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## Electronic Structure Investigation of Octahedral Complex and Nano ring by NBO Analysis: An EPR Study

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### ABSTRACT

To calculation non-bonded interaction of the  $[\text{CoCl}_6]^{3-}$  complex embedded in nano ring, we focus on the single wall boron-nitride  $\text{B}_{18}\text{N}_{18}$  nano ring. Thus, the geometry of  $\text{B}_{18}\text{N}_{18}$  nano ring has been optimized by B3LYP method with EPR-II (Electron paramagnetic resonance) basis set and geometry of the  $[\text{CoCl}_6]^{3-}$  complex has been optimized at B3LYP method with Aldrich's VTZ basis set and Stuttgart RSC 1997 Effective Core Potential. Also NBO (Natural Bond Orbital) analysis such as LUMO (lowest unoccupied molecular orbital) and the HOMO (highest occupied molecular orbital) for the lowest energy have been derived to estimate the structural stability and band gaps, Natural atomic orbitals, Fermi energy, absorption energy of the  $\text{B}_{18}\text{N}_{18}-[\text{CoCl}_6]^{3-}$  nano system can be distinguished based on these NBO data. Total atomic charges, Total atomic spin densities, Isotropic Fermi Contact Coupling and geometrical quantities of different loops of  $\text{B}_{18}\text{N}_{18}$  nano ring inclusive  $[\text{CoCl}_6]^{3-}$  embedded in the nano ring at the level of B3LYP theory and EPR-II basis set for B, N, Cl atoms and Aldrich's VTZ basis set and Stuttgart RSC 1997 Effective Core Potential for Co (III) have been calculated by Gaussian quantum chemistry package.

**Keywords:** Density functional theory; EPR-II; HOMO; LUMO; Nuclear independent chemical shift; NBO.

## 1. INTRODUCTION

To introduce physical properties of  $\text{B}_{24}\text{C}_{12}\text{N}_{24}$  molecule [1] and the  $\text{B}_{12}\text{N}_{12}$ ,  $\text{B}_{16}\text{N}_{16}$  and  $\text{B}_{28}\text{N}_{28}$  molecules, the experimental synthesis and various spectrometers are needed for their structural stabilities confirmation [2-4]. The schematic of  $\text{B}_{18}\text{N}_{18}$  is displayed in the Figure 1. In present work we presentation the non-bonded interaction of the  $[\text{CoCl}_6]^{3-}$  embedded in  $\text{B}_{18}\text{N}_{18}$  nano ring. The basically purpose of this investigation was the study of the electromagnetic interactions within the

$\text{B}_{18}\text{N}_{18}-[\text{CoCl}_6]^{3-}$  nano system. In chemistry, octahedral geometry describes the shape of compounds where six atoms or groups of atoms or ligands are symmetrically arranged around a central atom, defining the vertices of an octahedron compound. For further evaluation about electromagnetic interactions, stability structure of  $[\text{CoCl}_6]^{3-}$  complex under the different loops of nano ring have been determined. For further structural information, the lowest unoccupied molecular orbital and

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the highest occupied molecular orbital differences, namely band gaps and the hybrids on atom have been reported to explore the ability of the  $[\text{CoCl}_6]^{3-}$  to create a stable  $\text{B}_{18}\text{N}_{18}$ - $[\text{CoCl}_6]^{3-}$  nano system.

## 2. COMPUTATIONAL DETAILS

To determination electromagnetic interactions of the  $[\text{CoCl}_6]^{3-}$  complex including octahedral symmetric Co (III) coordination compounds and six  $\pi$ -acceptor ligands, the geometry of the  $[\text{CoCl}_6]^{3-}$  have been optimized at B3LYP method with Aldrich's VTZ basis set and Stuttgart RSC 1997 Effective Core Potential. The geometry of the  $\text{B}_{18}\text{N}_{18}$  nano ring and  $[\text{CoCl}_6]^{3-}$  complexes have been optimized at B3LYP method with EPR-II (Electron paramagnetic resonance) ba-

sis set using ab initio GAUSSIAN quantum chemical package. Vibrational frequencies have been calculated at B3LYP method with EPR-II basis set to analyze the thermochemical functions including enthalpies and Gibbs free energies [5]. The natural bond orbital (NBO) analysis [6, 7] has also been applied to study the intermolecular orbital interactions in the complexes [8]. Also, NBO data and  $\Delta E$  in  $[\text{CoCl}_6]^{3-}$  complex in different loops of the  $\text{B}_{18}\text{N}_{18}$  nano ring have been calculated.

## 3. RESULTS AND DISCUSSION

The geometry of the  $[\text{CoCl}_6]^{3-}$  complex including octahedral symmetric Co (III) coordination compounds and six  $\pi$ -donor ligands have been optimized at B3L-

**Table 1:** Optimized parameters of octahedral symmetric Co (III) coordination compounds and six  $\pi$ -donor ligands.

Compound	Bond ID	Bond lengths	Bond angles
$[\text{CoCl}_6]^{3-}$	Co(1)- Cl (2)	2.048	-
	Co(1)- Cl (3)	1.924	-
	Co(1)- Cl (4)	2.049	-
	Co(1)- Cl (5)	2.049	-
	Co(1)- Cl (6)	1.924	-
	Co(1)- Cl (7)	2.048	-
	Cl (2)-Co(1)- Cl (3)	-	90.000
	Cl (2)-Co(1)- Cl (4)	-	90.001
	Cl (2)-Co(1)- Cl (5)	-	89.999
	Cl (2)-Co(1)- Cl (6)	-	90.000
	Cl (2)-Co(1)- Cl (7)	-	179.998
	Cl (3)-Co(1)- Cl (4)	-	90.002
	Cl (3)-Co(1)- Cl (5)	-	89.998
	Cl (3)-Co(1)- Cl (6)	-	179.997
	Cl (3)-Co(1)- Cl (7)	-	90.000
	Cl (4)-Co(1)- Cl (5)	-	180.000
	Cl (4)-Co(1)- Cl (6)	-	90.002
	Cl (4)-Co(1)- Cl (7)	-	90.001
	Cl (5)-Co(1)- Cl (6)	-	89.998
Cl (5)-Co(1)- Cl (7)	-	89.999	
Cl (6)-Co(1)- Cl (7)	-	90.000	

\* See Figure 1 for more details.

**Table 2:** Natural atomic orbitals of  $[\text{CoCl}_6]^{3-}$  complex with six  $\pi$ -donor ligands.

Natural atomic orbital			
Atom	$[\text{CoCl}_6]^{3-}$		
	Atomic Orbital	Energy	Occ.
Co <sup>3+</sup> (1)	4s	1.62632	0.20611
	3dz <sup>2</sup>	0.38196	1.2198
	3dxy	0.35387	1.09592
	3dyz	0.35351	1.08186
	3dx <sup>2</sup> y <sup>2</sup>	0.32882	1.27044
	3dxz	0.23313	1.99444
Cl (2)	2s	-1.29779	1.98981
	2px	0.3623	1.99933
	2py	0.3626	1.97802
	2 pz	0.33289	1.89911
Cl (3)	2s	-1.3661	1.98486
	2px	0.30109	1.89182
	2py	0.3403	1.96424
	2 pz	0.33939	1.99917
Cl (4)	2s	-1.32367	1.98987
	2px	0.3385	1.98557
	2py	0.30771	1.87786
	2 pz	0.33891	1.98182
Cl (5)	2s	-1.32277	1.98986
	2px	0.33934	1.98561
	2py	0.3085	1.87798
	2 pz	0.33975	1.98184
Cl (6)	2s	-1.36678	1.98487
	2px	0.30051	1.89217
	2py	0.33971	1.96467
	2 pz	0.33886	1.99918
Cl (7)	2s	-1.29779	1.98981
	2px	0.3623	1.99933
	2py	0.3626	1.97802
	2 pz	0.33289	1.89911

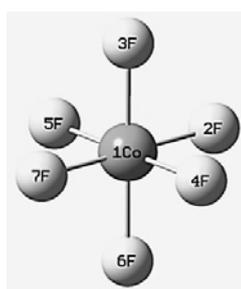
YP method with Aldrich's VTZ basis set and Stuttgart RSC 1997 Effective Core Potential. Optimized parameters of  $[\text{CoCl}_6]^{3-}$  such as bond lengths and bond angles have been reported in Table 1. We can view the Co-Cl (3) and Co-Cl (6) bond lengths are less than other bond lengths, because the octahedral symmet-

ric Co (III) coordination compounds and six  $\pi$ -donor ligands are High-spin  $d^6$  electronic configuration ( $S = 2$ ) exhibit the Elongation Jahn-Teller distortion [9].

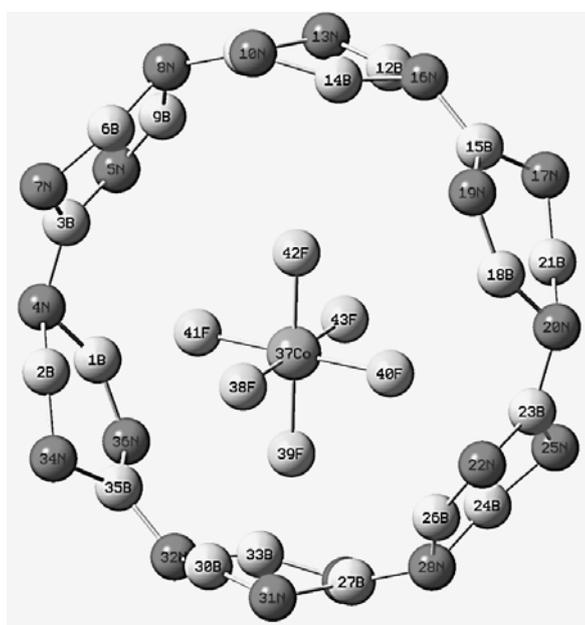
In accordance with the occupancy values of metal Co (III) in Table 2, it was elaborated that  $3d_{xz}$  orbital consists of two electrons and has the least value of

energy. The other d orbitals are single and 4S orbital has no electron.

Also, in accordance with the occupancy and energy values for 6 ligands of  $\pi$ -donor in atoms Cl (2), Cl (7) it was demonstrated that three non bonding electron pairs of Cl are in 2s and two 2p orbitals that have higher energy levels. For instance, in Cl (2),  $2p_z$  is single and has a lower energy level;  $2p_x$  and  $2p_y$  that have higher energy levels and are nearer to the metal d orbitals in energy, interfere to make molecular  $\pi$  orbitals and 2s orbitals interfere to make the  $\sigma$  molecular orbitals. In addition, related to Table 2 data, atoms Cl (4) – Cl (5), Cl (3) – Cl (6) and Cl (2) – Cl (7) that are in one direction related to Co (III), are the same in occupancy and energy levels (Figure 1-a). For further to determination non-bonded interaction of the  $[\text{CoCl}_6]^{3-}$  complex embedded in nano ring, we focus on the single



(a)



(b)

**Figure 1:** The optimized geometrical structure of the a)  $[\text{CoCl}_6]^{3-}$  complex and b)  $\text{B}_{18}\text{N}_{18}-[\text{CoCl}_6]^{3-}$  nano system at the level of B3LYP/EPR-III theory.

wall boron-nitride an armchair  $\text{B}_{18}\text{N}_{18}$  nanotube with chirality  $n = m = 6$ , and the schematic of optimized structure of the  $\text{B}_{18}\text{N}_{18}-[\text{CoCl}_6]^{3-}$  system have been displayed in Figure 1.

DFT (Density functional theory) calculations, as well as hybrid methods (B3LYP) for  $\text{B}_{18}\text{N}_{18}-[\text{CoCl}_6]^{3-}$  nano system have been carried out to study the non-bonded interaction. The geometry of  $\text{B}_{18}\text{N}_{18}$  nano ring has been optimized by B3LYP method with EPR-II basis set. The electromagnetic interactions of the  $[\text{CoCl}_6]^{3-}$  complex embedded in nano ring have been investigated at B3LYP in different loops of the  $\text{B}_{18}\text{N}_{18}$  nano ring. According to the frequency calculation at the level of B3LYP/EPR-II theory, obtaining thermo chemical functions such as  $\Delta G = -67.7929$  kcal/mol and  $\Delta H = -124.4012$  kcal/mol confirmed the structural stability of  $\text{B}_{18}\text{N}_{18}$  nano ring. The geometry of  $\text{B}_{18}\text{N}_{18}$  nano ring and  $[\text{CoCl}_6]^{3-}$  have been optimized by B3LYP method with EPR-II basis set for B, N, Cl atoms and Aldrich's VTZ basis set and Stuttgart RSC 1997 ECP (Effective core potential) for Co (III). So it is notable that the obtained energy of mentioned basis set and ECP for  $\text{B}_{18}\text{N}_{18}$  nano ring and  $[\text{CoCl}_6]^{3-}$  were  $-1434.1167014$  and  $-744.7157743$ , (Hartree) respectively. To investigate the non-bonded interaction on  $[\text{CoCl}_6]^{3-}$  with six different loops of  $\text{B}_{18}\text{N}_{18}$  nano ring, first the five hexagon loops have been frozen and the electrostatic interaction of  $[\text{CoCl}_6]^{3-}$  with the one remained active loop have been considered. Other loops have been examined one by one in the same way and the changes of all the following calculated quantities have been explored. In accordance with Figure (1-b), it is demonstrated that atoms Cl (42) and Cl (39) are exactly in central direction of loop 3, loop 6. For further structural information, the lowest unoccupied molecular orbital and the highest occupied molecular orbital differences, namely band gaps have been reported to explore the ability of the suitable  $[\text{CoCl}_6]^{3-}$  forms to create a stable  $\text{B}_{18}\text{N}_{18}-[\text{CoCl}_6]^{3-}$  system. So, quantities values such as the relative energies ( $\Delta E$ ), radial coordinate of dipole moment ( $r$ ), band gaps, Dipole orientation and NICS (Nuclear independent chemical shift) of  $\text{B}_{18}\text{N}_{18}-[\text{CoCl}_6]^{3-}$  system have been reported in Table 3.

Natural bond orbital (NBO) analysis of the  $[\text{CoCl}_6]^{3-}$  complex embedded in nano ring, such as ionization

**Table 3:** Relative energies ( $\Delta E$ ), radial coordinate of dipole moment ( $r$ ) and band gap of  $[\text{CoCl}_6]^{3-}$  under different loops of  $B_{18}N_{18}$  at EPR-II basis set for B,N,F atoms and Def2-TZVP basis set and Stuttgart RSC 1997 Effective Core Potential for Co (III).

Compound	Basis sets for $\text{Co}^{3+}$					
	Def2-TZVP, Stuttgart RSC 1997 ECP					
	band gap (a.u.)	$\Delta E$ (Hartree)	NICS	Dipole moment (Debye)	Dipole orientation	
$\theta$					$\phi$	
$[\text{CoCl}_6]^{3-}$	0.18716	-744.7157	-	0.0085	90	0
$B_{18}N_{18}$	0.16409	-1434.1167	-	0.0000	90	-
loop 1- $[\text{CoCl}_6]^{3-}$	0.00563	-983.4365	-9.8094	14.999	90	58.864
loop 2- $[\text{CoCl}_6]^{3-}$	0.04882	-983.5047	-9.8196	8.5251	90	136.0460
loop 3- $[\text{CoCl}_6]^{3-}$	0.05779	-983.4791	-9.8051	8.1247	90	165.6071
loop 4- $[\text{CoCl}_6]^{3-}$	0.03409	-983.4757	-9.8094	7.9953	90	113.1564
loop 5- $[\text{CoCl}_6]^{3-}$	0.04873	-983.5047	-9.8196	8.5441	90	44.02423
loop 6- $[\text{CoCl}_6]^{3-}$	0.15495	-983.4417	-9.8051	15.7468	90	0.540243

energy ( $I_E$ ); that the ionization energy ( $I_E$ ) of an atom or molecule refers to the energy required to remove a single electron from a single atom or molecule, electron affinity energy ( $E_{ca}$ ); that the electron affinity of an atom or molecule is defined as the amount of energy released when an electron is added to a neutral atom or molecule in the gaseous state to form a negative ion, energy gap or band gap ( $E_g$ ); that the band gap generally refers to the energy difference (in electron volts) between the top of the valence band and the bottom of the conduction band in insulators and semiconductors

have been reported in Table 4. This is equivalent to the energy required to free an outer shell electron from its orbit about the nucleus to become a mobile charge carrier, able to move freely within the solid material, so the band gap is a major factor determining the electrical conductivity of a solid. Substances with large band gaps are generally insulators, those with smaller band gaps are semiconductors, while conductors either have very small band gaps or none, because the valence and conduction bands overlap and Fermi energy ( $E_F$ ); that the Fermi energy also called electrochemical poten-

**Table 4:** Natural bond orbital (NBO) analysis of the  $[\text{CoCl}_6]^{3-}$  complex embedded in  $B_{18}N_{18}$  nano ring.

Compound	Basis sets for $\text{Co}^{3+}$					
	Aldrich's VTZ, Stuttgart RSC 1997 ECP					
	LUMO (ev)	HOMO(ev)	IE (ev)	$E_{ca}$ (ev)	$E_g$ (ev)	$E_F$ (ev)
$[\text{CoCl}_6]^{3-}$	10.73	5.64	-5.64	-10.73	5.09	8.185
$B_{18}N_{18}$	-3.4	-7.86	7.86	3.4	4.46	-5.63
1,2,4,34,35,36	5.46	5.31	-5.31	-5.46	0.15	5.385
3,5,6,7,8,9	5.84	4.52	-4.52	-5.84	1.32	5.18
10,11,12,13,14,16	5.86	4.29	-4.29	-5.86	1.57	5.075
15,17,18,19,20,21	5.46	4.53	-4.53	-5.46	0.93	4.995
22,23,24,25,26,28	5.85	4.52	-4.52	-5.85	1.33	5.185
27,29,30,31,32,33	7.71	3.49	-3.49	-7.71	4.22	5.6

**Table 5:** Different quantities of  $[\text{CoCl}_6]^{3-}$  under six different loops of  $\text{B}_{18}\text{N}_{18}$  nano system at the level of B3LYP theory and EPR-II basis set for B, N, Cl atoms and Aldrich's VTZ basis set and Stuttgart RSC 1997 Effective Core Potential for Co (III).

Different quantities of $[\text{CoCl}_6]^{3-}$ under different loops of $\text{B}_{18}\text{N}_{18}$ nano ring												
Total atomic charges												
Total atomic spin densities												
Isotropic Fermi Contact Coupling ( $10(-4) \text{ cm}^{-1}$ )												
loop 1- $[\text{CoCl}_6]^{3-}$												
B (1)	B (2)	N (4)	N (34)	B (35)	N (36)	Co (37)	Cl (38)	Cl (39)	Cl (40)	Cl (41)	Cl (42)	Cl (43)
-0.056	-0.056	-0.279	-0.106	-0.173	-0.106	1.504	-0.738	-0.538	-0.672	-0.467	-0.568	-0.738
0.109	0.109	0.222	0.025	0.658	0.025	2.548	0.112	-0.043	-0.030	0.204	-0.053	0.112
13.132	13.132	4.059	7.976	48.937	7.976	-0.035	16.769	10.678	7.966	16.731	8.412	16.769
Loop 2- $[\text{CoCl}_6]^{3-}$												
B (3)	B (5)	N (6)	N (7)	B (8)	N (9)	Co (37)	Cl (38)	Cl (39)	Cl (40)	Cl (41)	Cl (42)	Cl (43)
-0.048	-0.063	-0.013	-0.063	-0.206	-0.013	1.604	-0.741	-0.704	-0.750	-0.579	-0.677	-0.741
0.158	-0.013	0.027	-0.013	-0.005	0.027	3.256	0.150	0.085	0.104	-0.022	0.092	0.150
8.748	1.802	2.404	1.802	-0.271	2.404	-0.043	17.886	18.356	18.634	21.070	17.922	17.886
Loop 3- $[\text{CoCl}_6]^{3-}$												
B (10)	B (11)	N (12)	N (13)	B (14)	N (16)	Co (37)	Cl (38)	Cl (39)	Cl (40)	Cl (41)	Cl (42)	Cl (43)
-0.094	-0.039	-0.009	-0.094	-0.009	-0.215	1.592	-0.741	-0.675	-0.761	-0.763	-0.446	-0.741
0.010	-0.146	-0.018	0.010	-0.018	0.000	3.332	0.151	0.150	0.129	0.130	0.118	0.151
-1.325	-7.745	-2.249	-1.325	-2.249	-0.037	-0.044	16.980	21.832	17.440	18.511	22.132	16.980
Loop 4- $[\text{CoCl}_6]^{3-}$												
B (15)	B (17)	N (18)	N (19)	B (20)	N (21)	Co (37)	Cl (38)	Cl (39)	Cl (40)	Cl (41)	Cl (42)	Cl (43)
-0.028	-0.066	-0.020	-0.066	-0.211	-0.020	1.609	-0.778	-0.690	-0.541	-0.724	-0.681	-0.778
0.264	-0.024	0.066	-0.024	-0.132	0.066	3.280	0.102	0.114	-0.054	0.124	0.113	0.102
23.712	2.795	4.713	2.795	1.599	4.713	-0.044	18.263	20.625	7.814	18.297	21.969	18.263
Loop 5- $[\text{CoCl}_6]^{3-}$												
B (22)	B (23)	N (24)	N (25)	B (26)	N (28)	Co (37)	Cl (38)	Cl (39)	Cl (40)	Cl (41)	Cl (42)	Cl (43)
-0.063	-0.048	-0.013	-0.063	-0.013	-0.206	1.604	-0.741	-0.676	-0.579	-0.750	-0.704	-0.741
-0.013	0.159	0.028	-0.013	0.028	-0.005	3.256	0.150	0.092	-0.022	0.104	0.085	0.150
1.815	8.840	2.427	1.815	2.427	-0.268	-0.043	17.889	17.894	21.096	18.627	18.322	17.889
Loop 6- $[\text{CoCl}_6]^{3-}$												
B (27)	B (29)	N (30)	N (31)	B (32)	N (33)	Co (37)	Cl (38)	Cl (39)	Cl (40)	Cl (41)	Cl (42)	Cl (43)
-0.196	-0.107	-0.056	-0.107	-0.319	-0.057	1.550	-0.712	-0.379	-0.669	-0.616	-0.615	-0.712
-0.733	0.171	-0.109	0.172	-0.023	-0.109	3.306	0.180	0.241	0.223	0.285	0.212	0.181
-51.399	-7.266	-14.155	-7.211	-2.241	-14.169	-0.044	15.995	14.478	20.201	22.041	21.492	15.997

tial is a total energy level including kinetic energy and potential energy have been considered to justify the structural stability and semi-conducting properties of  $\text{B}_{18}\text{N}_{18}-[\text{CoCl}_6]^{3-}$  nano systems.

In accordance data of  $E_g$  in Table 4,  $[\text{CoCl}_6]^{3-}$  - loop 4 nano system is more conductor than other nano system and  $[\text{CoCl}_6]^{3-}$  alone is insulators. Also, total atomic charges; that provide a means of estimating partial atomic charges from calculations carried out by the methods of computational chemistry, spin densities; that Spin density is electron density applied to

free radicals. It is defined as the total electron density of electrons of one spin minus the total electron density of the electrons of the other spin. One of the ways to measure it experimentally is by electron spin resonance and isotropic Fermi contact coupling; that the Fermi contact interaction is the magnetic interaction between an electron and an atomic nucleus when the electron is inside that nucleus. So mentioned parameters of  $[\text{CoCl}_6]^{3-}$  under different loops of  $\text{B}_{18}\text{N}_{18}$  system at the level of B3LYP theory and EPR-II basis set for B, N, Cl atoms and Aldrich's VTZ basis set

**Table 6:** Geometrical quantities of different loops of  $B_{18}N_{18}$  nano ring inclusive embedded  $[CoCl_6]^{3-}$  in the nano ring at the level of B3LYP theory and EPR-II basis set for B, N, Cl atoms and Aldrich's VTZ basis set and Stuttgart RSC 1997 Effective Core Potential for Co (III).

Compound		Geometrical quantities			
$B_{18}N_{18}-[CoCl_6]^{3-}$		Bond ID	Bond Lengths (Å)	Angle ID	Bond Angles
loop 1	B(1)	r 1-4	1.414	1-4-2	91.014
	B(2)	r 4-2	1.414	4-2-34	147.316
	N(4)	r 2-34	1.293	2-34-35	103.620
	N(34)	r 1-36	1.293	34-35-36	125.522
	B(35)	r 35-36	1.459	35-36-1	103.620
	N(36)	r 34-35	1.459	36-1-4	147.316
loop 2	B(3)	r 3-5	1.459	9-8-6	91.019
	N(5)	r 3-7	1.459	8-6-7	147.318
	B(6)	r 5-9	1.293	6-7-3	103.607
	N(7)	r 6-7	1.293	7-3-5	125.530
	N(8)	r 8-9	1.414	3-5-9	103.607
	B(9)	r 6-8	1.414	5-9-8	147.318
Loop 3	N(10)	r 11-13	1.459	12-16-14	91.027
	B(11)	r 11-10	1.459	16-14-10	147.312
	B(12)	r 12-13	1.293	14-10-11	103.602
	N(13)	r 10-14	1.293	10-11-13	125.513
	B(14)	r 12-16	1.414	11-13-12	103.602
	N(16)	r 14-16	1.414	13-12-16	147.312
loop 4	B(15)	r 15-17	1.459	21-20-18	91.014
	N(17)	r 15-19	1.459	20-18-19	147.316
	B(18)	r 17-21	1.293	18-19-15	103.620
	N(19)	r 18-19	1.293	19-15-17	125.522
	N(20)	r 18-20	1.414	15-17-21	103.620
	B(21)	r 20-21	1.414	17-21-20	147.316
loop 5	N(22)	r 22-23	1.459	24-28-26	91.019
	B(23)	r 23-25	1.459	28-26-22	147.318
	B(24)	r 22-26	1.293	26-22-23	103.607
	N(25)	r 24-25	1.293	22-23-25	125.530
	B(26)	r 26-28	1.414	23-25-24	103.607
	N(28)	r 24-28	1.414	25-24-28	147.318
loop 6	B(27)	r 27-31	1.459	33-32-30	91.027
	N(29)	r 27-29	1.459	32-30-31	147.312
	B(30)	r 30-31	1.293	30-31-27	103.602
	N(31)	r 29-33	1.293	31-27-29	125.513
	N(32)	r 30-32	1.414	27-29-33	103.602
	B(33)	r 32-33	1.414	29-33-32	147.312

and Stuttgart RSC 1997 ECP for Co (III) have been reported in Table 5.

In accordance Table 5, it is clear that Sum of Mulliken charges and Sum of Mulliken spin densities of  $[CoCl_6]^{3-}$  under six different loops of  $B_{18}N_{18}$  nano ring

are -3.0 and 4.0 respectively.

Geometrical quantities of different loops of  $B_{18}N_{18}$  nano ring inclusive embedded  $[CoCl_6]^{3-}$  in the nano ring at the level of B3LYP theory and EPR-II basis set for B,N, Cl atoms and Aldrich's VTZ basis set and

Stuttgart RSC 1997 Effective Core Potential for Co (III) have been reported in Table 6.

#### 4. CONCLUSIONS

In this study, Density functional theory calculations with EPR-II basis sets have been used to determination electrostatic non-bonded interaction. Relative energies, HOMO-LUMO bond gaps, total atomic charges of complex in six different loops have been employed to detect and characterize the hyperfine structural properties of nano ring-complex system. In accordance with Table 1,  $[\text{CoCl}_6]^{3-}$  complex with weak field ligands exhibits the Jahn–Teller distortion. In accordance with Table 3, definition the band gap of  $[\text{CoCl}_6]^{3-}$  to 0.18716 a.u. and  $[\text{CoCl}_6]^{3-}$  is insulators. In accordance with NICS values of Table 3, it's elaborated that loops 1,3 and 5 have similar NICS values that is equal to -10.1058 and loops 2,4 and 6 have similar NICS values that is equal to -10.1189. So, that if the NICS values would be more negative, the aromaticity and magnetism of the loop is more.

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