

Supporting Information for Metallocene: Multi-layered Molecular Rotors

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Table S1. The C-M bond distances in Å, WBI values, and NPA charges of M atom in |e| of LM of M(Cp)₂^q, M(Bz)₂^q, and M(Cp)(Bz)^q were computed at the PBE0-D3/def2-TZVP level.

Species	B _{C-M}	WBI _{C-M}	Q _M
Mn(Cp) ₂ ⁻	2.065	0.45	-0.79
Fe(Cp) ₂	2.043	0.42	-0.54
Co(Cp) ₂ ⁺	2.036	0.41	-0.29
V(Bz) ₂ ⁻	2.174	0.43	-1.08
Cr(Bz) ₂	2.134	0.42	-1.22
Mn(Bz) ₂ ⁺	2.120	0.39	-0.72
Cr(Cp)(Bz) ⁻	2.169	0.38	-1.10
Mn(Cp)(Bz)	2.100	0.45	-0.74
Fe(Cp)(Bz) ⁺	2.055	0.45	-0.54

Table S2. The C-M bond distances in Å, WBI values, and NPA charges of M atom in |e| of TS of M(Cp)₂^q, M(Bz)₂^q, and M(Cp)(Bz)^q were computed at the PBE0-D3/def2-TZVP level.

Species	B _{C-M}	WBI _{C-M}	Q _M
Mn(Cp) ₂ ⁻	2.071	0.44	-0.78
Fe(Cp) ₂	2.046	0.42	-0.53
Co(Cp) ₂ ⁺	2.037	0.41	-0.28
V(Bz) ₂ ⁻	2.176	0.43	-1.08
Cr(Bz) ₂	2.137	0.42	-1.22
Mn(Bz) ₂ ⁺	2.122	0.39	-0.72
Cr(Cp)(Bz) ⁻	2.168	0.38	-1.10
Mn(Cp)(Bz)	2.100	0.42	-0.74
Fe(Cp)(Bz) ⁺	2.055	0.45	-0.54

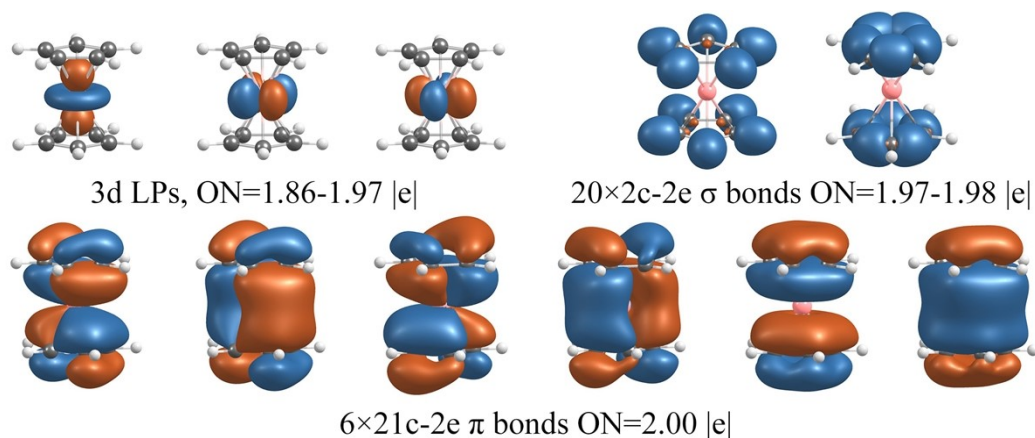


Figure S1. AdNDP analysis for the **TS** of $\text{Fe}(\text{Cp})_2$ computed at the PBE0-D3/def2-TZVP level. Occupation numbers (ON) in |e|.

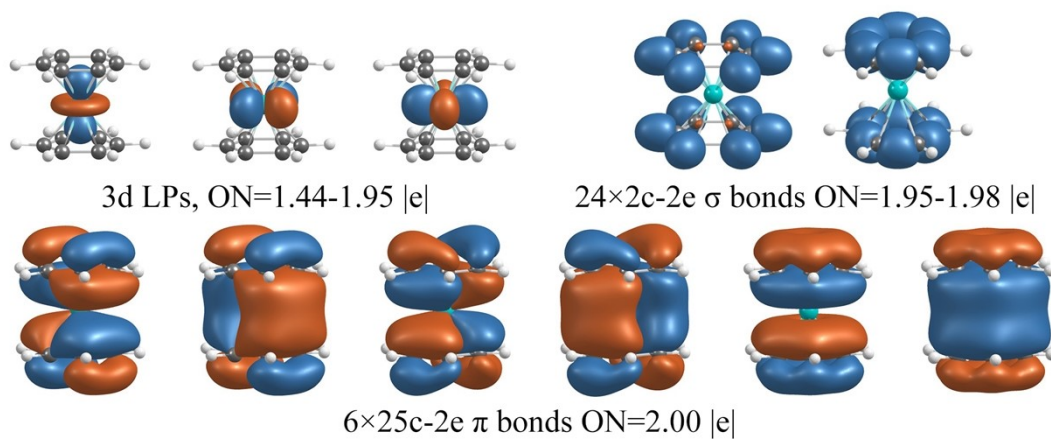


Figure S2. AdNDP analysis for the **LM** of $\text{Cr}(\text{Bz})_2$ computed at the PBE0-D3/def2-TZVP level. Occupation numbers (ON) in |e|.

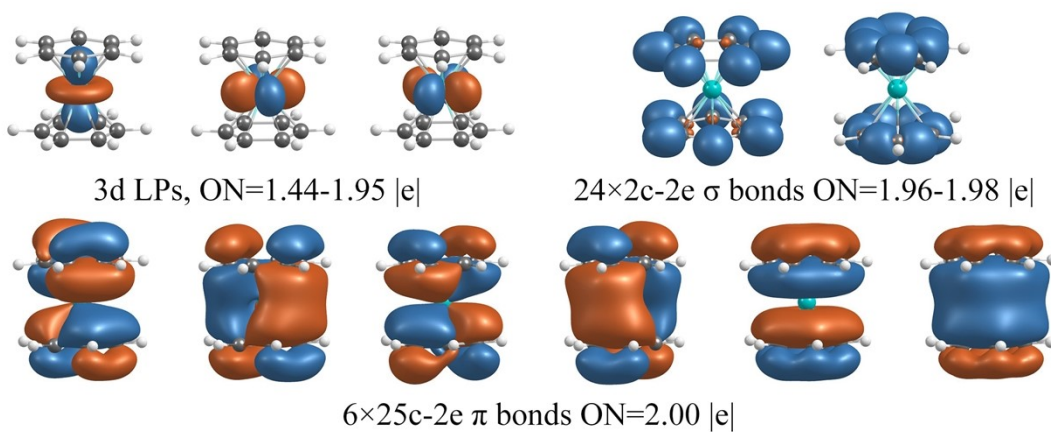


Figure S3. AdNDP analysis for the **TS** of $\text{Cr}(\text{Bz})_2$ computed at the PBE0-D3/def2-

TZVP level. Occupation numbers (ON) in |e|.

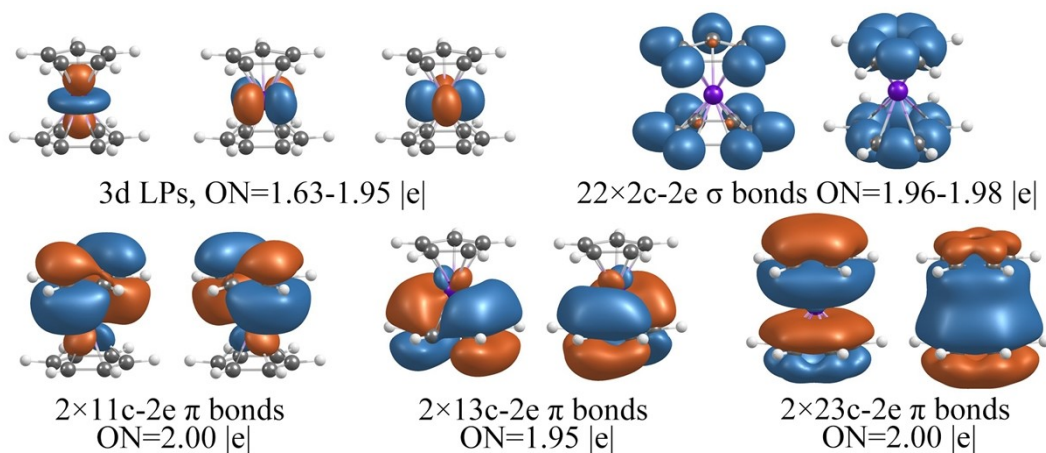


Figure S4. AdNDP analysis for the LM of Mn(Cp)(Bz) computed at the PBE0-D3/def2-TZVP level. Occupation numbers (ON) in |e|.

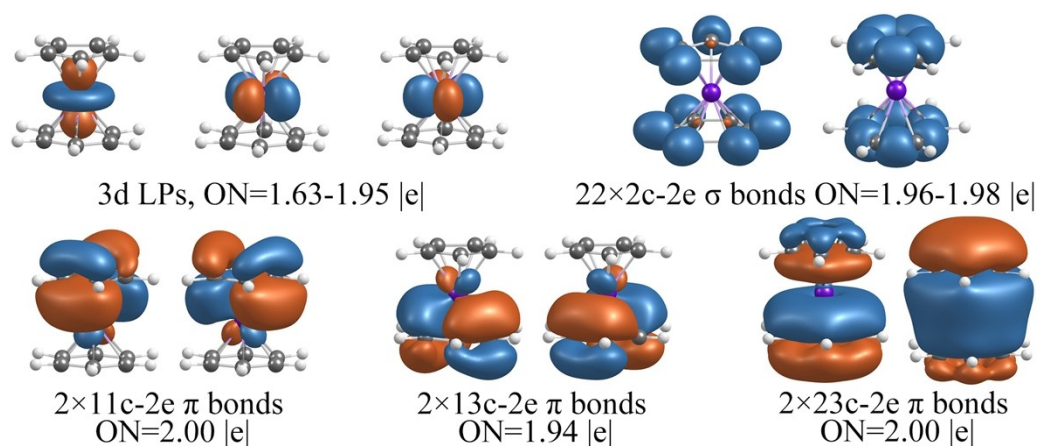


Figure S5. AdNDP analysis for the TS of Mn(Cp)(Bz) computed at the PBE0-D3/def2-TZVP level. Occupation numbers (ON) in |e|.

Table S3. EDA-NOCV results using Fe^{2+} and Cp_2^{2-} as interacting fragments at BP86-D3(BJ)/TZ2P. All values are in kcal/mol.

		$\text{Fe}(\text{Cp})_2 \rightarrow \text{Fe}^{2+} (\text{singlet}) + \text{Cp}_2^{2-} (\text{singlet})$		
		LM	TS	$\Delta E_{(\text{TS-LM})}$
ΔE_{eb}	energy barrier without ZPE	0.0	+1.0	+1.0
$\Delta E_{deform1}$	deformation energy of Cp_2^{2-}	0.0	-0.4	-0.4
$\Delta E_{deform2}$	deformation energy of Fe^{2+}	0.0	0.0	0.0
ΔE_{int}	–	-899.1	-897.6	+1.5
ΔE_{pauli}	–	+291.1	+287.7	-3.4
ΔE_{disp}	–	-2.8	-2.8	0.0
ΔE_{elstat}^a	–	-623.6 (52.5%)	-622.1 (52.6%)	+1.5
ΔE_{orba}	–	-563.8 (47.5%)	-560.4 (47.4%)	+3.4
$\Delta E_{orb(1)}^b$	$\text{Fe}^{2+} \leftarrow \text{Cp}_2^{2-}$ back-donation	-179.6 (31.8%)	-178.4 (31.8%)	–
$\Delta E_{orb(2)}^b$	$\text{Fe}^{2+} \leftarrow \text{Cp}_2^{2-}$ back-donation	-179.6 (31.8%)	-178.4 (31.8%)	–

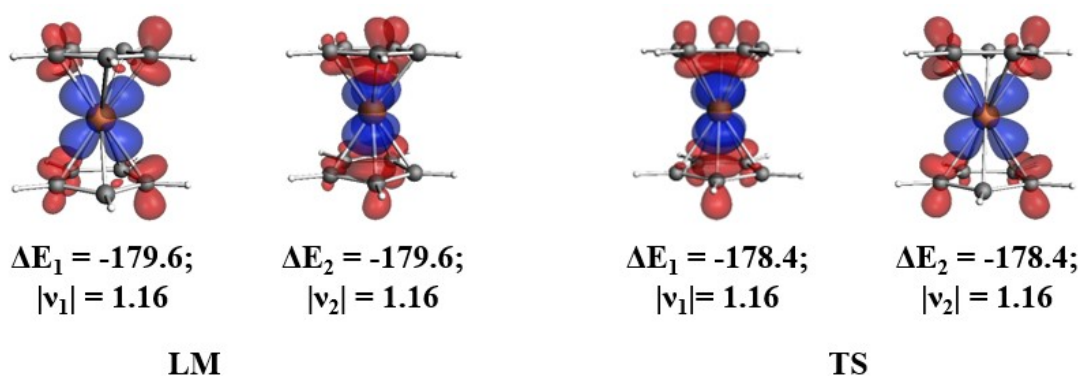


Figure S6. Deformation densities $\Delta\rho$ that are connected with the pairwise orbital interactions in $\text{Fe}(\text{Cp})_2$ at BP86-D3(BJ)/TZ2P. The charge flow of the electronic charge is red \rightarrow blue. The associated orbital interaction energies ΔE are given in kcal/mol. The eigenvalues ν indicate the size of the charge flow.

Table S4. EDA-NOCV results using Cr and Bz₂ as interacting fragments at BP86-D3(BJ)/TZ2P. All values are in kcal/mol.

		Cr(Bz) ₂ → Cr (singlet) + Bz ₂ (singlet)		
		LM	TS	$\Delta E_{(TS-LM)}$
ΔE_{eb}	energy barrier without ZPE	0.0	+1.6	+1.6
$\Delta E_{deform1}$	deformation energy of Bz ₂	0.0	-0.1	-0.1
$\Delta E_{deform2}$	deformation energy of Cr	0.0	0.0	0.0
ΔE_{int}	–	-272.1	-270.6	+1.5
ΔE_{pauli}	–	+377.7	+372.6	-5.1
ΔE_{disp}	–	-3.5	-3.5	0.0
ΔE_{elstat}^a	–	-258.5 (40.0%)	-255.8 (40.0%)	+2.7
ΔE_{orba}	–	-387.8 (60.0%)	-383.9 (60.0%)	+3.9
$\Delta E_{orb(1)b}$	Cr → Bz ₂ back-donation	-139.6 (36.0%)	-138.2 (36.0%)	–
$\Delta E_{orb(2)b}$	Cr → Bz ₂ back-donation	-139.6 (36.0%)	-138.2 (36.0%)	–

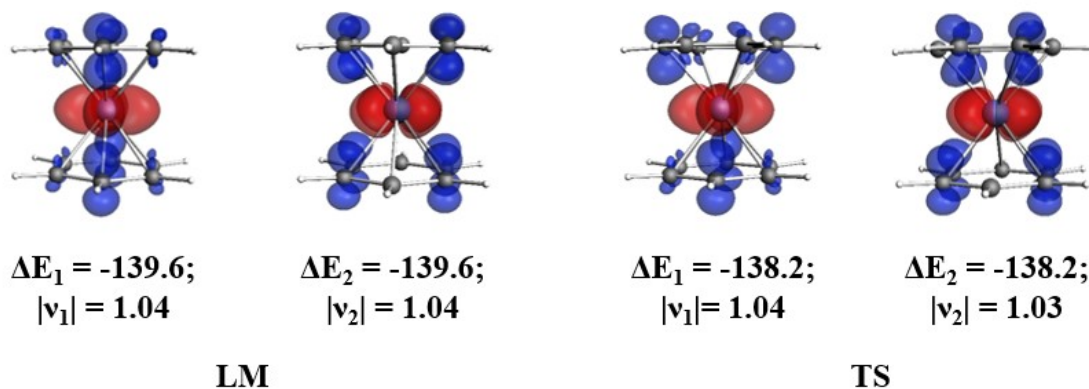


Figure S7. Deformation densities $\Delta\rho$ that are connected with the pairwise orbital interactions in Cr(Bz)₂ at BP86-D3(BJ)/TZ2P. The charge flow of the electronic charge is red → blue. The associated orbital interaction energies ΔE are given in kcal/mol. The eigenvalues v indicate the size of the charge flow.

Table S5. EDA-NOCV results using Mn^+ and $(\text{Cp})(\text{Bz})^-$ as interacting fragments at BP86-D3(BJ)/TZ2P. All values are in kcal/mol.

		$\text{Mn}(\text{Cp})(\text{Bz}) \rightarrow \text{Mn}^+ (\text{singlet})$ $+ (\text{Cp})(\text{Bz})^- (\text{singlet})$		
		LM	TS	$\Delta E_{(\text{TS-LM})}$
ΔE_{eb}	energy barrier without ZPE deformation	0.0	-0.1	-0.1
$\Delta E_{deform1}$	energy of $(\text{Cp})(\text{Bz})^-$ deformation	0.0	0.0	0.0
$\Delta E_{deform2}$	energy of Mn^+	0.0	0.0	0.0
ΔE_{int}	–	-392.8	-392.7	+0.1
ΔE_{pauli}	–	+325.6	+325.6	0.0
ΔE_{disp}	–	-2.4	-2.4	0.0
ΔE_{elstat}^a	–	-319.0 (44.6%)	-319.0 (44.6%)	0.0
ΔE_{orb}^a	–	-397.0 (55.4%)	-396.9 (55.4%)	+0.1
$\Delta E_{orb(1)b}$	$\text{Mn}^+ \leftarrow (\text{Cp})(\text{Bz})^-$ donation	-79.4 (20.0%)	-79.3 (20.0%)	–
$\Delta E_{orb(2)b}$	$\text{Mn}^+ \leftarrow (\text{Cp})(\text{Bz})^-$ donation	-79.3 (20.0%)	-79.3 (20.0%)	–
$\Delta E_{orb(3)b}$	$\text{Mn}^+ \leftarrow (\text{Cp})(\text{Bz})^-$ donation	-73.4 (18.5%)	-73.4 (18.5%)	–
$\Delta E_{orb(4)b}$	$\text{Mn}^+ \leftarrow (\text{Cp})(\text{Bz})^-$ donation	-73.2 (18.4%)	-73.3 (18.5%)	–

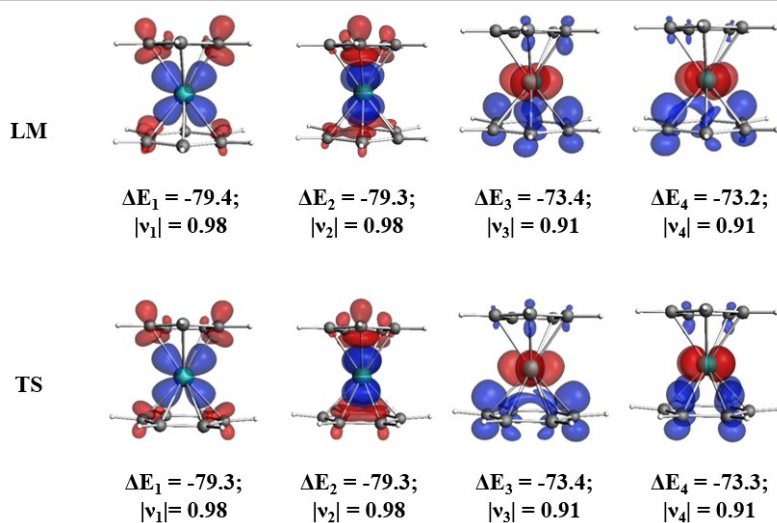


Figure S8. Deformation densities $\Delta\rho$ that are connected with the pairwise orbital interactions in $\text{Mn}(\text{Cp})(\text{Bz})$ at BP86-D3(BJ)/TZ2P. The charge flow of the electronic

charge is red \rightarrow blue. The associated orbital interaction energies ΔE are given in kcal/mol. The eigenvalues v indicate the size of the charge flow.

We also considered the neutral model for EDA-NOCV analysis. In this model, the $\text{Mn}(\text{Cp})(\text{Bz})$ was separated to be $\text{Mn}(\text{doublet}) + (\text{CpBz})(\text{doublet})$ while $\text{Fe}(\text{Cp})_2$ was decomposed to be $\text{Fe}(\text{triplet})$ and $(\text{Cp})_2(\text{triplet})$. Because EDA-NOCV analysis at BP86/TZ2P failed in calculating the neutral $\text{Mn}(\text{doublet})$ and $\text{Fe}(\text{triplet})$, we switched to B3LYP/TZ2P. As shown in Tables S6 and S7, the $|\Delta E_{\text{orb}}|$ in EDA-NOCV results using neutral fragments in both $\text{Mn}(\text{Cp})(\text{Bz})$ and $\text{Fe}(\text{Cp})_2$ is larger than that in corresponding ionic fragments. Those results suggest that the ionic fragments with dative scheme is more reasonable.

Table S6. EDA-NOCV results using Mn^+ and $(\text{Cp})(\text{Bz})^-$ and using Mn and $(\text{Cp})(\text{Bz})$ as interacting fragments at B3LYP(BJ)/TZ2P. All values are in kcal/mol.

	$\text{Mn}(\text{Cp})(\text{Bz}) \rightarrow \text{Mn}^+$ (singlet)		$\text{Mn}(\text{Cp})(\text{Bz}) \rightarrow \text{Mn}$ (doublet)	
	+ $(\text{Cp})(\text{Bz})^-$ (singlet)		+ $(\text{Cp})(\text{Bz})$ (doublet)	
	LM	TS	LM	TS
ΔE_{int}	-314.0	-313.5	-190.0	-187.4
ΔE_{Pauli}	+460.1	+567.6	+956.4	+1079.1
ΔE_{disp}	-2.4	-2.4	-2.4	-2.4
ΔE_{elstat}	-367.9	-401.3	-506.9	-565.0
ΔE_{orb}	-403.8	-477.4	-637.2	-699.1

Table S7. EDA-NOCV results using Fe^{2+} and $(\text{Cp})_2^{2-}$ and using Fe and $(\text{Cp})_2$ as interacting fragments at B3LYP(BJ)/TZ2P. All values are in kcal/mol.

	$\text{Fe}(\text{Cp})_2 \rightarrow \text{Fe}^{2+}$ (singlet)		+ $\text{Fe}(\text{Cp})_2 \rightarrow \text{Fe}$ (triplet)	
	+ $(\text{Cp})_2^{2-}$ (singlet)		+ $(\text{Cp})_2$ (triplet)	
	LM	TS	LM	TS
ΔE_{int}	-840.8	-839.5	-219.1	-218.7
ΔE_{Pauli}	+294.3	+290.7	+969.1	+880.8
ΔE_{disp}	-2.9	-2.9	-2.9	-2.9
ΔE_{elstat}	-620.6	-618.9	-543.9	-531.2
ΔE_{orb}	-511.6	-508.4	-650.4	-565.4

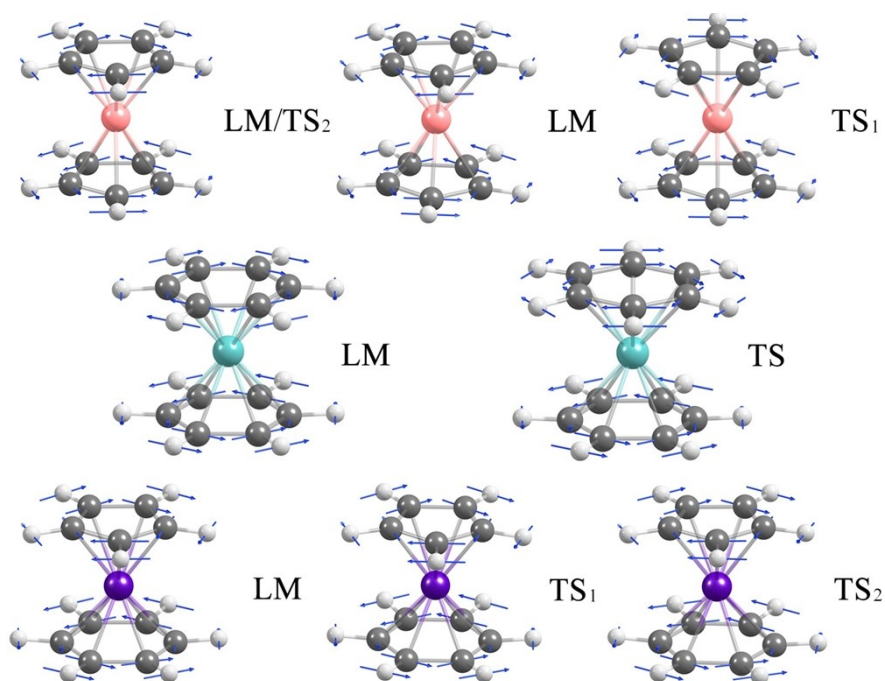


Figure S9. Displacement vectors of soft vibrational mode of the **LM** and imaginary soft vibrational mode of the **TS**. The order and name of complexes can be checked in Figure 1.

Table S8. Period (T_{rot} , s) and frequency (ν_{rot} , THz) associated with the rotation system of $\text{M}(\text{Cp})_2^q$, $\text{M}(\text{Bz})_2^q$ and $\text{M}(\text{Cp})(\text{Bz})^q$ at the PBE0-D3/def2-SVP level.

System	T_{rot} (s)	ν_{rot} (THz)
$\text{Mn}(\text{Cp})_2^-$	2.23264×10^{-12}	0.44790
$\text{Fe}(\text{Cp})_2$	6.05437×10^{-12}	0.16517
$\text{Co}(\text{Cp})_2^+$	2.13799×10^{-12}	0.46773
$\text{V}(\text{Bz})_2^-$	1.75759×10^{-12}	0.56896
$\text{Cr}(\text{Bz})_2$	1.72328×10^{-12}	0.58029
$\text{Mn}(\text{Bz})_2^+$	2.64859×10^{-12}	0.37756
$\text{Cr}(\text{Cp})(\text{Bz})^-$	5.96872×10^{-12}	0.16754
$\text{Mn}(\text{Cp})(\text{Bz})$	6.75813×10^{-12}	0.14797
$\text{Fe}(\text{Cp})(\text{Bz})^+$	9.72573×10^{-12}	0.10282

I. Coordinates obtained at the PBE0-D3/def2-TZVP level.

Fe(Cp)₂, LM

Frequencies = 13.6997 cm⁻¹

HF = -1650.2887743 a.u.

26	0.000000000	0.000000000	0.000000000
6	1.208332000	0.000000000	-1.647501000
6	0.373395000	1.149192000	-1.647501000
6	-0.977561000	0.710240000	-1.647501000
6	-0.977561000	-0.710240000	-1.647501000
6	0.373395000	-1.149192000	-1.647501000
1	2.287325000	0.000000000	-1.620124000
1	0.706822000	2.175376000	-1.620124000
1	-1.850485000	1.344456000	-1.620124000
1	-1.850485000	-1.344456000	-1.620124000
1	0.706822000	-2.175376000	-1.620124000
6	1.208332000	0.000000000	1.647501000
6	0.373395000	1.149192000	1.647501000
6	-0.977561000	0.710240000	1.647501000
6	-0.977561000	-0.710240000	1.647501000
6	0.373395000	-1.149192000	1.647501000
1	2.287325000	0.000000000	1.620124000
1	0.706822000	2.175376000	1.620124000
1	-1.850485000	1.344456000	1.620124000
1	-1.850485000	-1.344456000	1.620124000
1	0.706822000	-2.175376000	1.620124000

Fe(Cp)₂, TS

Frequencies = -54.2000 cm⁻¹

HF = -1650.2877382 a.u.

26	0.000000000	0.000000000	0.000000000
6	0.000000000	-1.207942000	-1.651384000
6	1.148821000	-0.373275000	-1.651384000
6	0.710011000	0.977246000	-1.651384000
6	-0.710011000	0.977246000	-1.651384000
6	-1.148821000	-0.373275000	-1.651384000
1	0.000000000	-2.286918000	-1.619650000
1	2.174988000	-0.706697000	-1.619650000
1	1.344217000	1.850156000	-1.619650000
1	-1.344217000	1.850156000	-1.619650000
1	-2.174988000	-0.706697000	-1.619650000
6	-0.710011000	-0.977246000	1.651384000
6	0.710011000	-0.977246000	1.651384000
6	1.148821000	0.373275000	1.651384000

6	0.000000000	1.207942000	1.651384000
6	-1.148821000	0.373275000	1.651384000
1	-1.344217000	-1.850156000	1.619650000
1	1.344217000	-1.850156000	1.619650000
1	2.174988000	0.706697000	1.619650000
1	0.000000000	2.286918000	1.619650000
1	-2.174988000	0.706697000	1.619650000

Mn(Cp)₂⁻, LM

Frequencies = 62.0042 cm⁻¹

HF = -1537.5688891 a.u.

25	0.000000000	0.000000000	0.000000000
6	-1.213889000	0.000000000	-1.670336000
6	-0.375112000	-1.154477000	-1.670336000
6	0.982056000	-0.713506000	-1.670336000
6	0.982056000	0.713506000	-1.670336000
6	-0.375112000	1.154477000	-1.670336000
1	-2.295787000	0.000000000	-1.667684000
1	-0.709437000	-2.183424000	-1.667684000
1	1.857331000	-1.349430000	-1.667684000
1	1.857331000	1.349430000	-1.667684000
1	-0.709437000	2.183424000	-1.667684000
6	-1.213889000	0.000000000	1.670336000
6	-0.375112000	-1.154477000	1.670336000
6	0.982056000	-0.713506000	1.670336000
6	0.982056000	0.713506000	1.670336000
6	-0.375112000	1.154477000	1.670336000
1	-2.295787000	0.000000000	1.667684000
1	-0.709437000	-2.183424000	1.667684000
1	1.857331000	-1.349430000	1.667684000
1	1.857331000	1.349430000	1.667684000
1	-0.709437000	2.183424000	1.667684000

Mn(Cp)₂⁻, TS

Frequencies = -59.7834 cm⁻¹

HF = -1537.5665772 a.u.

25	0.000000000	0.000000000	0.000000000
6	0.000000000	1.213407000	1.677847000
6	1.154019000	0.374963000	1.677847000
6	0.713223000	-0.981667000	1.677847000
6	-0.713223000	-0.981667000	1.677847000
6	-1.154019000	0.374963000	1.677847000
1	0.000000000	2.295251000	1.668058000
1	2.182914000	0.709272000	1.668058000

1	1.349115000	-1.856897000	1.668058000
1	-1.349115000	-1.856897000	1.668058000
1	-2.182914000	0.709272000	1.668058000
6	-0.713223000	0.981667000	-1.677847000
6	0.713223000	0.981667000	-1.677847000
6	1.154019000	-0.374963000	-1.677847000
6	0.000000000	-1.213407000	-1.677847000
6	-1.154019000	-0.374963000	-1.677847000
1	-1.349115000	1.856897000	-1.668058000
1	1.349115000	1.856897000	-1.668058000
1	2.182914000	-0.709272000	-1.668058000
1	0.000000000	-2.295251000	-1.668058000
1	-2.182914000	-0.709272000	-1.668058000

Co(Cp)₂⁺, LM

Frequencies = 46.1896 cm⁻¹

HF = -1769.1254591 a.u.

27	0.000000000	0.000000000	0.000000000
6	-0.294936000	-1.171409000	1.639091000
6	-1.205217000	-0.081484000	1.639091000
6	-0.449929000	1.121049000	1.639091000
6	0.927145000	0.774331000	1.639091000
6	1.022936000	-0.642486000	1.639091000
1	-0.558132000	-2.217873000	1.605854000
1	-2.281795000	-0.154546000	1.605854000
1	-0.852095000	2.122358000	1.605854000
1	1.755171000	1.466235000	1.605854000
1	1.936850000	-1.216175000	1.605854000
6	-0.449929000	-1.121049000	-1.639091000
6	-1.205217000	0.081484000	-1.639091000
6	-0.294936000	1.171409000	-1.639091000
6	1.022936000	0.642486000	-1.639091000
6	0.927145000	-0.774331000	-1.639091000
1	-0.852095000	-2.122358000	-1.605854000
1	-2.281795000	0.154546000	-1.605854000
1	-0.558132000	2.217873000	-1.605854000
1	1.936850000	1.216175000	-1.605854000
1	1.755171000	-1.466235000	-1.605854000

Co(Cp)₂⁺, TS

Frequencies = -25.8928 cm⁻¹

HF = -1769.1254061 a.u.

27	0.000000000	0.000000000	0.000000000
6	1.208024000	0.000000000	1.638675000

6	0.373300000	-1.148899000	1.638675000
6	-0.977312000	-0.710059000	1.638675000
6	-0.977312000	0.710059000	1.638675000
6	0.373300000	1.148899000	1.638675000
1	2.287077000	0.000000000	1.605135000
1	0.706746000	-2.175139000	1.605135000
1	-1.850284000	-1.344310000	1.605135000
1	-1.850284000	1.344310000	1.605135000
1	0.706746000	2.175139000	1.605135000
6	1.208024000	0.000000000	-1.638675000
6	0.373300000	-1.148899000	-1.638675000
6	-0.977312000	-0.710059000	-1.638675000
6	-0.977312000	0.710059000	-1.638675000
6	0.373300000	1.148899000	-1.638675000
1	2.287077000	0.000000000	-1.605135000
1	0.706746000	-2.175139000	-1.605135000
1	-1.850284000	-1.344310000	-1.605135000
1	-1.850284000	1.344310000	-1.605135000
1	0.706746000	2.175139000	-1.605135000

Co(Cp)₂⁺, TS

Frequencies = -44.1538 cm⁻¹

HF = -1769.1249558 a.u.

27	0.000000000	0.000000000	0.000000000
6	0.709958000	-0.977173000	-1.640322000
6	1.148736000	0.373247000	-1.640322000
6	0.000000000	1.207852000	-1.640322000
6	-1.148736000	0.373247000	-1.640322000
6	-0.709958000	-0.977173000	-1.640322000
1	1.344205000	-1.850140000	-1.603610000
1	2.174970000	0.706690000	-1.603610000
1	0.000000000	2.286898000	-1.603610000
1	-2.174970000	0.706690000	-1.603610000
1	-1.344205000	-1.850140000	-1.603610000
6	0.000000000	-1.207852000	1.640322000
6	1.148736000	-0.373247000	1.640322000
6	0.709958000	0.977173000	1.640322000
6	-0.709958000	0.977173000	1.640322000
6	-1.148736000	-0.373247000	1.640322000
1	0.000000000	-2.286898000	1.603610000
1	2.174970000	-0.706690000	1.603610000
1	1.344205000	1.850140000	1.603610000
1	-1.344205000	1.850140000	1.603610000
1	-2.174970000	-0.706690000	1.603610000

Cr(Bz)₂, LMFrequencies = 43.0210 cm⁻¹

HF = -1508.3976674 a.u.

24	0.000000000	0.000000000	0.000000000
6	-1.221456000	-0.705208000	1.601204000
6	-1.221456000	0.705208000	1.601204000
6	0.000000000	-1.410416000	1.601204000
1	-2.158823000	1.246397000	1.551696000
1	0.000000000	-2.492794000	1.551696000
6	0.000000000	1.410416000	1.601204000
6	1.221456000	-0.705208000	1.601204000
1	0.000000000	2.492794000	1.551696000
1	2.158823000	-1.246397000	1.551696000
6	1.221456000	0.705208000	1.601204000
1	2.158823000	1.246397000	1.551696000
1	-2.158823000	-1.246397000	1.551696000
6	1.221456000	-0.705208000	-1.601204000
6	1.221456000	0.705208000	-1.601204000
6	0.000000000	-1.410416000	-1.601204000
1	2.158823000	1.246397000	-1.551696000
1	0.000000000	-2.492794000	-1.551696000
6	0.000000000	1.410416000	-1.601204000
6	-1.221456000	-0.705208000	-1.601204000
1	0.000000000	2.492794000	-1.551696000
1	-2.158823000	-1.246397000	-1.551696000
6	-1.221456000	0.705208000	-1.601204000
1	-2.158823000	1.246397000	-1.551696000
1	2.158823000	-1.246397000	-1.551696000

Cr(Bz)₂, TSFrequencies = -64.6490 cm⁻¹

HF = -1508.3959912 a.u.

24	0.000000000	0.000000000	0.000000000
6	0.000000000	1.409970000	1.606411000
6	1.221069000	0.704985000	1.606411000
6	-1.221069000	0.704985000	1.606411000
1	2.158325000	1.246109000	1.555511000
1	-2.158325000	1.246109000	1.555511000
6	1.221069000	-0.704985000	1.606411000
6	-1.221069000	-0.704985000	1.606411000
1	2.158325000	-1.246109000	1.555511000
1	-2.158325000	-1.246109000	1.555511000
6	0.000000000	-1.409970000	1.606411000

1	0.000000000	-2.492219000	1.555511000
1	0.000000000	2.492219000	1.555511000
6	-0.704985000	-1.221069000	-1.606411000
6	0.704985000	-1.221069000	-1.606411000
6	-1.409970000	0.000000000	-1.606411000
1	1.246109000	-2.158325000	-1.555511000
1	-2.492219000	0.000000000	-1.555511000
6	1.409970000	0.000000000	-1.606411000
6	-0.704985000	1.221069000	-1.606411000
1	2.492219000	0.000000000	-1.555511000
1	-1.246109000	2.158325000	-1.555511000
6	0.704985000	1.221069000	-1.606411000
1	1.246109000	2.158325000	-1.555511000
1	-1.246109000	-2.158325000	-1.555511000

$V(\text{Bz})_2^-$, LM

Frequencies = 62.3332 cm^{-1}

HF = -1407.939375 a.u.

23	0.000000000	0.000000000	0.000000000
6	0.708112000	1.226485000	1.649188000
6	1.416223000	0.000000000	1.649188000
6	-0.708112000	1.226485000	1.649188000
1	2.503879000	0.000000000	1.613434000
1	-1.251939000	2.168422000	1.613434000
6	0.708112000	-1.226485000	1.649188000
6	-1.416223000	0.000000000	1.649188000
1	1.251939000	-2.168422000	1.613434000
1	-2.503879000	0.000000000	1.613434000
6	-0.708112000	-1.226485000	1.649188000
1	-1.251939000	-2.168422000	1.613434000
1	1.251939000	2.168422000	1.613434000
6	-1.416223000	0.000000000	-1.649188000
6	-0.708112000	-1.226485000	-1.649188000
6	-0.708112000	1.226485000	-1.649188000
1	-1.251939000	-2.168422000	-1.613434000
1	-1.251939000	2.168422000	-1.613434000
6	0.708112000	-1.226485000	-1.649188000
6	0.708112000	1.226485000	-1.649188000
1	1.251939000	-2.168422000	-1.613434000
1	1.251939000	2.168422000	-1.613434000
6	1.416223000	0.000000000	-1.649188000
1	2.503879000	0.000000000	-1.613434000
1	-2.503879000	0.000000000	-1.613434000

V(Bz)₂⁻, TS

Frequencies = -66.3346 cm⁻¹

HF = -1407.937265 a.u.

23	0.000000000	0.000000000	0.000000000
6	1.001208000	1.001208000	-1.652265000
6	-0.366467000	1.367675000	-1.652265000
6	1.367675000	-0.366467000	-1.652265000
1	-0.647935000	2.418125000	-1.612916000
1	2.418125000	-0.647935000	-1.612916000
6	-1.367675000	0.366467000	-1.652265000
6	0.366467000	-1.367675000	-1.652265000
1	-2.418125000	0.647935000	-1.612916000
1	0.647935000	-2.418125000	-1.612916000
6	-1.001208000	-1.001208000	-1.652265000
1	-1.770190000	-1.770190000	-1.612916000
1	1.770190000	1.770190000	-1.612916000
6	-0.366467000	-1.367675000	1.652265000
6	-1.367675000	-0.366467000	1.652265000
6	1.001208000	-1.001208000	1.652265000
1	-2.418125000	-0.647935000	1.612916000
1	1.770190000	-1.770190000	1.612916000
6	-1.001208000	1.001208000	1.652265000
6	1.367675000	0.366467000	1.652265000
1	-1.770190000	1.770190000	1.612916000
1	2.418125000	0.647935000	1.612916000
6	0.366467000	1.367675000	1.652265000
1	0.647935000	2.418125000	1.612916000
1	-0.647935000	-2.418125000	1.612916000

Mn(Bz)₂⁺, LM

Frequencies = 39.0068 cm⁻¹

HF = -1614.7283949 a.u.

25	0.000000000	0.000000000	0.000000000
6	0.702875000	1.217414000	1.586282000
6	1.405749000	0.000000000	1.586282000
6	-0.702875000	1.217414000	1.586282000
1	2.486193000	0.000000000	1.525140000
1	-1.243097000	2.153106000	1.525140000
6	0.702875000	-1.217414000	1.586282000
6	-1.405749000	0.000000000	1.586282000
1	1.243097000	-2.153106000	1.525140000
1	-2.486193000	0.000000000	1.525140000
6	-0.702875000	-1.217414000	1.586282000
1	-1.243097000	-2.153106000	1.525140000

1	1.243097000	2.153106000	1.525140000
6	-1.405749000	0.000000000	-1.586282000
6	-0.702875000	-1.217414000	-1.586282000
6	-0.702875000	1.217414000	-1.586282000
1	-1.243097000	-2.153106000	-1.525140000
1	-1.243097000	2.153106000	-1.525140000
6	0.702875000	-1.217414000	-1.586282000
6	0.702875000	1.217414000	-1.586282000
1	1.243097000	-2.153106000	-1.525140000
1	1.243097000	2.153106000	-1.525140000
6	1.405749000	0.000000000	-1.586282000
1	2.486193000	0.000000000	-1.525140000
1	-2.486193000	0.000000000	-1.525140000

Mn(Bz)₂⁺, TS

Frequencies = -60.8343 cm⁻¹

HF = -1614.727317 a.u.

25	0.000000000	0.000000000	0.000000000
6	-0.363777000	-1.357633000	1.590283000
6	-1.357633000	-0.363777000	1.590283000
6	0.993857000	-0.993857000	1.590283000
1	-2.401258000	-0.643415000	1.527290000
1	1.757843000	-1.757843000	1.527290000
6	-0.993857000	0.993857000	1.590283000
6	1.357633000	0.363777000	1.590283000
1	-1.757843000	1.757843000	1.527290000
1	2.401258000	0.643415000	1.527290000
6	0.363777000	1.357633000	1.590283000
1	0.643415000	2.401258000	1.527290000
1	-0.643415000	-2.401258000	1.527290000
6	0.993857000	0.993857000	-1.590283000
6	-0.363777000	1.357633000	-1.590283000
6	1.357633000	-0.363777000	-1.590283000
1	-0.643415000	2.401258000	-1.527290000
1	2.401258000	-0.643415000	-1.527290000
6	-1.357633000	0.363777000	-1.590283000
6	0.363777000	-1.357633000	-1.590283000
1	-2.401258000	0.643415000	-1.527290000
1	0.643415000	-2.401258000	-1.527290000
6	-0.993857000	-0.993857000	-1.590283000
1	-1.757843000	-1.757843000	-1.527290000
1	1.757843000	1.757843000	-1.527290000

Mn(Bz)(Cp), LM

Frequencies = 9.7139 cm⁻¹

HF = -1576.2456221 a.u.

25	-0.000310000	0.016490000	0.002307000
6	1.266439000	-1.504629000	0.617529000
6	1.167072000	-1.505863000	-0.788700000
6	0.097570000	-1.500365000	1.407168000
1	2.061282000	-1.414191000	-1.391981000
1	0.173529000	-1.412114000	2.483415000
6	-0.099987000	-1.503393000	-1.406739000
6	-1.170930000	-1.497134000	0.788703000
1	-0.175027000	-1.411014000	-2.482773000
1	-2.065232000	-1.407804000	1.392023000
6	-1.269197000	-1.499087000	-0.618556000
1	-2.238499000	-1.407429000	-1.091766000
1	2.236674000	-1.416226000	1.089438000
6	0.497090000	1.735347000	-1.098010000
6	-0.891717000	1.735781000	-0.808550000
6	-1.045928000	1.736059000	0.601611000
6	0.247553000	1.734667000	1.183703000
6	1.201203000	1.734533000	0.133360000
1	0.940217000	1.721677000	-2.082614000
1	-1.690970000	1.723619000	-1.534467000
1	-1.983101000	1.724414000	1.137658000
1	0.467809000	1.721927000	2.240619000
1	2.274498000	1.719693000	0.250624000

Mn(Bz)(Cp), TS

Frequencies = -26.7583 cm⁻¹

HF = -1576.2455632 a.u.

25	-0.015551000	-0.001518000	0.000000000
6	1.505799000	1.220296000	0.704854000
6	1.505799000	1.220296000	-0.704854000
6	1.502617000	-0.000539000	1.410387000
1	1.413822000	2.154571000	-1.243959000
1	1.412899000	0.000262000	2.489200000
6	1.502617000	-0.000539000	-1.410387000
6	1.499537000	-1.222559000	0.705549000
1	1.412899000	0.000262000	-2.489200000
1	1.410694000	-2.156664000	1.245136000
6	1.499537000	-1.222559000	-0.705549000
1	1.410694000	-2.156664000	-1.245136000
1	1.413822000	2.154571000	1.243959000
6	-1.733027000	0.374032000	-1.147693000
6	-1.736673000	-0.975205000	-0.709264000

6	-1.736673000	-0.975205000	0.709264000
6	-1.733027000	0.374032000	1.147693000
6	-1.730719000	1.207992000	0.000000000
1	-1.718758000	0.707682000	-2.174559000
1	-1.726587000	-1.848933000	-1.343755000
1	-1.726587000	-1.848933000	1.343755000
1	-1.718758000	0.707682000	2.174559000
1	-1.715502000	2.287705000	0.000000000

Mn(Bz)(Cp), TS

Frequencies = -28.5232 cm⁻¹

HF = -1576.2455376 a.u.

25	-0.015735000	0.001529000	0.000000000
6	1.498015000	-0.706555000	-1.221973000
6	1.493191000	-1.412265000	0.000000000
6	1.506480000	0.703808000	-1.221163000
1	1.402794000	-2.490892000	0.000000000
1	1.418534000	1.244535000	-2.154846000
6	1.498015000	-0.706555000	1.221973000
6	1.511627000	1.408200000	0.000000000
1	1.405023000	-1.245018000	2.156412000
1	1.425485000	2.487402000	0.000000000
6	1.506480000	0.703808000	1.221163000
1	1.418534000	1.244535000	2.154846000
1	1.405023000	-1.245018000	-2.156412000
6	-1.734540000	0.977151000	0.709327000
6	-1.734540000	0.977151000	-0.709327000
6	-1.733594000	-0.372172000	-1.147697000
6	-1.732799000	-1.206135000	0.000000000
6	-1.733594000	-0.372172000	1.147697000
1	-1.722699000	1.850844000	1.343820000
1	-1.722699000	1.850844000	-1.343820000
1	-1.720040000	-0.706022000	-2.174501000
1	-1.720991000	-2.285885000	0.000000000
1	-1.720040000	-0.706022000	2.174501000

Cr(Bz)(Cp)⁻, LM

Frequencies = 16.4655 cm⁻¹

HF = -1469.7253816 a.u.

24	-0.000170000	-0.012999000	0.002262000
6	1.274971000	-1.548918000	0.620307000
6	1.174283000	-1.550707000	-0.794644000
6	0.098931000	-1.543663000	1.415897000
1	2.071576000	-1.461067000	-1.400679000

1	0.175934000	-1.459993000	2.496411000
6	-0.100820000	-1.548526000	-1.415835000
6	-1.178247000	-1.540154000	0.794047000
1	-0.175988000	-1.458828000	-2.496021000
1	-2.076212000	-1.454585000	1.399563000
6	-1.277255000	-1.543036000	-0.622350000
1	-2.250191000	-1.454964000	-1.097639000
1	2.249311000	-1.463939000	1.093470000
6	0.497901000	1.786487000	-1.098878000
6	-0.892699000	1.788550000	-0.809646000
6	-1.047857000	1.789247000	0.602430000
6	0.247189000	1.788131000	1.186235000
6	1.202416000	1.786154000	0.134621000
1	0.942661000	1.782749000	-2.085181000
1	-1.693414000	1.787056000	-1.537234000
1	-1.987453000	1.788736000	1.138732000
1	0.467266000	1.786570000	2.245469000
1	2.277902000	1.782657000	0.252664000

Cr(Bz)(Cp)⁻, TS

Frequencies = -32.3892 cm⁻¹

HF = -1469.7252613 a.u.

24	0.013445000	0.004747000	0.000000000
6	1.540044000	-0.710575000	-1.229780000
6	1.533014000	-1.421083000	0.000000000
6	1.553119000	0.708659000	-1.228646000
1	1.442665000	-2.503690000	0.000000000
1	1.470914000	1.251961000	-2.165879000
6	1.540044000	-0.710575000	1.229780000
6	1.559582000	1.417302000	0.000000000
1	1.450526000	-1.250644000	2.168163000
1	1.479523000	2.500834000	0.000000000
6	1.553119000	0.708659000	1.228646000
1	1.470914000	1.251961000	2.165879000
1	1.450526000	-1.250644000	-2.168163000
6	-1.789808000	0.977522000	0.710287000
6	-1.789808000	0.977522000	-0.710287000
6	-1.785728000	-0.373634000	-1.149290000
6	-1.782944000	-1.208487000	0.000000000
6	-1.785728000	-0.373634000	1.149290000
1	-1.791133000	1.853084000	1.346032000
1	-1.791133000	1.853084000	-1.346032000
1	-1.782613000	-0.708415000	-2.178193000
1	-1.778017000	-2.290439000	0.000000000

1	-1.782613000	-0.708415000	2.178193000
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Cr(Bz)(Cp)⁻, TS

Frequencies = -28.2722 cm⁻¹

HF = -1469.7252887 a.u.

24	0.013304000	0.002389000	0.000000000
6	1.554749000	1.228353000	0.709122000
6	1.554749000	1.228353000	-0.709122000
6	1.546423000	0.000144000	1.419311000
1	1.471263000	2.166853000	-1.250093000
1	1.461038000	0.001927000	2.502403000
6	1.546423000	0.000144000	-1.419311000
6	1.538564000	-1.229913000	0.710191000
1	1.461038000	0.001927000	-2.502403000
1	1.450809000	-2.167226000	1.252264000
6	1.538564000	-1.229913000	-0.710191000
1	1.450809000	-2.167226000	-1.252264000
1	1.471263000	2.166853000	1.250093000
6	-1.787044000	0.373203000	-1.149316000
6	-1.786102000	-0.977848000	-0.710196000
6	-1.786102000	-0.977848000	0.710196000
6	-1.787044000	0.373203000	1.149316000
6	-1.787437000	1.208265000	0.000000000
1	-1.785428000	0.707574000	-2.178312000
1	-1.783784000	-1.853484000	-1.345885000
1	-1.783784000	-1.853484000	1.345885000
1	-1.785428000	0.707574000	2.178312000
1	-1.787964000	2.290243000	0.000000000

Fe(Bz)(Cp)⁺, LM

Frequencies = 20.5583 cm⁻¹

HF = -1688.7565966 a.u.

26	0.061098000	-0.000291000	-0.000323000
6	-1.486814000	1.354884000	-0.380148000
6	-1.482154000	1.009020000	0.982494000
6	-1.490539000	0.348044000	-1.361123000
1	-1.400736000	1.782066000	1.735206000
1	-1.411448000	0.613673000	-2.407172000
6	-1.481786000	-0.344334000	1.364443000
6	-1.489344000	-1.004861000	-0.979881000
1	-1.401541000	-0.610145000	2.410291000
1	-1.410901000	-1.777668000	-1.733173000
6	-1.485663000	-1.351471000	0.382754000
1	-1.407426000	-2.390303000	0.675185000

1	-1.405699000	2.393384000	-0.673136000
6	1.723928000	-1.202877000	0.110675000
6	1.723950000	-0.479427000	-1.109301000
6	1.725682000	0.904129000	-0.798089000
6	1.726376000	1.035739000	0.614198000
6	1.725474000	-0.266557000	1.175959000
1	1.696646000	-2.277570000	0.210409000
1	1.697658000	-0.906662000	-2.100533000
1	1.699833000	1.714646000	-1.510932000
1	1.701652000	1.964267000	1.164637000
1	1.699638000	-0.503132000	2.228971000

Fe(Bz)(Cp)⁺, TS

Frequencies = -24.7812 cm⁻¹

HF = -1688.7565148 a.u.

26	-0.060927000	-0.000011000	0.000000000
6	1.490524000	1.216155000	0.702733000
6	1.490524000	1.216155000	-0.702733000
6	1.487506000	-0.000963000	1.405788000
1	1.410696000	2.150702000	-1.242230000
1	1.408017000	-0.000556000	2.484867000
6	1.487506000	-0.000963000	-1.405788000
6	1.484250000	-1.218662000	0.703064000
1	1.408017000	-0.000556000	-2.484867000
1	1.404615000	-2.153003000	1.242653000
6	1.484250000	-1.218662000	-0.703064000
1	1.404615000	-2.153003000	-1.242653000
1	1.410696000	2.150702000	1.242230000
6	-1.724062000	0.374050000	-1.147318000
6	-1.725924000	-0.974756000	-0.709043000
6	-1.725924000	-0.974756000	0.709043000
6	-1.724062000	0.374050000	1.147318000
6	-1.722859000	1.207773000	0.000000000
1	-1.696297000	0.707698000	-2.173756000
1	-1.700648000	-1.848048000	-1.343407000
1	-1.700648000	-1.848048000	1.343407000
1	-1.696297000	0.707698000	2.173756000
1	-1.694689000	2.287069000	0.000000000

Fe(Bz)(Cp)⁺, TS

Frequencies = -26.3984 cm⁻¹

HF = -1688.7565026 a.u.

26	-0.061338000	0.000867000	0.000000000
6	1.484276000	-0.704758000	-1.217636000

6	1.481209000	-1.407923000	0.000000000
6	1.490236000	0.700986000	-1.217228000
1	1.400589000	-2.486813000	0.000000000
1	1.412005000	1.241057000	-2.151549000
6	1.484276000	-0.704758000	1.217636000
6	1.493919000	1.403492000	0.000000000
1	1.403530000	-1.243903000	2.152220000
1	1.417080000	2.482842000	0.000000000
6	1.490236000	0.700986000	1.217228000
1	1.412005000	1.241057000	2.151549000
1	1.403530000	-1.243903000	-2.152220000
6	-1.724655000	0.977560000	0.709067000
6	-1.724655000	0.977560000	-0.709067000
6	-1.724850000	-0.371256000	-1.147291000
6	-1.724995000	-1.205000000	0.000000000
6	-1.724850000	-0.371256000	1.147291000
1	-1.697741000	1.850954000	1.343222000
1	-1.697741000	1.850954000	-1.343222000
1	-1.697524000	-0.704671000	-2.173785000
1	-1.699069000	-2.284314000	0.000000000
1	-1.697524000	-0.704671000	2.173785000