Supporting information to

Dehalogenation of chloroalkanes by nickel(I) porphyrin derivatives, a computational study.

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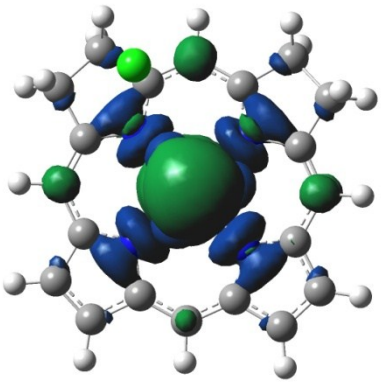
	[*L*-Ni···MeCl]$^-$	**[*L*-Ni···Me···Cl]$^{\ddagger-}$**	**[*L*-Ni-Me···Cl]$^-$**	**[*L*-Ni-Me]**
		B3LYP		
Ni-C [Å]	3.702 *(3.743)*	2.523 *(2.506)*	1.984 *(2.087)*	1.981 *(2.085)*
C-Cl [Å]	1.829 *(1.825)*	2.203 *(2.246)*	7.642 *(9.631)*	
N-C-Cl [deg]	179.0 *(165.2)*	179.4 *(178.2)*	109.6 *(74.5)*	
		M06-L		
Ni-C [Å]	3.101 *(3.268)*	2.507 *(2.437)*	1.956 *(2.087)*	1.955 *(2.084)*
C-Cl [Å]	1.818 *(1.800)*	2.159 *(2.228)*	3.857 *(8.524)*	
N-C-Cl [deg]	178.9 *(158.3)*	179.8 *(178.7)*	119.0 *(69.5)*	
		ωB97X-D		
Ni-C [Å]	3.274 *(3.236)*	2.416 *(2.434)*	1.996 *(2.063)*	1.993 *(2.066)*
C-Cl [Å]	1.813 *(1.808)*	2.191 *(2.179)*	3.971 *(5.537)*	
N-C-Cl [deg]	175.6 *(174.0)*	179.9 *(179.7)*	116.6 *(104.3)*	

S.II Spin Densities for [*L*-Ni] complexes

Low Spin [*iBCh*-Ni-Me···Cl]$^-$
4



Low Spin [*iBCh*-Ni-Me]
5

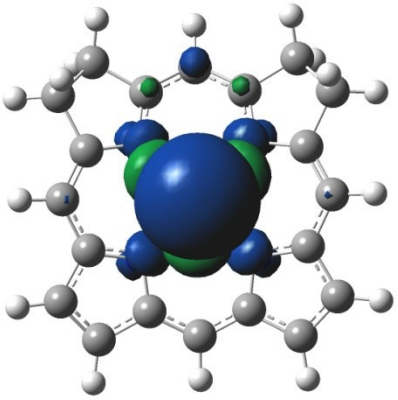
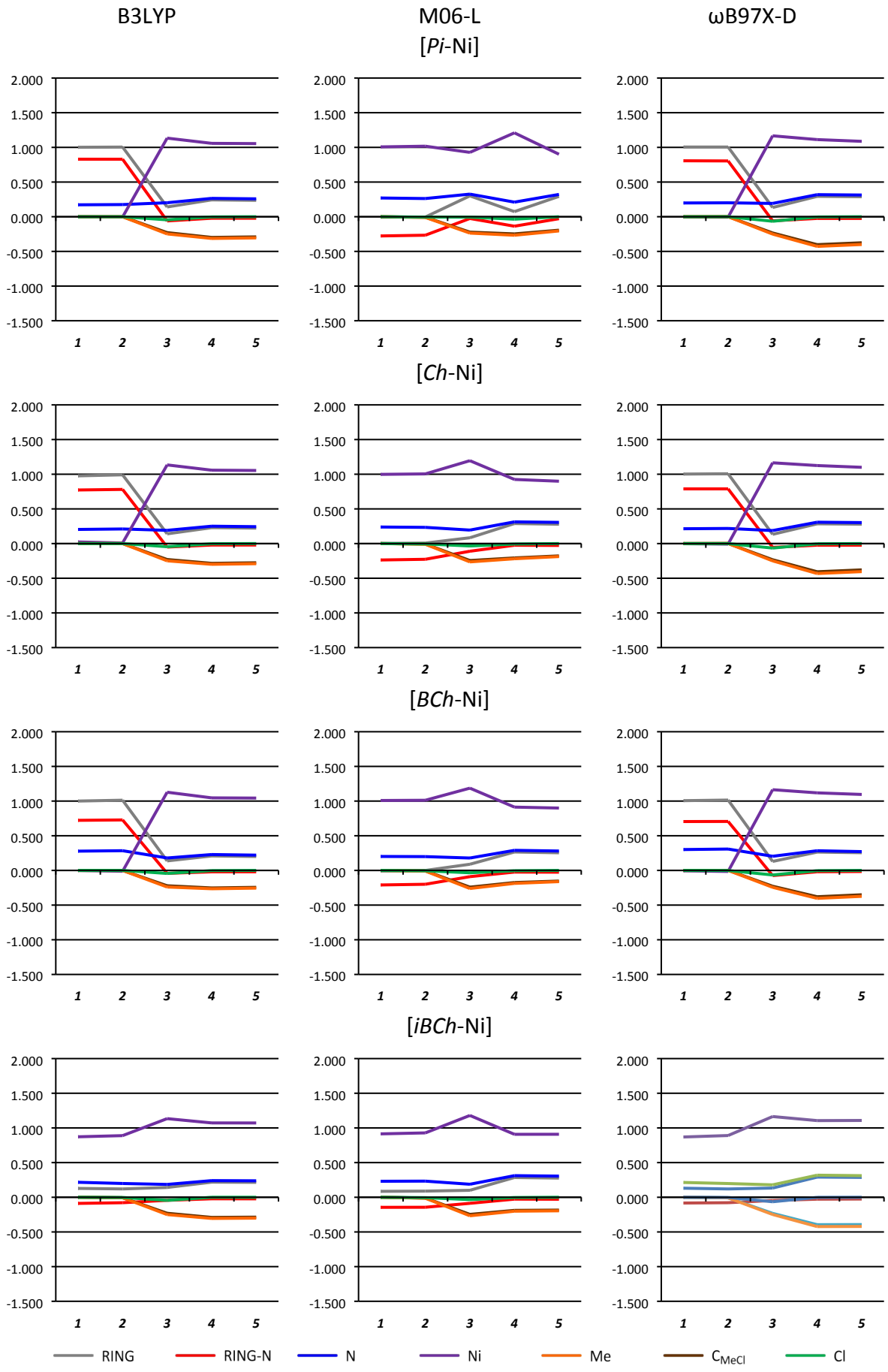


Figure S.1 Spin densities of low spin complex **4** and **5** for [*iBCh*-Ni] in ωB97X-D functional.


B3LYP
M06-L
ωB97X-D
[Pi-Ni]
[Ch-Ni]
[BCh-Ni]
[iBCh-Ni]
2.000
1.500
1.000
0.500
0.000
-0.500
-1.000
-1.500
1
2
3
4
5
RING
RING-N
N
Ni
Me
C_MeCl
Cl

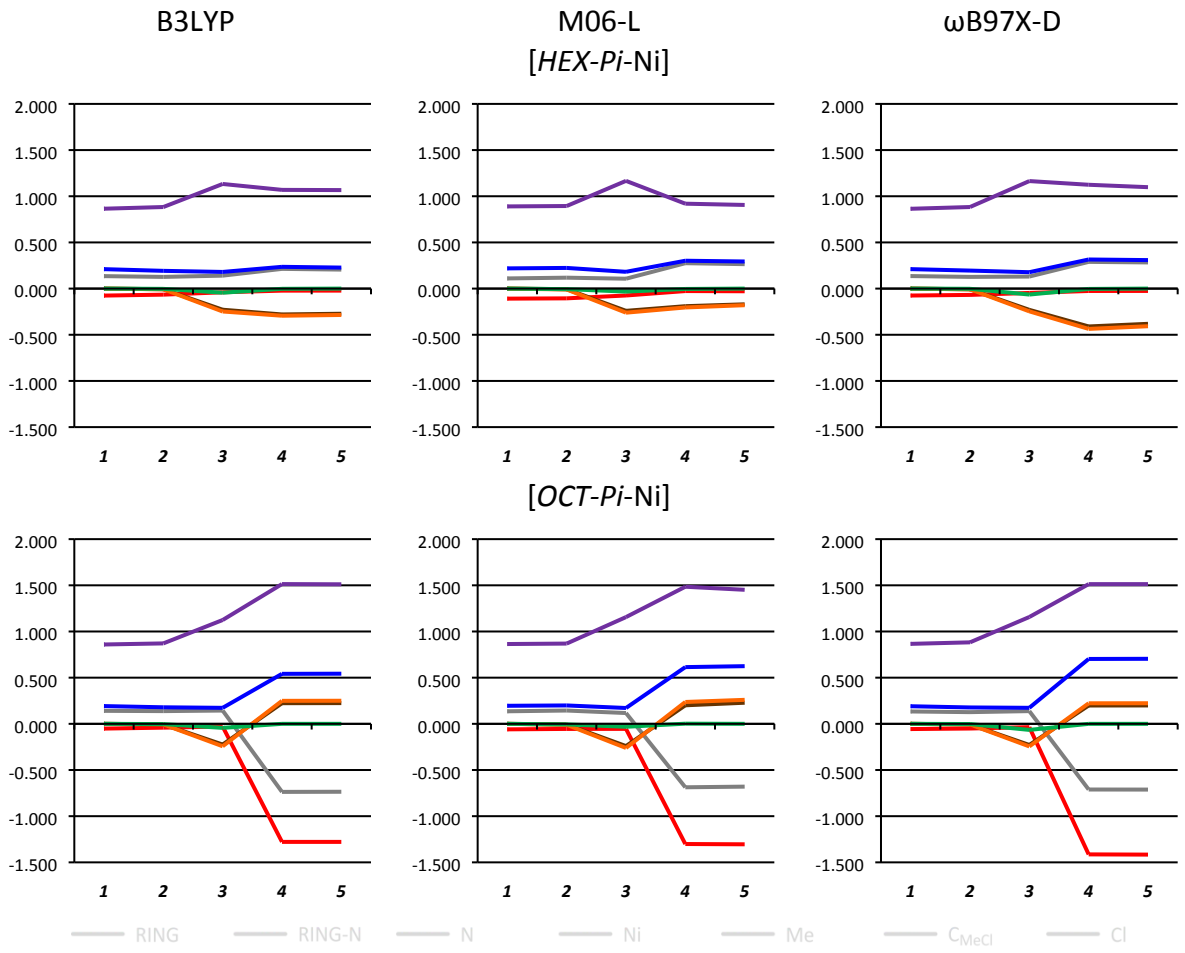


Figure S.2 Spin densities for LS complexes: RING - sum of all spin densities on ligand ring; RING-N - sum of all spin densities beside spin densities for N atoms on ligand ring; N - sum of all spin densities for all N atoms; Ni - spin densities on Ni atom; Me - sum of spin densities on CH_3 group from MeCl molecule; C_{MeCl} - spin densities on C atom from MeCl molecule; Cl - spin densities on Cl atom. The distribution of spin densities for single point M06 calculation are almost identical to the distribution of spin densities for M06-L functional and therefore has not been shown.

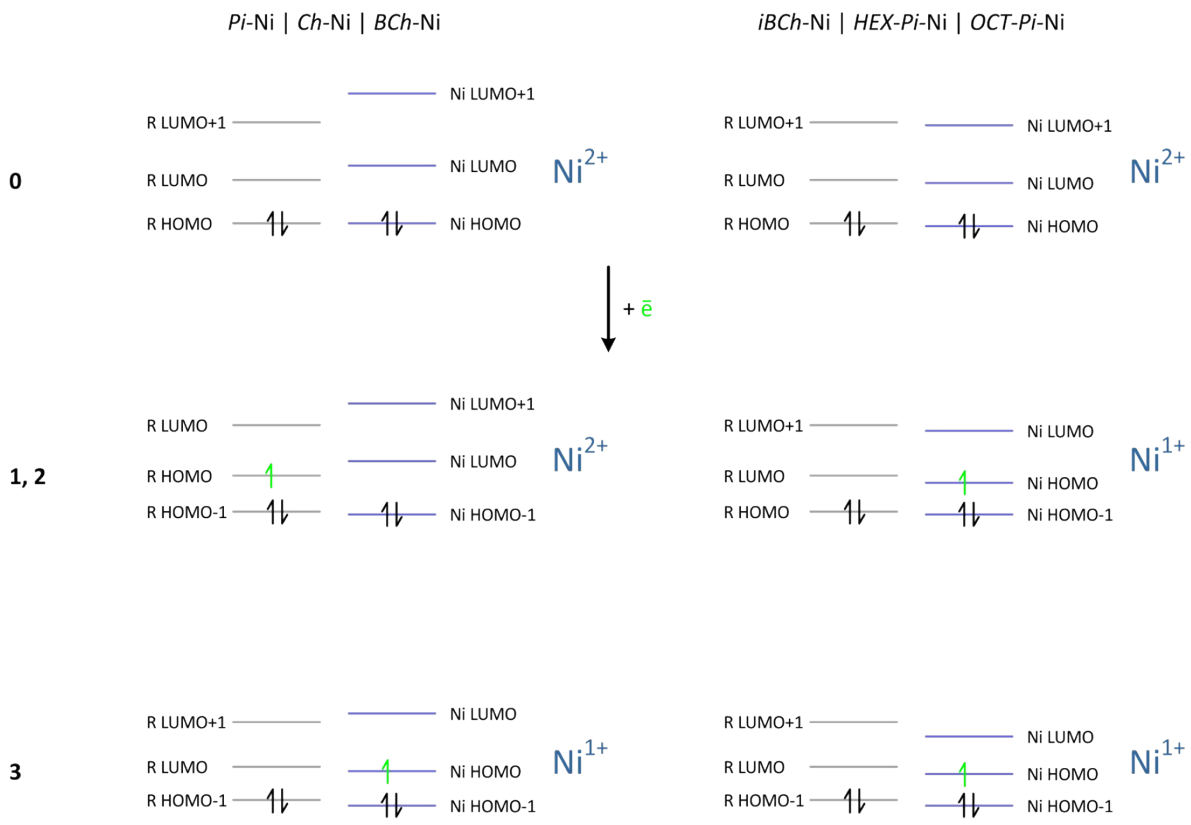


Figure S.3 Schematic diagram of differences in distribution of unpaired electron in B3LYP and ωB97X-D functionals for studied complexes. **0** - neutral complex before reduction; **1**,**2** - respectively anion complexes and anion reaction complex (with MeCl molecule) after reduction; **3** - transition state; R - ring orbitals; Ni - nickel orbitals

S.III Porphyrin derivative ligands geometries

Table S.2 Key geometric parameters for low spin and high spin (italic in parentheses) [*L*-Ni]$^-$ complex in B3LYP functional.

	[*L*-Ni···MeCl]$^-$ **2**	[*L*-Ni···Me···Cl]$^{‡-}$ **3**	[*L*-Ni-Me···Cl]$^-$ **4**	[*L*-Ni-Me] **5**
		[*OCT-Pi*-Ni]$^-$		
Ni-C [Å]	3.657 *(3.729)*	2.509 *(2.561)*	2.086 *(2.084)*	2.086 *(2.084)*
C-Cl [Å]	1.831 *(1.830)*	2.199 *(2.172)*	15.245 *(19.640)*	
N-C-Cl [deg]	173.8 *(176.4)*	179.7 *(179.3)*	164.5 *(163.5)*	
		[*HEX-Pi*-Ni]$^-$		
Ni-C [Å]	3.632 *(3.569)*	2.527 *(2.548)*	1.982 *(2.087)*	1.980 *(2.087)*
C-Cl [Å]	1.830 *(1.825)*	2.199 *(2.188)*	4.149 *(16.315)*	
N-C-Cl [deg]	178.9 *(176.4)*	179.5 *(179.5)*	172.3 *(176.3)*	
		[*iBCh*-Ni]$^-$		
Ni-C [Å]	3.702 *(3.743)*	2.523 *(2.506)*	1.984 *(2.087)*	1.981 *(2.085)*
C-Cl [Å]	1.829 *(1.825)*	2.203 *(2.246)*	7.642 *(9.631)*	
N-C-Cl [deg]	179.0 *(165.2)*	179.4 *(178.2)*	109.6 *(74.5)*	
		[*BCh*-Ni]$^-$		
Ni-C [Å]	3.684 *(3.535)*	2.509 *(2.551)*	1.980 *(2.088)*	1.977 *(2.089)*
C-Cl [Å]	1.828 *(1.826)*	2.212 *(2.190)*	4.151 *(18.423)*	
N-C-Cl [deg]	178.2 *(172.2)*	179.3 *(179.6)*	178.1 *(165.1)*	
		[*Ch*-Ni]$^-$		
Ni-C [Å]	3.699 *(3.516)*	2.519 *(3.321)*	1.984 *(2.122)*	1.981 *(2.120)*
C-Cl [Å]	1.828 *(1.826)*	2.212 *(2.313)*	4.140 *(15.191)*	
N-C-Cl [deg]	174.7 *(165.7)*	179.7 *(164.2)*	178.1 *(164.7)*	
		[*Pi*-Ni]$^-$		
Ni-C [Å]	3.546 *(3.643)*	2.514 *(3.432)*	1.985 *(2.129)*	1.983 *(2.092)*
C-Cl [Å]	1.828 *(1.826)*	2.217 *(2.294)*	4.138 *(21.974)*	
N-C-Cl [deg]	175.7 *(175.1)*	179.4 *(159.5)*	178.7 *(174.9)*	

Table S.3 Key geometric parameters for low spin and high spin (italic in parentheses) [*L*-Ni]$^-$ complex in M06-L functional.

	[*L*-Ni···MeCl]$^-$ **2**	[*L*-Ni···Me···Cl]$^{‡-}$ **3**	[*L*-Ni-Me···Cl]$^-$ **4**	[*L*-Ni-Me] **5**
		[*OCT-Pi*-Ni]$^-$		
Ni-C [Å]	3.091 *(3.101)*	2.510 *(2.547)*	2.085 *(2.082)*	2.085 *(2.084)*
C-Cl [Å]	1.821 *(1.824)*	2.142 *(2.115)*	4.711 *(4.705)*	
N-C-Cl [deg]	176.5 *(176.6)*	179.3 *(179.5)*	173.7 *(174.6)*	
		[*HEX-Pi*-Ni]$^-$		
Ni-C [Å]	3.103 *(3.120)*	2.515 *(2.499)*	1.957 *(2.084)*	1.955 *(2.086)*
C-Cl [Å]	1.819 *(1.809)*	2.147 *(2.163)*	3.899 *(4.771)*	
N-C-Cl [deg]	172.9 *(171.3)*	178.8 *(179.1)*	175.7 *(171.1)*	
		[*iBCh*-Ni]$^-$		
Ni-C [Å]	3.101 *(3.268)*	2.507 *(2.437)*	1.956 *(2.087)*	1.955 *(2.084)*
C-Cl [Å]	1.818 *(1.800)*	2.159 *(2.228)*	3.857 *(8.524)*	
N-C-Cl [deg]	178.9 *(158.3)*	179.8 *(178.7)*	119.0 *(69.5)*	
		[*BCh*-Ni]$^-$		
Ni-C [Å]	3.111 *(3.193)*	2.492 *(2.452)*	1.958 *(2.086)*	1.956 *(2.088)*
C-Cl [Å]	1.814 *(1.797)*	2.174 *(2.230)*	3.893 *(4.772)*	
N-C-Cl [deg]	172.8 *(179.6)*	179.8 *(152.3)*	178.5 *(176.8)*	
		[*Ch*-Ni]$^-$		
Ni-C [Å]	3.125 *(3.267)*	2.495 *(2.938)*	1.960 *(2.166)*	1.955 *(2.152)*
C-Cl [Å]	1.814 *(1.799)*	2.177 *(2.259)*	3.728 *(4.157)*	
N-C-Cl [deg]	172.6 *(157.0)*	179.1 *(157.2)*	178.4 *(179.5)*	
		[*Pi*-Ni]$^-$		
Ni-C [Å]	3.138 *(3.262)*	2.484 *(2.953)*	1.961 *(2.203)*	1.957 *(2.194)*
C-Cl [Å]	1.813 *(1.798)*	2.191 *(2.289)*	3.757 *(4.138)*	
N-C-Cl [deg]	173.7 *(150.7)*	179.1 *(170.8)*	179.3 *(177.3)*	

Table S.4 Key geometric parameters for low spin and high spin (italic in parentheses) [*L*-Ni]$^-$ complex in ωB97X-D functional.

	[*L*-Ni···MeCl]$^-$ **2**	[*L*-Ni···Me···Cl]$^{‡-}$ **3**	[*L*-Ni-Me···Cl]$^-$ **4**	[*L*-Ni-Me] **5**
		[*OCT-Pi*-Ni]$^-$		
Ni-C [Å]	3.349 *(3.403)*	2.401 *(2.435)*	2.061 *(2.059)*	2.064 *(2.061)*
C-Cl [Å]	1.813 *(1.813)*	2.198 *(2.165)*	4.628 *(4.599)*	
N-C-Cl [deg]	176.7 *(174.0)*	179.7 *(179.3)*	113.2 *(114.5)*	
		[*HEX-Pi*-Ni]$^-$		
Ni-C [Å]	3.284 *(3.415)*	2.419 *(2.433)*	1.996 *(2.063)*	1.986 *(2.065)*
C-Cl [Å]	1.814 *(1.810)*	2.187 *(2.173)*	3.744 *(4.571)*	
N-C-Cl [deg]	176.4 *(155.0)*	179.4 *(178.8)*	174.3 *(111.8)*	
		[*iBCh*-Ni]$^-$		
Ni-C [Å]	3.274 *(3.236)*	2.416 *(2.434)*	1.996 *(2.063)*	1.993 *(2.066)*
C-Cl [Å]	1.813 *(1.808)*	2.191 *(2.179)*	3.971 *(5.537)*	
N-C-Cl [deg]	175.6 *(174.0)*	179.9 *(179.7)*	116.6 *(104.3)*	
		[*BCh*-Ni]$^-$		
Ni-C [Å]	3.236 *(3.360)*	2.405 *(2.437)*	1.988 *(2.065)*	1.981 *(2.066)*
C-Cl [Å]	1.988 *(1.813)*	2.207 *(2.171)*	3.762 *(4.695)*	
N-C-Cl [deg]	171.0 *(176.9)*	179.1 *(178.9)*	179.2 *(177.2)*	
		[*Ch*-Ni]$^-$		
Ni-C [Å]	3.260 *(3.313)*	2.418 *(2.204)*	1.997 *(2.062)*	1.990 *(2.092)*
C-Cl [Å]	1.810 *(1.813)*	2.200 *(2.658)*	3.757 *(5.055)*	
N-C-Cl [deg]	172.7 *(173.6)*	179.1 *(171.5)*	179.8 *(106.1)*	
		[*Pi*-Ni]$^-$		
Ni-C [Å]	3.260 *(3.328)*	2.419 *(2.435)*	1.996 *(2.077)*	1.989 *(2.079)*
C-Cl [Å]	1.810 *(1.809)*	2.206 *(2.165)*	3.758 *(4.782)*	
N-C-Cl [deg]	169.4 *(167.2)*	179.1 *(179.3)*	179.3 *(108.2)*	

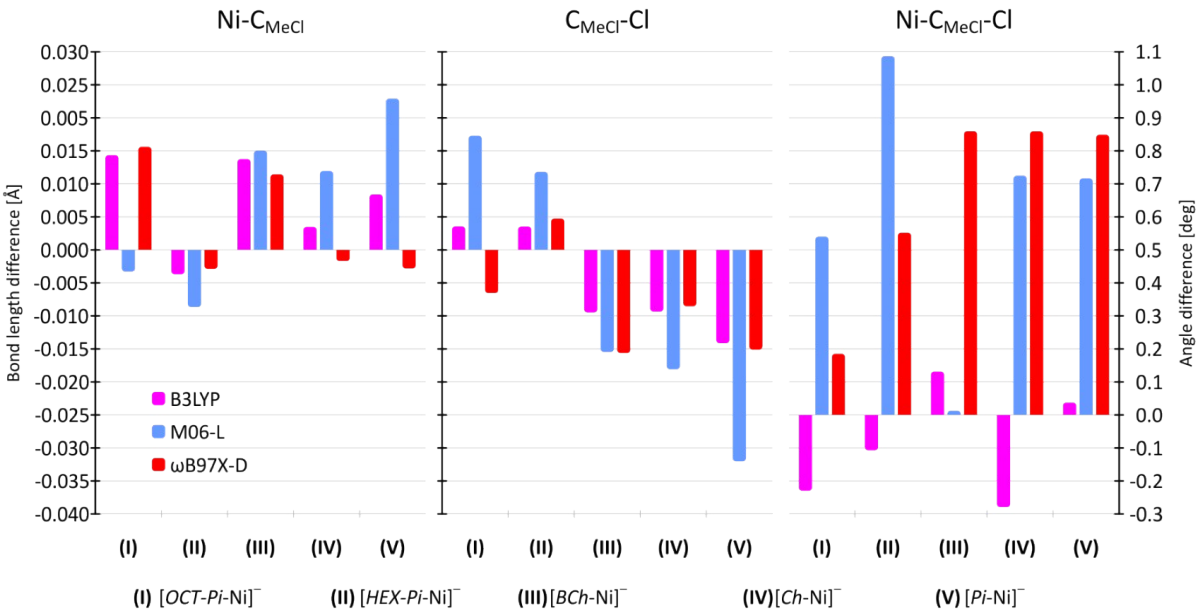


Figure S.4 Relative differences between porphyrin ligands and *iBCh*-Ni complex in transition state key distances Ni-C_{MeCl}, C_{MeCl}-Cl and angle Ni-C_{MeCl}-Cl.

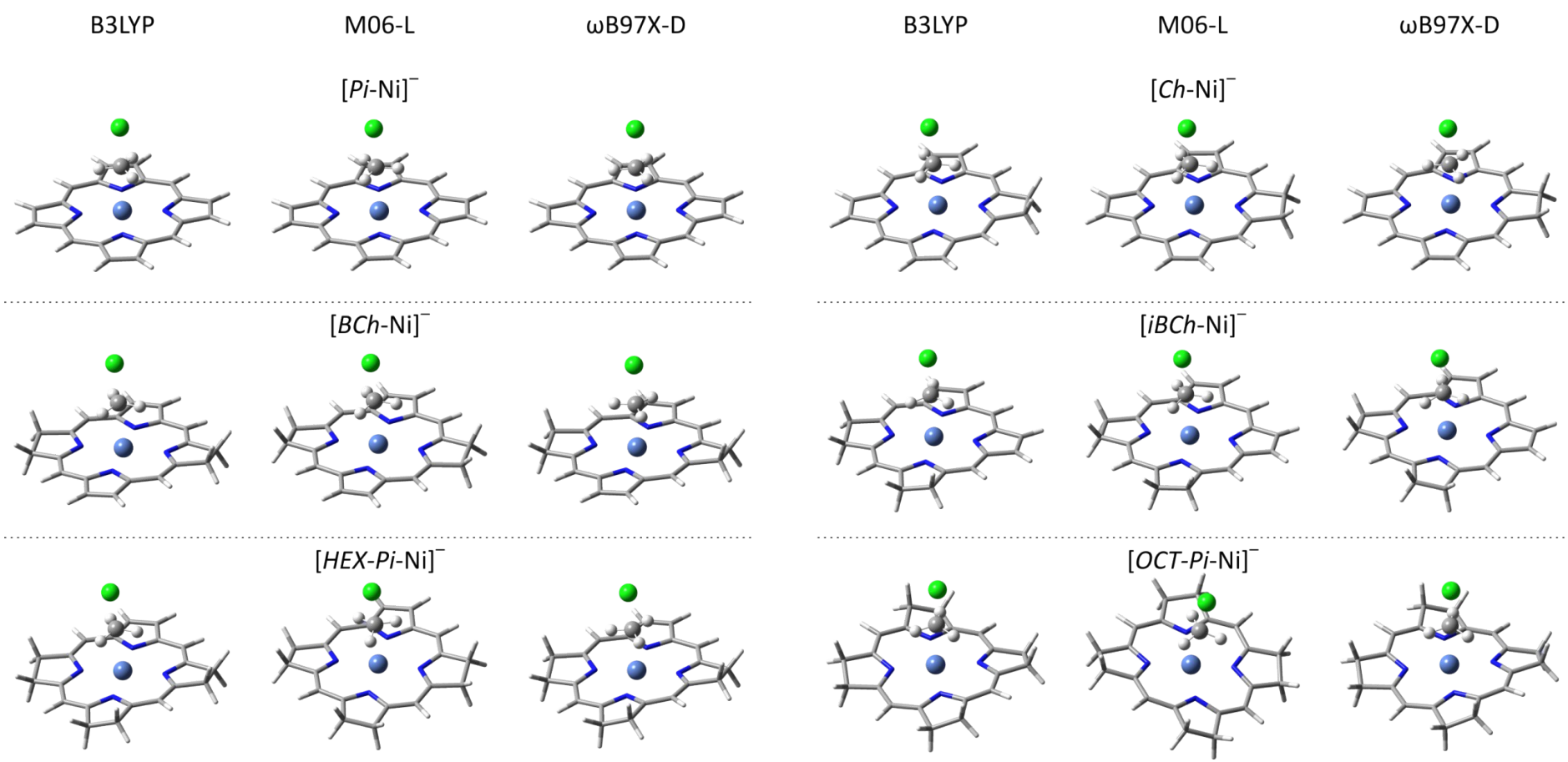


Figure S.5 LS-TS's structures for different porphyrin derivative ligands in B3LYP, M06-L and ωB97X-D functionals.

S.IV Superposition of [*BCh*-Ni]$^{-}$ and [*BCh*-Ni—Me—Cl]$^{‡-}$

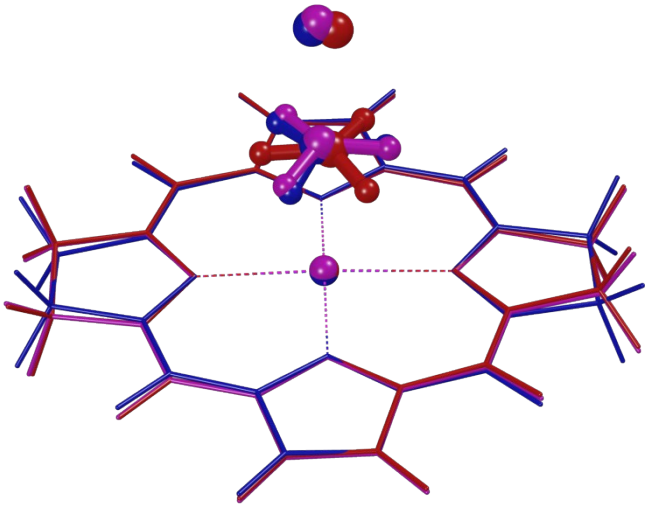


Figure S.6 Superposition of low spin [*BCh*-Ni—Me—Cl]$^{‡-}$ geometries from B3LYP (pink), M06-L (blue) and ωB97X-D (red) functionals. N and Ni atoms were used for superposition.

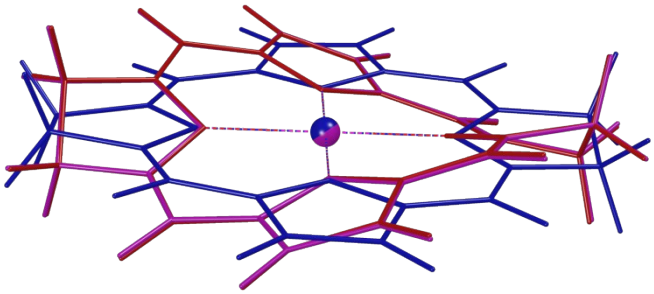


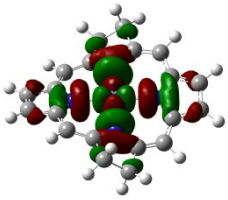
Figure S.7 Superposition of low spin [*BCh*-Ni]$^{-}$ geometries from B3LYP (pink), M06-L (blue) and ωB97X-D (red) functionals. N and Ni atoms were used for superposition.

S.V Molecular orbitals for [*BCh*-Ni]$^-$ and [*iBCh*-Ni]$^-$

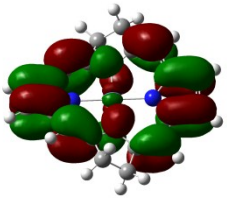
B3LYP

[*BCh*-Ni]$^-$

LUMO α

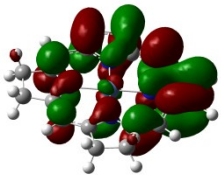


LUMO β

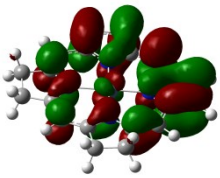


[*iBCh*-Ni]$^-$

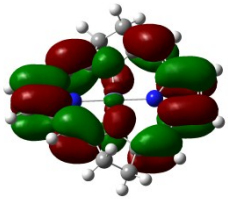
LUMO α



LUMO β



HOMO α



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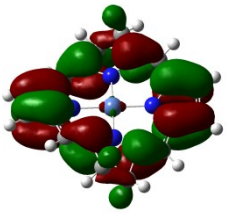

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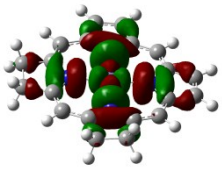

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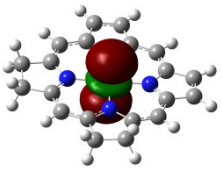
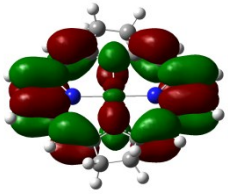


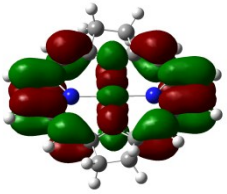
M06-L

[*iBCh*-Ni]$^-$

LUMO α

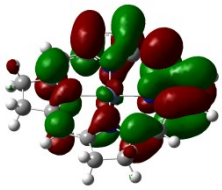


LUMO β

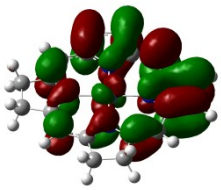


[*BCh*-Ni]$^-$

LUMO α



LUMO β



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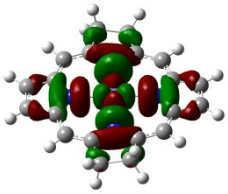

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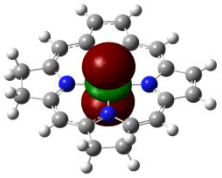

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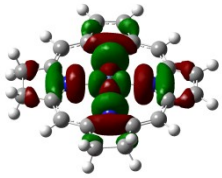

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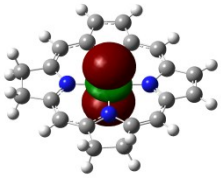


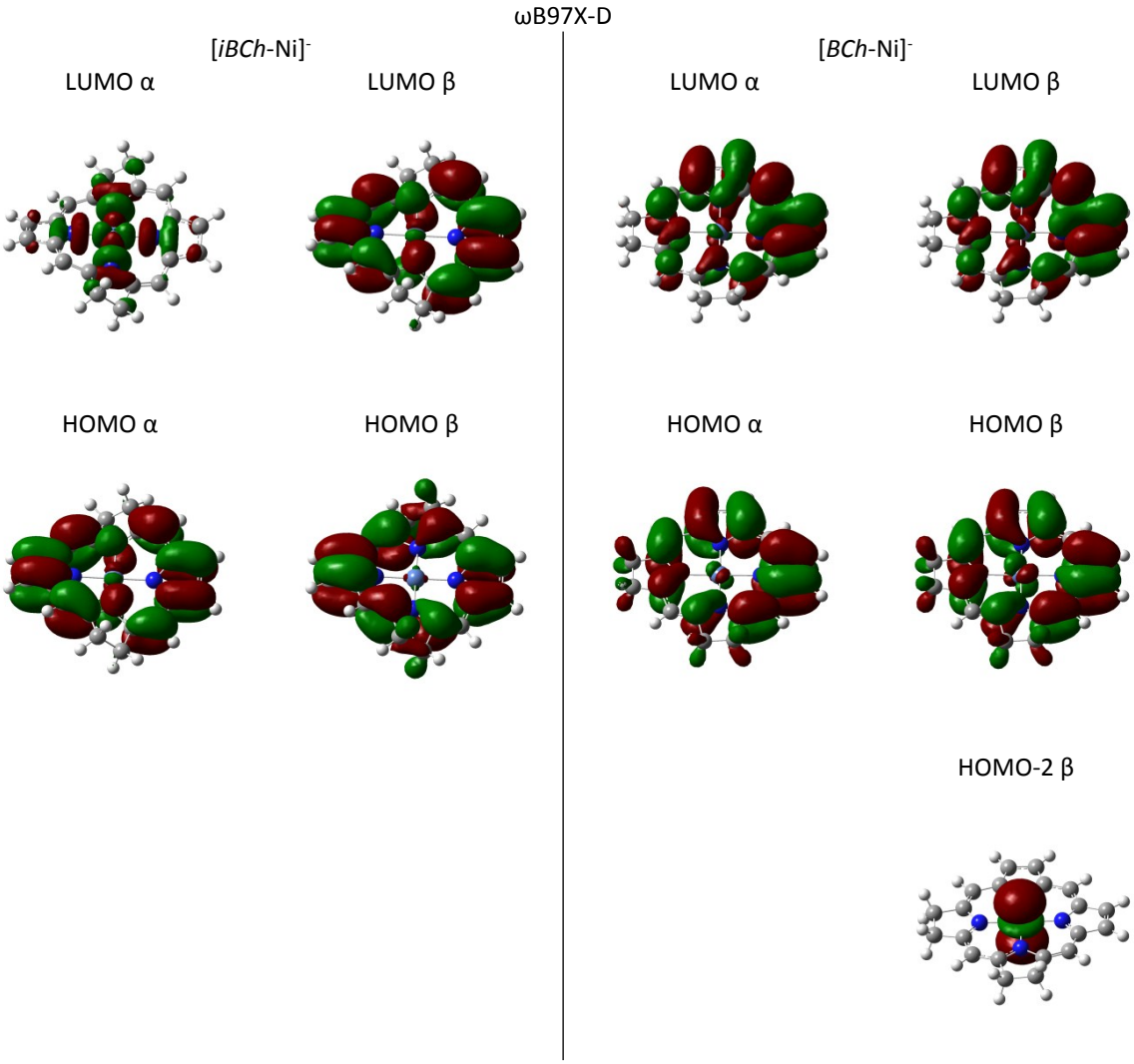


Figure S.8 Example of differences in molecular orbital shape in B3LYP, M06-L and ωB97X-D functionals for ionic form of complexes **1** between *BCh* and *iBCh* ligands where is visible change of spin distribution for Species **1** and **2**, see Figure S.2. Only M06-L functionals always places unpaired electron on Ni atom. It can be seen that with change of spin distribution in B3LYP and ωB97X-D functionals unpaired spin was moved from ligand ring to Ni atom. Moreover highest occupied Ni orbital for [*BCh*-Ni]$^-$ in ωB97X-D functional is HOMO-2 orbital instead of HOMO.

S.VI Energy analysis

Table S.5 Energy data for low spin - LS and high spin - *HS* (*italic*) pathways for different porphyrin derivative ligands in B3LYP, M06-L and ωB97X-D functionals and for M06 single point **3** and **5** energies on geometries from M06-L.

	[*L*-Ni]$^-$ + MeCl		[*L*-Ni···MeCl]$^-$		[*L*-Ni···Me···Cl]$^{‡-}$		[*L*-Ni-Me···Cl]$^-$		[*L*-Ni-Me] + Cl$^-$	
	1		**2**		**3**		**4**		**5**	
	LS	*HS*	LS	*HS*	LS	*HS*	LS	*HS*	LS	*HS*
					B3LYP					
[*OCT-Pi*-Ni]$^-$	0.00	*18.60*	6.19	*24.94*	15.04	*32.12*	-26.10	*-26.26*	-27.50	*-27.30*
[*HEX-Pi*-Ni]$^-$	0.00	*26.44*	5.33	*32.58*	15.15	*42.13*	-1.05	*-6.01*	-6.29	*-7.42*
[*iBCh*-Ni]$^-$	0.00	*20.33*	5.21	*26.44*	14.82	*47.34*	-2.34	*8.77*	-5.22	*3.83*
[*BCh*-Ni]$^-$	0.00	*6.90*	5.83	*13.29*	11.72	*33.13*	-4.93	*-0.50*	-10.19	*-1.91*
[*Ch*-Ni]$^-$	0.00	*6.51*	6.04	*12.75*	10.32	*31.31*	-6.55	*14.34*	-11.37	*13.93*
[*Pi*-Ni]$^-$	0.00	*6.52*	6.57	*12.96*	10.40	*30.02*	-4.81	*18.30*	-10.86	*21.69*
					M06-L					
[OCT-Pi-Ni]-	0.00	*20.65*	2.03	*22.89*	5.52	*26.33*	-27.44	*-27.46*	-33.19	*-32.78*
[HEX-Pi-Ni]-	0.00	*24.16*	1.74	*25.58*	7.36	*34.51*	-9.62	*-6.48*	-14.48	*-12.59*
[iBCh-Ni]-	0.00	*21.11*	2.46	*24.28*	8.11	*38.66*	-10.06	*3.67*	-12.70	*-1.41*
[BCh-Ni]-	0.00	*13.29*	2.33	*17.28*	9.04	*31.23*	-7.05	*3.41*	-13.14	*-0.42*
[Ch-Ni]-	0.00	*13.98*	2.26	*17.07*	9.02	*31.98*	-6.17	*14.17*	-11.57	*8.36*
[Pi-Ni]-	0.00	*13.82*	2.45	*17.99*	10.17	*36.07*	-3.01	*17.74*	-9.27	*12.19*
					ωB97X-D					
[OCT-Pi-Ni]-	0.00	*10.97*	1.43	*12.92*	15.14	*24.89*	-33.23	*-33.14*	-37.70	*-36.74*
[HEX-Pi-Ni]-	0.00	*22.53*	1.54	*24.82*	14.57	*40.93*	-4.09	*-5.63*	-8.43	*-11.36*
[iBCh-Ni]-	0.00	*34.46*	1.06	*36.53*	14.53	*45.62*	-3.60	*4.76*	-8.43	*-0.79*
[BCh-Ni]-	0.00	*25.74*	1.82	*21.59*	18.28	*33.19*	0.11	*1.10*	-4.66	*-2.84*
[Ch-Ni]-	0.00	*30.86*	1.15	*32.39*	13.19	*51.09*	-5.80	*15.66*	-10.46	*17.61*
[Pi-Ni]-	0.00	*26.27*	1.59	*26.63*	13.38	*40.88*	-5.34	*17.90*	-10.12	*11.72*
					M06					
[OCT-Pi-Ni]-	0.00				13.10				-1.97	
[HEX-Pi-Ni]-	0.00				13.71				-2.35	
[iBCh-Ni]-	0.00				15.19				-1.61	
[BCh-Ni]-	0.00				12.23				-2.56	
[Ch-Ni]-	0.00				12.26				-2.25	
[Pi-Ni]-	0.00				13.66				-19.88	

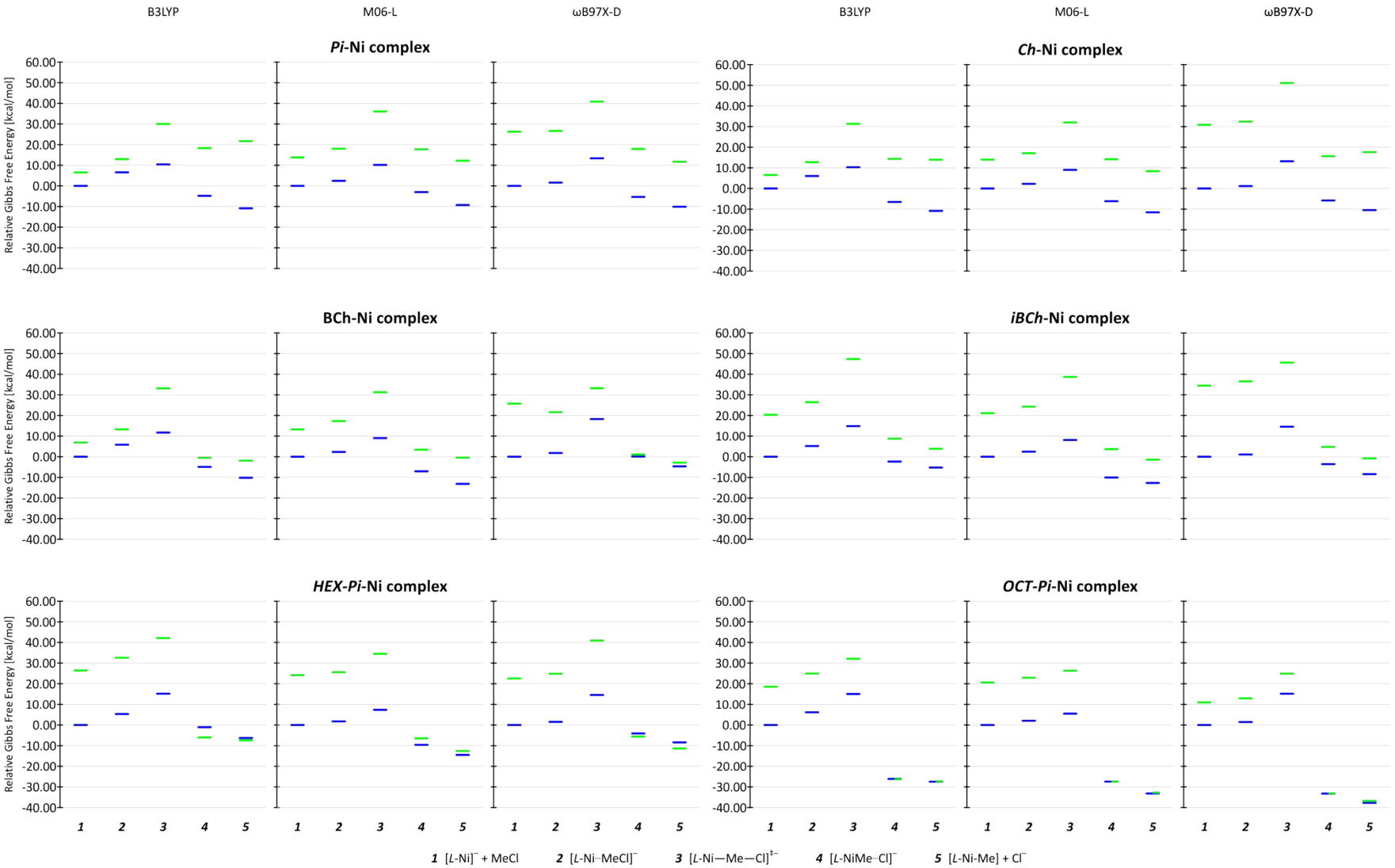


Figure S.9 Energy diagram for dehalogenation of MeCl by low spin (blue) and high spin (green) [*L*-Ni]$^{-}$ complexes in B3LYP, M06-L and ωB97X-D functionals with 6-311+G(d,p)/6-31+G(d,p) basis set in SMD solvent model for DMF. x marker - Single Point energy in ωB97X D functional on geometry from B3LYP functional, see also Table S.5.

S.VI.1 B3LYP-GD3BJ functional test

For all anion ligands [*L*-Ni]$^{-}$ and MeCl molecules (reactants **1**) as well as for LS-TS structures **3** Single Point (SP) calculation in B3LYP functionals with Grimme's empirical dispersion correction with Becke-Johnson damping (B3LYP-GD3BJ)[52] were performed. Adding dispersion correction from B3LYP-GD3BJ SP calculations to previously reported Gibbs Free Activation Energies from B3LYP functional decreased energy barriers by approximately 6-7 kcal/mol comparing to B3LYP functional without dispersion correction for all porphyrin ligands except for the [*Ch*-Ni] complex where activation energy in B3LYP-GD3BJ functional was only 0.51 kcal/mol and it was lower in energy by 9.81 kcal/mol comparing to B3LYP functional, see Figure S.10. Additional, the new SP B3LYP-GD3BJ reaction barrier for [i*BCh*-Ni]$^{-}$ complex (7.96 kcal/mol) after recalculation to reaction rate constant (9.2×10^{6} $M^{-1}s^{-1}$) shows similar values to reaction rate from M06-L functional which was in good arrangement with experimental data. Unfortunately, this simple test wasn't enough to unequivocally say that dispersion correction is the clue of difference between B3LYP and ωB97X-D functional but that possibility cannot be excluded.

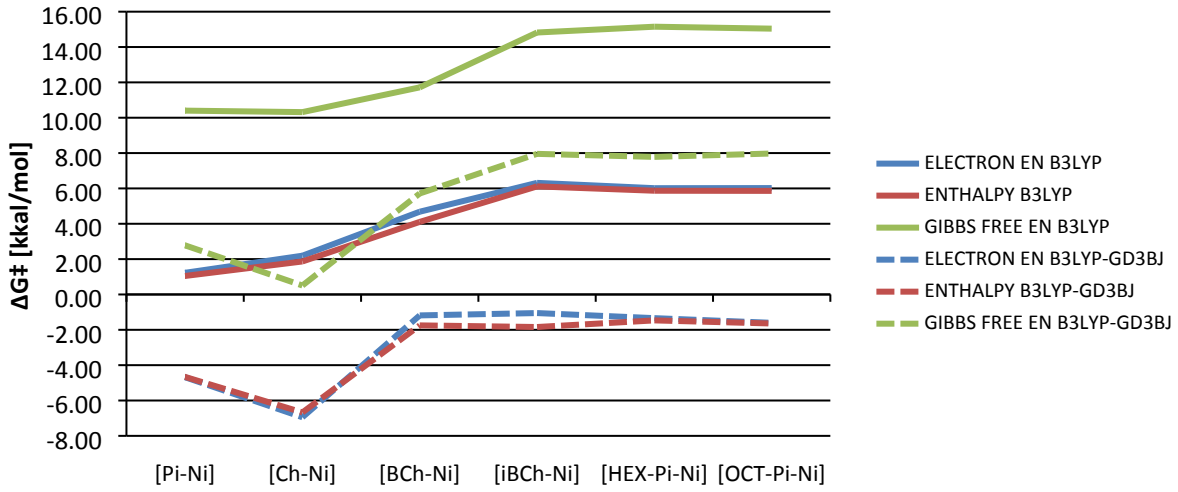


Figure S.10 Influence of Grimme's GD3BJ dispersion correction on low spin activation energies for B3LYP functional. Single point energies in B3LYP-GD3BJ on geometries from B3LYP.

S.VI.2 M06 family functionals test

Influence of Hartree-Fock Exchange Energy E_{ex}^{HF} were investigated for functionals from M06 family. Similar to case described above we used M06 geometries of [*L*-Ni]$^{-}$ and MeCl molecules (reactants **1**) as well as for LS-TS **3** to calculate SP calculation energy in M06 functional (which has 27% of E_{ex}^{HF})[1] which show no changes in for activation energy pattern for Electron Energy and Enthalpy while almost flat distribution of Gibbs Free Activation Energies with small peak for [*BCh*-Ni] complex exist, see Figure S.11. For M06-2X functional (54% of E_{ex}^{HF})[2] activation energy trend distortion are visible for [*iBCh*-Ni], [*HEX-Pi*-Ni] and [*OCT-Pi*-Ni] complexes while for rest of porphyrin ligands energy barrier is almost the same, see Figure S.12. And finally for M06-HF functional (100% of E_{ex}^{HF})[2,3] big fluctuation of activation energies between all porphyrin derivative ligands were present, see Figure S.12.

Therefore for M06 family functional there is no systematic dependence between activation energies and amount of E_{ex}^{HF} and any clear conclusion cannot be made after this analysis.

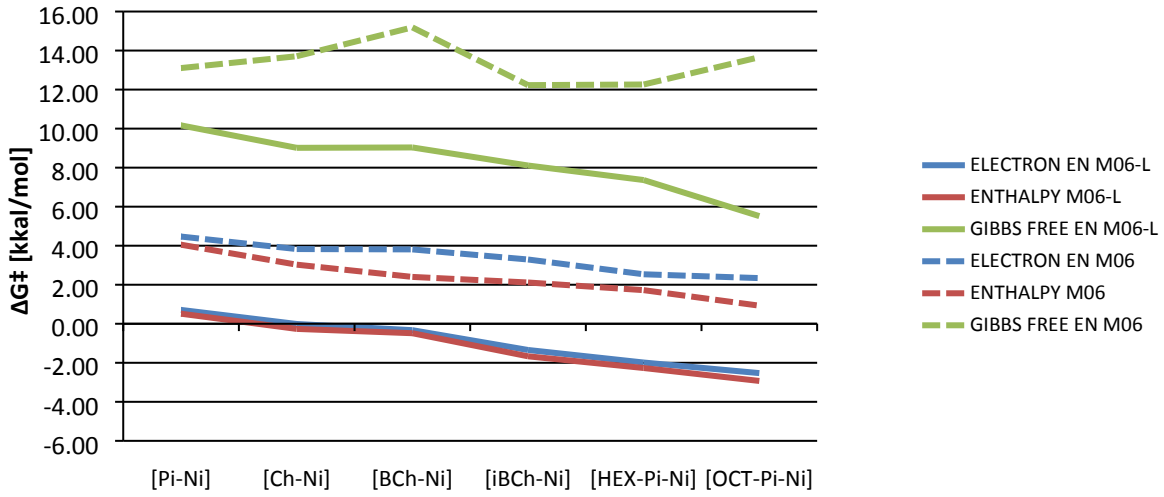


Figure S.11 Difference in low spin activation energies between M06-L and M06 functionals. Single point energies in M06 on geometries from M06-L.

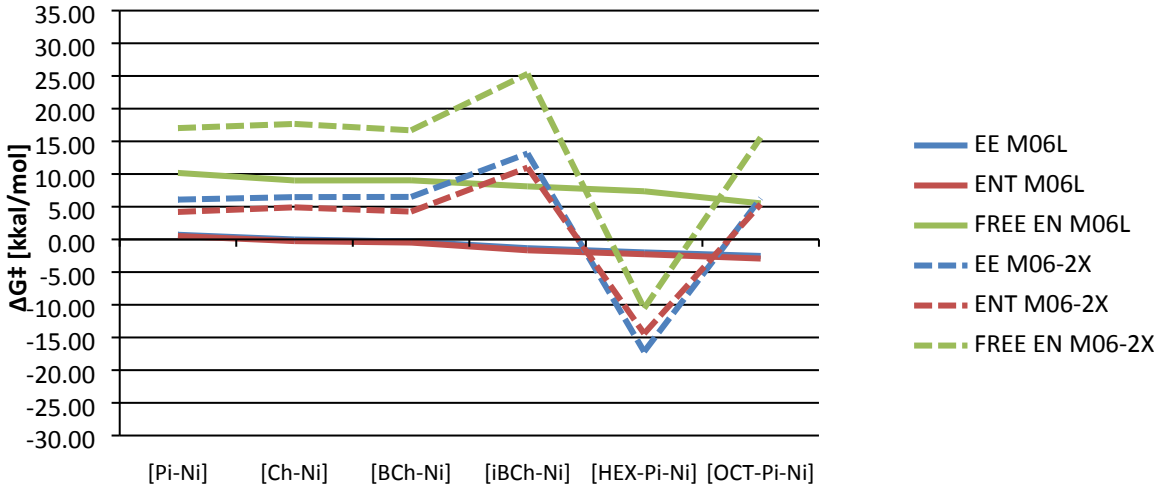


Figure S.12 Difference in low spin activation energies between M06-L and M06-2X functionals. Single point energies in M06-2X on geometries from M06-L.

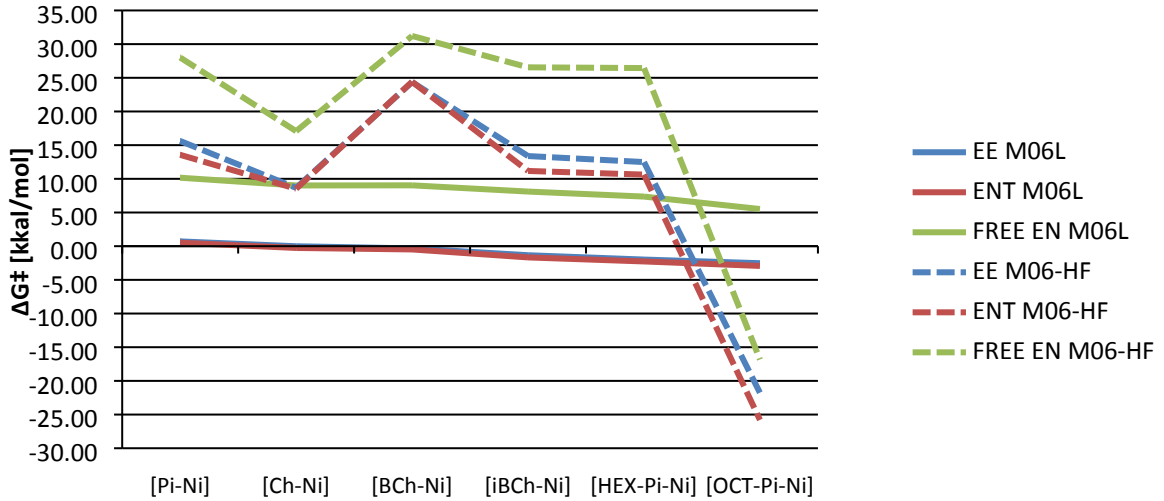


Figure S.13 Difference in low spin activation energies between M06-L and M06-HF functionals. Single point energies in M06-HF on geometries from M06-L.

S.VI.3 Hartree-Fock exchange energy test

The influence of amount of E_{ex}^{HF} for Gibbs Free Activation Energies of BCh-Ni complex (in range from 0% to 100% of E_{ex}^{HF}) was investigated for B3LYP functional (which by default has 20% of E_{ex}^{HF}) through SP calculations in Gaussian 09 Rev.D01 with different values of IOp (3/76) parameter. By changing values of IOp (3/76) parameter and leaving unchanged parameters for IOp (3/77) and IOp (3/78)[4] we were able to test influence of E_{ex}^{HF} on activation energy in studied reaction of [*BCh*-Ni] complex. Geometries of [*BCh*-Ni]$^-$ and MeCl molecules (reactants **1**) as well as for LS-TS **3** were used to perform SP calculation in B3LYP functional with E_{ex}^{HF} set in range from 0% to 100%.

Linear correlation between energy and amount of E_{ex}^{HF} were found for all separate molecules: [*BCh*-Ni]$^-$, MeCl, [*BCh*-Ni—Me—Cl]$^{‡-}$ see Figure S.14 to S.16. However the directional factor for plot for each molecule is different, see Figure S.17. Unfortunately no linear trend was found for activation energy vs. % E_{ex}^{HF}, see Figure S.18. Nevertheless tree different regions with linear correlation are present: for E_{ex}^{HF} from 0-20% and 40-50%, E_{ex}^{HF} 30% and 90-100% and 60-80% see Figure S.19, which source need further much deeper analysis. Therefore much better way to show fluctuation of energy of separate molecule should be correlation between increment of energy of each molecule vs. % E_{ex}^{HF}, see Figure S.20. And indeed with much more tight range small fluctuations of energy can be noticed and those fluctuation are responsible for bad linear correlation on Figure S.17. Because of big range on 0X axis, 40 a.u. for MeCl molecule (Figure S.14) and 250 a.u. for [*BCh*-Ni]$^-$ and [*BCh*-Ni—Me—Cl]$^{‡-}$ molecules (Figure S.15-S17) any small energy fluctuation were hidden. However, when energy range on 0X axis were smaller than 1 a.u. situation has become much more clear. At this moment it need to be pointed out that any energy change by 0.01 a.u. can caused difference in activation energy in by 6.27 kcal/mol.

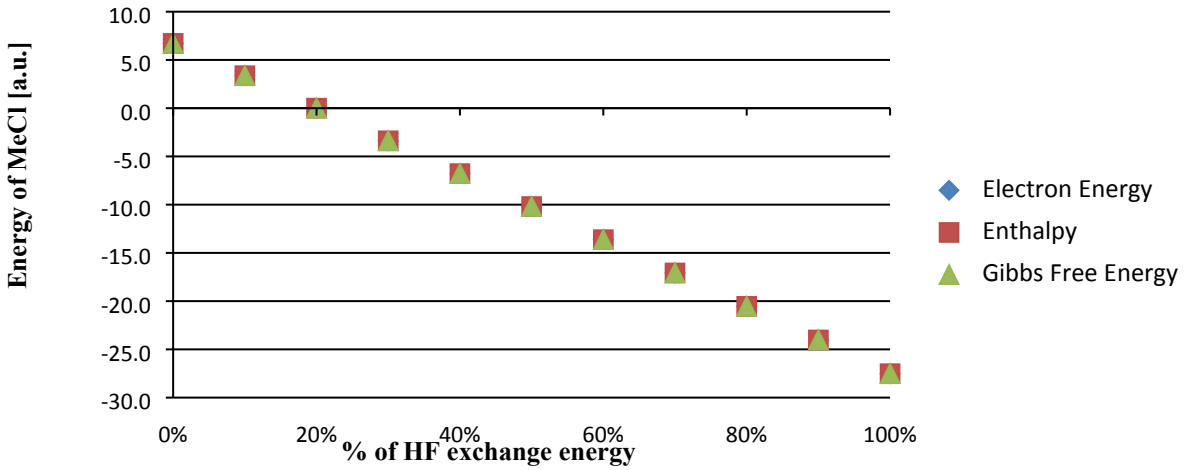


Figure S.14 Influence of Hartree-Fock exchange energy included in B3LYP functional on energy of MeCl for SP calculation of MeCl energy with geometry from default B3LYP functional. Energies from default B3LYP functional were taken as a 0.

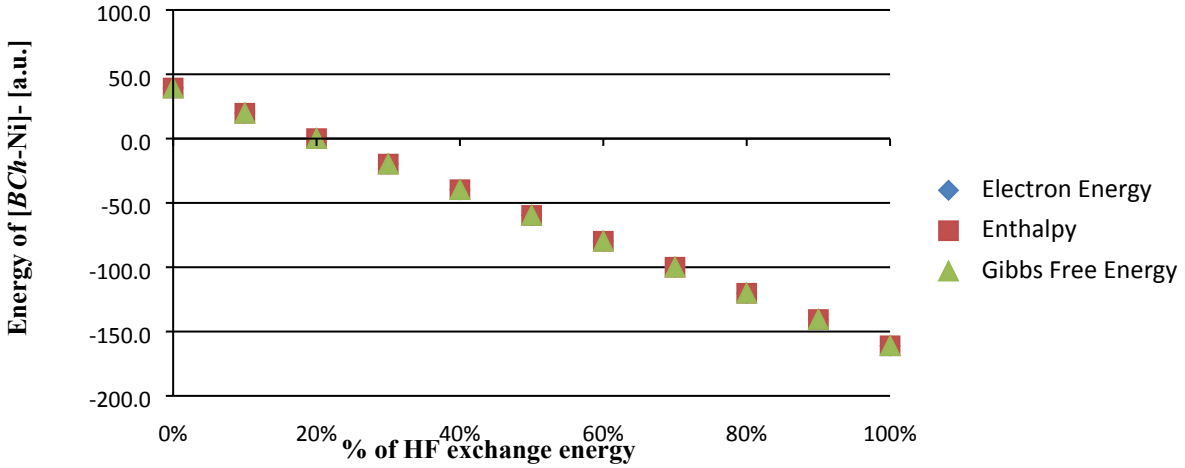


Figure S.15 Influence of Hartree-Fock exchange energy included in B3LYP functional on energy of [*BCh*-Ni]$^{-}$ complex for SP calculation of [*BCh*-Ni]$^{-}$ complex energy with geometry from default B3LYP functional. Energies from default B3LYP functional were taken as a 0.

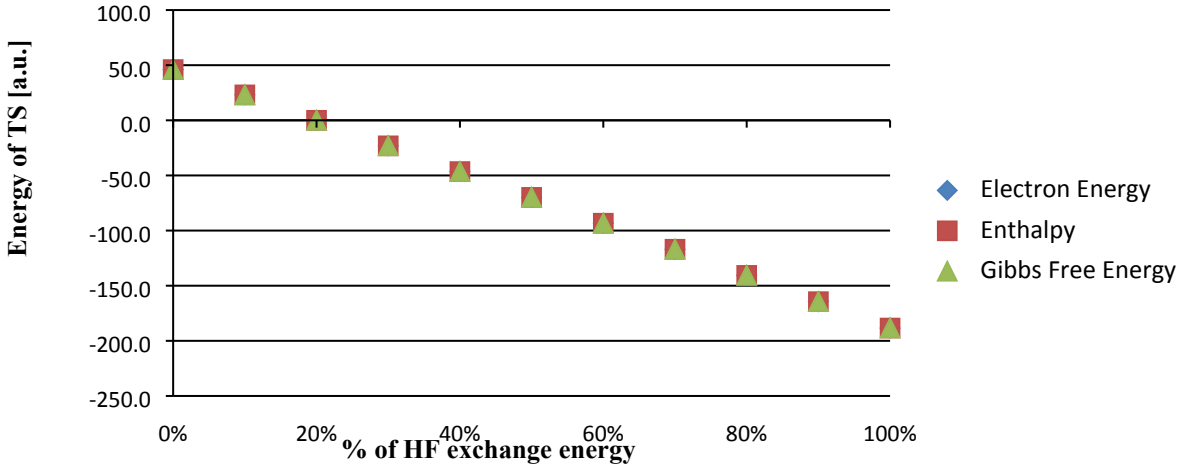


Figure S.16 Influence of Hartree-Fock exchange energy included in B3LYP functional on energy of [*BCh*-Ni−Me−Cl]$^{‡-}$ complex for SP calculation of [*BCh*-Ni−Me−Cl]$^{‡-}$ energy with geometry from default B3LYP functional. Energies from default B3LYP functional were taken as a 0.

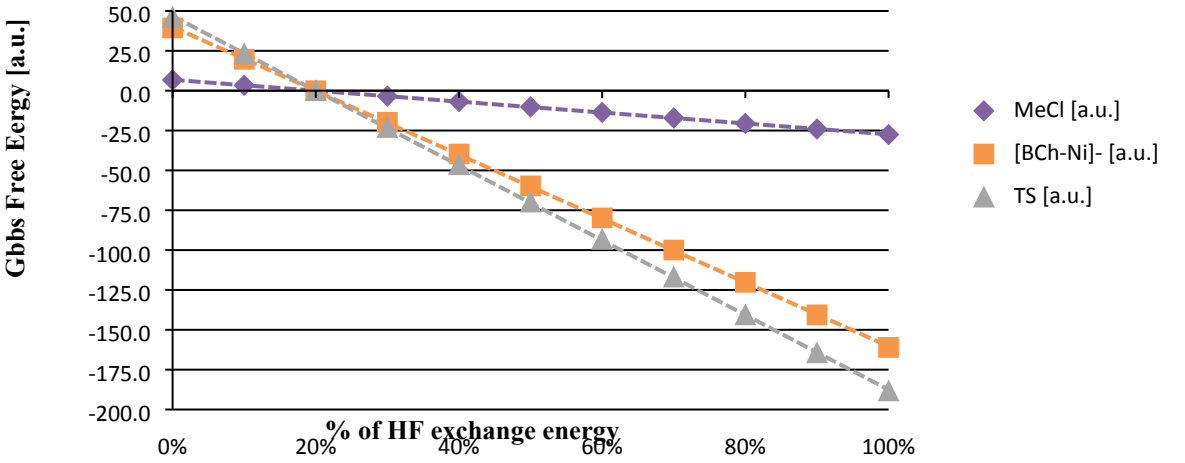


Figure S.17 Correlation of influence of Hartree-Fock exchange energy included in B3LYP functional on Gibbs Free Energy of MeCl, [*BCh*-Ni]$^{-}$ complex and [*BCh*-Ni−Me−Cl]$^{‡-}$ complex for SP calculation with geometry from default B3LYP functional. Dashed lines represented linear correlation for each species. Below legend correlation parameters are given for each species. Energies from default B3LYP functional were taken as a 0.

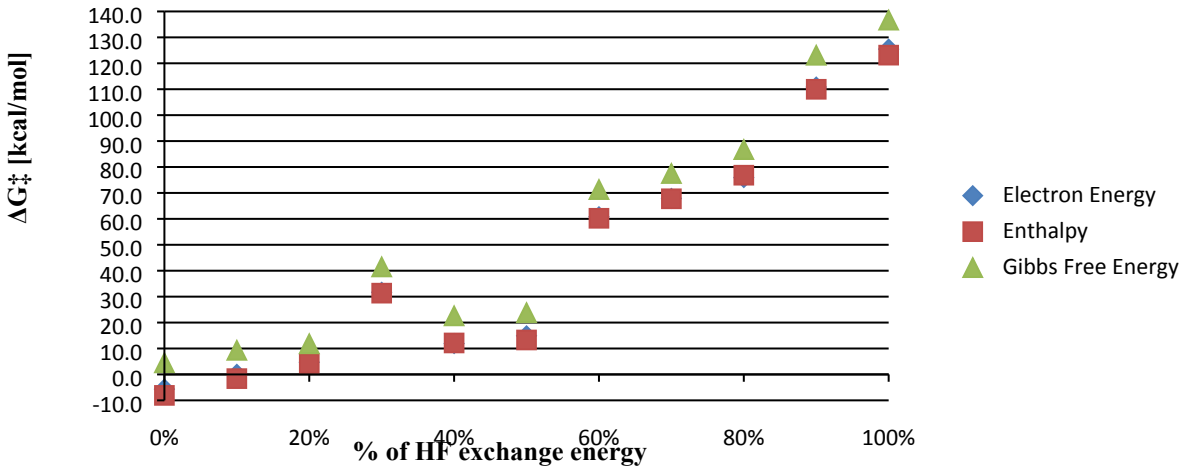


Figure S.18 Single point activation energies for MeCl dehalogenation by low spin [*BCh*-Ni]$^{-}$ complex for different amount of Hartree-Fock exchange energy in BLYP functional as a differences of energies between and [*BCh*-Ni−Me−Cl]$^{‡-}$ TS complex and sum of the energies of MeCl molecule and [*BCh*-Ni]$^{-}$ complex. Energies from default B3LYP functional were taken as a 0.

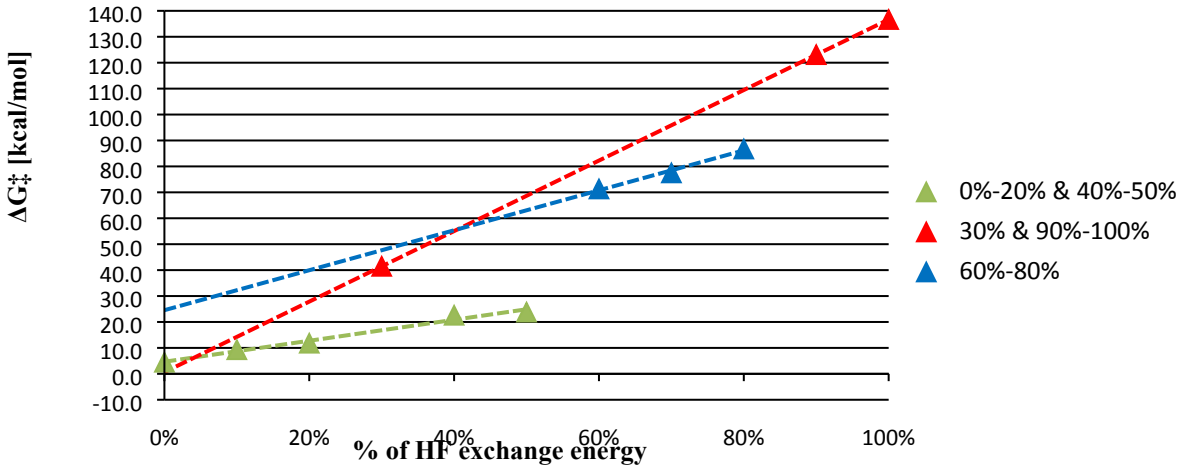


Figure S.19 Linear correlation regions for single point Gibbs Free Activation Energies for MeCl dehalogenation by low spin [*BCh*-Ni]$^{-}$ complex for different amount of Hartree-Fock exchange energy in B3LYP functional as a differences of energies between and [*BCh*-Ni−Me−Cl]$^{‡-}$ TS complex and sum of the energies of MeCl molecule and [*BCh*-Ni]$^{-}$ complex. Energies from default B3LYP functional were taken as a 0.

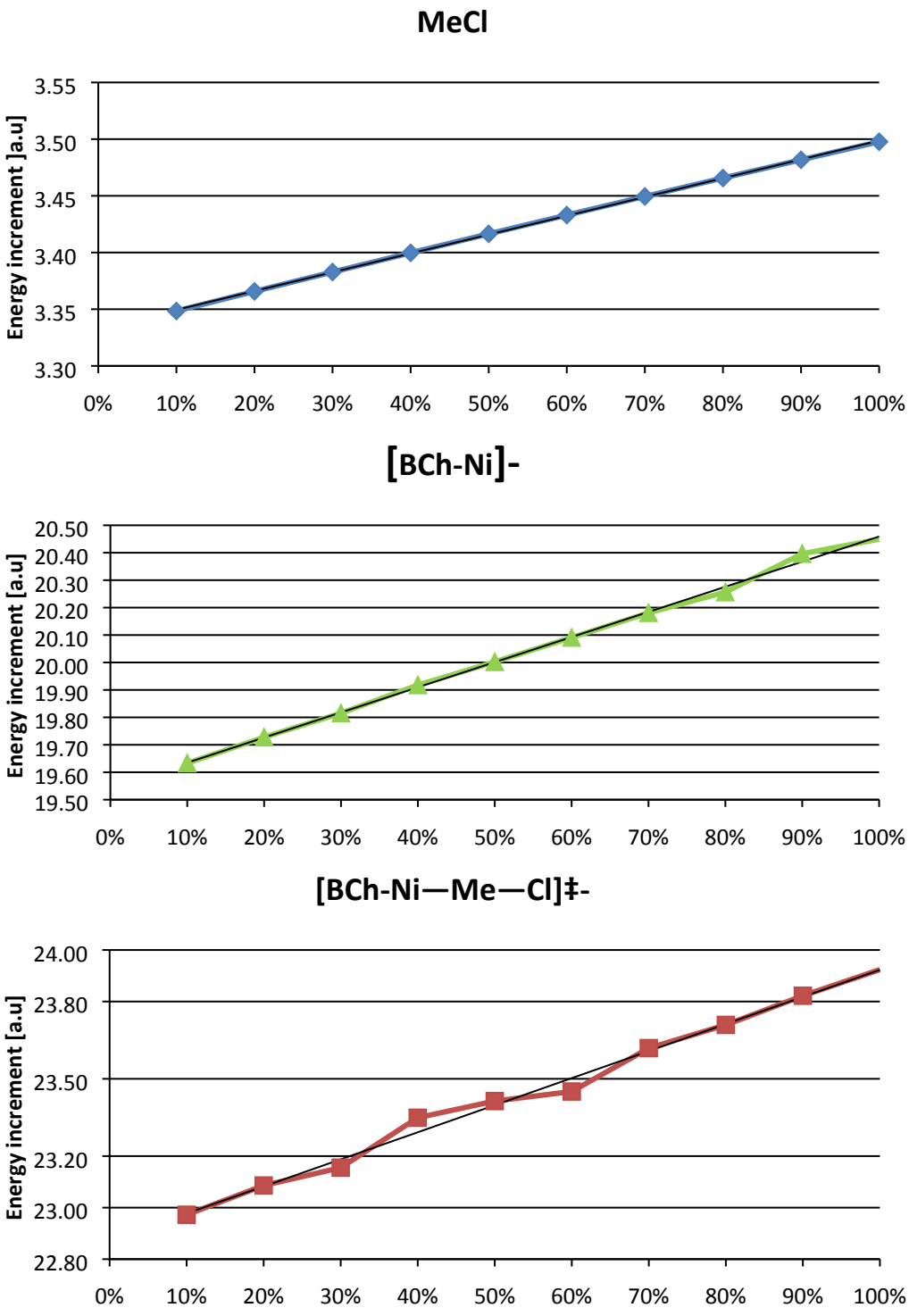


Figure S.20 Electron Energy increment MeCl, [*BCh*-Ni]$^{-}$ and [*BCh*-Ni−Me−Cl]$^{‡-}$ vs. % of E_{ex}^{HF}. Black lines shows linear correlation, R^2 values are given in top right corner of each plot.

S.VI.4 "Cross energy test"

The idea of "cross energy test" was to calculate SP energy of **1** and **3** in B3LYP functional with geometry from ωB97X-D functional and check the differences between energy of that single point and fully optimized **1** and **3** in B3LYP functional. Similar procedure was used for calculation of SP's in ωB97X-D functional with geometry from B3LYP functional. As it is visible on Figure S.6 the difference between B3LYP and ωB97X-D structure is in rotation by approx. 60° Me substituent from MeCl molecule. Therefore alternative geometry of **3** optimized in ωB97X-D functional also was tested.

As results in both functionals SP energies of **1** were very similar to energies of fully optimized structures. Similar situations can be observed for activation energies where SP structures (see Table S.6. for clarification) have higher electronic energy by less than 2 kcal/mol in B3LYP and less than 1 kcal/mol in ωB97X-D functional. This result suggests that the problem of higher activation barrier with the ωB97X-D functional is not connected with differences in geometry between TS structures in B3LYP and ωB97X-D functionals. However, it needs to be checked whether use of SMD solvation model is not responsible for this unusual behavior. Therefore, similar SP calculation for all complexes 1 and 2 were performed in gas phase (GP) with their geometries taken from structures optimized in SMD solvent models. As in the solution model, GP differences in electronic activation energies between B3LYP and ωB97X-D functionals are present. This result confirms our belief that the source of this unusual high energy barrier for ωB97X-D functional lies in ωB97X-D functional itself. All energy data are in Table S.6.

Table S.6 "Cross energy test" for *BCh*-Ni complex with Electronic Energies

DMF

[*BCh*-Ni]$^-$

	SP in B3LYP; Geometry from ωB97X-D	SP in ωB97X-D; Geometry from B3LYP
$\Delta E = E_{SP} - E_{OPT}$ [kcal/mol][a]	0.81	0.63

[*BCh*-Ni—Me—Cl]$^{‡-}$

	SP calculation in B3LYP; Geometry taken from structures optimized in ωB97X-D	SP calculation in B3LYP; Geometry taken from structures optimized in ωB97X-D with Me group rotated by 60°	SP calculation in ωB97X-D; Geometry taken from structures optimized in ωB97X-D with Me group rotated by 60°	SP calculation in ωB97X-D; Geometry taken from structures optimized in B3LYP
$\Delta E_{OPT}^{‡}$ [kcal/mol][b]		4.68		11.09
$\Delta E_{SP}^{‡}$ [kcal/mol][c]	6.21	6.43	11.36	12.05
$\Delta E = E_{SP}^{‡} - E_{OPT}^{‡}$ [kcal/mol][d]	1.52	1.75	0.27	0.95

GAS PHASE

[*BCh*-Ni]$^-$

	Difference between energy of SP calculation in B3LYP with geometry taken from structures optimized in ωB97X-D and energy of SP calculation in B3LYP with geometry taken from structures optimized in B3LYP	Difference between energy of SP calculation in ωB97X-D with geometry taken from structures optimized in B3LYP and energy of SP calculation in ωB97X-D with geometry from structures optimized in ωB97X-D
ΔE [kcal/mol]	0.66	0.76

[*BCh*-Ni—Me—Cl]$^{‡-}$

	SP in B3LYP; Geometry from B3LYP in DMF	SP in B3LYP; Geometry from ωB97X-D in DMF	SP in ωB97X-D; Geometry from ωB97X-D in DMF	SP in ωB97X-D; Geometry from B3LYP in DMF
$\Delta E_{SP}^{‡}$ [kcal/mol] = $E_{SP}^{‡}$ - ($E_{SP}^{[BCh\text{-}Ni]^-}$ + E_{OPT}^{MeCl})[e]	2.44	4.27	8.95	22.68

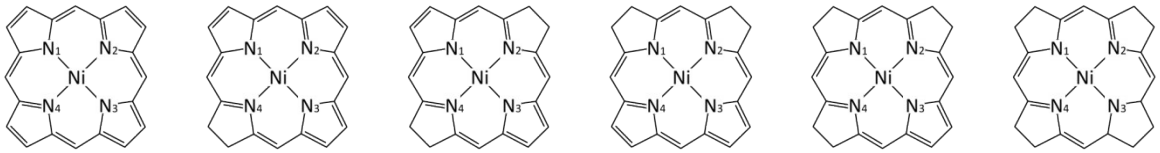
[a] Differences in Electron Energy between SP structure and fully optimized structure of complex **1**;
[b] Electron activation energy for fully optimizes complexes **1** and TS **3**;
[c] Electron activation energies between SP TS **3** and fully optimized complexes **1**;
[d] Differences in Electron activation energies between [c] and [b];
[e] As a reference: for B3LYP was taken sum of energy of SP [*BCh*-Ni]$^-$ in B3LYP with geometry from B3LYP in DMF and electron energy of MeCl molecule optimized in B3LYP Gas Phase, for ωB97X-D was taken sum of energy of SP [*BCh*-Ni]$^-$ in ωB97X-D with geometry from ωB97X-D in DMF and electron energy of MeCl optimized molecule in ωB97X-D Gas Phase.

S.VII Cl-KIEs

Table S.7 Chlorine kinetic isotope effects (Cl-KIE's) with corresponding Wiberg bond order for low spin pathway for different porphyrin derivative ligands in B3LYP, M06-L and ωB97X-D functionals.

	B3LYP		**M06-L**		**ωB97X-D**	
	Cl-KIE	*n(C-Cl)*	Cl-KIE	*n(C-Cl)*	Cl-KIE	*n(C-Cl)*
[*OCT-Pi*-Ni]$^-$	1.0089	*0.1136*	1.0100	*0.1218*	1.0096	*0.0980*
[*HEX-Pi*-Ni]$^-$	1.0095	*0.1127*	1.0101	*0.1210*	1.0096	*0.1006*
[*iBCh*-Ni]$^-$	1.0084	*0.1120*	1.0101	*0.1183*	1.0097	*0.0996*
[*BCh*-Ni]$^-$	1.0097	*0.1114*	1.0102	*0.1163*	1.0096	*0.0967*
[*Ch*-Ni]$^-$	1.0097	*0.1104*	1.0104	*0.1162*	1.0097	*0.0977*
[*Pi*-Ni]$^-$	1.0097	*0.1098*	1.0092	*0.1140*	1.0093	*0.0972*

S.VIII Ni-N distances



Pi-Ni *Ch*-Ni *BCh*-Ni *iBCh*-Ni *HEX-Pi*-Ni *OCT-Pi*-Ni

Figure S.21 Nitrogen atoms numbers in *L*-Ni complexes.

Table S.8 Ni-N distances for low spin [*L*-Ni] complex in B3LYP functional.

	[*L*-Ni]	**[*L*-Ni]$^-$**	**[*L*-Ni···MeCl]$^-$**	**[*L*-Ni···Me···Cl]$^{‡-}$**	**[*L*-Ni-Me···Cl]$^-$**	**[*L*-Ni-Me]**
		1	**2**	**3**	**4**	**5**
			[*OCT-Pi*-Ni]$^-$			
Ni-N1 [Å]	1.968	2.098	2.098	2.099	2.133	2.131
Ni-N2 [Å]	1.968	2.098	2.097	2.102	2.132	2.130
Ni-N3 [Å]	1.968	2.098	2.097	2.102	2.133	2.132
Ni-N4 [Å]	1.968	2.098	2.098	2.099	2.134	2.133
			[*HEX-Pi*-Ni]$^-$			
Ni-N1 [Å]	1.957	2.081	2.081	2.088	2.081	2.080
Ni-N2 [Å]	1.961	2.099	2.099	2.106	2.105	2.106
Ni-N3 [Å]	1.945	2.056	2.057	2.050	2.013	2.012
Ni-N4 [Å]	1.961	2.099	2.099	2.112	2.116	2.116
			[*iBCh*-Ni]$^-$			
Ni-N1 [Å]	1.968	2.081	2.081	2.089	2.093	2.099
Ni-N2 [Å]	1.968	2.080	2.080	2.089	2.086	2.097
Ni-N3 [Å]	1.954	2.062	2.063	2.063	2.042	2.042
Ni-N4 [Å]	1.954	2.062	2.062	2.061	2.049	2.044
			[*BCh*-Ni]$^-$			
Ni-N1 [Å]	1.948	1.959	1.960	2.034	2.006	2.004
Ni-N2 [Å]	1.978	1.968	1.969	2.119	2.136	2.137
Ni-N3 [Å]	1.948	1.959	1.960	2.034	2.002	2.000
Ni-N4 [Å]	1.977	1.967	1.968	2.125	2.148	2.149
			[*Ch*-Ni]$^-$			
Ni-N1 [Å]	1.963	1.989	1.980	2.041	2.025	2.023
Ni-N2 [Å]	1.971	1.982	1.974	2.069	2.064	2.064
Ni-N3 [Å]	1.963	1.983	1.975	2.042	2.021	2.020
Ni-N4 [Å]	1.991	1.993	1.983	2.101	2.125	2.125
			[*Pi*-Ni]$^-$			
Ni-N1 [Å]	1.979	1.997	1.997	2.049	2.044	2.046
Ni-N2 [Å]	1.979	1.985	1.984	2.052	2.040	2.040
Ni-N3 [Å]	1.979	1.997	1.997	2.049	2.044	2.043
Ni-N4 [Å]	1.979	1.985	1.984	2.048	2.050	2.050

Table S.9 Ni-N distances for low spin [*L*-Ni] complex in M06-L functional.

	[*L*-Ni]	[*L*-Ni]$^-$	[*L*-Ni···MeCl]$^-$	[*L*-Ni···Me···Cl]$^{‡-}$	[*L*-Ni-Me···Cl]$^-$	[*L*-Ni-Me]
		1	**2**	**3**	**4**	**5**
			[*OCT-Pi*-Ni]$^-$			
Ni-N1 [Å]	1.975	2.081	2.086	2.085	2.111	2.111
Ni-N2 [Å]	1.976	2.081	2.085	2.086	2.107	2.109
Ni-N3 [Å]	1.976	2.081	2.086	2.088	2.109	2.109
Ni-N4 [Å]	1.975	2.081	2.086	2.086	2.112	2.111
			[*HEX-Pi*-Ni]$^-$			
Ni-N1 [Å]	1.959	2.067	2.068	2.077	2.073	2.072
Ni-N2 [Å]	1.960	2.077	2.077	2.088	2.101	2.102
Ni-N3 [Å]	1.946	2.046	2.046	2.040	2.006	2.006
Ni-N4 [Å]	1.960	2.078	2.081	2.087	2.106	2.106
			[*iBCh*-Ni]$^-$			
Ni-N1 [Å]	1.966	2.063	2.064	2.074	2.087	2.089
Ni-N2 [Å]	1.966	2.063	2.063	2.073	2.077	2.087
Ni-N3 [Å]	1.952	2.048	2.047	2.048	2.034	2.033
Ni-N4 [Å]	1.952	2.048	2.048	2.051	2.040	2.035
			[*BCh*-Ni]$^-$			
Ni-N1 [Å]	1.947	2.035	2.037	2.029	2.000	1.997
Ni-N2 [Å]	1.969	2.073	2.073	2.094	2.122	2.125
Ni-N3 [Å]	1.947	2.035	2.035	2.028	1.996	1.994
Ni-N4 [Å]	1.969	2.073	2.076	2.097	2.129	2.132
			[*Ch*-Ni]$^-$			
Ni-N1 [Å]	1.956	2.036	2.036	2.032	2.018	2.014
Ni-N2 [Å]	1.961	2.042	2.042	2.051	2.057	2.060
Ni-N3 [Å]	1.956	2.035	2.035	2.032	2.010	2.009
Ni-N4 [Å]	1.978	2.053	2.057	2.077	2.110	2.111
			[*Pi*-Ni]$^-$			
Ni-N1 [Å]	1.972	2.029	2.030	2.034	2.039	2.038
Ni-N2 [Å]	1.973	2.029	2.030	2.033	2.033	2.033
Ni-N3 [Å]	1.972	2.029	2.029	2.034	2.033	2.033
Ni-N4 [Å]	1.973	2.029	2.031	2.037	2.039	2.039

Table S.10 Ni-N distances for low spin [*L*-Ni] complex in ωB97X-D functional.

	[*L*-Ni]	[*L*-Ni]$^-$	[*L*-Ni···MeCl]$^-$	[*L*-Ni···Me···Cl]$^{‡-}$	[*L*-Ni-Me···Cl]$^-$	[*L*-Ni-Me]
		1	**2**	**3**	**4**	**5**
			[*OCT-Pi*-Ni]$^-$			
Ni-N1 [Å]	1.948	2.085	2.084	2.084	2.116	2.116
Ni-N2 [Å]	1.947	2.086	2.084	2.087	2.119	2.116
Ni-N3 [Å]	1.948	2.085	2.085	2.088	2.115	2.116
Ni-N4 [Å]	1.948	2.087	2.086	2.084	2.113	2.114
			[*HEX-Pi*-Ni]$^-$			
Ni-N1 [Å]	1.937	2.067	2.069	2.073	2.055	2.057
Ni-N2 [Å]	1.942	2.088	2.086	2.093	2.087	2.084
Ni-N3 [Å]	1.931	2.051	2.050	2.043	2.008	2.004
Ni-N4 [Å]	1.942	2.087	2.088	2.089	2.077	2.079
			[*iBCh*-Ni]$^-$			
Ni-N1 [Å]	1.945	2.069	2.067	2.073	2.070	2.068
Ni-N2 [Å]	1.945	2.069	2.067	2.073	2.057	2.067
Ni-N3 [Å]	1.942	2.057	2.055	2.058	2.038	2.036
Ni-N4 [Å]	1.942	2.057	2.055	2.058	2.042	2.037
			[*BCh*-Ni]$^-$			
Ni-N1 [Å]	1.930	1.944	1.941	2.029	2.009	2.006
Ni-N2 [Å]	1.957	1.949	1.946	2.107	2.119	2.120
Ni-N3 [Å]	1.934	1.945	1.943	2.026	1.994	1.991
Ni-N4 [Å]	1.957	1.949	1.946	2.101	2.110	2.111
			[*Ch*-Ni]$^-$			
Ni-N1 [Å]	1.946	1.958	1.956	2.034	2.024	2.023
Ni-N2 [Å]	1.957	1.957	1.956	2.068	2.063	2.063
Ni-N3 [Å]	1.946	1.958	1.957	2.034	2.016	2.014
Ni-N4 [Å]	1.961	1.954	1.952	2.075	2.078	2.079
			[*Pi*-Ni]$^-$			
Ni-N1 [Å]	1.967	1.979	1.975	2.039	2.037	2.037
Ni-N2 [Å]	1.967	1.965	1.962	2.042	2.036	2.036
Ni-N3 [Å]	1.967	1.979	1.976	2.039	2.029	2.028
Ni-N4 [Å]	1.967	1.965	1.963	2.037	2.030	2.029

S.IX Existence of [*iBCh*-Ni]···Me• complex

In our research we found existence of [*iBCh*-Ni]···Me• complex as an alternative to the [*iBCh*-Ni-Me] complex. It needs to be pointed out that [*iBCh*-Ni]···Me• complex were fully optimized in solution (SMD solvent model) as a local minimum, without any constrains.

The nature of the [*iBCh*-Ni]···Me• complex was confirmed by spin distribution analysis. While in case of the [*iBCh*-Ni-Me] complex the unpaired electron is localized on the Ni atom, in [*iBCh*-Ni]···Me• it is always on C atom from Me group, see Table S.11 and compare with Figure S.2. It is visible that [*iBCh*-Ni]···Me• complex structure optimized in M06-L functional stands out from the rest cases. However for a SP calculation in M06-L functional with geometry from B3LYP we achieved similar spin distribution like in case of B3LYP and ωB97X-D functionals.

The main structural difference between both complexes was Ni-C_{Me} distance which was elongated to 3.132Å, 2.225Å and 2.787Å respectively in B3LYP, M06-L and ωB97X-D functionals. Also Ni-N distances in [*iBCh*-Ni]···Me• complex were more similar to distances in [*iBCh*-Ni] neutral complex rather than to distances in [*iBCh*-Ni-Me] complex, see Table S.12 and compare with Tables S.2 to S.4.

From the energetic point of view, the [*iBCh*-Ni]···Me• complexes were less preferred than [*iBCh*-Ni-Me] complexes, see Table S.14. Moreover, both [*iBCh*-Ni]···Me• complex fully optimized in M06-L functional as well as complex with optimized with frozen Ni-C_{Me} (3.138Å) in M06-L had a very similar energy.

Table S.11 Spin distribution between Ni and C_{Me} atoms in [*iBCh*-Ni]···Me• complex in B3LYP, M06-L, M06-L with geometry frozen Ni-C_{Me} bond and ωB97X-D functionals.

	B3LYP	M06-L	M06-L frozen	ωB97X-D
Ni	0.135	0.404	0.250	0.161
C_{Me}	1.043	0.611	1.029	0.995

Table S.12 Key distances for [*iBCh*-Ni]···Me• complex in B3LYP, M06-L and ωB97X-D functionals.

	B3LYP	M06-L	ωB97X-D
Ni-C [Å]	3.132	2.225	2.787
Ni-N1 [Å]	1.970	1.985	1.946
Ni-N2 [Å]	1.970	1.985	1.947
Ni-N3 [Å]	1.956	1.966	1.943
Ni-N4 [Å]	1.956	1.966	1.943

Table S.13 Energy difference between [*iBCh*-Ni-Me] and [*iBCh*-Ni]···Me• complexes in B3LYP, M06-L, M06-L with geometry frozen Ni-C_{Me} bond and ωB97X-D functionals.

	ΔG[kcal/mol]
B3LYP	8.87
M06-L	12.49
M06-L frozen	12.85
ωB97X-D	8.48

S.X Reduction potentials

Table S.14 Theoretical reduction potentials in V for [*L*-Ni$^{(II)}$]/[*L*-Ni$^{(I)}$]$^-$ reduction for studied complexes in DMF reported vs. ferrocenium/ferrocene ($Cp_2Fe^{+1/0}$) electrode in non-aqueous solvents.

	B3LYP	**M06-L**	**ωB97X-D**
[*Pi*-Ni$^{(II)}$]/[*Pi*-Ni$^{(I)}$]$^-$	-2.18	-1.49	-2.20
[*Ch*-Ni$^{(II)}$]/[*Ch*-Ni$^{(I)}$]$^-$	-2.10	-1.46	-2.13
[*BCh*-Ni$^{(II)}$]/[*BCh*-Ni$^{(I)}$]$^-$	-1.98	-1.44	-1.83
[*iBCh*-Ni$^{(II)}$]/[*iBCh*-Ni$^{(I)}$]$^-$	-1.87	-1.53	-2.07
[HEX-*Pi*-Ni$^{(II)}$]/[HEX-*Pi*-Ni$^{(I)}$]$^-$	-1.88	-1.55	-2.09
[OCT-*Pi*-Ni$^{(II)}$]/[OCT-*Pi*-Ni$^{(I)}$]$^-$	-1.94	-1.72	-2.08

[*iBCh*-Ni$^{(III)}$-Me] + e$^-$ $\rightarrow$ [*iBCh*-Ni$^{(II)}$-Me]$^-$ (1)

[*iBCh*-Ni$^{(I)}$]$^-$ + [*iBCh*-Ni$^{(III)}$-Me] $\rightarrow$ [*iBCh*-Ni$^{(II)}$] + [*iBCh*-Ni$^{(II)}$-Me]$^-$ (2)

Scheme S.1 Proposed pathways of reduction [iBCh-Ni$^{(III)}$-Me] complex: (1) by direct electron attachment, (2) use of [*iBCh*-Ni$^{(I)}$]$^-$ as a electron donor.

Table S.15 Theoretical reduction potentials in [V] of the reduction [*iBCh*-Ni$^{(III)}$-Me] by direct electron attachment to [*iBCh*-Ni$^{(II)}$-Me]$^-$ complex (1) for isobacteriochlorin complex in DMF reported vs. ferrocenium/ferrocene ($Cp_2Fe^{+1/0}$) electrode in non-aqueous solvents.

	B3LYP	**M06-L**	**ωB97X-D**
[*iBCh*-Ni$^{(III)}$-Me]/[*iBCh*-Ni$^{(II)}$-Me]$^-$	-2.64V	-2.34V	-2.79V

To estimate the Gibbs Free Energy ($\Delta G^{red(1)}$) between substrate and products in pathway (1) at first we had to estimate the Gibbs Free Energy of a single electron. We made this by calculating the difference in the Gibbs Free Energy between neutral ferrocene complex (Cp_2Fe) and cationic ferrocenium complex (Cp_2Fe^+) in each functionals: B3LYP, M06-L and ωB97X-D in SMD solvent model. As a result, we have noticed that reduced methyl-nickel anion complexes was more than 50 kcal/mol higher in energy than its neutral precursor. This implicate that direct electron reduction pathway is highly improbable. However, energy difference in pathway (2) was much smaller (16-19 kcal/mol) which makes it more probable than pathway (1). To fully answer if above statement is true a search of possible TS's between both forms of methyl-nickel complexes, as well as search of other possible reduction pathways will be done in the future.

Table S.16 Gibbs Free Energy difference between reduction products and substrates for pathway (1) and (2) for in DMF.

	B3LYP	**M06-L**	**ωB97X-D**
ΔG^{red1} [kcal/mol]	60.88	53.87	63.41
ΔG^{red2} [kcal/mol]	17.65	18.67	16.50

S.XI References

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S. XII Cartesian coordinates of Low Spin (LS) systems

Due to the fact that Low Spin (LS) complexes are more favorable energetically than High Spin (HS) complexes only Cartesian coordinates for LS complexes are provided. Cartesian coordinates for chloride ion (Cl^-) have been omitted.

S.IX.1 Nickel porphyrin (*Pi*) complexes

B3LYP/6-311+G(d,p)				M06-L/6-311+G(d,p)				ωB97X-D/6-311+G(d,p)			
[*Pi*-Ni]											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.83572922	C	0.00000000	0.00000000	4.82236602	C	0.00000000	0.00000000	4.81566159
C	4.83596239	0.00000000	4.83573276	C	4.82271902	0.00000000	4.82287232	C	4.81593423	0.00000000	4.81511714
C	4.83595335	0.00349761	0.00001093	C	4.82271442	-0.00129340	0.00050726	C	4.81593872	-0.00122716	-0.00054130
C	3.51142661	0.00287867	-0.40230648	C	3.50198345	-0.00094735	-0.40290655	C	3.49481349	-0.00069515	-0.39792461
C	3.09898206	0.00469055	-1.78322758	C	3.09146354	-0.00257119	-1.77587248	C	3.08576640	0.00131058	-1.77651449
C	1.73691086	0.00323721	-1.78327898	C	1.73147658	-0.00207056	-1.77600479	C	1.72972702	0.00135687	-1.77644230
C	1.32447827	0.00084510	-0.40223125	C	1.32074022	-0.00026338	-0.40301382	C	1.32098555	-0.00048628	-0.39757455
N	2.41789716	-0.00006590	0.43889700	N	2.41124187	0.00127099	0.43921283	N	2.40796033	-0.00225003	0.44105049
C	-0.40235981	-0.00020170	1.32443572	C	-0.40332779	0.00039943	1.32064840	C	-0.39743727	0.00013551	1.32100758
C	-1.78336494	-0.00072877	1.73674799	C	-1.77634285	0.00110724	1.73128564	C	-1.77625297	0.00009971	1.72973511
C	-1.78352626	-0.00094780	3.09884143	C	-1.77634840	0.00164105	3.09131042	C	-1.77650582	-0.00038080	3.08575535
C	-0.40257271	-0.00022746	3.51134766	C	-0.40342769	0.00081826	3.50180388	C	-0.39778188	-0.00001432	3.49476095
N	0.43868174	0.00060202	2.41786169	N	0.43881446	-0.00027765	2.41116802	N	0.44116079	0.00056182	2.40789500
C	1.32452667	0.00031574	5.23804581	C	1.32073222	-0.00084349	5.22577664	C	1.32111963	0.00049551	5.21303870
C	1.73697737	-0.00137348	6.61896203	C	1.73125237	-0.00006847	6.59874250	C	1.73017402	-0.00059135	6.59163266
C	3.09905122	-0.00132305	6.61900626	C	3.09124154	-0.00008519	6.59887291	C	3.08620768	-0.00019120	6.59156112
C	3.51147637	0.00032348	5.23795477	C	3.50197739	-0.00087142	5.22588025	C	3.49495412	0.00088726	5.21269001
N	2.41805758	0.00204084	4.39683335	N	2.41147446	-0.00226106	4.38365508	N	2.40797561	0.00186477	4.37406318
C	5.23833083	0.00050663	3.51130343	C	5.22605293	0.00015502	3.50222626	C	5.21336997	-0.00105708	3.49410485
C	6.61933325	0.00078708	3.09898008	C	6.59906702	0.00025364	3.09158246	C	6.59219120	-0.00196041	3.08538570
C	6.61948655	0.00243952	1.73688868	C	6.59906730	-0.00078771	1.73155887	C	6.59244637	-0.00210762	1.72936648
C	5.23852605	0.00258961	1.32439208	C	5.22614219	-0.00106407	1.32106976	C	5.21372360	-0.00174283	1.32035154
N	4.39728192	0.00101607	2.41788084	N	4.38390709	-0.00003785	2.41171145	N	4.37477798	-0.00153718	2.40722632
Ni	2.41797901	0.00089406	2.41786311	Ni	2.41136079	-0.00032074	2.41143529	Ni	2.40797050	-0.00037992	2.40755856
H	-0.76710598	0.00003587	-0.76738877	H	-0.76731417	-0.00037297	-0.76779263	H	-0.76724167	0.00055970	-0.76712816
H	-0.76715949	-0.00057274	5.60294508	H	-0.76746158	0.00039388	5.58989811	H	-0.76708029	-0.00069206	5.58282452
H	5.60305359	-0.00081820	5.60313680	H	5.59002737	0.00065759	5.59067110	H	5.58318004	-0.00025461	5.58224052
H	5.60311327	0.00480641	-0.76720343	H	5.59017998	-0.00197369	-0.76702235	H	5.58301863	-0.00078027	-0.76770665
H	1.05453952	0.00421463	-2.62394318	H	-2.61498009	0.00245813	3.77630948	H	-2.61587184	-0.00100453	3.76917382
H	3.78126575	0.00723283	-2.62391667	H	-2.61504215	0.00152774	1.04640448	H	-2.61553282	-0.00039227	1.04626918
H	-2.62431929	-0.00166054	3.78104112	H	1.04641337	-0.00325345	-2.61459195	H	1.04618943	0.00272163	-2.61572889
H	-2.62402577	-0.00137683	1.05440792	H	3.77649823	-0.00446031	-2.61443604	H	3.76907941	0.00297362	-2.61589386
H	7.46027209	0.00352985	1.05467964	H	3.77630253	0.00073615	7.43746348	H	3.76975203	-0.00087956	7.43084284
H	7.46000079	0.00045793	3.78131198	H	1.04621909	0.00115600	7.43730760	H	1.04685568	-0.00197199	7.43100851
H	3.78142501	-0.00268438	7.45966597	H	7.43769437	-0.00145370	1.04655366	H	7.43180662	-0.00212829	1.04594051
H	1.05469780	-0.00303854	7.45965623	H	7.43777283	0.00069189	3.77645421	H	7.43146457	-0.00168936	3.76886057
[*Pi*-Ni]$^-$											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.83726211	C	0.00000000	0.00000000	4.84332390	C	0.00000000	0.00000000	4.81273320
C	4.87745643	0.00000000	4.83664823	C	4.84335202	0.00000000	4.84400658	C	4.86407746	0.00000000	4.76402392
C	4.87745262	-0.00028310	-0.00061120	C	4.84335196	-0.00156656	0.00068276	C	4.76875794	-0.95518771	0.04772697
C	3.53756575	-0.00001084	-0.42359597	C	3.51867217	-0.00127476	-0.43582819	C	3.44488734	-0.76362296	-0.38542950
C	3.13093898	0.00241773	-1.78568139	C	3.10480604	-0.00305137	-1.81561621	C	3.03897222	-0.81218458	-1.73990233
C	1.74612267	0.00207549	-1.78552359	C	1.73910710	-0.00441536	-1.81583948	C	1.69559534	-0.48916130	-1.75873730
C	1.33986382	-0.00019968	-0.42312706	C	1.32483471	-0.00152216	-0.43612065	C	1.31609581	-0.27180464	-0.41323612
N	2.43873107	-0.00167833	0.42149775	N	2.42162204	-0.00012049	0.39324047	N	2.38878851	-0.43482472	0.43689926
C	-0.38984936	-0.00007032	1.31623396	C	-0.43635638	0.00121706	1.32471681	C	-0.38046041	0.06636033	1.30932629
C	-1.77568097	0.00020046	1.73975172	C	-1.81614901	0.00342719	1.73884898	C	-1.76132995	0.20012095	1.73218194
C	-1.77579632	-0.00029573	3.09747802	C	-1.81611200	0.00207029	3.10453121	C	-1.76763803	0.13901231	3.08006810
C	-0.39011390	-0.00018516	3.52116586	C	-0.43636760	0.00001175	3.51863942	C	-0.38691173	0.00527284	3.50358756
N	0.45410594	0.00002311	2.41864583	N	0.39284234	-0.00052725	2.42166448	N	0.45261015	-0.04579531	2.40663375
C	1.33988738	0.00027133	5.26024406	C	1.32468204	0.00000344	5.27983541	C	1.34439064	0.01332002	5.22482800
C	1.74651633	-0.00155641	6.62232875	C	1.73854612	0.00248084	6.65962403	C	1.75958645	0.15621942	6.56970626
C	3.13133282	-0.00111068	6.62216926	C	3.10424575	0.00354762	6.65985081	C	3.14025615	0.20875815	6.55059490
C	3.53758925	0.00062942	5.25977359	C	3.51852072	0.00124789	5.28013100	C	3.52832311	0.07691859	5.19642904
N	2.43872331	0.00171348	4.41514802	N	2.42173153	-0.00069224	4.45077010	N	2.42788145	-0.03959349	4.37459831
C	5.26730735	-0.00038652	3.52041633	C	5.27971115	-0.00157652	3.51928926	C	5.22460522	-0.27031116	3.47548658
C	6.65313872	-0.00119138	3.09689348	C	6.65950068	-0.00382137	3.10516420	C	6.59638615	-0.49324620	3.06062995
C	6.65325021	-0.00080904	1.73916830	C	6.65947294	-0.00315861	1.73947716	C	6.56352433	-0.81992585	1.75195462
C	5.26756589	-0.00043242	1.31548403	C	5.27973693	-0.00124764	1.32536367	C	5.17483222	-0.76502914	1.33710489
N	4.42334836	-0.00030930	2.41800635	N	4.45051885	-0.00033011	2.42233550	N	4.36360671	-0.43397285	2.40617797
Ni	2.43872825	-0.00005471	2.41832627	Ni	2.42167139	-0.00041880	2.42200268	Ni	2.40824243	-0.23857479	2.40611893
H	-0.77177378	0.00068508	-0.76349927	H	-0.76920308	0.00011303	-0.76934923	H	-0.76275597	0.10189243	-0.76558778

H	-0.77171250	-0.00066065	5.60077359	H	-0.76930219	0.00131994	5.61254730	H	-0.76725350	0.04864198	5.57899487
H	5.64922875	-0.00068792	5.60014885	H	5.61255855	0.00031617	5.61335209	H	5.64653590	0.10192188	5.50949718
H	5.64916612	0.00026510	-0.76412224	H	5.61265059	-0.00328800	-0.76854681	H	5.51601573	-1.20904852	-0.69759912
H	1.06835151	0.00364187	-2.63064959	H	1.06591275	-0.00613965	-2.66570368	H	-2.60907024	0.19353125	3.75986291
H	3.80841105	0.00448395	-2.63102750	H	3.77822329	-0.00408317	-2.66531439	H	-2.59703607	0.30861833	1.05185582
H	-2.61927497	-0.00067370	3.77746205	H	-2.66605415	0.00290961	3.77765037	H	1.02639274	-0.42238643	-2.60776115
H	-2.61907332	0.00022798	1.05971522	H	-2.66607430	0.00498422	1.06572628	H	3.69131176	-1.04605694	-2.57227811
H	7.49672632	-0.00075702	1.05918128	H	7.50944760	-0.00433195	1.06639970	H	7.38575109	-1.06478147	1.09079856
H	7.49653434	-0.00142655	3.77692697	H	7.50944809	-0.00496044	3.77826254	H	7.45106773	-0.41649252	3.72144621
H	3.80910282	-0.00230462	7.46729557	H	3.77743868	0.00513086	7.50971652	H	3.82609487	0.31140656	7.38257442
H	1.06904381	-0.00337467	7.46767671	H	1.06512498	0.00373992	7.50931995	H	1.09064474	0.22337309	7.41890077

MeCl

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08694599	H	0.00000000	0.00000000	1.08633125	H	0.00000000	0.00000000	1.08723601
H	1.01451467	0.00000000	-0.39014216	H	1.01688044	0.00000000	-0.38219087	H	1.01683743	0.00000000	-0.38486802
H	-0.56802896	0.84058499	-0.39014216	H	-0.55193887	0.85405463	-0.38219087	H	-0.55718534	0.85058971	-0.38486802
Cl	-0.81300034	-1.53061085	-0.55839644	Cl	-0.81461320	-1.49636904	-0.56408018	Cl	-0.81430307	-1.50687408	-0.56246966

[*Pi*-Ni···MeCl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.83745025	C	0.00000000	0.00000000	4.84335344	C	0.00000000	0.00000000	4.81225957
C	4.87737463	0.00000000	4.83536599	C	4.84376218	0.00000000	4.84343269	C	4.86304421	0.00000000	4.74896529
C	4.87353140	-0.19094956	0.00195431	C	4.84354806	0.00595378	0.00069586	C	4.72778382	-1.13734409	0.07555433
C	3.53427934	-0.15317880	-0.42161166	C	3.51859075	0.00608977	-0.43579962	C	3.41206294	-0.90725023	-0.36509937
C	3.12787882	-0.16100200	-1.78385743	C	3.10504473	-0.01476579	-1.81576455	C	3.00333181	-0.97659893	-1.71798884
C	1.74458578	-0.09638268	-1.78474216	C	1.73935423	-0.01638154	-1.81625085	C	1.67585847	-0.59309628	-1.74696993
C	1.33894462	-0.05419163	-0.42280682	C	1.32493404	0.00416779	-0.43655381	C	1.30631779	-0.32380166	-0.40799776
N	2.43673866	-0.08910603	0.42244440	N	2.42154837	0.01978206	0.39246725	N	2.37172752	-0.50996097	0.44619246
C	-0.38969544	0.01389726	1.31632582	C	-0.43676754	0.00605168	1.32490036	C	-0.38014001	0.08266646	1.30878752
C	-1.77528374	0.04086556	1.73996027	C	-1.81679863	-0.00400531	1.73879388	C	-1.75897660	0.23575316	1.73192239
C	-1.77552853	0.02790948	3.09764215	C	-1.81686004	-0.00457064	3.10451240	C	-1.76740409	0.16280386	3.07944796
C	-0.39001483	0.00050788	3.52120191	C	-0.43695168	0.00572257	3.51855356	C	-0.38854755	0.01012599	3.50315656
N	0.45400568	-0.00975824	2.41865935	N	0.39188004	0.01441695	2.42182170	N	0.44998391	-0.04506098	2.40637501
C	1.33996911	0.00414617	5.26042677	C	1.32492480	0.00193275	5.27983760	C	1.34562400	0.01790847	5.22138888
C	1.74706548	0.03196552	6.62211751	C	1.73912393	-0.01353142	6.65966521	C	1.76490678	0.17563725	6.56366221
C	3.13190629	0.04239042	6.62121307	C	3.10478872	-0.01462472	6.65941026	C	3.14514024	0.23808185	6.53873325
C	3.53765780	0.01630209	5.25888196	C	3.51857307	0.00010980	5.27931896	C	3.52903443	0.09387752	5.18443516
N	2.43844553	-0.00592417	4.41509082	N	2.42166647	0.01151608	4.45082000	N	2.42625420	-0.03672465	4.36860892
C	5.26641189	-0.05377704	3.51994366	C	5.28114743	0.01170889	3.51883362	C	5.21596847	-0.31146212	3.46728935
C	6.65164467	-0.09801882	3.09670922	C	6.66105142	-0.00319559	3.10475317	C	6.58006303	-0.58958150	3.06002170
C	6.65045760	-0.16234330	1.74048978	C	6.66083215	-0.00069209	1.73901759	C	6.53313689	-0.97804750	1.76859180
C	5.26465109	-0.15167442	1.31726931	C	5.28084998	0.01472568	1.32533205	C	5.14534544	-0.89932546	1.35372182
N	4.42172115	-0.08628768	2.41864305	N	4.45244594	0.02619358	2.42219096	N	4.34908866	-0.49299515	2.40668639
Ni	2.43769918	-0.04948318	2.41893514	Ni	2.42137697	0.02812622	2.42197532	Ni	2.39994419	-0.26397146	2.40606920
H	-0.77147419	0.02086610	-0.76351647	H	-0.76920424	-0.01162459	-0.76927682	H	-0.75908919	0.11532603	-0.76730767
H	-0.77177876	0.00935786	5.60083902	H	-0.76910632	-0.00815936	5.61274356	H	-0.76587304	0.05133681	5.57971732
H	5.64953791	0.01956151	5.59821489	H	5.61244694	-0.01258283	5.61320040	H	5.64886672	0.11005582	5.48971592
H	5.64434412	-0.24112186	-0.76083264	H	5.61246759	-0.00766011	-0.76881589	H	5.46299597	-1.45066328	-0.65908699
H	-2.61886807	0.03928017	3.77771638	H	-2.66674309	-0.01255986	3.77766269	H	-2.60887498	0.22310413	3.75871228
H	-2.61843158	0.06334859	1.05999159	H	-2.66655651	-0.01173083	1.06549569	H	-2.59296377	0.36002717	1.05218250
H	1.06733218	-0.08181115	-2.63016716	H	1.06644233	-0.03155834	-2.66620922	H	1.00999811	-0.52108733	-2.59820127
H	3.80461974	-0.20569489	-2.62861633	H	3.77854272	-0.02852838	-2.66529140	H	3.64408164	-1.26163693	-2.54338886
H	7.49306738	-0.21009592	1.06109931	H	3.77820654	-0.02544979	7.50904049	H	3.83330121	0.35180800	7.36735470
H	7.49552975	-0.08294096	3.77597024	H	1.06606651	-0.02341533	7.50959968	H	1.09875834	0.24721683	7.41469171
H	3.80995882	0.06255378	7.46587892	H	7.51053160	-0.01155330	1.06568253	H	7.34572870	-1.27905849	1.11880458
H	1.06996566	0.04496316	7.46767008	H	7.51092364	-0.01615713	3.77782135	H	7.43865216	-0.50836842	3.71523425
C	2.21129653	-3.57715160	2.13576863	C	2.32408760	-3.10818374	2.48464966	C	2.84663878	-3.42638023	3.06050173
H	3.18689256	-3.22764788	1.81425711	H	3.32486551	-2.69705866	2.58630620	H	3.07621674	-3.25610065	2.01247901
H	2.01484074	-3.30566742	3.16798768	H	1.69790032	-2.82546923	3.32592098	H	3.62573946	-3.02522850	3.70146588
H	1.42578599	-3.22135165	1.47750819	H	1.87325185	-2.80970236	1.54250561	H	1.87604554	-3.01282740	3.31954299
Cl	2.22167685	-5.40267128	2.03912909	Cl	2.46190215	-4.91597977	2.48318780	Cl	2.77445620	-5.21537386	3.32892766

[*Pi*-Ni—Me—Cl]$^{‡-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85705400	C	0.00000000	0.00000000	4.84166717	C	0.00000000	0.00000000	4.83742923
C	4.85775114	0.00000000	4.85713573	C	4.84215125	0.00000000	4.84148976	C	4.83773847	0.00000000	4.83734827
C	4.85775115	0.00000000	-0.00008027	C	4.84214926	0.00008892	0.00018362	C	4.83774044	0.00000000	0.00006304
C	3.52852063	-0.00289572	-0.43847158	C	3.51710261	0.00087158	-0.43737767	C	3.51246859	0.00542790	-0.43435846
C	3.11197498	0.00737820	-1.82903359	C	3.10364377	-0.00627445	-1.81848086	C	3.09897625	-0.00430385	-1.82306374
C	1.74548334	0.00611391	-1.82873801	C	1.73884109	-0.00443533	-1.81880122	C	1.73882616	-0.00475194	-1.82290783
C	1.32936262	-0.00506904	-0.43797247	C	1.32490164	0.00342116	-0.43792974	C	1.32547283	0.00420884	-0.43410795
N	2.42888262	-0.01214087	0.38153070	N	2.42102088	0.00877632	0.38735187	N	2.41884190	0.01287914	0.38137690
C	-0.43885594	0.00546634	1.32898206	C	-0.43844867	0.00669108	1.32475308	C	-0.43444663	0.00696244	1.32519630
C	-1.82932924	0.02792400	1.74524496	C	-1.81950305	0.00287032	1.73842132	C	-1.82316479	0.00315487	1.73862224
C	-1.82932978	0.02792846	3.11180896	C	-1.81950494	0.00289294	3.10324537	C	-1.82316405	0.00318503	3.09880631
C	-0.43885596	0.00546634	3.52807208	C	-0.43845150	0.00670709	3.51691516	C	-0.43444601	0.00697366	3.51223347
N	0.38098145	-0.00819245	2.42852690	N	0.38642035	0.01191740	2.42083451	N	0.38147354	0.01130726	2.41871405
C	1.32936194	-0.00508309	5.29502651	C	1.32490240	0.00339020	5.27959245	C	1.32547369	0.00415660	5.27153038
C	1.74548266	0.00611811	6.68579299	C	1.73883788	-0.00458957	6.66046505	C	1.73883404	-0.00488884	6.66032854
C	3.11197430	0.00736897	6.68608842	C	3.10364049	-0.00645954	6.66014840	C	3.09898410	-0.00447445	6.66047064
C	3.52852100	-0.00289660	5.29552741	C	3.51710326	0.00079588	5.27904851	C	3.51246425	0.00542898	5.27176382

N	2.42888288	-0.01218221	4.47552465	N	2.42102199	0.00879261	4.45431502	N	2.41883331	0.01284832	4.45603525
C	5.29673147	0.00416040	3.52805942	C	5.28060758	0.01070589	3.51685576	C	5.27259918	0.00740086	3.51213288
C	6.68739893	0.01788563	3.11180260	C	6.66157410	0.01081561	3.10326766	C	6.66143689	-0.00263846	3.09878923
C	6.68739846	0.01788828	1.74525360	C	6.66157297	0.01084200	1.73840562	C	6.66143216	-0.00264531	1.73862216
C	5.29673155	0.00416043	1.32899642	C	5.28060641	0.01074685	1.32481969	C	5.27259472	0.00740017	1.32528276
N	4.47706882	-0.00377798	2.42852814	N	4.45543687	0.01422046	2.42083841	N	4.45726758	0.01675169	2.41870886
Ni	2.43073550	-0.09568009	2.42852664	Ni	2.41889945	-0.04655220	2.42084125	Ni	2.42193848	-0.06007268	2.41871784
H	-0.76820187	0.00807348	-0.76895160	H	-0.76895721	-0.00676259	-0.76930835	H	-0.76839512	-0.00815207	-0.76870589
H	-0.76820163	0.00809020	5.62600543	H	-0.76895370	-0.00678764	5.61097888	H	-0.76839917	-0.00814612	5.60613232
H	5.62613332	0.00581582	5.62594797	H	5.61091876	-0.00716251	5.61096687	H	5.60613658	-0.01024046	5.60603722
H	5.62613417	0.00580978	-0.76889203	H	5.61091922	-0.00701147	-0.76929232	H	5.60614936	-0.01021200	-0.76861604
H	-2.67958468	0.04411127	3.78343900	H	-2.66897720	0.00029398	3.77657150	H	-2.67207270	0.00096638	3.77170045
H	-2.67958466	0.04410296	1.07361499	H	-2.66897428	0.00027250	1.06509341	H	-2.67207226	0.00091927	1.06572631
H	1.07366350	0.01487988	-2.67894943	H	1.06566943	-0.00783766	-2.66839002	H	1.06582707	-0.01083897	-2.67171350
H	3.78347043	0.01728737	-2.67948663	H	3.77717570	-0.01126045	-2.66777812	H	3.77184508	-0.00974095	-2.67197529
H	3.78346972	0.01728600	7.53654239	H	3.77716872	-0.01153803	7.50944817	H	3.77185883	-0.00999364	7.50937712
H	1.07366177	0.01490616	7.53600358	H	1.06566258	-0.00805852	7.51005128	H	1.06583886	-0.01101700	7.50913593
H	7.53774483	0.02769935	1.07361589	H	7.51105608	0.01068296	1.06508584	H	7.51027763	-0.00935611	1.06568260
H	7.53774480	0.02769551	3.78344090	H	7.51105819	0.01063744	3.77658592	H	7.51028416	-0.00935651	3.77172574
C	2.47662557	-2.60969964	2.42848725	C	2.35723661	-2.52968239	2.42098150	C	2.50658014	-2.47788890	2.41839049
H	3.00949904	-2.49392682	1.50220047	H	3.42802323	-2.40805588	2.42089726	H	3.04075852	-2.36919004	1.48965280
H	3.00949856	-2.49394295	3.35477647	H	1.82397121	-2.39325513	3.34684105	H	3.04104258	-2.36925665	3.34697291
H	1.40643050	-2.50402189	2.42848888	H	1.82381800	-2.39329288	1.49520599	H	1.43220351	-2.39874629	2.41855108
Cl	2.49395902	-4.82646296	2.42847178	Cl	2.33642578	-4.72043697	2.42103436	Cl	2.54777443	-4.68389323	2.41831914

[*Pi*-Ni-Me···Cl]⁻

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85339895	C	0.00000000	0.00000000	4.83849578	C	0.00000000	0.00000000	4.83392307
C	4.85364550	0.00000000	4.85310167	C	4.83847843	0.00000000	4.83674476	C	4.83406162	0.00000000	4.83417748
C	4.85365448	0.00026915	0.00032620	C	4.83792449	0.02033014	-0.00118204	C	4.83380831	0.00351218	0.00020692
C	3.52662809	0.00296159	-0.43304131	C	3.51455667	0.02651232	-0.43579164	C	3.51034161	0.01259424	-0.42852539
C	3.10983935	-0.00233379	-1.81969321	C	3.10041072	0.00953592	-1.81443949	C	3.09688926	-0.00118209	-1.81318821
C	1.74407743	-0.00154791	-1.81983366	C	1.73663137	0.00365954	-1.81410839	C	1.73722008	-0.00198480	-1.81337029
C	1.32715064	0.00432715	-0.43325628	C	1.32309885	0.01753765	-0.43527242	C	1.32338173	0.01009347	-0.42875013
N	2.42700885	0.01534210	0.38989028	N	2.41912456	0.04442505	0.38949645	N	2.41657313	0.02703633	0.39064641
C	-0.43452663	0.00540173	1.32670074	C	-0.43575462	0.00552784	1.32308671	C	-0.42834101	0.00694868	1.32348752
C	-1.82100963	0.00211110	1.74376564	C	-1.81418184	-0.01928040	1.73732208	C	-1.81300011	-0.01003913	1.73710671
C	-1.82100248	0.00206524	3.10963824	C	-1.81424424	-0.01699574	3.10120318	C	-1.81314522	-0.00877423	3.09672569
C	-0.43451589	0.00535810	3.52669187	C	-0.43586327	0.00838643	3.51542383	C	-0.42860476	0.00849922	3.51041181
N	0.38800991	0.01616091	2.42669388	N	0.38821782	0.03585993	2.41911764	N	0.39080427	0.02558242	2.41688754
C	1.32714579	0.00423409	5.28666945	C	1.32321419	0.00907106	5.27390480	C	1.32304010	0.00976517	5.26371356
C	1.74406850	-0.00136807	6.67325068	C	1.73794272	-0.01624729	6.65213122	C	1.73707150	-0.01370688	6.64797894
C	3.10982994	-0.00229048	6.67310538	C	3.10182592	-0.01864986	6.65155755	C	3.09678083	-0.01459139	6.64797249
C	3.52661052	0.00266875	5.28644680	C	3.51555031	0.00616674	5.27297955	C	3.51080896	0.00967884	5.26369799
N	2.42700431	0.01491965	4.46351459	N	2.41921279	0.03674134	4.44940617	N	2.41676036	0.03425849	4.44532320
C	5.28697596	0.00735995	3.52609755	C	5.27328750	0.01707263	3.51349060	C	5.26392635	0.01101416	3.51098720
C	6.67381861	0.00629763	3.10958165	C	6.65197185	0.00255890	3.09946033	C	6.64831046	-0.00982066	3.09689620
C	6.67382075	0.00643173	1.74385288	C	6.65182371	0.00847610	1.73568263	C	6.64812370	-0.01000491	1.73715404
C	5.28698009	0.00753185	1.32733717	C	5.27303309	0.02607209	1.32202131	C	5.26370653	0.01086330	1.32324976
N	4.46354559	0.01611140	2.42671727	N	4.44815076	0.04424721	2.41775356	N	4.44551613	0.03335700	2.41708658
Ni	2.42077291	-0.15909459	2.42663323	Ni	2.41562697	-0.11632969	2.42204971	Ni	2.42171887	-0.12148879	2.42265428
H	-0.76778472	-0.00951001	-0.76852648	H	-0.76837564	-0.02456998	-0.76858999	H	-0.76816556	-0.01726381	-0.76787034
H	-0.76779803	-0.00934423	5.62191299	H	-0.76835570	-0.02386908	5.60711806	H	-0.76821618	-0.02057216	5.60165865
H	5.62171832	-0.00919440	5.62133904	H	5.60733023	-0.02484418	5.60484709	H	5.60190924	-0.02282465	5.60223223
H	5.62173722	-0.00896095	-0.76790120	H	5.60636020	0.00357530	-0.76991386	H	5.60144214	-0.01460930	-0.76813532
H	-2.66936714	0.00143832	3.78308254	H	-2.66162655	-0.03132380	3.77607006	H	-2.65982568	-0.01961828	3.77165692
H	-2.66938045	0.00148760	1.07032645	H	-2.66153368	-0.03567151	1.06245858	H	-2.65965987	-0.02147708	1.06219567
H	1.07058849	-0.00299220	-2.66817105	H	1.06149800	-0.00868362	-2.66133309	H	1.06253057	-0.01123651	-2.66026133
H	3.78346487	-0.00471241	-2.66792185	H	3.77520303	0.00274773	-2.66200002	H	3.77174216	-0.00886175	-2.65995518
H	7.52205533	0.00706063	1.07021063	H	3.77699368	-0.03522363	7.49866501	H	3.77148049	-0.03071069	7.49473400
H	7.52204930	0.00683889	3.78322906	H	1.06340167	-0.03068948	7.49977229	H	1.06248023	-0.02985964	7.49480829
H	3.78345711	-0.00449779	7.52133356	H	7.49913346	0.00129618	1.06058060	H	7.49468777	-0.02392890	1.06214818
H	1.07057664	-0.00251563	7.52158586	H	7.49942515	-0.01019190	3.77430294	H	7.49510828	-0.02378018	3.77156222
C	2.34933401	-2.14308552	2.42584862	C	2.36228461	-2.07539259	2.47590036	C	2.49051235	-2.11522336	2.49319922
H	3.38973676	-2.45289159	2.42435380	H	3.36581268	-2.38532243	2.75682619	H	2.80420852	-2.40465085	1.49480420
H	1.81911221	-2.41140373	3.33391820	H	1.61406118	-2.32372481	3.22415721	H	3.21644722	-2.34143603	3.26785690
H	1.81673086	-2.41089555	1.51901793	H	2.08156997	-2.38530933	1.47232077	H	1.47346629	-2.40397778	2.74042086
Cl	2.10829082	-6.27409443	2.43318790	Cl	2.22406642	-5.82740529	2.60642164	Cl	2.60844969	-5.87024225	2.58113436

[*Pi*-Ni-Me]

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85349468	C	0.00000000	0.00000000	4.83816696	C	0.00000000	0.00000000	4.83367428
C	4.85369908	0.00000000	4.85385200	C	4.83841732	0.00000000	4.83616766	C	4.83387314	0.00000000	4.83370366
C	4.85353251	0.00797955	0.00094627	C	4.83795788	0.01429307	-0.00134519	C	4.83360932	0.00320636	-0.00009525
C	3.52652509	0.00774297	-0.43235984	C	3.51462721	0.02044213	-0.43559143	C	3.51020689	0.01199478	-0.42860631
C	3.11008060	0.00749158	-1.81910514	C	3.10032047	0.00345903	-1.81404487	C	3.09664185	-0.00157346	-1.81310527
C	1.74432518	0.00650441	-1.81958034	C	1.73659389	-0.00053246	-1.81361086	C	1.73701053	-0.00243795	-1.81316412
C	1.32713768	0.00610912	-0.43310333	C	1.32312058	0.01463046	-0.43491335	C	1.32325897	0.00943202	-0.42865044
N	2.42680700	0.01453516	0.39057857	N	2.41923823	0.04046760	0.39008092	N	2.41650178	0.02629655	0.39098461
C	-0.43427190	0.00481432	1.32675388	C	-0.43569532	0.00653322	1.32294188	C	-0.42816340	0.00709876	1.32340597
C	-1.82071616	0.00005177	1.74380168	C	-1.81406314	-0.01479462	1.73718355	C	-1.81272391	-0.00796970	1.73698519

C	-1.82080292	0.00121977	3.10968707
C	-0.43441614	0.00605108	3.52680108
N	0.38833280	0.01744854	2.42679223
C	1.32700300	0.00411904	5.28702992
C	1.74379414	-0.00343237	6.67356418
C	3.10957892	-0.00534894	6.67364418
C	3.52669793	0.00153812	5.28716345
N	2.42708459	0.01568904	4.46400806
C	5.28681214	0.00932538	3.52679885
C	6.67355801	0.01552203	3.11019140
C	6.67348603	0.01790117	1.74446416
C	5.28671679	0.01313562	1.32793093
N	4.46312453	0.01529137	2.42738598
Ni	2.42045235	-0.16090193	2.42875430
H	-0.76785264	-0.00818290	-0.76844568
H	-0.76786058	-0.00975785	5.62191188
H	5.62181091	-0.00785730	5.62202991
H	5.62163885	0.00529738	-0.76725096
H	-2.66913821	0.00080100	3.78315695
H	-2.66897123	-0.00093434	1.07022075
H	1.07095666	0.00904783	-2.66800868
H	3.78397309	0.01142127	-2.66710768
H	7.52159692	0.02551514	1.07072808
H	7.52172090	0.02038520	3.78389325
H	3.78310715	-0.00810595	7.52194287
H	1.07014752	-0.00468816	7.52176588
C	2.34244558	-2.14189074	2.44908123
H	3.37920317	-2.45897359	2.51111201
H	1.76032078	-2.39940392	3.32833916
H	1.86023718	-2.41853395	1.51661094

C	-1.81411526	-0.01348531	3.10104182
C	-0.43582540	0.00859630	3.51524710
N	0.38867420	0.03455014	2.41897446
C	1.32311250	0.00894646	5.27333629
C	1.73808654	-0.01709942	6.65131582
C	3.10193216	-0.01861930	6.65054097
C	3.51551948	0.00675885	5.27205808
N	2.41898061	0.03777441	4.44823501
C	5.27329315	0.01643319	3.51304953
C	6.65186847	-0.00117437	3.09909528
C	6.65176310	0.00328332	1.73536135
C	5.27312314	0.02266643	1.32166325
N	4.44801049	0.04456839	2.41735881
Ni	2.41604609	-0.11981533	2.42177308
H	-0.76828990	-0.02187059	-0.76870605
H	-0.76828021	-0.02249446	5.60684172
H	5.60709786	-0.02485731	5.60439437
H	5.60620744	-0.00401524	-0.77019702
H	-2.66143174	-0.02479681	3.77601129
H	-2.66136564	-0.02746773	1.06222478
H	1.06126210	-0.01058402	-2.66067186
H	3.77512823	-0.00308170	-2.66155418
H	3.77732468	-0.03437252	7.49745417
H	1.06362443	-0.03128916	7.49899400
H	7.49892782	-0.00529826	1.06014244
H	7.49915975	-0.01366030	3.77409748
C	2.37485762	-2.07556302	2.47152377
H	3.38974109	-2.38072439	2.71485563
H	1.65754454	-2.33818522	3.24425707
H	2.06202699	-2.38606272	1.47744267

C	-1.81289635	-0.00717984	3.09657642
C	-0.42847394	0.00845360	3.51028572
N	0.39131992	0.02466008	2.41680364
C	1.32297593	0.00925491	5.26321435
C	1.73706693	-0.01292952	6.64734236
C	3.09676209	-0.01355940	6.64728889
C	3.51072974	0.00953622	5.26312055
N	2.41665075	0.03324301	4.44446053
C	5.26356598	0.01069967	3.51061055
C	6.64780172	-0.00989010	3.09650813
C	6.64765642	-0.00965913	1.73678032
C	5.26339347	0.01069933	1.32285017
N	4.44483976	0.03292315	2.41668103
Ni	2.42176729	-0.12168373	2.42231503
H	-0.76819784	-0.01570003	-0.76784224
H	-0.76817837	-0.01887439	5.60147343
H	5.60174957	-0.02135538	5.60174968
H	5.60121248	-0.01378714	-0.76847760
H	-2.65952584	-0.01599083	3.77158481
H	-2.65930661	-0.01698320	1.06195345
H	1.06214092	-0.01041274	-2.65991078
H	3.77153313	-0.00789400	-2.65983460
H	3.77159182	-0.02759200	7.49397492
H	1.06239187	-0.02728816	7.49412649
H	7.49418298	-0.02199366	1.06171487
H	7.49454450	-0.02260376	3.77126057
C	2.49291746	-2.10860232	2.49128595
H	2.81495079	-2.40155920	1.49601335
H	3.21276843	-2.33783018	3.27143363
H	1.47525917	-2.40410557	2.73030352

S.IX.2 Nickel chlorin (*Ch*) complexes

B3LYP/6-311+G(d,p)				M06-L/6-311+G(d,p)				ωB97X-D/6-311+G(d,p)			
[*Ch*-Ni]											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84871371	C	0.00000000	0.00000000	4.83297772	C	0.00000000	0.00000000	4.83927233
C	4.83659396	0.00000000	4.70785091	C	4.82284212	0.00000000	4.67617242	C	4.81331965	0.00000000	4.64588771
C	4.59934689	-1.49630177	0.13878550	C	4.54931412	1.60181645	0.15711647	C	4.48875295	-1.73672974	0.19009056
C	3.31870542	-1.14914605	-0.30561820	C	3.27930767	1.24360347	-0.29417906	C	3.22932447	-1.32537624	-0.26520902
C	2.91127277	-1.19671230	-1.68751661	C	2.86914982	1.30494346	-1.66532193	C	2.82941745	-1.37258443	-1.64963241
C	1.64081595	-0.70018905	-1.73904417	C	1.61516163	0.77192462	-1.72409021	C	1.60153400	-0.79833689	-1.71888210
C	1.26261578	-0.39096234	-0.38551386	C	1.24995857	0.43100001	-0.38354408	C	1.23436950	-0.44702157	-0.37340381
N	2.31546580	-0.66139861	0.48271361	N	2.29050236	0.71562281	0.48714257	N	2.26589635	-0.76907516	0.50301033
C	-0.40447742	0.10454383	1.32974688	C	-0.40110434	-0.12014718	1.32372790	C	-0.40773819	0.12284139	1.33255191
C	-1.76137456	0.31307737	1.74013751	C	-1.74861085	-0.35038633	1.73453409	C	-1.75052590	0.36143151	1.73514233
C	-1.77330051	0.23808701	3.10843736	C	-1.76354332	-0.26491846	3.09817357	C	-1.76622684	0.27656492	3.10408613
C	-0.41784912	0.02090864	3.51906370	C	-0.41738577	-0.02704832	3.50910360	C	-0.42625270	0.02310940	3.50685024
N	0.41768016	-0.06828372	2.42448146	N	0.41757184	0.06949915	2.41643402	N	0.40408696	-0.07842486	2.41978622
C	1.32195353	-0.01493551	5.23359624	C	1.32190963	0.01545283	5.21726811	C	1.31313083	-0.01990446	5.21139470
C	1.77773419	0.16682320	6.58628500	C	1.77942796	-0.17786477	6.55887063	C	1.78354020	0.18896110	6.55450401
C	3.13959970	0.24352260	6.53433810	C	3.13926582	-0.26479878	6.50056982	C	3.13576147	0.28152318	6.48331033
C	3.51178073	0.06686513	5.15302685	C	3.50586070	-0.07742815	5.12858091	C	3.49080577	0.07882091	5.10060454
N	2.40646240	-0.08766312	4.36538049	N	2.39804075	0.08945197	4.34646163	N	2.39074992	-0.09894938	4.33485295
C	5.19709733	-0.38413996	3.44332146	C	5.17512027	0.41518360	3.42123111	C	5.14319341	-0.45654324	3.40456404
C	6.63750363	-0.56977136	3.02258624	C	6.59834237	0.62932859	2.99901008	C	6.56608198	-0.70159537	2.97410729
C	6.49061706	-1.50520031	1.82207050	C	6.43730478	1.58248366	1.82923758	C	6.37254870	-1.73068040	1.86722264
C	5.06153738	-1.24223801	1.40316474	C	5.02102064	1.32101000	1.41016970	C	4.95897895	-1.43957916	1.43447633
N	4.33055881	-0.68780983	2.42365846	N	4.29973251	0.73344349	2.41608484	N	4.25549727	-0.79912359	2.41993604
Ni	2.36451813	-0.37622304	2.42418368	Ni	2.35005522	0.40175376	2.41647754	Ni	2.32784972	-0.43656121	2.41953005
H	-0.74414088	0.16601669	-0.77254889	H	-0.74055727	-0.17724974	-0.77402588	H	-0.73339033	0.19715329	-0.77568150
H	-0.75868030	0.07223844	5.62150524	H	-0.75751863	-0.07841609	5.60692970	H	-0.75462304	0.08159478	5.61532453
H	5.62300096	0.18725844	5.43130568	H	5.61577374	-0.19503515	5.39100140	H	5.60954683	0.21311899	5.35039615
H	5.28892518	-1.91624975	-0.58586840	H	5.23299944	2.04822537	-0.55776714	H	5.15399706	-2.22103132	-0.51611566
H	0.99522494	-0.57265643	-2.59907876	H	-2.59832408	-0.37591919	3.77910521	H	-2.60232385	0.39591353	3.78131126
H	3.53582954	-1.55095425	-2.49794376	H	-2.57203231	-0.52642006	1.05350350	H	-2.57418154	0.54745735	1.05775785
H	-2.61132203	0.33992883	3.78660658	H	0.96956207	0.64097720	-2.58368613	H	0.97135712	-0.64285694	-2.58537204
H	-2.58994395	0.47326329	1.06166579	H	3.48389565	1.69086537	-2.46898579	H	3.43568603	-1.78029081	-2.44814188
H	7.19979043	-1.31924691	1.01262527	H	7.14454730	1.42879943	1.01191611	H	6.42441829	-2.75048236	2.26806398
H	7.05439077	0.39967153	2.71701413	H	7.02895484	-0.32650123	2.67305592	H	7.19541751	-1.03496566	3.80039948
H	3.84338335	0.38854303	7.34427630	H	3.84726991	-0.42118321	7.30494766	H	3.84884879	0.45049718	7.27976246
H	1.12482206	0.24927529	7.44629522	H	1.12680441	-0.26509515	7.41872219	H	1.14061871	0.27969063	7.42083430
H	6.59356602	-2.55558343	2.12689324	H	6.53379917	2.62667610	2.15423651	H	7.08177979	-1.64986671	1.04237612
H	7.25719296	-0.96255870	3.83144005	H	7.21882561	1.00506715	3.81488418	H	6.98671154	0.22925840	2.57389615
[*Ch*-Ni]$^-$											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84777964	C	0.00000000	0.00000000	4.85018628	C	0.00000000	0.00000000	4.82236725
C	4.88096512	0.00000000	4.71270244	C	4.84824955	0.00000000	4.83964729	C	4.86187583	0.00000000	4.59760602
C	4.65087917	-1.47247713	0.13272884	C	4.84690267	0.11783891	0.01204943	C	4.47010408	-1.91273774	0.22133121
C	3.35696795	-1.12857033	-0.33647511	C	3.51114644	0.08042962	-0.43189114	C	3.21435427	-1.46337274	-0.27354720
C	2.95387390	-1.17310792	-1.70003823	C	3.10413732	0.08002842	-1.81028139	C	2.82054891	-1.51204963	-1.63211493
C	1.65634335	-0.68564642	-1.74795670	C	1.73446768	0.04439318	-1.81528260	C	1.58553721	-0.89116836	-1.70803565
C	1.28322375	-0.38616359	-0.40829840	C	1.31936746	0.02590698	-0.44070627	C	1.24379115	-0.50870131	-0.38912065
N	2.34063388	-0.64823601	0.45688259	N	2.42307967	0.04632737	0.39010714	N	2.25879380	-0.85300306	0.49039563
C	-0.39639148	0.09557648	1.31996778	C	-0.43393087	-0.00746877	1.32775634	C	-0.38879267	0.13035455	1.31390745
C	-1.75536952	0.33599732	1.74331700	C	-1.80973871	-0.02108874	1.74079923	C	-1.74112968	0.40368244	1.73433827
C	-1.76779938	0.26469110	3.10587743	C	-1.80974085	-0.01908813	3.10939086	C	-1.76139076	0.30473441	3.08801062
C	-0.40912617	0.02203186	3.52857744	C	-0.43393099	-0.00539202	3.52240637	C	-0.40994710	0.02756269	3.50862953
N	0.42239889	-0.09635963	2.42406675	N	0.39875811	0.00129738	2.42507225	N	0.41829214	-0.08790177	2.41125859
C	1.34067844	-0.01703827	5.25420080	C	1.31945730	0.00825773	5.29132076	C	1.34398133	-0.01544102	5.21037705
C	1.78758678	0.14411833	6.59417276	C	1.73439075	0.00189777	6.66604295	C	1.80989062	0.21603471	6.52652678
C	3.17302779	0.19833403	6.54846853	C	3.10451347	0.00128566	6.66154946	C	3.18901397	0.30467071	6.44807877
C	3.54296551	0.04932629	5.18365885	C	3.51188301	0.00848438	5.28328635	C	3.53107972	0.09137185	5.09113475
N	2.42859778	-0.08515632	4.38765854	N	2.42362117	0.01482337	4.46088542	N	2.41197579	-0.10308568	4.33030224
C	5.23365720	-0.34894595	3.44538453	C	5.29324696	0.01351260	3.53580375	C	5.16272648	-0.49461087	3.37384530
C	6.67161550	-0.52596296	3.00300812	C	6.75821155	-0.04798131	3.17709944	C	6.57290025	-0.77066326	2.91079408
C	6.51041467	-1.52015705	1.85084243	C	6.75612504	0.19652367	1.67422452	C	6.33547376	-1.90826873	1.92177057
C	5.09684483	-1.22219159	1.39441609	C	5.29215430	0.11141361	1.31584344	C	4.93705673	-1.59053539	1.45015666
N	4.36094242	-0.63606403	2.40990651	N	4.49344349	0.05532772	2.42590602	N	4.24885342	-0.87669603	2.41204049
Ni	2.38610734	-0.36787462	2.42546011	Ni	2.44034795	0.02924937	2.42553619	Ni	2.33523998	-0.48072754	2.41104542
H	-0.74747395	0.16844823	-0.76972253	H	-0.77282765	-0.01011749	-0.76614848	H	-0.73147293	0.20759839	-0.77526023
H	-0.76053221	0.08798163	5.61810509	H	-0.77302171	-0.00609073	5.61619020	H	-0.75393745	0.09728316	5.59780013
H	5.67094644	0.17879707	5.43596943	H	5.61254803	-0.02585552	5.61381224	H	5.67211212	0.24107413	5.27848709
H	5.34100894	-1.91222383	-0.58114898	H	5.61057177	0.15939741	-0.76203493	H	5.11829689	-2.45425665	-0.46043257
H	1.00720922	-0.57943906	-2.60915182	H	1.06438213	0.03434099	-2.66773126	H	-2.59818828	0.43291315	3.76374348
H	3.57981280	-1.50472698	-2.52002484	H	3.77902205	0.10439660	-2.65879095	H	-2.56114829	0.61386169	1.05860632
H	-2.60567540	0.38889281	3.78170116	H	-2.65985148	-0.02576596	3.78257731	H	0.95781358	-0.74124384	-2.57824224
H	-2.58339707	0.51754662	1.06836275	H	-2.65982863	-0.03026599	1.06761644	H	3.40915917	-1.94240535	-2.43315688

H	7.24148645	-1.40709664	1.04649643	H	7.35590022	-0.52470103	1.11117061	H	6.34294745	-2.87420061	2.44316422
H	7.06815532	0.42976297	2.63163845	H	7.16412854	-1.03503846	3.43029103	H	7.24175917	-1.01845682	3.73710661
H	3.86991870	0.32481100	7.36845801	H	3.77950634	-0.00494161	7.51029299	H	3.89986237	0.47744221	7.24694165
H	1.13749809	0.22390345	7.45743132	H	1.06395750	-0.00407307	7.51825746	H	1.17466321	0.33240749	7.39640792
H	6.57367763	-2.55226752	2.22364617	H	7.14685422	1.18953006	1.42048795	H	7.05296411	-1.95415285	1.10037068
H	7.31988396	-0.86871969	3.81306359	H	7.34703690	0.68205472	3.74031522	H	6.97457229	0.10931795	2.39201888

MeCl

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08694599	H	0.00000000	0.00000000	1.08633125	H	0.00000000	0.00000000	1.08723601
H	1.01451467	0.00000000	-0.39014216	H	1.01688044	0.00000000	-0.38219087	H	1.01683743	0.00000000	-0.38486802
H	-0.56802896	0.84058499	-0.39014216	H	-0.55193887	0.85405463	-0.38219087	H	-0.55718534	0.85058971	-0.38486802
Cl	-0.81300034	-1.53061085	-0.55839644	Cl	-0.81461320	-1.49636904	-0.56408018	Cl	-0.81430307	-1.50687408	-0.56246966

[*Ch*-Ni···MeCl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84699866	C	0.00000000	0.00000000	4.84995743	C	0.00000000	0.00000000	4.82175296
C	4.87869674	0.00000000	4.66385716	C	4.84859629	0.00000000	4.83919540	C	4.86124644	0.00000000	4.59095070
C	4.55942274	-1.72931277	0.18193597	C	4.84712912	0.12057258	0.01236156	C	4.43377416	-1.98929735	0.25215012
C	3.28462839	-1.33371175	-0.30175239	C	3.51100394	0.08272634	-0.43128713	C	3.18473234	-1.52882790	-0.25050367
C	2.87946194	-1.39317864	-1.66391502	C	3.10490383	0.06191584	-1.81010259	C	2.78160331	-1.60917158	-1.60553129
C	1.61601895	-0.82327679	-1.72922132	C	1.73526680	0.02757038	-1.81543676	C	1.56052971	-0.96288141	-1.69325112
C	1.26126237	-0.46295147	-0.39963579	C	1.31947052	0.02954073	-0.44073338	C	1.23532658	-0.53332547	-0.38416508
N	2.29965019	-0.76814819	0.47417789	N	2.42265438	0.06368675	0.38999046	N	2.24784479	-0.87511299	0.49882350
C	-0.39418741	0.11826957	1.31931611	C	-0.43485970	-0.00116485	1.32776616	C	-0.38597610	0.15151472	1.31300551
C	-1.74651879	0.39334874	1.74351270	C	-1.81070188	-0.02897065	1.74064587	C	-1.74211438	0.40845588	1.73247296
C	-1.76420307	0.30445324	3.10527155	C	-1.81078742	-0.02631180	3.10929268	C	-1.76347221	0.30157667	3.08580641
C	-0.41217915	0.02598070	3.52827230	C	-0.43497920	0.00160552	3.52220237	C	-0.40898717	0.03992831	3.50735912
N	0.41643868	-0.10353627	2.42342768	N	0.39712835	0.01942310	2.42501841	N	0.42211988	-0.05523912	2.41115280
C	1.34390342	-0.01400531	5.24521841	C	1.31965641	0.00922731	5.29096462	C	1.34442896	-0.01197339	5.21072409
C	1.80413230	0.19024099	6.57488958	C	1.73476192	-0.01641078	6.66570733	C	1.81198331	0.22336529	6.52611177
C	3.18852979	0.26421292	6.51094871	C	3.10475921	-0.02031268	6.66085934	C	3.19104169	0.31606258	6.44495353
C	3.54568095	0.07520048	5.14768496	C	3.51184608	0.00542535	5.28233610	C	3.53146667	0.09892518	5.08794853
N	2.42367844	-0.09590753	4.37000550	N	2.42367548	0.02658400	4.46079638	N	2.41125053	-0.09943617	4.33066901
C	5.21009316	-0.42957300	3.41528750	C	5.29501747	0.02941710	3.53567996	C	5.15689429	-0.51040807	3.37228541
C	6.63651926	-0.67083132	2.96607714	C	6.76040897	-0.02913998	3.17740277	C	6.56290737	-0.79605610	2.90242208
C	6.43267161	-1.74170867	1.89024925	C	6.75805677	0.20672285	1.67295593	C	6.31624814	-1.95125597	1.93535480
C	5.02453532	-1.43072999	1.42639720	C	5.29349629	0.12575172	1.31607944	C	4.91376971	-1.64097992	1.46973251
N	4.31769833	-0.76321443	2.41162873	N	4.49566767	0.07839349	2.42660874	N	4.23611591	-0.90729158	2.42220228
Ni	2.36220104	-0.43511893	2.42537268	Ni	2.43903590	0.05593390	2.42604940	Ni	2.33154471	-0.47823432	2.41187269
H	-0.73778200	0.19523317	-0.77268363	H	-0.77237068	-0.02276345	-0.76637515	H	-0.73321128	0.19777486	-0.77624917
H	-0.75653425	0.10016415	5.61978331	H	-0.77255749	-0.01672902	5.61630804	H	-0.75511450	0.08712504	5.59729697
H	5.67880341	0.20967030	5.36731963	H	5.61216301	-0.03583422	5.61368245	H	5.67398331	0.25044335	5.26544433
H	5.22554172	-2.23248921	-0.51248173	H	5.61058545	0.15063592	-0.76248790	H	5.07308512	-2.55197501	-0.42081367
H	-2.60017948	0.44253132	3.78073547	H	-2.66088166	-0.04370386	3.78232811	H	-2.60381181	0.41239098	3.76019649
H	-2.56856118	0.60302965	1.06937635	H	-2.66069190	-0.04937490	1.06756686	H	-2.56431025	0.60825076	1.05618461
H	0.97592844	-0.70080276	-2.59500338	H	1.06561170	0.00350966	-2.66794982	H	0.93165897	-0.82406742	-2.56444941
H	3.48280138	-1.78761540	-2.47295042	H	3.78046237	0.07143279	-2.65837074	H	3.35409499	-2.07854554	-2.39626355
H	7.15804061	-1.71000639	1.07365780	H	7.35410252	-0.52066392	1.11382499	H	7.02650522	-2.01171309	1.10864304
H	7.05047695	0.24473075	2.52022255	H	7.17083482	-1.01242122	3.43758853	H	6.96143350	0.07340421	2.36395105
H	3.89253840	0.42196521	7.31935280	H	3.78004798	-0.04044671	7.50915623	H	3.90258067	0.49121521	7.24269020
H	1.16302071	0.29123177	7.44262735	H	1.06435191	-0.03363954	7.51779493	H	1.17801744	0.34187877	7.39662358
H	6.46885566	-2.74501899	2.33798677	H	7.15308254	1.19628191	1.41269265	H	6.32872486	-2.90809618	2.47298414
H	7.28939654	-0.97145480	3.78898614	H	7.34571653	0.70742950	3.73590599	H	7.23895265	-1.02979118	3.72701331
C	1.10710880	-3.91442198	2.42307231	C	2.37747919	-3.06797746	2.44883768	C	0.98108822	-3.44285791	2.52812217
H	2.15941798	-3.89239845	2.15860397	H	3.36650197	-2.62799182	2.54585358	H	1.97048356	-3.49727322	2.08313432
H	0.93421842	-3.46274589	3.39456647	H	1.75204979	-2.81596327	3.30040494	H	1.01841615	-2.96928437	3.50516158
H	0.49680522	-3.44958102	1.65607086	H	1.90794939	-2.77118882	1.51544046	H	0.28511332	-2.93014927	1.87161322
Cl	0.60649307	-5.66862738	2.53610946	Cl	2.57050663	-4.87143812	2.42142164	Cl	0.38455447	-5.13665820	2.75625546

[*Ch*-Ni—Me—Cl]$^{‡-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.86385153	C	0.00000000	0.00000000	4.84717462	C	0.00000000	0.00000000	4.85406015
C	4.86592584	0.00000000	4.84986601	C	4.84865191	0.00000000	4.83570748	C	4.84362657	0.00000000	4.83620829
C	4.86480824	-0.11340178	0.01256590	C	4.84768965	0.10247343	0.01129269	C	4.84236169	0.12821298	0.01697987
C	3.52121523	-0.08101427	-0.42211250	C	3.51102253	0.07253814	-0.42665440	C	3.49719085	0.10081774	-0.41327616
C	3.11047463	-0.07417545	-1.81347744	C	3.10321907	0.06511723	-1.80750562	C	3.08945007	0.09441662	-1.80603309
C	1.74240013	-0.03897413	-1.81888770	C	1.73588305	0.03654744	-1.81254785	C	1.72990556	0.05332800	-1.81273016
C	1.32133449	-0.02644023	-0.43367221	C	1.31902954	0.02771361	-0.43642195	C	1.30899252	0.03764014	-0.42840053
N	2.43218526	-0.05091617	0.39190178	N	2.42325412	0.05144569	0.39249859	N	2.42045535	0.07002679	0.39461899
C	-0.44739261	0.00994252	1.33309990	C	-0.44211719	-0.00136604	1.32776698	C	-0.45001576	-0.00695362	1.33577704
C	-1.83056296	0.03945765	1.74528998	C	-1.81809581	-0.02082571	1.73889790	C	-1.82475958	-0.02712561	1.74051190
C	-1.83060586	0.03543632	3.11855899	C	-1.81816894	-0.01749286	3.10828051	C	-1.82481807	-0.02282166	3.11353726
C	-0.44739507	0.00562822	3.53065312	C	-0.44221746	0.00199566	3.51944829	C	-0.45007086	-0.00241397	3.51824467
N	0.37423218	-0.01039670	2.43187692	N	0.38505903	0.01390013	2.42361358	N	0.36867560	0.00692413	2.42702251
C	1.32160712	-0.00706937	5.29736160	C	1.31927111	0.01046683	5.28359164	C	1.30940906	0.01636342	5.28240604
C	1.74338379	0.01351711	6.68228898	C	1.73619890	-0.00901486	6.65960854	C	1.73083849	-0.00288960	6.66657052
C	3.11186738	0.01575462	6.67627721	C	3.10382659	-0.01349565	6.65456555	C	3.09094169	-0.00465497	6.65961535
C	3.52213413	-0.00633261	5.28490999	C	3.51175140	0.00623061	5.27385312	C	3.49847169	0.01604596	5.26693717
N	2.43236529	-0.02185854	4.47145381	N	2.42378174	0.02502968	4.45484488	N	2.42119746	0.03492544	4.45937399
C	5.32515925	-0.01322196	3.54456358	C	5.30349769	0.02801192	3.53284558	C	5.29335893	0.02485227	3.53520719
C	6.80529773	0.04705001	3.19269307	C	6.77060252	-0.00595064	3.17971208	C	6.76793964	-0.03168239	3.18340441

C	6.80542505	-0.15262992	1.66843077	C	6.76798320	0.18166899	1.66732680	C	6.76699504	0.18541169	1.66867810
C	5.32481910	-0.10006691	1.31753177	C	5.30250036	0.10761590	1.31443114	C	5.29242857	0.12190286	1.31799884
N	4.54053757	-0.06008254	2.43136778	N	4.51118885	0.06255177	2.42383545	N	4.50838731	0.07593468	2.42712153
Ni	2.44064668	-0.12171417	2.43213456	Ni	2.43565160	-0.01697384	2.42337038	Ni	2.43605749	-0.02525946	2.42648742
H	-0.76686305	0.01532042	-0.77074300	H	-0.76896044	-0.01694287	-0.76967827	H	-0.76733426	-0.02049243	-0.77038549
H	-0.76694971	0.01271480	5.63455995	H	-0.76896910	-0.01472602	5.61689183	H	-0.76746061	-0.01622055	5.62444436
H	5.62113419	0.02950795	5.63135490	H	5.60831662	-0.02753267	5.61401053	H	5.59937240	-0.03751220	5.61634445
H	5.61943387	-0.14584881	-0.76937783	H	5.60698458	0.13144801	-0.76734029	H	5.59777250	0.16088572	-0.76369507
H	-2.68194712	0.05385068	3.78903007	H	-2.66831602	-0.02805803	3.78103276	H	-2.67550174	-0.03256031	3.78449387
H	-2.68189352	0.06098440	1.07489636	H	-2.66816727	-0.03420535	1.06609843	H	-2.67541104	-0.04005386	1.06956332
H	1.07424335	-0.02269707	-2.67204135	H	1.06547323	0.02403586	-2.66442076	H	1.06120625	0.03667588	-2.66500752
H	3.78491311	-0.09211435	-2.66158580	H	3.77904974	0.08078734	-2.65511647	H	3.76608786	0.11727692	-2.65169551
H	7.37370856	0.61367685	1.13237909	H	7.17740316	1.15423954	1.37024324	H	7.33965670	-0.56811900	1.12201020
H	7.21993005	1.02107023	3.47901499	H	7.33148329	0.76664327	3.71410408	H	7.17482992	-1.01087592	3.45739376
H	3.78688404	0.03326988	7.52392995	H	3.77978021	-0.02885987	7.50208376	H	3.76812755	-0.02003352	7.50500690
H	1.07536806	0.02952406	7.53555514	H	1.06563607	-0.02073943	7.51137512	H	1.06207297	-0.01657020	7.51884175
H	7.22468110	-1.12449034	1.38141634	H	7.34974907	-0.57484603	1.13231969	H	7.17020261	1.16598126	1.39420717
H	7.37756442	-0.71615203	3.72900039	H	7.20668729	-0.96666189	3.47732009	H	7.33833987	0.72380878	3.72972649
C	2.41786036	-2.64095967	2.44272549	C	2.42978151	-2.51178838	2.41036195	C	2.58249837	-2.43893481	2.41341891
H	3.48760416	-2.53001979	2.43776531	H	3.49697253	-2.36083716	2.40813696	H	3.11532565	-2.30797819	1.48655786
H	1.88917606	-2.51921562	3.37071671	H	1.89700242	-2.38228816	3.33771952	H	3.11229315	-2.32053388	3.34381361
H	1.88150272	-2.52876050	1.51799771	H	1.89200736	-2.37273345	1.48727720	H	1.50649497	-2.38270990	2.41207002
Cl	2.40832525	-4.85295453	2.45487552	Cl	2.45834167	-4.68848510	2.39890078	Cl	2.67958014	-4.63656454	2.39851842

[*Ch*-Ni-Me···Cl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85409546	C	0.00000000	0.00000000	4.83577817	C	0.00000000	0.00000000	4.84828722
C	4.86831429	0.00000000	4.83961204	C	4.85404042	0.00000000	4.82501119	C	4.84307013	0.00000000	4.82855680
C	4.86778639	-0.06712621	0.01353035	C	4.85299581	0.04570698	0.01269117	C	4.84059846	-0.12293242	0.01710109
C	3.52498102	-0.04913074	-0.40734407	C	3.51585125	0.03769856	-0.41027372	C	3.49795216	-0.07407782	-0.40293949
C	3.11293730	-0.05784554	-1.79407893	C	3.10662065	0.01596363	-1.78829099	C	3.08950712	-0.09242856	-1.79130729
C	1.74609800	-0.03810670	-1.80026595	C	1.74120341	0.00181710	-1.79387029	C	1.73105650	-0.05673900	-1.79832357
C	1.32142335	-0.01797351	-0.42033116	C	1.32014890	0.01598418	-0.42161825	C	1.30809058	-0.01922435	-0.41864130
N	2.43360336	-0.01540854	0.41133873	N	2.42557599	0.05178992	0.41083170	N	2.42093458	-0.01915860	0.40934693
C	-0.45011916	0.01711371	1.32854101	C	-0.45023093	0.01068308	1.32302425	C	-0.44756962	0.01660740	1.33351596
C	-1.82937717	0.02718141	1.74035409	C	-1.82350875	-0.01219529	1.73312602	C	-1.81802431	0.02023333	1.73741981
C	-1.82950638	0.02656745	3.11366212	C	-1.82375627	-0.00775166	3.10273864	C	-1.81833314	0.01789216	3.11073848
C	-0.45030919	0.01631741	3.52564930	C	-0.45059007	0.01569317	3.51299278	C	-0.44809696	0.01410744	3.51509110
N	0.37335665	0.01987440	2.42715643	N	0.37458756	0.04048183	2.41787419	N	0.37389142	0.01887044	2.42419143
C	1.32151605	-0.00761867	5.27440470	C	1.32005320	0.00250131	5.25839831	C	1.30835316	0.00157350	5.26718994
C	1.74670405	-0.01690974	6.65416580	C	1.74058025	-0.03359036	6.63015233	C	1.73327247	-0.01276813	6.64630906
C	3.11372778	-0.01510290	6.64784963	C	3.10621463	-0.03597882	6.62532547	C	3.09238039	-0.00837708	6.63848835
C	3.52558602	-0.00658672	5.26112719	C	3.51684931	0.00004731	5.24824260	C	3.49967545	0.00665801	5.25003666
N	2.43351378	0.00637608	4.44268739	N	2.42664512	0.03913392	4.42771940	N	2.42071264	0.02293343	4.43896808
C	5.33184776	0.00447488	3.53866510	C	5.31849903	0.02992155	3.52677610	C	5.29209334	-0.00864647	3.53091116
C	6.81073049	0.04355787	3.19218999	C	6.78486065	0.02112110	3.18010825	C	6.76450084	0.00967152	3.18079632
C	6.81103978	-0.08439202	1.66083550	C	6.78403488	0.06628057	1.65660452	C	6.75966660	-0.19797787	1.66609251
C	5.33189921	-0.04978216	1.31409707	C	5.31748566	0.05692489	1.31123482	C	5.29028379	-0.10368740	1.31439805
N	4.54652550	-0.01561945	2.42617593	N	4.52961158	0.05767675	2.41935617	N	4.50476438	-0.02130453	2.42156225
Ni	2.42795067	-0.17501570	2.42963948	Ni	2.42662462	-0.10834210	2.42272664	Ni	2.43070324	-0.14175324	2.42987705
H	-0.76096105	-0.00329663	-0.77583026	H	-0.76014484	-0.02686592	-0.77707391	H	-0.76481841	-0.00577018	-0.77224896
H	-0.76081008	-0.00753556	5.63004529	H	-0.76028066	-0.02686179	5.61276133	H	-0.76445395	-0.01377915	5.62081467
H	5.61690337	0.00488915	5.62705295	H	5.60440033	-0.02948447	5.61118305	H	5.59562191	-0.00099388	5.61165939
H	5.61573334	-0.09708245	-0.77394805	H	5.60360129	0.03838622	-0.77375144	H	5.59087917	-0.18763762	-0.76544707
H	-2.67945481	0.03236196	3.78534087	H	-2.67248104	-0.02137412	3.77628281	H	-2.66736636	0.01861316	3.78313169
H	-2.67916797	0.03402216	1.06847868	H	-2.67197337	-0.02914971	1.05931227	H	-2.66679367	0.02301946	1.06471574
H	1.07629005	-0.03481300	-2.65167894	H	1.06932585	-0.01456792	-2.64376936	H	1.06034946	-0.05807354	-2.64867565
H	3.79045988	-0.07450425	-2.63902851	H	3.78557539	0.01262819	-2.63265424	H	3.76859096	-0.12933704	-2.63384712
H	7.35279164	0.72494300	1.16181508	H	7.29523172	-0.78740346	1.20109917	H	7.14092094	-1.18461256	1.38364534
H	7.25190288	0.98774845	3.53106054	H	7.26669501	-0.87755465	3.57861119	H	7.30942180	-0.76588570	3.72422393
H	3.79143036	-0.01692525	7.49281494	H	3.78443027	-0.05829748	7.46994126	H	3.77252173	-0.01602810	7.48092451
H	1.07707872	-0.01977618	7.50571880	H	1.06816154	-0.05312797	7.47954364	H	1.06359277	-0.02407196	7.49736880
H	7.25481123	-1.02720975	1.32180517	H	7.26592091	0.96476812	1.25745792	H	7.34508320	0.54794217	1.12312320
H	7.35427725	-0.76412563	3.69184428	H	7.29705335	0.87455464	3.63524811	H	7.19647833	0.97519865	3.46358970
C	2.36152862	-2.15746366	2.45969938	C	2.39833239	-2.06748891	2.47189338	C	2.49912856	-2.13545071	2.51568066
H	3.40134015	-2.46495116	2.52142030	H	3.41906081	-2.36009755	2.70735836	H	2.81100823	-2.43350552	1.51930902
H	1.78334096	-2.41566150	3.34096251	H	1.68869932	-2.33521960	3.25058199	H	3.22488423	-2.35641538	3.29213516
H	1.88046528	-2.44189652	1.52950244	H	2.08034851	-2.38264195	1.48111962	H	1.48109372	-2.41761756	2.76599223
Cl	2.23397804	-6.29496839	2.38731047	Cl	2.44660883	-5.79369733	2.56776628	Cl	2.63424978	-5.88739960	2.66730466

[*Ch*-Ni-Me]

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85360410	C	0.00000000	0.00000000	4.83392142	C	0.00000000	0.00000000	4.84762098
C	4.86861204	0.00000000	4.83900172	C	4.85492340	0.00000000	4.82253297	C	4.84336776	0.00000000	4.82838260
C	4.86819803	-0.06660231	0.01345518	C	4.85439574	-0.00086868	0.01149615	C	4.84165139	-0.08841011	0.01676751
C	3.52532712	-0.05026392	-0.40696084	C	3.51687025	-0.00152770	-0.40952787	C	3.49864469	-0.05000829	-0.40237056
C	3.11312283	-0.06033818	-1.79349161	C	3.10671619	-0.03060540	-1.78678254	C	3.09035107	-0.06759276	-1.79058640
C	1.74629017	-0.04074700	-1.79965075	C	1.74131905	-0.03140867	-1.79183151	C	1.73168921	-0.04275873	-1.79755061
C	1.32153345	-0.01945350	-0.41985706	C	1.32061453	-0.00151090	-0.42003615	C	1.30830016	-0.01198674	-0.41797254
N	2.43378767	-0.01607150	0.41195561	N	2.42675736	0.03063792	0.41233494	N	2.42109928	-0.00597378	0.41046248
C	-0.45042001	0.01852239	1.32832960	C	-0.45149841	0.02072235	1.32219719	C	-0.44764360	0.01443588	1.33327811

C	-1.82967522	0.03104054	1.74008715
C	-1.82982318	0.03027239	3.11340365
C	-0.45064434	0.01759651	3.52536096
N	0.37313021	0.01998284	2.42693796
C	1.32165571	-0.00934772	5.27329221
C	1.74697434	-0.01927912	6.65294744
C	3.11396541	-0.01777963	6.64657370
C	3.52585172	-0.00850118	5.25997926
N	2.43364148	0.00466505	4.44130940
C	5.33250020	0.00709033	3.53822390
C	6.81118317	0.05064548	3.19178872
C	6.81185738	-0.07803270	1.66052319
C	5.33269416	-0.04702197	1.31385474
N	4.54713157	-0.01397715	2.42581795
Ni	2.42795615	-0.17413905	2.42884405
H	-0.76062889	-0.00222976	-0.77613494
H	-0.76041940	-0.00610177	5.62992824
H	5.61683860	0.00617092	5.62675718
H	5.61584553	-0.09530628	-0.77433675
H	-2.67965351	0.03855782	3.78520061
H	-2.67934091	0.04034852	1.06808773
H	1.07645042	-0.03699884	-2.65102941
H	3.79066158	-0.07632645	-2.63842933
H	7.35148412	0.73245979	1.16116969
H	7.24887416	0.99667866	3.52993068
H	3.79175575	-0.01886034	7.49146202
H	1.07734155	-0.02116918	7.50449013
H	7.25815874	-1.01977357	1.32172804
H	7.35776855	-0.75455605	3.69212846
C	2.36167163	-2.15365803	2.45273771
H	3.40286631	-2.46233105	2.48316797
H	1.80954031	-2.41753607	3.34932285
H	1.85450794	-2.43764427	1.53594800

C	-1.82492397	0.00791753	1.73222140
C	-1.82485419	0.00834694	3.10181155
C	-0.45145985	0.02219545	3.51170786
N	0.37375976	0.04427083	2.41673207
C	1.32038569	-0.00350673	5.25510609
C	1.74137601	-0.03807236	6.62656685
C	3.10695395	-0.03752907	6.62165020
C	3.51764019	-0.00360851	5.24471307
N	2.42704390	0.03225382	4.42376449
C	5.32026756	0.02521634	3.52454057
C	6.78667577	0.03140620	3.17897208
C	6.78659420	0.02160810	1.65480674
C	5.32018010	0.02201777	1.30926593
N	4.53172422	0.03955151	2.41677021
Ni	2.42688986	-0.11968485	2.42061560
H	-0.75911503	-0.02281083	-0.77819258
H	-0.75936376	-0.02370482	5.61181976
H	5.60469571	-0.02030961	5.60950479
H	5.60361207	-0.02205793	-0.77598190
H	-2.67345423	-0.00053856	3.77556843
H	-2.67354639	-0.00182883	1.05851769
H	1.06878857	-0.04582504	-2.64120494
H	3.78548990	-0.04580142	-2.63108987
H	7.28127389	-0.85902744	1.23288658
H	7.28976625	-0.83814670	3.61343569
H	3.78545396	-0.05622760	7.46608964
H	1.06894430	-0.05597657	7.47594639
H	7.28564309	0.89401313	1.22134768
H	7.27726058	0.91488317	3.59984808
C	2.38955046	-2.07414297	2.47153269
H	3.39885585	-2.37684375	2.74252253
H	1.65223068	-2.33807324	3.22559488
H	2.10415577	-2.39187000	1.47152497

C	-1.81810330	0.01616728	1.73711176
C	-1.81846283	0.01551563	3.11038297
C	-0.44827270	0.01367873	3.51475835
N	0.37401710	0.01864603	2.42393371
C	1.30850556	0.00122607	5.26582531
C	1.73337510	-0.01559873	6.64476185
C	3.09247407	-0.01281770	6.63715813
C	3.50001037	0.00493046	5.24900299
N	2.42098527	0.02358877	4.43737525
C	5.29318966	0.00078370	3.53104214
C	6.76588065	0.02215473	3.18262858
C	6.76297884	-0.14828034	1.66313353
C	5.29201470	-0.07177331	1.31377702
N	4.50594490	-0.00538913	2.42163373
Ni	2.43153417	-0.13559612	2.42931267
H	-0.76449319	-0.00767567	-0.77250318
H	-0.76399210	-0.01347825	5.62055578
H	5.59542916	-0.00379199	5.61193321
H	5.59201795	-0.14021282	-0.76663976
H	-2.66740994	0.01680420	3.78287848
H	-2.66676449	0.01840804	1.06429262
H	1.06091663	-0.04565363	-2.64783896
H	3.76988068	-0.09530944	-2.63309086
H	7.16513453	-1.11818179	1.35374324
H	7.30546214	-0.77047373	3.70669405
H	3.77262384	-0.02136238	7.47956655
H	1.06345607	-0.02677240	7.49562752
H	7.33179677	0.62419721	1.13981363
H	7.20317335	0.97696996	3.49154754
C	2.50821566	-2.12273922	2.50446054
H	2.83610393	-2.41864040	1.51203365
H	3.22342926	-2.34824934	3.29014257
H	1.48866720	-2.41539529	2.73845293

S.IX.3 Nickel bacteriochlorin (*BCh*) complexes

B3LYP/6-311+G(d,p)				M06-L/6-311+G(d,p)				ωB97X-D/6-311+G(d,p)			
[*BCh*-Ni]											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.81577180	C	0.00000000	0.00000000	4.80458954	C	0.00000000	0.00000000	4.79796350
C	4.84008500	0.00000000	4.55617063	C	4.82710354	0.00000000	4.56201274	C	4.85219093	0.00000000	4.46542322
C	4.35263829	-2.11748730	0.25819359	C	4.36878682	2.05326952	0.24235705	C	4.23557842	-2.24273049	0.26816542
C	3.11463996	-1.68487751	-0.22464284	C	3.12777095	1.63776860	-0.23707748	C	3.02173993	-1.78831550	-0.19466789
C	2.67794024	-1.80348755	-1.58475267	C	2.69217695	1.75737907	-1.58928053	C	2.56314260	-1.92260790	-1.56361637
C	1.49473048	-1.11243153	-1.68107074	C	1.50096205	1.08402236	-1.68081532	C	1.43855200	-1.17956278	-1.67109191
C	1.19500609	-0.62416513	-0.36721647	C	1.19845974	0.60644901	-0.37206884	C	1.16016575	-0.65244009	-0.34940678
N	2.19655886	-0.97045762	0.51262025	N	2.20353719	0.94061815	0.50513042	N	2.14467876	-1.02358449	0.52688426
C	-0.38867846	0.19781721	1.30282153	C	-0.38694132	-0.19461867	1.30000737	C	-0.38397430	0.17180865	1.32471587
C	-1.76159584	0.69732759	1.69860556	C	-1.75001740	-0.68295861	1.69690737	C	-1.77070995	0.62417147	1.70708474
C	-1.89014976	0.13519110	3.11769623	C	-1.87370150	-0.13202488	3.10746268	C	-1.89708335	0.04495920	3.11345176
C	-0.43663118	-0.01228325	3.51318592	C	-0.43257679	0.00925793	3.50433013	C	-0.44892231	-0.04493772	3.52404062
N	0.37021963	-0.08680513	2.40778974	N	0.37714145	0.08300182	2.40227466	N	0.36787115	-0.11183554	2.39712783
C	1.34777494	0.04259799	5.18227888	C	1.34258102	-0.03855432	5.17665893	C	1.36651130	0.05707157	5.15735306
C	1.83135841	0.35900449	6.49398318	C	1.81957737	-0.34312481	6.48520243	C	1.85684323	0.39611468	6.43606934
C	3.19743842	0.46425221	6.39633777	C	3.18390406	-0.44740690	6.39319150	C	3.23488348	0.48852023	6.31840493
C	3.53790114	0.15882043	5.03783629	C	3.52727630	-0.15289371	5.04116918	C	3.54576391	0.16843814	4.97984255
N	2.39958735	-0.08697356	4.30239534	N	2.39431249	0.08639920	4.29939340	N	2.40120262	-0.08860522	4.26765628
C	5.14077842	-0.57635039	3.34579459	C	5.13328302	0.55646038	3.34771496	C	5.13153688	-0.57737428	3.27578518
C	6.54909504	-0.92030620	2.91086708	C	6.53267385	0.88415135	2.91333882	C	6.51707656	-0.90408836	2.77784033
C	6.28779900	-2.04971279	1.90974029	C	6.28689343	1.98296086	1.89306327	C	6.22593307	-2.06662178	1.83282514
C	4.87280470	-1.73801771	1.47189450	C	4.88195791	1.68212636	1.45751518	C	4.79021345	-1.79328325	1.46079034
N	4.22400449	-0.97628077	2.40879528	N	4.22064284	0.94374868	2.40276707	N	4.17515865	-1.01525599	2.36235914
Ni	2.29773740	-0.53028384	2.40792053	Ni	2.29896703	0.51347537	2.40227495	Ni	2.27285056	-0.55803032	2.39580753
H	-0.70410623	0.24877732	-0.78752771	H	-0.71085413	-0.24071010	-0.78449546	H	-0.70872462	0.25548522	-0.77973892
H	-0.74201624	0.08509901	5.60330629	H	-0.74586417	-0.08451088	5.58895476	H	-0.73137777	0.07938687	5.59674404
H	5.66054784	0.25228643	5.22034831	H	5.64610549	-0.24312175	5.23193084	H	5.68270569	0.27864183	5.10717244
H	4.97962104	-2.70233942	-0.40727144	H	5.00649340	2.62143018	-0.42787244	H	4.84635426	-2.85439414	-0.38640839
H	-2.37263339	-0.85245419	3.10503062	H	-2.43381910	-0.76548990	3.79814364	H	-2.33991637	-0.95863450	3.07618949
H	-2.53996141	0.36504174	1.00836103	H	-1.76184275	-1.78135318	1.70217399	H	-2.52715997	0.27528068	1.00236673
H	0.86415625	-0.96905538	-2.54979664	H	0.86297895	0.94743496	-2.54540700	H	0.81439150	-1.01160615	-2.53930446
H	3.22449575	-2.32009561	-2.36403054	H	3.24802134	2.26274277	-2.36957021	H	3.07908654	-2.48999418	-2.32744522
H	-2.44618688	0.77330688	3.80777141	H	-2.35444925	0.85563518	3.10214587	H	-2.48697819	0.65553452	3.79867746
H	-1.76565347	1.79656933	1.71196387	H	-2.52730939	-0.35004033	1.00629253	H	-1.79631287	1.72176217	1.72375433
H	6.98619316	-2.08087202	1.07077487	H	6.98720492	1.99423091	1.05557846	H	6.28190664	-3.02970040	2.35702017
H	7.00412246	-0.05303993	2.41161471	H	6.98878781	0.00410992	2.43989278	H	7.20390188	-1.14757987	3.58980496
H	3.91486404	0.69480459	7.17412248	H	3.90187911	-0.66938626	7.17321237	H	3.96183228	0.72433289	7.08582845
H	1.20196615	0.51109850	7.36208015	H	1.18413056	-0.49118993	7.34976904	H	1.24231489	0.57245285	7.31031243
H	6.31368067	-3.02815216	2.41006831	H	6.32315746	2.97347664	2.36660013	H	6.87712000	-2.11543232	0.95876233
H	7.18780436	-1.19966484	3.75149039	H	7.17001736	1.17273014	3.75151017	H	6.92751246	-0.05121900	2.22214771
[*BCh*-Ni]$^{-}$											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.81451115	C	0.00000000	0.00000000	4.82839689	C	0.00000000	0.00000000	4.79304442
C	4.88058644	0.00000000	4.51547709	C	4.85919606	0.00000000	4.82495940	C	4.87533024	0.00000000	4.45230035
C	4.32818611	-2.25606455	0.29766848	C	4.84988006	0.30129816	0.00581470	C	4.25068253	-2.34711498	0.31924944
C	3.08905198	-1.79342163	-0.21640577	C	3.51872236	0.23502369	-0.44377752	C	3.02339742	-1.86843365	-0.19289501
C	2.65550004	-1.91821636	-1.55915723	C	3.11073358	0.25349318	-1.81392882	C	2.58504918	-2.00308081	-1.53247290
C	1.46864062	-1.19285517	-1.66660085	C	1.73641755	0.16369121	-1.81579534	C	1.42949884	-1.24650664	-1.64976161
C	1.18874559	-0.67661684	-0.37756410	C	1.33036112	0.09639385	-0.44658011	C	1.16927049	-0.70314179	-0.36841212
N	2.18639617	-1.03778740	0.50978235	N	2.42507999	0.14022109	0.38049332	N	2.15076562	-1.07879952	0.51827670
C	-0.37035820	0.21116481	1.29551288	C	-0.44294479	-0.04116900	1.30380210	C	-0.36425945	0.20341315	1.29822924
C	-1.72365618	0.74993351	1.71476630	C	-1.90297016	-0.18479803	1.66361868	C	-1.71507503	0.73824381	1.71398341
C	-1.87737552	0.11224921	3.10088852	C	-1.91056561	0.07130292	3.16454944	C	-1.87313458	0.08902419	3.08771524
C	-0.42734103	-0.02512478	3.51966956	C	-0.44465060	0.01416284	3.52454846	C	-0.42904193	-0.03578326	3.51124403
N	0.39030748	-0.09909133	2.40725051	N	0.35554202	0.01009563	2.41421222	N	0.39100949	-0.11459740	2.39503714
C	1.36710311	0.05932886	5.19030464	C	1.33361587	-0.01432071	5.27555325	C	1.37541126	0.06614929	5.16115790
C	1.85435127	0.39994567	6.47595922	C	1.74227415	-0.05577968	6.64500592	C	1.86524462	0.42335493	6.42817832
C	3.24183285	0.49588158	6.36690968	C	3.11947273	-0.05996151	6.64397763	C	3.25429966	0.51553256	6.30674431
C	3.56817104	0.17375292	5.02658222	C	3.52633082	-0.01669158	5.27404021	C	3.56274619	0.18122183	4.97763223
N	2.41833562	-0.08594392	4.30300754	N	2.42944940	0.00968619	4.44909241	N	2.41322158	-0.08858690	4.27010766
C	5.15399377	-0.60696037	3.32505740	C	5.30150497	0.06925796	3.52205695	C	5.13110500	-0.62166604	3.27886943
C	6.54888681	-0.98040979	2.86430605	C	6.76708959	0.03971982	3.15745710	C	6.51062271	-1.00210299	2.79602501
C	6.24885933	-2.18579482	1.96502760	C	6.75666445	0.37931090	1.67311750	C	6.19071855	-2.23040851	1.94613915
C	4.84686945	-1.85531435	1.49360428	C	5.29546017	0.26064928	1.30874680	C	4.78496515	-1.90878787	1.49471698
N	4.21221933	-1.03508260	2.40815849	N	4.49937721	0.14071767	2.41549173	N	4.17074904	-1.06588745	2.38217456
Ni	2.30204785	-0.56446945	2.40710444	Ni	2.42737906	0.07503273	2.41483057	Ni	2.28186799	-0.58619123	2.39430580
H	-0.69747438	0.26944946	-0.78777492	H	-0.76458275	-0.04353055	-0.77367236	H	-0.69699843	0.27556986	-0.78535346
H	-0.74270516	0.08310677	5.60270057	H	-0.76599053	-0.00222176	5.60193389	H	-0.73775149	0.08388605	5.58582850
H	5.71176028	0.27156412	5.15979397	H	5.62651264	-0.04403045	5.59589507	H	5.71323621	0.28614607	5.08148415
H	4.93753177	-2.88357086	-0.34629556	H	5.61317180	0.39210704	-0.76500933	H	4.84787416	-2.99603133	-0.31386847
H	-2.34356914	-0.88001503	3.01364897	H	-2.50329145	-0.65183676	3.73253429	H	-2.32546927	-0.90652849	2.98694250
H	-2.51582706	0.49309597	1.00721520	H	-2.24928475	-1.19823788	1.42347371	H	-2.50206080	0.48643247	1.00046895

H	0.83847667	-1.06184670	-2.53862603	H	1.06497044	0.14669871	-2.66742193	H	0.80293256	-1.10579293	-2.52233494
H	3.18943036	-2.45100770	-2.33746237	H	3.78098618	0.32368661	-2.66378341	H	3.10086471	-2.56703709	-2.30033796
H	-2.46509030	0.70202546	3.80860099	H	-2.31603771	1.06258301	3.40448637	H	-2.46919994	0.66837041	3.79548867
H	-1.68613371	1.84568481	1.80177731	H	-2.53705128	0.50232147	1.09553888	H	-1.67123052	1.83141870	1.80877719
H	6.94994424	-2.31959089	1.13757061	H	7.38689728	-0.27779798	1.06647048	H	6.18519511	-3.13625793	2.56680267
H	6.98594032	-0.16264486	2.27293013	H	7.17855381	-0.96080777	3.34199611	H	7.20471209	-1.18959274	3.61756311
H	3.96160453	0.72837949	7.14314212	H	3.79229541	-0.08802748	7.49422356	H	3.98053669	0.75754778	7.07384662
H	1.23534653	0.58169040	7.34686148	H	1.07053081	-0.08021874	7.49621526	H	1.25343981	0.61631349	7.30162597
H	6.24155864	-3.11125557	2.55920484	H	7.10671764	1.40290344	1.48834637	H	6.87229516	-2.39164156	1.10865428
H	7.22290871	-1.19353729	3.69758941	H	7.35654871	0.73368588	3.76403364	H	6.92565558	-0.20293125	2.16762859

MeCl

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08694599	H	0.00000000	0.00000000	1.08633125	H	0.00000000	0.00000000	1.08723601
H	1.01451467	0.00000000	-0.39014216	H	1.01688044	0.00000000	-0.38219087	H	1.01683743	0.00000000	-0.38486802
H	-0.56802896	0.84058499	-0.39014216	H	-0.55193887	0.85405463	-0.38219087	H	-0.55718534	0.85058971	-0.38486802
Cl	-0.81300034	-1.53061085	-0.55839644	Cl	-0.81461320	-1.49636904	-0.56408018	Cl	-0.81430307	-1.50687408	-0.56246966

[*BCh*-Ni···MeCl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.81464608	C	0.00000000	0.00000000	4.82846067	C	0.00000000	0.00000000	4.79280910
C	4.88097619	0.00000000	4.52103581	C	4.85937610	0.00000000	4.82382836	C	4.87279985	0.00000000	4.44809289
C	4.34055069	-2.23242060	0.28948780	C	4.84979087	0.30293481	0.00523771	C	4.21244875	-2.40938419	0.35881223
C	3.09722165	-1.77787376	-0.22130386	C	3.51834011	0.23631824	-0.44419054	C	2.99368312	-1.91859124	-0.16483474
C	2.66012822	-1.90905630	-1.56230406	C	3.11171332	0.23613819	-1.81519546	C	2.55114696	-2.07191728	-1.50061640
C	1.46797678	-1.19221492	-1.66721732	C	1.73738625	0.14739866	-1.81711475	C	1.40906328	-1.29615987	-1.63165983
C	1.18969656	-0.67398727	-0.37858482	C	1.33014878	0.09942524	-0.44719105	C	1.16020640	-0.72368602	-0.36124031
N	2.19185693	-1.02762940	0.50687731	N	2.42404305	0.15554078	0.37981583	N	2.13692473	-1.09875649	0.53043938
C	-0.36818814	0.21575582	1.29525322	C	-0.44367448	-0.03457249	1.30417049	C	-0.36203429	0.21870879	1.29607001
C	-1.71963515	0.75970728	1.71293905	C	-1.90294482	-0.18666207	1.66428381	C	-1.70725024	0.76693341	1.71158788
C	-1.87545139	0.12743588	3.10104173	C	-1.91185099	0.07075999	3.16506865	C	-1.87184829	0.11771186	3.08521599
C	-0.42584454	-0.01750987	3.51906165	C	-0.44561039	0.02118693	3.52468221	C	-0.42881631	-0.02174883	3.50941153
N	0.39206486	-0.09462265	2.40744979	N	0.35396010	0.02583482	2.41420873	N	0.39091612	-0.09996549	2.39522412
C	1.36659459	0.05129501	5.19294532	C	1.33388763	-0.01327488	5.27559792	C	1.37502947	0.06543659	5.16126205
C	1.85242316	0.38394838	6.48132870	C	1.74297745	-0.07562217	6.64444165	C	1.86668962	0.41140412	6.43170266
C	3.24018690	0.47754619	6.37476703	C	3.12008639	-0.08262030	6.64265627	C	3.25499389	0.50752283	6.30847794
C	3.56776724	0.16266552	5.03311918	C	3.52635134	-0.01942259	5.27291424	C	3.56167582	0.18636596	4.97492814
N	2.41875627	-0.09190272	4.30637376	N	2.42939107	0.02271930	4.44960643	N	2.41140247	-0.07758996	4.26796986
C	5.15816070	-0.59204258	3.32426753	C	5.30251053	0.08420054	3.52165331	C	5.12282788	-0.63156431	3.27797998
C	6.55560171	-0.94735570	2.85691117	C	6.76846952	0.05590688	3.15747847	C	6.49652002	-1.03807669	2.79983548
C	6.26601396	-2.14942452	1.95001890	C	6.75811832	0.38729744	1.67109388	C	6.15738894	-2.28353498	1.98188889
C	4.85876581	-1.83096726	1.48542248	C	5.29607797	0.27330548	1.30854492	C	4.75727196	-1.95082107	1.52164224
N	4.21844466	-1.02136062	2.40533037	N	4.50067604	0.16216206	2.41614502	N	4.15721630	-1.07844733	2.38961638
Ni	2.30476573	-0.56095080	2.40708332	Ni	2.42551895	0.09953864	2.41560177	Ni	2.27637293	-0.58076260	2.39620751
H	-0.69905920	0.26722723	-0.78712564	H	-0.76405539	-0.05409262	-0.77355434	H	-0.69405293	0.27599071	-0.78784683
H	-0.74356147	0.08460317	5.60182305	H	-0.76580351	-0.01204486	5.60212346	H	-0.73806631	0.08030818	5.58560876
H	5.71038567	0.27320116	5.16689246	H	5.62645125	-0.05448412	5.59434611	H	5.71292534	0.28407479	5.07508255
H	4.95378858	-2.85306366	-0.35739615	H	5.61334058	0.38240408	-0.76660961	H	4.79693062	-3.08424182	-0.25893982
H	-2.34815004	-0.86210558	3.01809778	H	-2.50116631	-0.65448295	3.73389471	H	-2.33483441	-0.87281036	2.98366166
H	-2.51237167	0.50257787	1.00609766	H	-2.24306590	-1.20247304	1.42516870	H	-2.49680222	0.52356027	0.99801057
H	0.83421952	-1.06695588	-2.53746035	H	1.06679649	0.11745038	-2.66906585	H	0.78330447	-1.16312029	-2.50602925
H	3.19489368	-2.44043312	-2.34099767	H	3.78291509	0.29267399	-2.66531684	H	3.05469000	-2.66084021	-2.25786088
H	-2.45865271	0.72316056	3.80754648	H	-2.32182983	1.06050958	3.40379241	H	-2.46209122	0.70245175	3.79342169
H	-1.67896716	1.85557783	1.79585554	H	-2.54126548	0.49612442	1.09572146	H	-1.65268439	1.85942935	1.80782054
H	6.96516861	-2.26919039	1.11878202	H	7.38462326	-0.27637713	1.06769665	H	6.13605968	-3.17165646	2.62767051
H	6.98218827	-0.12128700	2.26953718	H	7.18295559	-0.94200811	3.34889573	H	7.19170540	-1.21368023	3.62308535
H	3.95934125	0.70613762	7.15274485	H	3.79327272	-0.12534932	7.49201495	H	3.98231609	0.74324312	7.07647959
H	1.23241508	0.56228140	7.35221645	H	1.07157733	-0.11292574	7.49546465	H	1.25625893	0.59417156	7.30827404
H	6.27224744	-3.07947565	2.53684489	H	7.11296547	1.40799411	1.47988652	H	6.83682846	-2.47905775	1.15002690
H	7.23456828	-1.15842102	3.68670466	H	7.35548303	0.75559216	3.75994088	H	6.91877762	-0.26052675	2.14956139
C	0.91265664	-3.95234041	2.77274215	C	2.41185913	-3.01048300	2.35891265	C	1.98474498	-3.53457709	3.68573822
H	1.95560769	-4.03140906	2.48357183	H	3.39541409	-2.56020411	2.46433261	H	2.24559660	-3.57510029	2.63171541
H	0.80526362	-3.44483479	3.72603898	H	1.78376428	-2.78402256	3.21566864	H	2.81788937	-3.17537151	4.28191466
H	0.32316266	-3.47218227	1.99878839	H	1.93847562	-2.70176883	1.43149187	H	1.09882180	-2.92692773	3.84727946
Cl	0.27067315	-5.65078283	2.98104714	Cl	2.62832192	-4.81078981	2.29504387	Cl	1.60441681	-5.21998988	4.22598458

[*BCh*-Ni—Me—Cl]$^{‡-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.83574216	C	0.00000000	0.00000000	4.82408704	C	0.00000000	0.00000000	4.81867015
C	4.88033671	0.00000000	4.83041342	C	4.86016726	0.00000000	4.82353384	C	4.87984840	0.00000000	4.79600719
C	4.87326336	-0.26279371	0.00207887	C	4.85788577	0.14741369	0.00173830	C	4.83215668	-0.29110854	-0.01364618
C	3.53519216	-0.20204589	-0.43427334	C	3.52475079	0.11331773	-0.43882136	C	3.50697678	-0.21435241	-0.43194431
C	3.12233488	-0.20540494	-1.81521776	C	3.11598797	0.11186997	-1.81135601	C	3.08580037	-0.24092922	-1.81987758
C	1.74904258	-0.12375821	-1.81624044	C	1.74235288	0.07115896	-1.81206105	C	1.73005742	-0.15120137	-1.81610680
C	1.33733178	-0.07644327	-0.43586121	C	1.33258890	0.04958973	-0.44006947	C	1.32296346	-0.07784207	-0.42541035
N	2.43691121	-0.12286154	0.38569979	N	2.42852863	0.07886245	0.38522812	N	2.41932447	-0.11100481	0.38650366
C	-0.46347797	0.03101111	1.30483505	C	-0.45618219	-0.01250890	1.30302835	C	-0.45131800	0.03219899	1.31731571
C	-1.94109044	0.15478563	1.65564214	C	-1.92407936	-0.08068366	1.65293135	C	-1.92375260	0.15543173	1.65964915
C	-1.94727877	-0.04723108	3.18049673	C	-1.92511736	0.06036115	3.17134140	C	-1.93712457	-0.08445569	3.17186937
C	-0.46502345	-0.01311988	3.53117078	C	-0.45646661	0.01643453	3.52133937	C	-0.46276106	-0.02103631	3.53190934
N	0.31829008	-0.01876839	2.41795001	N	0.33470275	0.01304142	2.41201438	N	0.32681813	-0.01864844	2.40792382
C	1.33987378	0.01519635	5.27047660	C	1.33362603	-0.00449567	5.26428605	C	1.34721400	0.02818005	5.25804872

C	1.75450600	0.06452802	6.64991256	C	1.74313286	-0.03577931	6.63617149	C	1.75791871	0.06426002	6.62287920
C	3.13017526	0.06876733	6.64783816	C	3.11733839	-0.03754594	6.63583549	C	3.13886853	0.06594575	6.61659403
C	3.54127715	0.01697653	5.26734678	C	3.52664459	-0.00659679	5.26380717	C	3.53707498	0.02956453	5.24810940
N	2.43964032	-0.01261077	4.44846845	N	2.43009502	0.01632529	4.43958382	N	2.43821440	0.01207268	4.43580820
C	5.34290963	-0.06249534	3.52652119	C	5.31591275	0.04360029	3.52116616	C	5.33092916	-0.06342459	3.50622812
C	6.82410286	-0.02669402	3.17094615	C	6.78508168	0.03839916	3.16999247	C	6.80311489	-0.05432625	3.13236592
C	6.81863544	-0.31119339	1.65933485	C	6.78003817	0.22694620	1.65679125	C	6.77183169	-0.36398752	1.63300738
C	5.33898064	-0.22699891	1.30580092	C	5.31381122	0.14008341	1.30468751	C	5.29739025	-0.24314805	1.29861523
N	4.55778768	-0.13590203	2.41694750	N	4.52374382	0.07377067	2.41290605	N	4.53135506	-0.11783826	2.39118297
Ni	2.43330378	-0.15538418	2.41951484	Ni	2.42839223	-0.00934536	2.41187745	Ni	2.43088390	-0.12980864	2.41510977
H	-0.75381567	0.04064416	-0.78301480	H	-0.76023811	-0.02608420	-0.77838692	H	-0.75969199	0.03307395	-0.77667687
H	-0.75444308	0.00947835	5.61915650	H	-0.76045687	-0.00548917	5.60268717	H	-0.75289365	-0.00304081	5.60425367
H	5.63610119	0.04506459	5.61129170	H	5.62101148	-0.02459120	5.60136181	H	5.64038099	0.03074350	5.57359141
H	5.62585434	-0.33434189	-0.77988369	H	5.61771120	0.19047350	-0.77627630	H	5.58296739	-0.38948678	-0.79339821
H	-2.37713823	-1.01698105	3.46149227	H	-2.48520323	-0.72972206	3.68108389	H	-2.33893320	-1.07414165	3.41754855
H	-2.54969599	-0.57961777	1.11910955	H	-2.34922185	-1.03646433	1.32419628	H	-2.53025622	-0.55936232	1.09736195
H	1.07922384	-0.09866197	-2.66803823	H	1.06999384	0.05755137	-2.66270714	H	1.05267155	-0.13972402	-2.66144772
H	3.79170837	-0.25871740	-2.66607171	H	3.78877501	0.13839245	-2.66131058	H	3.75431855	-0.31671512	-2.66895696
H	-2.51141680	0.72184998	3.71692875	H	-2.36408030	1.01015771	3.49923239	H	-2.52542684	0.65391834	3.72233717
H	-2.31277229	1.14814632	1.37435517	H	-2.49536255	0.70184497	1.14389761	H	-2.27716794	1.16003791	1.39924812
H	7.41693948	0.40088952	1.08273417	H	7.36870882	-0.52525872	1.12255974	H	7.11373938	-1.38249358	1.41535380
H	7.24142466	0.96242897	3.39796176	H	7.24390374	-0.91163647	3.46878930	H	7.37562178	-0.78286823	3.71200876
H	3.80208408	0.10325674	7.49766105	H	3.79041706	-0.05755883	7.48578252	H	3.81249034	0.08865124	7.46541372
H	1.08488241	0.09566453	7.50166305	H	1.07042044	-0.05381046	7.48640773	H	1.09207913	0.08395819	7.47788252
H	7.20278335	-1.31351802	1.43150737	H	7.18331559	1.20226309	1.35939601	H	7.37937662	0.31865541	1.03303452
H	7.39916967	-0.75788182	3.74737195	H	7.32881496	0.82422812	3.70350350	H	7.23380753	0.93378764	3.33004722
C	2.31410357	-2.66066564	2.48982509	C	2.38470535	-2.50050949	2.37962403	C	2.49061189	-2.53267443	2.49772240
H	3.38691637	-2.58627066	2.47236259	H	3.45154912	-2.37985055	2.47677610	H	3.01454222	-2.45610903	1.55994287
H	1.79883233	-2.50179978	3.41984325	H	1.77408641	-2.36137348	3.25615657	H	3.03505079	-2.40507648	3.41808828
H	1.77234332	-2.55392923	1.56753307	H	1.93912789	-2.33510313	1.41271574	H	1.41635700	-2.44790721	2.50786814
Cl	2.23564697	-4.87054209	2.55341520	Cl	2.34402969	-4.67416223	2.34536974	Cl	2.51492519	-4.73872763	2.55362108

[*BCh*-Ni-Me···Cl]$^-$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.81856067	C	0.00000000	0.00000000	4.80496609	C	0.00000000	0.00000000	4.80622079
C	4.88826706	0.00000000	4.81170171	C	4.87125364	0.00000000	4.80272180	C	4.89286177	0.00000000	4.77078917
C	4.88097289	-0.26251399	0.00064972	C	4.86473836	0.24039862	0.00377155	C	4.82372050	-0.38018009	-0.01982971
C	3.54150909	-0.21575668	-0.41515026	C	3.53040145	0.18349196	-0.41531676	C	3.50143763	-0.29177176	-0.41643761
C	3.12246483	-0.24933483	-1.78902011	C	3.11804561	0.16680425	-1.78350504	C	3.07139292	-0.34295585	-1.80098766
C	1.75117501	-0.16773637	-1.78952385	C	1.74840889	0.09345921	-1.78485564	C	1.72269589	-0.22321646	-1.79578309
C	1.33778796	-0.08981498	-0.41564428	C	1.33399728	0.07160750	-0.41748518	C	1.31748892	-0.10934153	-0.40719912
N	2.44199667	-0.10948248	0.41151475	N	2.43091302	0.14220480	0.41301197	N	2.41776222	-0.13982362	0.40873785
C	-0.47285779	0.05228560	1.29763076	C	-0.47249244	-0.00724989	1.29592200	C	-0.45396432	0.05218099	1.31711313
C	-1.94842131	0.17166662	1.64516756	C	-1.93632111	-0.10699493	1.64468001	C	-1.92356992	0.18013088	1.65437472
C	-1.95483539	-0.01634388	3.17185362	C	-1.94031229	0.04584505	3.16237399	C	-1.94214427	-0.05614086	3.16648706
C	-0.47491148	0.00874024	3.52048261	C	-0.47311045	0.02999649	3.50989446	C	-0.47035454	-0.00476763	3.52872822
N	0.30822543	0.01539709	2.40958509	N	0.31265864	0.05057313	2.40201769	N	0.32259945	0.00485006	2.40186422
C	1.34079435	0.00406612	5.23360148	C	1.33601248	-0.01139076	5.22346054	C	1.35159918	0.01991247	5.22974944
C	1.75985866	0.02303721	6.60749328	C	1.75054297	-0.08252463	6.58900401	C	1.76772896	0.04832258	6.58449811
C	3.13361317	0.02796761	6.60498633	C	3.12235142	-0.08982037	6.58837709	C	3.15092093	0.05471167	6.57404627
C	3.54840688	0.00684086	5.22968149	C	3.53614931	-0.01847464	5.22265750	C	3.54706995	0.02563711	5.21332480
N	2.44334251	0.00494804	4.40372586	N	2.43601594	0.04601976	4.39653459	N	2.44314751	0.01678537	4.39854120
C	5.36082545	-0.04395993	3.51364191	C	5.34058730	0.08460576	3.50849562	C	5.34635876	-0.07048978	3.48932241
C	6.84033878	-0.01751929	3.16318636	C	6.80720844	0.08325017	3.15782361	C	6.81318635	-0.06943107	3.10528579
C	6.83610404	-0.26982984	1.64581940	C	6.80079482	0.31088292	1.64971882	C	6.77015511	-0.42701364	1.61778695
C	5.35727841	-0.20361939	1.29695474	C	5.33621548	0.22950657	1.29969954	C	5.29876501	-0.30063340	1.28866548
N	4.57665334	-0.10499051	2.40501465	N	4.55120031	0.15048268	2.40520568	N	4.53945822	-0.13562896	2.37383618
Ni	2.43123853	-0.21839037	2.41407818	Ni	2.43186995	-0.05401637	2.40347439	Ni	2.43126414	-0.19987833	2.41632025
H	-0.74328623	0.02380138	-0.79272072	H	-0.74402541	-0.05393323	-0.79139219	H	-0.75365964	0.02734436	-0.78154795
H	-0.74311907	-0.00616346	5.61178973	H	-0.74572346	-0.03102098	5.59603080	H	-0.74238649	-0.01065239	5.60081585
H	5.63281667	0.02815843	5.60309579	H	5.61866997	-0.05544232	5.59079582	H	5.64625737	0.03279013	5.55432092
H	5.62183502	-0.34646139	-0.79022534	H	5.61003903	0.28954472	-0.78671407	H	5.56277231	-0.51318567	-0.80441558
H	-2.39125971	-0.97889181	3.46499666	H	-2.48332288	-0.75038981	3.67966654	H	-2.35308188	-1.04105770	3.41398164
H	-2.54883986	-0.57294523	1.11424153	H	-2.33373281	-1.07633692	1.32291990	H	-2.52708927	-0.53504935	1.09006211
H	1.07792488	-0.15897323	-2.63820022	H	1.07460575	0.06261401	-2.63292256	H	1.04007546	-0.21594932	-2.63627063
H	3.79266133	-0.31962228	-2.63724032	H	3.79302744	0.20682066	-2.63025693	H	3.73847485	-0.45369760	-2.64666824
H	-2.50831788	0.76429371	3.70210527	H	-2.39294147	0.99083851	3.48403130	H	-2.52253475	0.69022647	3.71385120
H	-2.32386774	1.15957202	1.35167436	H	-2.52496476	0.65671008	1.12806572	H	-2.27030203	1.18491994	1.38693044
H	7.41595117	0.46832326	1.08366086	H	7.38768470	-0.42624178	1.09419148	H	7.09358156	-1.45725652	1.42988860
H	7.26877465	0.95977162	3.41631086	H	7.25757292	-0.87759923	3.43203364	H	7.39132055	-0.77688319	3.70414841
H	3.80793768	0.04592837	7.45266084	H	3.79769977	-0.13515930	7.43454793	H	3.82795998	0.07566853	7.41956061
H	1.08846088	0.03685151	7.45755297	H	1.07554770	-0.12136830	7.43578611	H	1.10334230	0.06351298	7.44008722
H	7.23757387	-1.25811352	1.39137877	H	7.19861180	1.29489828	1.37608793	H	7.37999140	0.22718758	0.98982908
H	7.40035141	-0.77065377	3.72554952	H	7.35351355	0.85160516	3.71260107	H	7.24056990	0.92656931	3.26570799
C	2.30444005	-2.19250428	2.49071118	C	2.41118258	-2.01210663	2.40619631	C	2.43246842	-2.18224885	2.56937693
H	3.33341858	-2.53219960	2.56786383	H	3.42481345	-2.31433792	2.66232265	H	2.72127139	-2.52757871	1.58112029
H	1.71326199	-2.41388278	3.37373301	H	1.68227797	-2.29982846	3.16021687	H	3.15818103	-2.40695064	3.34471495
H	1.82127180	-2.48931011	1.56524587	H	2.12000306	-2.31084894	1.40180495	H	1.40881531	-2.42399018	2.84058553
Cl	2.06387717	-6.33622773	2.51940046	Cl	2.27353281	-5.90257172	2.44459561	Cl	2.38219134	-5.93404152	2.84210061

[*BCh*-Ni-Me]

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.81770402
C	4.88885044	0.00000000	4.81126420
C	4.88222030	-0.25099395	0.00045610
C	3.54231944	-0.21052367	-0.41430449
C	3.12302709	-0.24718349	-1.78787811
C	1.75156633	-0.16924778	-1.78832530
C	1.33796460	-0.09018362	-0.41470361
N	2.44242399	-0.10629132	0.41265881
C	-0.47348291	0.05540539	1.29722647
C	-1.94894825	0.17695931	1.64410593
C	-1.95576351	-0.00227230	3.17196818
C	-0.47559598	0.01364931	3.51993110
N	0.30750969	0.01807783	2.40914107
C	1.34091610	-0.00036249	5.23199052
C	1.76001804	0.01396179	6.60581813
C	3.13371279	0.01834197	6.60347450
C	3.54881992	0.00193841	5.22831798
N	2.44370089	0.00261717	4.40196829
C	5.36219483	-0.03648672	3.51330792
C	6.84157420	-0.00269623	3.16327144
C	6.83865144	-0.24504862	1.64419905
C	5.35920660	-0.18933241	1.29635336
N	4.57819908	-0.09730348	2.40462841
Ni	2.43199494	-0.21517280	2.41341317
H	-0.74268079	0.02349327	-0.79327211
H	-0.74252761	-0.00472614	5.61148330
H	5.63268190	0.02800854	5.60331398
H	5.62277300	-0.33033169	-0.79116932
H	-2.40077783	-0.95869645	3.47198259
H	-2.54913032	-0.57099545	1.11749216
H	1.07823051	-0.16184099	-2.63693384
H	3.79346408	-0.31524733	-2.63607255
H	-2.50185314	0.78674295	3.69749623
H	-2.32472047	1.16274787	1.34443691
H	7.41088613	0.50279272	1.08705017
H	7.26682560	0.97407424	3.42322228
H	3.80802907	0.03490440	7.45117088
H	1.08845682	0.02679427	7.45575472
H	7.24974916	-1.22731794	1.38212946
H	7.40391090	-0.75775017	3.72081102
C	2.30867058	-2.18675364	2.48695066
H	3.33818869	-2.52697468	2.55959300
H	1.72157280	-2.41265017	3.37194042
H	1.82225686	-2.48530366	1.56330537

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.80369534
C	4.87222638	0.00000000	4.80270192
C	4.86944192	0.15009108	0.00156791
C	3.53424778	0.10458550	-0.41542016
C	3.12132849	0.07456717	-1.78299938
C	1.75057996	0.02909398	-1.78357361
C	1.33560202	0.03546416	-0.41638135
N	2.43393749	0.09637528	0.41360465
C	-0.47441861	0.01207023	1.29510982
C	-1.94169584	-0.03334324	1.64038585
C	-1.94241751	0.03779025	3.16447096
C	-0.47449143	0.03059021	3.50909676
N	0.31116227	0.04977393	2.40156907
C	1.33611329	-0.01021730	5.22093042
C	1.75058758	-0.07143558	6.58675721
C	3.12229162	-0.07613421	6.58656661
C	3.53664763	-0.01534561	5.22065484
N	2.43646208	0.04210044	4.39337895
C	5.34381969	0.06665074	3.50830466
C	6.81115291	0.06561626	3.16106827
C	6.80755095	0.22999152	1.64449525
C	5.34172591	0.16144754	1.29715203
N	4.55563670	0.11345120	2.40342515
Ni	2.43225250	-0.07728685	2.40340665
H	-0.74389287	-0.03950275	-0.79237039
H	-0.74464540	-0.02838167	5.59585989
H	5.61813652	-0.04390614	5.59291169
H	5.61435689	0.17409057	-0.79041130
H	-2.46182133	-0.80242378	3.63548869
H	-2.39589595	-0.95480993	1.26044612
H	1.07601716	0.00124798	-2.63110368
H	3.79702331	0.09034431	-2.62994114
H	-2.41952705	0.94806668	3.54348231
H	-2.48247360	0.79393041	1.17039000
H	7.37766856	-0.54379557	1.12188244
H	7.27446459	-0.87481062	3.47987049
H	3.79764446	-0.11239244	7.43313382
H	1.07525704	-0.10312886	7.43353579
H	7.22679069	1.19136287	1.32726033
H	7.34436639	0.86586791	3.68288105
C	2.39941811	-2.03305433	2.42231046
H	3.41358231	-2.33873796	2.67199185
H	1.67635968	-2.31221176	3.18527730
H	2.09811660	-2.34060211	1.42359324

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.80492570
C	4.89356341	0.00000000	4.76969721
C	4.82540572	-0.36950557	-0.02038910
C	3.50234865	-0.28738386	-0.41563302
C	3.07197238	-0.34247659	-1.79956630
C	1.72290784	-0.22658365	-1.79421816
C	1.31764330	-0.11058130	-0.40617185
N	2.41829263	-0.13704497	0.41012939
C	-0.45460369	0.05639219	1.31638442
C	-1.92382154	0.18854874	1.65295973
C	-1.94328392	-0.04218872	3.16604060
C	-0.47111734	0.00056663	3.52764598
N	0.32199869	0.00819608	2.40131238
C	1.35167305	0.01436799	5.22711780
C	1.76802752	0.03771244	6.58182096
C	3.15100738	0.04286590	6.57149717
C	3.54758429	0.01915437	5.21088928
N	2.44349722	0.01375753	4.39554318
C	5.34803688	-0.06184120	3.48810304
C	6.81455712	-0.04943658	3.10386567
C	6.77365792	-0.40382342	1.61556818
C	5.30137870	-0.28654594	1.28725125
N	4.54125440	-0.12768932	2.37290525
Ni	2.43201571	-0.19839535	2.41548305
H	-0.75305581	0.02686604	-0.78214954
H	-0.74159320	-0.00891622	5.60024356
H	5.64605498	0.03343402	5.55400758
H	5.56409443	-0.49859765	-0.80594017
H	-2.36180371	-1.02267258	3.41826989
H	-2.52850331	-0.52756604	1.09098791
H	1.04007163	-0.22163505	-2.63453347
H	3.73931277	-0.45192253	-2.64517512
H	-2.51752949	0.71095453	3.71058405
H	-2.26861457	1.19286566	1.38148375
H	7.10457677	-1.43121010	1.42491400
H	7.39843017	-0.75343423	3.70123023
H	3.82811043	0.06258244	7.41696439
H	1.10347893	0.05213145	7.43726628
H	7.37860391	0.25620488	0.98906097
H	7.23407476	0.94953160	3.26629021
C	2.43960539	-2.17361915	2.56271213
H	2.74232935	-2.51977109	1.57831976
H	3.15640563	-2.40147885	3.34616160
H	1.41463527	-2.42683417	2.82073305

S.IX.4 Nickel isobacteriochlorin (*iBCh*) complexes

B3LYP/6-311+G(d,p)				M06-L/6-311+G(d,p)				ωB97X-D/6-311+G(d,p)			
[*iBCh*-Ni]											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.81126378	C	0.00000000	0.00000000	4.80058290	C	0.00000000	0.00000000	4.79150373
C	4.85003600	0.00000000	4.52772256	C	4.83549477	0.00000000	4.54938246	C	4.83383263	0.00000000	4.46478629
C	4.31126130	2.12689769	0.19299624	C	4.35213950	2.01855135	0.17474016	C	4.22436156	2.25162434	0.21796331
C	3.06479617	1.79879971	-0.23551129	C	3.10192191	1.70441259	-0.25427368	C	2.99205185	1.90472593	-0.20390286
C	2.50027307	2.15605164	-1.59097653	C	2.55801959	2.04355990	-1.60981301	C	2.39836194	2.28038881	-1.53559350
C	1.46963457	1.04040627	-1.79443219	C	1.49447515	0.97340142	-1.79313529	C	1.42677228	1.12492803	-1.76457274
C	1.17612344	0.63341255	-0.36786286	C	1.18768658	0.59718122	-0.37404455	C	1.15327214	0.67789003	-0.35182909
N	2.15903903	1.01746381	0.47659429	N	2.18116695	0.96253315	0.46828149	N	2.11479485	1.07669981	0.49709535
C	-0.39878422	-0.14429378	1.31897226	C	-0.40102909	-0.13848229	1.31424542	C	-0.39150890	-0.14102482	1.31920091
C	-1.79668797	-0.57326529	1.70454222	C	-1.79178237	-0.54770079	1.69891781	C	-1.78214671	-0.57443853	1.70558189
C	-1.90665836	-0.02153639	3.12994348	C	-1.89178390	-0.01783593	3.11992715	C	-1.89870787	-0.00449588	3.11733061
C	-0.45236872	0.06244614	3.53198787	C	-0.44858902	0.05869775	3.51955852	C	-0.45086597	0.07317033	3.52339304
N	0.35990869	0.12977918	2.40353957	N	0.36437078	0.12075818	2.39904340	N	0.36290107	0.14648606	2.39249989
C	1.37128681	-0.08815241	5.15339876	C	1.36012113	-0.08066028	5.15090988	C	1.38092624	-0.10280755	5.12023259
C	1.85749098	-0.46158698	6.44693298	C	1.83750950	-0.43194060	6.44673528	C	1.87248326	-0.51061355	6.39462289
C	3.22591857	-0.55783566	6.34231637	C	3.20307307	-0.52600579	6.35342578	C	3.23668004	-0.60728921	6.27459468
C	3.56208069	-0.19706133	5.00144764	C	3.54680631	-0.18448146	5.01585739	C	3.55641520	-0.21834846	4.94510953
N	2.40363607	0.07932345	4.27710389	N	2.39859970	0.07833788	4.27834254	N	2.39323632	0.08113650	4.24359872
C	5.14526457	0.58396287	3.30548606	C	5.14176535	0.55570413	3.32066895	C	5.11420889	0.61560362	3.25949960
C	6.44063560	1.02841393	2.89889874	C	6.43893375	0.97524590	2.91418324	C	6.39563079	1.08039843	2.85604845
C	6.27120941	1.71513687	1.71883213	C	6.28552255	1.63148274	1.71914091	C	6.20632508	1.80282864	1.70407383
C	4.87844923	1.64170569	1.39646856	C	4.90153022	1.56238469	1.38688896	C	4.81476154	1.72993856	1.40339061
N	4.19282556	0.96171782	2.36044180	N	4.20032580	0.91448649	2.36344537	N	4.14985280	1.02088527	2.34287774
Ni	2.28216197	0.55095186	2.38431075	Ni	2.28864500	0.52215533	2.38103135	Ni	2.25743583	0.58605813	2.37342732
H	-0.70627329	-0.26132110	-0.78014020	H	-0.71308472	-0.24765528	-0.77911687	H	-0.70190709	-0.26808571	-0.78089461
H	-0.72515851	-0.08625685	5.61404124	H	-0.73144977	-0.08485549	5.59828934	H	-0.71944995	-0.08986736	5.59855934
H	5.67745339	-0.24048992	5.18895960	H	5.65708147	-0.22850607	5.22263636	H	5.66971650	-0.25773158	5.10920467
H	4.94763019	2.71254591	-0.46259884	H	5.00147093	2.57385493	-0.49500269	H	4.84103666	2.87391798	-0.42190699
H	-2.49193414	-0.64252069	3.81121976	H	-2.47840873	-0.63923375	3.79922128	H	-2.48939978	-0.61369302	3.80277400
H	-1.85223394	-1.67071243	1.69981623	H	-1.86544953	-1.64313434	1.67628560	H	-1.82346771	-1.67071176	1.71582622
H	1.90965725	0.18799061	-2.33038687	H	1.89709229	0.09799560	-2.31991630	H	1.90904714	0.30399825	-2.30980832
H	3.27062518	2.20628879	-2.36322375	H	3.33361468	2.05342999	-2.37797422	H	3.15650656	2.39361630	-2.31170876
H	-2.34994747	0.98359495	3.11888296	H	-2.33397310	0.98710129	3.12726817	H	-2.33075109	1.00319473	3.08824410
H	-2.55096740	-0.19584815	1.01087104	H	-2.54227988	-0.15735352	1.00861705	H	-2.53451983	-0.21141846	1.00390434
H	0.56837054	1.34516454	-2.33057534	H	0.60414395	1.29790772	-2.33550723	H	0.51208168	1.39595918	-2.29377833
H	2.00207809	3.13400104	-1.54233625	H	2.10181095	3.04201885	-1.58893844	H	1.85137370	3.22670350	-1.44401238
H	7.01966982	2.20626362	1.10940938	H	7.04115746	2.09941932	1.09997026	H	6.94260464	2.31920272	1.10147699
H	7.35210640	0.86536611	3.46098611	H	7.34173814	0.81837459	3.49197979	H	7.31547846	0.90440301	3.39985194
H	3.94573828	-0.81579311	7.10951827	H	3.92161190	-0.76837131	7.12703052	H	3.96299001	-0.88695973	7.02758451
H	1.23113037	-0.64837898	7.31038720	H	1.20215016	-0.60919438	7.30593062	H	1.25372804	-0.71642786	7.25870243
[*iBCh*-Ni]$^-$											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84367270	C	0.00000000	0.00000000	4.82968616	C	0.00000000	0.00000000	4.82618370
C	4.87793794	0.00000000	4.83478457	C	4.85984392	0.00000000	4.82563330	C	4.86508867	0.00000000	4.81423952
C	4.83986098	0.19712252	-0.03931644	C	4.82765108	0.13107441	-0.03230527	C	4.82440186	0.12258780	-0.04917898
C	3.54307531	0.18094447	-0.48389438	C	3.53136072	0.12571308	-0.47579125	C	3.53613829	0.12079136	-0.48624658
C	3.16701872	0.26254600	-1.95843323	C	3.16131091	0.19063113	-1.93913116	C	3.15991070	0.18574370	-1.95659995
C	1.65026839	0.02076642	-1.94050389	C	1.64817623	0.01470839	-1.92412221	C	1.63963759	0.01797789	-1.93113589
C	1.31855996	0.05218062	-0.45566978	C	1.31415910	0.03826903	-0.45344153	C	1.31827948	0.03779235	-0.44953966
N	2.42011095	0.10832832	0.31857549	N	2.41370796	0.07528733	0.33032897	N	2.41234514	0.07501280	0.32008491
C	-0.44487646	-0.00454386	1.32322857	C	-0.44438443	-0.00691244	1.31782704	C	-0.43605425	-0.00817485	1.32329920
C	-1.92526399	-0.08641601	1.66609042	C	-1.91166458	-0.07304955	1.66069482	C	-1.91299681	-0.07625975	1.65915846
C	-1.93463980	0.09934507	3.19072287	C	-1.91978171	0.06444484	3.17780400	C	-1.92638723	0.05219655	3.18337448
C	-0.45551968	0.03428895	3.55110206	C	-0.45285082	0.02032906	3.53674884	C	-0.45080954	0.01816484	3.54280190
N	0.33803077	0.03274223	2.41924240	N	0.34614630	0.02118776	2.41298711	N	0.34418778	0.02186326	2.41004800
C	1.35537847	-0.02661989	5.28267670	C	1.34571612	-0.01546324	5.26881406	C	1.36214927	-0.01166932	5.26398575
C	1.76806621	-0.07403314	6.66274723	C	1.75574901	-0.04238437	6.64064003	C	1.77091157	-0.03677700	6.64074752
C	3.14597789	-0.07523375	6.66190360	C	3.13094555	-0.04269711	6.64158613	C	3.14474163	-0.03808239	6.63940684
C	3.55541607	-0.02700711	5.28413243	C	3.53997519	-0.01507934	5.27127671	C	3.54904265	-0.01253533	5.26631972
N	2.43799425	-0.00052523	4.45960601	N	2.42951355	-0.00012350	4.44051375	N	2.43245338	0.00268780	4.44545408
C	5.31532597	0.05794182	3.50931703	C	5.29580249	0.03488230	3.50283458	C	5.30306808	0.03110112	3.49375559
C	6.68968079	0.09710795	3.08761139	C	6.66327157	0.05724313	3.08404015	C	6.67191327	0.05000979	3.07499827
C	6.67677852	0.15456387	1.71097308	C	6.65201953	0.09479282	1.70941878	C	6.65839279	0.08571667	1.70169708
C	5.29206839	0.14779318	1.31117750	C	5.27696282	0.09394763	1.30946994	C	5.27710281	0.08676034	1.30769779
N	4.47948006	0.08992570	2.40060511	N	4.45664073	0.05672400	2.39864924	N	4.47006661	0.05371723	2.38631627
Ni	2.41811618	0.06016268	2.39897930	Ni	2.40904667	0.04012711	2.39325733	Ni	2.41283487	0.04092884	2.38861767
H	-0.77089848	-0.04443278	-0.76531343	H	-0.77132632	-0.03263994	-0.76673312	H	-0.77185998	-0.03201603	-0.76463152
H	-0.75399763	-0.00328036	5.62777935	H	-0.75839917	-0.00156664	5.61055315	H	-0.75288163	-0.00326095	5.61128996
H	5.65110496	-0.02130673	5.60021774	H	5.63269107	-0.01326917	5.59258157	H	5.63895102	-0.01362045	5.57963085
H	5.61630723	0.25412303	-0.79908560	H	5.60259926	0.16967229	-0.79579355	H	5.60113945	0.15866131	-0.80984161
H	-2.51601120	-0.66481262	3.71574263	H	-2.48366102	-0.72701343	3.68121061	H	-2.47490706	-0.75523030	3.67582469
H	-2.32457490	-1.06346499	1.36568856	H	-2.33471550	-1.02736768	1.32417220	H	-2.32601953	-1.03061185	1.31513283

H	1.38203358	-0.95658966	-2.36107817	H	1.33191373	-0.93753837	-2.36693474	H	1.31539895	-0.93340741	-2.36641795
H	3.71392346	-0.47200904	-2.55753210	H	3.68092674	-0.57698808	-2.52084997	H	3.66661723	-0.59334773	-2.53245181
H	-2.35126525	1.07325993	3.47582984	H	-2.36376111	1.01309842	3.50183457	H	-2.37382119	0.99688305	3.50914162
H	-2.50385851	0.67293316	1.13042100	H	-2.47784010	0.71030102	1.14654359	H	-2.46741707	0.71798710	1.15110458
H	1.08192966	0.77371536	-2.49590081	H	1.11139361	0.79782959	-2.46934290	H	1.10557794	0.81357922	-2.45850153
H	3.41393923	1.25313974	-2.35984892	H	3.45850174	1.15542931	-2.36669540	H	3.45659556	1.15047512	-2.38091313
H	7.52333628	0.19755566	1.03494327	H	7.49878625	0.12152369	1.03183785	H	7.50404897	0.10918753	1.02417751
H	7.54799840	0.08397669	3.74983976	H	7.51950884	0.04671525	3.74973488	H	7.53002981	0.03894512	3.73717476
H	3.81695483	-0.10388511	7.51305791	H	3.80313063	-0.05855759	7.49268729	H	3.81620964	-0.05365471	7.49020586
H	1.09951202	-0.10126632	7.51582715	H	1.08413990	-0.05738879	7.49240843	H	1.10217775	-0.05139970	7.49356348

MeCl

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08694599	H	0.00000000	0.00000000	1.08633125	H	0.00000000	0.00000000	1.08723601
H	1.01451467	0.00000000	-0.39014216	H	1.01688044	0.00000000	-0.38219087	H	1.01683743	0.00000000	-0.38486802
H	-0.56802896	0.84058499	-0.39014216	H	-0.55193887	0.85405463	-0.38219087	H	-0.55718534	0.85058971	-0.38486802
Cl	-0.81300034	-1.53061085	-0.55839644	Cl	-0.81461320	-1.49636904	-0.56408018	Cl	-0.81430307	-1.50687408	-0.56246966

[*iBCh*-Ni···MeCl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84387991	C	0.00000000	0.00000000	4.82903742	C	0.00000000	0.00000000	4.82398831
C	4.87813691	0.00000000	4.83463438	C	4.86018965	0.00000000	4.81929968	C	4.86537444	0.00000000	4.80548709
C	4.83840667	0.21770071	-0.03812819	C	4.82287124	0.23997472	-0.03483646	C	4.81520400	0.28787542	-0.05106783
C	3.54171007	0.19629250	-0.48341412	C	3.52559982	0.23611006	-0.47640228	C	3.52554164	0.28689889	-0.48388872
C	3.16750882	0.27589021	-1.95876676	C	3.14817105	0.33486961	-1.93539890	C	3.13667748	0.40731327	-1.94623121
C	1.64632467	0.06243710	-1.94166273	C	1.65168855	0.05210055	-1.92331132	C	1.64744623	0.06278455	-1.92709577
C	1.31753987	0.06613495	-0.45593605	C	1.31268967	0.08230003	-0.45371363	C	1.31591066	0.09884547	-0.44805071
N	2.41899445	0.11654013	0.31848375	N	2.41011298	0.15638843	0.33013499	N	2.40499513	0.19232802	0.32344968
C	-0.44449118	-0.01439973	1.32331322	C	-0.44438023	-0.00645872	1.31842556	C	-0.43492388	-0.00665191	1.32401777
C	-1.92323858	-0.11488356	1.66766730	C	-1.90712418	-0.12883474	1.66620752	C	-1.90471887	-0.14926953	1.66776403
C	-1.93401712	0.09495790	3.18899690	C	-1.91899631	0.08070621	3.17467952	C	-1.92331007	0.09762049	3.17642354
C	-0.45557550	0.03059586	3.55104307	C	-0.45334185	0.03725275	3.53635856	C	-0.45058900	0.04696222	3.54126079
N	0.33820931	0.03043001	2.41936033	N	0.34536236	0.05326479	2.41252303	N	0.34486638	0.06763442	2.40861582
C	1.35555525	-0.02411088	5.28276223	C	1.34645296	-0.01967626	5.26735273	C	1.36309046	-0.02555434	5.25984440
C	1.76815615	-0.06928718	6.66308094	C	1.75812804	-0.08270945	6.63754690	C	1.77363769	-0.10936676	6.63371404
C	3.14606234	-0.07197598	6.66217247	C	3.13334416	-0.08404035	6.63666419	C	3.14742440	-0.10889475	6.63063034
C	3.55566358	-0.02656411	5.28427178	C	3.54066587	-0.02183071	5.26684919	C	3.54987483	-0.02505765	5.25924808
N	2.43834912	-0.00007284	4.45980815	N	2.42910559	0.01756712	4.43868603	N	2.43224262	0.02512270	4.44130597
C	5.31544620	0.06150566	3.50961735	C	5.29541862	0.06464580	3.49706914	C	5.30128635	0.07792320	3.48599604
C	6.68941936	0.10927977	3.08789009	C	6.66263586	0.09010489	3.07722535	C	6.66941442	0.09735853	3.06465523
C	6.67580477	0.17630593	1.71172414	C	6.65014546	0.15932290	1.70381385	C	6.65323990	0.17806723	1.69330214
C	5.29088106	0.16578477	1.31215773	C	5.27458819	0.17502423	1.30574456	C	5.27119953	0.20645325	1.30322864
N	4.47906918	0.09714970	2.40142843	N	4.45558477	0.11779497	2.39485287	N	4.46618663	0.14639740	2.38207646
Ni	2.41750416	0.05733398	2.39817956	Ni	2.40814223	0.10095973	2.39302473	Ni	2.41101337	0.13062565	2.38926385
H	-0.77090024	-0.04680961	-0.76540495	H	-0.76968457	-0.06641231	-0.76646092	H	-0.76860238	-0.07979594	-0.76426743
H	-0.75399623	-0.00327248	5.62807969	H	-0.75808661	-0.01789780	5.61013022	H	-0.75227662	-0.02182156	5.60930608
H	5.65114179	-0.02239239	5.60020106	H	5.63389600	-0.03626518	5.58466574	H	5.64043129	-0.04746906	5.56832126
H	5.61459448	0.28029296	-0.79784935	H	5.59655068	0.29844148	-0.79846220	H	5.58956275	0.35768277	-0.81173268
H	-2.52012015	-0.65659846	3.72638743	H	-2.49790020	-0.67254969	3.71733092	H	-2.50714380	-0.64042203	3.73188901
H	-2.30436517	-1.10479985	1.38580342	H	-2.27544093	-1.12327061	1.38360767	H	-2.23988822	-1.16121303	1.41212994
H	1.35484192	-0.89622663	-2.38816831	H	1.41335660	-0.93447876	-2.34073408	H	1.45326850	-0.94333798	-2.31680482
H	3.69914095	-0.47573016	-2.55096748	H	3.72075341	-0.36163051	-2.55511559	H	3.72970173	-0.25364147	-2.58299234
H	-2.34522329	1.07656223	3.45632608	H	-2.34589304	1.05450270	3.44469500	H	-2.33109507	1.08662453	3.41367041
H	-2.51667912	0.62404297	1.11984686	H	-2.51810105	0.59263059	1.11466964	H	-2.52103765	0.55136690	1.09823083
H	1.09252575	0.84280516	-2.47401470	H	1.06026757	0.77660514	-2.49194970	H	1.02566669	0.75839579	-2.49680296
H	3.43589861	1.25688866	-2.36868450	H	3.36716938	1.34051486	-2.31500843	H	3.30332057	1.43407332	-2.29096592
H	7.52199232	0.22723849	1.03577596	H	7.49647452	0.19696384	1.02619848	H	7.49757198	0.21522034	1.01472495
H	7.54827338	0.09539185	3.74948585	H	7.51973373	0.05842362	3.74117825	H	7.52880590	0.05426882	3.72388226
H	3.81711354	-0.09816619	7.51338030	H	3.80631334	-0.12460511	7.48632297	H	3.82005428	-0.16159784	7.47903033
H	1.09974139	-0.09400427	7.51637556	H	1.08773501	-0.12026901	7.48961051	H	1.10600340	-0.16104319	7.48596997
C	2.70246646	-3.59324388	1.85187620	C	2.00137674	-2.92249855	1.83806329	C	1.88911040	-3.02218401	1.67761188
H	3.69535742	-3.17120554	1.73497083	H	3.03414488	-2.67267123	1.61199354	H	2.92208462	-2.75856679	1.47088604
H	2.31854770	-3.42357790	2.85256864	H	1.77385001	-2.73476510	2.88359272	H	1.64016425	-2.83330330	2.71759641
H	2.02079522	-3.21415888	1.09727034	H	1.31572792	-2.39069109	1.18456020	H	1.21041617	-2.49901455	1.01046361
Cl	2.83887170	-5.40193304	1.61329609	Cl	1.78590666	-4.70266267	1.53740882	Cl	1.69934627	-4.80002121	1.37637793

[*iBCh*-Ni—Me—Cl]$^{‡-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84358606	C	0.00000000	0.00000000	4.82916533	C	0.00000000	0.00000000	4.82508043
C	4.87869909	0.00000000	4.82691474	C	4.86001252	0.00000000	4.82387782	C	4.86529717	0.00000000	4.80616514
C	4.83601071	-0.25848169	-0.04495093	C	4.82913873	-0.00927263	-0.03517232	C	4.81972071	0.22099787	-0.05393157
C	3.53908464	-0.24644414	-0.48850121	C	3.53299905	-0.01460712	-0.48080537	C	3.53170730	0.21491229	-0.48912593
C	3.15601965	-0.35646639	-1.95810441	C	3.16385800	-0.05893739	-1.94477439	C	3.14898954	0.30601249	-1.95482315
C	1.64917506	-0.05945848	-1.94177063	C	1.64531792	0.06494181	-1.92579864	C	1.63976392	0.06026256	-1.93061645
C	1.31697765	-0.07904424	-0.45772193	C	1.31438854	0.01641351	-0.45574564	C	1.31651548	0.07669828	-0.45055785
N	2.41780126	-0.15276095	0.31279182	N	2.41546123	0.00301467	0.32250617	N	2.40924503	0.14254887	0.31642311
C	-0.44389533	0.02001269	1.32369021	C	-0.44637545	-0.00447161	1.31803656	C	-0.43605817	-0.00379917	1.32360458
C	-1.91862422	0.15687816	1.66921171	C	-1.91451063	-0.04339713	1.65896827	C	-1.90940396	-0.10306621	1.66232076
C	-1.93532950	-0.07083442	3.18786637	C	-1.92193359	0.07345490	3.17821151	C	-1.92474324	0.07353877	3.18129811
C	-0.45722203	-0.03175807	3.55169862	C	-0.45583254	0.01866274	3.53681164	C	-0.45150361	0.03228399	3.54308747
N	0.33447431	-0.04565329	2.41989432	N	0.33956138	0.00964914	2.41310912	N	0.34156516	0.04775698	2.40956317
C	1.35654774	0.02598425	5.28084156	C	1.34647651	-0.00754367	5.26824565	C	1.36348065	-0.01197852	5.26146670

C	1.77158195	0.09519479	6.65883958	C	1.75651344	-0.01901588	6.64099275	C	1.77395146	-0.05340570	6.63618478
C	3.14938965	0.09574690	6.65555335	C	3.13107846	-0.01909036	6.64108838	C	3.14798607	-0.06059674	6.63195816
C	3.55713643	0.02630528	5.27915261	C	3.54018959	-0.00800294	5.27070160	C	3.55025941	-0.02010111	5.25998672
N	2.43827691	-0.01529801	4.45889787	N	2.42959604	-0.00065645	4.44301575	N	2.43211187	0.00941037	4.44294892
C	5.31525886	-0.06654754	3.50163477	C	5.29784665	0.01453567	3.50109381	C	5.30208781	0.06025507	3.48659773
C	6.68840727	-0.09411649	3.07782033	C	6.66506424	0.02285045	3.08179108	C	6.66903724	0.10094557	3.06760277
C	6.67506614	-0.16695562	1.70204993	C	6.65424804	0.02124588	1.70722283	C	6.65474210	0.17048814	1.69537962
C	5.29031765	-0.18170551	1.30422650	C	5.27848086	0.01142826	1.30752205	C	5.27424210	0.16737915	1.30260390
N	4.48064895	-0.12005478	2.39389978	N	4.46144249	0.01134744	2.39693443	N	4.46982038	0.10283750	2.38016545
Ni	2.42003571	-0.17018726	2.40152193	Ni	2.41151888	-0.04673303	2.39554129	Ni	2.41432218	0.00564745	2.38523017
H	-0.76991347	0.06290765	-0.76457962	H	-0.77220359	-0.00180257	-0.76615578	H	-0.77071047	-0.05628699	-0.76388090
H	-0.75288793	0.01573157	5.62820457	H	-0.75702574	0.00515077	5.61102615	H	-0.75164336	-0.01318778	5.61078046
H	5.65276660	0.03494881	5.59068026	H	5.63247978	-0.00370490	5.59111451	H	5.63989570	-0.02764025	5.57008733
H	5.61150309	-0.32919234	-0.80413757	H	5.60471257	-0.02319874	-0.79850193	H	5.59517513	0.27782741	-0.81413508
H	-2.35887955	-1.05057487	3.44191139	H	-2.48688520	-0.72413956	3.67036448	H	-2.48762377	-0.70585142	3.70095643
H	-2.53251410	-0.55644896	1.11090792	H	-2.35798580	-0.98193414	1.30597811	H	-2.28843138	-1.08312562	1.35253051
H	1.05218486	-0.78953848	-2.49702321	H	1.13386454	-0.73172728	-2.47537738	H	1.36905735	-0.91442540	-2.35113670
H	3.36197594	-1.36981616	-2.32452234	H	3.49601366	-1.00149077	-2.39481685	H	3.69549723	-0.42298860	-2.55833387
H	-2.51093783	0.68191180	3.73442118	H	-2.36214772	1.01813590	3.51737783	H	-2.35356397	1.03835858	3.47201185
H	-2.26697393	1.16205781	1.39951568	H	-2.45995202	0.76124008	1.15558565	H	-2.48965688	0.65357136	1.12732800
H	1.41845649	0.92893554	-2.35915446	H	1.29425867	1.00942743	-2.35806487	H	1.06382593	0.81767942	-2.46916935
H	3.72862458	0.33556934	-2.58250284	H	3.65553025	0.74120770	-2.50650142	H	3.39062594	1.30127943	-2.34253478
H	7.52100242	-0.20588224	1.02540367	H	7.50057138	0.02481862	1.02900592	H	7.49917907	0.21809995	1.01802729
H	7.54703027	-0.06146154	3.73882324	H	7.52093191	0.02892170	3.74770346	H	7.52724950	0.08265407	3.72923448
H	3.82138719	0.14048681	7.50500030	H	3.80372451	-0.02412325	7.49173549	H	3.82106935	-0.08741440	7.48099332
H	1.10416833	0.13866861	7.51191293	H	1.08487062	-0.02464508	7.49248101	H	1.10637085	-0.07516436	7.48941951
C	2.36107344	-2.69226957	2.42131367	C	2.32448341	-2.55197077	2.37876398	C	2.36216578	-2.40493401	2.22477446
H	3.33317613	-2.59856248	1.97147937	H	3.39267004	-2.43570396	2.46859744	H	3.39793025	-2.29969830	1.94789164
H	2.26976708	-2.55068772	3.48347264	H	1.72184056	-2.38692181	3.25664161	H	2.09509068	-2.35933560	3.26743088
H	1.48860599	-2.56698145	1.80545926	H	1.87585993	-2.37796801	1.41445924	H	1.60125546	-2.23882126	1.48098857
Cl	2.31754695	-4.89422629	2.45861933	Cl	2.24722766	-4.70932387	2.35867597	Cl	2.31719556	-4.59107363	2.08160865

[*iBCh*-Ni-Me···Cl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.83692958	C	0.00000000	0.00000000	4.82499335	C	0.00000000	0.00000000	4.81987560
C	4.87600640	0.00000000	4.80723166	C	4.85721779	0.00000000	4.80797974	C	4.86130465	0.00000000	4.78087093
C	4.81358575	-0.47173047	-0.04473516	C	4.80998531	-0.35303927	-0.03547161	C	4.77406510	-0.64875383	-0.03739739
C	3.51898260	-0.42652147	-0.48169799	C	3.51661850	-0.30591396	-0.47860006	C	3.49093575	-0.56510939	-0.46742074
C	3.12007518	-0.57945156	-1.93946717	C	3.13274067	-0.43108174	-1.93047235	C	3.07988566	-0.74944636	-1.91236070
C	1.64308713	-0.16571047	-1.93104841	C	1.63979309	-0.13491136	-1.92021164	C	1.63088371	-0.26702681	-1.91357332
C	1.31011474	-0.13826266	-0.45086236	C	1.30954436	-0.09113731	-0.45280157	C	1.30466777	-0.18582778	-0.44015225
N	2.40899247	-0.23858371	0.32279501	N	2.40952409	-0.14626702	0.32425527	N	2.38971656	-0.30729432	0.33492488
C	-0.43867012	0.03575405	1.32069149	C	-0.44193627	0.02589012	1.31578811	C	-0.42527916	0.04227413	1.32105482
C	-1.90817366	0.18493672	1.66819836	C	-1.90466517	0.10790005	1.66012922	C	-1.88643748	0.20712576	1.67146239
C	-1.92893009	-0.07601909	3.17978116	C	-1.91596461	-0.07788624	3.17095377	C	-1.91025141	-0.11290619	3.16427254
C	-0.45584029	-0.03142932	3.54813212	C	-0.45473509	-0.01856720	3.53473500	C	-0.44595926	-0.04166929	3.54001506
N	0.34149959	-0.02934398	2.41763056	N	0.34253134	0.00131684	2.41202707	N	0.35504213	-0.03517056	2.40740122
C	1.35485092	0.03926227	5.26460124	C	1.34461421	0.03598986	5.25801178	C	1.36196683	0.05911402	5.24523139
C	1.77383879	0.12241051	6.63587438	C	1.75893906	0.06924411	6.62564189	C	1.77820469	0.16789996	6.60923929
C	3.15100279	0.13120273	6.62875956	C	3.13294130	0.07528797	6.62221136	C	3.15227737	0.18326610	6.59809160
C	3.55813995	0.04868275	5.25719175	C	3.54111516	0.04191539	5.25537539	C	3.55063921	0.07690738	5.23304299
N	2.43637064	0.00555979	4.43635227	N	2.42775362	0.03632872	4.42961962	N	2.42861459	0.01384721	4.42013635
C	5.30303409	-0.11667803	3.48632324	C	5.28782358	-0.07973555	3.48863586	C	5.28167241	-0.16900459	3.46942885
C	6.66883013	-0.20154175	3.05984885	C	6.64839864	-0.17160971	3.06784011	C	6.63817977	-0.30774923	3.04998395
C	6.64895896	-0.34443824	1.69048694	C	6.63250176	-0.28076354	1.69879459	C	6.61122200	-0.50681387	1.69148440
C	5.26767919	-0.34074702	1.29558997	C	5.25971297	-0.24974876	1.29980088	C	5.23381557	-0.47962368	1.30344545
N	4.45973026	-0.19332338	2.38248295	N	4.44747185	-0.11134699	2.38577741	N	4.43770347	-0.26964539	2.37177244
Ni	2.41245517	-0.28181471	2.41524273	Ni	2.40940772	-0.20480116	2.41053132	Ni	2.39597462	-0.29036796	2.40487799
H	-0.76777998	0.07127489	-0.76478190	H	-0.77099414	0.03099338	-0.76569262	H	-0.76717606	0.08035310	-0.76375445
H	-0.74968566	0.00650872	5.62370593	H	-0.75454947	-0.01315682	5.60797703	H	-0.74878899	0.00158760	5.60714709
H	5.65185538	0.04394731	5.56776583	H	5.63114286	0.00914337	5.57268421	H	5.64070687	0.05569595	5.53748732
H	5.58321408	-0.61225768	-0.79903516	H	5.58073030	-0.47865987	-0.79226612	H	5.53699728	-0.84823866	-0.78484409
H	-2.34050858	-1.06673557	3.40905414	H	-2.33358274	-1.04916561	3.45966145	H	-2.28386625	-1.12710829	3.34433171
H	-2.52937854	-0.50545200	1.09088123	H	-2.48243932	-0.64504966	1.11680750	H	-2.51989312	-0.44395458	1.06512531
H	0.98787603	-0.84945841	-2.47784457	H	1.03541634	-0.88508795	-2.43868612	H	0.94152741	-0.93539831	-2.43481911
H	3.24045129	-1.62462327	-2.25053302	H	3.34649166	-1.44510004	-2.28782495	H	3.14575737	-1.80956925	-2.17995972
H	-2.51174637	0.65777917	3.74307718	H	-2.49548735	0.68204954	3.70226658	H	-2.51796621	0.57621531	3.75424724
H	-2.23747024	1.20221338	1.42145068	H	-2.30034894	1.08339486	1.35404426	H	-2.18448800	1.24240095	1.46920436
H	1.49388502	0.83563961	-2.35449304	H	1.39996060	0.83053717	-2.38127573	H	1.52645302	0.72915843	-2.35841334
H	3.74288873	0.03115353	-2.59873926	H	3.71058901	0.25127724	-2.55981533	H	3.72895405	-0.19342222	-2.59217479
H	7.48930182	-0.43996731	1.01340938	H	7.47308786	-0.37441205	1.02117393	H	7.44546096	-0.65717605	1.01748973
H	7.52888033	-0.15803118	3.71758783	H	7.50438771	-0.15833199	3.73256221	H	7.49931157	-0.26421806	3.70593726
H	3.82593090	0.18836874	7.47455809	H	3.80837416	0.09809228	7.46955878	H	3.83008596	0.25455805	7.44022027
H	1.10687211	0.17134807	7.48819921	H	1.08780543	0.08521686	7.47646419	H	1.11232579	0.22489354	7.46148091
C	2.26521587	-2.25399854	2.57283966	C	2.29263057	-2.15292993	2.54685684	C	2.23470740	-2.26713982	2.62930649
H	3.25229841	-2.58679301	2.87861448	H	3.26908016	-2.48307450	2.89460687	H	3.19108049	-2.56531752	3.04840339
H	1.50003651	-2.42527206	3.32363579	H	1.50114254	-2.34857692	3.26740693	H	1.39598164	-2.39505703	3.30799614
H	1.98212262	-2.59208328	1.58031380	H	2.05154412	-2.50208688	1.54202976	H	2.04981888	-2.63624056	1.62258466
Cl	-2.91011494	-4.84204723	-2.41920531	Cl	1.39200046	-4.19859919	-0.59625168	Cl	1.00731824	-4.32029436	-0.54020745

[*iBCh*-Ni-Me]

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.83790404
C	4.87548303	0.00000000	4.82268384
C	4.83470153	-0.15642611	-0.05017642
C	3.54058721	-0.14624625	-0.49119952
C	3.16327823	-0.21887509	-1.96175909
C	1.63823232	-0.04943616	-1.93777252
C	1.31490231	-0.04668070	-0.45470500
N	2.41958582	-0.07628178	0.31602681
C	-0.43992077	0.02117845	1.32036369
C	-1.91703425	0.10077915	1.65927203
C	-1.93137865	-0.03415940	3.18782030
C	-0.45487980	-0.00934736	3.54842620
N	0.34173353	-0.00450961	2.41757667
C	1.35321467	0.01612517	5.26942086
C	1.76798207	0.03878863	6.64432890
C	3.14495082	0.04065008	6.64210762
C	3.55619816	0.01805010	5.26964995
N	2.43700807	0.01364337	4.44356345
C	5.30703171	-0.03391149	3.49876612
C	6.67484062	-0.06322567	3.07246693
C	6.66111189	-0.10861665	1.69640946
C	5.28130707	-0.10569085	1.29731741
N	4.46809570	-0.04959226	2.38909705
Ni	2.42971783	-0.19531155	2.41188260
H	-0.77207818	0.02563580	-0.76370340
H	-0.75090698	-0.00269721	5.62364408
H	5.64876924	0.00749194	5.58700530
H	5.61170098	-0.20940486	-0.80826185
H	-2.38519551	-0.97756579	3.51221440
H	-2.48040203	-0.68514628	1.14671066
H	1.10288118	-0.85373335	-2.45210519
H	3.46292583	-1.18532760	-2.38259373
H	-2.47536170	0.77425050	3.68526570
H	-2.32274689	1.06080293	1.31904074
H	1.31247320	0.89397367	-2.39119138
H	3.67169733	0.55741074	-2.54151816
H	7.50474904	-0.13932862	1.01743748
H	7.53205706	-0.04895909	3.73509060
H	3.81736828	0.05791780	7.49161537
H	1.09806556	0.05362974	7.49560456
C	2.43687992	-2.17468090	2.49740460
H	3.21870344	-2.43593707	3.20303494
H	1.44153937	-2.44463687	2.83791632
H	2.64811203	-2.49620658	1.48166352

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.82408383
C	4.85737095	0.00000000	4.81239758
C	4.82322869	-0.09837482	-0.04383544
C	3.52896676	-0.08789317	-0.48694055
C	3.15547817	-0.14892310	-1.94598562
C	1.63768237	-0.03377515	-1.92417292
C	1.31159016	-0.02487098	-0.45483624
N	2.41461742	-0.02929239	0.32004298
C	-0.44286943	0.02113807	1.31560505
C	-1.90798112	0.06953091	1.65542141
C	-1.91877520	-0.02514003	3.17477830
C	-0.45496054	0.00146231	3.53394140
N	0.34240131	0.01777729	2.41106004
C	1.34417691	0.01369075	5.25747162
C	1.75674584	0.00810735	6.62615295
C	3.13036726	0.00971405	6.62504324
C	3.54073811	0.01582347	5.25855028
N	2.42812270	0.03450566	4.43074411
C	5.29075036	-0.01464458	3.49158890
C	6.65310482	-0.05034511	3.06926245
C	6.64148306	-0.07925723	1.69607472
C	5.26911017	-0.06047592	1.29589937
N	4.45274669	-0.00456529	2.38661591
Ni	2.42301837	-0.14954251	2.40579678
H	-0.77225761	0.00573736	-0.76509373
H	-0.75472958	-0.01552527	5.60684537
H	5.63019893	-0.01204799	5.57806975
H	5.59864908	-0.14569816	-0.80481544
H	-2.38193928	-0.95135819	3.53134887
H	-2.45176335	-0.74124850	1.16107220
H	1.12874593	-0.85925086	-2.43122781
H	3.49635641	-1.09167190	-2.38693009
H	-2.45851882	0.79637465	3.65482725
H	-2.34495365	1.00346166	1.28481923
H	1.27359364	0.88651565	-2.39395897
H	3.64069397	0.65145715	-2.51249745
H	7.48504324	-0.10996886	1.01642696
H	7.50778082	-0.05184257	3.73572487
H	3.80426921	0.00847440	7.47386740
H	1.08425554	0.00440363	7.47598073
C	2.43941044	-2.10320663	2.48219082
H	3.22542311	-2.37181360	3.18342719
H	1.44883918	-2.39028374	2.82824396
H	2.64829487	-2.43190705	1.46633463

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.81917656
C	4.86218476	0.00000000	4.78349157
C	4.78484963	-0.57022095	-0.04412477
C	3.49969889	-0.50762405	-0.47079573
C	3.08755896	-0.69779113	-1.91452122
C	1.63838498	-0.21727684	-1.91359142
C	1.30723388	-0.16431468	-0.43966206
N	2.39422412	-0.27519859	0.33498894
C	-0.42551031	0.04279594	1.32138360
C	-1.88694558	0.20729120	1.67012270
C	-1.91101736	-0.10089082	3.16536116
C	-0.44610464	-0.03573062	3.53953143
N	0.35559501	-0.03115585	2.40704704
C	1.36202122	0.05141361	5.24419622
C	1.77791338	0.14750848	6.60966374
C	3.15141620	0.15949053	6.59941669
C	3.55084158	0.06575995	5.23362072
N	2.42879643	0.01192317	4.41906177
C	5.28668099	-0.14280774	3.46989278
C	6.64448117	-0.25859160	3.04909863
C	6.62061915	-0.43070796	1.68668273
C	5.24380537	-0.41273585	1.29844318
N	4.44495913	-0.23132554	2.37009682
Ni	2.40818993	-0.27325508	2.40311805
H	-0.76667143	0.07987425	-0.76412510
H	-0.74908000	0.00100841	5.60609497
H	5.63905604	0.04799435	5.54314869
H	5.54980415	-0.74847367	-0.79473053
H	-2.29249772	-1.11027306	3.35555171
H	-2.51899605	-0.45033291	1.06907197
H	0.95148233	-0.87057352	-2.45603918
H	3.15259080	-1.76002988	-2.17557832
H	-2.51278130	0.59787207	3.74986507
H	-2.18664260	1.24005042	1.45767204
H	1.53968831	0.78971057	-2.33495454
H	3.73464723	-0.14618488	-2.59958307
H	7.45707797	-0.55642333	1.01045330
H	7.50471775	-0.21695872	3.70634118
H	3.82880858	0.22279262	7.44240991
H	1.11154453	0.20036076	7.46175620
C	2.35534695	-2.25534789	2.60163491
H	3.13040172	-2.48151905	3.32727541
H	1.34824598	-2.46285704	2.95214814
H	2.56335082	-2.62486271	1.60142016

S.IX.5 Nickel hexahydroporphyrin (*HEX-Pi*) complexes

B3LYP/6-311+G(d,p)				M06-L/6-311+G(d,p)				ωB97X-D/6-311+G(d,p)			
[*HEX-Pi*-Ni]											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.81924041	C	0.00000000	0.00000000	4.80743210	C	0.00000000	0.00000000	4.80102977
C	4.87823049	0.00000000	4.40985725	C	4.85502986	0.00000000	4.44822520	C	4.87876710	0.00000000	4.34117074
C	4.12782436	-2.43990436	0.32235173	C	4.19158734	2.31752952	0.28806803	C	4.04723711	-2.53055850	0.34727669
C	2.92094336	-1.98980541	-0.15381087	C	2.97643320	1.88860346	-0.18490889	C	2.85630222	-2.05839755	-0.12635193
C	2.37681296	-2.31366617	-1.52546883	C	2.45324789	2.19331018	-1.55628740	C	2.30048306	-2.38918863	-1.48508341
C	1.44674873	-1.11838859	-1.77520486	C	1.47678596	1.04681326	-1.77833518	C	1.40546558	-1.17827222	-1.75043180
C	1.13676159	-0.67917862	-0.36339559	C	1.15505492	0.64198328	-0.37129523	C	1.11221617	-0.71100416	-0.35033839
N	2.09366292	-1.12354519	0.50978658	N	2.12242518	1.06699276	0.49547503	N	2.05680979	-1.16354845	0.52738251
C	-0.39767629	0.14856094	1.33477145	C	-0.39738118	-0.15097050	1.32520852	C	-0.39276831	0.13742723	1.34101196
C	-1.79569876	0.58521525	1.71718625	C	-1.78290519	-0.58209537	1.71171108	C	-1.79095413	0.55783305	1.71729898
C	-1.91915053	0.01106503	3.13453817	C	-1.89973247	-0.01558665	3.11920050	C	-1.91541932	-0.01940969	3.12702510
C	-0.46739275	-0.06758642	3.55125009	C	-0.45895202	0.05989880	3.53326166	C	-0.46998083	-0.07974442	3.54838173
N	0.34820746	-0.13595603	2.40821419	N	0.35597290	0.12254269	2.40323693	N	0.34998656	-0.15116176	2.39805571
C	1.37901089	0.06570368	5.16581446	C	1.36497362	-0.05893002	5.16307074	C	1.39115175	0.07670413	5.13853400
C	1.89213850	0.42712703	6.43020539	C	1.86713007	-0.40694406	6.43435296	C	1.90728305	0.45280787	6.38256079
C	3.27895737	0.52114559	6.28854708	C	3.24599153	-0.50703853	6.30613648	C	3.29825225	0.53476455	6.22836203
C	3.57381559	0.17815912	4.95129369	C	3.55514396	-0.17440335	4.97075216	C	3.57241499	0.18029014	4.90359813
N	2.40948921	-0.09427821	4.25990857	N	2.40076891	0.09187093	4.26580546	N	2.40718167	-0.09719152	4.22873188
C	5.13920386	-0.60217651	3.22658391	C	5.13091815	0.58433006	3.25644758	C	5.12034420	-0.61304277	3.17402657
C	6.51023514	-0.94681923	2.68929915	C	6.50252129	0.90907881	2.74001321	C	6.47200514	-0.95881252	2.60523589
C	6.19006449	-2.15532053	1.80001821	C	6.20972296	2.07761570	1.81017270	C	6.13370184	-2.18706574	1.76089028
C	4.73390959	-1.90893399	1.46799827	C	4.77161397	1.83049510	1.45558763	C	4.67292154	-1.95778536	1.46620280
N	4.15357361	-1.08532950	2.34820941	N	4.16605173	1.04271565	2.35987658	N	4.11126332	-1.11681162	2.32047034
Ni	2.25221739	-0.60675497	2.39072034	Ni	2.26187629	0.57929971	2.38726274	Ni	2.23255586	-0.62844125	2.38051313
H	-0.69803513	0.29428135	-0.77585353	H	-0.70378112	-0.28029546	-0.77672361	H	-0.69823082	0.29762251	-0.77341171
H	-0.72024275	0.08394573	5.62830704	H	-0.72923991	-0.08185304	5.60883593	H	-0.71402480	0.08303944	5.61557854
H	5.71875994	0.30331567	5.02780893	H	5.69054416	-0.28860178	5.08018446	H	5.72632917	0.32096957	4.94019323
H	4.70849925	-3.11659741	-0.29473207	H	4.79093933	2.96191210	-0.34656759	H	4.61491345	-3.22613282	-0.25954210
H	-2.36286624	-0.99395236	3.09759012	H	-2.49947627	-0.61921885	3.80347947	H	-2.34330674	-1.02886133	3.08378799
H	-2.54863625	0.22384901	1.01309897	H	-1.83346709	-1.67988359	1.71700960	H	-2.53381263	0.19074345	1.00712170
H	0.54539807	-1.35551272	-2.34400054	H	1.96500394	0.21296113	-2.30007811	H	0.49590455	-1.39984519	-2.31000655
H	1.80231123	-3.24907690	-1.48192541	H	3.25161914	2.26497736	-2.29749533	H	1.70311579	-3.30633701	-1.41781219
H	-2.51790637	0.62076917	3.81473101	H	-2.34258497	0.98960506	3.08999365	H	-2.52242982	0.58315113	3.80452465
H	-1.84042373	1.68387260	1.72508014	H	-2.53857083	-0.22498241	1.00870827	H	-1.83802895	1.65462609	1.72476727
H	6.81066040	-2.23867538	0.90506795	H	6.84982034	2.13310223	0.92702618	H	6.23378327	-3.11415848	2.34029647
H	6.90217313	-0.12115680	2.07852825	H	6.90826835	0.06122482	2.17092315	H	7.21645821	-1.14134275	3.38173663
H	4.01501709	0.76487820	7.04552308	H	3.97917341	-0.74072416	7.06935322	H	4.04154851	0.78561033	6.97570773
H	1.29330205	0.62639554	7.31105660	H	1.25513505	-0.59976503	7.30782532	H	1.31734737	0.66540191	7.26614931
H	6.27710199	-3.09750344	2.36024047	H	6.29419817	3.03864184	2.33650208	H	6.72455852	-2.29069481	0.84930666
H	7.23118285	-1.15278477	3.48344451	H	7.20801322	1.13327742	3.54270849	H	6.83446571	-0.14752990	1.96138489
H	1.98000955	-0.31518113	-2.30187363	H	0.58345263	1.30982316	-2.34817579	H	1.95808295	-0.39623504	-2.28477173
H	3.16778826	-2.43637434	-2.26811636	H	1.92826753	3.15774357	-1.54579386	H	3.08616107	-2.54390325	-2.22553992
[*HEX-Pi*-Ni]$^-$											
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84710764	C	0.00000000	0.00000000	4.83292964	C	0.00000000	0.00000000	4.83061049
C	4.91340270	0.00000000	4.80264218	C	4.88449652	0.00000000	4.79736123	C	4.91695267	0.00000000	4.77243352
C	4.82201539	-0.45074469	-0.02300674	C	4.81163655	0.41956263	-0.01706717	C	4.79860327	-0.47351548	-0.03419357
C	3.51178599	-0.37475754	-0.46175624	C	3.50385860	0.34755950	-0.45948016	C	3.49267380	-0.39668417	-0.45925071
C	3.13843236	-0.49462286	-1.93202630	C	3.13435255	0.45835107	-1.91797873	C	3.11523644	-0.52140719	-1.92189960
C	1.64977784	-0.12155867	-1.93505465	C	1.64995125	0.11849153	-1.92136996	C	1.63918141	-0.12863899	-1.92258857
C	1.30232338	-0.11409441	-0.45377326	C	1.30143373	0.10824193	-0.45370808	C	1.29544829	-0.12085452	-0.44651180
N	2.41399251	-0.20974058	0.32999805	N	2.40836537	0.19438463	0.33665024	N	2.40294184	-0.22397263	0.33610820
C	-0.44182550	0.02313721	1.33629496	C	-0.43974080	-0.02493693	1.32700570	C	-0.43170268	0.01852394	1.34360689
C	-1.91676292	0.17682871	1.67934002	C	-1.90058191	-0.17514056	1.67460649	C	-1.90141514	0.17332251	1.68071516
C	-1.93965283	-0.09697635	3.19068152	C	-1.91917148	0.08885764	3.17464624	C	-1.93055878	-0.11354622	3.18273215
C	-0.46248978	-0.03667694	3.56424989	C	-0.45466255	0.03198682	3.54608436	C	-0.46068453	-0.04671408	3.56174938
N	0.33564933	-0.04993565	2.42042112	N	0.34766266	0.04365146	2.41381437	N	0.34248168	-0.06373006	2.41088615
C	1.35876659	0.02458850	5.29633151	C	1.34694809	-0.02245402	5.28214929	C	1.36829592	0.02918544	5.28184276
C	1.77428372	0.08797818	6.65417942	C	1.75992353	-0.08147013	6.63656883	C	1.77911684	0.09293415	6.62797099
C	3.17207273	0.09114683	6.64148237	C	3.15100403	-0.08477636	6.62634819	C	3.18071446	0.09203381	6.61164190
C	3.56316690	0.02610677	5.27647862	C	3.54433032	-0.02416714	5.26614963	C	3.55999727	0.02622313	5.25642568
N	2.45358634	-0.01250809	4.46184547	N	2.43965228	0.01236703	4.44541653	N	2.45460211	-0.01013850	4.44818781
C	5.35157843	-0.08920990	3.51382397	C	5.31983033	0.08545850	3.50626481	C	5.34643816	-0.08607759	3.49469470
C	6.82160325	-0.07024750	3.10897629	C	6.77893613	0.06884773	3.11013014	C	6.80716842	-0.06504373	3.07676000
C	6.76967879	-0.47919663	1.62928854	C	6.73707459	0.45512390	1.63727064	C	6.74161751	-0.48163983	1.60658757
C	5.28858928	-0.35391017	1.30153149	C	5.27111726	0.33256390	1.30062281	C	5.26306623	-0.36321832	1.29411083
N	4.53197191	-0.18046454	2.38896275	N	4.50054656	0.16966709	2.38939254	N	4.51548384	-0.18035355	2.36762319
Ni	2.43387273	-0.11316503	2.40849142	Ni	2.42406914	0.10484130	2.40115742	Ni	2.42920567	-0.12034851	2.40034094
H	-0.77286974	0.07404301	-0.76124718	H	-0.77283899	-0.06891045	-0.76316853	H	-0.77489958	0.08085992	-0.75758278
H	-0.75343737	0.01257238	5.63328420	H	-0.76006934	-0.01187819	5.61353805	H	-0.75149950	0.01333100	5.61876081
H	5.68136486	0.05839464	5.57248352	H	5.65608982	-0.05353459	5.56477516	H	5.68747881	0.06066530	5.53965562
H	5.58090685	-0.59347073	-0.78850356	H	5.57320364	0.55393531	-0.78283150	H	5.55575007	-0.62261947	-0.79931270

H	-2.34578416	-1.09498897	3.40248078	H	-2.52039497	-0.62958842	3.73977000	H	-2.32628038	-1.11668461	3.38032864
H	-2.54584801	-0.50471046	1.09801090	H	-2.23675772	-1.19184668	1.43019075	H	-2.52540414	-0.50078874	1.08771662
H	1.48209788	0.87549909	-2.36207541	H	1.45623590	-0.86814620	-2.36089857	H	1.48578936	0.87381455	-2.33741328
H	3.75406242	0.15416172	-2.56243602	H	3.73965803	-0.20504355	-2.54340275	H	3.74058907	0.11357106	-2.55414980
H	-2.54140486	0.62253672	3.75394288	H	-2.32992917	1.08227866	3.39748707	H	-2.53690868	0.59694202	3.74987573
H	-2.24487757	1.19791193	1.44109231	H	-2.53344122	0.50495159	1.09571946	H	-2.21593853	1.19815138	1.44778883
H	7.38798320	0.14578803	0.97711360	H	7.36051895	-0.17496497	0.99498832	H	7.05825565	-1.52067398	1.45419167
H	7.23474083	0.94075392	3.22280028	H	7.19865538	-0.93648390	3.24531141	H	7.42199837	-0.72927435	3.68918953
H	3.84621853	0.13251277	7.49041089	H	3.82727772	-0.12404493	7.47433274	H	3.85742669	0.13228039	7.45848544
H	1.11544948	0.12621613	7.51518815	H	1.09596160	-0.11660235	7.49440493	H	1.12235128	0.13267800	7.49038781
H	7.09286971	-1.51820226	1.47786858	H	7.07029376	1.48846078	1.47152201	H	7.34544108	0.14220593	0.94191201
H	7.43174972	-0.73897042	3.72355067	H	7.38451782	0.74280217	3.72344004	H	7.21437157	0.94760950	3.17863977
H	3.29958379	-1.52450762	-2.27534773	H	1.03602246	0.83047729	-2.48152749	H	3.26062019	-1.55675896	-2.24953020
H	1.02368254	-0.82128095	-2.49691040	H	3.32260898	1.47774084	-2.27786361	H	0.99987029	-0.81633351	-2.48144581

MeCl

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08694599	H	0.00000000	0.00000000	1.08633125	H	0.00000000	0.00000000	1.08723601
H	1.01451467	0.00000000	-0.39014216	H	1.01688044	0.00000000	-0.38219087	H	1.01683743	0.00000000	-0.38486802
H	-0.56802896	0.84058499	-0.39014216	H	-0.55193887	0.85405463	-0.38219087	H	-0.55718534	0.85058971	-0.38486802
Cl	-0.81300034	-1.53061085	-0.55839644	Cl	-0.81461320	-1.49636904	-0.56408018	Cl	-0.81430307	-1.50687408	-0.56246966

[*HEX-Pi*-Ni···MeCl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84719100	C	0.00000000	0.00000000	4.83259878	C	0.00000000	0.00000000	4.83100424
C	4.91334438	0.00000000	4.80268403	C	4.88462934	0.00000000	4.79603536	C	4.91617846	0.00000000	4.77602576
C	4.82430648	-0.42412106	-0.02566253	C	4.81216805	0.41549511	-0.01875743	C	4.80157072	-0.43030330	-0.03377053
C	3.51333055	-0.35783288	-0.46382736	C	3.50406854	0.34410636	-0.46108311	C	3.49601038	-0.34858996	-0.46026340
C	3.14122515	-0.47448764	-1.93460060	C	3.13650933	0.43850936	-1.92129669	C	3.11959248	-0.48547935	-1.92198294
C	1.64812574	-0.11920969	-1.93605072	C	1.65057854	0.10533317	-1.92222786	C	1.63824657	-0.11375575	-1.92373449
C	1.30233628	-0.11235369	-0.45445915	C	1.30134140	0.10996468	-0.45455555	C	1.29702575	-0.09898982	-0.44723818
N	2.41453251	-0.20451039	0.32875357	N	2.40752166	0.20460223	0.33548311	N	2.40674079	-0.17760780	0.33462197
C	-0.44120648	0.02460739	1.33650640	C	-0.44036662	-0.01683951	1.32736715	C	-0.43177867	0.01672308	1.34370534
C	-1.91514921	0.18439103	1.68048226	C	-1.89995115	-0.17754458	1.67607007	C	-1.90419100	0.14655832	1.67906171
C	-1.93858085	-0.10142711	3.18944857	C	-1.91988549	0.09565645	3.17440864	C	-1.92924612	-0.12794531	3.18348299
C	-0.46199070	-0.03717002	3.56410719	C	-0.45550179	0.04220801	3.54605774	C	-0.45980342	-0.04430247	3.56168455
N	0.33641964	-0.05061730	2.42043683	N	0.34632358	0.06196813	2.41359398	N	0.34349433	-0.04899195	2.41113697
C	1.35876909	0.02498998	5.29651757	C	1.34725114	-0.02470642	5.28171631	C	1.36774683	0.03218878	5.28323376
C	1.77428660	0.08441289	6.65462671	C	1.76051052	-0.10776313	6.63504149	C	1.77753663	0.07871837	6.63049115
C	3.17213015	0.08351040	6.64208335	C	3.15153973	-0.11403143	6.62407189	C	3.17911377	0.07362267	6.61522158
C	3.56312211	0.02285774	5.27678831	C	3.54427543	-0.03061381	5.26454160	C	3.55909249	0.02523270	5.25939436
N	2.45358431	-0.01122952	4.46205614	N	2.43964905	0.02296645	4.44571974	N	2.45444663	0.00246506	4.45005501
C	5.35175393	-0.07997242	3.51329220	C	5.32102850	0.10206114	3.50615177	C	5.34606493	-0.06863813	3.49726674
C	6.82180111	-0.05165964	3.10941574	C	6.78110143	0.09298467	3.11195359	C	6.80675295	-0.04855926	3.08056309
C	6.77259814	-0.44507129	1.62541140	C	6.73928205	0.45854863	1.63352231	C	6.74011890	-0.46905693	1.61188345
C	5.29049238	-0.32864066	1.29919996	C	5.27216438	0.34163583	1.29989432	C	5.26463163	-0.32690803	1.29543808
N	4.53277498	-0.16705420	2.38759315	N	4.50220490	0.18958494	2.39001795	N	4.51625856	-0.14227297	2.36794859
Ni	2.43461003	-0.11634335	2.40792515	Ni	2.42230321	0.12756236	2.40241985	Ni	2.42970720	-0.07892337	2.40133421
H	-0.77319173	0.07395316	-0.76093683	H	-0.77234282	-0.07859294	-0.76276025	H	-0.77682958	0.06189715	-0.75743067
H	-0.75363475	0.01100839	5.63316924	H	-0.75988836	-0.02149520	5.61320115	H	-0.75200136	0.00207782	5.61879041
H	5.68134886	0.05535164	5.57269937	H	5.65586634	-0.06178877	5.56321384	H	5.68652657	0.04540653	5.54446729
H	5.58416259	-0.55761737	-0.79185566	H	5.57424097	0.53767154	-0.78608950	H	5.55870912	-0.58332589	-0.79816512
H	-2.33896830	-1.10381492	3.39208281	H	-2.52133771	-0.61879682	3.74424611	H	-2.31579248	-1.13256998	3.39108297
H	-2.54904820	-0.48749713	1.09325744	H	-2.22638759	-1.19926142	1.43899544	H	-2.51420497	-0.54522591	1.09176260
H	1.46678808	0.87412725	-2.36603761	H	1.04022227	0.81528413	-2.48887255	H	1.46923944	0.88264500	-2.34696090
H	3.74895334	0.18570942	-2.56090255	H	3.33011571	1.45240001	-2.29356157	H	3.73586277	0.15498528	-2.55769488
H	-2.54482223	0.60980924	3.75826641	H	-2.33054768	1.09089160	3.38970708	H	-2.54164273	0.58218543	3.74462991
H	-2.23577738	1.21023368	1.45164152	H	-2.53942215	0.49262379	1.09296947	H	-2.23884391	1.16258519	1.43603984
H	7.38508316	0.19263892	0.98004224	H	7.35666268	-0.18613871	0.99977901	H	7.03761568	-1.51494207	1.46596661
H	7.23104517	0.95951012	3.23490566	H	7.21121040	-0.90529970	3.26419038	H	7.42285500	-0.70918065	3.69547978
H	3.84631902	0.12184058	7.49112816	H	3.82803512	-0.16968645	7.47096927	H	3.85535474	0.10120025	7.46294777
H	1.11555605	0.12136911	7.51576597	H	1.09690736	-0.15758389	7.49243098	H	1.12016854	0.10737344	7.49289198
H	7.10488040	-1.47935042	1.46192381	H	7.08067389	1.48625329	1.45121697	H	7.35755507	0.14062857	0.94668925
H	7.43395643	-0.72483799	3.71717346	H	7.37833237	0.78277730	3.71596574	H	7.21179239	0.96565725	3.17769554
H	3.31557723	-1.50019505	-2.28389879	H	3.73937629	-0.23549198	-2.53768628	H	3.27973374	-1.52053086	-2.24399477
H	1.02975422	-0.82876591	-2.49426008	H	1.45207657	-0.88415608	-2.35313005	H	1.00826109	-0.81588897	-2.47522959
C	2.40573009	-3.74613276	2.27545347	C	2.41717003	-2.97412588	2.30979815	C	2.81283369	-3.28847063	1.81934253
H	3.44864245	-3.44715431	2.29972889	H	3.40007756	-2.52759770	2.43374796	H	3.35794472	-2.80622351	1.01353210
H	1.88661013	-3.44127376	3.17811335	H	1.78193302	-2.76913000	3.16653992	H	3.24705531	-3.04828385	2.78542697
H	1.90786903	-3.37092580	1.38740329	H	1.95159023	-2.64593176	1.38533947	H	1.75898340	-3.02741598	1.79056618
Cl	2.35601746	-5.57445953	2.20245649	Cl	2.63481060	-4.77724441	2.20513359	Cl	2.94742296	-5.08132653	1.58062894

[*HEX-Pi*-Ni—Me—Cl]$^{‡-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.84593746	C	0.00000000	0.00000000	4.83240807	C	0.00000000	0.00000000	4.82969674
C	4.91720046	0.00000000	4.79239067	C	4.88689738	0.00000000	4.79179240	C	4.91969226	0.00000000	4.76158211
C	4.82008784	-0.47482394	-0.02965074	C	4.81053405	0.42124503	-0.02184922	C	4.78180329	-0.61084516	-0.02690815
C	3.50945099	-0.39942884	-0.46501367	C	3.50158097	0.37089253	-0.46172358	C	3.47992112	-0.49504034	-0.45305387
C	3.13337846	-0.51389543	-1.93406072	C	3.13010888	0.49258556	-1.91807465	C	3.09333497	-0.64484490	-1.90962532
C	1.64634262	-0.13534699	-1.93466511	C	1.64461794	0.15821064	-1.92189130	C	1.63715968	-0.18491322	-1.91860939
C	1.30064614	-0.12407080	-0.45378559	C	1.29881246	0.12986279	-0.45427110	C	1.29240234	-0.14589923	-0.44448232
N	2.41303043	-0.23107345	0.32696629	N	2.40617682	0.21864755	0.33268348	N	2.39868737	-0.26140818	0.33771046

C	-0.44355953	0.02843970	1.33685148	C	-0.44265320	-0.02902325	1.32772604	C	-0.43165604	0.02652332	1.34454898
C	-1.91651936	0.19617988	1.67859813	C	-1.90391877	-0.18072156	1.67095584	C	-1.89963893	0.18614791	1.68152433
C	-1.94440962	-0.07513104	3.19075369	C	-1.92618928	0.05247644	3.17681719	C	-1.93182326	-0.11293932	3.18121214
C	-0.46752018	-0.03494747	3.56524780	C	-0.46078876	0.02282838	3.54725328	C	-0.46368578	-0.04665303	3.56298465
N	0.32807399	-0.05698214	2.42067089	N	0.33768525	0.04315213	2.41437734	N	0.33837121	-0.06207564	2.41136041
C	1.36052989	0.02470289	5.29089982	C	1.34809012	-0.00348692	5.27984392	C	1.36997759	0.03888994	5.27669319
C	1.77973887	0.10573168	6.64535766	C	1.76315514	-0.06255618	6.63344433	C	1.78376040	0.12097224	6.61928038
C	3.17761756	0.11021947	6.62928622	C	3.15385620	-0.06847211	6.62167447	C	3.18588072	0.12475995	6.59994227
C	3.56643485	0.02656494	5.26585194	C	3.54638754	-0.00816360	5.26142873	C	3.56278701	0.04186277	5.24664639
N	2.45441608	-0.02369999	4.45571619	N	2.44043388	0.03493743	4.44465461	N	2.45506972	-0.00766115	4.44266357
C	5.35859123	-0.09568961	3.50568368	C	5.32688404	0.08156203	3.50174142	C	5.34800604	-0.11396643	3.48659458
C	6.82809954	-0.07218746	3.09974181	C	6.78541712	0.05686690	3.10458160	C	6.80591367	-0.12131049	3.06219893
C	6.77675131	-0.45438484	1.61206081	C	6.74364117	0.41852229	1.62471341	C	6.72848745	-0.59772401	1.61080970
C	5.29206925	-0.36467124	1.29309594	C	5.27437752	0.32412347	1.29550387	C	5.25327531	-0.46135167	1.29627120
N	4.54021622	-0.20372576	2.38237740	N	4.51024143	0.17327450	2.38545245	N	4.51480717	-0.22692585	2.36295007
Ni	2.42855507	-0.21043836	2.41470134	Ni	2.42588079	0.06782457	2.40453321	Ni	2.42648067	-0.20867948	2.40941091
H	-0.77157000	0.08192558	-0.76129239	H	-0.77186811	-0.07273729	-0.76335396	H	-0.77418252	0.08431325	-0.75734224
H	-0.74998663	0.02115207	5.63486047	H	-0.75705122	-0.02153078	5.61543100	H	-0.74862992	0.01262594	5.62013188
H	5.68324004	0.06966316	5.56291606	H	5.65643885	-0.06082368	5.56044779	H	5.69046463	0.06887147	5.52746544
H	5.57714759	-0.61433921	-0.79714247	H	5.57179843	0.54731185	-0.78889672	H	5.53207079	-0.80933141	-0.78705101
H	-2.36468178	-1.06661548	3.40443092	H	-2.50725077	-0.69418595	3.72606713	H	-2.32451121	-1.11906303	3.36904331
H	-2.54964217	-0.48076289	1.09660348	H	-2.24289955	-1.18937442	1.40086609	H	-2.52541355	-0.47940144	1.08120001
H	1.48040432	0.86124361	-2.36262675	H	1.03146222	0.88010527	-2.46954671	H	1.53264393	0.82024972	-2.34184949
H	3.75109771	0.13399635	-2.56286452	H	3.32257738	1.51386224	-2.26916254	H	3.74640215	-0.06105746	-2.56231420
H	-2.53542084	0.65455288	3.75196833	H	-2.36204336	1.02894970	3.42319361	H	-2.54049733	0.59150884	3.75301751
H	-2.23358078	1.21963737	1.43701555	H	-2.53052812	0.51550978	1.10483193	H	-2.20656854	1.21478792	1.45618665
H	7.37061201	0.20244050	0.96864338	H	7.34626115	-0.23877136	0.99014680	H	7.01809217	-1.65012124	1.50270746
H	7.24559835	0.93378724	3.23511665	H	7.20545098	-0.94502908	3.25944752	H	7.41832649	-0.76396488	3.69914295
H	3.85367568	0.16580281	7.47560742	H	3.83084742	-0.10974721	7.46867935	H	3.86423879	0.17784713	7.44449304
H	1.12279958	0.15814346	7.50680455	H	1.10023765	-0.09906529	7.49173928	H	1.12872048	0.17108964	7.48221606
H	7.12799559	-1.47956290	1.43450381	H	7.09941808	1.43970427	1.43540623	H	7.34423988	-0.01769053	0.91843473
H	7.43423975	-0.75645857	3.70096450	H	7.38972358	0.74308086	3.70522328	H	7.22030636	0.89199591	3.11811480
H	3.29105611	-1.54388889	-2.27794217	H	3.73316584	-0.16861565	-2.54738842	H	3.18767756	-1.69634904	-2.20265630
H	1.01596273	-0.83432556	-2.49225973	H	1.44442082	-0.82179726	-2.37219223	H	0.96708654	-0.84674900	-2.47198152
C	2.30278357	-2.73217163	2.50659121	C	2.51675811	-2.44414761	2.30781104	C	2.41571807	-2.62491423	2.53196316
H	3.37494707	-2.65599320	2.46400392	H	3.43417463	-2.28535554	2.85084767	H	2.95250464	-2.57303250	1.59911720
H	1.81131535	-2.55567484	3.44652352	H	1.58954645	-2.35068205	2.84944907	H	2.95324757	-2.47646344	3.45347374
H	1.74012244	-2.61864674	1.59748793	H	2.51063214	-2.22472627	1.25222090	H	1.34544572	-2.49952790	2.52726875
Cl	2.20956094	-4.92810937	2.58041871	Cl	2.59310823	-4.58590059	2.17853144	Cl	2.38227064	-4.80865315	2.63714487

[*HEX-Pi*-Ni-Me···Cl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.83462771	C	0.00000000	0.00000000	4.81817081	C	0.00000000	0.00000000	4.81989960
C	4.92314097	0.00000000	4.75955792	C	4.89677538	0.00000000	4.77688357	C	4.92423404	0.00000000	4.70375770
C	4.79193090	-0.68811340	-0.02346598	C	4.80733218	0.47931107	-0.01826883	C	4.70091006	-1.05130083	0.00801905
C	3.48482067	-0.57907139	-0.44687705	C	3.50018542	0.39558716	-0.44727035	C	3.41022679	-0.85946679	-0.41284318
C	3.08652410	-0.75503624	-1.89953616	C	3.12877943	0.48474276	-1.90283771	C	2.98171120	-1.09180904	-1.84208957
C	1.64226150	-0.24470330	-1.91562770	C	1.65256375	0.12194665	-1.90452658	C	1.62278167	-0.39996227	-1.89140164
C	1.29391245	-0.18381063	-0.44047695	C	1.29963952	0.12368269	-0.44190805	C	1.27365562	-0.26913934	-0.42759233
N	2.40336145	-0.31303765	0.34691294	N	2.40364363	0.24745891	0.34985146	N	2.36782465	-0.45202636	0.36635558
C	-0.44264793	0.04948376	1.33205794	C	-0.44987514	-0.00487343	1.32303430	C	-0.42805232	0.05690831	1.34128975
C	-1.90999779	0.23502761	1.67435291	C	-1.90862739	-0.15421458	1.66520896	C	-1.88528625	0.26807112	1.68347954
C	-1.94446263	-0.06312016	3.18030332	C	-1.93304288	0.08065039	3.17043236	C	-1.93090327	-0.09258980	3.16834857
C	-0.47186988	-0.02750270	3.55902334	C	-0.47044726	0.05125669	3.54065728	C	-0.46789386	-0.04535961	3.55835047
N	0.32859850	-0.03864875	2.41664356	N	0.32667802	0.08762414	2.40812869	N	0.33925049	-0.06228866	2.40786257
C	1.36153358	0.02608214	5.26212493	C	1.34946295	-0.02400789	5.25011519	C	1.37341928	0.04590806	5.24450799
C	1.79043795	0.10943144	6.60729715	C	1.76855154	-0.13470051	6.59409631	C	1.80369719	0.17290126	6.57281205
C	3.18760135	0.12024355	6.58446182	C	3.15831860	-0.14483171	6.58232105	C	3.20544781	0.18866342	6.53764813
C	3.57452779	0.03508102	5.22655943	C	3.55573099	-0.03403753	5.23180068	C	3.57193791	0.06301566	5.19025665
N	2.45525293	-0.00859249	4.41608117	N	2.44626919	0.05718393	4.41518783	N	2.45277099	-0.01414961	4.39656115
C	5.35956931	-0.13271733	3.47845304	C	5.34124305	0.12688453	3.49512149	C	5.33537247	-0.20390213	3.43807184
C	6.82167460	-0.13760107	3.05912967	C	6.79717250	0.13665442	3.09699631	C	6.77870923	-0.26711779	2.98455229
C	6.75288655	-0.62906245	1.60607741	C	6.74589456	0.49469930	1.61683180	C	6.66191841	-0.95508383	1.62445176
C	5.27350815	-0.51613286	1.28558050	C	5.27816289	0.39710401	1.29451502	C	5.19545088	-0.78770732	1.30058510
N	4.52979286	-0.27146891	2.36466261	N	4.52031161	0.24045370	2.38568011	N	4.48002904	-0.39898755	2.33937817
Ni	2.41548589	-0.31756539	2.42740008	Ni	2.42654701	0.01174621	2.40947945	Ni	2.40479557	-0.35896368	2.41873086
H	-0.76496174	0.09114188	-0.76571722	H	-0.76318890	-0.09499522	-0.76835548	H	-0.76352678	0.12213245	-0.76165265
H	-0.74119820	0.01339335	5.63083829	H	-0.74670753	-0.04240596	5.60899111	H	-0.73875525	0.01769417	5.61826008
H	5.68668393	0.08175530	5.53015203	H	5.65824464	-0.08310237	5.55012675	H	5.69903099	0.11564784	5.45852355
H	5.53461825	-0.90322172	-0.78634322	H	5.56040064	0.60498122	-0.79217083	H	5.42136717	-1.38351714	-0.73266819
H	-2.36132888	-1.05986661	3.37360475	H	-2.51132081	-0.66653719	3.72060869	H	-2.32363501	-1.10661966	3.30723636
H	-2.55118820	-0.41951136	1.07698816	H	-2.24333095	-1.16324719	1.39356763	H	-2.53919754	-0.33990945	1.05402616
H	1.57407346	0.76172184	-2.34785931	H	1.02516208	0.81537436	-2.47109319	H	1.70066751	0.60144926	-2.33032966
H	3.75633414	-0.21473684	-2.57362670	H	3.30360747	1.50438227	-2.26612965	H	3.71099209	-0.70285636	-2.55507049
H	-2.53698699	0.65521189	3.75338932	H	-2.36725441	1.05737964	3.41634724	H	-2.54132746	0.58723142	3.76638891
H	-2.20461831	1.26906516	1.45080453	H	-2.53112060	0.54150154	1.09504501	H	-2.13937592	1.32002972	1.50438029
H	7.36424514	-0.04606487	0.91105895	H	7.34093409	-0.16538455	0.97890550	H	6.88410433	-2.02790541	1.68447112
H	7.23411748	0.87813699	3.11156631	H	7.24212476	-0.85257072	3.25741542	H	7.41348661	-0.80121597	3.69442653
H	3.86843352	0.18136899	7.42571452	H	3.83619534	-0.21448969	7.42567771	H	3.89295642	0.27484028	7.37122507
H	1.13648109	0.16338152	7.47005832	H	1.10404259	-0.19778096	7.44855643	H	1.15691022	0.24909485	7.43925834
H	7.06301043	-1.67783098	1.50791887	H	7.09743025	1.51489540	1.41870119	H	7.30049609	-0.52879152	0.84737623

H	7.43486679	-0.77203181	3.70496279	H	7.38057647	0.84196138	3.69544795	H	7.18099041	0.74655835	2.87021098
H	3.14152483	-1.81837277	-2.16525334	H	3.74873903	-0.17447808	-2.51628074	H	2.88621455	-2.17044303	-2.01283617
H	0.95100814	-0.88513681	-2.46964245	H	1.47369235	-0.87483764	-2.32463431	H	0.85864063	-0.94935833	-2.44410704
C	2.26470390	-2.28307230	2.63781283	C	2.43914785	-1.94516183	2.36699347	C	2.33804494	-2.34067509	2.64616075
H	3.23476599	-2.60767088	3.00151532	H	3.45013813	-2.24081206	2.63960301	H	2.79523716	-2.71866645	1.73637990
H	1.46281416	-2.44080514	3.35195486	H	1.69497152	-2.27195412	3.08887290	H	2.90690750	-2.54506194	3.54725892
H	2.03326938	-2.64638672	1.64107466	H	2.18010720	-2.20775459	1.34340136	H	1.27633366	-2.55119217	2.73406093
Cl	2.10048381	-6.42801269	2.54197012	Cl	2.54811891	-5.82504140	2.00136071	Cl	2.14549483	-6.07920834	2.70556790

[*HEX*-*Pi*-Ni-Me]

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.83413168	C	0.00000000	0.00000000	4.81776291	C	0.00000000	0.00000000	4.81958942
C	4.92358863	0.00000000	4.75952116	C	4.89696431	0.00000000	4.77551001	C	4.92432279	0.00000000	4.69983969
C	4.79356091	-0.67963232	-0.02410963	C	4.80796794	0.47550704	-0.01944282	C	4.69849713	-1.06117075	0.00712293
C	3.48598836	-0.57411607	-0.44678359	C	3.50065938	0.39158332	-0.44776922	C	3.40818090	-0.86735948	-0.41287263
C	3.08843748	-0.74863663	-1.89981445	C	3.12910998	0.48164339	-1.90313732	C	2.97933515	-1.09653494	-1.84251646
C	1.64208157	-0.24458674	-1.91516111	C	1.65126194	0.12590458	-1.90465395	C	1.62193629	-0.40187992	-1.89074981
C	1.29404516	-0.18384574	-0.43997943	C	1.29958595	0.12330263	-0.44190655	C	1.27323708	-0.27195831	-0.42696968
N	2.40379335	-0.31151493	0.34752320	N	2.40420027	0.24422763	0.34980393	N	2.36660626	-0.45846724	0.36749521
C	-0.44294533	0.05197647	1.33174558	C	-0.44984493	-0.00482283	1.32296369	C	-0.42796023	0.05852651	1.34073964
C	-1.90985066	0.24070878	1.67367979	C	-1.90898416	-0.14946038	1.66519299	C	-1.88422593	0.27492720	1.68293901
C	-1.94509334	-0.05462328	3.18018260	C	-1.93244926	0.08744522	3.17001976	C	-1.93132603	-0.08407511	3.16811606
C	-0.47228205	-0.02428782	3.55859301	C	-0.47017121	0.05184419	3.54027586	C	-0.46816816	-0.04299400	3.55797574
N	0.32824248	-0.03665055	2.41640588	N	0.32739217	0.08520623	2.40785460	N	0.33928671	-0.06168131	2.40756816
C	1.36153912	0.02265585	5.26128384	C	1.34945772	-0.02561871	5.24906828	C	1.37340044	0.04397105	5.24346916
C	1.79042641	0.10181573	6.60660577	C	1.76913955	-0.13937476	6.59249638	C	1.80508311	0.16834022	6.57129868
C	3.18753134	0.11184245	6.58402551	C	3.15883889	-0.14894546	6.58034002	C	3.20676754	0.18455848	6.53490015
C	3.57482083	0.03067405	5.22609301	C	3.55596815	-0.03499368	5.23014699	C	3.57256055	0.06135549	5.18736012
N	2.45557466	-0.01010076	4.41511903	N	2.44591187	0.05830617	4.41381738	N	2.45242997	-0.01370814	4.39446660
C	5.36058031	-0.12719241	3.47810386	C	5.34192681	0.12820281	3.49395903	C	5.33458245	-0.20412824	3.43396889
C	6.82253776	-0.12522790	3.05854620	C	6.79786010	0.13965072	3.09632596	C	6.77741534	-0.26510889	2.97911231
C	6.75547340	-0.61276889	1.60408579	C	6.74645452	0.49576832	1.61572955	C	6.66073334	-0.95771111	1.62142252
C	5.27540037	-0.50652150	1.28468965	C	5.27904881	0.39593423	1.29320689	C	5.19359487	-0.79435411	1.29868043
N	4.53099405	-0.26636715	2.36424859	N	4.52099980	0.24031839	2.38450134	N	4.47823047	-0.40269228	2.33644039
Ni	2.41605215	-0.31480778	2.42710396	Ni	2.42767924	0.00955395	2.40833885	Ni	2.40155719	-0.35948592	2.42131532
H	-0.76448298	0.09163221	-0.76612466	H	-0.76343933	-0.09116022	-0.76854547	H	-0.76265897	0.12533425	-0.76196104
H	-0.74082706	0.01475753	5.63062629	H	-0.74656792	-0.04006145	5.60876541	H	-0.73839526	0.01960640	5.61817095
H	5.68660081	0.08232761	5.53054256	H	5.65817845	-0.08237556	5.54904460	H	5.69949935	0.11807465	5.45378067
H	5.53664712	-0.89025805	-0.78785245	H	5.56047514	0.60187814	-0.79372357	H	5.41868911	-1.39282969	-0.73405242
H	-2.36664502	-1.04894712	3.37585158	H	-2.51468839	-0.65562481	3.72155745	H	-2.32962461	-1.09572685	3.30847678
H	-2.55238120	-0.41344780	1.07731430	H	-2.24714096	-1.15769210	1.39462199	H	-2.54061222	-0.33078089	1.05391260
H	1.56898674	0.76105663	-2.34820420	H	1.02680178	0.82548086	-2.46687337	H	1.70194517	0.60000815	-2.32806079
H	3.75591363	-0.20340872	-2.57221849	H	3.30905238	1.50011022	-2.26690461	H	3.70941085	-0.70716717	-2.55438681
H	-2.53418929	0.66754102	3.75192939	H	-2.36132951	1.06685653	3.41438249	H	-2.53803408	0.59966517	3.76538001
H	-2.20239194	1.27485680	1.44823486	H	-2.52915240	0.54754949	1.09420595	H	-2.13392077	1.32776535	1.50308587
H	7.36305465	-0.02416544	0.91051672	H	7.34275539	-0.16387862	0.97852460	H	6.88599265	-2.02976594	1.68438600
H	7.23086836	0.89194221	3.11377199	H	7.24449547	-0.84859182	3.25837095	H	7.41463786	-0.79483397	3.69004442
H	3.86830965	0.17192167	7.42537176	H	3.83702985	-0.21900957	7.42336869	H	3.89494446	0.27100027	7.36784678
H	1.13629342	0.15520220	7.46924831	H	1.10491470	-0.20300730	7.44709758	H	1.15909650	0.24463141	7.43827954
H	7.07167056	-1.65939284	1.50226303	H	7.09639508	1.51623232	1.41657552	H	7.29711947	-0.53218322	0.84217141
H	7.43839711	-0.75886982	3.70261529	H	7.37982410	0.84672419	3.69398187	H	7.17657592	0.74927936	2.86084457
H	3.14870184	-1.81087321	-2.16881697	H	3.74593408	-0.18067111	-2.51644744	H	2.88199930	-2.17457461	-2.01608988
H	0.95317236	-0.88836079	-2.46827270	H	1.46623579	-0.86762970	-2.32968189	H	0.85640512	-0.94858173	-2.44418485
C	2.26600131	-2.27726714	2.64071793	C	2.44776135	-1.94500812	2.37037727	C	2.30645747	-2.32249594	2.70861281
H	3.23579890	-2.60312872	3.00492831	H	3.45803922	-2.23767684	2.64853879	H	2.55284932	-2.73813661	1.73498948
H	1.46430965	-2.43574917	3.35520346	H	1.70168361	-2.27125441	3.09081699	H	3.04176555	-2.53646217	3.47801960
H	2.03423189	-2.64423498	1.64491931	H	2.19359076	-2.21543793	1.34748412	H	1.28023141	-2.49946479	3.01862439

S.IX.6 Nickel octahydroporphyrin (*OCT-Pi*) complexes

[*OCT-Pi*-Ni]

B3LYP/6-311+G(d,p)				M06-L/6-311+G(d,p)				ωB97X-D/6-311+G(d,p)			
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.82644634	C	0.00000000	0.00000000	4.81570912	C	0.00000000	0.00000000	4.80550706
C	4.81105109	0.00000000	4.44046877	C	4.80620018	0.00000000	4.51003714	C	4.78702370	0.00000000	4.38215789
C	4.09733789	-2.52121321	0.38703453	C	4.23170425	2.27854016	0.30648586	C	4.01029224	-2.61405351	0.42493807
C	2.89043087	-2.05662344	-0.11044169	C	3.00570652	1.85971064	-0.17587046	C	2.81747539	-2.13037641	-0.07638087
C	2.33685637	-2.39280792	-1.48004946	C	2.47731909	2.17501565	-1.54738894	C	2.25464893	-2.47338027	-1.43508137
C	1.47104110	-1.15471351	-1.76185633	C	1.53258140	1.00168038	-1.78099913	C	1.43600308	-1.21572308	-1.73817330
C	1.13987388	-0.70376176	-0.35397348	C	1.17591740	0.62515682	-0.37030754	C	1.11759803	-0.73614930	-0.34208703
N	2.07604912	-1.16497185	0.52614621	N	2.13913171	1.04980172	0.49616454	N	2.03424798	-1.20847796	0.54377576
C	-0.39437583	0.23663473	1.30711182	C	-0.40068913	-0.21188558	1.30597719	C	-0.38729036	0.24698508	1.30288609
C	-1.73696939	0.81077469	1.71076769	C	-1.75005712	-0.73894233	1.70750749	C	-1.71599099	0.84018552	1.70669854
C	-1.90546785	0.21097342	3.11569469	C	-1.89357240	-0.15774046	3.10931793	C	-1.89684610	0.22871237	3.09838509
C	-0.46033040	0.00196214	3.51950311	C	-0.45424368	0.00537736	3.51025833	C	-0.45933710	0.00443095	3.50284700
N	0.33384614	-0.09431240	2.41330688	N	0.34338549	0.08867113	2.40788001	N	0.33326881	-0.09728374	2.40279293
C	1.33982355	0.00617654	5.17999820	C	1.33210065	-0.00240639	5.18518272	C	1.33843079	0.00704692	5.14785790
C	1.85768736	0.22091039	6.58763615	C	1.82379254	-0.17438039	6.59525954	C	1.86734099	0.23603471	6.54387851
C	3.24518549	0.81857982	6.30561246	C	3.21420472	-0.75327405	6.35956239	C	3.23849841	0.84532915	6.24002898
C	3.53985962	0.24036558	4.93669251	C	3.52861477	-0.21871213	4.99038589	C	3.52355325	0.24943670	4.88203300
N	2.37882068	-0.09201872	4.30019373	N	2.38128697	0.08367463	4.31909828	N	2.36424709	-0.09637433	4.26206200
C	5.07254039	-0.70726172	3.27803576	C	5.10038214	0.63177652	3.31629372	C	5.02937520	-0.73738236	3.23958723
C	6.44923688	-1.16226819	2.83880023	C	6.48498394	1.01790781	2.87666701	C	6.39164675	-1.21802464	2.79985744
C	6.09805218	-2.39733347	1.99416227	C	6.18809512	2.18834634	1.94615880	C	6.01727117	-2.47524664	2.01075452
C	4.68939587	-2.05834667	1.55117080	C	4.78859492	1.86559354	1.50235871	C	4.61467412	-2.13114315	1.56952721
N	4.12065122	-1.16630841	2.41389108	N	4.17457520	1.05305888	2.40860980	N	4.06614042	-1.20926565	2.40418200
Ni	2.22748742	-0.62917777	2.41328159	Ni	2.25977460	0.56863318	2.40784762	Ni	2.19966777	-0.65281982	2.40302058
H	-0.66899446	0.31374932	-0.79567355	H	-0.68644514	-0.28981363	-0.79062199	H	-0.66124610	0.32283000	-0.79817908
H	-0.73416665	0.08218589	5.62238389	H	-0.74174619	-0.06930635	5.60657012	H	-0.73043904	0.08879285	5.60382967
H	5.65763186	0.31310075	5.04408326	H	5.63894153	-0.28871469	5.14523778	H	5.64031971	0.32265381	4.97063468
H	4.65399174	-3.23213215	-0.21618488	H	4.82704408	2.92894984	-0.32822114	H	4.54916338	-3.35007749	-0.16371696
H	-2.43075768	-0.75515282	3.06341956	H	-2.45199393	-0.78581464	3.80743956	H	-2.42532211	-0.73314972	3.03328662
H	-2.53373913	0.54741655	1.01101141	H	-1.73715654	-1.83867595	1.74049598	H	-2.51465043	0.59755810	1.00315294
H	0.57837533	-1.35659563	-2.35870394	H	2.05745842	0.17202260	-2.27774271	H	0.53883887	-1.39746166	-2.33301463
H	1.71199222	-3.29770823	-1.42691989	H	3.27388883	2.27231519	-2.28886957	H	1.60040639	-3.35382261	-1.36126352
H	-2.44848330	0.85062462	3.81558423	H	-2.39543340	0.82080340	3.07602343	H	-2.43562122	0.86631494	3.80188257
H	-1.68172721	1.90910685	1.76269666	H	-2.53717252	-0.44370927	1.00964410	H	-1.63657026	1.93485192	1.77104688
H	6.77205780	-2.57258942	1.15222296	H	6.87922987	2.28841234	1.10590325	H	6.00043718	-3.35620869	2.66824251
H	6.92603905	-0.38938097	2.21641731	H	6.95685245	0.19097838	2.32526773	H	7.06324461	-1.40034683	3.64093844
H	3.19012334	1.91678327	6.25153793	H	3.96057856	-0.46124181	7.10208810	H	3.16856149	1.93991232	6.16482715
H	1.20370507	0.86377341	7.18164659	H	1.88833230	0.80090907	7.10036567	H	1.21429689	0.87684131	7.13939868
H	6.09380792	-3.30434746	2.61817281	H	6.20545518	3.13942053	2.49897465	H	6.67979986	-2.69048304	1.17021345
H	7.11178825	-1.36885093	3.68272155	H	7.13703560	1.26043064	3.71909846	H	6.86073998	-0.47232885	2.14215843
H	2.05785068	-0.38178106	-2.28177120	H	0.65313627	1.23814271	-2.38460663	H	2.04980264	-0.46970994	-2.26289165
H	3.12251739	-2.56986209	-2.21848807	H	1.92265794	3.12511203	-1.53548185	H	3.03370845	-2.68872079	-2.16887049
H	4.00639343	0.55652412	7.04436383	H	3.18146451	-1.85293639	6.34302944	H	4.00954556	0.60306799	6.97387882
H	1.95058823	-0.74295912	7.11141219	H	1.16299790	-0.80681622	7.19279948	H	1.97706927	-0.72380161	7.06864421

[*OCT-Pi*-Ni]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85838756	C	0.00000000	0.00000000	4.84279561	C	0.00000000	0.00000000	4.83821338
C	4.85828470	0.00000000	4.83312553	C	4.84310465	0.00000000	4.82256315	C	4.83855909	0.00000000	4.80779583
C	4.80235350	-0.73219974	0.03107529	C	4.79556221	0.67395708	0.02764279	C	4.77502355	-0.77877189	0.03337311
C	3.49445173	-0.60128376	-0.43209707	C	3.48995687	0.55422216	-0.43157294	C	3.47171091	-0.63913125	-0.42659718
C	3.10791584	-0.78998668	-1.89417099	C	3.10806817	0.72889946	-1.88309394	C	3.08342297	-0.83357381	-1.88224825
C	1.67557913	-0.23251762	-1.92933191	C	1.67231475	0.21570364	-1.91375591	C	1.66905977	-0.24822291	-1.92040759
C	1.30307533	-0.19964599	-0.45205911	C	1.30138527	0.18513544	-0.44926829	C	1.29770783	-0.21126433	-0.44802123
N	2.40263927	-0.34009602	0.33835613	N	2.39880374	0.31293161	0.34746841	N	2.38931762	-0.36295578	0.34132923
C	-0.45496859	0.06717915	1.31572658	C	-0.45219552	-0.06217341	1.31211274	C	-0.45180436	0.07161760	1.31181697
C	-1.91493134	0.31130323	1.67816932	C	-1.90205427	-0.28672876	1.67403325	C	-1.90556638	0.32427824	1.67251487
C	-1.94040982	-0.01540269	3.18036917	C	-1.92373359	0.01323787	3.16911990	C	-1.93318604	-0.01458403	3.16570427
C	-0.46011085	0.00042044	3.54275360	C	-0.45648563	-0.00101397	3.53078200	C	-0.45754117	0.00107309	3.52653768
N	0.32282299	-0.02803054	2.42928754	N	0.33341765	0.02622360	2.42148514	N	0.32368923	-0.02673162	2.41924672
C	1.31814709	0.00044801	5.31159566	C	1.31418531	-0.00003288	5.29372226	C	1.31497911	0.00190545	5.28651265
C	1.68840910	-0.01847816	6.78987213	C	1.68165971	0.01795890	6.75939189	C	1.68612424	-0.02025127	6.75938293
C	3.18975349	0.31102211	6.75687972	C	3.17737655	-0.27878677	6.73281821	C	3.17679524	0.32740275	6.72256216
C	3.54505836	0.06674182	5.29517144	C	3.53294761	-0.05950361	5.28062217	C	3.52945667	0.07369095	5.26692865
N	2.42772138	-0.02761143	4.52300549	N	2.42040762	0.02630594	4.49929728	N	2.41749673	-0.02362176	4.49799412
C	5.30358187	-0.19837075	3.52754225	C	5.28726807	0.18155551	3.51899369	C	5.27894686	-0.21200934	3.50756426
C	6.77899275	-0.23344258	3.14825773	C	6.75025756	0.21183981	3.14258942	C	6.74955176	-0.25705361	3.12980211
C	6.73640255	-0.78958226	1.71554282	C	6.71438558	0.72290933	1.70626463	C	6.70257207	-0.83270654	1.71145189
C	5.27247880	-0.59998225	1.33633234	C	5.26088276	0.55038373	1.33057530	C	5.24399796	-0.63822800	1.33330732
N	4.50766654	-0.33780059	2.43153740	N	4.48630905	0.30885171	2.42446386	N	4.48326372	-0.36096037	2.42013315
Ni	2.41508980	-0.18323339	2.43071010	Ni	2.40973996	0.16840080	2.42333323	Ni	2.40333306	-0.19334268	2.41971792
H	-0.76059968	0.10532737	-0.77189553	H	-0.76243991	-0.09692563	-0.77226755	H	-0.75911901	0.11190507	-0.77233497
H	-0.76786297	0.01353894	5.63023476	H	-0.76876382	-0.01260828	5.61486795	H	-0.76717361	0.01116154	5.61067508

H	5.63448228	0.10463743	5.58943836	H	5.61878228	-0.09546181	5.58174720	H	5.61560898	0.11014971	5.56238860
H	5.55387155	-0.95511379	-0.72455306	H	5.55038849	0.87981138	-0.73064686	H	5.52393042	-1.01454150	-0.72085142
H	-2.36231208	-1.01545727	3.36173082	H	-2.51002751	-0.70240389	3.75456151	H	-2.34811751	-1.01751454	3.33764945
H	-2.60598931	-0.29608148	1.08508488	H	-2.18571204	-1.32984381	1.47074621	H	-2.59860556	-0.27313570	1.07372911
H	0.98428463	-0.83371989	-2.52834977	H	1.61922475	-0.79811069	-2.33746356	H	0.96626845	-0.83409859	-2.51918820
H	3.12306381	-1.85957663	-2.15295507	H	3.78147035	0.19876644	-2.56435790	H	3.07526645	-1.90546999	-2.12470502
H	-2.52904344	0.69204527	3.77302576	H	-2.35446333	1.00467351	3.37292323	H	-2.52085354	0.68710426	3.76405187
H	-2.17694828	1.36460148	1.49708260	H	-2.58543607	0.33675284	1.08846670	H	-2.15327963	1.38095921	1.50063466
H	7.42115171	-0.28387676	1.02743801	H	7.39140562	0.19029113	1.03058493	H	6.94814680	-1.90380368	1.70952362
H	7.19574995	0.78501485	3.16543876	H	7.17491802	-0.80153462	3.19599613	H	7.34575831	-0.85315418	3.82618128
H	3.36972643	1.36511838	7.01662995	H	3.76432899	0.34919803	7.41092977	H	3.34290707	1.38616870	6.96584579
H	1.09747955	0.68590958	7.38390169	H	1.47720292	1.00985648	7.18880103	H	1.08763185	0.67330966	7.35643028
H	6.99464910	-1.85923851	1.69805970	H	6.99618253	1.78486891	1.65177793	H	7.38742368	-0.34113458	1.01501530
H	7.37973938	-0.83681390	3.83615283	H	7.34839572	0.83212215	3.81788838	H	7.16534027	0.76020148	3.13177210
H	1.65798127	0.78690443	-2.34368170	H	0.99362109	0.83434493	-2.50975695	H	1.67399233	0.77264454	-2.32753595
H	3.79288058	-0.28464536	-2.58237236	H	3.15936454	1.79151748	-2.16319085	H	3.77864767	-0.34884869	-2.57316163
H	3.78754790	-0.29423445	7.44573761	H	1.10016424	-0.69768880	7.34966494	H	1.52387617	-1.02747109	7.16818753
H	1.51142155	-1.02035643	7.20952944	H	3.38471609	-1.32004966	7.02016161	H	3.78343246	-0.26405175	7.41385623

MeCl

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08694599	H	0.00000000	0.00000000	1.08633125	H	0.00000000	0.00000000	1.08723601
H	1.01451467	0.00000000	-0.39014216	H	1.01688044	0.00000000	-0.38219087	H	1.01683743	0.00000000	-0.38486802
H	-0.56802896	0.84058499	-0.39014216	H	-0.55193887	0.85405463	-0.38219087	H	-0.55718534	0.85058971	-0.38486802
Cl	-0.81300034	-1.53061085	-0.55839644	Cl	-0.81461320	-1.49636904	-0.56408018	Cl	-0.81430307	-1.50687408	-0.56246966

[*OCT-Pi*-Ni···MeCl]$^{-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85821102	C	0.00000000	0.00000000	4.84302637	C	0.00000000	0.00000000	4.83764981
C	4.85818538	0.00000000	4.83021210	C	4.84251361	0.00000000	4.83728439	C	4.83731924	0.00000000	4.80797588
C	4.79606206	-0.77119958	0.03439873	C	4.83298598	0.31767709	0.00666492	C	4.76604282	-0.82886060	0.04268926
C	3.48848452	-0.63637295	-0.42897734	C	3.52368238	0.23067700	-0.45089244	C	3.46636930	-0.66911611	-0.42033446
C	3.10019946	-0.82715971	-1.89025725	C	3.17365265	0.12548296	-1.91751774	C	3.07549848	-0.87237156	-1.87418607
C	1.67508867	-0.25163531	-1.92806217	C	1.65755967	0.28931119	-1.91445763	C	1.66900926	-0.26857358	-1.91831468
C	1.30147278	-0.21275420	-0.45128877	C	1.30759844	0.12288164	-0.45378923	C	1.29778619	-0.21499012	-0.44655566
N	2.39865464	-0.36442852	0.34035910	N	2.41541943	0.16430387	0.33698362	N	2.38757109	-0.36950782	0.34429618
C	-0.45442869	0.07390721	1.31575125	C	-0.45194566	-0.06471374	1.31189551	C	-0.45192500	0.07165778	1.31185114
C	-1.91213703	0.32895919	1.67911658	C	-1.90594257	-0.26305657	1.67228171	C	-1.90762162	0.31100770	1.67340527
C	-1.94023004	-0.00766305	3.17904354	C	-1.92169089	0.02755981	3.16895044	C	-1.93220660	-0.03974196	3.16379259
C	-0.46017912	0.00287994	3.54244614	C	-0.45480499	-0.01290187	3.53011682	C	-0.45741970	-0.00346340	3.52626317
N	0.32283616	-0.02799133	2.42920792	N	0.33565281	-0.00108106	2.42149286	N	0.32453331	-0.01993058	2.41895744
C	1.31847468	0.00012869	5.31089464	C	1.31242691	0.01163578	5.29789271	C	1.31574762	0.01899570	5.28539398
C	1.69040696	-0.01917130	6.78862695	C	1.67395334	0.05752942	6.76443707	C	1.68767791	-0.00647365	6.75807484
C	3.18987104	0.31847292	6.75371838	C	3.17249702	-0.22438208	6.74908254	C	3.17682137	0.34746206	6.72134568
C	3.54523878	0.06943209	5.29290073	C	3.53058302	-0.03990197	5.29229203	C	3.52895248	0.09441572	5.26571752
N	2.42759113	-0.02719995	4.52158473	N	2.42072766	0.02693105	4.50640036	N	2.41669209	0.00153881	4.49658080
C	5.30211363	-0.20703194	3.52543351	C	5.29480461	0.12166344	3.52911650	C	5.27620791	-0.22839424	3.50972738
C	6.77697938	-0.24568781	3.14451314	C	6.76058900	0.08902713	3.16182164	C	6.74581861	-0.30561559	3.13363500
C	6.73238913	-0.81579358	1.71729295	C	6.74490638	0.47089999	1.68566760	C	6.68663934	-0.91207017	1.72910575
C	5.26810506	-0.62890536	1.33804034	C	5.28744327	0.31587508	1.31908465	C	5.23613973	-0.68076931	1.34193262
N	4.50488228	-0.35607917	2.43166672	N	4.50155428	0.20079148	2.42567688	N	4.47979566	-0.37188982	2.42226052
Ni	2.41292526	-0.19707888	2.43120639	Ni	2.41737834	0.11030324	2.42202664	Ni	2.40234264	-0.18065205	2.41963479
H	-0.75925909	0.11202944	-0.77224786	H	-0.76929676	-0.03935954	-0.77069214	H	-0.75923345	0.10780220	-0.77272789
H	-0.76767076	0.01346232	5.63022145	H	-0.77070274	0.00134109	5.61336768	H	-0.76688308	0.00019716	5.61047470
H	5.63509556	0.10943173	5.58510311	H	5.61427237	-0.07643060	5.60268806	H	5.61514573	0.10229278	5.56290218
H	5.54613020	-1.00217148	-0.72023870	H	5.60196232	0.38262448	-0.76262128	H	5.51078703	-1.08985198	-0.70733630
H	-2.36364379	-1.00863772	3.35252608	H	-2.51984803	-0.68162679	3.75030651	H	-2.33037907	-1.05114528	3.32621002
H	-2.60874134	-0.26760431	1.08158605	H	-2.20944076	-1.29927306	1.46165621	H	-2.59613092	-0.28664408	1.06970787
H	1.67145675	0.76773387	-2.34309716	H	1.35926087	1.28885660	-2.26339748	H	1.68776879	0.74865487	-2.33405040
H	3.79162243	-0.33415283	-2.58087839	H	3.69610349	0.86858580	-2.52904524	H	3.77715532	-0.40386229	-2.56971610
H	-2.52854171	0.69642046	3.77590679	H	-2.33513866	1.02475825	3.37990105	H	-2.53242467	0.64686330	3.76701137
H	-2.16391821	1.38615857	1.50591012	H	-2.57637287	0.37779167	1.09029380	H	-2.16275252	1.36738830	1.51048397
H	7.41662872	-0.31722210	1.02351677	H	7.40423854	-0.14264472	1.06301107	H	6.89513358	-1.99101162	1.75526449
H	7.19363330	0.77296999	3.15099243	H	7.16486927	-0.92291480	3.31143015	H	7.33368471	-0.89462773	3.84294551
H	3.36345275	1.37504598	7.00803316	H	3.75105822	0.42810978	7.41119891	H	3.33783357	1.40708674	6.96455054
H	1.09633025	0.68043044	7.38510057	H	1.45654322	1.05356252	7.17691540	H	1.08647259	0.68199258	7.35829694
H	6.99009898	-1.88570559	1.71006576	H	7.06319967	1.51333216	1.53788790	H	7.39063027	-0.46112047	1.02440748
H	7.37884413	-0.84213893	3.83744323	H	7.36680260	0.75603200	3.78345244	H	7.17739205	0.70502298	3.11029551
H	3.10111458	-1.89824281	-2.14355421	H	3.47237702	-0.85836413	-2.30804683	H	3.05291615	-1.94637191	-2.10633367
H	0.97691362	-0.84427084	-2.52764435	H	1.13515976	-0.42734568	-2.55684848	H	0.95883356	-0.85024074	-2.51247532
H	1.52021983	-1.02317361	7.20628721	H	1.09735266	-0.65479115	7.36353810	H	1.53041836	-1.01631842	7.16285099
H	3.79141564	-0.27987461	7.44529826	H	3.39105964	-1.25524986	7.06428575	H	3.78610870	-0.24129094	7.41262165
C	1.56183345	-3.74661469	2.20400233	C	2.59825794	-2.97467666	2.35644920	C	2.93463204	-3.24881529	3.65295628
H	2.58035962	-3.56015262	1.87999283	H	3.58118480	-2.53059552	2.48565222	H	3.20943859	-3.25535636	2.60235509
H	1.39997593	-3.40078430	3.21966916	H	1.95271043	-2.75466925	3.20196544	H	3.59046271	-2.60096697	4.22635875
H	0.84279291	-3.31070947	1.51876264	H	2.14451457	-2.65877877	1.42146394	H	1.89478179	-2.96358936	3.78201036
Cl	1.30157128	-5.55881248	2.19078565	Cl	2.81097511	-4.78145247	2.28289761	Cl	3.12746333	-4.93736421	4.28401686

[*OCT-Pi*-Ni—Me—Cl]$^{‡-}$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85800658	C	0.00000000	0.00000000	4.84272043	C	0.00000000	0.00000000	4.83724607
C	4.85785051	0.00000000	4.81184671	C	4.84241283	0.00000000	4.81089290	C	4.83701951	0.00000000	4.78977629

C	4.77791364	-0.87760121	0.03449886	C	4.78619595	0.73655939	0.02494772	C	4.73509136	-0.98553122	0.05542712
C	3.47342162	-0.71811611	-0.43049236	C	3.48084955	0.61116748	-0.43504456	C	3.43989656	-0.79864828	-0.41139156
C	3.07695118	-0.90946541	-1.88863781	C	3.09566233	0.78519014	-1.88524591	C	3.03827817	-1.01795918	-1.85891012
C	1.66875414	-0.29308368	-1.92797496	C	1.66449607	0.25806803	-1.91640770	C	1.65907438	-0.35428333	-1.91438884
C	1.29651943	-0.23920790	-0.45203598	C	1.29718073	0.21067219	-0.45181704	C	1.28938404	-0.26296972	-0.44497977
N	2.39115064	-0.41474541	0.33619956	N	2.39331200	0.35500339	0.34037122	N	2.37390666	-0.44480040	0.34515244
C	-0.45444504	0.08027434	1.31509933	C	-0.45461184	-0.06315069	1.31169613	C	-0.45000416	0.09345273	1.31069916
C	-1.90707707	0.35923247	1.67914735	C	-1.90193113	-0.30161613	1.67378915	C	-1.89738966	0.37296678	1.67339907
C	-1.94154886	0.02043537	3.17880739	C	-1.92597186	-0.00398848	3.16971105	C	-1.93273835	0.01425767	3.16198865
C	-0.46269021	0.00388632	3.54322106	C	-0.45927699	-0.00145511	3.53113706	C	-0.45890951	0.00924673	3.52606370
N	0.31730857	-0.03879955	2.42926310	N	0.32594683	0.03524415	2.42129566	N	0.32030688	-0.02247015	2.41892352
C	1.31914313	0.00176147	5.30816045	C	1.31430395	0.00983251	5.29341359	C	1.31564774	0.00956155	5.28314370
C	1.69756025	0.01591804	6.78349217	C	1.68575070	0.02004118	6.75746861	C	1.69406600	0.01427855	6.75331714
C	3.19659901	0.35569222	6.73530946	C	3.18028017	-0.28325868	6.72559314	C	3.18228378	0.37266595	6.70356472
C	3.54707942	0.07851057	5.27898941	C	3.53361496	-0.05526898	5.27439173	C	3.53080399	0.09355788	5.25257979
N	2.42572962	-0.04008226	4.51766265	N	2.41926984	0.04029724	4.50026884	N	2.41516701	-0.02217046	4.49311360
C	5.29759802	-0.23751303	3.51080001	C	5.28521576	0.20377500	3.50968223	C	5.26921323	-0.26303434	3.49607767
C	6.76990219	-0.28993271	3.12432109	C	6.74708803	0.24587132	3.13135337	C	6.73493638	-0.35460100	3.11205433
C	6.71752609	-0.90676128	1.71675470	C	6.70703260	0.78069816	1.70346012	C	6.66584651	-1.01826797	1.73346106
C	5.25546314	-0.71670784	1.33427413	C	5.25438992	0.60830870	1.32688690	C	5.21456024	-0.79850986	1.34592483
N	4.49897063	-0.41360753	2.42373869	N	4.48561496	0.35044598	2.41923294	N	4.46847979	-0.44461491	2.41928158
Ni	2.40262050	-0.30482381	2.43249739	Ni	2.40909581	0.14967989	2.41541912	Ni	2.38930094	-0.29928358	2.42402634
H	-0.75613372	0.12804176	-0.77243811	H	-0.76028855	-0.10981050	-0.77236212	H	-0.75499371	0.12644319	-0.77362194
H	-0.76578720	0.02630884	5.63116522	H	-0.76758958	-0.02124271	5.61539179	H	-0.76573758	0.01511773	5.61060917
H	5.63739735	0.12805286	5.56064699	H	5.61965584	-0.10923205	5.56621687	H	5.61802566	0.12617946	5.53717292
H	5.52236805	-1.13366163	-0.71710012	H	5.53894045	0.95167556	-0.73238184	H	5.47105542	-1.28625159	-0.68779001
H	-2.38080462	-0.97360549	3.35060784	H	-2.50287339	-0.72707007	3.75484646	H	-2.35543200	-0.98787269	3.31819607
H	-2.61205925	-0.22564982	1.08025556	H	-2.17383838	-1.34715632	1.46778912	H	-2.60146763	-0.20184345	1.06584117
H	1.69411420	0.72503187	-2.34486728	H	0.97851605	0.87660316	-2.50370881	H	1.72265912	0.65531425	-2.34372883
H	3.78108879	-0.44350073	-2.58475821	H	3.13701756	1.84907388	-2.16068274	H	3.75819039	-0.59686946	-2.56570506
H	-2.51722015	0.73349387	3.77692932	H	-2.36635116	0.98233346	3.37564677	H	-2.51522765	0.71239882	3.76896020
H	-2.14003228	1.42070309	1.50674127	H	-2.59014440	0.31689914	1.08899065	H	-2.12091777	1.43728474	1.51625930
H	7.40649589	-0.44049102	1.00582246	H	7.38514145	0.26337990	1.01752779	H	6.87136841	-2.09574983	1.80193763
H	7.18549773	0.72859413	3.09465240	H	7.17381387	-0.76709798	3.16841434	H	7.32771226	-0.91355047	3.84093390
H	3.37045997	1.41706647	6.96768046	H	3.77190319	0.33713183	7.40619914	H	3.34187300	1.43684998	6.92596706
H	1.10445159	0.72748159	7.36615077	H	1.48710371	1.01148687	7.18965663	H	1.09291126	0.71242989	7.34179530
H	6.96010826	-1.97986474	1.74593542	H	6.98149738	1.84506666	1.66674358	H	7.36583270	-0.59751009	1.00673435
H	7.37415177	-0.86327860	3.83400042	H	7.34320229	0.85720474	3.81610646	H	7.16381463	0.65492115	3.04432917
H	3.04582340	-1.98275703	-2.13013412	H	3.77431642	0.26356703	-2.56741624	H	2.96789944	-2.09535639	-2.06421598
H	0.95340702	-0.86722367	-2.52474799	H	1.61796204	-0.75219061	-2.34846869	H	0.92443182	-0.91311689	-2.50011966
H	1.53063199	-0.97907312	7.22250591	H	3.38407681	-1.32798849	7.00234964	H	1.54168424	-0.98790595	7.17729321
H	3.80244342	-0.22950391	7.43405718	H	1.10182465	-0.69502591	7.34544852	H	3.79653134	-0.20258040	7.40145534
C	2.22421751	-2.80041835	2.61353850	C	2.55498540	-2.34253142	2.15428401	C	2.21282525	-2.68742406	2.59664920
H	2.96856226	-2.78631458	1.83772854	H	3.55637303	-2.09668203	1.83874086	H	2.98640896	-2.69726198	1.84682838
H	2.53132062	-2.62898654	3.62982450	H	2.33703751	-2.30681787	3.20991254	H	2.48164295	-2.53112317	3.62810783
H	1.19627922	-2.62652761	2.34944529	H	1.74820598	-2.14628678	1.46686955	H	1.19013490	-2.53441417	2.29463296
Cl	2.07686599	-4.98948616	2.76342945	Cl	2.65635652	-4.46869071	1.91904518	Cl	2.06020919	-4.87462045	2.74942570

[*OCT-Pi*-Ni-Me···Cl]$^-$

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85574474	C	0.00000000	0.00000000	4.84014793	C	0.00000000	0.00000000	4.83821032
C	4.85591014	0.00000000	4.85578995	C	4.84010300	0.00000000	4.84078023	C	4.83762854	0.00000000	4.82942127
C	4.85593145	-0.00075640	-0.00012715	C	4.84042256	0.00099984	0.00044828	C	4.83277851	-0.22794209	-0.00173066
C	3.53850988	-0.00222191	-0.45618781	C	3.52618359	0.00574431	-0.45388445	C	3.51884888	-0.17813381	-0.45191894
C	3.19600511	0.05659608	-1.93454135	C	3.18186592	0.03779686	-1.91954469	C	3.17733401	-0.18096012	-1.92601607
C	1.65990005	0.06587098	-1.93410578	C	1.65882158	0.05525111	-1.91920167	C	1.65451230	-0.03242619	-1.92473878
C	1.31745267	0.00056472	-0.45594328	C	1.31432096	0.00973923	-0.45390360	C	1.31324751	-0.05621191	-0.45079577
N	2.42813384	-0.04297005	0.32235886	N	2.42032319	-0.01454458	0.33066858	N	2.41589602	-0.12601295	0.32775370
C	-0.45645236	-0.00454127	1.31732835	C	-0.45476001	-0.00101816	1.31411317	C	-0.45008553	0.02250915	1.31434288
C	-1.93480338	0.05302919	1.65979106	C	-1.92036525	0.02531049	1.65849288	C	-1.92182582	0.11398768	1.65418378
C	-1.93479688	0.05305317	3.19596022	C	-1.92017939	0.03162873	3.18167294	C	-1.92348002	0.07874036	3.18390492
C	-0.45644907	-0.00456088	3.53841608	C	-0.45465270	-0.00004838	3.52599907	C	-0.45042505	0.01353161	3.52332614
N	0.32194749	-0.04565778	2.42787380	N	0.32978541	-0.02015197	2.42005727	N	0.32774598	-0.02697247	2.41923907
C	1.31745539	0.00075703	5.31167899	C	1.31412012	0.00798236	5.29456213	C	1.31478833	-0.00655055	5.28668220
C	1.65990995	0.06582956	6.78983397	C	1.65819470	0.04706000	6.76003188	C	1.65835919	0.02608447	6.75985784
C	3.19601520	0.05730342	6.79021875	C	3.18129909	0.03250008	6.76066734	C	3.18602213	0.10701981	6.75294581
C	3.53849944	-0.00158206	5.31187709	C	3.52588183	0.00358409	5.29514025	C	3.52369420	0.01399488	5.28090921
N	2.42812836	-0.04248881	4.53334369	N	2.42034151	-0.01371628	4.51029226	N	2.41785709	-0.03614557	4.50541455
C	5.31165933	-0.00107911	3.53833415	C	5.29396756	0.00937594	3.52648387	C	5.28646553	-0.05271430	3.51530159
C	6.78999855	0.06024650	3.19588422	C	6.75941869	0.05315167	3.18238792	C	6.75804276	-0.00242322	3.16945306
C	6.79005236	0.05914394	1.65978596	C	6.75989784	0.04318913	1.65931016	C	6.75846241	-0.19545224	1.65223314
C	5.31169460	-0.00161185	1.31732286	C	5.29430776	0.00827160	1.31472846	C	5.28495215	-0.18642982	1.31125854
N	4.53310349	-0.04312818	2.42782673	N	4.50943155	-0.01312659	2.42051461	N	4.50616612	-0.13339358	2.41515301
Ni	2.42673816	-0.38400510	2.42788667	Ni	2.41773759	-0.30520387	2.42127439	Ni	2.41169324	-0.41334091	2.42451602
H	-0.76815499	0.03634910	-0.76836002	H	-0.76881260	0.01693865	-0.76931802	H	-0.76700657	0.04792539	-0.76838642
H	-0.76815881	0.03619266	5.62410505	H	-0.76904267	0.01686739	5.60923136	H	-0.76752723	0.02765971	5.60707680
H	5.62426547	0.03532733	5.62397296	H	5.60935146	0.01507609	5.60968728	H	5.60694032	0.05389214	5.59501061
H	5.62428168	0.03430474	-0.76833009	H	5.60957621	0.01603958	-0.76851434	H	5.59989520	-0.27341360	-0.77010158
H	-2.46193064	-0.80816305	3.62147802	H	-2.43695693	-0.83129392	3.61511561	H	-2.44280440	-0.79638302	3.58711457
H	-2.46189249	-0.80824288	1.23432521	H	-2.43086910	-0.84560181	1.23340954	H	-2.47110628	-0.71961268	1.20636784
H	1.24106975	0.97065283	-2.38830801	H	1.24128566	0.95363860	-2.38661858	H	1.32359934	0.91027431	-2.37255458

H	3.62673952	0.95120884	-2.39731568	H	3.62228710	0.91564792	-2.40397895	H	3.68945022	0.63330207	-2.44666278
H	-2.39609118	0.95129925	3.62085574	H	-2.39887273	0.92032618	3.60686545	H	-2.38413844	0.96405195	3.63211553
H	-2.39616495	0.95122656	1.23486803	H	-2.40562115	0.90626127	1.22496780	H	-2.34903729	1.03765916	1.25139906
H	7.24958813	0.95801485	1.23431059	H	7.27504807	-0.82605573	1.23629464	H	7.20173174	-1.15134979	1.35357277
H	7.24865302	0.96024042	3.61997430	H	7.28464798	-0.80308155	3.61889365	H	7.31192321	-0.77756963	3.70600907
H	3.62630939	0.95224582	7.25277423	H	3.61990560	0.91079072	7.24607136	H	3.55931108	1.04958455	7.16608932
H	1.24059779	0.97021973	7.24436121	H	1.23831587	0.94177628	7.23229574	H	1.18344319	0.87947184	7.25215155
H	7.31904568	-0.80121309	1.23482370	H	7.24096048	0.92542601	1.22385009	H	7.29142262	0.59341287	1.11447755
H	7.31976091	-0.79891641	3.62225989	H	7.22930532	0.94787707	3.60486814	H	7.17787732	0.96426249	3.46757808
H	3.61561402	-0.80827038	-2.46058255	H	3.60001885	-0.83593624	-2.43116158	H	3.50833718	-1.11856868	-2.38434439
H	1.22831797	-0.78812655	-2.46785407	H	1.21782853	-0.79708522	-2.44691445	H	1.14178016	-0.84056927	-2.45425177
H	1.22880856	-0.78860396	7.32327746	H	1.21928409	-0.80942599	7.28277488	H	1.28771058	-0.87985903	7.25057903
H	3.61609342	-0.80723210	7.31641665	H	3.60110201	-0.84098877	7.27124584	H	3.66366286	-0.70368307	7.31047096
C	2.40397855	-2.46972027	2.42834207	C	2.37866584	-2.38983202	2.42749608	C	2.39921061	-2.47383854	2.47539324
H	3.42075763	-2.88525444	2.42984928	H	3.38709273	-2.82814876	2.43477237	H	2.87759319	-2.89949583	1.58110143
H	1.88271678	-2.85850711	3.31384091	H	1.84737698	-2.77274216	3.31091077	H	2.95241725	-2.85215834	3.34744609
H	1.88522715	-2.85879630	1.54147759	H	1.85697250	-2.77974350	1.54137989	H	1.38072312	-2.88615959	2.52936244
Cl	-1.28165684	-17.11997395	4.47664315	Cl	1.77732876	-7.06146246	2.50528641	Cl	6.60712164	-4.31044492	3.06077741

[*OCT-Pi*-Ni-Me]

C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	4.85588010	C	0.00000000	0.00000000	4.84039877	C	0.00000000	0.00000000	4.83778002
C	4.85576044	0.00000000	4.84657434	C	4.84039789	0.00000000	4.84112414	C	4.83819129	0.00000000	4.82034606
C	4.85135504	-0.20139992	-0.00488633	C	4.83973468	0.05919487	0.00139020	C	4.82134300	-0.39992872	-0.00120608
C	3.53395074	-0.16739113	-0.45956188	C	3.52555079	0.05596369	-0.45295021	C	3.50930541	-0.32169231	-0.45152561
C	3.18803661	-0.16725026	-1.93801993	C	3.18118459	0.09910763	-1.91823576	C	3.16188687	-0.36131419	-1.92343550
C	1.66203874	0.00875327	-1.93426295	C	1.65827983	0.07497599	-1.91897753	C	1.65371572	-0.10495972	-1.92424199
C	1.31637481	-0.04761093	-0.45652982	C	1.31404931	0.02719573	-0.45381285	C	1.31054064	-0.10707191	-0.45067179
N	2.42497092	-0.13009143	0.32131080	N	2.41986560	0.01757741	0.33120348	N	2.40991284	-0.20875584	0.32813903
C	-0.45586879	0.00648193	1.31753815	C	-0.45447391	-0.00396448	1.31414716	C	-0.44766205	0.03855931	1.31480270
C	-1.93182457	0.10928279	1.66021138	C	-1.92016059	0.01573608	1.65859649	C	-1.91328229	0.19402688	1.65721508
C	-1.93455508	0.06969276	3.19587970	C	-1.91975997	0.03965739	3.18154360	C	-1.92359303	0.05821449	3.18083998
C	-0.45699528	-0.00515647	3.53875239	C	-0.45437385	0.00356541	3.52616184	C	-0.45127540	0.00351762	3.52376700
N	0.32078363	-0.05917157	2.42821308	N	0.33022729	-0.01809106	2.42007464	N	0.32787371	-0.04039157	2.41936878
C	1.31805214	-0.00067264	5.31005048	C	1.31416830	0.00354577	5.29497070	C	1.31643398	0.00579010	5.28426976
C	1.66368971	0.07677725	6.78689063	C	1.65856716	0.03958987	6.76040851	C	1.66433528	0.06454261	6.75523408
C	3.19947831	0.10982810	6.78154944	C	3.18151485	0.01570263	6.76103509	C	3.18774700	0.20306901	6.73922641
C	3.53911866	0.00876730	5.30475756	C	3.52618254	-0.00398773	5.29540074	C	3.52525195	0.04233166	5.27301475
N	2.42710358	-0.05458516	4.53004751	N	2.42037318	-0.01809872	4.51053477	N	2.41735395	-0.03884589	4.50166660
C	5.30949097	-0.04718507	3.52927270	C	5.29440868	0.02722544	3.52714279	C	5.28457105	-0.11179885	3.50871920
C	6.78691858	0.00449969	3.18155590	C	6.75962307	0.07505848	3.18313423	C	6.75682959	-0.11343811	3.15999032
C	6.78761377	-0.15835133	1.65410093	C	6.75911158	0.09912905	1.66022727	C	6.74964946	-0.37309851	1.65232050
C	5.30836851	-0.16264044	1.31151831	C	5.29387889	0.05598402	1.31564170	C	5.27669386	-0.32792283	1.31017430
N	4.52938767	-0.12611098	2.42208644	N	4.50955847	0.01759769	2.42120863	N	4.50163213	-0.21352909	2.41168723
Ni	2.41802839	-0.42922932	2.43167799	Ni	2.42115111	-0.29119208	2.41961678	Ni	2.40194061	-0.46143556	2.42878188
H	-0.76678610	0.06309523	-0.76793321	H	-0.76909015	0.00969134	-0.76913121	H	-0.76505999	0.07538649	-0.76814539
H	-0.76721059	0.04707699	5.62456503	H	-0.76909076	0.01814956	5.60937284	H	-0.76652500	0.03533029	5.60738811
H	5.62531941	0.06004743	5.61196589	H	5.60941393	0.00969647	5.61032872	H	5.60920272	0.07649590	5.58245976
H	5.61899391	-0.23214282	-0.77389107	H	5.60863252	0.08905879	-0.76739369	H	5.58548345	-0.49414288	-0.76821822
H	-2.46438431	-0.80257329	3.59555165	H	-2.44331194	-0.81310028	3.62662652	H	-2.41539036	-0.86209237	3.51388394
H	-2.49245966	-0.71685846	1.20946587	H	-2.42363660	-0.86467234	1.24446457	H	-2.51650018	-0.56323648	1.14907955
H	1.35200400	0.97087867	-2.35895350	H	1.21503860	0.95698654	-2.39334220	H	1.39549059	0.86342264	-2.36573361
H	3.71450662	0.63263594	-2.46847692	H	3.59593537	0.99768170	-2.38740157	H	3.72982294	0.38665410	-2.48315530
H	-2.39479265	0.95608401	3.64534236	H	-2.39159931	0.93763965	3.59488964	H	-2.41617306	0.89208210	3.68805236
H	-2.35565733	1.03764064	1.26105314	H	-2.41282773	0.88693197	1.21426598	H	-2.27205876	1.17358320	1.32382019
H	7.31188885	0.64977769	1.13386970	H	7.28504936	-0.75295013	1.21634603	H	7.15876726	-1.35653658	1.39693231
H	7.21831597	0.96064855	3.50031615	H	7.28127248	-0.79387887	3.59868670	H	7.29358478	-0.87677748	3.72989146
H	3.60381934	1.03503182	7.20724750	H	3.62575010	0.88691353	7.25376319	H	3.52021683	1.18486038	7.09285469
H	1.21912945	0.96684010	7.24491469	H	1.24512628	0.93754019	7.23222609	H	1.15720223	0.89855497	7.24765536
H	7.25122392	-1.09896507	1.33367986	H	7.22835514	0.99767584	1.24550668	H	7.31071945	0.37096859	1.08062952
H	7.34076468	-0.78462586	3.70068902	H	7.23387071	0.95711534	3.62640769	H	7.20119487	0.85478799	3.41398730
H	3.49810973	-1.11386063	-2.39667480	H	3.62518576	-0.75294193	-2.44412038	H	3.41812792	-1.34225997	-2.33787989
H	1.13465913	-0.77167097	-2.49244564	H	1.24284691	-0.79400943	-2.44064373	H	1.08341876	-0.86869955	-2.46001945
H	1.26073231	-0.79175681	7.32024078	H	1.21343010	-0.81320373	7.28385653	H	1.33465252	-0.85528093	7.25026160
H	3.64732035	-0.72003731	7.33909341	H	3.59559576	-0.86469143	7.26457825	H	3.69930510	-0.55058640	7.34405239
C	2.37028788	-2.51401849	2.46092507	C	2.42728131	-2.37655314	2.41352816	C	2.35607024	-2.52387273	2.50749624
H	3.38244688	-2.94030945	2.44364847	H	3.41609837	-2.77747333	2.67875417	H	2.89873202	-2.96891929	1.66053517
H	1.86683433	-2.88638277	3.36371226	H	1.70439657	-2.78172834	3.13646267	H	2.82889080	-2.89675572	3.42796521
H	1.82706334	-2.91020458	1.59194424	H	2.16200188	-2.77750218	1.42473563	H	1.32992053	-2.91851465	2.48165423