Standard redox potential of $[Co(bpy)_3]^{2+/3+}$ and $[Co(phen)_3]^{2+/3+}$ redox couples using a density functional theory protocol.

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Supporting information

Table S1 Triplet state spin contamination

CAM-B3LYP	Spin	S(S+1)	S^2
Def2-SVP	1	2.00	2.001385
Def2-TZVP	1	2.00	2.002777
TPSSh			
Def2-SVP	1	2.00	2.000199
Def2-TZVP	1	2.00	2.000252

Geometric parameters of the $[Co(bpy)_3]^{3+} \rightarrow [Co(bpy)_3]^{2+}$***. The structures were optimized at the TPSSh/def2TZVP level. Where Atom 1 is Cobalt and atoms 2-7 are Nitrogen atoms.***

singlet - [Co(bpy)3]3+

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.9607	-DE/DX = 0.0
R2	R(1,3)	1.9607	-DE/DX = 0.0
R3	R(1,4)	1.9606	-DE/DX = 0.0
R4	R(1,5)	1.9606	-DE/DX = 0.0
R5	R(1,6)	1.9606	-DE/DX = 0.0
R6	R(1,7)	1.9608	-DE/DX = 0.0
A1	A(2,1,3)	82.5641	-DE/DX = 0.0
A2	A(2,1,4)	88.0032	-DE/DX = 0.0
A3	A(2,1,5)	94.7633	-DE/DX = 0.0
A4	A(2,1,7)	94.7627	-DE/DX = 0.0
A5	A(3,1,4)	94.7723	-DE/DX = 0.0
A6	A(3,1,6)	94.771	-DE/DX = 0.0
A7	A(3,1,7)	87.9907	-DE/DX = 0.0
A8	A(4,1,5)	82.5651	-DE/DX = 0.0
A9	A(4,1,6)	94.7771	-DE/DX = 0.0
A10	A(5,1,6)	88.01	-DE/DX = 0.0
A11	A(5,1,7)	94.7801	-DE/DX = 0.0
A12	A(6,1,7)	82.5646	-DE/DX = 0.0

doublet - [Co(bpy)3]2+

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	2.2102	-DE/DX = 0.0
R2	R(1,3)	1.9899	-DE/DX = 0.0
R3	R(1,4)	1.9686	-DE/DX = 0.0
R4	R(1,5)	1.9686	-DE/DX = 0.0
R5	R(1,6)	2.2097	-DE/DX = 0.0
R6	R(1,7)	1.9897	-DE/DX = 0.0

! A1	A(2,1,3)	78.2073	-DE/DX =	0.0 !
! A2	A(2,1,4)	89.3014	-DE/DX =	0.0 !
! A3	A(2,1,5)	95.3125	-DE/DX =	0.0 !
! A4	A(2,1,7)	97.3382	-DE/DX =	0.0 !
! A5	A(3,1,4)	95.0382	-DE/DX =	0.0 !
! A6	A(3,1,6)	97.3376	-DE/DX =	0.0 !
! A7	A(3,1,7)	88.7251	-DE/DX =	0.0 !
! A8	A(4,1,5)	81.8585	-DE/DX =	0.0 !
! A9	A(4,1,6)	95.3412	-DE/DX =	0.0 !
! A10	A(5,1,6)	89.3366	-DE/DX =	0.0 !
! A11	A(5,1,7)	95.0506	-DE/DX =	0.0 !
! A12	A(6,1,7)	78.2129	-DE/DX =	0.0 !

quartet - [Co(bpy)3]2+

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	
! R1	R(1,2)	2.1536	-DE/DX =	0.0 !
! R2	R(1,3)	2.1544	-DE/DX =	0.0 !
! R3	R(1,4)	2.1545	-DE/DX =	0.0 !
! R4	R(1,5)	2.1536	-DE/DX =	0.0 !
! R5	R(1,6)	2.1542	-DE/DX =	0.0 !
! R6	R(1,7)	2.1538	-DE/DX =	0.0 !
! A1	A(2,1,3)	76.1671	-DE/DX =	0.0 !
! A2	A(2,1,4)	88.5322	-DE/DX =	0.0 !
! A3	A(2,1,5)	97.9413	-DE/DX =	0.0 !
! A4	A(2,1,7)	97.9446	-DE/DX =	0.0 !
! A5	A(3,1,4)	97.8492	-DE/DX =	0.0001 !
! A6	A(3,1,6)	97.8746	-DE/DX =	0.0 !
! A7	A(3,1,7)	88.5332	-DE/DX =	0.0 !
! A8	A(4,1,5)	76.1727	-DE/DX =	0.0 !
! A9	A(4,1,6)	97.8494	-DE/DX =	0.0 !
! A10	A(5,1,6)	88.5106	-DE/DX =	0.0 !
! A11	A(5,1,7)	97.9388	-DE/DX =	0.0 !
! A12	A(6,1,7)	76.1649	-DE/DX =	0.0 !

Atomic contributions to molecular orbitals from Gaussian (Version=ES64L-G16RevC.02)

{singlet - [Co(bpy)3]3+

 Atomic contributions to Alpha molecular orbitals:
 Alpha occ 126 OE=-0.619 is C16-p=0.0885
 Alpha occ 127 OE=-0.611 is C12-p=0.0512
 Alpha occ 128 OE=-0.609 is C20-p=0.1035
 Alpha occ 129 OE=-0.609 is C38-p=0.1141 C48-p=0.1088
 Alpha occ 130 OE=-0.595 is Co1-d=0.5064
 Alpha occ 131 OE=-0.595 is Co1-d=0.5066
 Alpha occ 132 OE=-0.593 is Co1-d=0.5300
 Alpha occ 133 OE=-0.566 is C10-p=0.0450
 Alpha occ 134 OE=-0.564 is C28-p=0.0914
 Alpha occ 135 OE=-0.564 is C10-p=0.0721
 Alpha vir 136 OE=-0.428 is Co1-d=0.5955
 Alpha vir 137 OE=-0.428 is Co1-d=0.5957
 Alpha vir 138 OE=-0.415 is C17-p=0.0731
 Alpha vir 139 OE=-0.415 is C35-p=0.0649
 Alpha vir 140 OE=-0.411 is C53-p=0.0388
 Alpha vir 141 OE=-0.386 is C44-p=0.0542
 Alpha vir 142 OE=-0.376 is C60-p=0.0513
 Alpha vir 143 OE=-0.374 is C14-p=0.1108 C18-p=0.1025
 Alpha vir 144 OE=-0.374 is C32-p=0.1050
 Alpha vir 145 OE=-0.368 is C24-p=0.0747
}

{doublet - [Co(bpy)3]2+

 Atomic contributions to Alpha molecular orbitals:
 Alpha occ 127 OE=-0.488 is N6-p=0.0886
 Alpha occ 128 OE=-0.488 is C12-p=0.1194 C48-p=0.1193 N2-p=0.1113 N6-p=0.1106 C50-p=0.1033
 Alpha occ 129 OE=-0.487 is N2-p=0.1181 C12-p=0.1174 N6-p=0.1171 C48-p=0.1161
 Alpha occ 130 OE=-0.450 is Co1-d=0.3286
 Alpha occ 131 OE=-0.450 is Co1-d=0.2360
 Alpha occ 132 OE=-0.445 is C46-p=0.0807
 Alpha occ 133 OE=-0.442 is Co1-d=0.2561
 Alpha occ 134 OE=-0.424 is Co1-d=0.8567
 Alpha occ 135 OE=-0.421 is Co1-d=0.8735
 Alpha occ 136 OE=-0.377 is Co1-d=0.5712
 Alpha vir 137 OE=-0.295 is C34-p=0.1095 C35-p=0.1095 N4-p=0.1049 N5-p=0.1049
 Alpha vir 138 OE=-0.291 is C53-p=0.0702
 Alpha vir 139 OE=-0.288 is Co1-d=0.0610
 Alpha vir 140 OE=-0.282 is Co1-d=0.5824
 Alpha vir 141 OE=-0.267 is C42-p=0.0756
 Alpha vir 142 OE=-0.258 is C32-p=0.0855
 Alpha vir 143 OE=-0.256 is C24-p=0.0888

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 Alpha vir 144 OE=-0.253 is C38-p=0.0643
 Alpha vir 145 OE=-0.247 is C44-p=0.0918
 Alpha vir 146 OE=-0.246 is C8-p=0.0980

 Atomic contributions to Beta  molecular orbitals:
 Beta  occ 126 OE=-0.493 is C18-p=0.1023 C54-p=0.1023
 Beta  occ 127 OE=-0.487 is C48-p=0.1258 C12-p=0.1210 N6-p=0.1143 N2-p=0.1100 C50-p=0.1062 C14
 Beta  occ 128 OE=-0.487 is C12-p=0.1313 C48-p=0.1261 N2-p=0.1100 N6-p=0.1055
 Beta  occ 129 OE=-0.485 is N2-p=0.1674 N6-p=0.1663
 Beta  occ 130 OE=-0.450 is C40-p=0.1305 C28-p=0.1305 C32-p=0.1196 C36-p=0.1196 C42-p=0.1018 C
 Beta  occ 131 OE=-0.445 is C46-p=0.0674
 Beta  occ 132 OE=-0.445 is C10-p=0.0812
 Beta  occ 133 OE=-0.421 is Co1-d=0.8310
 Beta  occ 134 OE=-0.410 is Co1-d=0.8623
 Beta  occ 135 OE=-0.408 is Co1-d=0.8939
 Beta  vir 136 OE=-0.294 is C34-p=0.1123 C35-p=0.1122 N4-p=0.1063 N5-p=0.1063 C28-p=0.1039 C40
 Beta  vir 137 OE=-0.290 is C53-p=0.0680
 Beta  vir 138 OE=-0.287 is C17-p=0.0663
 Beta  vir 139 OE=-0.267 is C42-p=0.0741
 Beta  vir 140 OE=-0.258 is C32-p=0.0867
 Beta  vir 141 OE=-0.256 is C24-p=0.0846
 Beta  vir 142 OE=-0.253 is C38-p=0.0625
 Beta  vir 143 OE=-0.252 is Co1-d=0.6494
 Beta  vir 144 OE=-0.248 is C44-p=0.0869
 Beta  vir 145 OE=-0.245 is C8-p=0.0925
}

{quartet - [Co(bpy)3]2+

 Atomic contributions to Alpha molecular orbitals:
 Alpha occ 128 OE=-0.488 is C30-p=0.1037 C12-p=0.1031
 Alpha occ 129 OE=-0.488 is C56-p=0.0986
 Alpha occ 130 OE=-0.487 is N5-p=0.0549
 Alpha occ 131 OE=-0.470 is Co1-d=0.6480
 Alpha occ 132 OE=-0.470 is Co1-d=0.6480
 Alpha occ 133 OE=-0.444 is C46-p=0.0476
 Alpha occ 134 OE=-0.443 is C58-p=0.0803
 Alpha occ 135 OE=-0.443 is C22-p=0.0963
 Alpha occ 136 OE=-0.416 is Co1-d=0.3914 N4-p=0.1175 N7-p=0.1148
 Alpha occ 137 OE=-0.416 is Co1-d=0.3914 N2-p=0.1060 N6-p=0.1000
 Alpha vir 138 OE=-0.289 is C35-p=0.0773
 Alpha vir 139 OE=-0.289 is C17-p=0.0643
 Alpha vir 140 OE=-0.286 is C46-p=0.0407
 Alpha vir 141 OE=-0.263 is C42-p=0.0547
 Alpha vir 142 OE=-0.255 is C18-p=0.1046 C14-p=0.1004
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 Alpha vir 143 OE=-0.255 is C54-p=0.1064 C50-p=0.1025
 Alpha vir 144 OE=-0.250 is C26-p=0.0479
 Alpha vir 145 OE=-0.245 is C38-p=0.0717
 Alpha vir 146 OE=-0.245 is C20-p=0.0905
 Alpha vir 147 OE=-0.206 is C40-p=0.0516

 Atomic contributions to Beta  molecular orbitals:
 Beta  occ 125 OE=-0.494 is C8-p=0.0741
 Beta  occ 126 OE=-0.494 is C44-p=0.0800
 Beta  occ 127 OE=-0.486 is C12-p=0.1022
 Beta  occ 128 OE=-0.486 is C48-p=0.1037
 Beta  occ 129 OE=-0.485 is N6-p=0.0623
 Beta  occ 130 OE=-0.444 is C46-p=0.0468
 Beta  occ 131 OE=-0.443 is C58-p=0.0785
 Beta  occ 132 OE=-0.443 is C22-p=0.0948
 Beta  occ 133 OE=-0.426 is Co1-d=0.8618
 Beta  occ 134 OE=-0.426 is Co1-d=0.8618
 Beta  vir 135 OE=-0.302 is Co1-d=0.8805
 Beta  vir 136 OE=-0.289 is C35-p=0.0718
 Beta  vir 137 OE=-0.289 is C17-p=0.0711
 Beta  vir 138 OE=-0.285 is C46-p=0.0417
 Beta  vir 139 OE=-0.263 is C42-p=0.0544
 Beta  vir 140 OE=-0.255 is C18-p=0.1024
 Beta  vir 141 OE=-0.255 is C54-p=0.1041
 Beta  vir 142 OE=-0.246 is Co1-d=0.0690
 Beta  vir 143 OE=-0.244 is C26-p=0.0691
 Beta  vir 144 OE=-0.244 is C20-p=0.0900
}
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NATURAL LOCALIZED MOLECULAR ORBITAL (NLMO) ANALYSIS

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For convenience, I will just provide two text files containing the NLMOs of the doublet an

{doublet - [Co(bpy)3]2+

Read the text file: Co_bpy3_2plus_B3LYP_GD3BJ_LANL2DZ_doublet_NBO.txt
Analyse the alpha and beta spin localized orbitals. Which is the probable SOMO. Focus on t
}

{quartet - [Co(bpy)3]2+

Read the text file: Co_bpy3_2plus_B3LYP_GD3BJ_LANL2DZ_quartet_NBO.txt
Analyse the alpha and beta spin localized orbitals. Focus on the active orbitals
}
```

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

{singlet - [Co(bpy)3]3+

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
from unit 2 to unit 1				
44. LP (1) N 2	131. LV (1)Co 1	106.63	0.15	0.112
44. LP (1) N 2	132. LV (2)Co 1	0.21	0.15	0.005
44. LP (1) N 2	133. LV (3)Co 1	24.20	1.01	0.140
44. LP (1) N 2	218. RY (4)Co 1	1.70	5.93	0.090
44. LP (1) N 2	225. RY (11)Co 1	0.06	1.66	0.009
44. LP (1) N 2	226. RY (12)Co 1	0.06	1.66	0.009
45. LP (1) N 3	131. LV (1)Co 1	22.81	0.15	0.052
45. LP (1) N 3	132. LV (2)Co 1	84.02	0.15	0.100
45. LP (1) N 3	133. LV (3)Co 1	24.19	1.01	0.140
45. LP (1) N 3	218. RY (4)Co 1	1.70	5.93	0.090
45. LP (1) N 3	226. RY (12)Co 1	0.12	1.66	0.013
from unit 3 to unit 1				
46. LP (1) N 4	131. LV (1)Co 1	30.81	0.15	0.060
46. LP (1) N 4	132. LV (2)Co 1	76.02	0.15	0.095
46. LP (1) N 4	133. LV (3)Co 1	24.19	1.01	0.140
46. LP (1) N 4	218. RY (4)Co 1	1.70	5.93	0.090
46. LP (1) N 4	225. RY (11)Co 1	0.11	1.66	0.012
47. LP (1) N 5	131. LV (1)Co 1	22.72	0.15	0.052
47. LP (1) N 5	132. LV (2)Co 1	84.11	0.15	0.100
47. LP (1) N 5	133. LV (3)Co 1	24.19	1.01	0.140
47. LP (1) N 5	218. RY (4)Co 1	1.70	5.93	0.090
47. LP (1) N 5	226. RY (12)Co 1	0.12	1.66	0.012
from unit 4 to unit 1				
48. LP (1) N 6	131. LV (1)Co 1	106.64	0.15	0.112
48. LP (1) N 6	132. LV (2)Co 1	0.20	0.15	0.005
48. LP (1) N 6	133. LV (3)Co 1	24.20	1.01	0.140
48. LP (1) N 6	218. RY (4)Co 1	1.70	5.93	0.090
48. LP (1) N 6	225. RY (11)Co 1	0.08	1.66	0.010
49. LP (1) N 7	131. LV (1)Co 1	30.91	0.15	0.061
49. LP (1) N 7	132. LV (2)Co 1	75.93	0.15	0.095
49. LP (1) N 7	133. LV (3)Co 1	24.19	1.01	0.140
49. LP (1) N 7	218. RY (4)Co 1	1.70	5.93	0.090
49. LP (1) N 7	225. RY (11)Co 1	0.12	1.66	0.012

}

{doublet - [Co(bpy)3]2+

Alpha Spin

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
from unit 2 to unit 1				
45. LP (1) N 2	133. LV (2)Co 1	6.49	0.71	0.086
45. LP (1) N 2	218. RY (4)Co 1	0.26	6.83	0.053
45. LP (1) N 2	225. RY (11)Co 1	0.05	2.32	0.013
46. LP (1) N 3	132. LV (1)Co 1	25.82	0.20	0.091
46. LP (1) N 3	133. LV (2)Co 1	10.66	0.73	0.112
46. LP (1) N 3	218. RY (4)Co 1	0.36	6.85	0.063
46. LP (1) N 3	225. RY (11)Co 1	0.22	2.34	0.029
from unit 3 to unit 1				
47. LP (1) N 4	132. LV (1)Co 1	26.43	0.21	0.093
47. LP (1) N 4	133. LV (2)Co 1	10.97	0.74	0.114
47. LP (1) N 4	218. RY (4)Co 1	0.40	6.85	0.066
47. LP (1) N 4	225. RY (11)Co 1	0.20	2.34	0.028
48. LP (1) N 5	132. LV (1)Co 1	26.41	0.21	0.093
48. LP (1) N 5	133. LV (2)Co 1	10.97	0.74	0.113
48. LP (1) N 5	218. RY (4)Co 1	0.40	6.85	0.066
48. LP (1) N 5	225. RY (11)Co 1	0.20	2.34	0.028
from unit 4 to unit 1				
49. LP (1) N 6	133. LV (2)Co 1	6.50	0.71	0.086
49. LP (1) N 6	218. RY (4)Co 1	0.26	6.83	0.053
49. LP (1) N 6	225. RY (11)Co 1	0.05	2.32	0.013
50. LP (1) N 7	132. LV (1)Co 1	25.83	0.20	0.091
50. LP (1) N 7	133. LV (2)Co 1	10.66	0.73	0.112
50. LP (1) N 7	218. RY (4)Co 1	0.36	6.85	0.063
50. LP (1) N 7	225. RY (11)Co 1	0.22	2.34	0.029

Beta-spin

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
from unit 2 to unit 1				
44. LP (1) N 2	132. LV (2)Co 1	9.79	0.29	0.068

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   44. LP ( 1) N  2          133. LV ( 3)Co  1          7.97    0.70   0.094
   44. LP ( 1) N  2          218. RY ( 4)Co  1          0.19    6.80   0.045
   44. LP ( 1) N  2          225. RY (11)Co  1          0.08    2.36   0.018
   45. LP ( 1) N  3          131. LV ( 1)Co  1         22.50    0.25   0.094
   45. LP ( 1) N  3          132. LV ( 2)Co  1          7.86    0.33   0.064
   45. LP ( 1) N  3          133. LV ( 3)Co  1          9.21    0.73   0.104
   45. LP ( 1) N  3          218. RY ( 4)Co  1          0.29    6.84   0.056
   45. LP ( 1) N  3          225. RY (11)Co  1          0.12    2.40   0.021

 from unit  3 to unit  1
   46. LP ( 1) N  4          131. LV ( 1)Co  1         23.44    0.25   0.096
   46. LP ( 1) N  4          132. LV ( 2)Co  1          7.91    0.33   0.065
   46. LP ( 1) N  4          133. LV ( 3)Co  1          9.44    0.73   0.105
   46. LP ( 1) N  4          216. RY ( 2)Co  1          0.03    1.07   0.007
   46. LP ( 1) N  4          218. RY ( 4)Co  1          0.31    6.84   0.058
   46. LP ( 1) N  4          225. RY (11)Co  1          0.10    2.40   0.020
   47. LP ( 1) N  5          131. LV ( 1)Co  1         23.43    0.25   0.096
   47. LP ( 1) N  5          132. LV ( 2)Co  1          7.91    0.33   0.065
   47. LP ( 1) N  5          133. LV ( 3)Co  1          9.44    0.73   0.105
   47. LP ( 1) N  5          216. RY ( 2)Co  1          0.03    1.07   0.007
   47. LP ( 1) N  5          218. RY ( 4)Co  1          0.31    6.84   0.058
   47. LP ( 1) N  5          225. RY (11)Co  1          0.10    2.40   0.020

 from unit  4 to unit  1
   48. LP ( 1) N  6          132. LV ( 2)Co  1          9.81    0.29   0.068
   48. LP ( 1) N  6          133. LV ( 3)Co  1          7.97    0.70   0.094
   48. LP ( 1) N  6          218. RY ( 4)Co  1          0.19    6.80   0.045
   48. LP ( 1) N  6          225. RY (11)Co  1          0.08    2.36   0.018
   49. LP ( 1) N  7          131. LV ( 1)Co  1         22.51    0.25   0.094
   49. LP ( 1) N  7          132. LV ( 2)Co  1          7.86    0.33   0.064
   49. LP ( 1) N  7          133. LV ( 3)Co  1          9.21    0.73   0.104
   49. LP ( 1) N  7          218. RY ( 4)Co  1          0.29    6.84   0.056
   49. LP ( 1) N  7          225. RY (11)Co  1          0.12    2.40   0.021
}

{quartet - [Co(bpy)3]2+

Alpha Spin

                                                      E(2) E(NL)-E(L) F(L,NL)
      Donor (L) NBO              Acceptor (NL) NBO     kcal/mol   a.u.    a.u.
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 from unit  2 to unit  1
   46. LP ( 1) N  2          133. LV ( 1)Co  1          9.56    0.59   0.095
   46. LP ( 1) N  2          218. RY ( 4)Co  1          0.41    6.29   0.064
```

46. LP (1) N 2	224. RY (10)Co 1	0.03	1.40	0.008
47. LP (1) N 3	133. LV (1)Co 1	9.55	0.59	0.095
47. LP (1) N 3	218. RY (4)Co 1	0.41	6.29	0.064
47. LP (1) N 3	224. RY (10)Co 1	0.03	1.40	0.008
from unit 3 to unit 1				
48. LP (1) N 4	133. LV (1)Co 1	9.56	0.59	0.095
48. LP (1) N 4	218. RY (4)Co 1	0.41	6.29	0.064
48. LP (1) N 4	224. RY (10)Co 1	0.03	1.40	0.008
49. LP (1) N 5	133. LV (1)Co 1	9.56	0.59	0.095
49. LP (1) N 5	218. RY (4)Co 1	0.41	6.29	0.064
49. LP (1) N 5	224. RY (10)Co 1	0.03	1.40	0.008
from unit 4 to unit 1				
50. LP (1) N 6	133. LV (1)Co 1	9.56	0.59	0.095
50. LP (1) N 6	218. RY (4)Co 1	0.41	6.29	0.064
50. LP (1) N 6	224. RY (10)Co 1	0.03	1.40	0.008
51. LP (1) N 7	133. LV (1)Co 1	9.56	0.59	0.095
51. LP (1) N 7	218. RY (4)Co 1	0.41	6.29	0.064
51. LP (1) N 7	224. RY (10)Co 1	0.03	1.40	0.008

Beta-spin

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
from unit 2 to unit 1				
43. LP (1) N 2	130. LV (1)Co 1	11.83	0.29	0.074
43. LP (1) N 2	131. LV (2)Co 1	3.02	0.29	0.037
43. LP (1) N 2	132. LV (3)Co 1	9.53	0.60	0.095
43. LP (1) N 2	218. RY (4)Co 1	0.32	6.24	0.057
44. LP (1) N 3	131. LV (2)Co 1	14.83	0.29	0.083
44. LP (1) N 3	132. LV (3)Co 1	9.53	0.60	0.095
44. LP (1) N 3	218. RY (4)Co 1	0.32	6.24	0.057
from unit 3 to unit 1				
45. LP (1) N 4	130. LV (1)Co 1	10.72	0.29	0.071
45. LP (1) N 4	131. LV (2)Co 1	4.13	0.29	0.044
45. LP (1) N 4	132. LV (3)Co 1	9.53	0.60	0.095
45. LP (1) N 4	218. RY (4)Co 1	0.32	6.24	0.057
46. LP (1) N 5	130. LV (1)Co 1	0.05	0.29	0.005
46. LP (1) N 5	131. LV (2)Co 1	14.80	0.29	0.083
46. LP (1) N 5	132. LV (3)Co 1	9.53	0.60	0.095
46. LP (1) N 5	218. RY (4)Co 1	0.32	6.24	0.057
from unit 4 to unit 1				

```
   47. LP ( 1) N  6          130. LV ( 1)Co  1          11.54    0.29   0.073
   47. LP ( 1) N  6          131. LV ( 2)Co  1           3.31    0.29   0.039
   47. LP ( 1) N  6          132. LV ( 3)Co  1           9.53    0.60   0.095
   47. LP ( 1) N  6          218. RY ( 4)Co  1           0.32    6.24   0.057
   48. LP ( 1) N  7          130. LV ( 1)Co  1          10.39    0.29   0.069
   48. LP ( 1) N  7          131. LV ( 2)Co  1           4.46    0.29   0.045
   48. LP ( 1) N  7          132. LV ( 3)Co  1           9.53    0.60   0.095
   48. LP ( 1) N  7          218. RY ( 4)Co  1           0.32    6.24   0.057
}
```

Geometric parameters of the $[Co(phen)_3]^{3+}$ ***and*** $[Co(phen)_3]^{2+}$***. The structures were optimized at the TPSSh/def2TZVP level. Where Atom 1 is Cobalt and atoms 2-7 are Nitrogen atoms.***

```
{singlet - [Co(phen)3]3+
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
-------------------------------------------------------------------------------
Bond lengths:
! R1    R(1,2)                  1.9601         calculate D2E/DX2 analytically  !
! R2    R(1,3)                  1.9602         calculate D2E/DX2 analytically  !
! R3    R(1,4)                  1.9602         calculate D2E/DX2 analytically  !
! R4    R(1,5)                  1.9602         calculate D2E/DX2 analytically  !
! R5    R(1,6)                  1.9601         calculate D2E/DX2 analytically  !
! R6    R(1,7)                  1.9601         calculate D2E/DX2 analytically  !

Bond Angles:
! A1    A(2,1,3)               84.8759         calculate D2E/DX2 analytically  !
! A2    A(2,1,4)               93.5006         calculate D2E/DX2 analytically  !
! A3    A(2,1,6)               93.4927         calculate D2E/DX2 analytically  !
! A4    A(2,1,7)               88.1699         calculate D2E/DX2 analytically  !
! A5    A(3,1,4)               88.1604         calculate D2E/DX2 analytically  !
! A6    A(3,1,5)               93.498          calculate D2E/DX2 analytically  !
! A7    A(3,1,7)               93.5092         calculate D2E/DX2 analytically  !
! A8    A(4,1,5)               84.8738         calculate D2E/DX2 analytically  !
! A9    A(4,1,6)               93.4936         calculate D2E/DX2 analytically  !
! A10   A(5,1,6)               88.1747         calculate D2E/DX2 analytically  !
! A11   A(5,1,7)               93.4974         calculate D2E/DX2 analytically  !
! A12   A(6,1,7)               84.8787         calculate D2E/DX2 analytically  !
}
```

{doublet - [Co(phen)3]2+

Optimized Parameters (Angstroms and Degrees)				
Name	Definition	Value	Derivative Info.	
Bond lengths:				
R1	R(1,2)	1.9829	-DE/DX =	0.0
R2	R(1,3)	2.2347	-DE/DX =	0.0
R3	R(1,4)	1.9897	-DE/DX =	0.0
R4	R(1,5)	1.9897	-DE/DX =	0.0
R5	R(1,6)	2.2346	-DE/DX =	0.0
R6	R(1,7)	1.9829	-DE/DX =	0.0
Bond Angles:				
A1	A(2,1,3)	80.4407	-DE/DX =	0.0
A2	A(2,1,4)	93.6526	-DE/DX =	0.0
A3	A(2,1,6)	96.8864	-DE/DX =	0.0
A4	A(2,1,7)	89.4765	-DE/DX =	0.0
A5	A(3,1,4)	88.7125	-DE/DX =	0.0
A6	A(3,1,5)	94.0633	-DE/DX =	0.0
A7	A(3,1,7)	96.8863	-DE/DX =	0.0
A8	A(4,1,5)	83.7059	-DE/DX =	0.0
A9	A(4,1,6)	94.0643	-DE/DX =	0.0
A10	A(5,1,6)	88.7137	-DE/DX =	0.0
A11	A(5,1,7)	93.6529	-DE/DX =	0.0
A12	A(6,1,7)	80.441	-DE/DX =	0.0

}

{quartet - [Co(phen)3]2+

Optimized Parameters (Angstroms and Degrees)				
Name	Definition	Value	Derivative Info.	
Bond lengths:				
R1	R(1,2)	2.1406	-DE/DX =	0.0
R2	R(1,3)	2.1406	-DE/DX =	0.0
R3	R(1,4)	2.1406	-DE/DX =	0.0
R4	R(1,5)	2.1404	-DE/DX =	0.0
R5	R(1,6)	2.1406	-DE/DX =	0.0
R6	R(1,7)	2.1402	-DE/DX =	0.0

```
 Bond Angles:
 ! A1    A(2,1,3)              79.1446         -DE/DX =    0.0              !
 ! A2    A(2,1,4)              96.261          -DE/DX =    0.0              !
 ! A3    A(2,1,6)              96.186          -DE/DX =    0.0              !
 ! A4    A(2,1,7)              88.6618         -DE/DX =    0.0              !
 ! A5    A(3,1,4)              88.6374         -DE/DX =    0.0              !
 ! A6    A(3,1,5)              96.2502         -DE/DX =    0.0              !
 ! A7    A(3,1,7)              96.2976         -DE/DX =    0.0              !
 ! A8    A(4,1,5)              79.1527         -DE/DX =    0.0              !
 ! A9    A(4,1,6)              96.2284         -DE/DX =    0.0              !
 ! A10   A(5,1,6)              88.7266         -DE/DX =    0.0              !
 ! A11   A(5,1,7)              96.2389         -DE/DX =    0.0              !
 ! A12   A(6,1,7)              79.1554         -DE/DX =    0.0              !
}
```

Atomic contributions to molecular orbitals for $[Co(phen)_3]^{3+}$ ***and*** $[Co(phen)_3]^{2+}$

```
{singlet - [Co(phen)3]3+

 Atomic contributions to Alpha molecular orbitals:
 Alpha occ 144 OE=-0.608 is C29-p=0.0790
 Alpha occ 145 OE=-0.594 is Co13-d=0.5947
 Alpha occ 146 OE=-0.594 is Co13-d=0.5947
 Alpha occ 147 OE=-0.590 is Co13-d=0.5833
 Alpha occ 148 OE=-0.559 is Co13-d=0.0545
 Alpha occ 149 OE=-0.558 is C5-p=0.1039
 Alpha occ 150 OE=-0.558 is C18-p=0.1055 C23-p=0.1018
 Alpha occ 151 OE=-0.544 is C50-p=0.0781
 Alpha occ 152 OE=-0.539 is C49-p=0.1474 C50-p=0.1446
 Alpha occ 153 OE=-0.539 is C58-p=0.1444 C57-p=0.1412
 Alpha vir 154 OE=-0.419 is Co13-d=0.6095
 Alpha vir 155 OE=-0.419 is Co13-d=0.6095
 Alpha vir 156 OE=-0.404 is C11-p=0.0740
 Alpha vir 157 OE=-0.404 is C22-p=0.0749
 Alpha vir 158 OE=-0.399 is N25-p=0.0367
 Alpha vir 159 OE=-0.393 is C9-p=0.0526
 Alpha vir 160 OE=-0.386 is C9-p=0.0932
 Alpha vir 161 OE=-0.386 is C24-p=0.0950
 Alpha vir 162 OE=-0.354 is C1-p=0.0479
 Alpha vir 163 OE=-0.344 is C1-p=0.0959
}

{doublet - [Co(phen)3]2+
```

```
 Atomic contributions to Alpha molecular orbitals:
 Alpha occ 145 OE=-0.451 is Co13-d=0.4439
 Alpha occ 146 OE=-0.449 is C35-p=0.1506 C28-p=0.1506
 Alpha occ 147 OE=-0.444 is C23-p=0.0920
 Alpha occ 148 OE=-0.440 is Co13-d=0.2762
 Alpha occ 149 OE=-0.435 is C49-p=0.1974 C50-p=0.1974 Co13-d=0.1452
 Alpha occ 150 OE=-0.430 is C57-p=0.1096 C41-p=0.1094
 Alpha occ 151 OE=-0.425 is Co13-d=0.1440
 Alpha occ 152 OE=-0.415 is Co13-d=0.6952
 Alpha occ 153 OE=-0.414 is Co13-d=0.8509
 Alpha occ 154 OE=-0.373 is Co13-d=0.5772
 Alpha vir 155 OE=-0.287 is N33-p=0.1091 N26-p=0.1091 C36-p=0.1002 C29-p=0.1002
 Alpha vir 156 OE=-0.285 is C17-p=0.0898
 Alpha vir 157 OE=-0.281 is C6-p=0.0696
 Alpha vir 158 OE=-0.279 is C27-p=0.1150 C34-p=0.1149
 Alpha vir 159 OE=-0.277 is Co13-d=0.6231
 Alpha vir 160 OE=-0.272 is C19-p=0.0725
 Alpha vir 161 OE=-0.272 is C11-p=0.0722
 Alpha vir 162 OE=-0.239 is C37-p=0.0778
 Alpha vir 163 OE=-0.232 is C37-p=0.0725
 Alpha vir 164 OE=-0.229 is C12-p=0.0775

 Atomic contributions to Beta  molecular orbitals:
 Beta  occ 144 OE=-0.480 is N8-p=0.1964 N25-p=0.1955
 Beta  occ 145 OE=-0.449 is C35-p=0.1460 C28-p=0.1460
 Beta  occ 146 OE=-0.446 is C23-p=0.0712
 Beta  occ 147 OE=-0.444 is C10-p=0.0939
 Beta  occ 148 OE=-0.434 is C49-p=0.2159 C50-p=0.2159
 Beta  occ 149 OE=-0.431 is Co13-d=0.1424 C58-p=0.1004
 Beta  occ 150 OE=-0.429 is C41-p=0.1143 C57-p=0.1138
 Beta  occ 151 OE=-0.412 is Co13-d=0.6911
 Beta  occ 152 OE=-0.403 is Co13-d=0.8225
 Beta  occ 153 OE=-0.402 is Co13-d=0.8915
 Beta  vir 154 OE=-0.286 is N26-p=0.1118 N33-p=0.1118 C29-p=0.1011 C36-p=0.1010
 Beta  vir 155 OE=-0.284 is C17-p=0.0901
 Beta  vir 156 OE=-0.280 is C6-p=0.0743
 Beta  vir 157 OE=-0.279 is C27-p=0.1171 C34-p=0.1171
 Beta  vir 158 OE=-0.273 is C19-p=0.0697
 Beta  vir 159 OE=-0.272 is C11-p=0.0733
 Beta  vir 160 OE=-0.245 is Co13-d=0.6999
 Beta  vir 161 OE=-0.239 is C37-p=0.0773
 Beta  vir 162 OE=-0.232 is C37-p=0.0728
 Beta  vir 163 OE=-0.229 is C12-p=0.0772
}
```

```
{quartet - [Co(phen)3]2+

 Atomic contributions to Alpha molecular orbitals:
 Alpha occ 146 OE=-0.471 is Co13-d=0.7545
 Alpha occ 147 OE=-0.471 is Co13-d=0.7540
 Alpha occ 148 OE=-0.444 is C10-p=0.0572
 Alpha occ 149 OE=-0.443 is C10-p=0.1123 C5-p=0.1122
 Alpha occ 150 OE=-0.443 is C28-p=0.0881
 Alpha occ 151 OE=-0.428 is C41-p=0.0722
 Alpha occ 152 OE=-0.426 is C42-p=0.1407 C41-p=0.1405
 Alpha occ 153 OE=-0.426 is C50-p=0.1113 C49-p=0.1085 C57-p=0.1035 C58-p=0.1005
 Alpha occ 154 OE=-0.412 is Co13-d=0.3839 N8-p=0.1052 N25-p=0.1009
 Alpha occ 155 OE=-0.412 is Co13-d=0.3840 N26-p=0.1162 N14-p=0.1141
 Alpha vir 156 OE=-0.283 is N8-p=0.0757
 Alpha vir 157 OE=-0.283 is C22-p=0.0665
 Alpha vir 158 OE=-0.279 is N26-p=0.0375
 Alpha vir 159 OE=-0.275 is C9-p=0.0497
 Alpha vir 160 OE=-0.271 is C34-p=0.0920
 Alpha vir 161 OE=-0.271 is C4-p=0.0780
 Alpha vir 162 OE=-0.236 is C12-p=0.0486
 Alpha vir 163 OE=-0.229 is C21-p=0.0989
 Alpha vir 164 OE=-0.229 is C12-p=0.0931
 Alpha vir 165 OE=-0.208 is C7-p=0.0581

 Atomic contributions to Beta  molecular orbitals:
 Beta  occ 143 OE=-0.490 is N26-p=0.0775
 Beta  occ 144 OE=-0.484 is N8-p=0.0683
 Beta  occ 145 OE=-0.444 is C10-p=0.0568
 Beta  occ 146 OE=-0.443 is C10-p=0.0869
 Beta  occ 147 OE=-0.443 is C28-p=0.1078 C35-p=0.1075
 Beta  occ 148 OE=-0.431 is Co13-d=0.2820
 Beta  occ 149 OE=-0.431 is Co13-d=0.2818 C58-p=0.1065 C57-p=0.1045
 Beta  occ 150 OE=-0.428 is C58-p=0.0712
 Beta  occ 151 OE=-0.417 is Co13-d=0.5863
 Beta  occ 152 OE=-0.417 is Co13-d=0.5865
 Beta  vir 153 OE=-0.298 is Co13-d=0.8290
 Beta  vir 154 OE=-0.282 is N3-p=0.0757
 Beta  vir 155 OE=-0.282 is N25-p=0.0627
 Beta  vir 156 OE=-0.278 is N33-p=0.0382
 Beta  vir 157 OE=-0.272 is Co13-d=0.1029
 Beta  vir 158 OE=-0.271 is C34-p=0.0921
 Beta  vir 159 OE=-0.271 is C4-p=0.0783
 Beta  vir 160 OE=-0.236 is C21-p=0.0515
 Beta  vir 161 OE=-0.236 is Co13-d=0.6829
 Beta  vir 162 OE=-0.236 is Co13-d=0.6792
```

}

SECOND ORDER PERTURBATION THEORY ANALYSIS E(2)

{singlet - [Co(phen)3]3+

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
from unit 2 to unit 1				
50. LP (1) N 2	149. LV (1)Co 1	7.25	0.15	0.029
50. LP (1) N 2	150. LV (2)Co 1	96.70	0.15	0.107
50. LP (1) N 2	151. LV (3)Co 1	24.15	0.99	0.138
50. LP (1) N 2	248. RY (4)Co 1	1.66	5.77	0.087
50. LP (1) N 2	256. RY (12)Co 1	0.12	1.65	0.012
51. LP (1) N 3	149. LV (1)Co 1	51.30	0.15	0.078
51. LP (1) N 3	150. LV (2)Co 1	52.63	0.15	0.079
51. LP (1) N 3	151. LV (3)Co 1	24.15	0.99	0.138
51. LP (1) N 3	248. RY (4)Co 1	1.66	5.77	0.087
51. LP (1) N 3	255. RY (11)Co 1	0.11	1.65	0.012
from unit 3 to unit 1				
52. LP (1) N 4	149. LV (1)Co 1	97.27	0.15	0.107
52. LP (1) N 4	150. LV (2)Co 1	6.69	0.15	0.028
52. LP (1) N 4	151. LV (3)Co 1	24.15	0.99	0.138
52. LP (1) N 4	248. RY (4)Co 1	1.66	5.77	0.087
52. LP (1) N 4	255. RY (11)Co 1	0.06	1.65	0.009
52. LP (1) N 4	256. RY (12)Co 1	0.07	1.65	0.010
53. LP (1) N 5	149. LV (1)Co 1	7.30	0.15	0.029
53. LP (1) N 5	150. LV (2)Co 1	96.64	0.15	0.107
53. LP (1) N 5	151. LV (3)Co 1	24.15	0.99	0.138
53. LP (1) N 5	248. RY (4)Co 1	1.66	5.77	0.087
53. LP (1) N 5	256. RY (12)Co 1	0.13	1.65	0.013
from unit 4 to unit 1				
54. LP (1) N 6	149. LV (1)Co 1	51.43	0.15	0.078
54. LP (1) N 6	150. LV (2)Co 1	52.54	0.15	0.079
54. LP (1) N 6	151. LV (3)Co 1	24.15	0.99	0.138
54. LP (1) N 6	248. RY (4)Co 1	1.66	5.77	0.087
54. LP (1) N 6	255. RY (11)Co 1	0.12	1.65	0.013
55. LP (1) N 7	149. LV (1)Co 1	97.32	0.15	0.107

55. LP (1) N 7	150. LV (2)Co 1	6.64	0.15	0.028
55. LP (1) N 7	151. LV (3)Co 1	24.15	0.99	0.138
55. LP (1) N 7	248. RY (4)Co 1	1.66	5.77	0.087
55. LP (1) N 7	255. RY (11)Co 1	0.08	1.65	0.010

}

{doublet - [Co(phen)3]2+

Alpha Spin

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
from unit 2 to unit 1				
51. LP (1) N 2	150. LV (1)Co 1	26.35	0.20	0.093
51. LP (1) N 2	151. LV (2)Co 1	10.91	0.73	0.113
51. LP (1) N 2	248. RY (4)Co 1	0.38	6.80	0.064
51. LP (1) N 2	255. RY (11)Co 1	0.22	2.33	0.029
52. LP (1) N 3	151. LV (2)Co 1	6.51	0.71	0.086
52. LP (1) N 3	248. RY (4)Co 1	0.26	6.77	0.053
52. LP (1) N 3	255. RY (11)Co 1	0.04	2.30	0.012
from unit 3 to unit 1				
53. LP (1) N 4	150. LV (1)Co 1	25.55	0.21	0.091
53. LP (1) N 4	151. LV (2)Co 1	10.89	0.73	0.113
53. LP (1) N 4	248. RY (4)Co 1	0.37	6.80	0.063
53. LP (1) N 4	255. RY (11)Co 1	0.19	2.33	0.026
54. LP (1) N 5	150. LV (1)Co 1	25.55	0.21	0.091
54. LP (1) N 5	151. LV (2)Co 1	10.89	0.73	0.113
54. LP (1) N 5	248. RY (4)Co 1	0.37	6.80	0.063
54. LP (1) N 5	255. RY (11)Co 1	0.19	2.33	0.026
from unit 4 to unit 1				
55. LP (1) N 6	151. LV (2)Co 1	6.51	0.71	0.086
55. LP (1) N 6	248. RY (4)Co 1	0.26	6.77	0.053
55. LP (1) N 6	255. RY (11)Co 1	0.04	2.30	0.012
56. LP (1) N 7	150. LV (1)Co 1	26.35	0.20	0.093
56. LP (1) N 7	151. LV (2)Co 1	10.91	0.73	0.113
56. LP (1) N 7	248. RY (4)Co 1	0.38	6.80	0.064
56. LP (1) N 7	255. RY (11)Co 1	0.22	2.33	0.029

Beta-spin

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.

```
 from unit  2 to unit  1
  50. LP ( 1) N  2          149. LV ( 1)Co  1          22.96    0.25   0.095
  50. LP ( 1) N  2          150. LV ( 2)Co  1           8.40    0.33   0.067
  50. LP ( 1) N  2          151. LV ( 3)Co  1           9.20    0.73   0.103
  50. LP ( 1) N  2          248. RY ( 4)Co  1           0.29    6.77   0.056
  50. LP ( 1) N  2          255. RY (11)Co  1           0.11    2.39   0.021
  51. LP ( 1) N  3          150. LV ( 2)Co  1           9.09    0.30   0.065
  51. LP ( 1) N  3          151. LV ( 3)Co  1           8.16    0.69   0.095
  51. LP ( 1) N  3          248. RY ( 4)Co  1           0.18    6.73   0.044
  51. LP ( 1) N  3          255. RY (11)Co  1           0.07    2.35   0.017

 from unit  3 to unit  1
    52. LP ( 1) N  4          149. LV ( 1)Co  1          22.64    0.25   0.095
    52. LP ( 1) N  4          150. LV ( 2)Co  1           8.03    0.33   0.065
    52. LP ( 1) N  4          151. LV ( 3)Co  1           9.23    0.73   0.104
    52. LP ( 1) N  4          248. RY ( 4)Co  1           0.29    6.77   0.056
    52. LP ( 1) N  4          255. RY (11)Co  1           0.09    2.39   0.019
    53. LP ( 1) N  5          149. LV ( 1)Co  1          22.64    0.25   0.095
    53. LP ( 1) N  5          150. LV ( 2)Co  1           8.03    0.33   0.065
    53. LP ( 1) N  5          151. LV ( 3)Co  1           9.23    0.73   0.104
    53. LP ( 1) N  5          248. RY ( 4)Co  1           0.29    6.77   0.056
    53. LP ( 1) N  5          255. RY (11)Co  1           0.09    2.39   0.019

 from unit  4 to unit  1
    54. LP ( 1) N  6          150. LV ( 2)Co  1           9.09    0.30   0.065
    54. LP ( 1) N  6          151. LV ( 3)Co  1           8.16    0.69   0.095
    54. LP ( 1) N  6          248. RY ( 4)Co  1           0.18    6.73   0.044
    54. LP ( 1) N  6          255. RY (11)Co  1           0.07    2.35   0.017
    55. LP ( 1) N  7          149. LV ( 1)Co  1          22.96    0.25   0.095
    55. LP ( 1) N  7          150. LV ( 2)Co  1           8.40    0.33   0.067
    55. LP ( 1) N  7          151. LV ( 3)Co  1           9.20    0.73   0.103
    55. LP ( 1) N  7          248. RY ( 4)Co  1           0.29    6.77   0.056
    55. LP ( 1) N  7          255. RY (11)Co  1           0.11    2.39   0.021
}

{quartet - [Co(phen)3]3+

Alpha Spin:

                                                          E(2) E(NL)-E(L) F(L,NL)
      Donor (L) NBO              Acceptor (NL) NBO      kcal/mol   a.u.    a.u.
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 from unit  2 to unit  1
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Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
52. LP (1) N 2	151. LV (1)Co 1	9.60	0.58	0.094
52. LP (1) N 2	248. RY (4)Co 1	0.40	6.22	0.063
53. LP (1) N 3	151. LV (1)Co 1	9.60	0.58	0.094
53. LP (1) N 3	248. RY (4)Co 1	0.40	6.22	0.063
53. LP (1) N 3	256. RY (12)Co 1	0.03	1.57	0.008
from unit 3 to unit 1				
51. LP (1) N 4	148. LV (1)Co 1	12.86	0.29	0.077
51. LP (1) N 4	149. LV (2)Co 1	1.53	0.29	0.027
51. LP (1) N 4	150. LV (3)Co 1	9.55	0.59	0.095
51. LP (1) N 4	248. RY (4)Co 1	0.32	6.18	0.056
52. LP (1) N 5	148. LV (1)Co 1	8.01	0.29	0.061
52. LP (1) N 5	149. LV (2)Co 1	6.38	0.29	0.054
52. LP (1) N 5	150. LV (3)Co 1	9.56	0.59	0.095
52. LP (1) N 5	248. RY (4)Co 1	0.32	6.18	0.056
from unit 4 to unit 1				
56. LP (1) N 6	151. LV (1)Co 1	9.60	0.58	0.094
56. LP (1) N 6	248. RY (4)Co 1	0.40	6.22	0.063
57. LP (1) N 7	151. LV (1)Co 1	9.61	0.58	0.095
57. LP (1) N 7	248. RY (4)Co 1	0.40	6.22	0.063

Beta-spin:

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
from unit 2 to unit 1				
49. LP (1) N 2	148. LV (1)Co 1	8.20	0.29	0.062
49. LP (1) N 2	149. LV (2)Co 1	6.19	0.29	0.054
49. LP (1) N 2	150. LV (3)Co 1	9.55	0.59	0.095
49. LP (1) N 2	248. RY (4)Co 1	0.32	6.18	0.056
50. LP (1) N 3	148. LV (1)Co 1	0.60	0.29	0.017
50. LP (1) N 3	149. LV (2)Co 1	13.79	0.29	0.080
50. LP (1) N 3	150. LV (3)Co 1	9.56	0.59	0.095
50. LP (1) N 3	248. RY (4)Co 1	0.32	6.18	0.056
from unit 3 to unit 1				
54. LP (1) N 4	151. LV (1)Co 1	9.60	0.58	0.094
54. LP (1) N 4	248. RY (4)Co 1	0.40	6.22	0.063
54. LP (1) N 4	255. RY (11)Co 1	0.03	1.57	0.008
55. LP (1) N 5	151. LV (1)Co 1	9.61	0.58	0.095
55. LP (1) N 5	248. RY (4)Co 1	0.40	6.22	0.063
from unit 4 to unit 1				

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   53. LP ( 1) N  6          148. LV ( 1)Co  1          0.52    0.29   0.016
   53. LP ( 1) N  6          149. LV ( 2)Co  1         13.86    0.29   0.080
   53. LP ( 1) N  6          150. LV ( 3)Co  1          9.55    0.59   0.095
   53. LP ( 1) N  6          248. RY ( 4)Co  1          0.32    6.18   0.056
   54. LP ( 1) N  7          148. LV ( 1)Co  1         12.99    0.29   0.078
   54. LP ( 1) N  7          149. LV ( 2)Co  1          1.41    0.29   0.026
   54. LP ( 1) N  7          150. LV ( 3)Co  1          9.56    0.59   0.095
   54. LP ( 1) N  7          248. RY ( 4)Co  1          0.32    6.18   0.056
}
```