



## Quantum Mechanical Investigation of Bond Gaps of $\Pi$ -acceptor Ligand Alone and Affected Nanoring Field: EPR and NMR study

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### ABSTRACT

We studied non-bonded interaction of the  $[\text{Co}(\text{CN})_6]^{3-}$  complex Situated  $\text{B}_{24}\text{N}_{24}$  nanoring. Early, the geometry of  $[\text{Co}(\text{CN})_6]^{3-}$  and  $\text{B}_{24}\text{N}_{24}$  have been optimized at B3LYP method with Def2-SV(P)/ LANL2DZ(ECP) and EPR-II basis set respectively. To confirmation the structural stability of the  $\text{B}_{24}\text{N}_{24}$ - $[\text{Co}(\text{CN})_6]^{3-}$  nano system, delocalization of electrons between donor and acceptor bonds and LUMO and HOMO for the lowest energy have been computed by DFT/ B3LYP method. Then we investigated NBO data such as coefficients and hybrids of orbitals, second order perturbation theory analysis of fock matrix, and  ${}^n\text{E}$  in different loops of the nanoring have been calculated at B3LYP method.

**Key words:** DFT, ECP, EPR-II basis set, HOMO, LUMO, NICS.

### INTRODUCTION

There has been a noticeable regard in experimental researches of  $\text{B}_n\text{N}_m$  nanoring.  $\text{B}_n\text{N}_m$  have been provided by reaction of  $\text{BCl}_3$  with  $\text{NH}_3$  in a laser beam<sup>1,2</sup>. The experimental data of synthesis and various spectrometers are requirement to guess structural stabilities and consider physical chemistry properties of such molecules of  $\text{B}_{24}\text{C}_{12}\text{N}_{24}$  molecule<sup>3</sup> and the  $\text{B}_{12}\text{N}_{12}$ ,  $\text{B}_{16}\text{N}_{16}$  and  $\text{B}_{28}\text{N}_{28}$  molecules<sup>4-6</sup>. In present work we have utilize single wall  $\text{B}_{24}\text{N}_{24}$  borane nitride nanoring. The schematic of  $\text{B}_{24}\text{N}_{24}$  is displayed in the Figure 1. After valence bond theory was corroborated, Molecular orbital

theory had been prospered. Thus, we presentation the non-bonded interaction of the  $[\text{Co}(\text{CN})_6]^{3-}$  Situated  $\text{B}_{24}\text{N}_{24}$  nano ring. The basically purpose of this investigation was the study of the electromagnetic interactions within the  $\text{B}_{24}\text{N}_{24}$ - $[\text{Co}(\text{CN})_6]^{3-}$  system. For further evaluation about electromagnetic interactions, stability structure of  $[\text{Co}(\text{CN})_6]^{3-}$  complex affected various loops of nano ring have been computed. For further structural data, bond gaps and the hybrids on atom have been reported to estimate the structural ability of the  $[\text{Co}(\text{CN})_6]^{3-}$  to make a stable  $\text{B}_{24}\text{N}_{24}$ - $[\text{Co}(\text{CN})_6]^{3-}$  system.

### Computational details

To determination electromagnetic interactions of the  $[\text{Co}(\text{CN})_6]^{3-}$  complex inclusive Co (III) and six  $\pi$ -acceptor ligands, the geometry of the  $[\text{Co}(\text{CN})_6]^{3-}$  was optimized at DFT/B3LYP method with Def2-SV(P) basis set and LANL2DZ Effective Core Potential. Also, the geometry of the mix of  $\text{B}_{24}\text{N}_{24}$  nanoring and  $[\text{Co}(\text{CN})_6]^{3-}$  complex was optimized at DFT/B3LYP method with EPR-II basis set. Thermochemical properties were determined at B3LYP/EPR-II basis set to analyze the enthalpies and Gibbs free energies<sup>7</sup>. The natural bond orbital (NBO) calculations<sup>8,9</sup> has been used to theoretical predictions the intermolecular orbital interactions in the  $[\text{Co}(\text{CN})_6]^{3-}$  and  $\text{B}_{24}\text{N}_{24}-[\text{Co}(\text{CN})_6]^{3-}$ <sup>10</sup>. So, NBO data including coefficients and hybrids of orbitals of

atoms, donor-acceptor bonds and  $\pi$ E in  $[\text{Co}(\text{CN})_6]^{3-}$  complex affected various loops of the  $\text{B}_{24}\text{N}_{24}$  nanoring have been determined.

### RESULTS AND DISCUSSION

To calculate the non-bonded interaction of  $\text{B}_{24}\text{N}_{24}-[\text{Co}(\text{CN})_6]^{3-}$  nano system, the structure of the  $\text{B}_{24}\text{N}_{24}$  have been optimized at B3LYP/EPR-II basis set and structure of the  $[\text{Co}(\text{CN})_6]^{3-}$  complex including cyanide that known as six  $\text{\AA}$ -acceptor ligands, have been optimized at B3LYP/Def2-SV(P) basis set and LANL2DZ ECP. The non-bonded electromagnetic interactions of the  $[\text{Co}(\text{CN})_6]^{3-}$  complex Situated nanoring have been investigated at B3LYP in different loops of the  $\text{B}_{24}\text{N}_{24}$  nanoring.

**Table 1: Optimal quantities of  $[\text{Co}(\text{CN})_6]^{3-}$ .**

Compound	Bond ID	bond length	bond angle
$[\text{Co}(\text{CN})_6]^{3-}$	Co(1)-C(2)	1.957632	-
	Co(1)-C(3)	1.958069	-
	Co(1)-C(4)	1.957556	-
	Co(1)-C(5)	1.957584	-
	Co(1)-C(6)	1.957485	-
	Co(1)-C(7)	1.957629	-
	C(2)-N(11)	1.180025	-
	C(3)-N(8)	1.179911	-
	C(4)-N(12)	1.179998	-
	C(5)-N(10)	1.180055	-
	C(6)-N(13)	1.179861	-
	C(7)-N(9)	1.180024	-
	C(2)-Co(1)-C(3)	-	90.02
	C(2)-Co(1)-C(4)	-	90.0163
	C(2)-Co(1)-C(5)	-	89.9842
	C(2)-Co(1)-C(6)	-	89.9782
	C(2)-Co(1)-C(7)	-	179.9811
	C(3)-Co(1)-C(4)	-	89.817
	C(3)-Co(1)-C(5)	-	90.1773
	C(3)-Co(1)-C(6)	-	179.9773
	C(3)-Co(1)-C(7)	-	89.9877
	C(4)-Co(1)-C(5)	-	179.9942
	C(4)-Co(1)-C(6)	-	89.9782
	C(4)-Co(1)-C(7)	-	89.9665
	C(5)-Co(1)-C(6)	-	89.8001
	C(5)-Co(1)-C(7)	-	90.033
	C(6)-Co(1)-C(7)	-	90.014

\* See Figure 1 for more details

**Table 2: Natural atomic orbitals of  $[\text{Co}(\text{CN})_6]^{3-}$  complex**

Atom	Natural atomic orbital $[\text{CoF}_6]^{3-}$		
	Atomic Orbital	Occupancy	Energy
Co <sup>3+</sup> (1)	4s	0.46228	2.90416
	3dyz	1.84859	0.10792
	3dxy	1.73218	0.11879
	3dz <sup>2</sup>	1.68785	0.12323
	3dx <sup>2</sup> y <sup>2</sup>	1.41028	0.14943
	3dxz	1.06674	0.18220
	C (2)	2s	1.25718
2px		0.82429	0.33754
2py		0.98223	0.48570
C (3)	2pz	0.81132	0.32525
	2s	1.25730	0.22404
	2px	0.89856	0.40722
C (4)	2py	0.81923	0.33271
	2pz	0.89995	0.40823
	2s	1.25716	0.22399
C (5)	2px	0.89507	0.40400
	2py	0.81626	0.32990
	2pz	0.90656	0.41453
C (6)	2s	1.25716	0.22389
	2px	0.89526	0.40429
	2py	0.81626	0.32996
C (7)	2pz	0.90628	0.41436
	2s	1.25697	0.22387
	2px	0.89884	0.40752
N (8)	2py	0.81930	0.33276
	2pz	0.89969	0.40810
	2s	1.25717	0.22396
N (9)	2px	0.82428	0.33752
	2py	0.98225	0.48576
	2pz	0.81131	0.32525
N (10)	2s	1.58723	-0.18862
	2px	1.40270	0.20756
	2py	1.24637	0.24158
N (11)	2pz	1.40643	0.20663
	2s	1.58725	-0.18838
	2px	1.25623	0.23963
N (12)	2py	1.56854	0.17157
	2pz	1.23059	0.24522
	2s	1.58726	-0.18837
N (13)	2px	1.39603	0.20922
	2py	1.24036	0.24311
	2pz	1.41899	0.20415

N (11)	2s	1.58725	-0.18841
	2px	1.25623	0.23960
	2py	1.56853	0.17156
	2pz	1.23061	0.24519
N (12)	2s	1.58724	-0.18845
	2px	1.39563	0.20925
	2py	1.24032	0.24305
	2pz	1.41942	0.20395
N (13)	2s	1.58716	-0.18836
	2px	1.40311	0.20764
	2py	1.24641	0.24176
	2pz	1.40595	0.20693

Optimized parameters of  $[\text{Co}(\text{CN})_6]^{3-}$  consists bond lengths and bond angles have been reported in Table 1. We can get all of the Co-C bond lengths are the same in values and all of the C-N bond lengths are same to other, because the octahedral compounds that are Low-spin  $d^6$  electronic configuration such as Co (III) with six  $\Pi$ -acceptor ligands no indicate the Jahn–Teller distortion. But the octahedral compounds that are High-spin  $d^6$  electronic configuration such as Co (III) with six  $\sigma$ -donor ligands indicate the Jahn–Teller distortion<sup>11</sup>. Pursuant the occupancy and energy values of Co (III) metal in Table 2, we can get that  $3d_{yz}$ ,  $3d_{xy}$ ,  $3d_{z^2}$  orbitals include two electrons and the least value of energy. The other d orbitals and 4s orbital include no electron. Also, Pursuant the occupancy and energy values of 6  $\Pi$ -acceptor ligands it was demonstrated that 2s orbital of N atom participate to creation the  $\sigma$  molecular orbitals and one non bonding electron pairs of N situate in 2p orbital that has higher energy level. For instance, in N(8) and N(13) that are in same position relative to the Co (III),  $2p_y$  has a higher energy levels and  $2p_x$  and  $2p_z$  have lower energy levels. In addition, pursuant Table 2 data, atom pairs N(8)-N(13), N(9)-N(11), N(10)-N(12) in  $[\text{Co}(\text{CN})_6]^{3-}$  complex that are in same position relative to Co (III), have the same occupancy and energy levels (Fig. 1). The energy level difference of metal-ligands bonding in  $[\text{Co}(\text{CN})_6]^{3-}$  complex have been reported in Table 3. We can understand, the size of  $\sigma$  is determined by the ligand field strength. (CN)<sup>-</sup> ligand is a strong field ligand that increase  $\sigma$  more than F<sup>-</sup> ligand as weak field ligand. Determination of second order perturbation theory analysis of fock matrix of C and N atoms at the level of B3LYP/EPR-II basis set and Co (III) atom at the level of B3LYP/Def2-SV(P)/LANL2DZ (ECP)

Table 3: Molecular orbital diagram of  $[\text{Co}(\text{CN})_6]^{3-}$  complex.

Compound	Molecular orbital diagram			
	Natural Bond Orbitals		Occupancy	Energy (a.u.)
$[\text{Co}(\text{CN})_6]^{3-}$	BD*( 1)Co 1- C 6	$\Pi^*_{t1u}$	0.43225	1.40362
	BD*( 1)Co 1- C 5	$\sigma^*_{t2g}$	0.43283	1.40319
	BD*( 3) C 5- N10	n.b.	0.05113	0.50551
	BD*( 3) C 6- N13	n.b.	0.05112	0.50548
	BD*( 3) C 7- N 9	n.b.	0.05105	0.50547
	BD*( 3) C 2- N11	n.b.	0.05105	0.50546
	BD*( 3) C 3- N 8	n.b.	0.05107	0.50544
	BD*( 3) C 4- N12	n.b.	0.05113	0.50543
	LP ( 1) C 3	$\sigma^*_{a1g}$	1.50469	0.35364
	LP ( 1) C 7	$\Pi_{t1u}$	1.50443	0.35360
	LP ( 1) C 4	$\sigma^*_{eg}$	1.50444	0.35359
	LP ( 1)Co 1	$\Pi_{t2g}$	1.91544	0.10051
	BD ( 1)Co 1- C 5	$\sigma_{eg}$	1.91189	-0.05029
	BD ( 1)Co 1- C 2	$\sigma_{t1u}$	1.91190	-0.05030
	BD ( 1)Co 1- C 6	$\sigma_{a1g}$	1.91188	-0.05039
	$\Delta_{oct}$		0.25308 a.u.	

Table 4: Natural bond orbital (NBO) analysis of  $[\text{Co}(\text{CN})_6]^{3-}$ 

Compound	Natural bond orbital (NBO) analysis				
	Donor NBO (i)	Acceptor NBO (j)	E(2)kcal/mol	E(j)-E(i)a.u.	F(i,j)a.u.
$[\text{Co}(\text{CN})_6]^{3-}$	BD ( 1)Co 1- C 2	BD*( 1)Co 1- C 5	1.65	1.45	0.048
	BD ( 1)Co 1- C 2	BD*( 1)Co 1- C 6	1.65	1.45	0.048
	BD ( 1)Co 1- C 2	BD*( 3) C 6- N13	2.23	0.56	0.032
	BD ( 1)Co 1- C 5	BD*( 1)Co 1- C 6	1.66	1.45	0.048
	BD ( 1)Co 1- C 5	BD*( 3) C 2- N11	1.24	0.56	0.024
	BD ( 1)Co 1- C 6	BD*( 1)Co 1- C 5	1.67	1.45	0.048
	BD ( 1)Co 1- C 6	BD*( 3) C 2- N11	1.06	0.56	0.022
	BD ( 1)Co 1- C 6	BD*( 3) C 5- N10	2.27	0.56	0.032
	BD ( 2) C 6- N13	BD*( 3) C 5- N10	0.6	0.43	0.014
	LP ( 1)Co 1	BD*( 3) C 6- N13	2.04	0.4	0.026
	BD ( 1)Co 1- C 5	BD*( 3) C 3- N 8	2.25	0.56	0.032
	LP ( 1)Co 1	BD*( 3) C 3- N 8	0.13	0.4	0.007
	BD ( 1)Co 1- C 2	BD*( 3) C 4- N12	2.29	0.56	0.032
	LP ( 1)Co 1	BD*( 3) C 4- N12	1.59	0.4	0.023
	BD ( 1)Co 1- C 5	BD*( 3) C 7- N 9	1.3	0.56	0.024
	BD ( 1)Co 1- C 6	BD*( 3) C 7- N 9	1.02	0.56	0.021
	LP ( 1)Co 1	BD*( 2) C 7- N 9	3.73	0.4	0.035
	LP ( 1) C 3	BD*( 1)Co 1- C 5	345.09	1.05	0.546
	LP ( 1) C 3	BD*( 1)Co 1- C 6	585.34	1.05	0.711
	LP ( 1) C 3	BD*( 3) C 2- N11	4.15	0.15	0.025
	LP ( 1) C 3	BD*( 3) C 5- N10	10.16	0.15	0.04
	LP ( 1) C 3	BD*( 3) C 7- N 9	3.82	0.15	0.024

have been shown in Table 4. Also Bond orbital, Coefficients and Hybrids of  $[\text{Co}(\text{CN})_6]^{3-}$  complex have been shown in Table 5. In accordance with data of Table 5, we can get that the bonding and anti-bonding coefficients of orbitals of Co-C and Co-N bonds were 0.8 and 0.7 respectively. To calculation non-bonded interaction of the  $[\text{Co}(\text{CN})_6]^{3-}$  complex Situated in nano ring field, we attend on the  $\text{B}_{24}\text{N}_{24}$  nano ring and optimized structure of the  $\text{B}_{24}\text{N}_{24}-[\text{Co}(\text{CN})_6]^{3-}$  system have been displayed in Fig.1. The geometry of  $\text{B}_{24}\text{N}_{24}$

nano ring has been optimized at B3LYP method with EPR-II basis set. According to the frequency calculation for  $\text{B}_{24}\text{N}_{24}$  nano rings, thermochemical quantities were equal to  $\Delta G = -97.6323205765$  kcal/mol and  $\Delta H = -166.384143925$  kcal/mol, corroborated the structural stability of nano rings. Dipole moments of alone complex and complex affected various loops of nanoring have been shown in Table 6. The geometry of mix of  $\text{B}_{24}\text{N}_{24}$  and  $[\text{Co}(\text{CN})_6]^{3-}$  complex have been optimized at B3LYP method with EPR-II basis set for B,N,C atoms and

**Table 5: Bond orbital, Coefficients, Hybrids of  $[\text{Co}(\text{CN})_6]^{3-}$  at NBO studies**

Compound	Natural bond orbital (NBO) analysis	
	Bond orbital	Coefficients/ Hybrids
$[\text{Co}(\text{C})_6]^{3-}$	BD ( 1)Co 1- C 2	0.5127*Co 1(sp <sup>0.00d 2.00</sup> ) + 0.8586*C 2(sp <sup>0.79d 0.00</sup> )
	BD ( 1)Co 1- C 5	0.5127*Co 1(sp <sup>0.00d 2.00</sup> ) + 0.8585*C 5(sp <sup>0.79d 0.00</sup> )
	BD ( 1)Co 1- C 6	0.5128*Co 1(sp <sup>0.00d 2.00</sup> ) + 0.8585*C 6(sp <sup>0.79d 0.00</sup> )
	LP ( 1)Co 1	(sp <sup>0.00d 1.00</sup> )
	LP ( 1) C 3	(sp <sup>1.10d 0.00</sup> )
	BD*( 1)Co 1- C 5	0.8585*Co 1(sp <sup>0.00d 2.00</sup> ) -0.5127*C 5(sp <sup>0.79d 0.00</sup> )
	BD*( 1)Co 1- C 6	0.8585*Co 1(sp <sup>0.00d 2.00</sup> ) -0.5128*C 6(sp <sup>0.79d 0.00</sup> )
	BD*( 3) C 2- N11	0.7800*C 2(sp <sup>1.00d 0.00</sup> ) -0.6258*N11(sp <sup>1.00d 0.00</sup> )
	BD*( 3) C 3- N 8	0.7800*C 3(sp <sup>1.00d 0.00</sup> ) -0.6258*N 8(sp <sup>1.00d 0.00</sup> )
	BD*( 3) C 4- N12	0.7800*C 4(sp <sup>1.00d 0.00</sup> ) -0.6258*N12(sp <sup>1.00d 0.00</sup> )
	BD*( 3) C 5- N10	0.7800*C 5(sp <sup>1.00d 0.00</sup> ) -0.6258*N10(sp <sup>1.00d 0.00</sup> )
	BD*( 3) C 6- N13	0.7800*C 6(sp <sup>1.00d 0.00</sup> ) -0.6258*N13(sp <sup>1.00d 0.00</sup> )
	BD*( 3) C 7- N 9	0.7800*C 7(sp <sup>1.00d 0.00</sup> ) -0.6258*N 9(sp <sup>1.00d 0.00</sup> )

**Table 6: Changes in the relative energies ( $\Delta E$ ), dipole moment (r), nuclear repulsion energy and bond gap of alone  $[\text{Co}(\text{CN})_6]^{3-}$  and affected various loops of  $\text{B}_{24}\text{N}_{24}$**

Compound	Basis sets for $\text{Co}^{3+}$				
	Def2-SV(P) , LANL2DZ ECP				
$\text{B}_{24}\text{N}_{24}-[\text{Co}(\text{CN})_6]^{3-}$	band gap (Hartree)	$\Delta E$ (Hartree)	Dipole moment (Debye)	NICS	nuclear repulsion energy (Hartree)
$[\text{Co}(\text{CN})_6]^{3-}$	0.25308	-701.17098	0.0017	*	748.95533
loop 1- $[\text{Co}(\text{CN})_6]^{3-}$	0.02448	-940.01508	4.9114	-10.1058	1219.24152
loop 2- $[\text{Co}(\text{CN})_6]^{3-}$	0.0329	-940.03334	5.3568	-10.1189	1212.20610
loop 3- $[\text{Co}(\text{CN})_6]^{3-}$	0.0237	-940.01497	5.0787	-10.1058	1219.24129
loop 4- $[\text{Co}(\text{CN})_6]^{3-}$	0.03195	-940.03336	5.3016	-10.1189	1212.20822
loop 5- $[\text{Co}(\text{CN})_6]^{3-}$	0.03372	-940.01429	5.5595	-10.1058	1219.25988
loop 6- $[\text{Co}(\text{CN})_6]^{3-}$	0.03481	-940.03316	5.5523	-10.1189	1212.18374
loop 7- $[\text{Co}(\text{CN})_6]^{3-}$	0.02262	-940.01477	4.6646	-10.1058	1219.25565
loop 8- $[\text{Co}(\text{CN})_6]^{3-}$	0.0313	-940.03326	5.3537	-10.1189	1212.18442

Table 7. Total atomic charges of alone  $[\text{Co}(\text{CN})_6]^{3-}$  and affected various loops of  $\text{B}_{24}\text{N}_{24}$ 

Compound	Basis sets for $\text{Co}^{3+}$ Def2-SV(P), LANL2DZ ECP												
	Total atomic charges												
$[\text{Co}(\text{CN})_6]^{3-}$	Co (1)	C (2)	C (3)	C (4)	C (5)	C (6)	C (7)	N (8)	N (9)	N (10)	N (11)	N (12)	N (13)
$\text{B}_{24}\text{N}_{24}$ - $[\text{Co}(\text{CN})_6]^{3-}$	2.560	-0.343	-0.345	-0.344	-0.343	-0.342	-0.343	-0.582	-0.5829	-0.582	-0.582	-0.582	-0.583
loop 1- $[\text{Co}(\text{CN})_6]^{3-}$	Co (49)	C (50)	C (51)	C (52)	C (53)	C (54)	C (55)	N (56)	N (57)	N (58)	N (59)	N (60)	N (61)
loop 2- $[\text{Co}(\text{CN})_6]^{3-}$	2.6770	-0.388	-0.267	-0.394	-0.378	-0.744	-0.388	-0.576	-0.551	-0.559	-0.551	-0.548	-0.131
loop 3- $[\text{Co}(\text{CN})_6]^{3-}$	2.6006	-0.363	-0.370	-0.335	-0.457	-0.401	-0.363	-0.552	-0.551	-0.394	-0.551	-0.557	-0.504
loop 4- $[\text{Co}(\text{CN})_6]^{3-}$	2.6786	-0.386	-0.379	-0.266	-0.743	-0.391	-0.387	-0.559	-0.551	-0.132	-0.553	-0.575	-0.550
loop 5- $[\text{Co}(\text{CN})_6]^{3-}$	2.6020	-0.362	-0.457	-0.370	-0.401	-0.335	-0.362	-0.395	-0.552	-0.505	-0.552	-0.553	-0.557
loop 6- $[\text{Co}(\text{CN})_6]^{3-}$	2.6802	-0.391	-0.747	-0.380	-0.395	-0.271	-0.390	-0.125	-0.545	-0.544	-0.541	-0.554	-0.570
loop 7- $[\text{Co}(\text{CN})_6]^{3-}$	2.5993	-0.363	-0.402	-0.456	-0.336	-0.370	-0.363	-0.500	-0.550	-0.555	-0.550	-0.395	-0.550
loop 8- $[\text{Co}(\text{CN})_6]^{3-}$	2.6779	-0.386	-0.392	-0.747	-0.268	-0.379	-0.385	-0.551	-0.555	-0.580	-0.553	-0.130	-0.559
loop 8- $[\text{Co}(\text{CN})_6]^{3-}$	2.5979	-0.361	-0.334	-0.400	-0.367	-0.453	-0.361	-0.557	-0.553	-0.554	-0.553	-0.505	-0.397

Def2-SV(P) basis set and LANL2DZ ECP for Co (III). According to the electron paramagnetic resonance (EPR) calculate, it is noteworthy that the energy obtained from the mentioned basis set and ECP for alone  $\text{B}_{24}\text{N}_{24}$  nanoring and alone  $[\text{Co}(\text{CN})_6]^{3-}$  complex were equal to -1911.727563 and -701.1710148 (Hartree) respectively. To describes the non-bonded interaction of  $[\text{Co}(\text{CN})_6]^{3-}$  affected eight various loops of  $\text{B}_{24}\text{N}_{24}$  nano ring, we focus on quantities values such as the relative energies ( $E$ ), dipole moment ( $r$ ), nuclear repulsion energy, NICS and bond gap that mentioned values have been displayed in Table 6. Atomic charge is the physical property of matter that causes it to experience a force when close to other electrically charged matter. So, total atomic charge of alone  $[\text{Co}(\text{CN})_6]^{3-}$  complex atoms and under different loops of  $\text{B}_{24}\text{N}_{24}$  nanoring, have been reported in Table 7. Also, Bond Length, Total atomic charges and Dipole orientation of atoms of different loops of nanorings have been displayed in Table 8. Magnetic Resonance parameters of  $[\text{Co}(\text{CN})_6]^{3-}$  complexes under three CSGT, GIAO, IGAIM methods have been shown in Table 9.

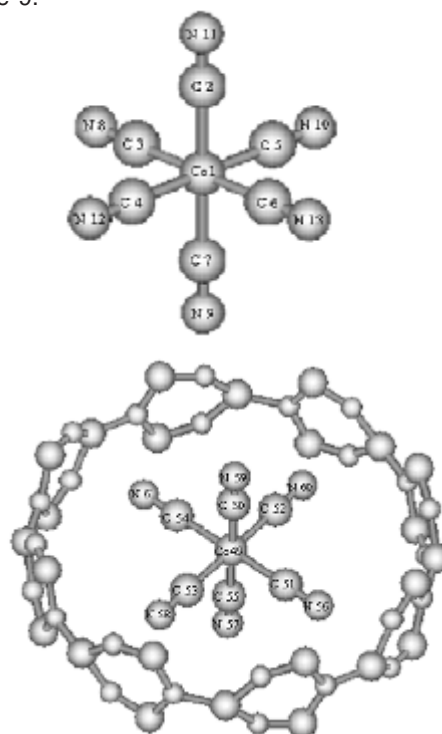
Fig. 1: Optimal structure of  $[\text{Co}(\text{CN})_6]^{3-}$  stand alone and situated  $\text{B}_{24}\text{N}_{24}$  nanoring

Table 8: Bond Length, Atomic charges & Dipole orientation of the sides of various loops of  $B_{24}N_{24}$ .

Compound $B_{24}N_{24} [Co(CN)_6]^{3-}$	Basis sets of Co (III) Def2-SV(P), LANL2DZ ECP				Dipole orientation $\theta$ $\varphi$
	Bond ID (Å)	Bond Length	Total atomic charges		
loop 1	B(1)	$r_{1-2}$	1.303	0.029792	90.0174.2630
	N(2)	$r_{1-32}$	1.417	-0.059818	
	B(3)	$r_{2-3}$	1.466	0.030860	
	N(32)	$r_{3-34}$	1.466	-0.166730	
	B(33)	$r_{32-33}$	1.417	0.029797	
	N(34)	$r_{33-34}$	1.303	-0.059851	
loop 2	N(4)	$r_{4-5}$	1.417	-0.143033	90.0147.1122
	B(5)	$r_{4-35}$	1.417	-0.003640	
	N(6)	$r_{5-6}$	1.303	-0.036094	
	B(7)	$r_{6-7}$	1.466	0.025729	
	B(35)	$r_{7-36}$	1.466	-0.003627	
	N(36)	$r_{35-36}$	1.303	-0.036107	
loop 3	N(8)	$r_{8-9}$	1.417	-0.166571	90.094.6723
	B(9)	$r_{8-37}$	1.417	0.028774	
	N(10)	$r_{9-10}$	1.303	-0.058331	
	B(11)	$r_{10-11}$	1.466	0.023939	
	B(37)	$r_{11-38}$	1.466	0.028554	
	N(38)	$r_{37-38}$	1.303	-0.058119	
loop 4	N(12)	$r_{12-13}$	1.417	-0.141968	90.057.3710
	B(13)	$r_{12-39}$	1.417	-0.003813	
	N(14)	$r_{13-14}$	1.303	-0.035563	
	B(15)	$r_{14-15}$	1.466	0.026477	
	B(39)	$r_{15-40}$	1.466	-0.003821	
	N(40)	$r_{39-40}$	1.303	-0.035568	
loop 5	N(16)	$r_{16-17}$	1.417	-0.176228	90.03.9639
	B(17)	$r_{16-41}$	1.417	0.027328	
	N(18)	$r_{17-18}$	1.303	-0.066071	
	B(19)	$r_{18-19}$	1.466	0.025758	
	B(41)	$r_{19-42}$	1.466	0.028672	
	N(42)	$r_{41-42}$	1.303	-0.061409	
loop 6	N(20)	$r_{20-21}$	1.417	-0.145945	90.033.7029
	B(21)	$r_{20-43}$	1.417	-0.004382	
	N(22)	$r_{21-22}$	1.303	-0.038261	
	B(23)	$r_{22-23}$	1.466	0.027356	
	B(43)	$r_{23-44}$	1.466	-0.004393	
	N(44)	$r_{43-44}$	1.303	-0.038252	
loop 7	N(24)	$r_{24-25}$	1.417	-0.167045	90.082.9711
	B(25)	$r_{24-45}$	1.417	0.032748	
	N(26)	$r_{25-26}$	1.303	-0.057311	
	B(27)	$r_{26-27}$	1.466	0.030136	
	B(45)	$r_{27-46}$	1.466	0.034124	
	N(46)	$r_{45-46}$	1.303	-0.059718	
loop 8	N(28)	$r_{28-29}$	1.417	-0.141699	90.0122.8949
	B(29)	$r_{28-47}$	1.417	-0.004621	
	N(30)	$r_{29-30}$	1.303	-0.035262	
	B(31)	$r_{30-31}$	1.466	0.025256	
	B(47)	$r_{31-48}$	1.466	-0.004614	
	N(48)	$r_{47-48}$	1.303	-0.035254	



**Table 9: Nuclear Magnetic Resonance parameters of  $[\text{Co}(\text{CN})_6]^{3-}$  complex at three CSGT, GIAO, IGAIM methods**

Compound	NMR parameters (ppm)						
	Isotropic	anisotropy	$\Delta\sigma$	$\delta$	$\eta$	$\Omega$	$\hat{\epsilon}$
$[\text{Co}(\text{CN})_6]^{3-}$				CSGT GIAOI GAIM			
Co(1)	-7827.8043	15.4186	15.4186	10.2791	0.734364	10.2791	-0.39844
	-7827.8043	15.4186	15.4186	10.2791	0.734364	10.2791	-0.39844
	-7860.7339	16.0271	16.0271	10.6848	0.851658	10.6848	-0.22248
C(2)	35.7915	349.7468	349.7469	233.1646	0.001602	233.1646	-1.4976
	35.7915	349.7468	349.7469	233.1646	0.001602	233.1646	-1.4976
	19.0814	373.804	373.804	249.2026	0.000786	249.2026	-1.49882
C(3)	35.8802	349.5784	349.5784	233.0522	0.000275	233.0522	-1.49959
	35.8802	349.5784	349.5784	233.0522	0.000275	233.0522	-1.49959
	19.1472	373.7295	373.7295	249.153	7.14E-05	249.153	-1.49989
C(4)	35.8283	349.6323	349.6323	233.0881	0.000297	233.0881	-1.49956
	35.8283	349.6323	349.6323	233.0881	0.000297	233.0881	-1.49956
	19.0861	373.7933	373.7934	249.1956	5.26E-05	249.1956	-1.49992
C(5)	35.808	349.6633	349.6633	233.1089	0.000288	233.1089	-1.49957
	35.808	349.6633	349.6633	233.1089	0.000288	233.1089	-1.49957
	19.064	373.8239	373.8239	249.216	8.83E-05	249.216	-1.49987
C(6)	35.8821	349.5573	349.5574	233.0382	0.000264	233.0382	-1.4996
	35.8821	349.5573	349.5574	233.0382	0.000264	233.0382	-1.4996
	19.1366	373.7248	373.7248	249.1499	0.000134	249.1499	-1.4998
C(7)	35.7907	349.7474	349.7474	233.165	0.001602	233.165	-1.4976
	35.7907	349.7474	349.7474	233.165	0.001602	233.165	-1.4976
	19.0811	373.804	373.804	249.2026	0.000786	249.2026	-1.49882
N(8)	-33.9122	527.9381	527.9381	351.9587	0.000605	351.9587	-1.49909
	-33.9122	527.9381	527.9381	351.9587	0.000605	351.9587	-1.49909
	-43.2697	546.1166	546.1166	364.0778	6.54E-05	364.0778	-1.4999
N(9)	-34.1079	528.12	528.12	352.08	0.001431	352.08	-1.49785
	-34.1079	528.12	528.12	352.08	0.001431	352.08	-1.49785
	-43.363	546.2229	546.2229	364.1486	0.000444	364.1486	-1.49933
N(10)	-34.1006	528.0967	528.0967	352.0645	0.000689	352.0645	-1.49897
	-34.1006	528.0967	528.0967	352.0645	0.000689	352.0645	-1.49897
	-43.3832	546.2333	546.2334	364.1556	0.000105	364.1556	-1.49984
N(11)	-34.1084	528.1192	528.1192	352.0794	0.00143	352.0794	-1.49786
	-34.1084	528.1192	528.1192	352.0794	0.00143	352.0794	-1.49786
	-43.3629	546.2218	546.2219	364.1479	0.000443	364.1479	-1.49934
N(12)	-34.063	528.0556	528.0557	352.0371	0.00073	352.0371	-1.49891
	-34.063	528.0556	528.0557	352.0371	0.00073	352.0371	-1.49891
	-43.3477	546.193	546.193	364.1286	3.05E-05	364.1286	-1.49995
N(13)	-33.9229	527.9167	527.9167	351.9444	0.000552	351.9444	-1.49917
	-33.9229	527.9167	527.9167	351.9444	0.000552	351.9444	-1.49917
	-43.2617	546.0694	546.0694	364.0463	7.72E-05	364.0463	-1.49988



### CONCLUSION

In this study, Density functional theory calculations with EPR basis sets have been employed to determination non-bonded interaction. In accordance with Table 3, definition the magnitude of  $\pi$  under strong field ligands, such as (CN)<sup>-</sup>, equal to 0.25308 a.u. . In accordance with Table 1, [Co(CN)<sub>6</sub>]<sup>3-</sup> complex with strong field ligands no exhibit the Jahn–Teller distortion. It has been displayed at Table 5 that the bonding coefficients of s, p and d orbitals were 0.3 and anti-bonding coefficients of Co-C bonds were 0.8 and Co-N bonds were 0.7. In accordance with NICS values of Table 6, it's displayed that loops 1,3 and 5 have

similar NICS values and equal to -10.1058 and loops 2,4 and 6 have similar NICS values and equal to -10.1189. So, the more negative NICS values, the aromaticity and magnetism that loops most. According to different NMR methods of Table 9, characterize that CSGT and GIAO methods have similar quantity.

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