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Metal carbonyl derivatives of CB_6 and NB_6 species: molecular rotors with hypercoordinated units

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Calculation procedure

The density functional theory (DFT) calculations were performed with the B3LYP[S1] and PBE0[S2] functionals and valence-split basis set 6-311+G(df)[S3] using the Gaussian-16[S4] program package. The stationary points on the potential energy surfaces (PESs) were located with full geometry optimizations, identified by calculating the matrix of second derivatives (force constants) and checked for the stabilities of Hartree-Fock solutions. The AIM (Atoms in molecules[S5]) analysis was carried out using the AIMAll Professional program.[S6] The drawings were made using the program suite ChemCraft[S7] with calculated atomic coordinates as the input parameters.

References to calculation procedure

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Table S1 Energy parameters* of the systems **5 - 7** calculated using B3LYP and PBE0 (values in italic) methods with 6-311+G(df) basis set.

System	$E_{tot.}$	ZPE	ΔE	λ	ω_1	Δ_{H-L}
5a (X=C, M=Ni)	-1922.089325	0.044563	0	0	23.1	3.1
	-1921.312227	*0.045905*	*0*	*0*	*23.8*	*3.7*
5b (X=C, M=Ni)	-1922.088933	0.044497	0.25	1	*i*24.0	3.0
	-1921.311784	*0.045831*	*0.28*	*1*	*i26.3*	*3.6*
5a (X=N, M=Co)	-1813.166017	0.041860	0	0	12.0	3.3
	-1812.382856	*0.043446*	*0*	*0*	*16.7*	*3.8*
5b (X=N, M=Co)	-1813.165894	0.041754	0.08	1	*i*14.0	3.3
	-1812.382639	*0.043373*	*0.14*	*1*	*i19.2*	*3.8*
6a (X=C, M=Fe)	-1790.901117	0.055069	0	0	22.4	4.8
	-1790.026699	*0.056611*	*0*	*0*	*26.1*	*5.3*
6b (X=C, M=Fe)	-1790.900683	0.054992	0.27	1	*i*22.7	4.8
	-1790.026098	*0.056514*	*0.38*	*1*	*i27.3*	*5.3*
6a (X=N, M=Mn)	-1694.791282	0.051803	0	0	25.7	4.2
	-1693.912541	*0.053541*	*0*	*0*	*28.0*	*4.7*
6b (X=N, M=Mn)	-1694.790716	0.051698	0.36	1	*i*25.9	4.1
	-1693.911867	*0.053414*	*0.42*	*1*	*i29.2*	*4.7*
7a (X=C, M=Cr)	-1685.023599	0.063253	0	0	3.2	4.5
	-1684.054683	*0.065108*	*0*	*0*	*6.9*	*5.0*
7b (X=C, M=Cr)	-1685.023599	0.063253	0	0	3.3	4.5
	-1684.054680	*0.065097*	*0*	*0*	*4.9*	*5.0*
7c (X=C, M=Cr)	-1685.023599	0.063251	0	1	*i*0.1	4.5
	-1684.054678	*0.065090*	*0*	*1*	*i4.4*	*4.5*
7a (X=N, M=V)	-1601.181594	0.059251	0	0	1.8	3.8
	-1600.205044	*0.061190*	*0*	*0*	*8.6*	*4.3*
7b (X=N, M=V)	-1601.181595	0.059256	0	0	4.8	3.8
	-1600.205042	*0.061183*	*0*	*0*	*2.2*	*4.3*
7c (X=N, M=V)	-1601.181594	0.059246	0	1	*i*0.4	3.8
	-1600.205041	*0.061177*	*0*	*1*	*i3.0*	*4.3*

*$E_{tot.}$ (a.u.) – total energy; ZPE (a.u.) – harmonic zero-point energy correction; ΔE (kcal·mol^{-1}) – relative energy; λ – number of negative hessian eigenvalues; ω_1 (cm^{-1}) – value of the lowest harmonic vibration frequencies; Δ_{H-L}, (eV) - HOMO–LUMO energy gap.

Table S2 AIM parameters (a.u.)* for the bond critical point (BCP) corresponding to the bonds in systems **5a** – **7a** calculated using B3LYP and PBE0 (values in italic) methods with 6-311+G(df) basis set.

System	Bond	$\rho(r)$	$\nabla^2\rho(r)$	$V_b(r)$	$G_b(r)$	$H_b(r)$	$-G(r)/V(r)$
5a (X=C, M=Ni)	C…B	0.145	-0.081	-0.167	0.073	-0.094	0.44
		0.144	*-0.082*	*-0.168*	*0.074*	*-0.094*	*0.44*
	C,,,.Ni	0.086	0.274	-0.114	0.091	-0.023	0.80
		0.095	*0.300*	*-0.131*	*0.103*	*-0.028*	*0.79*
5a (X=N, M=Co)	N…B	0.130	0.042	-0.160	0.086	-0.075	0.54
		0.130	*0.037*	*-0.163*	*0.086*	*-0.077*	*0.53*
	N,,,.Co	0.108	0.449	-0.166	0.139	-0.027	0.84
		0.119	*0.479*	*-0.189*	*0.154*	*-0.035*	*0.81*
6a (X=C, M=Fe)	C…B	0.147	-0.066	-0.173	0.078	-0.095	0.45
		0.146	*-0.069*	*-0.174*	*0.078*	*-0.096*	*0.45*
	C,,,.Fe	0.087	0.278	-0.113	0.091	-0.022	0.81
		0.096	*0.298*	*-0.129*	*0.102*	*-0.027*	*0.79*
6a (X=N, M=Mn)	N…B	0.130	0.048	-0.160	0.086	-0.074	0.54
		0.130	*0.041*	*-0.162*	*0.086*	*-0.076*	*0.53*
	N,,,.Mn	0.102	0.389	-0.149	0.123	-0.026	0.83
		0.112	*0.417*	*-0.172*	*0.138*	*-0.034*	*0.80*
7a (X=C, M=Cr)	C…B	0.149	-0.072	-0.177	0.080	-0.098	0.45
		0.148	*-0.076*	*-0.178*	*0.079*	*-0.098*	*0.44*
	C,,,.Cr	0.081	0.243	-0.098	0.079	-0.019	0.81
		0.089	*0.262*	*-0.114*	*0.090*	*-0.024*	*0.79*
7a (X=N, M=V)	N…B	0.132	0.040	-0.164	0.087	-0.077	0.53
		0.132	*0.033*	*-0.165*	*0.087*	*-0.078*	*0.53*
	N,,,.V	0.088	0.318	-0.121	0.100	-0.021	0.83
		0.095	*0.344*	*-0.137*	*0.111*	*-0.025*	*0.81*

[a]$\rho(r)$ - electron density; $\nabla^2\rho(r)$ - Laplacian of the electron density; H(r) - total electron energy density; V(r) - potential electron energy density; G(r) - kinetic electron energy density.

Figure S1

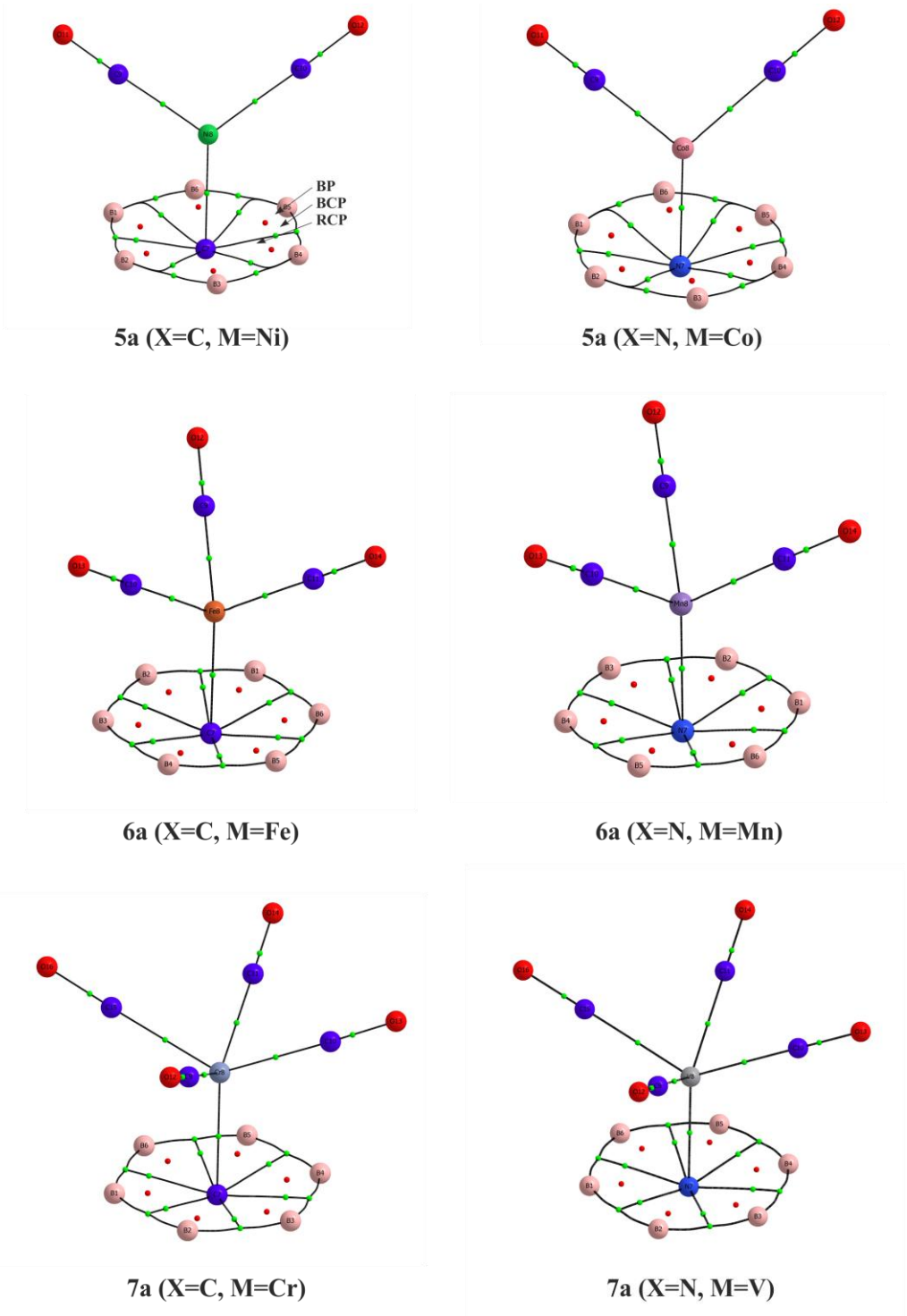

Figure S1 The Bader molecular graphs of structures **5a - 7a**. BP designates the Bader bond path, CP – the bond path critical point, RCP – ring critical point.

Atomic coordinates of optimized structures 5 - 7 calculated by B3LYP/6-311+G(df) and PBE0/6-311+G(df) methods

5a (X=C, M=Ni)
[B3LYP/6-311+G(df)]
C_{2v}

B	0.813549000000	1.355275000000	-1.491942000000
B	-0.813549000000	1.355275000000	-1.491942000000
B	-1.616499000000	0.000000000000	-1.543938000000
B	-0.813549000000	-1.355275000000	-1.491942000000
B	0.813549000000	-1.355275000000	-1.491942000000
B	1.616499000000	0.000000000000	-1.543938000000
C	0.000000000000	0.000000000000	-1.757535000000
Ni	0.000000000000	0.000000000000	0.240757000000
C	0.000000000000	1.426393000000	1.340147000000
C	0.000000000000	-1.426393000000	1.340147000000
O	0.000000000000	2.302248000000	2.062530000000
O	0.000000000000	-2.302248000000	2.062530000000

5a (X=C, M=Ni)
[PBE0/6-311+G(df)]
C_{2v}

B	0.811584000000	1.356081000000	-1.438442000000
B	-0.811584000000	1.356081000000	-1.438442000000
B	-1.615729000000	0.000000000000	-1.492344000000
B	-0.811584000000	-1.356081000000	-1.438442000000
B	0.811584000000	-1.356081000000	-1.438442000000
B	1.615729000000	0.000000000000	-1.492344000000
C	0.000000000000	0.000000000000	-1.742665000000
Ni	0.000000000000	0.000000000000	0.218064000000
C	0.000000000000	1.409267000000	1.307857000000
C	0.000000000000	-1.409267000000	1.307857000000
O	0.000000000000	2.288789000000	2.021761000000
O	0.000000000000	-2.288789000000	2.021761000000

5b (X=C, M=Ni)
[B3LYP/6-311+G(df)]
C_{2v}

B	1.403280000000	0.780721000000	-1.526934000000
B	0.000000000000	1.566015000000	-1.481599000000
B	-1.403280000000	0.780721000000	-1.526934000000
B	-1.403280000000	-0.780721000000	-1.526934000000
B	0.000000000000	-1.566015000000	-1.481599000000
B	1.403280000000	-0.780721000000	-1.526934000000
C	0.000000000000	0.000000000000	-1.760451000000
Ni	0.000000000000	0.000000000000	0.238088000000
C	0.000000000000	1.421505000000	1.342752000000
C	0.000000000000	-1.421505000000	1.342752000000
O	0.000000000000	2.292292000000	2.071118000000
O	0.000000000000	-2.292292000000	2.071118000000

5b (X=C, M=Ni)
[PBE0/6-311+G(df)]
C_{2v}

B	1.402095000000	0.782101000000	-1.475727000000
B	0.000000000000	1.565325000000	-1.426528000000
B	-1.402095000000	0.782101000000	-1.475727000000
B	-1.402095000000	-0.782101000000	-1.475727000000
B	0.000000000000	-1.565325000000	-1.426528000000
B	1.402095000000	-0.782101000000	-1.475727000000
C	0.000000000000	0.000000000000	-1.745031000000
Ni	0.000000000000	0.000000000000	0.216603000000
C	0.000000000000	1.405344000000	1.310328000000
C	0.000000000000	-1.405344000000	1.310328000000
O	0.000000000000	2.280893000000	2.028823000000
O	0.000000000000	-2.280893000000	2.028823000000

6a (X=C, M=Fe)
[B3LYP/6-311+G(df)]
C_{3v}

B	0.798499000000	1.373059000000	-1.644869000000
B	-0.798499000000	1.373059000000	-1.644869000000
B	-1.588354000000	0.004991000000	-1.644869000000
B	-0.789855000000	-1.378050000000	-1.644869000000
B	0.789855000000	-1.378050000000	-1.644869000000
B	1.588354000000	0.004991000000	-1.644869000000
C	0.000000000000	0.000000000000	-1.904592000000
Fe	0.000000000000	0.000000000000	0.116564000000
C	0.000000000000	1.546828000000	1.030653000000
C	-1.339592000000	-0.773414000000	1.030653000000
C	1.339592000000	-0.773414000000	1.030653000000
O	0.000000000000	2.514430000000	1.632967000000
O	-2.177560000000	-1.257215000000	1.632967000000
O	2.177560000000	-1.257215000000	1.632967000000

6a (X=C, M=Fe)
[PBE0/6-311+G(df)]
C_{3v}

B	0.798650000000	1.373297000000	-1.593229000000
B	-0.798650000000	1.373297000000	-1.593229000000
B	-1.588635000000	0.005003000000	-1.593229000000
B	-0.789985000000	-1.378300000000	-1.593229000000
B	0.789985000000	-1.378300000000	-1.593229000000
B	1.588635000000	0.005003000000	-1.593229000000
C	0.000000000000	0.000000000000	-1.884817000000
Fe	0.000000000000	0.000000000000	0.098685000000
C	0.000000000000	1.526917000000	1.003832000000
C	-1.322349000000	-0.763458000000	1.003832000000
C	1.322349000000	-0.763458000000	1.003832000000
O	0.000000000000	2.493619000000	1.602958000000
O	-2.159538000000	-1.246810000000	1.602958000000
O	2.159538000000	-1.246810000000	1.602958000000

6b (X=C, M=Fe)
[B3LYP/6-311+G(df)]
C_{3v}

B	0.000000000000	1.587478000000	-1.662193000000
B	-1.376065000000	0.794471000000	-1.632223000000
B	-1.374796000000	-0.793739000000	-1.662193000000
B	0.000000000000	-1.588943000000	-1.632223000000
B	1.374796000000	-0.793739000000	-1.662193000000
B	1.376065000000	0.794471000000	-1.632223000000
C	0.000000000000	0.000000000000	-1.904629000000
Fe	0.000000000000	0.000000000000	0.117325000000
C	0.000000000000	1.546212000000	1.032188000000
C	-1.339059000000	-0.773106000000	1.032188000000
C	1.339059000000	-0.773106000000	1.032188000000
O	0.000000000000	2.514157000000	1.633925000000
O	-2.177324000000	-1.257078000000	1.633925000000
O	2.177324000000	-1.257078000000	1.633925000000

6b (X=C, M=Fe)
[PBE0/6-311+G(df)]
C_{3v}

B	0.000000000000	1.587331000000	-1.607392000000
B	-1.376707000000	0.794842000000	-1.582530000000
B	-1.374669000000	-0.793666000000	-1.607392000000
B	0.000000000000	-1.589684000000	-1.582530000000
B	1.374669000000	-0.793666000000	-1.607392000000
B	1.376707000000	0.794842000000	-1.582530000000
C	0.000000000000	0.000000000000	-1.884994000000
Fe	0.000000000000	0.000000000000	0.099675000000
C	0.000000000000	1.526344000000	1.005241000000
C	-1.321853000000	-0.763172000000	1.005241000000
C	1.321853000000	-0.763172000000	1.005241000000
O	0.000000000000	2.493848000000	1.603038000000
O	-2.159736000000	-1.246924000000	1.603038000000
O	2.159736000000	-1.246924000000	1.603038000000

7a (X=C, M=Cr)
[B3LYP/6-311+G(df)]
C_{2v}

B	-1.376591000000	0.795269000000	1.825675000000
B	0.000000000000	1.590270000000	1.818974000000
B	1.376591000000	0.795269000000	1.825675000000
B	1.376591000000	-0.795269000000	1.825675000000
B	0.000000000000	-1.590270000000	1.818974000000
B	-1.376591000000	-0.795269000000	1.825675000000
C	0.000000000000	0.000000000000	2.020895000000
Cr	0.000000000000	0.000000000000	-0.060807000000
C	0.000000000000	1.720040000000	-0.865721000000
C	1.712079000000	0.000000000000	-0.879092000000
C	0.000000000000	-1.720040000000	-0.865721000000
O	0.000000000000	2.739378000000	-1.378913000000
O	2.728494000000	0.000000000000	-1.398056000000
O	0.000000000000	-2.739378000000	-1.378913000000
C	-1.712079000000	0.000000000000	-0.879092000000
O	-2.728494000000	0.000000000000	-1.398056000000

7a (X=C, M=Cr)
[PBE0/6-311+G(df)]
C_{2v}

B	1.377076000000	0.795781000000	-1.772490000000
B	0.000000000000	1.591293000000	-1.765789000000
B	-1.377076000000	0.795781000000	-1.772490000000
B	-1.377076000000	-0.795781000000	-1.772490000000
B	0.000000000000	-1.591293000000	-1.765789000000
B	1.377076000000	-0.795781000000	-1.772490000000
C	0.000000000000	0.000000000000	-2.004462000000
Cr	0.000000000000	0.000000000000	0.037991000000
C	0.000000000000	1.687600000000	0.843157000000
C	-1.680169000000	0.000000000000	0.855433000000
C	0.000000000000	-1.687600000000	0.843157000000
O	0.000000000000	2.702506000000	1.360875000000
O	-2.691991000000	0.000000000000	1.379100000000
O	0.000000000000	-2.702506000000	1.360875000000
C	1.680169000000	0.000000000000	0.855433000000
O	2.691991000000	0.000000000000	1.379100000000

7b (X=C, M=Cr)
[B3LYP/6-311+G(df)]
C_{2v}

B	1.377485000000	0.794413000000	-1.820527000000
B	1.377485000000	-0.794413000000	-1.820527000000
B	0.000000000000	-1.589608000000	-1.828913000000
C	0.000000000000	0.000000000000	-2.020706000000
B	0.000000000000	1.589608000000	-1.828913000000
B	-1.377485000000	0.794413000000	-1.820527000000
B	-1.377485000000	-0.794413000000	-1.820527000000
Cr	0.000000000000	0.000000000000	0.060957000000
C	1.213916000000	1.213183000000	0.872372000000
C	-1.213916000000	1.213183000000	0.872372000000
C	-1.213916000000	-1.213183000000	0.872372000000
O	1.932640000000	1.934061000000	1.388250000000
O	-1.932640000000	1.934061000000	1.388250000000
O	-1.932640000000	-1.934061000000	1.388250000000
C	1.213916000000	-1.213183000000	0.872372000000
O	1.932640000000	-1.934061000000	1.388250000000

7b (X=C, M=Cr)
[PBE0/6-311+G(df)]
C_{2v}

B	1.378324000000	0.794672000000	-1.767461000000
B	1.378324000000	-0.794672000000	-1.767461000000
B	0.000000000000	-1.590197000000	-1.776027000000
C	0.000000000000	0.000000000000	-2.004736000000
B	0.000000000000	1.590197000000	-1.776027000000
B	-1.378324000000	0.794672000000	-1.767461000000
B	-1.378324000000	-0.794672000000	-1.767461000000
Cr	0.000000000000	0.000000000000	0.037942000000
C	1.190923000000	1.190490000000	0.849345000000
C	-1.190923000000	1.190490000000	0.849345000000
C	-1.190923000000	-1.190490000000	0.849345000000
O	1.906157000000	1.908178000000	1.370094000000
O	-1.906157000000	1.908178000000	1.370094000000
O	-1.906157000000	-1.908178000000	1.370094000000
C	1.190923000000	-1.190490000000	0.849345000000
O	1.906157000000	-1.908178000000	1.370094000000

7c (X=C, M=Cr)
[B3LYP/6-311+G(df)]
C_2

B	0.569171000000	1.484626000000	-1.822395000000
B	-1.001589000000	1.234378000000	-1.828399000000
B	-1.570315000000	-0.250718000000	-1.819337000000
C	0.000000000000	0.000000000000	-2.020827000000
Cr	0.000000000000	0.000000000000	0.060825000000
C	0.000000000000	1.714057000000	0.875794000000
C	-1.718158000000	-0.000768000000	0.868960000000
C	0.000000000000	-1.714057000000	0.875794000000
O	-0.001514000000	2.731188000000	1.393336000000
O	-2.736812000000	0.000206000000	1.383504000000
O	0.001514000000	-2.731188000000	1.393336000000
C	1.718158000000	0.000768000000	0.868960000000
O	2.736812000000	-0.000206000000	1.383504000000
B	1.570315000000	0.250718000000	-1.819337000000
B	1.001589000000	-1.234378000000	-1.828399000000
B	-0.569171000000	-1.484626000000	-1.822395000000

7c (X=C, M=Cr)
[PBE0/6-311+G(df)]
C_2

B	-1.775843000000	1.560288000000	-0.307716000000
B	-1.767052000000	1.046831000000	1.198490000000
B	-1.767698000000	-0.512408000000	1.506263000000
C	-2.004898000000	0.000247000000	0.000240000000
Cr	0.037785000000	-0.000005000000	-0.000006000000
C	0.849468000000	1.382751000000	0.960891000000
C	0.849576000000	-0.960455000000	1.382866000000
C	0.848873000000	-1.382945000000	-0.961090000000
O	1.370484000000	2.215784000000	1.537503000000
O	1.370670000000	-1.539908000000	2.213875000000
O	1.369542000000	-2.216107000000	-1.537831000000
C	0.849469000000	0.960243000000	-1.383070000000
O	1.370507000000	1.539564000000	-2.214206000000
B	-1.767928000000	0.512833000000	-1.505838000000
B	-1.767619000000	-1.046407000000	-1.198064000000
B	-1.776142000000	-1.559854000000	0.308143000000

5a (X=N, M=Co)
[B3LYP/6-311+G(df)]
C_{2v}

B	0.811366000000	1.354549000000	-1.418026000000
B	-0.811366000000	1.354549000000	-1.418026000000
B	-1.649033000000	0.000000000000	-1.407463000000
B	-0.811366000000	-1.354549000000	-1.418026000000
B	0.811366000000	-1.354549000000	-1.418026000000
B	1.649033000000	0.000000000000	-1.407463000000
N	0.000000000000	0.000000000000	-1.749551000000
Co	0.000000000000	0.000000000000	0.167572000000
C	0.000000000000	1.309853000000	1.350606000000
C	0.000000000000	-1.309853000000	1.350606000000
O	0.000000000000	2.152254000000	2.121893000000
O	0.000000000000	-2.152254000000	2.121893000000

5a (X=N, M=Co)
[PBE0/6-311+G(df)]
C_{2v}

B	0.809718000000	1.355389000000	-1.378262000000
B	-0.809718000000	1.355389000000	-1.378262000000
B	-1.644720000000	0.000000000000	-1.364134000000
B	-0.809718000000	-1.355389000000	-1.378262000000
B	0.809718000000	-1.355389000000	-1.378262000000
B	1.644720000000	0.000000000000	-1.364134000000
N	0.000000000000	0.000000000000	-1.735880000000
Co	0.000000000000	0.000000000000	0.148712000000
C	0.000000000000	1.293160000000	1.322770000000
C	0.000000000000	-1.293160000000	1.322770000000
O	0.000000000000	2.133913000000	2.091830000000
O	0.000000000000	-2.133913000000	2.091830000000

5b (X=N, M=Co)
[B3LYP/6-311+G(df)]
C_{2v}

B	1.422610000000	0.791604000000	-1.409477000000
B	0.000000000000	1.551750000000	-1.423384000000
B	-1.422610000000	0.791604000000	-1.409477000000
B	-1.422610000000	-0.791604000000	-1.409477000000
B	0.000000000000	-1.551750000000	-1.423384000000
B	1.422610000000	-0.791604000000	-1.409477000000
N	0.000000000000	0.000000000000	-1.750520000000
Co	0.000000000000	0.000000000000	0.166554000000
C	0.000000000000	1.308976000000	1.350886000000
C	0.000000000000	-1.308976000000	1.350886000000
O	0.000000000000	2.150426000000	2.123091000000
O	0.000000000000	-2.150426000000	2.123091000000

5b (X=N, M=Co)
[PBE0/6-311+G(df)]
C_{2v}

B	1.418467000000	0.791734000000	-1.367627000000
B	0.000000000000	1.553951000000	-1.386879000000
B	-1.418467000000	0.791734000000	-1.367627000000
B	-1.418467000000	-0.791734000000	-1.367627000000
B	0.000000000000	-1.553951000000	-1.386879000000
B	1.418467000000	-0.791734000000	-1.367627000000
N	0.000000000000	0.000000000000	-1.737035000000
Co	0.000000000000	0.000000000000	0.147904000000
C	0.000000000000	1.291713000000	1.323607000000
C	0.000000000000	-1.291713000000	1.323607000000
O	0.000000000000	2.131140000000	2.093993000000
O	0.000000000000	-2.131140000000	2.093993000000

6a (X=N, M=Mn)
[B3LYP/6-311+G(df)]
C_{3v}

B	1.599389000000	0.006345000000	-1.606683000000
B	0.805189000000	1.381939000000	-1.606683000000
B	-0.805189000000	1.381939000000	-1.606683000000
B	-1.599389000000	0.006345000000	-1.606683000000
B	-0.794200000000	-1.388284000000	-1.606683000000
B	0.794200000000	-1.388284000000	-1.606683000000
N	0.000000000000	0.000000000000	-1.896154000000
Mn	0.000000000000	0.000000000000	0.072028000000
C	0.000000000000	1.521845000000	1.067534000000
C	-1.317956000000	-0.760922000000	1.067534000000
C	1.317956000000	-0.760922000000	1.067534000000
O	0.000000000000	2.485564000000	1.685718000000
O	-2.152562000000	-1.242782000000	1.685718000000
O	2.152562000000	-1.242782000000	1.685718000000

6a (X=N, M=Mn)
[PBE0/6-311+G(df)]
C_{3v}

B	1.598390000000	0.005976000000	-1.556413000000
B	0.804370000000	1.381259000000	-1.556413000000
B	-0.804370000000	1.381259000000	-1.556413000000
B	-1.598390000000	0.005976000000	-1.556413000000
B	-0.794020000000	-1.387234000000	-1.556413000000
B	0.794020000000	-1.387234000000	-1.556413000000
N	0.000000000000	0.000000000000	-1.880638000000
Mn	0.000000000000	0.000000000000	0.053524000000
C	0.000000000000	1.502535000000	1.040585000000
C	-1.301233000000	-0.751267000000	1.040585000000
C	1.301233000000	-0.751267000000	1.040585000000
O	0.000000000000	2.463878000000	1.657843000000
O	-2.133781000000	-1.231939000000	1.657843000000
O	2.133781000000	-1.231939000000	1.657843000000

6b (X=N, M=Mn)
[B3LYP/6-311+G(df)]
C_{3v}

B	1.396314000000	0.806162000000	-1.596008000000
B	0.000000000000	1.586177000000	-1.619809000000
B	-1.396314000000	0.806162000000	-1.596008000000
B	-1.373670000000	-0.793089000000	-1.619809000000
B	0.000000000000	-1.612324000000	-1.596008000000
B	1.373670000000	-0.793089000000	-1.619809000000
N	0.000000000000	0.000000000000	-1.896492000000
Mn	0.000000000000	0.000000000000	0.072879000000
C	0.000000000000	1.520930000000	1.068810000000
C	-1.317164000000	-0.760465000000	1.068810000000
C	1.317164000000	-0.760465000000	1.068810000000
O	0.000000000000	2.485606000000	1.685506000000
O	-2.152598000000	-1.242803000000	1.685506000000
O	2.152598000000	-1.242803000000	1.685506000000

6b (X=N, M=Mn)
[PBE0/6-311+G(df)]
C_{3v}

B	1.395059000000	0.805437000000	-1.550602000000
B	0.000000000000	1.585691000000	-1.564660000000
B	-1.395059000000	0.805437000000	-1.550602000000
B	-1.373249000000	-0.792845000000	-1.564660000000
B	0.000000000000	-1.610875000000	-1.550602000000
B	1.373249000000	-0.792845000000	-1.564660000000
N	0.000000000000	0.000000000000	-1.881576000000
Mn	0.000000000000	0.000000000000	0.054327000000
C	0.000000000000	1.501232000000	1.041932000000
C	-1.300105000000	-0.750616000000	1.041932000000
C	1.300105000000	-0.750616000000	1.041932000000
O	0.000000000000	2.463497000000	1.657793000000
O	-2.133451000000	-1.231748000000	1.657793000000
O	2.133451000000	-1.231748000000	1.657793000000

7a (X=N, M=V)
[B3LYP/6-311+G(df)]
C_{2v}

B	-1.383823000000	0.802457000000	1.806417000000
B	0.000000000000	1.601145000000	1.838271000000
B	1.383823000000	0.802457000000	1.806417000000
B	1.383823000000	-0.802457000000	1.806417000000
B	0.000000000000	-1.601145000000	1.838271000000
B	-1.383823000000	-0.802457000000	1.806417000000
N	0.000000000000	0.000000000000	2.026198000000
V	0.000000000000	0.000000000000	-0.023773000000
C	0.000000000000	1.756468000000	-0.923616000000
C	1.755329000000	0.000000000000	-0.921824000000
C	0.000000000000	-1.756468000000	-0.923616000000
O	0.000000000000	2.777505000000	-1.437924000000
O	2.776224000000	0.000000000000	-1.437224000000
O	0.000000000000	-2.777505000000	-1.437924000000
C	-1.755329000000	0.000000000000	-0.921824000000
O	-2.776224000000	0.000000000000	-1.437224000000

7a (X=N, M=V)
[PBE0/6-311+G(df)]
C_{2v}

B	1.382797000000	0.802235000000	-1.752906000000
B	0.000000000000	1.601409000000	-1.784464000000
B	-1.382797000000	0.802235000000	-1.752906000000
B	-1.382797000000	-0.802235000000	-1.752906000000
B	0.000000000000	-1.601409000000	-1.784464000000
B	1.382797000000	-0.802235000000	-1.752906000000
N	0.000000000000	0.000000000000	-2.016740000000
V	0.000000000000	0.000000000000	0.005779000000
C	0.000000000000	1.725731000000	0.900280000000
C	-1.725402000000	0.000000000000	0.897118000000
C	0.000000000000	-1.725731000000	0.900280000000
O	0.000000000000	2.742988000000	1.417632000000
O	-2.742939000000	0.000000000000	1.414759000000
O	0.000000000000	-2.742988000000	1.417632000000
C	1.725402000000	0.000000000000	0.897118000000
O	2.742939000000	0.000000000000	1.414759000000

7b (X=N, M=V)
[B3LYP/6-311+G(df)]
C_{2v}

B	1.387244000000	0.798044000000	-1.828093000000
B	1.387244000000	-0.798044000000	-1.828093000000
B	0.000000000000	-1.599536000000	-1.793258000000
N	0.000000000000	0.000000000000	-2.027503000000
B	0.000000000000	1.599536000000	-1.793258000000
B	-1.387244000000	0.798044000000	-1.828093000000
B	-1.387244000000	-0.798044000000	-1.828093000000
V	0.000000000000	0.000000000000	0.023340000000
C	1.242587000000	1.240377000000	0.922704000000
C	-1.242587000000	1.240377000000	0.922704000000
C	-1.242587000000	-1.240377000000	0.922704000000
O	1.964097000000	1.962725000000	1.437664000000
O	-1.964097000000	1.962725000000	1.437664000000
O	-1.964097000000	-1.962725000000	1.437664000000
C	1.242587000000	-1.240377000000	0.922704000000
O	1.964097000000	-1.962725000000	1.437664000000

7b (X=N, M=V)
[PBE0/6-311+G(df)]
C_{2v}

B	1.386445000000	0.797543000000	-1.777525000000
B	1.386445000000	-0.797543000000	-1.777525000000
B	0.000000000000	-1.599000000000	-1.740307000000
N	0.000000000000	0.000000000000	-2.017659000000
B	0.000000000000	1.599000000000	-1.740307000000
B	-1.386445000000	0.797543000000	-1.777525000000
B	-1.386445000000	-0.797543000000	-1.777525000000
V	0.000000000000	0.000000000000	0.005054000000
C	1.220907000000	1.218642000000	0.899354000000
C	-1.220907000000	1.218642000000	0.899354000000
C	-1.220907000000	-1.218642000000	0.899354000000
O	1.939488000000	1.938051000000	1.418013000000
O	-1.939488000000	1.938051000000	1.418013000000
O	-1.939488000000	-1.938051000000	1.418013000000
C	1.220907000000	-1.218642000000	0.899354000000
O	1.939488000000	-1.938051000000	1.418013000000

7c (X=N, M=V)
[B3LYP/6-311+G(df)]
C$_2$

B	0.669103000000	1.453121000000	-1.814539000000
B	-0.928236000000	1.302462000000	-1.799220000000
B	-1.594019000000	-0.151512000000	-1.836652000000
N	0.000000000000	0.000000000000	-2.026267000000
V	0.000000000000	0.000000000000	0.023932000000
C	0.000000000000	1.755750000000	0.922217000000
C	-1.756396000000	-0.001427000000	0.923199000000
C	0.000000000000	-1.755750000000	0.922217000000
O	-0.000951000000	2.776710000000	1.437336000000
O	-2.777636000000	-0.001524000000	1.437199000000
O	0.000951000000	-2.776710000000	1.437336000000
C	1.756396000000	0.001427000000	0.923199000000
O	2.777636000000	0.001524000000	1.437199000000
B	1.594019000000	0.151512000000	-1.836652000000
B	0.928236000000	-1.302462000000	-1.799220000000
B	-0.669103000000	-1.453121000000	-1.814539000000

7c (X=N, M=V)
[PBE0/6-311+G(df)]
C$_2$

B	-1.745700000000	0.356429000000	-1.558987000000
B	-1.784811000000	1.528776000000	-0.472560000000
B	-1.762374000000	1.175779000000	1.083715000000
N	-2.017536000000	-0.000054000000	-0.000320000000
V	0.004996000000	-0.000004000000	-0.000023000000
C	0.900417000000	1.591157000000	-0.666656000000
C	0.897472000000	0.668151000000	1.590323000000
C	0.900245000000	-1.591096000000	0.666990000000
O	1.418602000000	2.528742000000	-1.060264000000
O	1.416060000000	1.061169000000	2.528360000000
O	1.418322000000	-2.528651000000	1.060816000000
C	0.898112000000	-0.668127000000	-1.590044000000
O	1.417053000000	-1.061126000000	-2.527890000000
B	-1.762038000000	-1.175653000000	-1.084132000000
B	-1.784802000000	-1.529106000000	0.472016000000
B	-1.746263000000	-0.356449000000	1.558130000000