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Complexes of Cobaltocene: A Effective Atomic Softness and Fukui Function Based Study

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ABSTRACT

Atomic descriptor such as effective atomic softness ($E^{\ddagger}_{n}$ and $E^{\ddagger}_{m}$), fukui function (f^{-} and f^{+}) and their difference ($\Delta E^{\ddagger}_{nm}$ and $\Delta f^{-}f^{+}$) of complexes of Lewis acids [thiocyanate and selenocyanate of Ni(II), Cu(II), Zn(II), Fe(II) and Co(II)] and Lewis bases [$Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$] have been evaluated**.** All molecular geometries were minimized by quantum mechanic especially at PM3 method was used to calculate ionization potential (IP), electron affinity (EA), partial charge (q) and total number of electrons of a molecule (N). $E^{\ddagger}_{n}$, $E^{\ddagger}_{m}$, f^{-} and f^{+} were used to predict the chemical reactivity and site selectivity, while $\Delta E^{\ddagger}_{nm}$ and $\Delta f^{-}f^{+}$ used to predict stability of complexes. $\Delta E^{\ddagger}_{nm}$ and $\Delta f^{-}f^{+}$ values of complexes of $Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$ with thiocyanate and selenocyanate of Ni(II) are higher than thiocyanate and selenocyanate of Cu(II), Zn(II), Fe(II) and Co(II) hence former complexes have higher stability than later.

Key words: effective atomic softness, fukui function, PM3, cobaltocene

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INTRODUCTION

Computational chemistry methods have been introduced that allow analysis of reaction mechanisms and prediction of the reactivity in synthetic chemistry. Therefore, computational chemistry is used to predict the reactivates of a wide variety of compounds [1, 2]. The successful synthesis of a new compound is generally valued much more highly than the result of bonding analysis of a molecule. This is why chemistry has acquired during its history, the character of being an engineering discipline. Development of quantum chemistry has however given a new concept by which the metal-ligand bonding has been described in terms of quantum chemical parameters [3]. In the last decade, there has been a phenomenal advancement in theoretical inorganic chemistry [4]. Commercial programs incorporating the latest methods have become widely available, and are capable of providing more information about molecular orbitals with a simple input of chemical formula [5, 6]. In this paper a theoretical basis for the concepts of chemical reactivity, selectivity and stability of molecular complexes has been discussed. The objective of the work is to study the stability of complex formed between Lewis acids (thiocyanate of Ni(II), Cu(II), Zn(II), Fe(II) and Co(II)) and Lewis bases ($Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$). For this we have used two principles: one is based on softness parameters and their difference $\Delta E^{\ddagger}_{nm}$ [7] and other is on Fukui functions and their difference $\Delta f^- f^+$ [8]. Finally a comparative study has also been made to compare the measuring power of these quantum chemical parameters.

MATERIALS AND METHOD

The study materials of this paper are thiocyanate of Ni(II), Cu(II), Zn(II), Fe(II) and Co(II), and their complexes with $Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$. These compounds, which are study material of this paper, are listed in Table-1. These compounds have been prepared and studied by us in our earlier work [9]. For present study the molecular modeling and geometry optimization [10, 11] of all the compounds were carried out with CAChe Pro software by applying semiempirical PM3 metho0ds [12, 13]. The atomic softness and Fukui function of every atom of all the derivatives has been done by softness calculator developed by us using the equations given below.

The softness of an atom in a molecule was described by Klopman [7] and modified by Singh et. al.[14]. The Klopman equation is given by:

$$E_m^{\ddagger} = IP_m - a^2\ IP_m - EA_m\ - \\ -\left[\frac{\chi_r\ C_r^{m\ 2}}{R_r}\right]\left(1-\frac{1}{\in}\right)\left[q_r + 2b^2\chi_r\ C_r^{m\ 2}\right] \qquad (1)$$

$$E_n^{\ddagger} = IP_n - b^2\ IP_n - EA_n\ - \\ -\left[\frac{\chi_s\ C_s^{n\ 2}}{R_s}\right]\left(1-\frac{1}{\in}\right)\left[q_s - 2b^2\chi_s\ C_s^{n\ 2}\right] \qquad (2)$$

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where, $E^{\ddagger}_n$ is softness of Lewis acid, $E^{\ddagger}_m$ is softness of Lewis base, IP is ionization potential of atom, EA is electron affinity of atom, $\in$ is dielectric constant of the medium in which reaction is carried out [15], R is radius of atom and q is charge of atom, C is electron density, $\chi = q - (q - 1)(k)^{3/2}$ and k = 0.75, a and b are variational parameter defined as $a^2 + b^2 = 1$. The $\Delta E^{\ddagger}_{nm}$ values derived from the difference in softness values of nucleophiles and electrophiles. Higher is the –ve value of $\Delta E^{\ddagger}_{nm}$ greater will the stability of complex [16].

$$\Delta E^{\ddagger}_{nm} = \left| E^{\ddagger}_n - E^{\ddagger}_m \right| \qquad (3)$$

The Fukui function [17] of an atom in a molecule is evaluated by Eq.-4 and 5.

$$f^- = q(N) - q(N - 1) \qquad (4)$$

$$f^+ = q(N + 1) - q(N) \qquad (5)$$

where, f^- is fukui function values of Lewis acid, f^+ is fukui function values of Lewis base, q is partial charge of the atom in a molecule, N is total number of electrons of a molecule. The metal-ligand interaction has also been examined in terms of Fukui function values of the Lewis acids and Lewis bases. For drawing the relative stability of metal ligand bond, the difference in Fukui function values $\Delta f^- f^+$ has been evaluated which is represented by

$$\Delta f^- f^+ = \left| f^- - f^+ \right| \qquad (6)$$

RESULTS AND DISCUSSION

Cobaltocenylene bis mercury (II) thiocyanate (compound I) and cobaltocenylene bis mercury (II) selenocyanate (compound II) co-ordinate to metal ions through their *N* atoms. In order to study the matter of describing the stability of bond formed between a nucleophile and electrophile three principles have been prominently used, one is based on softness parameters and the other is on Fukui function. The $\Delta E^{\ddagger}_{nm}$ values derived from the difference in softness values of nucleophiles and Lewis acids have widely been used for describing relative stability. The higher is the value greater is the stability. The $\Delta f^- f^+$ values derived from the difference in Fukui function of Lewis bases and Lewis acids have widely been used for describing relative stability. The negative higher is the value greater is the stability.

Effective atomic softness and stability of metal-ligand bond

It is well established that the stability of the compound formed between metal halide and ligand, depends upon the values of deference between softness values $E^{\ddagger}_n$ of metal halide and softness values $E^{\ddagger}_m$ of ligand, $\Delta E^{\ddagger}_{nm}$ represents the difference. The higher is the value of $\Delta E^{\ddagger}_{nm}$ greater is the stability of compound [7, 14]. The softness $E^{\ddagger}_n$ of metal (Fe, Co, Ni, Cu, Zn) in their halides and the softness $E^{\ddagger}_m$ at nitrogen atom in cobaltocenylene bis mercury (II) thiocyanate derivatives for Fe, Co, Ni, Cu and Zn are presented in table 2. The $\Delta E^{\ddagger}_{nm}$ values derived as per Eq.-3 have also been derived and are included in the same. At last we find that in thiocyanate derivatives, the stability order of $\Delta E^{\ddagger}_{nm}$ value in respect of metal atom is

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Ni > Cu > Co > Fe > Zn

The softness $E^{\ddagger}_{n}$ of metal (Fe, Co, Ni, Cu, Zn) in their halides and the softness $E^{\ddagger}_{m}$ at nitrogen atom in cobaltocenylene bis mercury (II) selenocyanate derivatives for Fe, Co, Ni, Cu and Zn are presented table 3. The $\Delta E^{\ddagger}_{nm}$ values derived as per Eq.-3 have been also derived and are included in the same. In selenocyanate derivatives, the stability order of $\Delta E^{\ddagger}_{nm}$ values in respect of metal atom is

Ni > Fe > Co > Cu > Zn

$\Delta E^{\ddagger}_{nm}$ values of complexes of $Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$ with thiocyanate and selenocyanate of Ni(II) are higher than thiocyanate and selenocyanate of Cu(II), Zn(II), Fe(II) and Co(II) hence former complexes have higher stability than later.

Fukui function and stability of metal ligand bond

Various global and local quantities used to analyze the chemical reactivity have been discussed in the literature [18]. It is well known that chemical reactivity of any molecular system depends on the surrounding solvent medium [19]. Fukui function is one of the widely used local density functional descriptors to model chemical reactivity and site selectivity [20, 21]. The atom with the highest fukui function is highly reactive compared to the other atoms in the molecule. For drawing the relative stability of the metal-ligand bond, the difference in Fukui function $\Delta f^{-}f^{+}$ values has also been used. The Fukui function f^{-} of metal (Fe, Co, Ni, Cu, Zn) in their halides and the Fukui function f^{+} at nitrogen atom in cobaltocenylene bis mercury (II) thiocyanate derivatives for Fe, Co, Ni, Cu and Zn are presented in table 4. The $\Delta f^{-}f^{+}$ values derived as per Eq.-6 have also been derived and are included in the same. At last we find that in thiocyanate derivatives, the stability order of the $\Delta f^{-}f^{+}$ values in respect of metal is

Ni > Cu > Co > Fe > Zn

The Fukui function f^{-} of metal (Fe, Co, Ni, Cu, Zn) in their halides and Fukui function f^{+} at nitrogen atom in cobaltocenylene bis mercury (II) selenocyanate derivatives for Fe, Co, Ni, Cu and Zn are presented in table 5. The $\Delta f^{-}f^{+}$ values derived as per Eq.-6 have been also derived and are included in the same. In selenocyanate derivatives, the stability order of the $\Delta f^{-}f^{+}$ values in respect of metal atom is

Ni > Fe > Co > Cu > Zn

$\Delta f^{-}f^{+}$ values of complexes of $Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$ with thiocyanate and selenocyanate of Ni(II) are higher than thiocyanate and selenocyanate of Cu(II), Zn(II), Fe(II) and Co(II) hence former complexes have higher stability than later.

CONCLUSION

It is evident from the present investigation that

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1. □ $E^{\ddagger}_{nm}$ values of complexes of $Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$ with thiocyanate and selenocyanate of Ni(II) are higher than thiocyanate and selenocyanate of Cu(II), Zn(II), Fe(II) and Co(II) hence former complexes have higher stability than later.

2. $\Delta f^- f^+$ values of complexes of $Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$ with thiocyanate and selenocyanate of Ni(II) are also higher than thiocyanate and selenocyanate of Cu(II), Zn(II), Fe(II) and Co(II) hence former complexes have higher stability than later.

3. Comparative study of $\Delta E^{\ddagger}_{nm}$ and $\Delta f^- f^+$ values of complexes of $Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$ with thiocyanate and selenocyanate of Ni(II), Cu(II), Zn(II), Fe(II) and Co(II) has shown that thiocyanate and selenocyanate of Ni(II) formed most stable complexes with $Co(C_5H_4)_2$-$(HgSCN)_2$ and $Co(C_5H_4)_2$-$(HgSeCN)_2$ with are higher than thiocyanate and selenocyanate of Cu(II), Zn(II), Fe(II).

4. The present research was a theoretical basis for the concepts of chemical reactivity, selectivity and stability of molecular complexes and boosts a phenomenal advancement in theoretical inorganic chemistry. So this study will provide a gateway to save the time, money and efforts in search of desire complex compounds of synthetic importance in synthetic inorganic and inorganic medicinal chemistry.

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Table 1: List of compounds

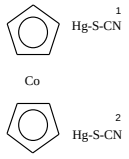
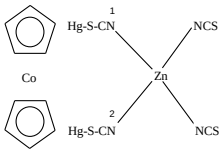
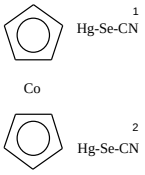
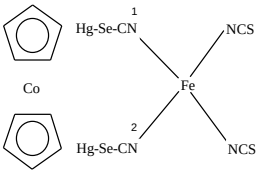
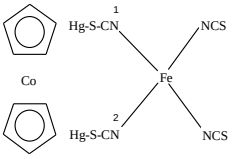
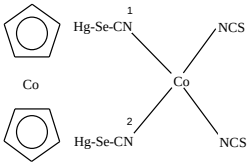
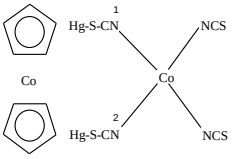
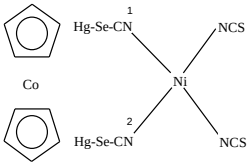
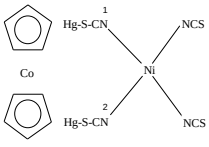
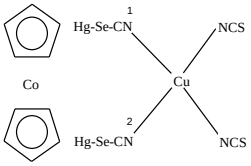
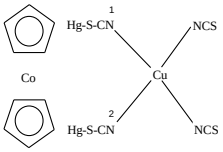
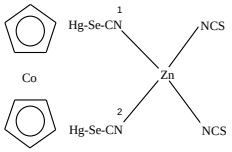
S.N.	Compound	S.N	Compound
1	 **$Co(C_5H_4)_2$-(Hg-S-CN)$_2$** Cobaltocenylene bis mercury (II) thiocyanate	7	 **$Co(C_5H_4)_2$-(Hg-S-CN)$_2$. Zn(NCS)$_2$** Complex of compound I with zinc thiocyanate
2	 **$Co(C_5H_4)_2$-(Hg-Se-CN)$_2$** Cobaltocenylene bis mercury (II) selenocyanate	8	 **$Co(C_5H_4)_2$-(Hg-Se-CN)$_2$. Fe(NCS)$_2$** Complex of compound II with iron selenocyanate
3	 **$Co(C_5H_4)_2$-(Hg-S-CN)$_2$. Fe(NCS)$_2$** Complex of compound I with iron thiocyanate	9	 **$Co(C_5H_4)_2$-(Hg-Se-CN)$_2$. Co(NCS)$_2$** Complex of compound II with cobalt selenocyanate
4	 **$Co(C_5H_4)_2$-(Hg-S-CN)$_2$ .Co(NCS)$_2$** Complex of compound I with cobalt thiocyanate	10	 **$Co(C_5H_4)_2$-(Hg-Se-CN)$_2$. Ni (NCS)$_2$** Complex of compound II with nickel selenocyanate
5	 **$Co(C_5H_4)_2$-(Hg S CN)$_2$. Ni(NCS)$_2$** Complex of compound I with nickel thiocyanate	11	 **$Co(C_5H_4)_2$-(Hg-Se-CN)$_2$. Cu(NCS)$_2$** Complex of compound II with copper selenocyanate
6	 **$Co(C_5H_4)_2$-(Hg S CN)$_2$. Cu(NCS)$_2$** Complex of compound I with copper thiocyanate	12	 **$Co(C_5H_4)_2$-(Hg-Se-CN)$_2$. Zn(NCS)$_2$** Complex of compound II with zink selenocyanate

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Table 2: $\Delta E^{\ddagger}_{nm}$ values derived from $E^{\ddagger}_{m}$ of nitrogen atom of cobaltocene derivatives and $E^{\ddagger}_{n}$ of electrophile (thiocyanate)

Compd.	Atom	$E^{\ddagger}_{m}$	Fe atom $E^{\ddagger}_{n}$ = 322.9577	Co atom $E^{\ddagger}_{n}$ = 511.5822	Ni atom $E^{\ddagger}_{n}$ = 485.5022	Cu atom $E^{\ddagger}_{n}$ = 1330.395	Zn atom $E^{\ddagger}_{n}$ = 7.51189
			$\Delta E^{\ddagger}_{nm}$	$\Delta E^{\ddagger}_{nm}$	$\Delta E^{\ddagger}_{nm}$	$\Delta E^{\ddagger}_{nm}$	$\Delta E^{\ddagger}_{nm}$
III	N_1	- 19.9114	342.8691	531.4936	505.4136	1350.3064	27.42329
	N_2	- 14.9447	337.9024	526.5269	500.4469	1345.3397	22.45659
IV	N_1	- 18.1563	341.114	529.7385	503.65383	1348.5513	25.66819
	N_2	- 22.1613	345.119	533.7435	507.6635	1352.5563	29.67319
V	N_1	- 34.2658	357.2235	545.848	519.768	1364.6608	41.77769
	N_2	- 31.5318	354.4895	543.114	517.034	1361.9268	39.04369
VI	N_1	- 18.6068	341.5645	530.189	504.109	1349.0018	26.11869
	N_2	- 24.322	347.2797	535.9042	509.8242	1354.717	31.83389
VII	N_1	- 13.6952	336.6529	525.2774	499.1974	1344.0902	21.20709
	N_2	- 11.1958	334.1535	522.778	496.698	1341.5908	18.70769

$E^{\ddagger}_{n}$ is softness of Lewis acid, $E^{\ddagger}_{m}$ is softness of Lewis base and $\Delta E^{\ddagger}_{nm}$ is their difference

Table 3: $\Delta E^{\ddagger}_{nm}$ values derived from $E^{\ddagger}_{m}$ of nitrogen atom of cobaltocene derivatives and $E^{\ddagger}_{n}$ of electrophile (selenocyanate)

Compd.	Atom	$E^{\ddagger}_{m}$	Fe atom $E^{\ddagger}_{n}$= 331.617	Co atom $E^{\ddagger}_{n}$= 551.634	Ni atom $E^{\ddagger}_{n}$= 535.5858	Cu atom $E^{\ddagger}_{n}$= 1353.74	Zn atom $E^{\ddagger}_{n}$= 7.978725
			$\Delta E^{\ddagger}_{nm}$	$\Delta E^{\ddagger}_{nm}$	$\Delta E^{\ddagger}_{nm}$	$\Delta E^{\ddagger}_{nm}$	$\Delta E^{\ddagger}_{nm}$
III	N_1	- 20.6437	352.2607	572.2777	556.2295	1374.3837	28.622125
	N_2	- 20.3129	315.9299	571.9469	555.8987	1374.0529	28.291625
IV	N_1	- 18.0364	349.6534	569.6704	553.6222	1371.7764	26.015125
	N_2	- 21.1294	352.7464	572.7634	556.7152	1374.8694	29.108125
V	N_1	- 33.5819	365.1989	585.2159	569.1677	1387.3219	41.560625
	N_2	- 29.2107	360.8277	580.8447	564.7965	1382.9507	37.189425
VI	N_1	- 15.0539	346.6709	566.6879	550.6397	1368.7939	23.032625
	N_2	- 13.9326	345.5496	565.5666	549.5184	1367.6726	21.911325
VII	N_1	- 12.3089	343.9259	563.9429	547.8947	1366.0489	20.287625
	N_2	- 9.6931	341.3101	561.3271	545.2789	1363.4331	17.671825

$E^{\ddagger}_{n}$ is softness of Lewis acid, $E^{\ddagger}_{m}$ is softness of Lewis base and $\Delta E^{\ddagger}_{nm}$ is their difference

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Table 4: $\Delta f^- f^+$ values derived from f^+ of nitrogen atom of cobaltocene derivatives and f^- of electrophile (thiocyanate)

Compd.	Atom	f^+	Fe atom f^- = 0.274142	Co atom f^- = 0.29043	Ni atom f^- = 0.252014	Cu atom f^- = 0.354421	Zn atom f^- = 0.05870
			$\Delta f^- f^+$	$\Delta f^- f^+$	$\Delta f^- f^+$	$\Delta f^- f^+$	$\Delta f^- f^+$
III	N_1	0.765371	- 0.491229	- 0.474941	- 0.513357	- 0.41095	- 0.706671
	N_2	0.729857	- 0.455715	- 0.439427	- 0.477843	- 0.375436	- 0.671157
IV	N_1	0.758157	- 0.484015	- 0.467727	- 0.506143	- 0.403736	- 0.699457
	N_2	0.785329	- 0.511187	- 0.494899	- 0.533315	- 0.430908	- 0.726629
V	N_1	0.866443	- 0.592301	- 0.576013	- 0.614429	- 0.512022	- 0.807743
	N_2	0.850871	- 0.576729	- 0.560441	- 0.598857	- 0.496450	- 0.792171
VI	N_1	0.762243	- 0.488101	- 0.471813	- 0.510229	- 0.407822	- 0.703543
	N_2	0.800243	- 0.526101	- 0.509813	- 0.548229	- 0.445822	- 0.741543
VII	N_1	0.725886	- 0.451744	- 0.435456	- 0.473872	- 0.371465	- 0.667186
	N_2	0.706514	- 0.432372	- 0.416084	- 0.45450	- 0.352093	- 0.647814

f^- is fukui function values of Lewis acid, f^+ is fukui function values of Lewis base and is $\Delta f^- f^+$ their difference

Table 5: $\Delta f^- f^+$ values derived from f^+ of nitrogen atom of cobaltocene derivatives and f^- of electrophile (selenocyanate)

Compd.	Atom	f^+	Fe atom f^- = 0.277212	Co atom f^- = 0.291478	Ni atom f^- = 0.261311	Cu atom f^- = 0.359076	Zn atom f^- = 0.05980
			$\Delta f^- f^+$	$\Delta f^- f^+$	$\Delta f^- f^+$	$\Delta f^- f^+$	$\Delta f^- f^+$
III	N_1	0.77350	- 0.496288	- 0.482022	- 0.512189	- 0.414424	- 0.71370
	N_2	0.771257	- 0.494045	- 0.479772	- 0.509939	- 0.412174	- 0.71145
IV	N_1	0.757486	- 0.480274	- 0.466008	- 0.496175	- 0.39841	- 0.697686
	N_2	0.778657	- 0.501445	- 0.487179	- 0.517346	- 0.419581	- 0.718857
V	N_1	0.869671	- 0.592459	- 0.578193	- 0.60836	- 0.510595	- 0.809871
	N_2	0.844614	- 0.567402	- 0.553136	- 0.583303	- 0.485538	- 0.784814
VI	N_1	0.736243	- 0.459031	- 0.444765	- 0.474932	- 0.377167	- 0.676443
	N_2	0.72790	- 0.450688	- 0.436422	- 0.466589	- 0.368824	- 0.66810
VII	N_1	0.723614	- 0.446402	- 0.432136	- 0.462303	- 0.364538	- 0.663814
	N_2	0.703086	- 0.425874	- 0.41160	- 0.44177	- 0.34401	- 0.643286

f^- is fukui function values of Lewis acid, f^+ is fukui function values of Lewis base and is $\Delta f^- f^+$ their difference

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