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Molecular Mechanics Based Study On Atomic And Molecular Orbitals Of Cobaltocene

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ABSTRACT

2pz orbitals of ten carbon atoms of two $C_5H_5^-$ are involved in bonding with, nine cobalt orbitals. The coefficient of eigen vector of 2pz of carbon are in the range 0.70-1.88. The major involvements are in molecular orbitals 28-54. The nine atomic orbitals which are involved in bonding are one 4s, there 4p and five d. The coefficients of eigen vector are in the range 1.50-4.42. The highest value is of 4s and lowest of $3dz^2$. The involvements of d orbitals are in MOs 23-31 and of 4s and 4p in the MOs 36-56. The MOs involving d orbitals have eigen values in the range -0.49 to -0.35 (e.V), that is in bonding range whereas 4s and 4p orbitals are in the range -0.08 to 2.04, which is anti bonding range. Energy levels diagram giving full quantitative details of involvement of atomic orbitals in molecular orbitals have been drawn population analysis showing extent of involvement of electrons is also presented.

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KEYWORDS

Energy level;
Eigen vector;
Eigen values;
Cobaltocene;
Population analysis;
Molecular orbitals.

INTRODUCTION

$M(C_5H_5)_2$[M(cp) M=Fe, Co, Mn] are the derivatives of cyclopentadiene and have a sandwich structure. They are offen called metallocenes. The structures of metallocen have been extensively studied and are reported in most of the organometallic chemistry books[1, 2]. However the calculations of relative energy levels and magnitude of contribution of atomic orbitals in the formation of MO is still a subject of study[2]. We in a recent publication[3] have evaluated the contribution of atomic orbitals in ferrocene on quantitative basis with the help of computational chemistry[4]. In this paper we present a similar study on cobaltocene. The main focus will be on the study of eigen values and eigen vector values of cobaltocene.

MATERIAL AND METHOD

The study material of this paper is cobaltocene. The 3D modeling and geometry optimization of cobaltocene have been done by CAChe software using molecular mechanics with EHT option[5]. The

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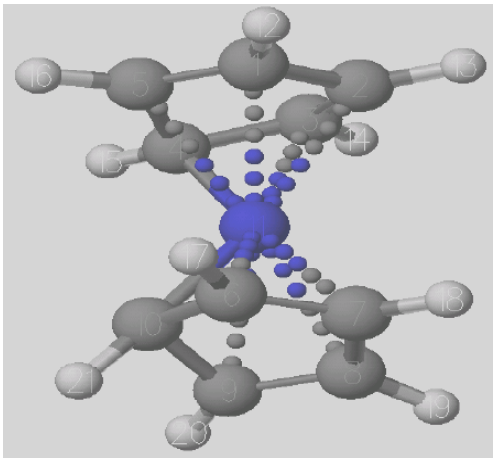

1-10 Carbon, 11 Cobalt, 12-21 Hydrogen

Figure 1 : 3D Structure of cobaltocene

3D structure is shown in the figure 1. Eigen values and eigenvectors values have been obtained with the same software, using the same option. With the help of these values, eigenvector analysis and magnitude of contribution of atomic orbital in MO formation have been made and discussed. The theory on which various calculations are made is defined elsewhere[6].

RESULT AND DISCUSSION

The molecular orbitals of cobaltocene figure 1 are formed by linear combination of 50 orbitals of two $C_5H_5^-$ anion and 9 orbital of cobalt, as detailed in TABLE 1. The 59 atomic orbitals give LCAO approximation to 59 molecular orbitals. The eigen values of MOs are included in TABLE 2. The atomic orbitals are represented by χ and MOs by ϕ. 1-40χ are atomic orbitals of carbon, 41-49 of cobalt and 50-59χ of hydrogen.

The orbitals involved in σ bonding are not of interest, hence shall remain out of our discussion. The 2pz orbitals of ten carbons[7] and nine orbital of cobalt, that is in total 19 orbitals, are relevant to our discussion in respect of bonding between cobalt orbital and 2pz orbitals of $C_5H_5^-$. These atomic orbit-

TABLE 1 : Atomic orbitals(χ) of cobaltocene

(χ)	Atom	AO	(χ)	Atom	AO
1	1C	2s	31	8C	2py
2	1C	2px	32	8C	2pz
3	1C	2py	33	9C	2s
4	1C	2pz	34	9C	2px
5	2C	2s	35	9C	2py
6	2C	2px	36	9C	2pz
7	2C	2py	37	10C	2s
8	2C	2pz	38	10C	2px
9	3C	2s	39	10C	2py
10	3C	2px	40	10C	2pz
11	3C	2py	41	11Co	4s
12	3C	2pz	42	11Co	4px
13	4C	2s	43	11Co	4py
14	4C	2px	44	11Co	4pz
15	4C	2py	45	11Co	$3dx^2$-y^2
16	4C	2pz	46	11Co	$3dz^2$
17	5C	2s	47	11Co	3dxy
18	5C	2px	48	11Co	3dxz
19	5C	2py	49	11Co	3dyz
20	5C	2pz	50	12H	1s
21	6C	2s	51	13H	1s
22	6C	2px	52	14H	1s
23	6C	2py	53	15H	1s
24	6C	2pz	54	16H	1s
25	7C	2s	55	17H	1s
26	7C	2px	56	18H	1s
27	7C	2py	57	19H	1s
28	7C	2pz	58	20H	1s
29	8C	2s	59	21H	1s
30	8C	2px			

TABLE 2 : Eigen values of MO (Φ) of cobaltocene

MO(Φ)	Eigen values(eV)	MO(Φ)	Eigen values(eV)
1	-1.1027	31	-0.3583
2	-1.0916	32	-0.2812
3	-0.9068	33	-0.2718
4	-0.9022	34	-0.2345
5	-0.8721	35	-0.2311
6	-0.867	36	-0.0875
7	-0.6877	37	-0.053
8	-0.682	38	0.0158
9	-0.6797	39	0.0917
10	-0.6779	40	0.0954
11	-0.6064	41	0.1197
12	-0.6014	42	0.2197
13	-0.561	43	0.2847
14	-0.5479	44	0.2875
15	-0.5443	45	0.2982
16	-0.5355	46	0.3228
17	-0.5234	47	0.3621
18	-0.5171	48	0.4308
19	-0.511	49	0.4363
20	-0.5093	50	0.455
21	-0.5079	51	0.5015
22	-0.5073	52	0.7381
23	-0.4935	53	0.7600
24	-0.4798	54	1.0022
25	-0.4753	55	1.0718
26	-0.4716	56	2.0412
27	-0.4627	57	2.0771
28	-0.4495	58	2.2583
29	-0.4374	59	2.2719
30	-0.3906		

TABLE 3 : Eigen vector values of orbitals of cobalt in cobaltocene and their summation values

MOs	4s	4px	4py	4pz	$3dx^2-y^2$	$3dz^2$	3dxy	3dxz	3dyz
	χ_{41}	χ_{42}	χ_{43}	χ_{44}	χ_{45}	χ_{46}	χ_{47}	χ_{48}	χ_{49}
ϕ_{23}	-	-	-	-	0.2507	0.4737	0.2664	0.2327	-
ϕ_{24}	-	-	-	-	0.5537	-	0.4186	-	0.2781
ϕ_{25}	-	-	-	-	-	0.5281	-	0.3033	0.5717
ϕ_{26}	-	-	-	-	0.2652	-	0.5281	0.3717	0.3035
ϕ_{28}	-	-	-	-	-	-	0.2339	-	0.2297
ϕ_{30}	-	-	-	-	-	0.5131	0.2416	0.3996	-
$\phi_{3?}$	-	-	-	-	0.3741	-	-	0.3523	0.4225
ϕ_{36}	0.3346	0.9288		0.4070	-	-	-	-	-
ϕ_{37}	0.3259	-	0.8777	0.5655	-	-	-	-	-
ϕ_{38}	0.6188	-	-	0.2691	-	-	-	-	-
ϕ_{41}?	0.3195	-	0.3626	0.4823	-	-	-	-	-
ϕ_{42}	0.3148	-	0.3549	0.3479	-	-	-	-	-
ϕ_{46}?	0.2767	0.3026	-	0.3002	-	-	-	-	-
ϕ_{47}?	0.3329	-	0.2698	0.2911	-	-	-	-	-
ϕ_{50}	0.7239	-	0.2913	0.3794	-	-	-	-	-
$\phi_{5?}$?	0.5741	0.5317	0.3413	0.7871	-	-	-	-	-
ϕ_{54}	-	0.2380	0.2945	0.2227	-	-	-	-	-
ϕ_{55}	0.3738	0.2889	0.3878	-	-	-	-	-	-
ϕ_{56}	0.2297	-	-	-	-	-	-	-	-
Summation Values	4.4247	2.2900	3.1799	4.0523	1.4437	1.5086	1.6886	1.6596	1.8055

N.B.: - Orbitals having eigen vector values above 0.22 have only been considered

TABLE 4 : Eigen vector values of 2pz orbitals of carbon atoms of both the $C_5H_5^-$ and their summation values

MOS	1C	2C	3C	4C	5C	6C	7C	8C	9C	10C
	χ_4	χ_8	χ_{12}	χ_{16}	χ_{20}	χ_{24}	χ_{28}	χ_{32}	χ_{36}	χ_{40}
ϕ_{23}	-	-	-	0.2610	-	-	-	-	-	-
ϕ_{24}	-	-	-	-	-	-	-	-	-	-
ϕ_{25}	-	-	-	-	-	-	-	-	-	-
ϕ_{26}	-	-	-	-	-	-	-	-	-	-
ϕ_{28}	0.2825	-	0.2548	-		0.2836	0.2755	-	0.2362	-
ϕ_{30}	0.2899	-	0.2750	-	0.2474	0.2537	-	0.2649	-	-
ϕ_{31}	0.2835	0.3653	-	0.2853	0.2495	-	0.2476	-	-	-
ϕ_{36}	-	0.2348	-		-	-	-	0.2304	-	-
ϕ_{37}	-	-	-	0.2413	-	-	0.2212	-	-	-
ϕ_{38}	-	-	-	0.1591	-	0.1146	-	0.1874	0.2835	-
ϕ_{41}	0.2925	-	-	0.5471	0.2847	-	-	-	-	-
ϕ_{42}	-	-	-	-	-	-	-	-	-	-
ϕ_{46}	-	-	-	-	-	0.2580	-	-	0.260	-
ϕ_{47}	-	-	-	0.3743	-	-	-	-	-	-
ϕ_{50}	-	-	-	0.2733	-	-	-	-	-	0.2233
ϕ_{51}	-	-	-	-	-	-	-	-	-	0.5771
ϕ_{54}	-	-	-	-	0.2218	-	-	-	-	-
ϕ_{55}	-	-	-	-	-	-	-	-	-	-
ϕ_{56}	-	-	-	-	-	-	-	-	-	-
Summation Values	1.1484	0.6001	0.5298	1.8804	1.0307	0.9099	0.7443	0.6827	0.8057	0.80040

als are χ_4, χ_8, χ_{12}, χ_{16}, χ_{20}, χ_{24}, χ_{28}, χ_{32}, χ_{36}, χ_{40} of carbon and χ_{41}-χ_{49} of cobalt. The coefficients of these orbitals are the eigen vector values of χ which have been evaluated by molecular mechanics method using cache software. They express the forms of molecular orbital that is the extent of involvement of χ in the formation of ϕ. These values are included in TABLE 3, for metal orbitals and TABLE 4 for 2pz orbitals of carbon. The zero or near zero values have been excluded from the TABLES.

The first seven molecular orbitals, that is $\phi_{23\text{-}26}$, ϕ_{28}, ϕ_{30}, and $_{31}$, have contributions from 3d orbitals of the metal and the remaining twelve molecular orbitals(ϕ_{36}-ϕ_{38}, ϕ_{41}-ϕ_{42}, ϕ_{46}-ϕ_{47}, ϕ_{50}-ϕ_{51}, ϕ_{54}-ϕ_{55}, ϕ_{56}) have contribution from vacant 4s, and 4px, 4py and 4pz orbitals of the metal in TABLE 3. To examine the extent of involvement of 3d, 4s and 4p orbitals in the formation of molecular orbitals the values of coefficient of each orbital have been added to see the total involvement in all the 19 molecular orbitals. The summation values are placed at the bottom of the TABLE 3. The total contribution from each atomic orbital is also shown in figure 2. It is clearly indicated that 4s orbital has the maximum involvement out of 4s and 4p orbitals, and 3dyz orbital has the maximum involvement from the 3d orbitals. The sequence from the two series is as below.

4s, 4pz>4py>4px, 3dyz>3dxy>3dxz>$3dz^2$>$3dx^2$-y^2

Eigen values

The eigen values of 59 molecular orbitals of cobaltocene are listed in TABLE 2, out of which we shall discuss only 19 molecular orbitals described in TABLE 3 and 4. The first seven MOs are formed by various 3d orbitals and 2pz orbitals $C_5H_5^-$ ion. These orbitals are the most stable molecular orbitals between cobalt and 2pz orbitals of $C_5H_5^-$. They have their energies in the range -0.4935 to -0.3583e.V. The contribution of 3d metal and 2pz of carbon in the formation of ϕ_{23}-ϕ_{31} MOs is described as below.

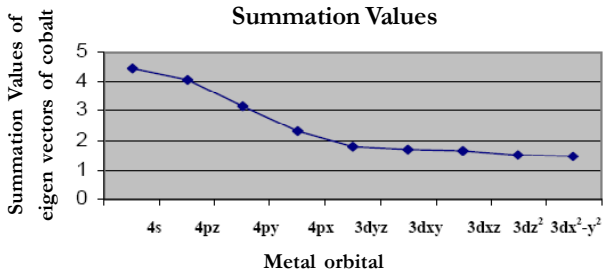

Figure 2 : Graph showing involvement of 3d, 4s only

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Figure 3 : Energy level diagram of cobaltocene

Molecular orbital (Φ)	Eigen values(e.v)	Energy levels	Atomic orbitals (χ)
56	2.0412	-	Co(4s)
55	1.0718	-	Co(4s,4px,4py)
54	1.0022	-	Co(4px,4py,4pz),C(2pz)
51	0.5015	-	Co(4s,4px,4py,4pz),C(2pz)
50	0.455	-	Co(4s,4py,4pz),C(2pz)
47	0.3621	-	Co(4s,4py,4pz),C(2pz)
46	0.3228	-	Co(4s,4px,4pz),C(2pz)
42	0.2197	-	Co(4s,4py,4pz)
41	0.1197	-	Co(4s,4py,4pz),C(2pz)
38	0.0158	-	Co(4s,4pz),C(2pz),
37	-0.053	-	Co(4s,4py,4pz), C(2pz),
36	-0.0875	-	Co(4s,4px,4pz),C(2pz) Co(4s,4py,4pz)
31	-0.3583	-	Co(3dx2-y2, 3dxz,3dyz) C(2pz)
30	-0.3906	-	Co(3dz2,3dxy3dxz),C(2pz)
29	-0.4374	-	Co(3dxy,3dyz), C(2pz), Co(3dx2-y2, 3dxy, 3dxz,3dyz)
23	-0.4935	-	Co(3dz2,3dxz,3dyz), Co(3dx2-y2,3dxy,3dyz)

ϕ_{23} - $\chi_{46},\chi_{47},\chi_{45},\chi_{48},\chi_{16}$,
ϕ_{24} - χ_{45},χ_{47},
ϕ_{25} - $\chi_{49},\chi_{46},\chi_{48}$,
ϕ_{26} - $\chi_{47},\chi_{48},\chi_{49}, \chi_{45}$,
ϕ_{28} - $\chi_{47},\chi_{49}, \chi_{24}, \chi_{4},\chi_{28}, \chi_{12},\chi_{36}$.
ϕ_{30} - $\chi_{46},\chi_{48},\chi_{47},\chi_{4},\chi_{12}, \chi_{32},\chi_{24}, \chi_{20}$,
ϕ_{31} - $\chi_{49},\chi_{45},\chi_{48}, \chi_{8}, \chi_{16},\chi_{4},\chi_{20}, \chi_{28}$,

The next twelve molecular orbitals are formed by interaction of 4s, 4px, 4py, and 4pz orbitals of metal and 2pz orbitals of carbon. These MOs are comparatively less stable and have their energies between -0.0875 and 2.0412e.V. The contribution of various atomic orbitals in the formation of molecular orbitals is presented below.

ϕ_{36} - $\chi_{42}, \chi_{44}, \chi_{41}, \chi_{8}, \chi_{32}$,
ϕ_{37} - $\chi_{43}, \chi_{44}, \chi_{41}, \chi_{16}, \chi_{28}$,
ϕ_{38} - $\chi_{41}, \chi_{44}, \chi_{36}, \chi_{32}, \chi_{16}, \chi_{24}$,
ϕ_{41} - $\chi_{44}, \chi_{43}, \chi_{41}, \chi_{16}, \chi_{4}, \chi_{20}$,
ϕ_{42} - $\chi_{43}, \chi_{44}, \chi_{41}$,
ϕ_{46} - $\chi_{42}, \chi_{44}, \chi_{41}, \chi_{36}, \chi_{24}$,
ϕ_{47} - $\chi_{41}, \chi_{44}, \chi_{43}, \chi_{16}$,
ϕ_{50} - $\chi_{41}, \chi_{44}, \chi_{43}, \chi_{16}, \chi_{40}$,
ϕ_{51} - $\chi_{44}, \chi_{41}, \chi_{42, 43}, \chi_{40}$,
ϕ_{54} - $\chi_{43}, \chi_{42}, \chi_{44}, \chi_{20}$,
ϕ_{55} - $\chi_{43}, \chi_{41}, \chi_{42}$,
ϕ_{56} - χ_{41}

Energy level diagram has been drawn for representing molecular orbital, their eigen values and involvement of atomic orbitals and is shown in figure 3.

TABLE 5 : contribution of electron in MO-23

χ	Atomic orbital	Eigen vector(c_{ri})	No. of electrons(n_i)	$n_{ri}=n_i c^2_{ri}$
3	1C-2py	0.1894	2	0.0717448
4	1C-2pz	0.1117	2	0.0249538
10	3C-2px	0.1792	2	0.0642252
14	4C-2px	0.1665	2	0.0554446
16	4C-2pz	0.2610	2	0.136242
24	6C-2pz	0.1332	2	0.0354844
32	8C-2pz	0.1701	2	0.057868
35	9C-2py	0.2135	2	0.0911644
36	9C-2pz	0.1118	2	0.0249984
45	11CO-3dx²-y²	0.2507	2	0.125701
46	11CO-3dz²	0.4737	2	0.4487834
47	11CO-3dxy	0.2664	2	0.141938
48	11CO-3dxz	0.2327	2	0.1082986
49	11CO-3dyz	0.1436	2	0.041242
50	12H-1s	0.1046	2	0.0218824

TABLE 6 : contribution of electron in MO-24

χ	Atomic orbital	Eigen vector(c_{ri})	No. of electrons(n_i)	$n_{ri}=n_i c^2_{ri}$
10	3C-2px	0.1183	2	0.0279898
12	3C-2pz	0.1153	2	0.0265882
14	4C-2px	0.1642	2	0.0539232
19	5C-2py	0.1184	2	0.0280372
22	6C-2px	0.1162	2	0.0270048
23	6C-2py	0.1573	2	0.0494866
24	6C-2pz	0.1220	2	0.029768
26	7C-2px	0.1660	2	0.055112
31	8C-2py	0.1793	2	0.064297
32	8C-2pz	0.1060	2	0.022472
34	9C-2px	0.1445	2	0.0417604
38	10C-2px	0.1349	2	0.036396
39	10C-2py	0.1000	2	0.02
45	11CO-3dx²-y²	0.5537	2	0.6131674
46	11CO-3dz²	0.1378	2	0.0379776
47	11CO-3dxy	0.4186	2	0.350452
48	11CO-3dxz	0.1448	2	0.041934
49	11CO-3dyz	0.2781	2	0.1546792
59	21H-1s	0.1015	2	0.0206046

Population analysis

The contribution of electrons in each occupied MO is calculated by using the population analysis method, introduced by Mulliken. This method apportions the electrons of n-electron molecule into net population n_r in the bas is function χ_r. Let there be n_i electrons in the MO ϕ_i(n_i=0, 1, 2) and let $n_{r,i}$ symbolize the contribution of electrons in the MO ϕ_i to the net population in χ_r, we have

$$n_{r,i} = n_i c^2_{ri} \quad \text{.....} \quad (1)$$

Where, c_{ri} is the coefficient of atomic orbitals for the i^{th} MO

TABLE 7 : Contribution of electron in MO-25

χ	Atomic orbital	Eigen vector(c_{ri})	No. of electrons(n_i)	$n_{ri}=n_ic^2_{ri}$
10	3C-2px	0.1254	2	0.0314504
16	4C-2pz	0.1338	2	0.0358048
24	6C-2pz	0.1464	2	0.042866
30	8C-2px	0.1343	2	0.036073
35	9C-2py	0.1092	2	0.0238492
39	10C-2py	0.1935	2	0.0748846
41	11CO-4s	0.1198	2	0.028704
46	11CO-3dz^2	0.5218	2	0.5445504
48	11CO-3dxz	0.3033	2	0.1839818
49	11CO-3dyz	0.5717	2	0.6536818
53	15H-1s	0.1298	2	0.033696

TABLE 8 : Contribution of electron in MO-26

χ	Atomic orbital	Eigen vector(c_{ri})	No. of electrons(n_i)	$n_{ri}=n_ic^2_{ri}$
2	1C-2px	0.1738	2	0.0604128
6	2C-2px	0.1271	2	0.0323088
8	2C-2pz	0.1818	2	0.0661024
16	4C-2pz	0.1756	2	0.0616708
34	9C-2px	0.2568	2	0.1318924
38	10C-2px	0.1466	2	0.0429832
39	10C-2py	01383	2	0.0382538
40	10C-2pz	0.1472	2	0.0433356
45	11CO-3dx^2-y^2	0.2652	2	0.140662
46	11CO-3dz^2	0.1081	2	0.0467424
47	11CO-3dxy	0.5281	2	0.5577792
48	11CO-3dxz	0.3717	2	0.2763218
49	11CO-3dyz	0.3035	2	0.1842246

TABLE 9 : Contribution of electron in MO-27

χ	Atomic orbital	Eigen vector(c_{ri})	No. of electrons(n_i)	$n_{ri}=n_ic^2_{ri}$
7	2C-2py	0.1239	2	0.030702
8	2C-2pz	0.3281	2	0.21530
11	3C-2py	0.1108	2	0.024554
12	3C-2pz	0.2463	2	0.121328
14	4C-2px	0.1247	2	0.0311
16	4C-2pz	0.2716	2	0.147334
18	5C-2px	0.1760	2	0.061952
19	5C-2py	0.2181	2	0.095136
20	5C-2pz	0.1675	2	0.056112
22	6C-2px	0.1482	2	0.043926
24	6C-2pz	0.2369	2	0.112244
27	7C-2py	0.1709	2	0.058414
28	7C-2pz	0.2131	2	0.090824
38	10C-2px	0.1430	2	0.040898
40	10C-2pz	0.1374	2	0.037758
45	11CO-3dx^2-y^2	0.1445	2	0.04176
47	11CO-3dxy	0.2931	2	0.171816
48	11CO-3dxz	0.2063	2	0.08512
59	21H-1s	0.1796	2	0.064512

(r =1-30).

Equation-1, has been solved for 59 electrons of 30 molecular orbitals in cobaltocene, each MO has two electrons except the MO-30 which has one electron. The coefficient of atomic orbitals that is c_{ri} is the eigen vector value. Since our interest is only in MO-23-30, we have tabulated the results of these MOs in TABLES 5-12. The result of solution of equation-1 for MOs of 23-30 clearly indicates that main contribution of electrons in MO-23 is from 2pz orbitals of 4c, and 9c and from Co it is from 3dz^2, 3dx^2-y^2, 3dxy, 3dxz. In MO-24 it is from 3dx^2-y^2, 3dxy, and 3dyz of cobalt. Briefly the contribution of electrons in other MOs can be presented as below: -

MO-25 - Co-3dyz, 3dz^2, 3dxz

TABLE 10 : Contribution of electron in MO-28

χ	Atomic orbital	Eigen vector(c_{ri})	No. of electrons(n_i)	$n_{ri}=n_ic^2_{ri}$
4	1C-2pz	0.2825	2	0.1596124
11	3C-2py	0.1404	2	0.0394244
12	3C-2pz	0.2548	2	0.129846
14	4C-2px	0.1343	2	0.036073
15	4C-2py	0.1270	2	0.032258
16	4C-2pz	0.1501	2	0.04506
18	5C-2px	0.1116	2	0.0249092
19	5C-2py	0.1774	2	0.0629416
20	5C-2pz	0.1591	2	0.0499912
23	6C-2py	0.1134	2	0.0257192
24	6C-2pz	0.2836	2	0.160858
26	7C-2px	0.1105	2	0.0244204
28	7C-2pz	0.2755	2	0.1518006
32	8C-2pz	0.2290	2	0.0567846
34	9C-2px	0.2130	2	0.104882
35	9C-2py	0.2130	2	0.090738
36	9C-2pz	0.2362	2	0.1115808
45	11CO-3dx^2-y^2	0.1103	2	0.0243322
46	11CO-3dz^2	0.1402	2	0.039312
47	11CO-3dxy	0.2339	2	0.1094184

TABLE 11 : Contribution of electron in MO-29

χ	Atomic orbital	Eigen vector(c_{ri})	No. of electrons(n_i)	$n_{ri}=n_ic^2_{ri}$
8	2C-2pz	0.2024	2	0.081932
12	3C-2pz	0.1605	2	0.05152
20	5C-2pz	0.1336	2	0.035698
22	6C-2px	0.1780	2	0.063368
23	6C-2py	0.1788	2	0.063938
24	6C-2pz	0.1537	2	0.047248
26	7C-2px	0.1194	2	0.028512
28	7C-2pz	0.1515	2	0.045904
30	8C-2px	0.1932	2	0.074652
34	9C-2px	0.2557	2	0.130764
38	10C-2px	0.3190	2	0.203522
39	10C-2py	0.3829	2	0.293224
40	10C-2pz	0.3061	2	0.187394
46	11CO-3dz^2	0.2052	2	0.084214
47	11CO-3dxy	0.2116	2	0.08955
48	11CO-3dxz	0.1243	2	0.0309
56	18H-1s	0.1009	2	0.020362
59	21H-1s	0.1658	2	0.05498

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TABLE 12 : Contribution of electron in MO-30

χ	Atomic orbital	Eigen vector(c_{ri})	No. of electrons(n_i)	$n_{ri}=n_ic^2_{ri}$
4	1C-2pz	0.2899	1	0.2899
11	3C-2py	0.1280	1	0.1280
12	3C-2pz	0.2750	1	0.2750
16	4C-2pz	0.1276	1	0.1276
19	5C-2py	0.1543	1	0.1543
20	5C-2pz	0.2474	1	0.2474
22	6C-2px	0.1130	1	0.1130
23	6C-2py	0.1436	1	0.1436
24	6C-2pz	0.2537	1	0.2537
30	8C-2px	0.1087	1	0.1087
31	8C-2py	0.1916	1	0.1916
32	8C-2pz	0.2649	1	0.2649
34	9C-2px	0.1309	1	0.1309
36	9C-2pz	0.1558	1	0.1558
40	10C-2pz	0.2073	1	0.2073
46	11CO-3dz^2	0.5131	1	0.5131
47	11CO-3dxy	0.2416	1	0.2416
48	11CO-3dxz	0.3996	1	0.3996
49	11CO-3dyz	0.1363	1	0.1363

MO-26 - 9c - 2px, Co- 3dxy, 3dxz, 3dyz, 3dx^2-y^2

MO-27 - 2c-2pz, 4c-2pz, 3c-2pz, 6c-2pz, 7c-2pz, 5c-2py, 11Co-3dxy

MO-28 - 6c - 2pz, 1c-2pz, 7c-2pz, 3c-2pz, 9c-2pz, 9c-2px, Co-3dxy

MO-29 - 10c-2py, 10c-2px, 10c-2pz, 9c-2px, 11Co-3dxy

MO-30 - 1c- 2pz, 3c-2pz, 8c-2pz, 6c-2pz, 5c-2pz, Co-3dz^2, 3dxz, 3dxy

The results very clearly indicate that only 2pz orbitals of carbon of $C_5H_5^-$, and 3d orbitals of cobalt provide electrons to molecular orbitals 23-30.

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