-ClPy forms more stable complex with acceptor compared to the o-BrPy. Figure 4 shows all the essential parameters used to compute the interaction energy (E_{int}) of meta-derivative complexes with $C_2H_5SnCl_3$ acceptor.
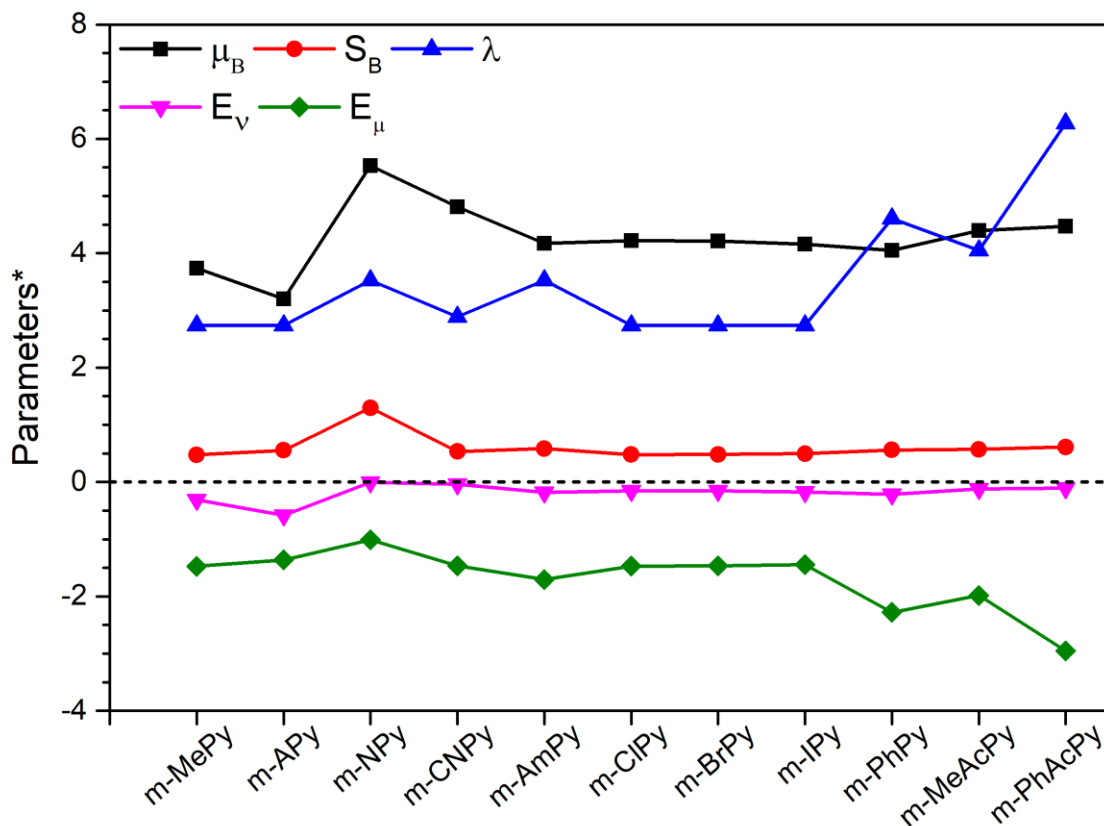
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*Chemical potential (μ_B)   Effective number of valence electron (λ)
Change in energy at constant external potential (E_v) Global softness (S_B)
Change in energy at constant chemical potential (E_μ)

Figure 4: All the essential parameters, chemical potential (μ_B), effective number of valence electron (λ), change in energy at constant external potential (E_v), global softness (S_B), and change in energy at constant chemical potential (E_μ), used to compute the (E_{int}) for meta-derivative donor molecule with $C_2H_5SnCl_3$ acceptor. The value of chemical potential and global softness parameter (S_A) of acceptor molecule are same as mentioned in figure caption 2.

As we move from ortho- to meta-derivative complexes, the essential parameters does not show any marked deviation, that is, all essential parameters can be mapped one by one with each other. For example, the global softness parameter (S_B) of all the donor molecule is similar to each other except for case of o-NPy derivative which ended up at higher side parameter compared to others. Similarly, the chemical potential of m-NPy derivative is highest among others.

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3.3 Interaction of para-derivatives of donors with ethyl tin (IV) chloride:

The interaction energy of para derivatives of donors with acceptor $C_2H_5SnCl_3$ is shown in Figure 5. The interaction energy of p-PhAcPy and acceptor $C_2H_5SnCl_3$ is lowest among others, as in the case of ortho- and meta-derivatives, resulting in the formation of most stable complex.
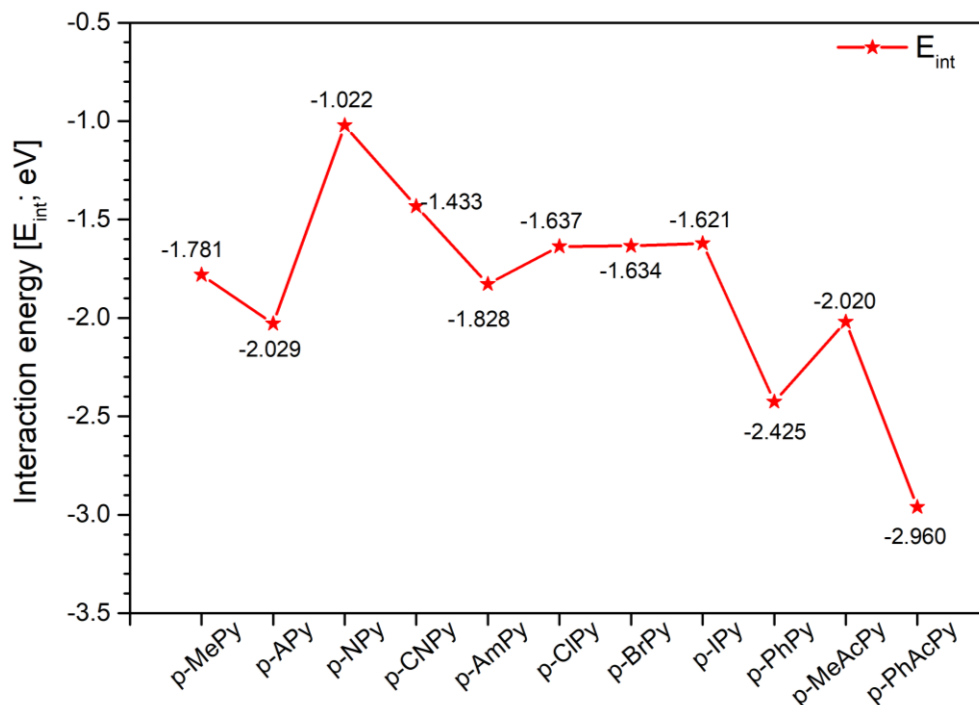
Figure 5: Variation of interaction energy (E_{int}) of ethyl tin (IV) chloride with para-derivatives of pyridine.

Again, in case of para-derivative complexes, the value of interaction energy of p-NPy with acceptor $C_2H_5SnCl_3$ is highest, resulting in the formation of least stable complex with acceptor. The exact order of stability of complex formation donor with acceptor is as follows

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

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Broadly, the stability order of para-derivative complexes is similar compared to ortho- and meta-derivative complexes; however a slight change in the stability order can be observed. For example, p-APy form more stable complex with acceptor compared to the o-MeAcPy, which is opposite to the ortho- and meta-derivative complexes. In addition, essential parameters used to compute the interaction energy (E_{int}) of para-derivative complexes with $C_2H_5SnCl_3$ acceptor are shown in Figure 6.
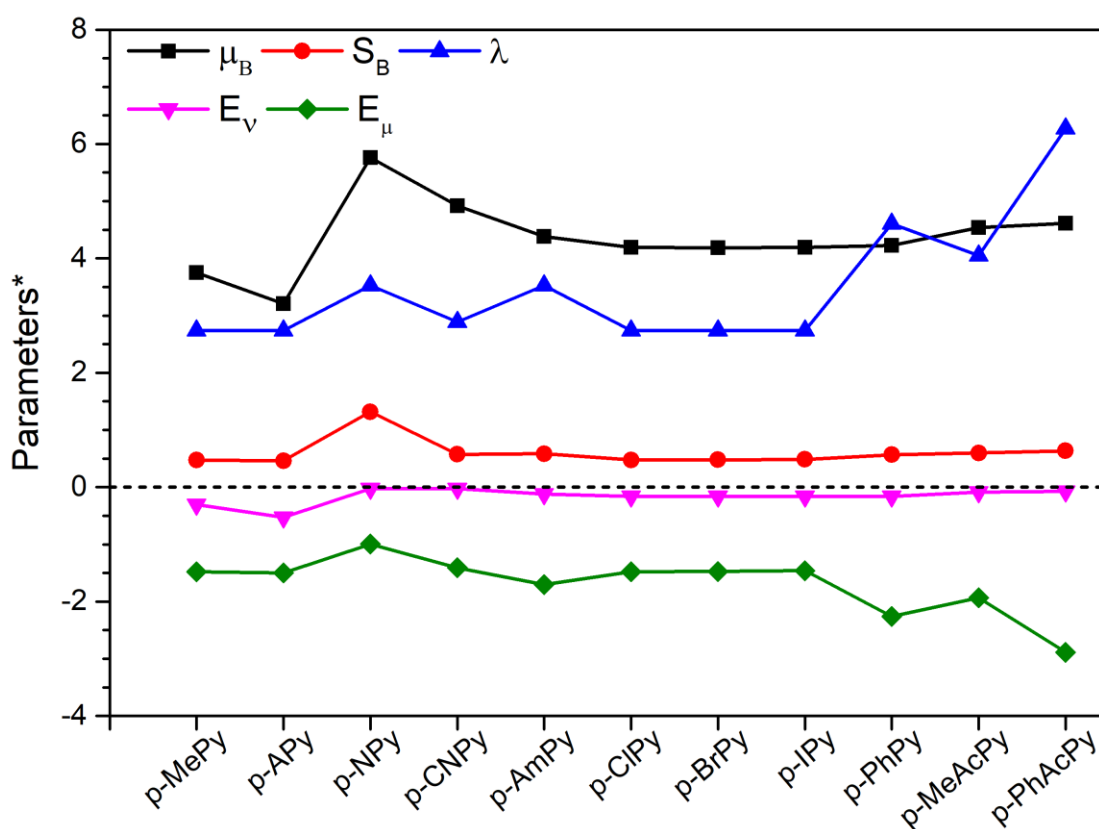
*Chemical potential (μ_B) Effective number of valence electron (λ)
Change in energy at constant external potential (E_v) Global softness (S_B)
Change in energy at constant chemical potential (E_μ)

Figure 6: All the essential parameters, chemical potential (μ_B), effective number of valence electron (λ), change in energy at constant external potential (E_v), global softness (S_B), and change in energy at constant chemical potential (E_μ), used to compute the (E_{int}) for para-derivative donor molecule with $C_2H_5SnCl_3$ acceptor. The value of chemical potential and global softness parameter (S_A) of acceptor molecule are same as mentioned in figure caption 2.

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Here in this also, the global softness parameter (S_B) of p-NPy derivative is highest. Similarly, the chemical potential of p-NPy derivative is highest among others.

3.4 A comparative analysis of ortho-, meta-, and para-derivative complexes:

As we have discussed earlier that PhAcPy and NPy derivatives form thermodynamically most stable and least stable complexes with ethyl tin (IV) chloride respectively. And therefore, we will be considering these two examples as a representative case to analyze the effect of ortho,
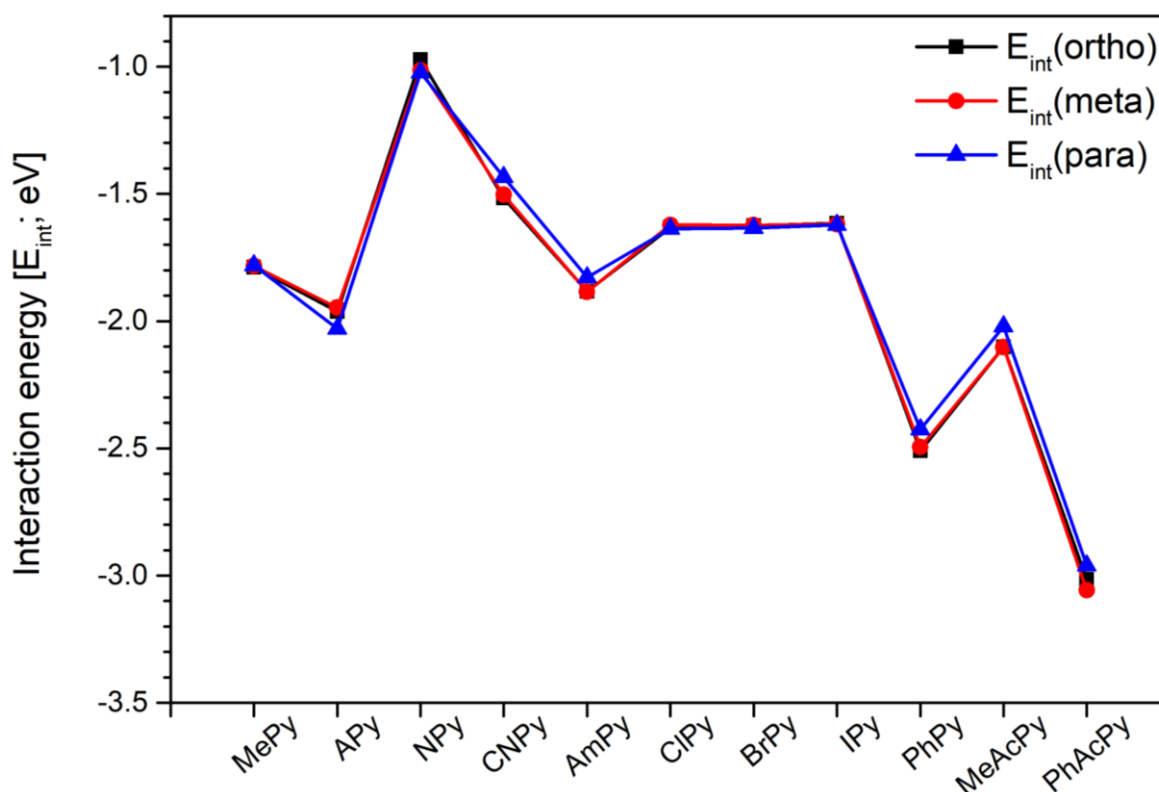
meta, and para substitution on their stability.

Figure 7: Interaction energy of ortho-, meta-, and para-derivatives of pyridine (donor) with ethyl tin (IV) chloride (acceptor).

Figure 7 shows the interaction energy (E_{int}) of donor-acceptor complexes along with their

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ortho, meta, and para derivatives. As can be seen from Figure 7, the interaction energy of ortho, and meta derivative complexes is close to each other compared to the para derivative complex.

To analyze further, we have plotted interaction energy of ortho-, meta-, and para-derivative donor-acceptor complexes with reference to ortho-derivative complexes. Figure 8 shows the relative interaction energy $(E_{int}\text{-}E_{int}(ortho))$ of all the studied complexes with respect to ortho-derivative complex. As can be seen from figure 8 that the meta derivative complex of PhAcPy is thermodynamically most stable compared to its ortho- and para-derivative complexes.
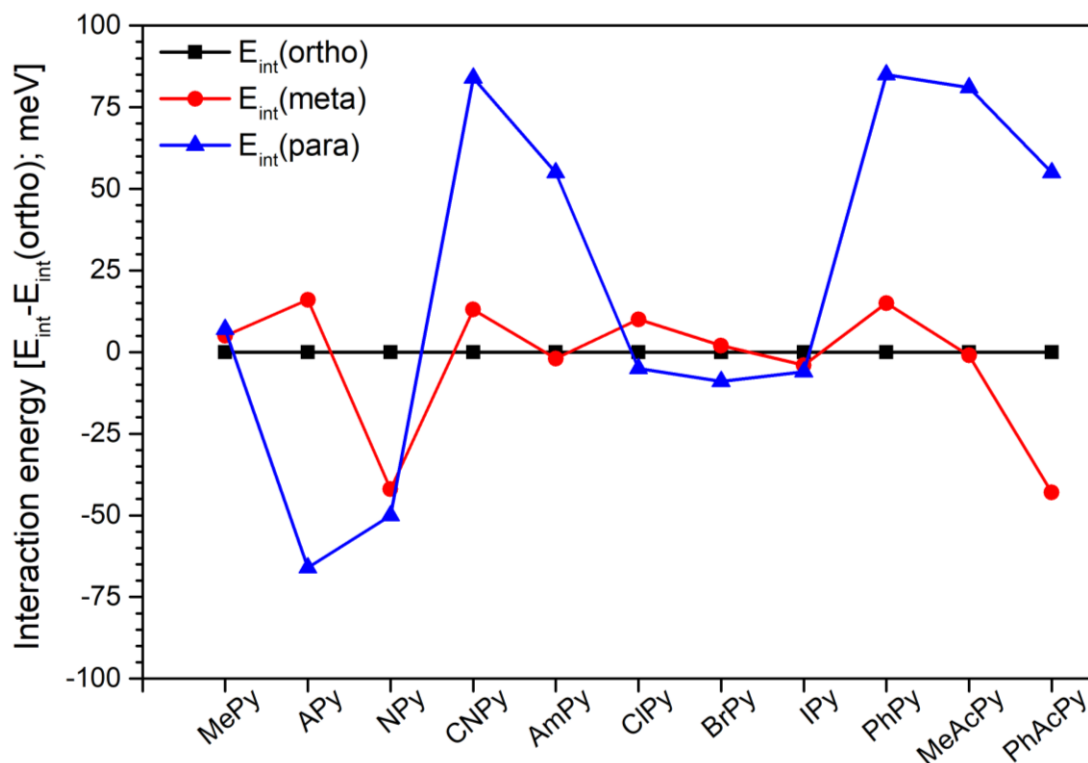
However, in the case of NPy derivative complex, the para and meta complexes are energetically degenerate.

Figure 8: Relative interaction energy $(E_{int}\text{-}E_{int}(ortho))$ of ortho-, meta-, and para-derivatives of pyridine (donor) with ethyl tin (IV) chloride (acceptor).

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Its ortho-derivative complex destabilizes compared to the meta- and para-derivative complexes. In the case of PhAcPy derivative complex, we can observe good resolution in terms of their thermodynamic stability; however for NPy derivative complex, the meta and para-derivative are energetically degenerate.

In summary, the interaction energy (E_{int}) of the subject line molecules depends on two factors: (a) change in energy at constant external potential (ΔE_v) and (b) change in energy at constant chemical potential(ΔE_μ). The value of (ΔE_v) effectively depends on the difference in chemical potential of the donor and acceptor molecules. As the donor interacts with the acceptor molecule, a positive charge is left behind at the donor molecule, the functional groups which has the tendency of donating electrons, for example, amino (-NH$_2$) group would stabilize this positive charge (on donor atom) resulting in felicitating the donor-acceptor-interaction. The Figures 2, 4 and 6 reflect the same, as aminopyridine has the lowest (E_v) value. The functional group that destabilizes the positive charge on donor molecules, for example, Nitro- and cyano- has the highest values. Another factor determining the interaction energy value is a change in energy at a constant chemical potential and the value effectively depends on the number of valence electrons on the donor species. Since phenylacetatopyridine (PhAcPy) has the highest number of valence electrons (74), it shows the lowest (E_μ) value and PhAcPy derivative complexes shows the highest stability in terms of interaction energy (E_{int}). The interaction energy has a synergistic effect of charge compensation by functional groups and a number of valence electrons on the functional group.

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4. Conclusions

The organotin derivative complexes encompass a broad range of technological and industrial applications. In this study, we have systematically studied the stability of commercially important organotin derivative complexes based in their interaction energy parameter using first-principle density functional theory calculations. Among all the donor-acceptor interactions, the interaction energy of PhAcPy-derivative with acceptor $C_2H_5SnCl_3$ is the lowest, which indicates that PhAcPy-derivative forms the most stable complex among others. The NPy-derivative has highest interaction energy with acceptor $C_2H_5SnCl_3$ resulting in the formation of least stable complex. The high global softness parameter of NPy-derivative indicates its hard nature also reflected through its high chemical potential value. The PhAcPy-derivative complex shows good resolution of thermodynamic stability on ortho, meta, and para substitution; however the meta and para derivative complexes of NPy are energetically degenerate. The first-principle based interaction energy parameter can be used for the further exploration of these materials in the synthesis of technological and industrially important organotin complexes.

Conflict of interest

There are no conflicts to declare.

Supporting Information

Not applicable

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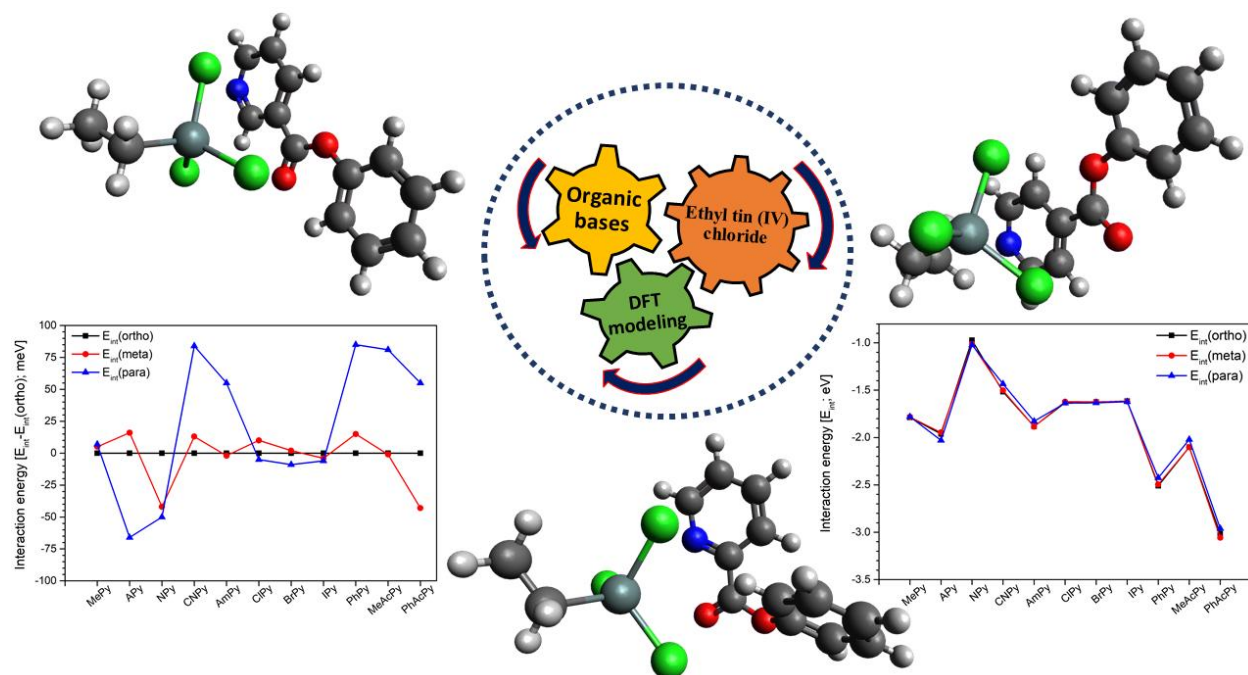
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20-word summary:

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