Design, Synthesis, and Evaluation of Nickel Dipyridylmethane Complexes for Coordination-Induced Spin State Switching (CISSS)

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S1 Computational Details

S1.1 General Procedures

All calculations were conducted with Gaussian 09, Revision D.01.[1] Geometry optimizations were performed at the PBE[2,3]/def2-SVP[4,5] level of theory. Harmonic frequency analyses were carried out at the same level to confirm that a minimum was reached and to obtain values for the entropy and the thermal correction to enthalpy. Single point energies were calculated at the optimized geometries using B3LYP[6]/def2-TZVP[4,5]. These methods were chosen because they have shown best performance in predicting experimental data for porphyrin-based CISSS-systems.[7]

S1.2 Comparison of Calculated and Crystal Structures

The optimized structures for the complexes **1a** and **1a**$(py)_2$ (see section S1.10.17) were superimposed with the solid state molecular structures (see section S3) using the program Mercury 3.5.1. The root mean square deviations (RMSD) of 0.15 Å and 0.21 Å, respectively, indicate the calculated and the single crystal molecular structures being in good agreement and PBE/def2-SVP being sufficient for geometry optimization.

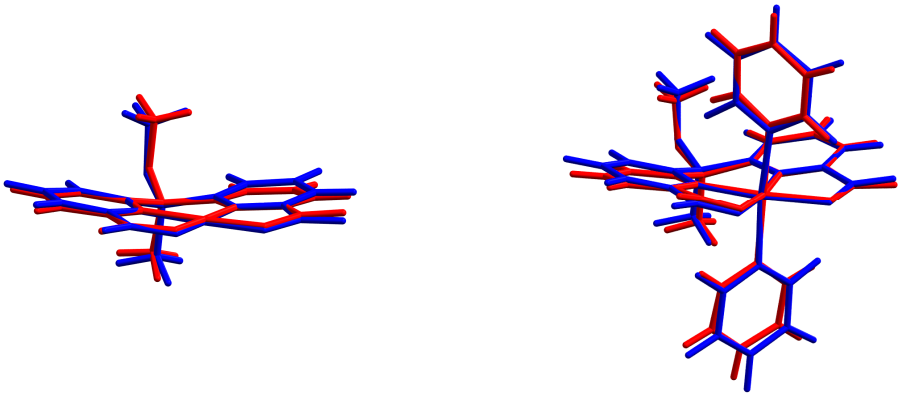


Figure S1: Overlay of solid state structures (red) with the calculated structures (blue, PBE/def2-SVP) for complexes **1a** (left) and **1a**$(py)_2$ (right).

S1.3 Binding Enthalpy of Pyridine to Different Nickel Complexes

Binding enthalpies $\Delta H_{Ni\text{-}Py}$ of pyridine to the nickel complexes with dipyridylmethanes containing different ligating anionic residues were determinded as the difference between the enthalpy of the triplet pentacoordinate complex (H_{NiPy}) and the sum of the enthalpies of the singlet tetracoordinate complex (H_{Ni}) and the non-binding pyridine (H_{Py}). Enthalpies H were determined by revising the electronic energies E_{elec} extracted from the single point energy calculations by the addition of the zero point energy and the thermal correction from harmonic frequency analyses H_{corr} (in Gaussian: thermal correction to enthalpy).

$$H = E_{elec} + H_{corr} \quad \text{(S1)}$$

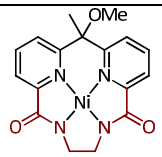
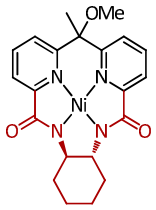
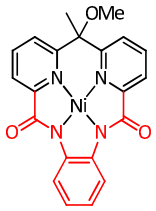
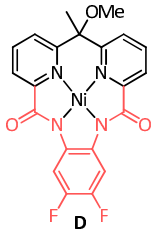
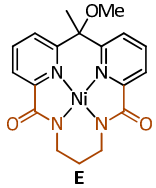
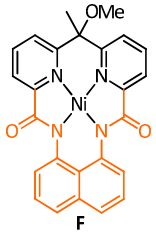
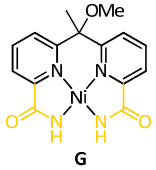
$$\Delta H_{Ni\text{-}Py} = H_{NiPy} - (H_{Ni} + H_{Py}) \quad \text{(S2)}$$

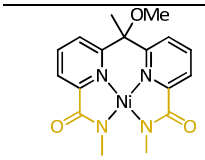
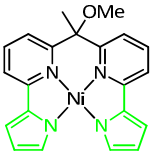
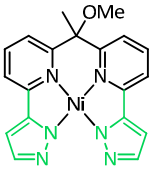
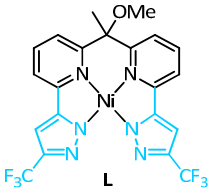
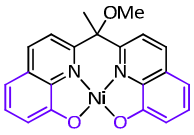
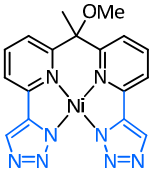
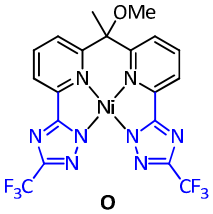
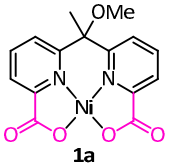
Where the binding enthalpy is negative, the coordination of pyridine is favored.

$E_{elec,Py}$ = -248.37686420 Hartree

$H_{corr,Py}$ = 0.091702 Hartree

Table S1. Absolute energies (E_{elec}) and corrections to enthalpy (H_{corr}) of tetracoordinate nickel dipyridylmethane complexes and pentacoordinate pyridine adducts as well as the hereby calculated binding enthalpies of pyridine to the complexes ($\Delta H_{Ni\text{-}Py}$).

	$E_{elec,Ni}$ / Hartree	$H_{corr,Ni}$ / Hartree	$E_{elec,NiPy}$ / Hartree	$H_{corr,NiPy}$ / Hartree	$\Delta H_{Ni\text{-}Py}$ / kcal·mol^{-1}
 **A**	-2611.01474264	0.328866	-2859.35871418	0.420712	+20.7
 **B**	-2767.10938902	0.423455	-3015.45533049	0.515356	+19.5
 **C**	-2763.51015677	0.354444	-3011.85696642	0.446492	+19.1
 **D**	-2962.06697249	0.340117	-3210.41465826	0.432313	+18.6
 **E**	-2650.27579139	0.358619	-2898.71369402	0.450925	+9.8
 **F**	-2917.18983459	0.403142	-3165.55500907	0.495775	+8.2
 **G**	-2533.58622008	0.293594	-2781.95339133	0.386453	+6.8

	$E_{elec,Ni}$ / Hartree	$H_{corr,Ni}$ / Hartree	$E_{elec,NiPy}$ / Hartree	$H_{corr,NiPy}$ / Hartree	$\Delta H_{Ni\text{-}Py}$ / kcal·mol^{-1}
 **H**	-2612.21506135	0.350541	-2860.58829618	0.443274	+2.9
 **I**	-2614.15809462	0.365778	-2862.53389931	0.458787	+1.5
 **J**	-2646.21739490	0.342405	-2894.59592763	0.435374	-0.3
 **K**	-2646.27339024	0.343411	-2894.65245306	0.436495	-0.5
 **L**	-3320.60913089	0.359231	-3568.99137492	0.452311	-2.5
 **M**	-2653.95410417	0.342153	-2902.33676685	0.435173	-2.8
 **N**	-2678.28234085	0.318432	-2926.66655702	0.411826	-3.6
 **O**	-3352.72392728	0.336675	-3601.11023590	0.430032	-4.9
 **1a**	-2573.34788283	0.268795	-2821.73421271	0.361986	-5.0

S1.4 Coordination Isomers of the Pentacoordinate Complexes

The two sides of the square planar complexes are diastereotopic. Therefore, there are two possibilities for the coordination of the first pyridine (compare Figure S3). According to the calculations, the coordination on the side of the methyl group is favored by 0.2 to 2.6 kcal·mol^{-1} (concerning the relevant complexes with negative binding enthalpies). Nevertheless, we used the isomer where pyridine coordinates from the methoxy side for the classification of the residues because in future LD-CISSS complexes the azopyridine is also supposed to bind from this side.

S1.5 Comparison of Binding Enthalpies in Low and High Spin Complexes

To show that spin state switching indeed takes place when a fifth ligand coordinates to the square planar nickel complex, singlet and triplet state complexes were compared. For this purpose, fully relaxed structures for each spin state were calculated (Figure S2). Interatomic distances between nickel and the pyridine nitrogen in singlet states are too long for actual coordinative bonds; i.e., the pyridine only weakly interacts with the nickel atom.

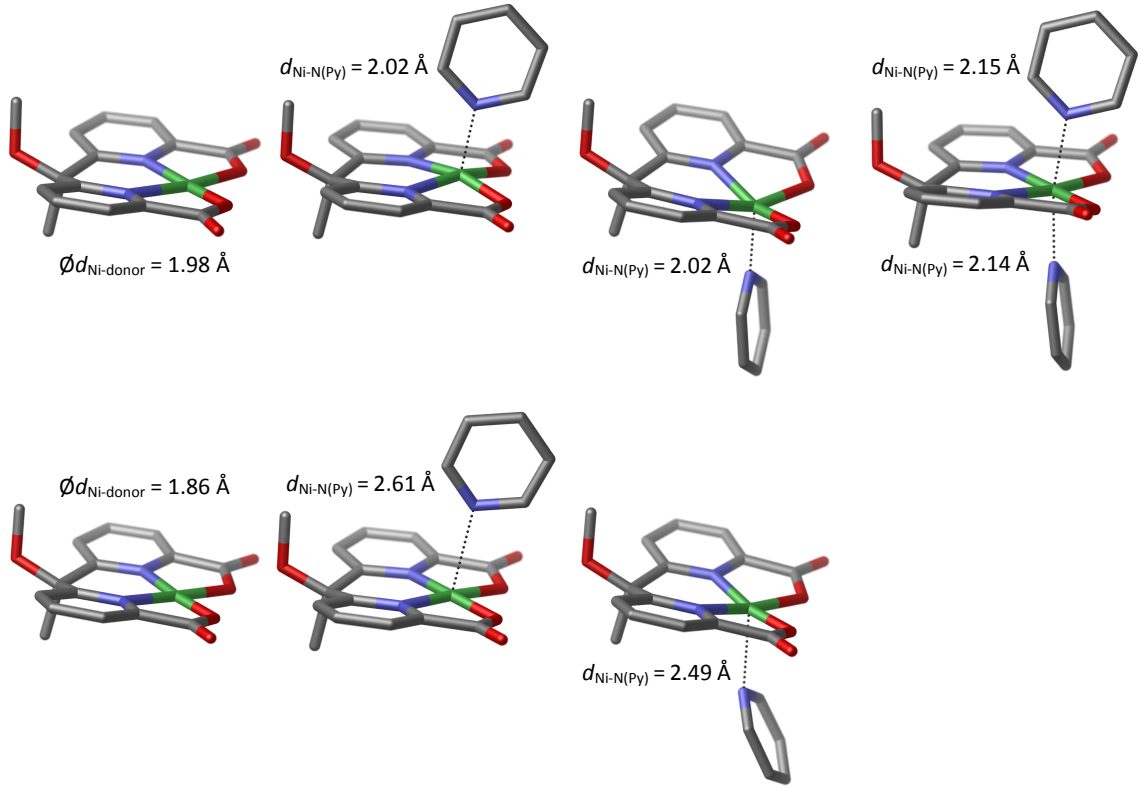


Figure S2. Optimized structures of complex **1a** in its square planar, the two square pyramidal and octahedral form with selected bond length. Triplet states are presented at the top and singlet states at the bottom. An appropriate structure for the singlet octahedral complex could not be obtained because the geometry optimization did not converge.

The results of the binding enthalpy calculations show that the complex does not bind pyridine in its diamagnetic state (Figure S3). Thus, spin state switching takes place with the formation of the square pyramidal complex. The sum of the binding enthalpies in the square pyramidal complexes is $\Sigma\Delta H_{Ni\text{-}Py}$ = -10.8 kcal·mol^{-1}. Since the binding enthalpy of two pyridine molecules in the octahedral complex amounts to $\Delta H_{Ni\text{-}2Py}$ = -13.0 kcal·mol^{-1}, the coordination of the second pyridine is facilitated by a cooperative effect of 2.2 kcal·mol^{-1}.

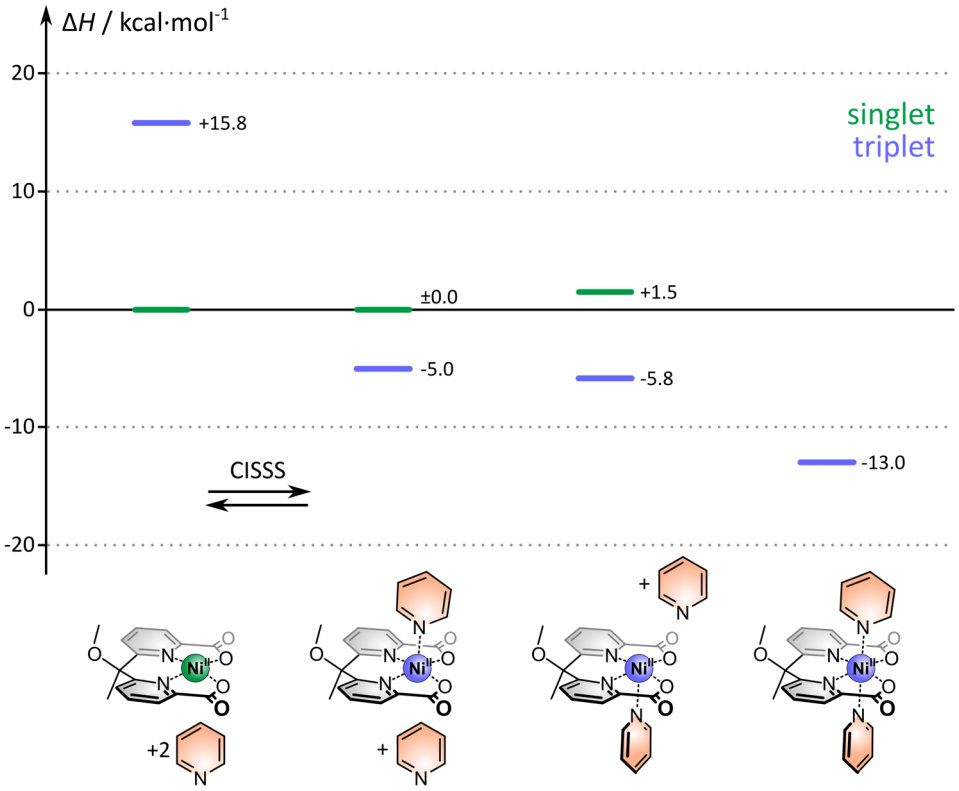


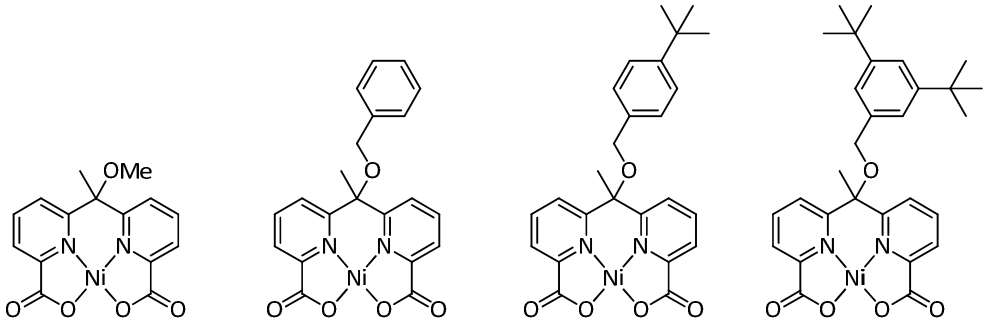
Figure S3. Enthalpies of different pyridine adducts of nickel complex **1a** relative to the diamagnetic square planar complex including two non-coordinating pyridine molecules. Spin state switching takes place with the association of the first pyridine.

Table S2. Absolute energies (E_{elec}) and corrections to enthalpy (H_{corr}) of singulet and triplet states of the tetracoordinate nickel dipyridylmethane complex **1a** and the penta- and hexacoordinate pyridine adducts as well as the hereby calculated enthalpies relative to the square planar complex in singlet state and two non-coordinating pyridine molecules (ΔH).

	E_{elec} / Hartree	H_{corr} / Hartree	ΔH / kcal·mol^{-1}
1a, S = 0	-2573.34788283	0.268795	
1a, S = 1	-2573.32463078	0.270667	+15.8
1a(py), S = 1 MeO-side coordination	-2821.73421271	0.361986	-5.0
1a(py), S = 0 MeO-side coordination	-2821.72676541	0.362535	±0.0
1a(py), S = 1 Me-side coordination	-2821.73072161	0.362156	-5.8
1a(py), S = 0 Me-side coordination	-2821.72429288	0.362467	+1.5
1a$(py)_2$, S = 1	-3070.12608411	0.455952	-13.0

S1.6 Substitution of the Methyl by Benzyl Groups

To enhance the solubility of complex **1a** in non-coordinating solvents the methyl group was substituted by different benzyl groups (**1b**-**1d**). According to the calculations, the influence of this substitution on the binding enthalpies is negligible (Figure S4).



	1a	**1b**	**1c**	**1d**
$\Delta H_{Ni\text{-}Py}$ / kcal·mol^{-1}	-5.0/-5.8	-5.2/-5.9	-5.0/-5.8	-4.9/-5.6
$\Delta H_{Ni\text{-}2Py}$ / kcal·mol^{-1}	-13.0	-13.1	-12.9	-12.9

Figure S4. Nickel dipyridylmethane complexes **1a-d** with different residues on the hydroxy group and binding enthalpies of one ($\Delta H_{Ni\text{-}Py}$) or two pyridines ($\Delta H_{Ni\text{-}2Py}$).

Table S3. Absolute energies (E_{elec}) and corrections to enthalpy (H_{corr}) of singlet and triplet states of the tetracoordinate nickel dipyridylmethane complex **1a** and the penta- and hexacoordinate pyridine adducts as well as the hereby calculated binding enthalpies relative to the square planar complex in singlet state and two unbound pyridine molecules (ΔH).

	E_{elec} / Hartree	H_{corr} / Hartree	ΔH / kcal·mol^{-1}
1b	-2804.48028703	0.352709	
1b(py) BnO-side coordination	-3052.86673350	0.445748	-5.2
1b(py) Me-side coordination	-3052.86799159	0.445883	-5.9
1b(py)$_2$	-3301.25856285	0.539772	-13.1
1c	-2961.78933607	0.466937	
1c(py) ^{t}BuBnO-side coordination	-3210.17574499	0.560155	-5.0
1c(py) Me-side coordination	-3210.17703795	0.560165	-5.8
1c(py)$_2$	-3458.56749057	0.654133	-12.9
1d	-3119.09777153	0.581297	
1d(py) ^{t}Bu$_2$BnO-side coordination	-3367.48391289	0.674432	-4.9
1d(py) Me-side coordination	-3367.48515437	0.674549	-5.6
1d(py)$_2$	-3615.87567993	0.768362	-12.9
1e	-2848.63908457	0.472018	
1e(py) MeO-side coordination	-3097.02488662	0.565084	-4.8
1e(py) Oct-side coordination	-3097.02655033	0.565328	-5.6
1e(py)$_2$	-3345.41679195	0.659148	-12.7

S1.7 Solvent Coordination

The pyridine titration was performed in dichloromethane as a solvent. To determine if the solvent has an effect on the coordination and the magnetism, several DCM adducts were calculated.

Without the presence of pyridine, the coordination of DCM is disfavored: In the low spin state it decoordinates, in the high spin state the binding enthalpy is positive (Figure S5). Thus, the tetracoordinate state is favored.

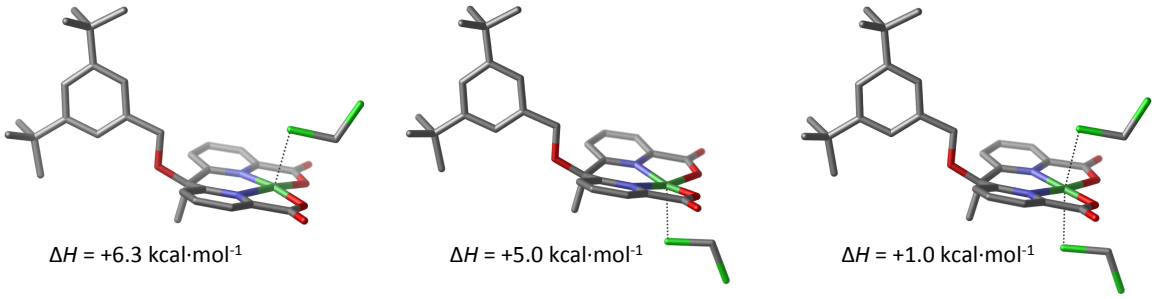


Figure S5. Optimized structures of dichloromethane adducts of complex **1d** in triplet state with the corresponding binding enthalpies for the dashed bonds.

When one pyridine molecule is already coordinated, the coordination of a DCM molecule at the sixth coordination site stabilizes the high spin state by 3.8 or 3.3 kcal·mol^{-1}, respectively (Figure S6). The DCM coordination competes with the binding a second pyridine (see section S2).

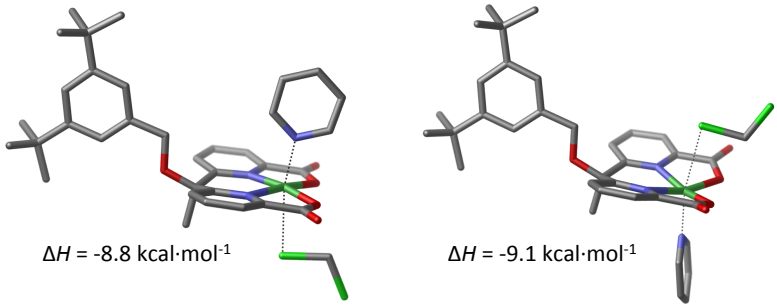


Figure S6. Optimized structures of pyridine-dichloromethane-adducts of complex **1d** in triplet state with the corresponding binding enthalpies for the dashed bonds.

Table S4. Absolute energies (E_{elec}) and corrections to enthalpy (H_{corr}) of dichloromethane and pyridine adducts in triplet state of the nickel dipyridylmethane complex **1d** and as well as the hereby calculated binding enthalpies relative to the square planar complex in singlet state and the unbound ligands (ΔH).

	E_{elec} / Hartree	H_{corr} / Hartree	ΔH / kcal·mol^{-1}
dcm	-959.77647823	0.032880	
1d(dcm) $^{t}Bu_2BnO$-side coordination	-4078.86538323	0.615357	+6.3
1d(dcm) Me-side coordination	-4078.86745288	0.615357	+5.0
1d$(dcm)_2$	-5038.65240375	0.650401	+1.0
1d(py)(dcm) $^{t}Bu_2BnO$-side coordination of py	-4327.26865255	0.709400	-8.8
1d(py)(dcm) Me-side coordination of py	-4327.26920133	0.709464	-9.1

S1.8 Dimers

Evans susceptibility measurements show that a solution of complex **1d** in DCM without any additional ligands is already slightly paramagnetic (see section S2). The reason for the observed paramagnetism is most probably the presence of dimers. In analogy to the solid state structure **1a**$_2$(EtOH)$_3$ (see section S3.3), dimers where the nickel ion in one complex is coordinated by a carbonyl oxygen of a second complex have been calculated. These calculated structures with up to two ligands differ from the solid state structure where three ligands (solvent molecules) are bound to the nickel atoms and the coordinating complex is oriented perpendicular to the other. In contrast, in the calculations the complexes are almost parallel to each other (Figure S7). For the dimer with one singlet and one triplet nickel center without any additional ligands **1d**$_2$ (= ^{1}Ni^{3}Ni), four isomers (depending upon the relative orientation of the two monomeric subunits) are possible. Of these, the one with the methyl groups pointing towards each other is the lowest in energy (Figure S7 top left) and was thus chosen as a starting point for the other structures.

Table S5. Absolute energies (E_{elec}) and corrections to enthalpy (H_{corr}) enthalpies for dimers potentially appearing in the pyridine titration of **1d** as well as the hereby calculated binding enthalpies relative to the square planar complex in singlet state and the non-coordinating ligands (ΔH). The complex is abbreviated with Ni, pyridine with py, and dichloromethane with dcm. The multiplicity of each nickel(II) ion is given as a superscript number.

	E_{elec} / Hartree	H_{corr} / Hartree	ΔH / kcal·mol^{-1}
py	-248.37686	0.09170	
dcm	-959.77648	0.03288	
Ni	-3119.09777	0.58130	±0.0
^{1}Ni^{3}Ni	-6238.21371	1.16387	-10.6
^{1}Ni^{3}Ni(dcm)	-7197.99693	1.19901	-13.4
^{1}Ni^{3}Ni(py)	-6486.60745	1.25794	-19.7
^{3}Ni$_2$	-6238.21152	1.16339	-9.5
^{3}Ni$_2$(dcm)	-7197.99343	1.19831	-11.7
^{3}Ni$_2$(dcm)$_2$	-8157.77550	1.23322	-13.9
^{3}Ni$_2$(py)	-6486.60529	1.25733	-18.7
^{3}Ni$_2$(py)(dcm)	-7446.38767	1.29224	-21.2
^{3}Ni$_2$(py)$_2$	-6734.99774	1.35104	-27.2
^{3}Ni$_2$(py)$_3$	-6983.38768	1.44566	-33.6

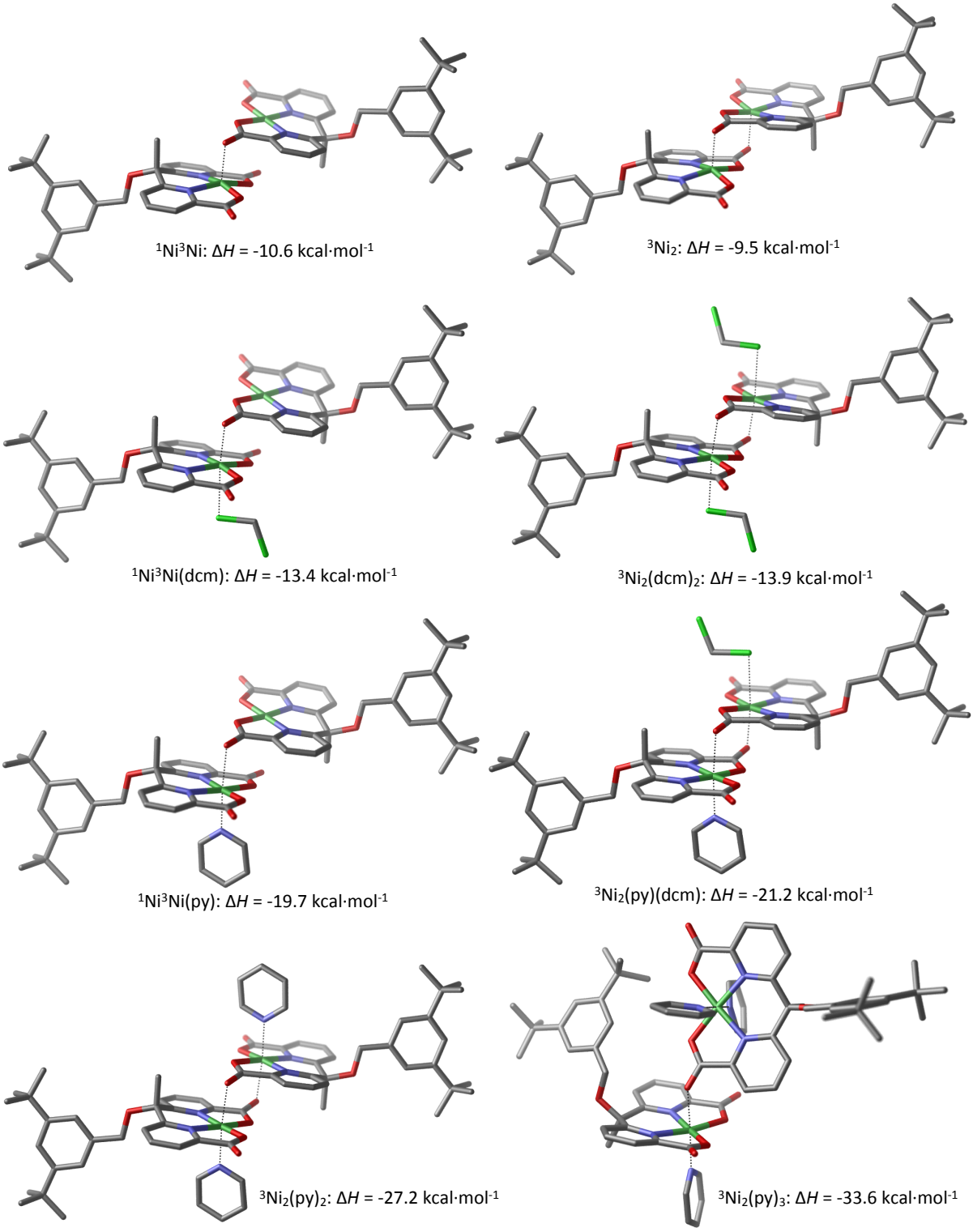


Figure S7. DFT-optimized structures of dimers of complex **1d** with the corresponding binding enthalpies for all dashed bonds. The two complexes on the top left can also exist in quintet states (not shown), which are slightly higher in energy.

S1.9 Reaction Enthalpies

For the species Ni(py) and Ni(py)(dcm), where two isomers can exist, average values are considered.

Table S6. Calculated reaction enthalpies for selected association steps potentially taking place in the pyridine titration.

Reaction	ΔH / kcal·mol^{-1}
$Ni + py \rightarrow Ni(py)$	-5.3
$Ni + py + dcm \rightarrow Ni(py)(dcm)$	-8.9
$Ni(py) + py \rightarrow Ni(py)_2$	-7.6
$Ni(py)(dcm) + py \rightarrow Ni(py)_2 + dcm$	-3.9
$2\ Ni \rightarrow {}^1Ni^3Ni$	-10.6
$2\ Ni \rightarrow {}^3Ni_2$	-9.5
$2\ Ni + dcm \rightarrow {}^1Ni^3Ni(dcm)$	-13.4
$2\ Ni + dcm \rightarrow {}^3Ni_2(dcm)$	-11.7
$2\ Ni + 2\ dcm \rightarrow {}^3Ni_2(dcm)_2$	-13.9
${}^1Ni^3Ni + py \rightarrow {}^1Ni^3Ni(py)$	-9.1
${}^3Ni_2 + py \rightarrow {}^3Ni_2(py)$	-9.2
${}^1Ni^3Ni(dcm) + py \rightarrow {}^3Ni_2(py)(dcm)$	-7.8
${}^3Ni_2(dcm) + py \rightarrow {}^3Ni_2(py)(dcm)$	-9.5
${}^3Ni_2(dcm)_2 + py \rightarrow {}^3Ni_2(py)(dcm) + dcm$	-7.3
${}^1Ni^3Ni(py) + py \rightarrow {}^3Ni_2(py)_2$	-7.5
${}^3Ni_2(py) + py \rightarrow {}^3Ni_2(py)_2$	-8.5
${}^3Ni_2(py)(dcm) + py \rightarrow {}^3Ni_2(py)_2 + dcm$	-6.1
${}^3Ni_2(py)_2 + py \rightarrow {}^3Ni_2(py)_3$	-6.4
${}^3Ni_2(py)_3 + py \rightarrow 2\ Ni(py)_2$	+7.9
${}^3Ni_2(py) + 3\ py \rightarrow 2Ni(py)_2$	-7.0
${}^3Ni_2(py)(dcm) + 3\ py \rightarrow 2Ni(py)_2 + dcm$	-4.6

S1.10 XYZ Atomic Coordinates of the PBE/def2-SVP Optimized Ligand and Complexes

S1.10.1 Pyridine

C	-1.205650	0.676271	0.000000
C	-1.147329	-0.728028	0.000000
C	0.000002	1.393404	0.000000
C	1.205652	0.676268	0.000000
C	1.147327	-0.728031	0.000000
N	-0.000002	-1.425803	0.000000
H	-2.080780	-1.320515	0.000000
H	0.000003	2.494678	0.000000
H	-2.177144	1.193838	0.000000
H	2.080777	-1.320519	0.000000
H	2.177148	1.193832	0.000000

S1.10.2 Ethylenediamido-substituted nickel(II) dipyridylmethane A

A			
C	1.175875	1.723351	0.082018
C	1.590070	-3.060103	-0.085210
C	0.636111	-4.071931	-0.266105
C	-0.728558	-3.739561	-0.262885
C	-1.086347	-2.403902	-0.094392
C	2.232193	-0.651646	0.447136
C	1.914384	0.833562	0.143049
N	-0.142113	-1.425215	0.069341
N	0.640482	1.281532	0.095646
C	2.980262	1.751620	0.054637
C	2.715885	3.121060	-0.090608
C	1.383596	3.563092	-0.136588
C	0.366107	2.616772	-0.036662
C	2.454287	-0.754775	1.974698
O	3.488028	-0.999060	-0.140245
C	-2.527727	-1.919336	-0.054467
C	-1.111559	2.962179	-0.129526
N	-2.522220	-0.568230	0.065723
O	-3.495091	-2.686783	-0.120256
N	-1.835903	1.823502	0.018825
O	-1.518005	4.111068	-0.339336
H	2.756213	-1.786153	2.240600
H	1.518596	-0.502239	2.509883
Ni	-0.906919	0.261645	0.124498
C	3.542038	-0.973436	-1.562712
H	3.251130	-0.052637	2.287237
H	2.665188	-3.284816	-0.054569
H	4.008818	1.368864	0.109199
H	4.577619	-1.248222	-1.840131
H	3.316649	0.035122	-1.975713
H	2.841993	-1.704258	-2.026088
C	-3.690976	0.292094	0.213141
C	-3.267502	1.701437	-0.248936
H	-4.005590	0.316316	1.282590
H	-4.553074	-0.104306	-0.365399
H	-3.843499	2.503985	0.260943
H	-3.453006	1.822563	-1.341795
H	0.959453	-5.115511	-0.398645
H	-1.537560	-4.475223	-0.383254
H	3.548079	3.837442	-0.164296
H	1.092701	4.617468	-0.254061

A(py)			
C	-1.392540	1.795424	-0.442010
C	-2.580847	2.529651	-0.244609
C	-3.818271	1.868877	-0.325554
C	-3.862058	0.493244	-0.616682
C	-2.651835	-0.196644	-0.739059
C	-0.052167	2.566038	-0.642877
C	1.318578	1.827505	-0.547539
N	-1.465231	0.464542	-0.633869
N	1.414108	0.493404	-0.694427
C	2.499522	2.599342	-0.472398
C	3.743593	1.968287	-0.626766
C	3.803894	0.582267	-0.861187
C	2.607014	-0.141125	-0.864365
C	-0.117395	3.134784	-2.081567
O	-0.032748	3.715212	0.209876
C	-2.555285	-1.695931	-1.083796
C	2.555661	-1.670796	-1.066910
N	-1.300664	-2.144854	-0.850346
O	-3.537118	-2.294769	-1.550314
N	1.291025	-2.105757	-0.882009
O	3.583050	-2.299394	-1.365226
H	4.742551	0.035297	-1.033087
H	-1.028936	3.751516	-2.201238
H	-0.144010	2.308711	-2.817808
Ni	-0.008903	-0.820087	-0.337777
N	0.046780	-0.731244	1.687687
C	-1.093562	-0.899808	2.394665
C	-1.100356	-1.044689	3.786929
C	0.119474	-1.020471	4.479907
C	1.302228	-0.849953	3.744542
C	1.222861	-0.710061	2.354063
H	2.285406	-0.829645	4.237031
C	0.040297	3.436883	1.599439
H	0.771226	3.764417	-2.280996
H	0.007740	4.412892	2.121000
H	0.986274	2.916753	1.876093
H	-0.815365	2.815385	1.950574
H	-2.027049	-0.929980	1.811029
H	-2.056134	-1.180789	4.313732
H	0.148363	-1.137161	5.573826
C	-0.744007	-3.392833	-1.351419
C	0.776752	-3.456480	-0.983380
H	-0.871108	-3.431744	-2.459090
H	-1.275409	-4.287720	-0.953585
H	1.344248	-4.062713	-1.724178
H	0.895743	-3.976046	-0.001719
H	-4.799710	-0.065322	-0.752922
H	-2.522867	3.612869	-0.064744
H	-4.750508	2.436898	-0.182260
H	2.424853	3.685360	-0.317169
H	4.667944	2.564693	-0.578385
H	2.129143	-0.583323	1.741153

S1.10.3 *trans*-Cyclohexylenediamido-substituted nickel(II) dipyridylmethane B

B			
C	1.177445	-1.721459	0.128694
C	1.594351	-3.064200	0.029372
C	0.645840	-4.083442	-0.134447
C	-0.716707	-3.749029	-0.188685
C	-1.076796	-2.408379	-0.070651
C	2.234960	-0.637381	0.443818
C	1.911902	0.832745	0.085444
N	-0.139747	-1.422229	0.081369
N	0.636760	1.281128	0.061210
C	2.976740	1.745061	-0.057330
C	2.712531	3.113231	-0.213168
C	1.381356	3.559742	-0.204254
C	0.365248	2.616137	-0.070516
C	2.469697	-0.676595	1.972542
O	3.486755	-1.007555	-0.138941
C	-2.510729	-1.919082	-0.173269
C	-1.108896	2.982068	-0.008919
N	-2.539910	-0.579656	0.053615
O	-3.446365	-2.680799	-0.450551
N	-1.841581	1.839670	-0.010226
O	-1.488846	4.159359	0.039644
H	2.770067	-1.696612	2.280725
H	1.539665	-0.397128	2.504218
Ni	-0.916619	0.265156	0.101268
C	3.526181	-1.049899	-1.561409
H	3.271655	0.035504	2.247010
H	2.669112	-3.284666	0.090166
H	4.005232	1.359689	-0.025001
H	4.563110	-1.322059	-1.836423
H	3.280554	-0.066167	-2.020349
H	2.833196	-1.813094	-1.981144
C	-3.677207	0.292610	-0.242911
C	-3.282563	1.714649	0.208302
H	0.971636	-5.131351	-0.217562
H	-1.523122	-4.484310	-0.326969
H	3.543958	3.825455	-0.325733
H	1.088854	4.616626	-0.290851
C	-5.033741	-0.095857	0.379282
H	-3.792655	0.321133	-1.354349
C	-5.965145	1.142420	0.466813
H	-4.856838	-0.515810	1.391659
H	-5.484675	-0.911040	-0.218853
C	-4.196390	2.749275	-0.478448
C	-5.639831	2.192058	-0.610846
H	-3.784286	2.987970	-1.480747
H	-4.170494	3.695996	0.094576
H	-5.773661	1.725789	-1.610976
H	-6.371148	3.025172	-0.567328
H	-5.869293	1.617870	1.466985
H	-7.025110	0.825148	0.385091
H	-3.45645	1.766039	1.311364

B(py)			
C	1.320944	-1.803028	0.362115
C	1.724976	-3.157467	0.355381
C	0.749596	-4.163839	0.286895
C	-0.614197	-3.819802	0.230356
C	-0.951870	-2.463426	0.187077
C	2.376351	-0.704236	0.690540
C	2.083187	0.798710	0.394834
N	0.014402	-1.507196	0.240705
N	0.821371	1.258369	0.288731
C	3.152345	1.717487	0.423477
C	2.876057	3.095485	0.413264
C	1.543976	3.542258	0.394183
C	0.525532	2.587937	0.301000
C	2.602263	-0.791558	2.219731
O	3.633427	-1.066826	0.108778
C	-2.408630	-1.971746	0.041972
C	-0.973860	2.939147	0.325751
N	-2.432018	-0.619599	-0.007085
O	-3.334435	-2.796732	-0.013963
N	-1.711128	1.901863	-0.133797
O	-1.340957	4.035687	0.781382
H	2.889345	-1.823446	2.500644
H	1.675213	-0.517677	2.758966
Ni	-0.747575	0.226766	-0.298691
C	3.671144	-1.058347	-1.309857
H	3.411323	-0.098723	2.521457
H	4.183905	1.342388	0.487177
H	4.705972	-1.322485	-1.601434
H	3.424845	-0.057174	-1.731699
H	2.974296	-1.805238	-1.755511
C	-3.554408	0.268916	-0.261831
C	-3.134722	1.724842	0.131878
H	-1.427575	-4.559541	0.203139
C	-4.893387	-0.075955	0.425513
H	-3.724747	0.276404	-1.368846
C	-5.818105	1.167054	0.504754
H	-4.681521	-0.459560	1.445455
H	-5.374560	-0.912324	-0.118621
C	-4.086187	2.729014	-0.553063
C	-5.533859	2.177279	-0.620529
H	-3.705508	2.934746	-1.576726
H	-4.034632	3.689892	-0.003104
H	-5.703394	1.675488	-1.598233
H	-6.264239	3.011972	-0.581106
H	-5.680885	1.678798	1.481712
H	-6.881393	0.850408	0.477885
H	-3.279632	1.815617	1.236670
N	-0.259092	0.134756	-2.274433
C	-0.103256	-1.029548	-2.942786
C	0.095299	-1.084176	-4.327592
C	0.137713	0.114136	-5.055929
C	-0.026052	1.322420	-4.361870
C	-0.226005	1.291029	-2.976826
H	-0.007407	2.290027	-4.884395
H	-0.391532	2.208886	-2.392163
H	-0.147879	-1.950255	-2.340430
H	0.290229	0.105873	-6.145810
H	0.209444	-2.060139	-4.821698
H	1.055948	-5.221521	0.288368
H	2.795094	-3.400451	0.423324
H	3.705716	3.818689	0.443765
H	1.263185	4.604096	0.451265

S1.10.4 Phenylenediamido-substituted nickel(II) dipyridylmethane C

C			
C	-2.217922	1.329398	0.103174
C	-2.990032	2.504957	-0.018356
C	-2.356857	3.745440	-0.163095
C	-0.953075	3.805221	-0.169583
C	-0.237414	2.615703	-0.046131
C	-2.940980	0.000057	0.424396
C	-2.217940	-1.329357	0.103378
N	-0.870491	1.408165	0.078937
N	-0.870517	-1.408137	0.078908
C	-2.990084	-2.504932	-0.017842
C	-2.356947	-3.745450	-0.162427
C	-0.953165	-3.805218	-0.169377
C	-0.237473	-2.615695	-0.046186
C	-3.211976	0.000202	1.948269
O	-4.232625	-0.000003	-0.186498
C	1.278190	2.560611	-0.049926
C	1.278128	-2.560616	-0.050250
N	1.669895	1.255138	0.036232
O	1.974059	3.578823	-0.132092
N	1.669865	-1.255164	0.036080
O	1.973975	-3.578828	-0.132624
H	-3.791395	0.901558	2.226524
H	-2.254430	0.000236	2.503863
N	0.335225	-0.000002	0.108199
C	-4.249703	-0.000103	-1.610394
H	-3.791416	-0.901093	2.226682
H	-4.084857	2.418811	0.014324
H	-4.084900	-2.418753	0.014958
H	-5.315213	-0.000878	-1.909367
H	-3.757244	-0.901868	-2.038514
H	-3.758524	0.902305	-2.038631
C	2.965408	0.716127	0.005324
C	2.965391	-0.716178	0.005214
H	-2.957420	4.662405	-0.261507
H	-0.381047	4.739425	-0.268030
H	-2.957537	-4.662359	-0.261195
H	-0.381162	-4.739424	-0.267960
C	4.179791	1.425763	-0.033276
C	4.179756	-1.425840	-0.033491
C	5.385407	-0.703131	-0.068073
C	5.385424	0.703030	-0.067967
H	4.155435	2.523069	-0.039134
H	6.339989	1.250722	-0.096774
H	6.339958	-1.250843	-0.096965
H	4.155370	-2.523144	-0.039519

C(py)			
C	-2.213383	-1.356231	-0.772545
C	-2.983947	-2.539215	-0.759346
C	-2.334289	-3.783489	-0.719936
C	-0.928712	-3.840689	-0.703818
C	-0.216507	-2.637297	-0.669021
C	-2.923511	0.000099	-1.069856
C	-2.213420	1.356412	-0.772357
N	-0.872683	-1.441820	-0.691478
N	-0.872727	1.441998	-0.691232
C	-2.984007	2.539388	-0.759024
C	-2.334358	3.783657	-0.719375
C	-0.928782	3.840873	-0.703178
C	-0.216571	2.637475	-0.668603
C	-3.199416	0.000185	-2.593190
O	-4.216675	0.000038	-0.456509
C	1.320302	-2.580083	-0.641865
C	1.320230	2.580259	-0.641511
N	1.731876	-1.289589	-0.471184
O	1.988955	-3.612973	-0.786175
N	1.731778	1.289694	-0.471329
O	1.988884	3.613190	-0.785464
H	-0.362976	4.783911	-0.714124
H	-3.779344	-0.900729	-2.872437
H	-2.244133	0.000220	-3.152420
Ni	0.333937	0.000040	-0.167188
N	-0.059241	-0.000291	1.841774
C	-0.087894	-1.161030	2.534573
C	-0.148567	-1.205318	3.932238
C	-0.178429	-0.000559	4.650425
C	-0.148884	1.204340	3.932457
C	-0.088212	1.160315	2.534783
H	-0.166037	2.177420	4.444704
C	-4.215627	-0.000163	0.963443
H	-3.779349	0.901123	-2.872355
H	-5.276057	-0.000009	1.281229
H	-3.716141	0.902105	1.385101
H	-3.716468	-0.902735	1.384834
H	-0.054812	-2.087027	1.938944
H	-0.165470	-2.178497	4.444305
H	-0.219720	-0.000663	5.750126
C	3.000841	-0.727555	-0.506095
C	3.000802	0.727745	-0.506111
H	-0.362884	-4.783714	-0.714988
H	-4.080099	-2.467618	-0.805591
H	-2.928167	-4.710445	-0.717319
H	-4.080151	2.467776	-0.805343
H	-2.928240	4.710610	-0.716565
H	-0.055389	2.086436	1.939328
C	4.227895	-1.423785	-0.571604
C	5.430268	-0.704810	-0.630166
C	5.430230	0.705124	-0.630159
C	4.227817	1.424037	-0.571605
H	4.204862	-2.522012	-0.587198
H	6.385000	1.251433	-0.681879
H	6.385071	-1.251062	-0.681885
H	4.204748	2.522263	-0.587191

S1.10.5 4,5-Difluorophenylenediamido-substituted nickel(II) dipyridylmethane D

D			
C	2.653119	-1.330053	0.099821
C	3.424956	-2.505624	-0.024593
C	2.791353	-3.746442	-0.164333
C	1.387620	-3.807270	-0.163704
C	0.672047	-2.617889	-0.038018
C	3.378120	-0.000048	0.415406
C	2.653136	1.329996	0.099939
N	1.305956	-1.409884	0.082559
N	1.305975	1.409842	0.082615
C	3.424995	2.505565	-0.024366
C	2.791414	3.746396	-0.164076
C	1.387681	3.807241	-0.163510
C	0.672087	2.617863	-0.037933
C	3.660334	-0.000121	1.937360
O	4.664683	-0.000001	-0.204976
C	-0.843034	-2.561902	-0.035148
C	-0.842995	2.561874	-0.035379
N	-1.231482	-1.255642	0.052147
O	-1.545947	-3.575311	-0.114745
N	-1.231463	1.255628	0.052035
O	-1.545896	3.575329	-0.114495
H	4.242027	-0.901344	2.211191
H	2.707310	-0.000126	2.500658
Ni	0.102571	-0.000014	0.117812
C	4.671340	0.000143	-1.629172
H	4.242065	0.901053	2.211271
H	4.519920	-2.419264	0.001873
H	4.519956	2.419187	0.002135
H	5.734615	0.000644	-1.935793
H	4.176089	0.902129	-2.053543
H	4.176886	-0.902194	-2.053725
C	-2.523578	-0.715859	0.024413
C	-2.523568	0.715864	0.024362
H	3.391735	-4.663245	-0.265002
H	0.816589	-4.742464	-0.258378
H	3.391812	4.663198	-0.264664
H	0.816666	4.742440	-0.258221
C	-3.736839	-1.428105	-0.013180
C	-3.736817	1.428126	-0.013309
C	-4.934033	0.705021	-0.046404
C	-4.934044	-0.704984	-0.046335
H	-3.739843	-2.525216	-0.021072
F	-6.112144	-1.352397	-0.080618
F	-6.112123	1.352449	-0.080750
H	-3.739804	2.525236	-0.021322

D(py)			
C	-8.532559	-5.643166	-0.738748
C	-9.304509	-6.823967	-0.680443
C	-8.653324	-8.066030	-0.608288
C	-7.247636	-8.126298	-0.625445
C	-6.533149	-6.925160	-0.654474
C	-9.222752	-4.290702	-1.102531
C	-8.535777	-2.930178	-0.763850
N	-7.190322	-5.731487	-0.683878
N	-7.193736	-2.837723	-0.711812
C	-9.310463	-1.750342	-0.726467
C	-8.662118	-0.505626	-0.678221
C	-7.256601	-0.442395	-0.698158
C	-6.539320	-1.642199	-0.705327
C	-9.363862	-4.304971	-2.644473
O	-10.567329	-4.287661	-0.612449
C	-4.996366	-6.870547	-0.726283
C	-5.002465	-1.694684	-0.777203
N	-4.576557	-5.572956	-0.664565
O	-4.332607	-7.907390	-0.856884
N	-4.579640	-2.989870	-0.690497
O	-4.341124	-0.659060	-0.928160
H	-6.697140	0.504224	-0.715903
H	-9.916068	-5.210341	-2.962891
H	-8.362862	-4.307498	-3.116607
Ni	-5.953879	-4.279139	-0.282800
N	-6.070022	-4.259287	1.748738
C	-4.890208	-4.247992	2.411422
C	-4.815593	-4.233529	3.808640
C	-6.002786	-4.230624	4.556491
C	-7.224980	-4.242497	3.868203
C	-7.212119	-4.256741	2.468401
H	-8.184884	-4.240925	4.405296
C	-10.720983	-4.275367	0.796100
H	-9.919065	-3.407269	-2.978973
H	-11.809782	-4.273059	0.996712
H	-10.275819	-3.366475	1.262922
H	-10.276814	-5.176544	1.278583
C	-3.318505	-5.010328	-0.795331
C	-3.320259	-3.552030	-0.810199
H	-6.685890	-9.071729	-0.624713
H	-10.400785	-6.756461	-0.726599
H	-9.247360	-8.991791	-0.563687
H	-10.406610	-1.821266	-0.770434
H	-9.258305	0.419406	-0.650292
H	-8.150494	-4.266644	1.893268
C	-2.096960	-5.708427	-0.931934
C	-0.911457	-4.987950	-1.079195
C	-0.913167	-3.574397	-1.093801
C	-2.100412	-2.853922	-0.961297
H	-2.091981	-6.806527	-0.934408
H	-2.098079	-1.756091	-0.986319
F	0.259888	-2.931589	-1.239486
F	0.263160	-5.630782	-1.211552
H	-3.981500	-4.250709	1.787979
H	-3.830609	-4.224655	4.297522
H	-5.975747	-4.219300	5.656549

S1.10.6 Propylenediamido-substituted nickel(II) dipyridylmethane E

E			
C	1.759376	-1.311018	0.132850
C	2.563151	-2.464108	0.025705
C	1.982170	-3.711916	-0.229029
C	0.588715	-3.787819	-0.343521
C	-0.154890	-2.616848	-0.204192
C	2.444326	0.000131	0.549271
C	1.759297	1.311163	0.132568
N	0.412520	-1.394895	0.014227
N	0.412385	1.394998	0.014367
C	2.562995	2.464258	0.025020
C	1.981882	3.712052	-0.229505
C	0.588379	3.787939	-0.343371
C	-0.155134	2.616929	-0.203833
C	2.527973	0.000348	2.093649
O	3.803349	0.000105	0.099631
C	-1.651897	-2.625820	-0.242033
C	-1.652149	2.625795	-0.241673
N	-2.144921	-1.376098	-0.031530
O	-2.296527	-3.671461	-0.411137
N	-2.145051	1.375952	-0.031578
O	-2.296822	3.671426	-0.410658
H	0.029672	4.718256	-0.522548
H	3.068563	-0.901640	2.439789
H	1.508428	0.000506	2.525144
Ni	-0.878955	-0.000015	0.041820
C	4.008968	-0.000161	-1.309742
H	3.068736	0.902329	2.439534
H	5.105295	0.000026	-1.462030
H	3.580277	0.901043	-1.801718
H	3.580647	-0.901753	-1.801326
C	-3.592936	-1.260999	0.016783
C	-3.593039	1.260344	0.015799
H	0.030103	-4.718147	-0.522947
H	3.647176	-2.353621	0.162892
H	2.610935	-4.610265	-0.321688
H	3.647075	2.353811	0.161780
H	2.610602	4.610401	-0.322481
C	-4.045540	-0.000071	0.739672
H	-3.996236	-2.172616	0.508758
H	-4.015772	-1.267372	-1.017484
H	-3.653591	0.000415	1.780405
H	-5.153427	-0.000145	0.807574
H	-4.015143	1.265458	-1.018783
H	-3.997006	2.172296	0.506577

E(py)			
C	1.980500	1.346081	-0.485212
C	2.771545	2.505706	-0.326092
C	2.167961	3.769206	-0.378125
C	0.785584	3.858506	-0.594648
C	0.051126	2.671820	-0.699128
C	2.725210	-0.000944	-0.668503
C	1.979325	-1.347393	-0.485767
N	0.645413	1.450318	-0.634327
N	0.644154	-1.450470	-0.635078
C	2.769388	-2.507725	-0.326964
C	2.164753	-3.770709	-0.379368
C	0.782295	-3.858785	-0.595860
C	0.048845	-2.671450	-0.700054
C	3.245654	-0.000877	-2.126940
O	3.904270	-0.001619	0.146836
C	-1.461612	2.704071	-0.882973
C	-1.463960	-2.702410	-0.883699
N	-1.995966	1.463802	-0.807184
O	-2.035649	3.793069	-1.067354
N	-1.997282	-1.461759	-0.807273
O	-2.038887	-3.790883	-1.068454
H	0.231376	-4.806540	-0.682960
H	3.863123	0.900132	-2.307337
H	2.394943	-0.000371	-2.835099
Ni	-0.762158	0.000512	-0.404985
N	-0.759882	-0.000346	1.637439
C	-0.839346	1.160725	2.324922
C	-0.993248	1.204019	3.715847
C	-1.072176	-0.000720	4.429940
C	-0.994055	-1.205264	3.715449
C	-0.840123	-1.161573	2.324531
H	-1.056461	-2.178745	4.223370
C	3.675782	-0.001771	1.548396
H	3.862319	-0.902371	-2.307660
H	4.671994	-0.002190	2.031247
H	3.115860	-0.904288	1.884831
H	3.116486	0.901031	1.885100
H	-0.786157	2.085479	1.730547
H	-1.055001	2.177347	4.224147
H	-1.197341	-0.000845	5.523358
C	-3.429949	1.302605	-0.945417
C	-3.431105	-1.299221	-0.945320
H	0.235501	4.806763	-0.681557
H	3.856295	2.394673	-0.189049
H	2.779622	4.677525	-0.263417
H	3.854228	-2.397652	-0.189868
H	2.775671	-4.679568	-0.264972
H	-0.787650	-2.086144	1.729806
C	-3.812191	0.001837	-1.668229
H	-3.846539	2.184174	-1.482202
H	-3.913605	1.308488	0.063846
H	-3.351537	0.001587	-2.680363
H	-4.913608	0.002336	-1.818232
H	-3.914610	-1.304474	0.064019
H	-3.848628	-2.180446	-1.481945

S1.10.7 1,8-Naphthalenediamido-substituted nickel(II) dipyridylmethane F

F			
C	1.699675	-1.316146	0.032042
C	2.496249	-2.443571	-0.247428
C	1.906545	-3.626202	-0.714529
C	0.514407	-3.676452	-0.844370
C	-0.225232	-2.541381	-0.506495
C	2.359325	-0.073132	0.645162
C	1.704983	1.267453	0.281280
N	0.354401	-1.376672	-0.103668
N	0.379395	1.351518	0.016929
C	2.501294	2.427674	0.322068
C	1.939638	3.678789	0.032466
C	0.578605	3.745570	-0.279120
C	-0.169533	2.564416	-0.256403
C	2.306027	-0.229109	2.181663
O	3.750803	-0.044086	0.317650
C	-1.718810	-2.572730	-0.432377
C	-1.643110	2.587398	-0.495450
N	-2.201949	-1.369593	0.038611
O	-2.338784	-3.606523	-0.704584
N	-2.233071	1.371890	-0.200809
O	-2.162304	3.653300	-0.859827
H	0.044132	4.673786	-0.526438
H	2.820594	-1.163121	2.479317
H	1.252674	-0.269864	2.519729
Ni	-0.935864	-0.003087	0.014534
C	4.094780	0.126723	-1.055169
H	2.809720	0.631695	2.662205
H	5.197013	0.040553	-1.107993
H	3.796639	1.123383	-1.448564
H	3.644159	-0.652478	-1.708616
C	-3.525988	-1.246081	0.482329
C	-3.633772	1.243409	-0.092455
H	-0.045789	-4.566790	-1.164904
H	3.577794	-2.373597	-0.072449
H	2.530087	-4.501838	-0.949883
H	3.562275	2.321173	0.584953
H	2.561737	4.586194	0.054336
C	-4.234842	0.002143	0.360899
C	-4.492616	2.336117	-0.351031
C	-5.874070	2.288732	-0.075494
C	-6.443163	1.158688	0.479565
C	-5.645242	0.001174	0.702490
C	-6.256815	-1.161763	1.250692
C	-5.520688	-2.318568	1.441800
C	-4.172677	-2.365091	1.041771
H	-3.620085	-3.307176	1.124927
H	-5.986078	-3.216809	1.875790
H	-7.325626	-1.118110	1.510528
H	-7.512286	1.121582	0.739286
H	-6.486396	3.178719	-0.288703
H	-4.053172	3.253279	-0.750323

F(py)			
C	1.859447	-1.355269	0.098480
C	2.641626	-2.493746	-0.188140
C	2.010092	-3.731229	-0.381684
C	0.618691	-3.819713	-0.252979
C	-0.100663	-2.648451	0.023881
C	2.572208	-0.057253	0.538188
C	1.865836	1.302989	0.316362
N	0.517381	-1.452036	0.172562
N	0.523112	1.403492	0.234212
C	2.667871	2.463428	0.348909
C	2.059578	3.725812	0.312285
C	0.664137	3.809597	0.260833
C	-0.077395	2.619568	0.222574
C	2.801137	-0.191813	2.062551
O	3.888379	-0.010408	-0.028651
C	-1.602941	-2.704039	0.232568
C	-1.593264	2.686360	0.176707
N	-2.167075	-1.463239	0.399205
O	-2.129411	-3.830913	0.244471
N	-2.191122	1.451830	0.176390
O	-2.101476	3.822522	0.168097
H	0.104666	4.755490	0.250902
H	3.374700	-1.115461	2.272186
H	1.829135	-0.243300	2.589260
Ni	-0.896653	-0.017443	-0.024839
C	3.962035	0.145648	-1.437209
H	3.370157	0.680851	2.437397
H	5.037365	0.131353	-1.700159
H	3.529369	1.113799	-1.779317
H	3.454426	-0.681779	-1.983783
C	-3.531819	-1.286080	0.681821
C	-3.582329	1.277388	0.110626
H	0.052776	-4.757388	-0.345009
H	3.735383	-2.397853	-0.221871
H	2.610126	-4.625850	-0.609257
H	3.758934	2.354239	0.419697
H	2.676855	4.637120	0.337063
C	-4.205244	-0.007201	0.448153
C	-4.411299	2.363551	-0.250342
C	-5.815703	2.290838	-0.220424
C	-6.431834	1.135878	0.220481
C	-5.658164	-0.009364	0.569060
C	-6.360471	-1.153631	1.045350
C	-5.673518	-2.301622	1.390426
C	-4.283956	-2.370176	1.186904
H	-3.758906	-3.311490	1.373784
H	-6.205090	-3.180877	1.786593
H	-7.456130	-1.093292	1.134816
H	-7.527051	1.072220	0.314442
H	-6.408590	3.172623	-0.509790
H	-3.923429	3.309559	-0.503779
N	-0.924112	-0.079049	-2.061422
C	0.157743	0.140760	-2.837193
C	0.096523	0.136651	-4.235575
C	-1.137444	-0.104524	-4.857469
C	-2.261084	-0.330998	-4.049643
C	-2.115602	-0.310678	-2.657394
H	-2.972493	-0.480542	-1.987461
H	-3.252155	-0.522993	-4.485372
H	-1.221735	-0.114364	-5.954739
H	1.007945	0.322402	-4.822455
H	1.105345	0.329151	-2.309622

S1.10.8 Bis(amido)-substituted nickel(II) dipyridylmethane G

G			
C	-0.683501	1.033195	0.560844
C	0.475393	1.825051	0.429866
C	1.726863	1.224248	0.246844
C	1.802320	-0.175216	0.221855
C	0.626417	-0.906600	0.366868
C	-2.002816	1.744398	0.915655
C	-3.322145	1.032959	0.561388
N	-0.597165	-0.317645	0.520272
N	-3.408308	-0.317915	0.521336
C	-4.481206	1.824598	0.430647
C	-5.732689	1.223541	0.248508
C	-5.807970	-0.175940	0.224151
C	-4.631881	-0.907102	0.368804
C	-2.002564	1.950699	2.449214
O	-2.003032	3.062509	0.358827
C	0.610039	-2.416541	0.383558
C	-4.615188	-2.417040	0.385389
N	-0.664336	-2.844008	0.540046
O	1.641313	-3.089531	0.273702
N	-3.340637	-2.844264	0.541104
O	-5.646509	-3.090219	0.277116
H	2.737457	-0.741971	0.100751
H	-6.743080	-0.742874	0.103686
H	-1.100733	2.517177	2.751654
H	-2.002395	0.969372	2.961708
Ni	-2.002589	-1.578439	0.579821
C	-2.003309	3.145885	-1.062832
H	-2.904381	2.517034	2.751962
H	0.367178	2.916552	0.489948
H	2.629791	1.843852	0.138427
H	-4.373133	2.916137	0.490291
H	-6.635746	1.842980	0.140220
H	-2.002746	4.224541	-1.310759
H	-2.905309	2.675820	-1.514320
H	-1.102064	2.674786	-1.514741
H	-0.770721	-3.864829	0.547428
H	-3.234088	-3.865069	0.548442

G(py)			
C	-1.211560	1.786368	0.146497
C	-2.305203	2.525768	0.649352
C	-3.612954	2.094808	0.393436
C	-3.808569	0.937312	-0.370401
C	-2.682962	0.227585	-0.802422
C	0.184160	2.448208	0.246324
C	1.473731	1.604112	0.100107
N	-1.415875	0.640918	-0.535041
N	1.496423	0.424057	-0.552002
C	2.675060	2.202624	0.541683
C	3.902464	1.589660	0.261601
C	3.911738	0.392306	-0.465083
C	2.686188	-0.166831	-0.842536
C	0.232861	3.499171	-0.890023
O	0.257605	3.208860	1.460334
C	-2.844759	-1.068380	-1.592404
C	2.645992	-1.490455	-1.601384
N	-1.656927	-1.672180	-1.785906
O	-3.981728	-1.426933	-1.946639
N	1.380449	-1.916044	-1.773311
O	3.713608	-2.019471	-1.957773
H	4.824076	-0.147040	-0.759068
H	-0.621148	4.197285	-0.795257
H	0.177820	2.996771	-1.874792
Ni	-0.066849	-0.869821	-0.953659
N	-0.129972	-1.720810	0.904356
C	-1.312376	-2.035280	1.478169
C	-1.400222	-2.750183	2.678883
C	-0.219757	-3.163568	3.313437
C	1.006739	-2.840758	2.714652
C	1.007700	-2.122701	1.512712
H	1.963050	-3.144826	3.164670
C	0.236179	2.447027	2.659044
H	1.176833	4.074791	-0.832900
H	0.287942	3.171121	3.494832
H	1.104557	1.753249	2.733710
H	-0.697727	1.848523	2.762145
H	-2.217372	-1.709468	0.944389
H	-2.389451	-2.981118	3.100309
H	-0.2551660	-3.731636	4.255438
H	-4.794644	0.539172	-0.650983
H	-2.106624	3.447019	1.214304
H	-4.469471	2.670564	0.777261
H	2.622040	3.157514	1.082752
H	4.842184	2.054420	0.598256
H	1.950242	-1.864872	1.007494
H	1.347008	-2.820295	-2.260406
H	-1.760592	-2.561393	-2.290489

S1.10.9 Bis(methylamido)-substituted nickel(II) dipyridylmethane H

H			
C	-0.709658	0.995739	0.720061
C	0.453459	1.787890	0.805609
C	1.720131	1.200208	0.708583
C	1.800719	-0.185465	0.521273
C	0.616719	-0.917823	0.446692
C	-2.059190	1.709228	0.915229
C	-3.317334	0.967787	0.438703
N	-0.618049	-0.344437	0.547270
N	-3.398297	-0.378904	0.551237
C	-4.449781	1.721958	0.074545
C	-5.671572	1.082926	-0.176031
C	-5.752011	-0.305773	-0.007735
C	-4.600018	-0.998310	0.363062
C	-2.243863	1.962069	2.430251
O	-2.003844	3.010942	0.324432
C	0.616263	-2.393304	0.178244
C	-4.609031	-2.463052	0.696817
N	-0.653679	-2.880116	0.166796
O	1.664545	-3.010413	-0.061601
N	-3.350882	-2.890273	0.983879
O	-5.661848	-3.112258	0.771482
H	2.742881	-0.743708	0.418844
H	-6.675872	-0.889757	-0.131060
H	-1.383909	2.536424	2.825342
H	-2.315097	0.998620	2.970579
Ni	-1.997880	-1.643595	0.609058
C	-1.781704	3.057675	-1.081253
H	-3.172772	2.540418	2.598433
H	0.332880	2.871284	0.944495
H	2.627587	1.819074	0.775446
H	-4.353760	2.814904	0.024475
H	-6.554138	1.670205	-0.471372
H	-1.842250	4.124435	-1.369953
H	-2.549636	2.488296	-1.651230
H	-0.778163	2.668251	-1.363070
C	-0.806213	-4.242513	-0.316808
H	-0.009228	-4.460624	-1.057655
H	-1.797058	-4.368420	-0.790524
H	-0.705884	-5.000841	0.490436
C	-3.240293	-4.209795	1.580405
H	-3.349959	-5.032166	0.839635
H	-4.050784	-4.350437	2.327074
H	-2.261488	-4.315010	2.082317

H(py)			
C	-1.183067	1.742559	0.243037
C	-2.254257	2.457515	0.822513
C	-3.564916	1.988472	0.668228
C	-3.785148	0.829076	-0.084537
C	-2.674533	0.153176	-0.605565
C	0.193822	2.438608	0.207047
C	1.485035	1.606151	0.027787
N	-1.403741	0.590913	-0.421358
N	1.491237	0.364263	-0.500927
C	2.695794	2.270551	0.325507
C	3.919105	1.657144	0.032040
C	3.911933	0.388214	-0.556184
C	2.678460	-0.232633	-0.792063
C	0.134634	3.416337	-0.992418
O	0.333661	3.277844	1.362469
C	-2.867155	-1.102326	-1.432430
C	2.654641	-1.642220	-1.345694
N	-1.694348	-1.701423	-1.747849
O	-4.024801	-1.448591	-1.740443
N	1.405296	-2.151400	-1.428739
O	3.734664	-2.201739	-1.620931
H	4.815166	-0.172165	-0.837558
H	-0.725371	4.103399	-0.873731
H	0.014912	2.851796	-1.936927
Ni	-0.081166	-0.960170	-0.830288
N	-0.217416	-1.758599	1.048882
C	-1.386192	-2.260957	1.505671
C	-1.490254	-2.931492	2.730998
C	-0.341513	-3.094043	3.518292
C	0.871723	-2.576184	3.041668
C	0.891391	-1.920574	1.805026
H	1.804675	-2.680737	3.614563
C	0.434221	2.598137	2.605543
H	1.066853	4.011095	-1.044177
H	0.503793	3.378889	3.387354
H	1.342187	1.955274	2.663108
H	-0.456855	1.962836	2.813506
H	-2.262781	-2.127256	0.854352
H	-2.466566	-3.322910	3.051959
H	-0.389322	-3.619545	4.484140
H	-4.778763	0.410417	-0.299691
H	-2.039420	3.392216	1.358222
H	-4.406189	2.540468	1.115421
H	2.650638	3.272864	0.773243
H	4.865803	2.173304	0.255048
H	1.827837	-1.515344	1.394060
C	-1.807695	-2.886422	-2.576953
H	-0.976599	-2.930141	-3.307623
H	-2.778815	-2.890101	-3.114950
H	-1.766802	-3.824177	-1.975314
C	1.334084	-3.553888	-1.789623
H	1.170917	-3.698060	-2.882037
H	0.488945	-4.043691	-1.265622
H	2.284049	-4.072641	-1.538078

S1.10.10 Bis(pyrrolido)-substituted nickel(II) dipyridylmethane I

I

C	1.309311	1.290176	0.256508
C	2.451849	2.108277	0.302732
C	3.728457	1.530242	0.202154
C	3.839529	0.15123	0.062145
C	2.667819	-0.637298	0.029548
C	-0.046016	1.991256	0.467451
C	-1.317732	1.269237	-0.012172
N	1.410049	-0.052519	0.128219
N	-1.412929	-0.076666	0.070514
C	-2.432695	2.059664	-0.339898
C	-3.670524	1.443193	-0.592748
C	-3.783245	0.061952	-0.469011
C	-2.644257	-0.694129	-0.114157
C	-0.219263	2.211962	1.989240
O	0.004799	3.305619	-0.095419
C	2.626606	-2.054346	-0.125805
C	-2.613790	-2.099343	0.139204
N	1.354351	-2.599804	-0.107848
C	3.574767	-3.059859	-0.421007
N	-1.359478	-2.593166	0.454996
C	-3.583270	-3.112680	0.312182
H	4.815831	-0.346202	-0.017882
H	-4.737012	-0.458458	-0.632239
H	0.642971	2.781269	2.386259
H	-0.279564	1.236062	2.507965
Ni	0.003532	-1.345204	0.189272
C	0.202329	3.382806	-1.503260
H	-1.150357	2.780360	2.177538
H	2.315993	3.190944	0.421218
H	4.627794	2.163645	0.237003
H	-2.317756	3.150517	-0.357441
H	-4.545912	2.052474	-0.864481
H	0.147959	4.456940	-1.765647
H	-0.583172	2.835393	-2.070370
H	1.196652	2.989316	-1.810437
C	1.472716	-3.919066	-0.411015
C	2.834136	-4.245199	-0.603341
C	-1.513928	-3.884760	0.845037
C	-2.877983	-4.246352	0.766774
H	-4.664658	-3.020664	0.155470
H	-3.298124	-5.223352	1.034254
H	-0.665695	-4.485500	1.190961
H	0.596216	-4.568590	-0.504541
H	4.659793	-2.931797	-0.514444
H	3.224581	-5.237164	-0.860399

I(py)

C	-1.284342	4.181717	1.405744
C	-2.283639	5.005427	1.960461
C	-3.633203	4.642085	1.808699
C	-3.957083	3.487958	1.104215
C	-2.914074	2.679479	0.586149
C	0.146989	4.772040	1.381055
C	1.395594	3.869765	1.215952
N	-1.593238	3.036206	0.765839
N	1.343730	2.669150	0.602975
C	2.623661	4.452713	1.585610
C	3.821460	3.785165	1.276930
C	3.773429	2.569087	0.605467
C	2.512468	2.010476	0.276217
C	0.170669	5.746626	0.176819
O	0.326950	5.606006	2.535008
C	-3.135251	1.451904	-0.129877
C	2.353131	0.741373	-0.381138
N	-2.021894	0.723091	-0.508505
C	-4.316442	0.796142	-0.561121
N	1.064759	0.279971	-0.582845
C	3.290676	-0.203640	-0.871431
H	4.689433	2.028261	0.330496
H	-0.647170	6.485925	0.276240
H	0.034124	5.184059	-0.766526
Ni	-0.321034	1.468721	0.246016
N	-0.366687	0.522380	2.057895
C	0.772829	0.044870	2.604565
C	0.785940	-0.661025	3.813782
C	-0.425159	-0.887879	4.483082
C	-1.607069	-0.400291	3.907440
C	-1.536321	0.296961	2.695040
C	0.347438	4.928214	3.782663
H	1.140909	6.278160	0.141202
H	0.492906	5.703047	4.560257
H	1.183280	4.195035	3.848945
H	-0.607974	4.393045	3.986161
H	1.699108	0.224137	2.036933
H	1.741315	-1.030204	4.214248
H	-5.001528	3.184955	0.947283
H	-1.990956	5.933664	2.467164
H	-4.426707	5.277825	2.231303
H	2.622553	5.432430	2.079919
H	4.789290	4.231716	1.553052
C	-3.889129	-0.370304	-1.227248
H	-5.349413	1.140235	-0.426180
C	-2.476464	-0.374106	-1.162618
H	-1.784001	-1.120675	-1.571415
H	-4.519929	-1.124946	-1.713232
C	2.529335	-1.273135	-1.383318
H	4.383895	-0.111857	-0.867861
C	1.171772	-0.934331	-1.175087
H	0.282319	-1.526149	-1.425598
H	2.905953	-2.188240	-1.856931
H	-0.448381	-1.441716	5.434037
H	-2.585508	-0.559125	4.383737
H	-2.443660	0.676682	2.199932

S1.10.11 Bis(pyrazolato)-substituted nickel(II) dipyridylmethane J

J			
C	1.318715	1.282243	0.171392
C	2.459723	2.105067	0.113159
C	3.727336	1.529783	-0.052014
C	3.834986	0.142938	-0.137190
C	2.668505	-0.641778	-0.052747
C	-0.020258	1.980357	0.471896
C	-1.321674	1.273375	0.052070
N	1.416991	-0.063544	0.091146
N	-1.420680	-0.074246	0.082205
C	-2.448319	2.084092	-0.182264
C	-3.699556	1.490521	-0.402950
C	-3.811661	0.102299	-0.347761
C	-2.661868	-0.667791	-0.086041
C	-0.097262	2.169312	2.005963
O	0.001094	3.305351	-0.068769
C	2.629518	-2.072701	-0.095458
C	-2.631190	-2.091725	0.071096
N	1.372630	-2.618392	0.042296
C	3.543970	-3.131889	-0.261922
N	-1.379503	-2.612321	0.313845
C	-3.559152	-3.149697	0.147784
H	4.805836	-0.356963	-0.256923
H	-4.773741	-0.407981	-0.492154
H	0.786635	2.734779	2.358452
H	-0.119130	1.181798	2.505669
Ni	0.000274	-1.370380	0.194749
C	0.095128	3.409651	-1.486087
H	-1.015896	2.728860	2.267637
H	2.326997	3.190162	0.210089
H	4.623679	2.1659930	-0.104691
H	-2.324420	3.173904	-0.158984
H	-4.583569	2.116184	-0.598142
H	0.041531	4.489988	-1.721489
H	-0.739985	2.888670	-2.004837
H	1.055875	3.006178	-1.876203
N	1.413914	-3.932405	-0.032431
C	2.716867	-4.270040	-0.213232
N	-1.437176	-3.906324	0.546632
C	-2.745849	-4.258226	0.451673
H	-4.646082	-3.112671	0.016366
H	-3.040481	-5.302935	0.614892
H	4.629230	-3.078597	-0.401276
H	2.996358	-5.327760	-0.302624

J(py)			
C	-1.298908	4.200028	1.400295
C	-2.299175	5.040757	1.931292
C	-3.646071	4.667369	1.807704
C	-3.970065	3.483072	1.149634
C	-2.929111	2.668665	0.649680
C	0.135983	4.785181	1.362025
C	1.381232	3.867537	1.260833
N	-1.609635	3.034026	0.800318
N	1.335169	2.662644	0.658457
C	2.605680	4.435680	1.670133
C	3.800508	3.741947	1.425723
C	3.756518	2.514926	0.767830
C	2.503190	1.984691	0.387488
C	0.182687	5.699578	0.113297
O	0.304903	5.673313	2.477408
C	-3.152351	1.417041	-0.033499
C	2.344364	0.721448	-0.292286
N	-2.043856	0.699063	-0.409570
C	-4.300968	0.685128	-0.410099
N	1.062478	0.302959	-0.551013
C	3.235557	-0.268003	-0.765381
H	4.671328	1.951215	0.538630
H	-0.632370	6.446905	0.165235
H	0.057453	5.092434	-0.803548
Ni	-0.334394	1.463309	0.252158
N	-0.395686	0.380102	1.960689
C	-0.576160	-0.951406	1.802549
C	-0.636524	-1.817344	2.901765
C	-0.506236	-1.294161	4.196473
C	-0.31863	0.087868	4.348611
C	-0.269813	0.889667	3.202030
H	-0.210794	0.546826	5.342291
C	0.298722	5.065082	3.759673
H	1.156258	6.224439	0.067704
H	0.440597	5.879351	4.496443
H	1.126806	4.329793	3.882140
H	-0.666509	4.553774	3.979379
H	-0.671374	-1.308615	0.762145
H	-0.784529	-2.893537	2.731204
H	-0.549840	-1.954013	5.076493
H	-5.013579	3.167360	1.013253
H	-2.006864	5.988239	2.401511
H	-4.438589	5.315014	2.213285
H	2.603994	5.425367	2.144361
H	4.764023	4.174002	1.737105
H	-0.125072	1.979579	3.271597
C	-3.760053	-0.473324	-0.996205
N	-2.399960	-0.450053	-0.973138
C	2.372034	-1.251945	-1.279502
N	1.068350	-0.893491	-1.128155
H	-5.355466	0.954151	-0.282056
H	4.331065	-0.268866	-0.742304
H	-4.286900	-1.330208	-1.437405
H	2.626535	-2.208573	-1.755456

S1.10.12 Bis(imidazolato)-substituted nickel(II) dipyridylmethane K

K			
C	1.313409	1.283237	0.213745
C	2.462359	2.095815	0.201576
C	3.733255	1.515144	0.060692
C	3.836879	0.131228	-0.053054
C	2.659525	-0.637909	-0.017544
C	-0.030749	1.988592	0.470105
C	-1.317586	1.267961	0.032342
N	1.409132	-0.061623	0.107858
N	-1.410927	-0.079441	0.090868
C	-2.447389	2.060153	-0.242413
C	-3.693685	1.450832	-0.464174
C	-3.800189	0.065004	-0.371386
C	-2.643743	-0.68075	-0.080128
C	-0.148614	2.210304	1.997306
O	0.002901	3.301585	-0.095342
C	2.616942	-2.065956	-0.123508
C	-2.609312	-2.100390	0.122548
N	1.364232	-2.627406	-0.051742
N	3.604381	-2.943155	-0.357752
N	-1.369120	-2.621124	0.406283
N	-3.612662	-2.986750	0.203907
H	4.792983	-0.398663	-0.164864
H	-4.745480	-0.479848	-0.501329
H	0.726810	2.781667	2.361062
H	-0.187800	1.235540	2.520207
Ni	0.002983	-1.368972	0.194422
C	0.142310	3.378184	-1.510817
H	-1.072378	2.778129	2.220040
H	2.333507	3.180862	0.307192
H	4.632654	2.149209	0.044795
H	-2.332361	3.151416	-0.244470
H	-4.577735	2.067325	-0.687058
H	0.088893	4.453061	-1.769587
H	-0.672117	2.840462	-2.045354
H	1.118359	2.974380	-1.860343
C	1.567942	-3.958801	-0.275219
C	2.953855	-4.134382	-0.453186
C	-1.601804	-3.932483	0.704289
C	-2.988557	-4.139564	0.570128
H	3.488063	-5.073608	-0.651366
H	0.753092	-4.686952	-0.325467
H	-0.811580	-4.619865	1.022153
H	-3.544237	-5.072266	0.737744

K(py)			
C	1.525051	1.198916	-1.308167
C	0.509224	2.012768	-0.766746
C	-0.837571	1.661654	-0.964490
C	-1.148069	0.521656	-1.700973
C	-0.088098	-0.271271	-2.192555
C	2.960330	1.779301	-1.272360
C	4.202112	0.870403	-1.446692
N	1.226306	0.067389	-1.977752
N	4.149243	-0.303519	-2.108489
C	5.434301	1.416339	-1.033028
C	6.629093	0.745490	-1.346085
C	6.578624	-0.441755	-2.071486
C	5.314613	-0.952807	-2.438786
C	3.023628	2.802525	-2.434403
O	3.117951	2.561639	-0.081131
C	-0.303085	-1.494366	-2.929861
C	5.153577	-2.190016	-3.166484
N	0.791028	-2.234437	-3.305186
N	-1.490409	-2.023628	-3.291656
N	3.881743	-2.634910	-3.430998
N	6.136353	-2.996398	-3.619164
H	7.471388	-1.007509	-2.372174
H	2.210604	3.545726	-2.325696
H	2.907024	2.281830	-3.404146
Ni	2.491957	-1.492733	-2.542028
N	2.441726	-2.508747	-0.764087
C	1.272042	-2.721382	-0.122129
C	1.191140	-3.458007	1.065886
C	2.362968	-4.000494	1.612084
C	3.574275	-3.785233	0.939679
C	3.571406	-3.036938	-0.243781
C	3.097585	1.831798	1.137195
H	3.998943	3.325775	-2.422712
H	3.221791	2.572331	1.950810
H	3.928244	1.092271	1.198185
H	2.134421	1.293133	1.288567
H	0.370425	-2.297443	-0.589962
H	0.212466	-3.603536	1.545749
H	-2.176547	0.199142	-1.914860
H	0.791322	2.926316	-0.227566
H	-1.637857	2.295299	-0.551631
H	5.437799	2.374755	-0.497835
H	7.596164	1.167861	-1.031809
C	-1.141048	-3.165956	-3.939792
C	0.262470	-3.310362	-3.949372
H	0.886420	-4.105312	-4.376210
H	-1.892195	-3.839409	-4.376093
C	5.459405	-4.015169	-4.211465
C	4.068573	-3.807105	-4.096451
H	3.231914	-4.421843	-4.450745
H	5.978981	-4.853073	-4.697322
H	2.331676	-4.586923	2.542996
H	4.522283	-4.195006	1.317345
H	4.500020	-2.863442	-0.808802

S1.10.13 Bis(trifluormethylpyrazolato)-substituted nickel(II) dipyridylmethane L

L

C	2.234452	1.301337	0.097308
C	3.375257	2.123516	0.026005
C	4.640358	1.549880	-0.156435
C	4.747257	0.162600	-0.247693
C	3.582043	-0.619514	-0.151685
C	0.900108	2.000823	0.414209
C	-0.407215	1.291509	0.017645
N	2.333331	-0.044141	0.011605
N	-0.506823	-0.056000	0.051417
C	-1.538631	2.100406	-0.199612
C	-2.792930	1.507034	-0.397458
C	-2.904100	0.118233	-0.336996
C	-1.749704	-0.648133	-0.094761
C	0.845561	2.196968	1.948762
O	0.913161	3.321492	-0.133487
C	3.540825	-2.052885	-0.203891
C	-1.714593	-2.074561	0.064682
N	2.285024	-2.597375	-0.049154
C	4.449212	-3.107863	-0.397995
N	-0.456922	-2.593093	0.281488
C	-2.638506	-3.129709	0.159968
H	5.716458	-0.336810	-0.381740
H	-3.868442	-0.392552	-0.463119
H	1.734199	2.764630	2.285259
H	0.830655	1.212975	2.455567
Ni	0.917768	-1.348718	0.136307
C	0.987056	3.419080	-1.553259
H	-0.068575	2.758861	2.220657
H	3.243386	3.208551	0.125897
H	5.535773	2.186275	-0.218386
H	-1.414446	3.190376	-0.182068
H	-3.680172	2.132016	-0.578748
H	0.925634	4.497819	-1.793007
H	0.147111	2.891916	-2.057625
H	1.943958	3.017812	-1.954710
N	2.317272	-3.907964	-0.138548
C	3.615310	-4.242135	-0.345995
N	-0.503186	-3.884391	0.516546
C	-1.812197	-4.234307	0.447532
H	-3.727254	-3.108902	0.051930
H	5.531126	-3.069592	-0.557699
C	4.015835	-5.679621	-0.509492
C	-2.236585	-5.654209	0.686507
F	3.690728	-6.432113	0.564779
F	5.362952	-5.769843	-0.678947
F	3.434267	-6.252428	-1.588882
F	-1.963252	-6.066573	1.947213
F	-1.633514	-6.520941	-0.155305
F	-3.579808	-5.773253	0.504965

L(py)

C	-17.034387	6.821353	2.496604
C	-18.036828	7.663746	3.020817
C	-19.383513	7.296438	2.886918
C	-19.706811	6.113703	2.224050
C	-18.664466	5.298982	1.733104
C	-15.597758	7.402619	2.473637
C	-14.354708	6.482483	2.372845
N	-17.345735	5.656919	1.893084
N	-14.398336	5.282727	1.759386
C	-13.130943	7.043258	2.794031
C	-11.936264	6.350477	2.550757
C	-11.978564	5.129590	1.879647
C	-13.230171	4.608274	1.488579
C	-15.539414	8.326621	1.231931
O	-15.434728	8.279882	3.596751
C	-18.886485	4.046222	1.045330
C	-13.389338	3.350905	0.791732
N	-17.777168	3.331316	0.665147
C	-20.033108	3.314947	0.675034
N	-14.671390	2.940708	0.519423
C	-12.498959	2.368437	0.312937
H	-16.352198	9.076278	1.284178
H	-15.659443	7.728465	0.308492
Ni	-16.068335	4.094715	1.338069
N	-16.130491	2.981162	3.030496
C	-16.311153	1.651082	2.860422
C	-16.370957	0.774262	3.950973
C	-16.239897	1.285639	5.250039
C	-16.052105	2.666246	5.415263
C	-16.003731	3.479182	4.276863
H	-15.943806	3.115582	6.413210
C	-15.453722	7.661632	4.874880
H	-14.564376	8.849489	1.198070
H	-15.319298	8.470336	5.618829
H	-14.626904	6.925477	5.000068
H	-16.420959	7.148646	5.080964
H	-20.750300	5.802373	2.078108
H	-13.133585	8.028330	3.277899
H	-15.858507	4.568221	4.357689
C	-19.485442	2.159123	0.088236
N	-18.126677	2.184232	0.102297
C	-13.368139	1.398039	-0.219345
N	-14.670974	1.756759	-0.074100
H	-21.090426	3.566563	0.804053
H	-11.404884	2.350150	0.337726
C	-20.224611	0.993561	-0.496574
C	-13.002933	0.095926	-0.865715
F	-19.893686	-0.176740	0.102901
F	-19.989153	0.837406	-1.820226
F	-21.566436	1.160842	-0.342454
F	-13.478264	-0.008788	-2.127439
F	-11.650222	-0.039430	-0.927824
F	-13.480098	-0.970762	-0.175555
H	-11.063406	4.566930	1.649435
H	-10.974012	6.777484	2.872171
H	-20.176620	7.946295	3.287235
H	-17.744561	8.608639	3.496390
H	-16.408652	1.299614	1.818686
H	-16.519201	-0.299887	3.768834
H	-16.283123	0.617503	6.123691

S1.10.14 Bis(quinolinolato)-substituted nickel(II) dipyridylmethane M

M

C	-0.974104	1.415281	0.308790
C	-1.454174	0.106148	0.014054
C	0.389151	1.644722	0.422042
C	1.328831	0.585473	0.260619
N	0.898588	-0.655887	-0.004098
C	-0.453486	-0.902890	-0.133320
C	-2.812792	-0.278704	-0.144414
C	-3.113345	-1.612554	-0.438672
C	-2.120645	-2.608509	-0.584092
C	-0.759407	-2.270727	-0.432323
H	0.783183	2.648386	0.633875
H	-1.689362	2.242540	0.439494
H	-4.167982	-1.905648	-0.562812
H	-3.608453	0.472465	-0.034887
H	-2.388692	-3.649551	-0.814575
C	2.823364	0.943242	0.241736
C	3.135366	1.513636	-1.163185
H	2.477638	2.379589	-1.371280
H	4.191050	1.844218	-1.208077
H	2.965747	0.736453	-1.932638
O	3.075206	2.021865	1.146483
C	3.822965	-0.195602	0.497780
C	5.152533	0.153647	0.873674
C	6.140852	-0.812793	0.988291
N	3.512641	-1.475028	0.247773
C	4.484833	-2.450483	0.343443
C	5.837251	-2.178139	0.715068
C	6.741489	-3.272378	0.777276
C	4.008515	-3.765872	0.032197
C	4.940246	-4.822628	0.104553
C	6.279090	-4.556647	0.472440
H	5.366208	1.214405	1.065139
H	7.163314	-0.529397	1.283765
H	4.606550	-5.843943	-0.128467
H	6.984281	-5.401625	0.520254
H	7.789117	-3.098297	1.062660
O	0.255054	-3.095587	-0.543061
O	2.743159	-3.876771	-0.297137
Ni	1.869388	-2.231825	-0.181657
C	2.856011	1.734249	2.522678
H	1.802350	1.438961	2.727955
H	3.079448	2.665920	3.076756
H	3.525315	0.926396	2.895562

M(py)

C	12.020048	6.334468	-2.290369
C	11.464714	5.021228	-2.287214
C	13.393150	6.519442	-2.329974
C	14.270060	5.392108	-2.348911
N	13.765839	4.156157	-2.312599
C	12.413602	3.943870	-2.289651
C	10.078261	4.716910	-2.287371
C	9.680335	3.376395	-2.300505
C	10.603380	2.310122	-2.305143
C	12.000999	2.547203	-2.293873
H	13.831247	7.526651	-2.360172
H	11.344480	7.204986	-2.275628
H	8.604248	3.138588	-2.306851
H	9.339586	5.531996	-2.282721
H	10.258463	1.265608	-2.319580
C	15.772703	5.662532	-2.598954
C	15.923780	5.916583	-4.118629
H	15.251411	6.738103	-4.433781
H	16.969077	6.197187	-4.352820
H	15.661913	5.000305	-4.681178
O	16.136272	6.908906	-1.982749
C	16.823736	4.588944	-2.229977
C	18.182263	5.013665	-2.110437
C	19.194605	4.078885	-1.960668
N	16.526066	3.288042	-2.181364
C	17.507284	2.342449	-2.050037
C	18.897218	2.684666	-1.942197
C	19.856258	1.644020	-1.833826
C	17.047874	0.960346	-2.054724
C	18.055210	-0.031990	-1.953961
C	19.417611	0.316272	-1.846023
H	18.401574	6.089472	-2.153696
H	20.242446	4.407571	-1.869028
H	17.741821	-1.086459	-1.965570
H	20.161402	-0.493201	-1.768252
H	20.924496	1.891941	-1.747789
O	12.907088	1.615934	-2.297004
O	15.776429	0.712737	-2.158984
Ni	14.721772	2.404222	-2.020588
C	14.278173	1.825744	2.730203
C	14.017407	0.799581	1.810284
C	14.177593	1.052517	0.442599
C	14.693243	3.075325	2.245594
C	14.829987	3.249630	0.863318
N	14.576679	2.260138	-0.015992
H	14.910537	3.911139	2.926533
H	15.153204	4.211832	0.435506
H	13.690427	-0.196398	2.142599
H	14.159998	1.654666	3.811085
H	13.990086	0.291037	-0.328900
C	16.078104	6.930789	-0.566722
H	16.372886	7.950505	-0.251657
H	16.782234	6.201114	-0.103345
H	15.051360	6.726306	-0.183705

S1.10.15 Bis(triazolato)-substituted nickel(II) dipyridylmethane N

N			
C	1.317394	1.285676	0.178838
C	2.460400	2.106062	0.134290
C	3.728066	1.532240	-0.030988
C	3.834979	0.145912	-0.133905
C	2.667400	-0.635844	-0.065147
C	-0.022006	1.984814	0.473818
C	-1.321339	1.275829	0.051968
N	1.416907	-0.059439	0.083423
N	-1.421757	-0.071874	0.086995
C	-2.449044	2.082665	-0.188296
C	-3.699505	1.487617	-0.406645
C	-3.811866	0.099186	-0.341687
C	-2.661887	-0.666186	-0.075334
C	-0.105168	2.176613	2.007578
O	0.000998	3.306900	-0.069808
C	2.620212	-2.066426	-0.134208
C	-2.624709	-2.089110	0.099675
N	1.364196	-2.612124	-0.006404
C	3.470995	-3.159037	-0.337947
N	-1.372309	-2.606670	0.336103
C	-3.495881	-3.176471	0.235825
H	4.805532	-0.354047	-0.256248
H	-4.773819	-0.412652	-0.481671
H	0.776929	2.743635	2.361863
H	-0.129251	1.191363	2.511563
Ni	0.000564	-1.359840	0.185931
C	0.103903	3.408707	-1.487486
H	-1.024424	2.737598	2.263673
H	2.328314	3.190568	0.240104
H	4.625067	2.168178	-0.071185
H	-2.326130	3.172823	-0.171735
H	-4.583400	2.111732	-0.606484
H	0.045147	4.488019	-1.725300
H	-0.724269	2.881252	-2.010708
H	1.069738	3.010584	-1.870201
N	1.429026	-3.930922	-0.131822
N	2.703541	-4.276699	-0.330490
N	-1.458784	-3.901660	0.605115
N	-2.744192	-4.260651	0.549479
H	-4.586623	-3.235672	0.140699
H	4.555938	-3.201977	-0.490925

N(py)			
C	-1.298100	4.211180	1.398859
C	-2.299346	5.051645	1.927580
C	-3.646068	4.678437	1.806942
C	-3.970844	3.492321	1.151434
C	-2.929753	2.679775	0.652943
C	0.136673	4.796166	1.363222
C	1.381058	3.877964	1.261269
N	-1.610256	3.043493	0.801334
N	1.336280	2.672254	0.658859
C	2.605861	4.443768	1.671598
C	3.800695	3.749615	1.430976
C	3.757401	2.521878	0.773255
C	2.504769	1.995160	0.391211
C	0.185067	5.712720	0.115725
O	0.304625	5.680597	2.480039
C	-3.148859	1.428501	-0.031225
C	2.341957	0.734249	-0.290950
N	-2.048350	0.713113	-0.425110
C	-4.253373	0.650156	-0.418961
N	1.066736	0.317836	-0.570622
C	3.177996	-0.289543	-0.769719
H	4.671968	1.957125	0.545106
H	-0.629288	6.460640	0.168598
H	0.060813	5.108750	-0.803360
Ni	-0.333790	1.481205	0.238013
N	-0.395291	0.369792	1.932979
C	-0.577763	-0.960339	1.765236
C	-0.637257	-1.834446	2.858043
C	-0.503839	-1.320487	4.155742
C	-0.313972	0.060206	4.318078
C	-0.266174	0.870552	3.177828
H	-0.203594	0.511495	5.314908
C	0.296254	5.070171	3.762082
H	1.158624	6.237689	0.072804
H	0.437286	5.883496	4.499766
H	1.123788	4.334450	3.884844
H	-0.669334	4.558837	3.979589
H	-0.675968	-1.313766	0.724316
H	-0.787054	-2.908732	2.678210
H	-0.546735	-1.986741	5.030879
H	-5.014319	3.175922	1.015415
H	-2.006904	5.999708	2.396703
H	-4.437934	5.326988	2.211902
H	2.604150	5.433313	2.146266
H	4.763562	4.181279	1.744321
H	-0.119470	1.959618	3.255891
N	-3.780506	-0.475135	-1.002434
N	-2.441227	-0.423863	-0.986992
N	2.388530	-1.256941	-1.290478
N	1.111179	-0.875500	-1.150774
H	-5.329291	0.837172	-0.313477
H	4.271717	-0.375864	-0.768043

S1.10.16 Bis(trifluormethyltriazolato)-substituted nickel(II) dipyridylmethane O

O			
C	2.235910	1.254699	0.012156
C	3.374568	2.062711	-0.180027
C	4.625853	1.474590	-0.405710
C	4.729636	0.082051	-0.410088
C	3.568036	-0.672377	-0.196821
C	0.931003	1.967230	0.410875
C	-0.403533	1.261158	0.111222
N	2.331118	-0.093134	-0.005079
N	-0.505340	-0.085958	0.088593
C	-1.549794	2.075120	0.011725
C	-2.816664	1.493929	-0.128834
C	-2.926015	0.101916	-0.142273
C	-1.755250	-0.658709	-0.020916
C	0.989997	2.179041	1.943697
O	0.912628	3.280673	-0.150422
C	3.521989	-2.110527	-0.126832
C	-1.710636	-2.097713	0.026388
N	2.286487	-2.646978	0.105331
N	4.470951	-3.048269	-0.204672
N	-0.465000	-2.641730	0.169898
N	-2.666297	-3.031270	-0.008601
H	5.678145	-0.451475	-0.561468
H	-3.884991	-0.426777	-0.232263
H	1.905025	2.743050	2.207911
H	1.004462	1.201305	2.462508
Ni	0.913566	-1.399268	0.153189
C	0.855993	3.363384	-1.572570
H	0.103137	2.752034	2.275758
H	3.253480	3.152384	-0.128265
H	5.514475	2.104244	-0.562208
H	-1.419822	3.163817	0.063614
H	-3.711638	2.128291	-0.213817
H	0.855714	4.441993	-1.819684
H	-0.067718	2.901416	-1.986189
H	1.734946	2.885308	-2.058919
N	2.407994	-3.966131	0.183576
C	3.729945	-4.167176	-0.005520
N	-0.586440	-3.961881	0.229824
C	-1.918593	-4.155700	0.122582
C	4.347628	-5.543374	0.005624
C	-2.537258	-5.531513	0.127869
F	5.307954	-5.634124	0.958031
F	4.940319	-5.818563	-1.181993
F	3.430751	-6.495264	0.245176
F	-1.623618	-6.483818	0.378537
F	-3.115138	-5.808781	-1.067345
F	-3.509036	-5.619884	1.067623

O(py)			
C	-17.038664	6.784959	2.465848
C	-18.047910	7.617393	2.995798
C	-19.392911	7.238023	2.880594
C	-19.714198	6.048212	2.225486
C	-18.662927	5.254955	1.732814
C	-15.607398	7.376689	2.427455
C	-14.363747	6.460045	2.311919
N	-17.347553	5.615397	1.871083
N	-14.412465	5.251965	1.715306
C	-13.131168	7.024238	2.705702
C	-11.937896	6.331715	2.455766
C	-11.986591	5.099793	1.801697
C	-13.245471	4.585501	1.444272
C	-15.568211	8.302027	1.185751
O	-15.435828	8.253080	3.548596
C	-18.882184	3.994738	1.048189
C	-13.411449	3.312310	0.768619
N	-17.796664	3.280374	0.638802
N	-20.041738	3.376926	0.767791
N	-14.674222	2.886525	0.486232
N	-12.472114	2.434079	0.379820
H	-11.091443	4.513254	1.552300
H	-16.383678	9.047922	1.248479
H	-15.695791	7.705568	0.262213
Ni	-16.078190	4.043575	1.296743
N	-16.132971	2.944452	2.999551
C	-16.314375	1.612847	2.843607
C	-16.368622	0.746162	3.942164
C	-16.230923	1.270352	5.235375
C	-16.042359	2.652329	5.386409
C	-15.999793	3.454716	4.240414
H	-15.928820	3.110980	6.379424
C	-15.434221	7.633972	4.826829
H	-14.596594	8.830399	1.141533
H	-15.291006	8.442627	5.568952
H	-14.603590	6.900096	4.939496
H	-16.396963	7.118397	5.047167
H	-16.416341	1.250244	1.806773
H	-16.517469	-0.329716	3.771427
H	-16.269520	0.610663	6.115523
H	-20.746185	5.700849	2.077667
H	-17.759514	8.566474	3.466110
H	-20.185542	7.883488	3.288878
H	-13.128459	8.014319	3.180006
H	-10.973241	6.766788	2.758598
H	-15.854199	4.544294	4.310388
C	-19.584597	2.246825	0.180900
N	-18.238153	2.145382	0.089324
C	-13.248227	1.455720	-0.140866
N	-14.581139	1.682536	-0.085533
C	-20.511565	1.196391	-0.373346
C	-12.667824	0.184015	-0.702773
F	-19.849372	0.064866	-0.681526
F	-21.134115	1.629430	-1.498607
F	-21.482534	0.883325	0.519092
F	-11.720831	0.443392	-1.635486
F	-12.070342	-0.551995	0.271600
F	-13.614974	-0.584299	-1.271574

S1.10.17 Bis(carboxylato)-substituted nickel(II) dipyridylmethane with MeO-substituent 1a

1a, S = 0

C	1.314427	1.302314	0.111937
C	2.483185	2.078083	-0.013632
C	3.726614	1.461588	-0.205199
C	3.785074	0.061509	-0.244992
C	2.599953	-0.656766	-0.106683
C	-0.000285	2.017333	0.472369
C	-1.314841	1.301839	0.112491
N	1.388234	-0.048913	0.056220
N	-1.388138	-0.049375	0.055930
C	-2.483960	2.077246	-0.011980
C	-3.727245	1.460413	-0.203384
C	-3.785153	0.060337	-0.244187
C	-2.599697	-0.657574	-0.106862
C	0.000057	2.212920	2.007380
O	-0.000530	3.336021	-0.077030
C	2.534152	-2.171653	-0.094056
C	-2.533323	-2.172440	-0.095282
O	1.306036	-2.607385	0.044915
O	3.544784	-2.856307	-0.194055
O	-1.305033	-2.607803	0.043303
O	-3.543692	-2.857415	-0.195755
H	4.714251	-0.513456	-0.372867
H	-4.714155	-0.514907	-0.372086
H	0.901556	2.778372	2.312584
H	0.000488	1.229070	2.514906
Ni	0.000252	-1.287531	0.097237
C	-0.001346	3.427716	-1.498897
H	-0.901604	2.777839	2.313089
H	2.389807	3.170655	0.055478
H	4.637096	2.070825	-0.308936
H	-2.390960	3.169812	0.057896
H	-4.638019	2.069359	-0.306255
H	0.004106	4.507664	-1.740137
H	-0.905803	2.964537	-1.952432
H	0.897325	2.955027	-1.954091

1a, S = 1

C	1.335334	1.291516	0.115697
C	2.482727	2.097500	-0.033541
C	3.736166	1.498137	-0.220638
C	3.830691	0.101083	-0.245160
C	2.658359	-0.643084	-0.088356
C	-0.000283	1.987368	0.472653
C	-1.335808	1.291114	0.116158
N	1.447663	-0.053458	0.086482
N	-1.447707	-0.053881	0.086576
C	-2.483520	2.096776	-0.032401
C	-3.736830	1.497078	-0.219265
C	-3.830899	0.100002	-0.244221
C	-2.658273	-0.643833	-0.088023
C	-0.000022	2.174827	2.008589
O	-0.000526	3.311039	-0.069786
C	2.670415	-2.177286	-0.077671
C	-2.669855	-2.178042	-0.077574
O	1.478090	-2.698764	-0.034243
O	3.747111	-2.765353	-0.113717
O	-1.477374	-2.699180	-0.034352
O	-3.746355	-2.766443	-0.114082
H	4.774257	-0.449688	-0.369815
H	-4.774325	-0.451040	-0.368735
H	0.901323	2.738488	2.317685
H	0.000264	1.188486	2.511121
Ni	0.000182	-1.469005	0.102447
C	-0.000876	3.411577	-1.490714
H	-0.901457	2.738145	2.318042
H	2.374317	3.189314	0.017150
H	4.633724	2.125448	-0.334996
H	-2.375437	3.188611	0.018602
H	-4.634632	2.124133	-0.333109
H	0.000487	4.493035	-1.725688
H	-0.903069	2.948374	-1.948782
H	0.899755	2.945959	-1.949400

1a(py), MeO-side coordination, S = 1

C	-1.286171	4.244835	1.366083
C	-2.325388	5.034867	1.901094
C	-3.655298	4.607579	1.781918
C	-3.930791	3.408806	1.111184
C	-2.856877	2.664897	0.612117
C	0.140906	4.848217	1.341517
C	1.373400	3.915611	1.232498
N	-1.572028	3.076534	0.754593
N	1.304086	2.716988	0.616471
C	2.621667	4.423580	1.649998
C	3.788330	3.683399	1.412576
C	3.695315	2.456952	0.741749
C	2.428855	2.003328	0.359575
C	0.192949	5.779557	0.107028
O	0.305436	5.716895	2.470030
C	-3.074160	1.349703	-0.156607
C	2.241864	0.681242	-0.405647
O	-1.975751	0.768801	-0.527487
O	-4.231502	0.979092	-0.358169
O	1.004733	0.394627	-0.667456
O	3.247755	0.036751	-0.706004
H	4.559675	1.825561	0.489743
H	-0.621006	6.527702	0.167209
H	0.071239	5.187606	-0.820266
Ni	-0.320896	1.591059	0.200679
N	-0.382912	0.448690	1.862641
C	-0.578871	-0.868138	1.626577
C	-0.646905	-1.799067	2.670291
C	-0.507602	-1.354985	3.993153
C	-0.303225	0.013311	4.227968
C	-0.247539	0.881614	3.131686
H	-0.187821	0.409505	5.247363
C	0.293303	5.091774	3.745055
H	1.166471	6.305793	0.073528
H	0.429097	5.897099	4.492290
H	1.121537	4.356230	3.864432
H	-0.670954	4.574402	3.954084
H	-0.681799	-1.152696	0.568643
H	-0.808167	-2.861365	2.437074
H	-0.557278	-2.065831	4.831990
H	-4.943683	3.013418	0.947039
H	-2.072555	5.987608	2.386383
H	-4.469421	5.220237	2.199419
H	2.658775	5.406638	2.139285
H	4.764291	4.075208	1.738841
H	-0.088653	1.963738	3.266751

1a(py), MeO-side coordination, S = 0

C	-1.241314	4.327024	1.305059
C	-2.297695	5.082899	1.849460
C	-3.614873	4.609013	1.786571
C	-3.858918	3.385078	1.147790
C	-2.778985	2.684236	0.616168
C	0.160428	4.962318	1.257988
C	1.370045	4.016117	1.145233
N	-1.494357	3.138794	0.706765
N	1.264687	2.810089	0.538595
C	2.631531	4.496118	1.547665
C	3.783976	3.728645	1.333090
C	3.656532	2.490726	0.687323
C	2.386607	2.069194	0.300564
C	0.192571	5.878608	0.012204
O	0.333773	5.836421	2.376599
C	-2.920771	1.374849	-0.135184
C	2.127210	0.772599	-0.441381
O	-1.765009	0.917549	-0.546164
O	-4.018220	0.858198	-0.316705
O	0.855284	0.603247	-0.704180
O	3.042853	0.014755	-0.743358
H	4.502235	1.826046	0.456524
H	-0.625563	6.622030	0.072735
H	0.063777	5.270298	-0.903835
Ni	-0.279080	1.892667	0.050178
N	-0.338556	0.377555	2.178212
C	-0.461273	-0.901988	1.777775
C	-0.616993	-1.965889	2.680923
C	-0.648917	-1.686944	4.054938
C	-0.523327	-0.353759	4.474828
C	-0.370454	0.638919	3.494792
H	-0.543395	-0.085187	5.541957
C	0.337890	5.220926	3.659687
H	1.162559	6.409803	-0.038415
H	0.501906	6.032441	4.394159
H	1.154361	4.471792	3.767282
H	-0.629071	4.720081	3.891740
H	-0.432359	-1.066036	0.687342
H	-0.712892	-2.995488	2.305257
H	-0.771006	-2.497435	4.790306
H	-4.857872	2.939407	1.030315
H	-2.058465	6.052112	2.308717
H	-4.437517	5.198009	2.219342
H	2.682867	5.487653	2.018444
H	4.767489	4.102900	1.654913
H	-0.269270	1.700986	3.786700

1a(py), Me-side coordination, S = 1

C	-1.853114	1.340487	0.047259
C	-2.638032	2.479207	-0.228777
C	-2.016002	3.709572	-0.483746
C	-0.618550	3.785024	-0.457450
C	0.102944	2.626979	-0.147771
C	-2.578303	0.018062	0.399464
C	-1.866440	-1.317528	0.070967
N	-0.508715	1.443560	0.109345
N	-0.523029	-1.432948	0.133398
C	-2.663634	-2.452670	-0.183231
C	-2.054909	-3.693524	-0.418482
C	-0.658352	-3.782248	-0.394473
C	0.075345	-2.626816	-0.104471
C	-2.850625	0.032133	1.920096
O	-3.875993	0.020078	-0.209288
C	1.638808	2.636789	-0.070676
C	1.610396	-2.652334	-0.030551
O	2.155240	1.495095	0.256102
O	2.226197	3.693274	-0.311187
O	2.139376	-1.515002	0.294877
O	2.187693	-3.715147	-0.266847
H	-0.095050	-4.708422	-0.579174
H	-3.422890	0.940984	2.189864
H	-1.893656	0.026072	2.475224
Ni	0.875664	0.002074	0.532162
C	-3.920574	0.006160	-1.633415
H	-3.440032	-0.861766	2.202481
H	-4.992788	0.021550	-1.908128
H	-3.455056	-0.906929	-2.065877
H	-3.424390	0.893646	-2.084669
H	-0.045378	4.702492	-0.654989
H	-3.732087	2.383177	-0.229404
H	-2.626093	4.600282	-0.700314
H	-3.756639	-2.345308	-0.183250
H	-2.674450	-4.581534	-0.618592
N	0.989075	0.045606	2.544068
C	1.002917	1.226083	3.200928
C	1.253303	1.315351	4.574657
C	1.505264	0.139695	5.296959
C	1.498998	-1.083088	4.610236
C	1.240580	-1.088264	3.234688
H	0.817325	2.125654	2.595983
H	1.711501	0.176980	6.377369
H	1.257941	2.300820	5.062411
H	1.255552	-2.019673	2.650851
H	1.702004	-2.032456	5.126553

1a(py), Me-side coordination, S = 0

C	-1.937449	1.324901	-0.082935
C	-2.696613	2.479472	-0.352959
C	-2.066095	3.718780	-0.529727
C	-0.671316	3.785243	-0.411468
C	0.029972	2.614840	-0.128957
C	-2.677370	0.014770	0.242538
C	-1.925429	-1.297205	-0.046395
N	-0.589528	1.407182	0.024443
N	-0.576741	-1.364446	0.061860
C	-2.674314	-2.465623	-0.283811
C	-2.032800	-3.703612	-0.427175
C	-0.637360	-3.754177	-0.308813
C	0.053516	-2.570208	-0.059166
C	-2.985921	0.034810	1.757208
O	-3.948224	-0.000429	-0.411333
C	1.532432	2.569414	0.065306
C	1.555735	-2.505795	0.131588
O	1.953811	1.362157	0.341762
O	2.218380	3.584086	-0.015913
O	1.966314	-1.287654	0.374340
O	2.250856	-3.515986	0.076693
H	-0.043762	-4.676730	-0.392082
H	-3.576958	0.937742	2.005278
H	-2.036413	0.047229	2.327640
Ni	0.626213	0.031059	0.359923
C	-3.933618	-0.020405	-1.836153
H	-3.568817	-0.865933	2.031107
H	-4.993180	-0.029738	-2.155843
H	-3.429272	-0.924582	-2.243447
H	-3.437513	0.876508	-2.268831
H	-0.086051	4.710586	-0.519185
H	-3.789788	2.382023	-0.402065
H	-2.662004	4.618499	-0.744980
H	-3.768333	-2.379388	-0.334712
H	-2.620723	-4.614223	-0.617057
N	0.676222	0.060966	2.849427
C	1.023966	1.220662	3.435209
C	1.713140	1.287881	4.654561
C	2.063257	0.089215	5.293230
C	1.707698	-1.123898	4.685583
C	1.018833	-1.084797	3.464839
H	0.745762	2.145267	2.901013
H	2.612175	0.100270	6.247474
H	1.976089	2.264978	5.086208
H	0.736321	-2.021709	2.954765
H	1.966243	-2.090769	5.142193

1a(py)$_2$, S = 1

C	-1.284220	4.248219	1.341545
C	-2.304854	5.015146	1.943337
C	-3.625683	4.546105	1.933370
C	-3.908706	3.323912	1.312084
C	-2.856839	2.619211	0.714954
C	0.138880	4.862685	1.278350
C	1.373001	3.924993	1.207216
N	-1.580999	3.081115	0.733309
N	1.317619	2.718048	0.606581
C	2.604603	4.427506	1.678835
C	3.767718	3.656522	1.547534
C	3.684193	2.398916	0.938509
C	2.437578	1.963639	0.473549
C	0.184414	5.767440	0.026937
O	0.305117	5.761293	2.386796
C	-3.116605	1.292531	-0.027032
C	2.294233	0.607840	-0.246872
O	-2.068965	0.783056	-0.585661
O	-4.274511	0.862883	-0.043094
O	1.106239	0.368036	-0.694446
O	3.305479	-0.093497	-0.353674
H	4.540702	1.725204	0.790916
H	-0.632441	6.513579	0.075785
H	0.063886	5.155603	-0.886632
Ni	-0.314072	1.705540	-0.083983
N	-0.400619	0.496039	1.693157
C	-0.609107	-0.818304	1.470616
C	-0.671595	-1.748774	2.516661
C	-0.512178	-1.302472	3.836299
C	-0.295234	0.064763	4.062772
C	-0.247459	0.925702	2.958428
H	-0.164173	0.464473	5.079139
C	0.305573	5.179057	3.683366
H	1.155422	6.298003	-0.017153
H	0.441843	6.012288	4.399561
H	1.137957	4.452980	3.824144
H	-0.652572	4.663210	3.919372
H	-0.731126	-1.110099	0.417234
H	-0.843973	-2.810673	2.289115
H	-0.556195	-2.010449	4.678161
H	-4.912576	2.879043	1.251646
H	-2.045428	5.979031	2.401674
H	-4.424715	5.139814	2.404274
H	2.631296	5.426607	2.134513
H	4.730313	4.044096	1.916142
H	-0.078786	2.007510	3.091559
N	-0.283427	2.564454	-2.044962
C	-1.428023	2.966982	-2.633879
C	-1.482694	3.405407	-3.963214
C	-0.302163	3.422598	-4.719843
C	0.887125	2.998003	-4.110556
C	0.850321	2.575364	-2.775106
H	-2.336767	2.921451	-2.016828
H	-0.310359	3.755327	-5.769150
H	-2.444951	3.718826	-4.393744
H	1.757431	2.212435	-2.271544
H	1.839731	2.981832	-4.659895

S1.10.18 Bis(carboxylato)-substituted nickel(II) dipyridylmethane with BnO-substituent 1b

1b

C	1.338827	1.280341	0.090173
C	2.515539	2.038683	-0.064549
C	3.751222	1.400781	-0.237171
C	3.793733	-0.000457	-0.226993
C	2.600993	-0.699986	-0.061226
C	0.031021	2.015455	0.434908
C	-1.290063	1.311965	0.075142
N	1.396853	-0.072629	0.081451
N	-1.379925	-0.039333	0.066033
C	-2.446748	2.097822	-0.092696
C	-3.695109	1.489189	-0.279176
C	-3.770851	0.089399	-0.269381
C	-2.596911	-0.638081	-0.090123
C	0.024685	2.226695	1.968039
O	0.050248	3.326260	-0.127778
C	2.516920	-2.212496	0.007709
C	-2.549568	-2.152187	-0.020181
O	1.283589	-2.627874	0.162765
O	3.519072	-2.912603	-0.066437
O	-1.328285	-2.596785	0.148471
O	-3.567206	-2.828279	-0.105382
H	4.716295	-0.589828	-0.335629
H	-4.705804	-0.478068	-0.388226
H	0.932141	2.782367	2.273659
H	0.009665	1.247118	2.483427
Ni	-0.006733	-1.291793	0.162887
C	0.058880	3.417243	-1.551177
H	-0.872393	2.804512	2.263079
H	2.437536	3.134343	-0.032888
H	4.668061	1.995659	-0.365014
H	-2.343623	3.191358	-0.060205
H	-4.596135	2.105541	-0.417293
C	0.065517	4.868984	-1.977186
H	-0.832001	2.902086	-1.982632
H	0.951616	2.896700	-1.972270
C	0.075283	5.177964	-3.353488
C	0.081143	6.511487	-3.784133
C	0.077467	7.556837	-2.844583
C	0.067956	7.255924	-1.474897
C	0.061984	5.919439	-1.041023
H	0.054636	5.681208	0.031792
H	0.065161	8.068516	-0.732008
H	0.082084	8.604241	-3.182755
H	0.088666	6.737250	-4.861525
H	0.078253	4.364083	-4.097148

1b(py), BnO-side coordination

C	-0.972152	4.225381	1.517792
C	-1.853852	5.085605	2.205611
C	-3.228080	4.806450	2.216435
C	-3.704939	3.688021	1.520650
C	-2.779617	2.868953	0.865634
C	0.501856	4.673407	1.350393
C	1.606324	3.617993	1.090176
N	-1.449506	3.134400	0.883261
N	1.341164	2.477285	0.420253
C	2.937656	3.955259	1.413584
C	3.982725	3.104395	1.025857
C	3.686294	1.942950	0.300912
C	2.346129	1.659579	0.018936
C	0.524353	5.628688	0.133165
O	0.878856	5.485089	2.467385
C	-3.220522	1.635409	0.058154
C	1.936151	0.418047	-0.792110
O	-2.237964	0.966856	-0.460588
O	-4.426482	1.402417	-0.034521
O	0.654864	0.287056	-0.943092
O	2.827647	-0.313609	-1.224800
H	4.444209	1.236046	-0.066619
H	-0.192262	6.457535	0.292722
H	0.239729	5.077580	-0.783462
Ni	-0.435178	1.562252	0.120911
N	-0.457167	0.335697	1.723745
C	-0.796738	-0.942206	1.441210
C	-0.863853	-1.921964	2.439251
C	-0.571366	-1.569528	3.764606
C	-0.220200	-0.240805	4.048073
C	-0.175710	0.680812	2.995644
H	0.017445	0.083872	5.071571
C	0.939261	4.843968	3.734586
H	1.541313	6.046316	0.001632
H	-1.013350	-1.155504	0.383733
H	-1.143995	-2.950217	2.168882
H	-0.616421	-2.320383	4.568089
H	-4.767324	3.412592	1.451849
H	-1.450842	5.977091	2.705970
H	-3.919657	5.473171	2.754529
H	3.137304	4.893844	1.948900
H	5.022990	3.361621	1.278890
H	0.094003	1.735244	3.169198
C	1.384146	5.829314	4.793957
H	1.648503	3.981349	3.706096
H	-0.058006	4.422738	4.010684
C	1.531204	5.389133	6.125643
C	1.940593	6.277490	7.129392
C	2.209364	7.621021	6.815770
C	2.064791	8.064831	5.493364
C	1.654092	7.175386	4.486095
H	1.323021	4.336662	6.380064
H	2.531337	8.318994	7.603572
H	2.051389	5.919273	8.164431
H	1.539430	7.518552	3.448444
H	2.273291	9.115526	5.238694

1b(py), Me-side coordination

C	-1.863465	-0.063891	1.678067
C	-2.734964	0.247651	2.741951
C	-2.211129	0.509788	4.016263
C	-0.825787	0.453528	4.208099
C	-0.018093	0.103204	3.120533
C	-2.479212	-0.414254	0.301612
C	-1.647076	-0.107732	-0.969840
N	-0.534984	-0.159846	1.894347
N	-0.304179	-0.246966	-0.971459
C	-2.329460	0.202420	-2.164533
C	-1.603797	0.404480	-3.347396
C	-0.209202	0.291125	-3.320198
C	0.406289	-0.041920	-2.108715
C	-2.782045	-1.928832	0.300824
O	-3.757153	0.221109	0.184422
C	1.508127	-0.017781	3.262074
C	1.931887	-0.198201	-2.004056
O	2.107156	-0.397312	2.178149
O	2.012931	0.237896	4.356903
O	2.347602	-0.517421	-0.819020
O	2.606581	-0.021238	-3.020068
H	0.439855	0.441062	-4.195075
H	-3.441986	-2.179662	1.153922
H	-1.839100	-2.500210	0.391067
Ni	0.951096	-0.668497	0.585707
C	-3.781167	1.646777	0.163241
H	-3.287925	-2.209626	-0.643391
H	-0.326702	0.655538	5.166955
H	-3.817356	0.268038	2.555812
H	-2.887860	0.755342	4.849384
H	-3.425233	0.276292	-2.154383
H	-2.133323	0.649347	-4.281168
N	0.999670	-2.681297	0.665083
C	0.979789	-3.317976	1.856705
C	1.191063	-4.696440	1.971712
C	1.438409	-5.445322	0.811918
C	1.466371	-4.779900	-0.422318
C	1.245749	-3.398283	-0.453569
H	0.803248	-2.692263	2.743593
H	1.614582	-6.530121	0.870062
H	1.169580	-5.167239	2.965166
H	1.284892	-2.833424	-1.395962
H	1.666821	-5.317760	-1.360177
C	-5.135036	2.138027	-0.301387
H	-2.986743	2.047881	-0.508461
H	-3.562741	2.058740	1.176849
C	-5.347272	3.525285	-0.443945
C	-6.590297	4.016875	-0.864622
C	-7.437459	1.747824	-1.007520
C	-7.641628	3.128139	-1.148522
H	-4.527662	4.228989	-0.223670
C	-6.191446	1.253198	-0.585792
H	-8.255765	1.044442	-1.226628
H	-6.027123	0.172563	-0.471118
H	-8.617984	3.514010	-1.479228
H	-6.740077	5.102115	-0.973022

1b(py)$_2$

C	-0.120307	4.217480	2.683957
C	0.500964	4.959670	3.711277
C	0.480633	4.476444	5.027144
C	-0.169825	3.266921	5.298383
C	-0.782771	2.586452	4.239660
C	-0.181306	4.845307	1.266370
C	-0.246197	3.918936	0.023149
N	-0.754379	3.061196	2.968830
N	-0.860581	2.718575	0.065995
C	0.242874	4.424356	-1.200509
C	0.114513	3.660929	-2.369234
C	-0.508803	2.409590	-2.298894
C	-0.990969	1.972152	-1.059547
C	-1.434879	5.747227	1.226006
O	0.924966	5.746917	1.112082
C	-1.552115	1.272766	4.484995
C	-1.728332	0.624113	-0.931121
O	-2.112926	0.781139	3.429837
O	-1.584245	0.835158	5.639484
O	-2.191277	0.383274	0.250811
O	-1.832541	-0.070494	-1.947200
H	-0.655059	1.742514	-3.160809
H	-1.392265	6.484039	2.051685
H	-2.345575	5.129555	1.337202
Ni	-1.580876	1.705772	1.684960
N	0.180213	0.472524	1.782381
C	-0.061047	-0.839163	1.986747
C	0.971787	-1.784374	2.047966
C	2.297769	-1.356156	1.891706
C	2.543736	0.008408	1.679184
C	1.451577	0.884729	1.632216
H	3.565833	0.394114	1.550756
C	2.228576	5.178972	1.105078
H	-1.478568	6.286845	0.259928
H	-1.118536	-1.116385	2.107199
H	0.729168	-2.843480	2.216878
H	3.129566	-2.075976	1.934709
H	-0.240465	2.813929	6.297937
H	0.982713	5.915797	3.465707
H	0.967190	5.050231	5.831250
H	0.709563	5.418639	-1.220140
H	0.497431	4.050010	-3.325541
H	1.599720	1.965100	1.466441
N	-3.532134	2.585343	1.639524
C	-4.127851	2.985536	2.781514
C	-5.454698	3.432313	2.827562
C	-6.201373	3.460867	1.640905
C	-5.584976	3.039070	0.454290
C	-4.252648	2.607528	0.499759
H	-3.518586	2.930506	3.694967
H	-7.248601	3.800166	1.642311
H	-5.891240	3.743129	3.787944
H	-3.743996	2.246372	-0.405217
H	-6.126456	3.031789	-0.502909
C	3.269782	6.268928	0.971413
H	2.339992	4.453275	0.263957
H	2.414006	4.601047	2.042240
C	4.634163	5.913158	0.936039
C	5.625483	6.896266	0.815472
C	5.267224	8.252589	0.727987
C	3.912324	8.612941	0.761392
C	2.917176	7.628053	0.882023
H	1.854071	7.905806	0.906990
H	3.622238	9.672907	0.692607
H	6.045349	9.025364	0.633773
H	6.686153	6.602436	0.789606
H	4.924069	4.851527	1.004220

S1.10.19 Bis(carboxylato)-substituted nickel(II) dipyridylmethane with ^{t}BuBnO-substituent 1c

1c

C	1.338534	1.276458	0.090163
C	2.514944	2.035095	-0.065540
C	3.750507	1.397455	-0.239596
C	3.793291	-0.003811	-0.230111
C	2.600856	-0.703621	-0.063526
C	0.031089	2.011647	0.436212
C	-1.290121	1.307895	0.077347
N	1.396783	-0.076465	0.080744
N	-1.380034	-0.043363	0.067851
C	-2.446874	2.093867	-0.089595
C	-3.695340	1.485300	-0.275241
C	-3.771155	0.085480	-0.265776
C	-2.597124	-0.642095	-0.087681
C	0.026011	2.221557	1.969617
O	0.049776	3.322252	-0.125534
C	2.517027	-2.216144	0.004542
C	-2.549697	-2.156194	-0.018473
O	1.283902	-2.631804	0.160375
O	3.519144	-2.916198	-0.071535
O	-1.328260	-2.600892	0.148704
O	-3.567339	-2.832379	-0.103721
H	4.715817	-0.592992	-0.340029
H	-4.706193	-0.481936	-0.384158
H	0.933647	2.777214	2.274720
H	0.011431	1.241681	2.484472
Ni	-0.006651	-1.295779	0.162716
C	0.057369	3.413048	-1.549876
H	-0.870769	2.799327	2.265649
H	2.436294	3.130717	-0.033868
H	4.667112	1.992529	-0.368255
H	-2.343181	3.187368	-0.057452
H	-4.596440	2.101702	-0.412700
C	0.064417	4.864192	-1.974627
H	-0.834007	2.897107	-1.979487
H	0.949441	2.890937	-1.970507
C	0.076226	5.185094	-3.344453
C	0.082564	6.520403	-3.772495
C	0.077513	7.590760	-2.852434
C	0.065706	7.252688	-1.481595
C	0.059290	5.920239	-1.045234
H	0.050476	5.690872	0.029677
H	0.061559	8.050087	-0.722200
H	0.091759	6.720414	-4.852707
H	0.080629	4.379227	-4.097028
C	0.084262	9.070167	-3.287153
C	0.101077	9.225464	-4.819117
H	1.003513	8.767536	-5.272652
H	0.105248	10.301088	-5.088191
H	-0.792554	8.769918	-5.292083
C	-1.184239	9.768763	-2.741234
H	-2.103553	9.294890	-3.141622
H	-1.193923	10.838911	-3.035679
H	-1.237337	9.725649	-1.634981
C	1.342548	9.765311	-2.713764
H	1.361912	10.835248	-3.008380
H	2.269069	9.288461	-3.093434
H	1.371190	9.722771	-1.606581

1c(py), ^{t}BuBnO-side coordination

C	-1.102225	4.218019	5.214170
C	-0.412229	5.074044	6.098266
C	-0.401778	4.790724	7.471603
C	-1.099863	3.672329	7.945284
C	-1.757057	2.857611	7.017702
C	-1.268364	4.671083	3.741529
C	-1.530656	3.619335	2.634073
N	-1.739247	3.127165	5.688418
N	-2.205597	2.480726	2.895583
C	-1.204256	3.958496	1.303955
C	-1.594548	3.111898	0.256407
C	-2.324892	1.952845	0.549070
C	-2.609276	1.667170	1.888213
C	-2.484819	5.627690	3.721959
O	-0.151086	5.482458	3.367564
C	-2.567230	1.624591	7.454958
C	-3.425497	0.427851	2.294479
O	-3.088293	0.960616	6.470513
O	-2.659809	1.387657	8.660208
O	-3.576549	0.293314	3.575408
O	-3.861829	-0.299078	1.400828
H	-2.694730	1.249535	-0.211055
H	-2.324211	6.454167	4.441069
H	-3.402230	5.076854	4.004575
Ni	-2.507119	1.561056	4.669090
N	-0.907711	0.330221	4.684571
C	-1.193093	-0.948221	5.019671
C	-0.197480	-1.930757	5.081877
C	1.128405	-1.580559	4.789043
C	1.414812	-0.251259	4.442518
C	0.364700	0.673246	4.402832
H	2.438789	0.071804	4.204746
C	1.116680	4.840491	3.305150
H	-2.615361	6.048723	2.706270
H	-2.250865	-1.159611	5.236729
H	-0.470120	-2.959372	5.358480
H	1.930020	-2.333635	4.830241
H	-1.168864	3.393766	9.006834
H	0.090076	5.965369	5.697309
H	0.137999	5.454109	8.165087
H	-0.664391	4.895136	1.107466
H	-1.339140	3.370534	-0.782936
H	0.540679	1.728240	4.136906
C	2.173202	5.826615	2.858058
H	1.085052	3.977470	2.596364
H	1.393275	4.418827	4.302034
C	3.509363	5.407263	2.726461
C	4.509240	6.299598	2.312592
C	4.216898	7.647524	2.013341
C	2.871674	8.053656	2.150640
C	1.866807	7.167728	2.563936
H	3.781290	4.362227	2.950388
H	5.538203	5.924878	2.224527
H	0.828348	7.513784	2.662544
H	2.590303	9.095022	1.929540
C	5.287935	8.656721	1.553330
C	6.690125	8.023938	1.479332
H	7.025910	7.643377	2.465388
H	7.427693	8.782911	1.148634
H	6.730044	7.186146	0.753831
C	5.340163	9.838853	2.550783
H	5.605396	9.490214	3.569606

H	4.368231	10.367332	2.618499
H	6.102601	10.579958	2.232531
C	4.918540	9.186123	0.146680
H	3.930581	9.688410	0.139415
H	5.672445	9.923292	-0.199957
H	4.881754	8.359934	-0.592251

1c(py), Me-side coordination

C	-1.852889	-0.057089	1.676274
C	-2.717529	0.261156	2.743809
C	-2.185346	0.532427	4.012685
C	-0.798634	0.478897	4.195527
C	0.001997	0.121353	3.105130
C	-2.478200	-0.415134	0.306079
C	-1.653056	-0.118376	-0.972218
N	-0.522989	-0.150860	1.884373
N	-0.310812	-0.264324	-0.981944
C	-2.341680	0.188945	-2.164080
C	-1.622882	0.379829	-3.352921
C	-0.228812	0.258422	-3.334621
C	0.393066	-0.070091	-2.125209
C	-2.783085	-1.929373	0.316700
O	-3.755511	0.221135	0.193601
C	1.529223	0.002599	3.237053
C	1.918501	-0.233040	-2.029688
O	2.120924	-0.386478	2.152486
O	2.041664	0.268840	4.325857
O	2.340918	-0.543539	-0.844681
O	2.587198	-0.068538	-3.051792
H	0.415085	0.399072	-4.214829
H	-3.438093	-2.173635	1.175479
H	-1.840610	-2.501964	0.404255
Ni	0.953320	-0.674310	0.571137
C	-3.777012	1.647236	0.165471
H	-3.295734	-2.215036	-0.622393
H	-0.293241	0.688450	5.149445
H	-3.801054	0.279905	2.564061
H	-2.856645	0.783272	4.848631
H	-3.436905	0.269680	-2.147160
H	-2.157314	0.622470	-4.284481
N	0.999649	-2.686048	0.673455
C	0.986379	-3.309355	1.872220
C	1.196341	-4.686773	2.001359
C	1.435157	-5.448998	0.848508
C	1.456220	-4.797475	-0.393256
C	1.237466	-3.415963	-0.438636
H	0.816295	-2.673633	2.753231
H	1.610058	-6.533358	0.917710
H	1.180435	-5.146330	3.000170
H	1.271562	-2.861688	-1.387481
H	1.649840	-5.346150	-1.326273
C	-5.130380	2.138046	-0.297225
H	-2.983004	2.041834	-0.511171
H	-3.552964	2.064085	1.175751
C	-5.370129	3.525061	-0.384198
C	-6.610382	4.011579	-0.808462
C	-7.416567	1.760466	-1.070147
C	-7.669273	3.142475	-1.164254
H	-4.572350	4.237351	-0.115985
C	-6.171729	1.263317	-0.644201
H	-8.202056	1.037590	-1.331213
H	-6.005071	0.178980	-0.574602
H	-6.755432	5.101708	-0.862549
C	-9.021869	3.722525	-1.622886
C	-9.620212	4.582041	-0.483384
H	-8.951622	5.419908	-0.201247
H	-9.796288	3.971315	0.425449
H	-10.591291	5.018874	-0.796757
C	-8.803102	4.606225	-2.874187
H	-8.109490	5.447020	-2.672891
H	-9.765898	5.041599	-3.214017
H	-8.380421	4.014041	-3.711257
C	-10.036274	2.620511	-1.980794
H	-10.991379	3.080594	-2.305763
H	-10.262440	1.966781	-1.113959
H	-9.677269	1.979771	-2.811771

1c(py)$_2$

C	-0.124465	4.222687	2.674640
C	0.498893	4.968598	3.698073
C	0.484056	4.488503	5.015066
C	-0.162490	3.277954	5.291323
C	-0.776958	2.593322	4.236245
C	-0.190522	4.847829	1.255946
C	-0.260830	3.919195	0.014696
N	-0.754505	3.065448	2.964267
N	-0.872344	2.717558	0.062086
C	0.221438	4.423914	-1.211973
C	0.088851	3.658813	-2.379042
C	-0.531367	2.406155	-2.304050
C	-1.006204	1.969133	-1.061766
C	-1.444045	5.750067	1.218766
O	0.915587	5.748022	1.096088
C	-1.540490	1.277320	4.486938
C	-1.738275	0.618769	-0.927601
O	-2.102239	0.780788	3.434566
O	-1.567726	0.842274	5.642567
O	-2.193384	0.377510	0.257279
O	-1.846156	-0.077348	-1.942319
H	-0.680194	1.737543	-3.164331
H	-1.397889	6.488462	2.042842
H	-2.354718	5.133143	1.334549
Ni	-1.581122	1.704928	1.686148
N	0.185694	0.479838	1.777210
C	-0.048084	-0.832285	1.987321
C	0.989596	-1.772373	2.045570
C	2.312598	-1.338418	1.880037
C	2.550767	0.026559	1.661446
C	1.454193	0.897547	1.618066
H	3.570175	0.416817	1.525598
C	2.218653	5.176558	1.085668
H	-1.491120	6.288021	0.251918
H	-1.103508	-1.114030	2.115287
H	0.753024	-2.832040	2.219501
H	3.148054	-2.054141	1.920562
H	-0.228437	2.826981	6.292107
H	0.978668	5.924526	3.447848
H	0.972163	5.065200	5.816154
H	0.686708	5.418816	-1.234520
H	0.466412	4.047356	-3.337704
H	1.596400	1.977985	1.447797
N	-3.535925	2.577295	1.648056
C	-4.127738	2.978011	2.791862
C	-5.456275	3.419166	2.843301
C	-6.208898	3.441354	1.660277
C	-5.596465	3.019192	0.471745

C	-4.262079	2.593510	0.511788
H	-3.513747	2.928295	3.702450
H	-7.257593	3.776061	1.665960
H	-5.889404	3.730643	3.805017
H	-3.756296	2.232260	-0.394753
H	-6.142566	3.007100	-0.482780
C	3.261786	6.264410	0.960637
H	2.326967	4.456234	0.239434
H	2.400805	4.590961	2.018687
C	4.625198	5.918939	0.936232
C	5.618480	6.902402	0.823991
C	5.292965	8.272378	0.730591
C	3.920598	8.603882	0.754032
C	2.921719	7.626099	0.866341
H	1.861342	7.915474	0.881315
H	3.611538	9.658631	0.682513
H	6.669280	6.581630	0.810486
H	4.923805	4.859729	1.007295
C	6.357316	9.380850	0.606689
C	7.790251	8.815975	0.619677
H	7.972543	8.126566	-0.229591
H	8.012642	8.271885	1.560100
H	8.521462	9.645241	0.535336
C	6.146805	10.142775	-0.723813
H	6.894822	10.956306	-0.827986
H	5.140351	10.603374	-0.781394
H	6.256090	9.462724	-1.593072
C	6.213022	10.365237	1.792024
H	6.969173	11.174173	1.716596
H	6.360742	9.846624	2.761127
H	5.213128	10.842761	1.814851

S1.10.20 Bis(carboxylato)-substituted nickel(II) dipyridylmethane with $^{t}Bu_2BnO$-substituent 1d

1d

C	1.456459	1.225400	-2.764285
C	1.212484	1.926914	-3.961019
C	0.945070	1.230663	-5.147321
C	0.949997	-0.171106	-5.122377
C	1.206805	-0.812935	-3.913536
C	1.898806	2.022558	-1.523826
C	1.641985	1.384436	-0.146529
N	1.442854	-0.128526	-2.756048
N	1.649635	0.039118	0.008615
C	1.556174	2.224282	0.980840
C	1.470573	1.675325	2.267359
C	1.498513	0.280960	2.409256
C	1.592178	-0.501412	1.261038
C	3.428141	2.227474	-1.644146
O	1.336261	3.331724	-1.565723
C	1.281578	-2.319734	-3.761599
C	1.668437	-2.015795	1.280685
O	1.534961	-2.675334	-2.525889
O	1.127060	-3.067560	-4.719247
O	1.739667	-2.518535	0.072543
O	1.670996	-2.642205	2.333182
H	0.770034	-0.803803	-6.004181
H	1.456762	-0.241117	3.376703
H	3.663583	2.735264	-2.599290
H	3.942959	1.247831	-1.617724
Ni	1.640102	-1.278405	-1.306355
C	-0.085535	3.426370	-1.471954
H	3.789794	2.849218	-0.802524
H	1.252225	3.024876	-3.937396
H	0.748395	1.781016	-6.079688
H	1.569910	3.311769	0.823861
H	1.395611	2.333775	3.145815
C	-0.512813	4.878401	-1.465608
H	-0.446918	2.922797	-0.543408
H	-0.571924	2.892788	-2.321984
C	-1.885973	5.175368	-1.557285
C	-2.344815	6.504851	-1.529835
C	-1.378366	7.526901	-1.410265
C	0.003078	7.266701	-1.320899
C	0.421836	5.920071	-1.351731
H	1.485387	5.658552	-1.296102
H	-1.721303	8.572936	-1.388904
H	-2.601063	4.344962	-1.653046
C	-3.840981	6.871595	-1.625243
C	-4.738159	5.628308	-1.772572
H	-4.501692	5.052159	-2.690296
H	-5.800589	5.937803	-1.841477
H	-4.649528	4.944915	-0.903599
C	-4.263578	7.626324	-0.342023
H	-5.335824	7.908253	-0.394009
H	-3.678827	8.556765	-0.197295
H	-4.118723	6.994326	0.557708
C	-4.069196	7.780636	-2.856549
H	-5.140231	8.060153	-2.938269
H	-3.777534	7.263633	-3.793351
H	-3.483264	8.719350	-2.793975
C	0.998336	8.440044	-1.193636
C	0.875563	9.353295	-2.436968
H	1.112487	8.795704	-3.365924
H	1.579242	10.208257	-2.360595
H	-0.146057	9.768978	-2.545754
C	0.668078	9.255924	0.079019
H	1.368248	10.110781	0.183736
H	-0.360537	9.667607	0.052269
H	0.755386	8.627757	0.988905
C	2.457220	7.956989	-1.091328
H	3.135947	8.828824	-0.997629
H	2.770243	7.387832	-1.989978
H	2.618667	7.313896	-0.202514

1d(py), $^{t}Bu_2BnO$-side coordination

C	-1.347413	4.233130	5.720291
C	-0.675234	5.103060	6.604557
C	-0.684378	4.836003	7.981147
C	-1.384189	3.719838	8.457533
C	-2.023019	2.890796	7.529865
C	-1.495515	4.667912	4.240321
C	-1.733129	3.601008	3.141566
N	-1.986055	3.144656	6.197868
N	-2.404941	2.461308	3.406047
C	-1.387913	3.926517	1.812802
C	-1.756841	3.065206	0.769512
C	-2.484443	1.904986	1.064523
C	-2.787723	1.633187	2.402399
C	-2.720111	5.613217	4.192908
O	-0.380687	5.484267	3.871883
C	-2.833765	1.658980	7.969315
C	-3.602013	0.393410	2.811015
O	-3.335842	0.980402	6.984966
O	-2.944162	1.436105	9.175770
O	-3.772720	0.273712	4.090969
O	-4.018883	-0.347798	1.919787
H	-2.837885	1.190397	0.307121
H	-2.576470	6.448786	4.905055
H	-3.636512	5.057372	4.468934
Ni	-2.729128	1.562075	5.185733
N	-1.122075	0.341988	5.242158
C	-1.405207	-0.933888	5.588768
C	-0.404986	-1.909505	5.679144
C	0.923334	-1.554943	5.403017
C	1.207403	-0.228350	5.044431
C	0.152659	0.689236	4.976424
H	2.233115	0.098050	4.818987
C	0.894174	4.853687	3.835428
H	-2.839729	6.022077	3.170936
H	-2.465033	-1.148902	5.791791
H	-0.675970	-2.936217	5.964321
H	1.728608	-2.302561	5.466453
H	-1.468133	3.453669	9.521180
H	-0.171273	5.992238	6.200962
H	-0.158453	5.510201	8.674856
H	-0.850450	4.864072	1.614161
H	-1.486920	3.313152	-0.268779
H	0.326917	1.741844	4.700065
C	1.951895	5.839607	3.384642
H	0.879595	3.978155	3.142173
H	1.160445	4.451940	4.843417
C	3.273113	5.384453	3.214511
C	4.295685	6.258771	2.803020
C	3.946717	7.606405	2.567299
C	2.636089	8.095990	2.727831
C	1.640464	7.186959	3.142597
H	3.495968	4.324682	3.408454
H	4.733512	8.304811	2.243080

H	0.601913	7.509678	3.282585
C	5.755428	5.798547	2.602566
C	5.942713	4.301355	2.910472
H	5.324415	3.661270	2.248661
H	7.001988	4.014646	2.751288
H	5.688513	4.059695	3.962600
C	6.172578	6.046705	1.133140
H	5.529866	5.473591	0.434242
H	7.224101	5.730646	0.970243
H	6.097931	7.117428	0.857250
C	6.681002	6.606353	3.543718
H	7.737375	6.292176	3.411648
H	6.405929	6.447425	4.606268
H	6.628742	7.694982	3.342239
C	2.333574	9.583646	2.448655
C	3.208688	10.467238	3.369433
H	4.290782	10.293943	3.204019
H	3.009051	11.542266	3.178728
H	2.994814	10.262971	4.438316
C	2.658102	9.902237	0.969455
H	2.038874	9.287698	0.284643
H	2.455040	10.971045	0.749390
H	3.722092	9.706933	0.727431
C	0.855907	9.935279	2.705436
H	0.171941	9.357363	2.051491
H	0.562442	9.750243	3.758697
H	0.683871	11.010716	2.497236

1d(py), Me-side coordination

C	-1.826154	-0.027332	1.708264
C	-2.651938	0.307955	2.800946
C	-2.074834	0.598928	4.045549
C	-0.682446	0.548164	4.179385
C	0.078632	0.172783	3.066851
C	-2.499933	-0.406207	0.366999
C	-1.719137	-0.128090	-0.943108
N	-0.489645	-0.118948	1.870270
N	-0.379392	-0.288822	-0.998701
C	-2.445972	0.175192	-2.113044
C	-1.767759	0.344121	-3.328745
C	-0.375650	0.205034	-3.359083
C	0.285259	-0.116325	-2.168586
C	-2.801505	-1.920581	0.410503
O	-3.780548	0.227115	0.290162
C	1.609643	0.055904	3.145645
C	1.811307	-0.294769	-2.125351
O	2.161863	-0.353332	2.047806
O	2.160991	0.341999	4.210188
O	2.273035	-0.590130	-0.951168
O	2.444515	-0.155106	-3.173417
H	0.237931	0.327151	-4.263380
H	-3.423632	-2.153344	1.296503
H	-1.855405	-2.490672	0.470703
Ni	0.936845	-0.675817	0.517062
C	-3.805442	1.653333	0.241729
H	-3.348351	-2.220004	-0.504714
H	-0.143113	0.772832	5.111015
H	-3.741163	0.323696	2.660006
H	-2.715857	0.862792	4.901038
H	-3.538826	0.270946	-2.059323
H	-2.332307	0.583718	-4.243181
N	0.980384	-2.684557	0.667860
C	1.004809	-3.279249	1.880865
C	1.212958	-4.654301	2.035778
C	1.409427	-5.444915	0.894113
C	1.391748	-4.823069	-0.362822
C	1.177596	-3.441939	-0.433883
H	0.867142	-2.622132	2.751804
H	1.581659	-6.528248	0.983281
H	1.228573	-5.089940	3.045256
H	1.182844	-2.910308	-1.396159
H	1.551578	-5.394691	-1.288431
C	-5.150495	2.141488	-0.254582
H	-2.998253	2.039167	-0.423825
H	-3.601133	2.082445	1.250819
C	-5.365015	3.529379	-0.355771
C	-6.591707	4.043311	-0.813331
C	-7.420561	1.723313	-1.070835
C	-7.597953	3.117141	-1.165502
H	-4.550627	4.211482	-0.070214
C	-6.175118	1.248930	-0.607349
H	-5.980110	0.174597	-0.505193
H	-8.563439	3.503618	-1.526784
C	-6.864434	5.556914	-0.943334
C	-5.663858	6.407388	-0.487793
H	-4.758075	6.207500	-1.095507
H	-5.411041	6.230523	0.577414
H	-5.903426	7.484441	-0.597220
C	-7.165742	5.894688	-2.423130
H	-6.303051	5.642450	-3.072899
H	-7.376503	6.978303	-2.539047
H	-8.046412	5.339054	-2.802637
C	-8.084346	5.935046	-0.069395
H	-8.999327	5.389719	-0.375633
H	-7.895641	5.703722	0.998727
H	-8.298510	7.020911	-0.152497
C	-8.570754	0.773360	-1.467638
C	-9.808032	1.068234	-0.586177
H	-10.648026	0.396016	-0.859478
H	-9.578668	0.911760	0.487517
H	-10.162740	2.111534	-0.705066
C	-8.932741	1.000127	-2.955062
H	-8.064053	0.791945	-3.612473
H	-9.762245	0.328256	-3.259674
H	-9.257684	2.042011	-3.148412
C	-8.190873	-0.708152	-1.283729
H	-9.044463	-1.353854	-1.573662
H	-7.939073	-0.943015	-0.229738
H	-7.326819	-0.996966	-1.915966

1d(py)$_2$

C	-0.117632	4.229594	2.666108
C	0.509256	4.976470	3.686680
C	0.496119	4.499115	5.004690
C	-0.152031	3.290314	5.284858
C	-0.769256	2.604246	4.232354
C	-0.187244	4.852156	1.246433
C	-0.258232	3.920892	0.007223
N	-0.748660	3.073784	2.959395
N	-0.867860	2.718440	0.058015
C	0.221397	4.423787	-1.221212
C	0.088341	3.655948	-2.386412
C	-0.529643	2.402382	-2.307855
C	-1.002112	1.967328	-1.063986
C	-1.443022	5.751439	1.210067
O	0.916107	5.754309	1.082843
C	-1.533436	1.289428	4.487047
C	-1.732130	0.616276	-0.925819
O	-2.095222	0.789784	3.436158
O	-1.560803	0.857781	5.643974
O	-2.186177	0.377495	0.259978
O	-1.839639	-0.082753	-1.938596
H	-0.678518	1.731651	-3.166475
H	-1.397068	6.491070	2.033048
H	-2.352209	5.132772	1.328056
Ni	-1.575033	1.709603	1.685072
N	0.193228	0.486815	1.779152
C	-0.038857	-0.824979	1.993099
C	1.000056	-1.763510	2.054377
C	2.322519	-1.328279	1.887825
C	2.558906	0.036343	1.665138
C	1.461194	0.905771	1.618942
H	3.577797	0.427623	1.528299
C	2.221247	5.187019	1.069810
H	-1.492488	6.288114	0.242627
H	-1.093942	-1.107730	2.121676
H	0.764857	-2.822962	2.231467
H	3.158918	-2.042767	1.930721
H	-0.216975	2.841700	6.286764
H	0.990463	5.930890	3.433501
H	0.986894	5.076573	5.803608
H	0.685075	5.419377	-1.246311
H	0.463858	4.043005	-3.346485
H	1.602089	1.985872	1.445482
N	-3.530752	2.579822	1.645361
C	-4.122181	2.983525	2.788313
C	-5.451139	3.423474	2.839273
C	-6.204577	3.441203	1.656692
C	-5.592518	3.015947	0.469072
C	-4.257669	2.591743	0.509544
H	-3.507457	2.937359	3.698592
H	-7.253603	3.774883	1.662037
H	-5.883930	3.737551	3.800297
H	-3.752082	2.228214	-0.396195
H	-6.139249	3.000349	-0.485042
C	3.266221	6.276514	0.951773
H	2.331180	4.471693	0.219736
H	2.403638	4.596428	1.999510
C	4.624297	5.906032	0.925471
C	5.640145	6.873264	0.820798
C	5.247248	8.227149	0.742446
C	3.899075	8.633702	0.763855
C	2.911016	7.632255	0.869975
H	1.844686	7.887778	0.890698
H	6.029649	8.997814	0.664100
H	4.881540	4.838255	0.990222
C	7.139588	6.508375	0.790429
C	7.372752	4.989744	0.897442
H	6.907181	4.438292	0.055354
H	6.974006	4.575207	1.845669
H	8.459972	4.773082	0.873205
C	7.857733	7.193125	1.977899
H	7.441396	6.849579	2.946728
H	7.758023	8.296313	1.941941
H	8.941584	6.954189	1.965552
C	7.758542	7.001299	-0.539544
H	8.840535	6.756529	-0.578525
H	7.658787	8.098498	-0.660641
H	7.266581	6.520952	-1.409760
C	3.549841	10.134534	0.670942
C	4.089850	10.702815	-0.663443
H	5.189517	10.591216	-0.746157
H	3.855222	11.784394	-0.748461
H	3.633187	10.183526	-1.530556
C	4.203974	10.887680	1.853833
H	5.307174	10.781056	1.853429
H	3.972085	11.971866	1.799971
H	3.829838	10.504722	2.825124
C	2.030537	10.382530	0.721810
H	1.824184	11.469963	0.653475
H	1.582905	10.018398	1.668715
H	1.501853	9.890867	-0.119726

1d(dcm), ^{t}Bu$_2$BnO-side coordination

C	-1.257701	4.221636	5.725846
C	-0.641239	5.127966	6.614290
C	-0.643732	4.863396	7.990618
C	-1.276050	3.706608	8.463859
C	-1.861638	2.844302	7.532643
C	-1.397230	4.643721	4.242475
C	-1.569943	3.563232	3.146067
N	-1.841202	3.102341	6.201181
N	-2.193183	2.394359	3.399609
C	-1.210357	3.899200	1.823696
C	-1.513220	3.018625	0.776074
C	-2.185340	1.822801	1.059429
C	-2.503453	1.542084	2.391178
C	-2.657496	5.539466	4.166393
O	-0.307714	5.496982	3.890715
C	-2.575215	1.557399	7.966742
C	-3.232898	0.252622	2.789439
O	-3.030757	0.847246	6.974665
O	-2.657985	1.302586	9.166456
O	-3.408806	0.121950	4.073215
O	-3.578570	-0.529031	1.905849
H	-2.477721	1.086418	0.297060
H	-2.561796	6.382613	4.877477
H	-3.557386	4.949337	4.425457
Ni	-2.542992	1.510795	5.178751
C	0.990747	4.906877	3.889689
H	-2.771704	5.940691	3.140872
H	-1.341385	3.432788	9.526749
H	-0.181186	6.040522	6.210827
H	-0.161381	5.567003	8.686562
H	-0.709500	4.858624	1.634915
H	-1.231737	3.275983	-0.256699
C	2.022290	5.911841	3.423421

H	1.012918	4.008766	3.227687
H	1.253534	4.543834	4.912310
C	3.354774	5.485085	3.266594
C	4.358717	6.377016	2.847661
C	3.979470	7.712329	2.589460
C	2.656775	8.173324	2.735177
C	1.680272	7.247667	3.158997
H	3.601448	4.434029	3.477874
H	4.751779	8.424068	2.259304
H	0.633944	7.549447	3.288225
C	5.830207	5.948524	2.664409
C	6.049294	4.459410	2.990064
H	5.451433	3.797917	2.330632
H	7.116120	4.195349	2.842741
H	5.792026	4.222555	4.042420
C	6.254788	6.191165	1.196218
H	5.632425	5.595417	0.497824
H	7.314824	5.898003	1.046441
H	6.158005	7.256847	0.907820
C	6.727379	6.788281	3.605158
H	7.792379	6.500282	3.483717
H	6.448450	6.631216	4.666979
H	6.648427	7.873435	3.393669
C	2.321573	9.648963	2.430653
C	3.171057	10.566995	3.341656
H	4.257658	10.416891	3.183458
H	2.947000	11.634054	3.134132
H	2.957290	10.373474	4.412550
C	2.646647	9.951458	0.948173
H	2.045481	9.311889	0.270200
H	2.420642	11.011667	0.709517
H	3.716063	9.776570	0.714824
C	0.834799	9.970522	2.674275
H	0.167903	9.366457	2.026278
H	0.540060	9.795626	3.728975
H	0.638958	11.038197	2.447880
Cl	-0.487954	0.104887	5.255751
C	-1.414184	-1.409792	5.763567
Cl	-0.332243	-2.777240	5.986683
H	-2.139066	-1.584094	4.948015
H	-1.922930	-1.125475	6.702514

1d(dcm), Me-side coordination

C	-2.054461	-0.145930	1.538802
C	-2.996808	0.225734	2.520379
C	-2.572010	0.477284	3.832318
C	-1.214014	0.347596	4.148318
C	-0.331477	-0.034745	3.133713
C	-2.576576	-0.541806	0.135113
C	-1.645728	-0.358748	-1.089070
N	-0.752680	-0.277189	1.867551
N	-0.310423	-0.520241	-0.983969
C	-2.236177	-0.161590	-2.354612
C	-1.427986	-0.113872	-3.499015
C	-0.043130	-0.272332	-3.365760
C	0.480040	-0.475555	-2.085281
C	-2.940187	-2.043616	0.198712
O	-3.811846	0.133099	-0.111646
C	1.168180	-0.214372	3.401909
C	1.983540	-0.676713	-1.857698
O	1.858670	-0.520609	2.341917
O	1.587296	-0.060118	4.547191
O	2.313857	-0.797993	-0.604639
O	2.731019	-0.705850	-2.833158
H	0.661933	-0.256077	-4.209330
H	-3.659965	-2.222016	1.020871
H	-2.030242	-2.647390	0.378935
Ni	0.813036	-0.756420	0.681418
C	-3.765535	1.555562	-0.216339
H	-3.397467	-2.359319	-0.758948
H	-0.796608	0.519519	5.150908
H	-4.057001	0.297337	2.242077
H	-3.304740	0.767322	4.601091
H	-3.327912	-0.062344	-2.424038
H	-1.885400	0.040402	-4.488488
C	-5.146481	2.103613	-0.506837
H	-3.059875	1.867517	-1.022078
H	-3.374054	2.005618	0.726729
C	-5.293243	3.493323	-0.679686
C	-6.551361	4.062531	-0.947174
C	-7.547873	1.795954	-0.866976
C	-7.657984	3.190019	-1.034216
H	-4.401411	4.132939	-0.603232
C	-6.268310	1.264686	-0.601057
H	-6.120239	0.186890	-0.463426
H	-8.649629	3.619917	-1.244085
C	-6.754418	5.578792	-1.150554
C	-5.439949	6.368001	-1.003271
H	-4.683448	6.057915	-1.752538
H	-4.994989	6.250415	0.005809
H	-5.630992	7.449534	-1.155594
C	-7.314821	5.831304	-2.570821
H	-6.612846	5.463738	-3.346772
H	-7.472586	6.917187	-2.737863
H	-8.287211	5.323367	-2.729868
C	-7.757711	6.108559	-0.098327
H	-8.745224	5.612163	-0.179516
H	-7.380349	5.941755	0.931099
H	-7.919133	7.198477	-0.232079
C	-8.805735	0.908680	-0.981703
C	-9.841839	1.347097	0.080712
H	-10.759067	0.726397	0.006886
H	-9.433353	1.234910	1.105713
H	-10.143358	2.405966	-0.046684
C	-9.417237	1.069335	-2.394113
H	-8.696846	0.757685	-3.177672
H	-10.327686	0.442607	-2.495965
H	-9.707221	2.118551	-2.602287
C	-8.489583	-0.582485	-0.759650
H	-9.419205	-1.180327	-0.849543
H	-8.069422	-0.771505	0.248966
H	-7.771722	-0.970962	-1.510161
Cl	0.947526	-3.202730	0.939881
C	2.778224	-3.162262	1.209804
Cl	3.427103	-4.775030	1.459833
H	2.910320	-2.516972	2.097353
H	3.179287	-2.687128	0.296047

1d(dcm)$_2$

C	-0.063536	4.495694	2.664793
C	0.531816	5.258238	3.692071
C	0.470092	4.807394	5.017303
C	-0.195091	3.608150	5.300992
C	-0.762916	2.897800	4.239147
C	-0.115044	5.109205	1.242977
C	-0.211366	4.178045	0.007827

N	-0.692099	3.339954	2.959211
N	-0.817629	2.975255	0.066813
C	0.232269	4.685523	-1.231939
C	0.047057	3.932291	-2.398616
C	-0.587007	2.686546	-2.313652
C	-1.005482	2.239689	-1.056782
C	-1.359216	6.027864	1.207018
O	1.001113	5.987010	1.074890
C	-1.508248	1.579354	4.475710
C	-1.711083	0.888723	-0.890793
O	-1.934400	1.006592	3.384970
O	-1.641378	1.171793	5.627966
O	-2.013064	0.594489	0.342759
O	-1.928691	0.206889	-1.890362
H	-0.780708	2.035608	-3.178258
H	-1.295501	6.774202	2.022398
H	-2.280627	5.429355	1.339628
Ni	-1.438684	1.958573	1.693276
Cl	0.798972	0.559711	1.811614
C	2.293407	5.383709	1.064014
H	-1.409426	6.556023	0.235267
H	-0.301195	3.188851	6.311787
H	1.025349	6.205391	3.435145
H	0.934828	5.398400	5.821496
H	0.708592	5.675016	-1.262051
H	0.392880	4.324387	-3.367450
Cl	-3.851336	2.833446	1.624437
C	3.366354	6.442116	0.923457
H	2.375979	4.650792	0.226483
H	2.461358	4.801775	2.001479
C	4.712140	6.030540	0.882768
C	5.754583	6.966679	0.758711
C	5.400771	8.331131	0.676671
C	4.065842	8.778124	0.712598
C	3.049828	7.807197	0.837136
H	1.992348	8.096312	0.868813
H	6.204770	9.077263	0.582288
H	4.938120	4.956071	0.951106
C	7.241625	6.555683	0.710866
C	7.428916	5.031178	0.821601
H	6.934635	4.490577	-0.011058
H	7.031243	4.632646	1.777025
H	8.508376	4.780714	0.782860
C	7.995152	7.223372	1.886021
H	7.580279	6.897304	2.861463
H	7.929708	8.329020	1.845608
H	9.070673	6.950252	1.861886
C	7.857919	7.024061	-0.629184
H	8.930819	6.744359	-0.681383
H	7.792044	8.123486	-0.753461
H	7.339351	6.556402	-1.490802
C	3.761059	10.288403	0.617163
C	4.307129	10.837023	-0.722947
H	5.402236	10.692648	-0.814282
H	4.104313	11.924934	-0.808296
H	3.828131	10.330205	-1.585369
C	4.447281	11.024416	1.792794
H	5.546906	10.886079	1.782992
H	4.246312	12.114671	1.738551
H	4.070712	10.654312	2.768141
C	2.250395	10.583047	0.679494
H	2.077381	11.676023	0.607948
H	1.799467	10.237433	1.631825
H	1.699792	10.104656	-0.155683
C	-4.567414	1.163431	1.893768
Cl	-6.326684	1.208546	1.964823
H	-4.128448	0.818329	2.847421
H	-4.209703	0.561120	1.039394
C	-0.081930	-1.028393	2.047109
Cl	1.035264	-2.389482	2.149297
H	-0.751731	-1.120254	1.173061
H	-0.656380	-0.909174	2.983036

1d(py)(dcm), $^{t}Bu_2BnO$-side coordination of py

C	-1.297773	4.369932	5.786797
C	-0.532973	5.145882	6.683742
C	-0.475614	4.786537	8.037417
C	-1.198063	3.671069	8.479705
C	-1.930079	2.937399	7.540234
C	-1.488650	4.908150	4.345532
C	-1.841841	3.932022	3.193734
N	-1.961891	3.282788	6.229146
N	-2.560850	2.812230	3.413918
C	-1.537106	4.329295	1.874253
C	-1.993434	3.560286	0.794779
C	-2.765503	2.419236	1.046739
C	-3.026075	2.072818	2.376548
C	-2.645409	5.933746	4.413482
O	-0.336662	5.673622	3.976113
C	-2.768335	1.717940	7.957989
C	-3.889123	0.849429	2.726224
O	-3.355968	1.113241	6.970359
O	-2.824852	1.431730	9.154501
O	-4.002615	0.625448	4.000569
O	-4.397062	0.211588	1.803309
H	-3.187744	1.776123	0.261181
H	-2.414598	6.711119	5.167334
H	-3.587732	5.427376	4.696196
Ni	-2.898222	1.850787	5.155886
N	-1.317602	0.549781	5.033666
C	-1.620023	-0.740752	5.294530
C	-0.648091	-1.748438	5.261033
C	0.675958	-1.409638	4.947337
C	0.982546	-0.067414	4.677322
C	-0.046920	0.879905	4.732708
H	2.005712	0.248439	4.426599
C	0.888255	4.963024	3.840286
H	-2.778392	6.414709	3.425063
H	-2.674413	-0.945015	5.531075
H	-0.936599	-2.786572	5.480013
H	1.460062	-2.181350	4.913487
H	-1.231619	3.335377	9.526234
H	-0.007812	6.034354	6.306552
H	0.120688	5.387808	8.741109
H	-0.958522	5.249337	1.712833
H	-1.756212	3.864732	-0.236382
H	0.147685	1.945577	4.530082
C	1.991275	5.897755	3.390015
H	0.776595	4.133807	3.099527
H	1.175692	4.484862	4.807496
C	3.309422	5.406998	3.332631
C	4.371636	6.224045	2.904437
C	4.065960	7.552664	2.538108
C	2.760172	8.078597	2.588531
C	1.723456	7.225603	3.021645
H	3.498269	4.365447	3.632410
H	4.885401	8.206828	2.202649

H	0.688196	7.580942	3.088436
C	5.829886	5.724090	2.829497
C	5.965949	4.254871	3.271828
H	5.373553	3.572239	2.629072
H	7.026125	3.937671	3.202081
H	5.645167	4.106192	4.323084
C	6.336660	5.839532	1.371921
H	5.721661	5.222096	0.685976
H	7.387867	5.490955	1.298195
H	6.304585	6.884224	1.003196
C	6.716836	6.591909	3.754273
H	7.771917	6.249741	3.712301
H	6.376585	6.526967	4.807842
H	6.700270	7.660628	3.461246
C	2.506241	9.544792	2.176670
C	3.343417	10.482671	3.079074
H	4.429616	10.280011	2.992183
H	3.176857	11.543092	2.796808
H	3.063300	10.364007	4.145566
C	2.926936	9.740334	0.700396
H	2.339352	9.082165	0.028360
H	2.758436	10.791111	0.384545
H	3.999583	9.510455	0.542834
C	1.024017	9.939886	2.314127
H	0.368025	9.322324	1.667784
H	0.665690	9.844800	3.359035
H	0.887953	10.997647	2.010246
Cl	-5.375379	3.188937	5.459796
C	-6.173963	1.611856	5.898100
Cl	-7.906300	1.803159	6.208721
H	-5.647986	1.251383	6.800070
H	-5.996043	0.941302	5.038145

1d(py)(dcm), Me-side coordination of py

C	-2.006662	0.008225	1.396788
C	-2.993434	0.303863	2.360930
C	-2.616178	0.558998	3.686659
C	-1.259841	0.515930	4.029590
C	-0.332319	0.196879	3.032124
C	-2.470459	-0.361627	-0.035341
C	-1.527296	-0.051421	-1.225088
N	-0.708374	-0.062790	1.755242
N	-0.186482	-0.112878	-1.094899
C	-2.106968	0.183565	-2.489610
C	-1.283155	0.396946	-3.603490
C	0.106580	0.374695	-3.437529
C	0.619159	0.109132	-2.163182
C	-2.741275	-1.882754	-0.048757
O	-3.743458	0.244522	-0.282050
C	1.170553	0.127858	3.339769
C	2.132627	0.061789	-1.908336
O	1.903893	-0.220220	2.326050
O	1.547711	0.396510	4.481424
O	2.456771	-0.273694	-0.697711
O	2.892333	0.337766	-2.839080
H	0.826828	0.550248	-4.249582
H	-3.476330	-2.139022	0.738804
H	-1.801008	-2.434332	0.139248
Ni	0.920835	-0.421849	0.586957
C	-3.791498	1.669951	-0.325413
H	-3.147523	-2.182923	-1.034225
H	-0.872423	0.715359	5.039090
H	-4.048990	0.321098	2.057853
H	-3.383027	0.791673	4.441655
H	-3.201484	0.188808	-2.581933
H	-1.731490	0.582908	-4.591753
N	1.007133	-2.460765	0.635256
C	0.918134	-3.121132	1.809868
C	1.121191	-4.502461	1.910541
C	1.434920	-5.229022	0.752795
C	1.534464	-4.539537	-0.464367
C	1.316719	-3.156839	-0.479734
H	0.692310	-2.512111	2.696918
H	1.606075	-6.315236	0.799565
H	1.041224	-4.992500	2.891660
H	1.406399	-2.575299	-1.408463
H	1.787669	-5.059417	-1.399635
C	-5.211786	2.136642	-0.563441
H	-3.127939	2.062183	-1.131714
H	-3.407662	2.105887	0.626909
C	-5.458100	3.520466	-0.646522
C	-6.756235	4.015375	-0.866308
C	-7.590177	1.683914	-0.924193
C	-7.800363	3.074351	-0.999808
H	-4.612326	4.215124	-0.535688
C	-6.273392	1.228484	-0.702416
H	-6.047603	0.157499	-0.634626
H	-8.822774	3.444693	-1.171662
C	-7.067100	5.523984	-0.964127
C	-5.804964	6.391767	-0.801302
H	-5.053016	6.183291	-1.589261
H	-5.321325	6.241649	0.185332
H	-6.074748	7.464605	-0.876864
C	-7.689565	5.829759	-2.347521
H	-6.991202	5.562110	-3.166435
H	-7.923522	6.911123	-2.436010
H	-8.631523	5.269094	-2.512533
C	-8.068707	5.913220	0.149476
H	-9.020238	5.351168	0.066319
H	-7.644830	5.711490	1.154284
H	-8.311995	6.994646	0.091066
C	-8.783621	0.717721	-1.086039
C	-9.825880	0.999775	0.022615
H	-10.697565	0.320522	-0.082320
H	-9.388151	0.842935	1.029544
H	-10.205058	2.040295	-0.020503
C	-9.435103	0.935788	-2.472585
H	-8.712458	0.731300	-3.288703
H	-10.302854	0.256170	-2.604101
H	-9.800596	1.974238	-2.599731
C	-8.355807	-0.758148	-0.982057
H	-9.239812	-1.415601	-1.109251
H	-7.907106	-0.991663	0.004680
H	-7.622062	-1.032377	-1.766848
Cl	1.354448	2.495880	0.600550
C	3.129117	2.247790	0.908355
Cl	3.966109	3.773809	1.246945
H	3.194009	1.565533	1.775648
H	3.540397	1.776808	-0.001100

1d$_2$, S = 1 + S = 0

Ni	-0.839567	8.439657	10.772921
N	-0.352422	10.211245	10.535788
N	0.769955	7.859672	11.524893
O	-2.521902	8.916674	10.150870
O	-1.470381	6.691807	11.087616

C	-1.410365	10.980836	10.148684
C	0.863346	10.771312	10.726720
C	1.918169	8.553474	11.666840
C	0.715966	6.552227	11.918439
C	-2.683392	10.195452	9.906808
C	-0.575730	5.888805	11.543301
C	-1.303451	12.357052	9.968501
C	1.029447	12.160135	10.552608
C	2.112947	9.907556	10.962707
C	3.029176	7.956882	12.297143
C	1.786265	5.900873	12.527007
O	-3.712158	10.734414	9.517677
O	-0.720241	4.638713	11.617484
C	-0.057365	12.962927	10.184689
C	2.700332	9.580633	9.568032
O	3.103042	10.673540	11.647039
C	2.961521	6.632646	12.744427
Ni	0.240649	3.866174	9.930189
C	2.794121	11.073008	12.980278
N	-1.249357	4.372345	8.662706
N	-0.401118	1.975483	10.076675
O	1.016792	5.619493	9.285767
O	1.863678	3.170352	10.818248
C	-1.052698	5.598297	8.117160
C	-2.373148	3.676767	8.400962
C	-1.575462	1.459484	9.664445
C	0.547330	1.192775	10.645406
C	0.220733	6.321739	8.551750
C	1.834708	1.900508	11.094818
C	-1.981596	6.186059	7.254252
C	-3.348043	4.212281	7.532541
C	-2.719721	2.379052	9.173876
C	-1.832682	0.082024	9.827940
C	0.356871	-0.180472	10.825705
O	0.373017	7.510976	8.219260
O	2.704948	1.237003	11.659142
C	-3.146022	5.470195	6.950196
O	-3.641540	1.602619	8.403358
C	-3.496840	2.824645	10.435132
C	-0.856216	-0.741639	10.406032
H	2.033870	12.582167	10.695447
H	0.075301	14.047567	10.054441
H	-3.909231	5.896076	6.281149
H	-1.770245	7.194008	6.871582
H	-2.805488	-0.321140	9.515496
H	-1.052980	-1.817355	10.534451
H	1.167799	-0.752636	11.298862
H	-2.206661	12.901382	9.655461
H	3.951333	8.546332	12.395043
H	1.694007	4.830659	12.758282
H	2.001321	8.926811	9.003828
H	3.662260	9.047844	9.698397
H	2.878688	10.519911	9.009065
H	3.833865	6.162076	13.221335
H	-4.269883	3.643446	7.350622
C	-3.171766	1.080627	7.163679
H	-4.387289	3.409878	10.133755
H	-2.845245	3.457100	11.069432
H	-3.823702	1.933846	11.006266
C	-4.228711	0.195001	6.538304
H	-2.231772	0.497365	7.308751
H	-2.913918	1.909859	6.461877
C	-3.906298	-0.519699	5.368780
C	-4.854737	-1.344401	4.736756
C	-6.138023	-1.430380	5.319358
C	-6.494498	-0.731259	6.488881
C	-5.515203	0.086516	7.090473
C	-4.542614	-2.143281	3.453639
C	-3.093963	-1.934855	2.973862
H	-2.354362	-2.265910	3.730933
H	-2.886376	-0.873311	2.729244
H	-2.913615	-2.527409	2.054060
C	-4.750224	-3.652602	3.724731
H	-4.543110	-4.243361	2.808086
H	-5.788345	-3.878016	4.040524
H	-4.070254	-4.010916	4.524329
C	-5.497013	-1.686805	2.324098
H	-5.295691	-2.255329	1.392131
H	-5.364748	-0.608041	2.103349
H	-6.560634	-1.847155	2.591031
C	-7.918285	-0.878093	7.066925
C	-8.950549	-0.413713	6.011744
H	-8.792941	0.650624	5.742757
H	-9.982812	-0.518490	6.406300
H	-8.886313	-1.009263	5.079199
C	-8.176326	-2.362380	7.421067
H	-8.086900	-3.021241	6.534236
H	-9.198932	-2.491121	7.833413
H	-7.452490	-2.721602	8.180767
C	-8.118305	-0.035951	8.341068
H	-7.971748	1.046283	8.149849
H	-7.424231	-0.338338	9.151074
H	-9.151371	-0.169252	8.721548
H	-6.891670	-2.072856	4.838156
H	-2.892079	-0.423371	4.953312
H	-5.732623	0.653462	8.003613
C	4.005071	11.702683	13.635181
H	2.456879	10.195145	13.581640
H	1.943502	11.796143	12.986938
C	5.236532	11.798877	12.968003
C	6.357047	12.379293	13.599044
C	6.196524	12.854611	14.914989
C	4.972400	12.776354	15.614178
C	3.878928	12.193205	14.948919
H	2.904483	12.110341	15.452915
H	7.062711	13.306517	15.422574
H	5.301031	11.412317	11.943792
C	7.728667	12.498479	12.900646
C	7.697908	11.951232	11.461459
H	6.973236	12.498903	10.825542
H	7.434936	10.874513	11.432384
H	8.698301	12.060650	10.995696
C	8.149531	13.986696	12.844324
H	7.414533	14.586986	12.270321
H	9.138131	14.091588	12.350615
H	8.231922	14.433006	13.855475
C	8.780778	11.696228	13.703609
H	8.508360	10.622374	13.754953
H	8.879398	12.068026	14.743132
H	9.778250	11.774180	13.222825
C	4.880026	13.314949	17.057430
C	3.465266	13.165655	17.647713
H	2.709216	13.724996	17.059980
H	3.445237	13.567382	18.680921
H	3.146573	12.104715	17.700235
C	5.865618	12.530872	17.956905
H	6.912533	12.629073	17.606877
H	5.616529	11.450304	17.972616

H	5.823091	12.908150	18.999981
C	5.253629	14.816686	17.070720
H	4.557172	15.406056	16.440085
H	6.280523	14.992627	16.692596
H	5.204871	15.218964	18.104025

$1d_2$, 2 · S = 1

Ni	0.227083	8.214980	10.742631
N	0.968168	10.069566	10.709095
N	1.793784	7.498997	11.795003
O	-1.454717	9.080988	10.231845
O	-0.593272	6.413318	11.320384
C	0.013926	10.953382	10.330878
C	2.213152	10.475588	11.021433
C	2.975121	8.109138	12.007649
C	1.598190	6.219863	12.207227
C	-1.372406	10.363453	10.030817
C	0.280477	5.610529	11.769091
C	0.279201	12.322190	10.232444
C	2.546210	11.843831	10.936301
C	3.331696	9.448096	11.313442
C	3.998015	7.439107	12.714033
C	2.575336	5.493673	12.892830
O	-2.267263	11.119965	9.655118
O	0.169235	4.341625	11.798500
C	1.570813	12.770113	10.540479
C	3.939374	9.061035	9.944203
O	4.376906	10.095982	12.042260
C	3.791625	6.131499	13.169417
Ni	0.833023	3.666283	9.948507
C	4.063533	10.535098	13.362160
N	-0.733687	4.382143	8.896048
N	0.092062	1.811650	9.982051
O	1.653282	5.467969	9.370726
O	2.514839	2.800414	10.459504
C	-0.538164	5.661286	8.483820
C	-1.914976	3.771921	8.683366
C	-1.152869	1.405530	9.669625
C	1.046344	0.927909	10.360343
C	0.779497	6.270704	8.921991
C	2.432603	1.517945	10.660535
C	-1.515337	6.387410	7.798185
C	-2.937892	4.441882	7.976946
C	-2.271478	2.432934	9.377553
C	-1.485823	0.037260	9.754727
C	0.781171	-0.440920	10.458755
O	0.890660	7.539614	8.892579
O	3.327487	0.761496	11.036296
C	-2.731576	5.749503	7.521564
O	-3.316589	1.784962	8.648669
C	-2.879270	2.819941	10.746757
C	-0.510380	-0.888946	10.150616
H	3.572278	12.160517	11.167444
H	-3.532584	6.280439	6.985476
H	-1.315215	7.435146	7.536733
H	-2.511849	-0.279508	9.523511
H	-0.766482	-1.957524	10.220341
H	1.600441	-1.101074	10.777932
H	4.962052	7.945028	12.859605
H	2.375156	4.445948	13.154282
H	3.177896	8.528579	9.340218
H	4.810235	8.394953	10.098960
H	4.269244	9.973924	9.411158
H	4.592614	5.600506	13.705478
H	-3.901891	3.935896	7.831346
C	-3.003100	1.345895	7.328779
H	-3.750179	3.485948	10.591948
H	-2.117872	3.352462	11.350788
H	-3.209094	1.907022	11.279779
C	-4.150560	0.539198	6.759417
H	-2.073114	0.730402	7.324864
H	-2.795124	2.221233	6.666898
C	-3.956668	-0.144860	5.544203
C	-4.995666	-0.888420	4.955392
C	-6.235944	-0.924455	5.628793
C	-6.464109	-0.255403	6.847249
C	-5.397164	0.480918	7.403213
C	-4.823625	-1.656325	3.627689
C	-3.408437	-1.497915	3.040498
H	-2.628947	-1.887969	3.726102
H	-3.169244	-0.439380	2.812161
H	-3.329550	-2.067096	2.092219
C	-5.080380	-3.162944	3.870505
H	-4.969974	-3.731998	2.923874
H	-6.101439	-3.352415	4.257733
H	-4.359773	-3.576704	4.605068
C	-5.840898	-1.120958	2.591662
H	-5.734768	-1.662928	1.628809
H	-5.679962	-0.040995	2.397532
H	-6.887232	-1.248696	2.934188
C	-7.847570	-0.345845	7.525907
C	-8.926889	0.210553	6.566725
H	-8.728446	1.272764	6.317125
H	-9.931136	0.150324	7.035776
H	-8.967627	-0.356527	5.615341
C	-8.161853	-1.825711	7.851650
H	-8.181175	-2.455602	6.939759
H	-9.154519	-1.912687	8.340865
H	-7.402762	-2.251745	8.538922
C	-7.906019	0.459957	8.837222
H	-7.709971	1.538399	8.670096
H	-7.175370	0.090277	9.584824
H	-8.915363	0.371795	9.288039
H	-7.059010	-1.504484	5.183078
H	-2.970691	-0.090302	5.059304
H	-5.514016	1.019929	8.351124
C	5.211161	11.341574	13.931497
H	3.855407	9.659798	14.024042
H	3.133666	11.150771	13.366100
C	6.457724	11.399719	13.287610
C	7.524818	12.135846	13.843545
C	7.296841	12.804849	15.062064
C	6.056608	12.768950	15.735554
C	5.017460	12.025575	15.146774
H	4.031513	11.971124	15.631743
H	8.120026	13.384729	15.507756
H	6.574426	10.860754	12.339654
C	8.908240	12.226134	13.164787
C	8.966451	11.420460	11.853383
H	8.235837	11.790371	11.105861
H	8.770191	10.342041	12.020406
H	9.975789	11.508465	11.402520
C	9.222735	13.705984	12.839173
H	8.463663	14.132207	12.151997
H	10.215380	13.792852	12.349896
H	9.242221	14.335779	13.751126
C	9.987546	11.669460	14.123822

H	9.788951	10.607254	14.373326
H	10.028454	12.236432	15.075263
H	10.991765	11.729574	13.654696
C	5.884771	13.536803	17.063314
C	4.469644	13.378450	17.650669
H	3.690091	13.768549	16.965161
H	4.390895	13.947621	18.598965
H	4.230430	12.319922	17.879020
C	6.902137	13.001332	18.099195
H	7.948438	13.129012	17.756543
H	6.741153	11.921373	18.293308
H	6.796165	13.543276	19.062079
C	6.141584	15.043417	16.820530
H	5.420923	15.457244	16.086056
H	7.162614	15.232845	16.433201
H	6.031309	15.612441	17.767193
H	-0.540042	12.982410	9.913333
H	1.826996	13.838670	10.470729

1d$_2$(dcm), S =1 + S = 0

Ni	-0.775976	8.148631	10.971422
N	-0.386358	9.950663	10.787487
N	0.903782	7.612295	11.587652
O	-2.513635	8.568913	10.473950
O	-1.297087	6.356618	11.208111
C	-1.499108	10.682648	10.490981
C	0.811363	10.561594	10.930657
C	2.020934	8.359666	11.710953
C	0.937753	6.284404	11.907490
C	-2.747383	9.847046	10.292464
C	-0.338408	5.573242	11.564790
C	-1.465729	12.067851	10.357032
C	0.903560	11.962022	10.800945
C	2.111627	9.752399	11.065114
C	3.191153	7.792761	12.255114
C	2.070965	5.660568	12.424511
O	-3.821077	10.351005	9.986901
O	-0.416648	4.319716	11.574604
C	-0.238044	12.724423	10.524859
C	2.641127	9.519614	9.628418
O	3.096790	10.539842	11.731536
C	3.214871	6.444218	12.629900
Ni	0.430452	3.635901	9.740152
C	2.837107	10.871720	13.094684
N	-1.174745	4.223884	8.667248
N	-0.247951	1.768624	9.972341
O	1.114709	5.487254	9.209894
O	2.072350	2.922423	10.646178
C	-1.020139	5.471093	8.158890
C	-2.306167	3.528380	8.445055
C	-1.451901	1.275839	9.626308
C	0.708176	0.971194	10.505297
C	0.267228	6.198181	8.538930
C	2.029660	1.645494	10.896581
C	-2.001374	6.081051	7.372958
C	-3.330552	4.082989	7.647487
C	-2.611059	2.209410	9.199978
C	-1.728538	-0.095997	9.809201
C	0.498177	-0.396629	10.705235
O	0.393160	7.393760	8.224987
O	2.920058	0.956641	11.395679
C	-3.172189	5.362740	7.101779
O	-3.564771	1.450359	8.450776
C	-3.330302	2.627492	10.504385
C	-0.742846	-0.936740	10.343866
H	1.893671	12.426923	10.905813
H	-0.162566	13.818045	10.428492
H	-3.972738	5.802855	6.487947
H	-1.820336	7.104911	7.018204
H	-2.723757	-0.479003	9.545502
H	-0.953505	-2.008016	10.486301
H	1.318263	-0.982179	11.144783
H	-2.409730	12.578856	10.116710
H	4.085634	8.425110	12.341453
H	2.044903	4.575170	12.597366
H	1.947584	8.858092	9.066357
H	3.634646	9.033553	9.684707
H	2.744183	10.491574	9.107725
H	4.132502	5.998941	13.042125
H	-4.253706	3.508868	7.490678
C	-3.135834	0.955816	7.185512
H	-4.230059	3.224383	10.258744
H	-2.644737	3.241103	11.121245
H	-3.635085	1.725212	11.069546
C	-4.255626	0.186941	6.517333
H	-2.243414	0.295855	7.300762
H	-2.812486	1.797189	6.526154
C	-3.982398	-0.496032	5.316644
C	-4.988718	-1.211681	4.642957
C	-6.279214	-1.221045	5.215729
C	-6.587440	-0.551799	6.416019
C	-5.550355	0.155043	7.059905
C	-4.731420	-1.974574	3.326282
C	-3.267615	-1.859571	2.860925
H	-2.561333	-2.280345	3.605159
H	-2.975555	-0.808068	2.663926
H	-3.128007	-2.423929	1.916670
C	-5.057303	-3.473549	3.530105
H	-4.887868	-4.038335	2.589659
H	-6.112666	-3.631636	3.829494
H	-4.414334	-3.917517	4.317220
C	-5.639648	-1.396479	2.214628
H	-5.475352	-1.937170	1.259170
H	-5.423317	-0.322456	2.042510
H	-6.714367	-1.486274	2.469893
C	-8.022735	-0.610519	6.981233
C	-9.006667	-0.016794	5.944873
H	-8.759534	1.041073	5.721698
H	-10.046250	-0.051863	6.332591
H	-8.987587	-0.575730	4.987956
C	-8.402382	-2.083540	7.265505
H	-8.362501	-2.705208	6.348788
H	-9.434176	-2.146987	7.670057
H	-7.714446	-2.535736	8.008663
C	-8.164083	0.186090	8.291995
H	-7.928747	1.260454	8.151506
H	-7.503074	-0.208123	9.090127
H	-9.207545	0.119798	8.661693
H	-7.077603	-1.778039	4.701238
H	-2.960396	-0.462163	4.910598
H	-5.728706	0.691793	7.999412
C	4.000781	11.647958	13.672333
H	2.668120	9.943318	13.692763
H	1.901133	11.472163	13.185100
C	5.241649	11.702493	13.016880
C	6.327622	12.402681	13.581904
C	6.124250	13.040083	14.821795

C	4.890216	13.008528	15.506442
C	3.831197	12.301930	14.907275
H	2.848803	12.253631	15.399919
H	6.962303	13.592464	15.274604
H	5.337320	11.195200	12.049119
C	7.704554	12.489820	12.889697
C	7.735745	11.717070	11.557677
H	7.003775	12.117846	10.827632
H	7.524050	10.637948	11.699747
H	8.741687	11.800189	11.098471
C	8.036988	13.972689	12.597539
H	7.276944	14.426503	11.929369
H	9.025510	14.057455	12.099712
H	8.074982	14.579138	13.524539
C	8.786263	11.892847	13.821375
H	8.575957	10.826989	14.044452
H	8.845676	12.432830	14.787416
H	9.785940	11.952080	13.342673
C	4.744037	13.745154	16.854792
C	3.333702	13.591051	17.454696
H	2.551647	14.010004	16.789326
H	3.274356	14.136172	18.418357
H	3.082323	12.530304	17.658400
C	5.765622	13.171149	17.865519
H	6.809803	13.294004	17.514797
H	5.592633	12.088896	18.034929
H	5.677351	13.690231	18.842639
C	5.018278	15.253566	16.644412
H	4.296433	15.693151	15.926249
H	6.038061	15.438716	16.251734
H	4.924081	15.802205	17.604731
Cl	1.756268	2.874358	7.447652
C	3.280576	3.711304	7.984153
Cl	4.601900	3.504726	6.824066
H	3.014593	4.777658	8.090363
H	3.536414	3.267838	8.963556

1d$_2$(dcm), 2 · S =1

Ni	-0.363912	7.906482	10.411381
N	0.206009	9.822582	10.399630
N	1.225439	7.338273	11.524165
O	-2.079739	8.609563	9.769353
O	-1.054156	6.064765	11.004136
C	-0.813986	10.614929	9.990612
C	1.382978	10.345962	10.793858
C	2.344008	8.047236	11.765336
C	1.131405	6.044974	11.926600
C	-2.111008	9.896677	9.587550
C	-0.129340	5.329401	11.475387
C	-0.691146	12.006765	9.948050
C	1.570688	11.743899	10.771764
C	2.589481	9.427752	11.104306
C	3.409358	7.461665	12.484079
C	2.155994	5.398907	12.623775
O	-3.047553	10.568575	9.156360
O	-0.149087	4.061866	11.520824
C	0.524377	12.576437	10.349208
C	3.274671	9.134712	9.748831
O	3.543000	10.157743	11.879422
C	3.309292	6.135851	12.923641
Ni	0.544445	3.361036	9.642795
C	3.147117	10.530417	13.197535
N	-1.062057	4.050387	8.636772
N	-0.201936	1.523866	9.855404
O	1.299853	5.219123	9.098026
O	2.195350	2.562847	10.429531
C	-0.897952	5.325838	8.203208
C	-2.222146	3.403407	8.424881
C	-1.435293	1.090050	9.536788
C	0.737285	0.678229	10.341079
C	0.393796	5.986530	8.644398
C	2.104864	1.287955	10.677786
C	-1.885030	6.009528	7.489219
C	-3.250822	4.025354	7.682198
C	-2.561065	2.083368	9.163835
C	-1.765471	-0.271284	9.706317
C	0.473549	-0.682150	10.527330
O	0.462124	7.257022	8.610788
O	2.985386	0.553657	11.125617
C	-3.074567	5.327447	7.200941
O	-3.576337	1.385883	8.439002
C	-3.207157	2.517358	10.501789
C	-0.801067	-1.161525	10.198415
H	2.541381	12.160738	11.072422
H	0.667435	13.667973	10.330239
H	-3.879799	5.821733	6.636979
H	-1.715305	7.058591	7.213044
H	-2.783448	-0.607640	9.467044
H	-1.053784	-2.224832	10.331769
H	1.281520	-1.310525	10.928559
H	-1.556314	12.588012	9.597924
H	4.321732	8.049870	12.652739
H	2.040622	4.335274	12.872853
H	2.590228	8.542217	9.109802
H	4.204026	8.557668	9.920468
H	3.526516	10.088023	9.244714
H	4.144187	5.670805	13.469408
H	-4.195856	3.487116	7.528101
C	-3.217047	0.894808	7.150573
H	-4.080980	3.167319	10.301833
H	-2.463814	3.081032	11.099844
H	-3.539040	1.622622	11.063540
C	-4.395178	0.191211	6.511365
H	-2.353478	0.191764	7.221725
H	-2.877661	1.732618	6.494512
C	-4.196076	-0.484976	5.292561
C	-5.257734	-1.142514	4.645004
C	-6.526909	-1.098867	5.261992
C	-6.761341	-0.434782	6.481826
C	-5.670270	0.212022	7.099074
C	-5.079809	-1.902235	3.313332
C	-3.632769	-1.831819	2.790216
H	-2.912104	-2.284828	3.501014
H	-3.313030	-0.788505	2.592685
H	-3.550743	-2.389915	1.835604
C	-5.446604	-3.391089	3.522141
H	-5.329181	-3.955554	2.573598
H	-6.494999	-3.516516	3.859064
H	-4.790257	-3.859689	4.283486
C	-6.012290	-1.286769	2.242794
H	-5.903086	-1.824937	1.278159
H	-5.768906	-0.218798	2.069216
H	-7.078576	-1.344671	2.539448
C	-8.177517	-0.435012	7.096013
C	-9.166961	0.218699	6.102016
H	-8.877654	1.266826	5.883474
H	-10.193195	0.227081	6.525053

H	-9.206879	-0.326936	5.138110
C	-8.614996	-1.892778	7.375018
H	-8.634927	-2.503668	6.450365
H	-9.634440	-1.914311	7.813787
H	-7.924284	-2.385746	8.089151
C	-8.237256	0.348417	8.420852
H	-7.956467	1.412549	8.286152
H	-7.569997	-0.087694	9.191540
H	-9.269970	0.325947	8.824445
H	-7.368736	-1.609246	4.768609
H	-3.188084	-0.493279	4.851824
H	-5.790316	0.740643	8.052473
C	4.118313	11.538466	13.775029
H	3.099685	9.632612	13.859508
H	2.118416	10.962132	13.192717
C	5.258956	11.949435	13.067085
C	6.156486	12.885325	13.623012
C	5.867962	13.390320	14.905681
C	4.730781	12.998826	15.645417
C	3.861943	12.062425	15.056388
H	2.963066	11.726063	15.594144
H	6.559605	14.120837	15.352869
H	5.431636	11.519358	12.073140
C	7.425812	13.356334	12.881396
C	7.559079	12.713096	11.488270
H	6.701544	12.964988	10.831964
H	7.634094	11.608424	11.546436
H	8.478576	13.082651	10.990751
C	7.378856	14.892702	12.703185
H	6.494634	15.198469	12.107540
H	8.287834	15.249245	12.175157
H	7.328746	15.422381	13.675577
C	8.672669	12.972721	13.714274
H	8.733723	11.874359	13.855059
H	8.658250	13.440235	14.719085
H	9.599741	13.305455	13.202333
C	4.482247	13.598446	17.045675
C	3.197661	13.050339	17.694805
H	2.295708	13.288865	17.095223
H	3.058496	13.505073	18.696514
H	3.239227	11.950822	17.833267
C	5.676345	13.255461	17.968307
H	6.630882	13.662317	17.578901
H	5.796284	12.157885	18.072680
H	5.518784	13.681648	18.980988
C	4.346949	15.135536	16.927504
H	3.494761	15.410613	16.273189
H	5.259686	15.600737	16.504544
H	4.172410	15.587244	17.926335
Cl	1.727719	2.587525	7.258608
C	3.333908	3.303833	7.725421
Cl	4.624925	2.842010	6.606527
H	3.193888	4.398054	7.716022
H	3.537515	2.932752	8.747868

1d$_2$(dcm)$_2$, 2 · S =1

Ni	0.210782	8.238747	10.831656
N	1.000546	10.062773	10.653758
N	1.821010	7.480537	11.785313
O	-1.428865	9.097229	10.085820
O	-0.583065	6.398295	11.350555
C	0.073229	10.944617	10.211570
C	2.244379	10.461102	10.979034
C	3.001133	8.091845	11.992473
C	1.632926	6.195779	12.180120
C	-1.309850	10.375118	9.867352
C	0.308839	5.585110	11.759610
C	0.361011	12.306128	10.076617
C	2.597558	11.822480	10.864545
C	3.355214	9.431270	11.297555
C	4.030831	7.419744	12.688096
C	2.619268	5.463587	12.846307
O	-2.175291	11.140533	9.442737
O	0.196646	4.322635	11.768064
C	1.645900	12.749000	10.416381
C	3.971526	9.035679	9.933799
O	4.395311	10.082079	12.029995
C	3.832608	6.105753	13.127758
Ni	0.849630	3.641916	9.859504
C	4.067314	10.527550	13.343904
N	-0.760628	4.400038	8.905911
N	0.059942	1.817860	10.037552
O	1.643415	5.482391	9.340678
O	2.489296	2.783515	10.605467
C	-0.572573	5.684792	8.511068
C	-1.940718	3.788677	8.698718
C	-1.183891	1.419493	9.712318
C	0.987246	0.936085	10.479889
C	0.751478	6.295523	8.931594
C	2.370282	1.505654	10.824134
C	-1.558916	6.416930	7.844826
C	-2.970409	4.460718	8.003026
C	-2.294757	2.449259	9.393669
C	-1.537060	0.058125	9.826960
C	0.699469	-0.425415	10.614999
O	0.863610	7.558010	8.923120
O	3.235678	0.740338	11.249023
C	-2.772218	5.774705	7.563339
O	-3.334745	1.798353	8.661163
C	-2.911210	2.844857	10.757361
C	-0.585403	-0.868337	10.275248
H	3.621659	12.132584	11.112676
H	-3.577063	6.307363	7.034553
H	-1.367661	7.470244	7.599778
H	-2.561162	-0.252008	9.578867
H	-0.855993	-1.931775	10.365430
H	1.498457	-1.083832	10.984823
H	4.991810	7.930242	12.838388
H	2.427982	4.410272	13.091328
H	3.209132	8.503888	9.330351
H	4.840425	8.368874	10.096854
H	4.306251	9.944407	9.396772
H	4.637454	5.573047	13.656494
H	-3.931362	3.950183	7.852705
C	-3.006605	1.352856	7.347302
H	-3.780127	3.511613	10.594202
H	-2.148900	3.376704	11.360867
H	-3.245942	1.936126	11.294379
C	-4.149400	0.547441	6.766837
H	-2.078303	0.734366	7.359431
H	-2.786805	2.224713	6.684623
C	-3.955468	-0.109997	5.536943
C	-4.989034	-0.855488	4.941129
C	-6.224081	-0.920853	5.622136
C	-6.452178	-0.278270	6.854667
C	-5.390749	0.460997	7.417355
C	-4.816919	-1.595482	3.597716

C	-3.408036	-1.408197	3.003868
H	-2.618873	-1.801699	3.676304
H	-3.183483	-0.342596	2.794290
H	-3.329041	-1.957909	2.044196
C	-5.053134	-3.109472	3.814121
H	-4.942763	-3.659720	2.856438
H	-6.068825	-3.318926	4.205202
H	-4.321958	-3.527323	4.535793
C	-5.848119	-1.053352	2.579108
H	-5.742673	-1.576034	1.605573
H	-5.701404	0.031866	2.403832
H	-6.890371	-1.199857	2.926517
C	-7.829022	-0.400167	7.541822
C	-8.923949	0.156856	6.600897
H	-8.743849	1.226474	6.369663
H	-9.923664	0.072328	7.075862
H	-8.963017	-0.392891	5.639337
C	-8.119184	-1.889782	7.844727
H	-8.136035	-2.504011	6.922253
H	-9.106600	-1.999866	8.339896
H	-7.348343	-2.316123	8.518606
C	-7.888654	0.382374	8.867158
H	-7.707638	1.465926	8.716926
H	-7.147971	0.009540	9.603247
H	-8.893530	0.273398	9.323403
H	-7.042569	-1.502934	5.170759
H	-2.973884	-0.033257	5.046130
H	-5.508271	0.981550	8.375386
C	5.210058	11.333202	13.924134
H	3.847811	9.655664	14.006644
H	3.138886	11.145853	13.331925
C	6.451370	11.419597	13.273539
C	7.512775	12.159051	13.836023
C	7.284699	12.801854	15.068445
C	6.049685	12.736559	15.749517
C	5.016138	11.990879	15.153903
H	4.034583	11.914173	15.644776
H	8.103184	13.384040	15.519690
H	6.568886	10.898847	12.315614
C	8.889597	12.280851	13.148812
C	8.949263	11.497919	11.823709
H	8.208585	11.870522	11.087497
H	8.768262	10.414408	11.974257
H	9.954144	11.606774	11.367446
C	9.179653	13.770397	12.845461
H	8.408788	14.196480	12.171447
H	10.167066	13.880403	12.350268
H	9.196455	14.384905	13.767748
C	9.984571	11.724184	14.089893
H	9.804556	10.654619	14.321437
H	10.023596	12.274216	15.051294
H	10.984279	11.808655	13.614902
C	5.877629	13.476740	17.092833
C	4.468858	13.289328	17.686908
H	3.679537	13.682569	17.014503
H	4.389896	13.839206	18.646488
H	4.244512	12.223730	17.896718
C	6.909062	12.934911	18.111367
H	7.951236	13.081461	17.763738
H	6.762493	11.849711	18.286872
H	6.803729	13.457767	19.084820
C	6.113588	14.990734	16.876185
H	5.382247	15.408382	16.154562
H	7.129192	15.200291	16.484934
H	6.003273	15.541095	17.833809
H	-0.437985	12.964603	9.706917
H	1.916501	13.812444	10.326310
Cl	-0.899004	9.006463	13.247349
C	-2.528015	8.327469	12.802950
Cl	-3.780632	8.769309	13.972095
Cl	1.959305	2.874462	7.444077
C	3.588419	3.553438	7.888249
Cl	4.841001	3.110923	6.719336
H	-2.401532	7.232001	12.771905
H	-2.754931	8.733770	11.799216
H	3.815219	3.147487	8.892154
H	3.462090	4.648930	7.918805

1d$_2$(py)(dcm), 2 · S =1

Ni	0.234806	8.235335	10.811011
N	0.999124	10.074742	10.663064
N	1.844906	7.495235	11.779054
O	-1.411946	9.085468	10.056140
O	-0.546247	6.397875	11.321640
C	0.062732	10.950590	10.228057
C	2.233716	10.486894	11.006820
C	3.018010	8.116892	11.995881
C	1.669049	6.204334	12.157753
C	-1.308476	10.366967	9.859543
C	0.349219	5.580516	11.734143
C	0.330552	12.318671	10.119956
C	2.566940	11.855337	10.919387
C	3.356852	9.467396	11.315423
C	4.053380	7.448833	12.685814
C	2.662578	5.475519	12.817714
O	-2.179225	11.128939	9.437004
O	0.243274	4.325825	11.743685
C	1.605164	12.775327	10.479246
C	3.979411	9.095163	9.948345
O	4.388796	10.124490	12.055944
C	3.867869	6.127218	13.109234
Ni	1.028622	3.602706	9.738849
C	4.056737	10.547692	13.375562
N	-0.644234	4.378934	8.894635
N	0.196050	1.817261	10.083530
O	1.749909	5.509202	9.326446
O	2.607404	2.813481	10.712089
C	-0.478940	5.670714	8.513020
C	-1.827975	3.762843	8.719936
C	-1.049528	1.409482	9.776704
C	1.110827	0.959591	10.594278
C	0.841892	6.301516	8.925924
C	2.478154	1.551087	10.979598
C	-1.488339	6.398767	7.875576
C	-2.877595	4.427871	8.047468
C	-2.164353	2.430335	9.439144
C	-1.408173	0.055262	9.949678
C	0.815186	-0.393127	10.793397
O	0.922585	7.569198	8.921483
O	3.309932	0.804198	11.500573
C	-2.698966	5.745506	7.609025
O	-3.210312	1.761138	8.727014
C	-2.770310	2.849599	10.800428
C	-0.462908	-0.851876	10.448736
H	3.584335	12.176228	11.180712
H	-3.518747	6.273649	7.098809
H	-1.315565	7.458457	7.644452

H	-2.432843	-0.262473	9.712977
H	-0.736580	-1.909945	10.583427
H	1.603198	-1.030197	11.220075
H	5.008582	7.967547	12.844532
H	2.482189	4.416615	13.045910
H	3.225268	8.556861	9.340043
H	4.857136	8.438820	10.106356
H	4.301166	10.014120	9.420626
H	4.677421	5.596594	13.633058
H	-3.837844	3.910578	7.915595
C	-2.891134	1.291871	7.423478
H	-3.643312	3.509962	10.632793
H	-2.001464	3.396488	11.382793
H	-3.095412	1.950018	11.358473
C	-4.063069	0.535339	6.834231
H	-1.993884	0.627904	7.450490
H	-2.626655	2.148040	6.754880
C	-3.892969	-0.119266	5.599487
C	-4.952013	-0.823447	4.998319
C	-6.188501	-0.849870	5.679280
C	-6.393429	-0.208500	6.916566
C	-5.306336	0.488151	7.484655
C	-4.805225	-1.561388	3.650671
C	-3.394253	-1.408884	3.051776
H	-2.613322	-1.827872	3.718499
H	-3.142655	-0.348138	2.847719
H	-3.334429	-1.954751	2.088494
C	-5.080305	-3.069460	3.862169
H	-4.986441	-3.619371	2.902470
H	-6.100244	-3.253072	4.255045
H	-4.359146	-3.508674	4.581229
C	-5.825120	-0.988076	2.637890
H	-5.736189	-1.508167	1.661298
H	-5.651721	0.094058	2.467913
H	-6.869672	-1.109994	2.987650
C	-7.773455	-0.287129	7.603680
C	-8.848558	0.314417	6.667352
H	-8.631384	1.378734	6.443559
H	-9.850239	0.261521	7.142672
H	-8.907519	-0.226822	5.701937
C	-8.115017	-1.767793	7.896480
H	-8.152965	-2.375419	6.970208
H	-9.105762	-1.846557	8.390915
H	-7.359896	-2.224804	8.568060
C	-7.805163	0.487582	8.934557
H	-7.587110	1.565276	8.791946
H	-7.077442	0.084131	9.667321
H	-8.813023	0.409892	9.390589
H	-7.027393	-1.399315	5.224378
H	-2.909185	-0.073907	5.108980
H	-5.403810	1.004903	8.446986
C	5.191404	11.357985	13.965186
H	3.848336	9.664487	14.026743
H	3.121410	11.155577	13.374014
C	6.437720	11.447949	13.324460
C	7.493375	12.188489	13.895965
C	7.254748	12.829652	15.127286
C	6.014502	12.761259	15.798429
C	4.986965	12.014317	15.193981
H	4.001670	11.935273	15.676915
H	8.068602	13.412789	15.585740
H	6.562543	10.929082	12.366417
C	8.875481	12.313318	13.219963
C	8.947675	11.530107	11.895596
H	8.212380	11.901040	11.153197
H	8.766878	10.446432	12.045155
H	9.956253	11.640537	11.447773
C	9.164831	13.803394	12.918576
H	8.398686	14.227443	12.237939
H	10.156286	13.915800	12.431933
H	9.171933	14.418006	13.840917
C	9.964198	11.759327	14.169802
H	9.784519	10.689460	14.400220
H	9.994285	12.309629	15.131369
H	10.967570	11.845908	13.702841
C	5.830840	13.499860	17.141106
C	4.417676	13.309979	17.723834
H	3.633239	13.702876	17.045573
H	4.330264	13.858549	18.683484
H	4.193042	12.243821	17.930323
C	6.854869	12.958265	18.167179
H	7.899480	13.105714	17.827291
H	6.707745	11.872837	18.340771
H	6.741826	13.480405	19.140193
C	6.066609	15.014401	16.928086
H	5.340291	15.431905	16.201312
H	7.084886	15.225484	16.544635
H	5.948426	15.563704	17.885421
N	1.916801	3.012186	7.933780
C	3.258905	3.139782	7.861702
C	1.239838	2.600042	6.845257
C	3.969049	2.860150	6.686790
C	3.266801	2.432012	5.551009
C	1.872918	2.296657	5.633328
H	1.277042	1.961780	4.771675
H	0.146368	2.513383	6.952980
H	3.754075	3.452037	8.794238
H	3.798035	2.204331	4.614157
H	5.062489	2.976336	6.672774
H	-0.475618	12.970661	9.754366
H	1.860191	13.844269	10.410526
Cl	-0.934431	8.998614	13.241500
C	-2.526434	8.269632	12.755175
Cl	-3.798479	8.572723	13.950686
H	-2.344082	7.186366	12.652119
H	-2.780386	8.723516	11.779397

1d$_2$(py), S = 1 + S = 0

Ni	1.814242	2.022876	0.028183
N	3.256551	2.700751	-0.916677
N	2.594200	0.392841	0.499823
O	0.965474	3.647758	-0.288701
O	0.339668	1.475161	1.052223
C	3.061639	4.002626	-1.276962
C	4.411435	2.073726	-1.236188
C	3.791141	-0.098155	0.113517
C	1.781096	-0.356173	1.302028
C	1.692257	4.541204	-0.914794
C	0.433059	0.270220	1.516225
C	4.032509	4.744798	-1.943860
C	5.427316	2.776650	-1.914518
C	4.579730	0.559484	-1.031299
C	4.237494	-1.338542	0.611131
C	2.153772	-1.602151	1.802301
O	1.349422	5.680967	-1.207867
O	-0.508643	-0.359556	2.041552
C	5.247915	4.121534	-2.261293
C	4.086857	-0.121408	-2.331639

O	5.967885	0.245803	-0.915560
C	3.425474	-2.088266	1.471006
Ni	-1.407105	-1.651085	0.409536
C	6.644220	0.754082	0.232337
N	-2.209412	0.028926	-0.383091
N	-2.967817	-1.984733	1.623541
O	0.146591	-1.162753	-0.848194
O	-0.619309	-3.258620	1.355605
C	-1.419836	0.560868	-1.348544
C	-3.380972	0.609379	-0.058267
C	-4.092403	-1.255633	1.748774
C	-2.815438	-3.157938	2.282820
C	-0.055829	-0.103209	-1.552422
C	-1.455007	-3.862835	2.142367
C	-1.793351	1.698723	-2.069793
C	-3.824875	1.748534	-0.764459
C	-4.174607	0.193980	1.208150
C	-5.155996	-1.734182	2.544526
C	-3.830738	-3.683716	3.088789
O	0.756217	0.448480	-2.318980
O	-1.269169	-4.902794	2.779379
C	-3.030597	2.288305	-1.783839
O	-5.553338	0.545342	1.033370
C	-3.645137	1.099660	2.345015
C	-5.026636	-2.963284	3.205998
H	6.346701	2.233779	-2.174291
H	6.045291	4.668469	-2.786762
H	-3.366480	3.183826	-2.328590
H	-1.088155	2.093913	-2.813653
H	-6.061718	-1.121617	2.651611
H	-5.854148	-3.342500	3.825706
H	-3.634336	-4.636913	3.600326
H	3.790584	5.787828	-2.195980
H	5.215102	-1.713211	0.277550
H	1.418722	-2.177008	2.384040
H	2.992458	0.031914	-2.450870
H	4.292207	-1.207929	-2.269808
H	4.627729	0.300231	-3.201353
H	3.768279	-3.063625	1.847331
H	-4.777818	2.214833	-0.479358
C	-6.262021	-0.154505	0.019782
H	-3.762543	2.163432	2.060769
H	-2.570854	0.883899	2.509749
H	-4.213938	0.905031	3.275160
C	-7.706860	0.296660	-0.021108
H	-6.219660	-1.256413	0.196774
H	-5.789993	0.019837	-0.978485
C	-8.599445	-0.369724	-0.882300
C	-9.948275	0.018942	-0.973179
C	-10.372790	1.098344	-0.168143
C	-9.508362	1.786074	0.705732
C	-8.163098	1.366115	0.765868
C	-10.959888	-0.684807	-1.902353
C	-10.317472	-1.834399	-2.701308
H	-9.907914	-2.622507	-2.037195
H	-9.499090	-1.475951	-3.358418
H	-11.078675	-2.312025	-3.351008
C	-12.113255	-1.271557	-1.053801
H	-12.858108	-1.773698	-1.705931
H	-12.645832	-0.486969	-0.480138
H	-11.733539	-2.019138	-0.327831
C	-11.531578	0.342912	-2.908190
H	-12.267294	-0.142373	-3.583076
H	-10.725831	0.777715	-3.534035
H	-12.047587	1.179463	-2.396236
C	-10.047736	2.955900	1.556117
C	-10.611622	4.052720	0.621510
H	-9.823746	4.444303	-0.053653
H	-11.007473	4.902552	1.215891
H	-11.438892	3.673187	-0.011007
C	-11.175451	2.438956	2.481293
H	-12.019229	2.009317	1.905029
H	-11.578781	3.267001	3.100934
H	-10.799417	1.651045	3.165255
C	-8.952690	3.587978	2.435865
H	-8.120418	3.999566	1.829880
H	-8.525646	2.859565	3.154447
H	-9.380093	4.424435	3.025380
H	-11.426158	1.413999	-0.225994
H	-8.222858	-1.207825	-1.487735
H	-7.442912	1.860768	1.428621
C	8.084953	0.290697	0.235601
H	6.135388	0.409687	1.165340
H	6.606873	1.869030	0.253573
C	8.524366	-0.738619	-0.612793
C	9.862050	-1.183700	-0.577558
C	10.737025	-0.562804	0.335578
C	10.330399	0.476210	1.200355
C	8.988219	0.892774	1.131948
H	8.625793	1.702677	1.782290
H	11.785220	-0.898075	0.373988
H	7.799353	-1.177329	-1.309178
C	10.383055	-2.308949	-1.496749
C	9.275859	-2.877647	-2.404130
H	8.856022	-2.106140	-3.080797
H	8.440858	-3.310103	-1.816564
H	9.689283	-3.687033	-3.039618
C	11.510603	-1.751709	-2.398425
H	11.138699	-0.921466	-3.032796
H	11.901024	-2.546649	-3.067738
H	12.362248	-1.364892	-1.803842
C	10.939496	-3.464101	-0.630506
H	10.150159	-3.887496	0.023491
H	11.771956	-3.130566	0.020725
H	11.325580	-4.281158	-1.275117
C	11.354202	1.113812	2.163267
C	10.728657	2.222420	3.030668
H	10.326338	3.052926	2.415667
H	11.498212	2.652043	3.703455
H	9.908308	1.836911	3.669604
C	11.919839	0.023549	3.104554
H	12.426214	-0.786732	2.542904
H	11.112380	-0.439067	3.707796
H	12.662597	0.461930	3.803280
C	12.508780	1.735640	1.341640
H	12.131943	2.525812	0.660684
H	13.030683	0.979170	0.722085
H	13.261974	2.194141	2.015917
N	-2.083463	-2.931202	-1.093589
C	-1.225146	-3.903931	-1.467004
C	-3.256426	-2.808818	-1.743262
C	-1.516977	-4.789910	-2.512164
C	-2.737359	-4.664908	-3.191535
C	-3.626436	-3.654046	-2.797026
H	-4.596482	-3.515791	-3.296571
H	-3.922196	-1.998954	-1.403147
H	-0.296184	-3.964868	-0.880157
H	-2.993889	-5.346808	-4.016750

H	-0.789553	-5.569053	-2.782474

$1d_2$(py), 2 · S = 1

Ni	-0.398470	7.934779	10.374335
N	0.187407	9.847294	10.376612
N	1.183988	7.347264	11.487630
O	-2.102193	8.661690	9.703206
O	-1.111980	6.111442	10.956533
C	-0.823158	10.652309	9.968783
C	1.365003	10.358190	10.786375
C	2.309745	8.042493	11.734623
C	1.077310	6.049911	11.871905
C	-2.120294	9.949575	9.537599
C	-0.196853	5.350807	11.422660
C	-0.691082	12.043974	9.946926
C	1.561561	11.755121	10.785799
C	2.564622	9.427567	11.087512
C	3.370885	7.438610	12.443337
C	2.098104	5.385235	12.557864
O	-3.043083	10.637356	9.099023
O	-0.239066	4.091856	11.464739
C	0.523813	12.600478	10.367380
C	3.246776	9.144231	9.728717
O	3.524325	10.144262	11.869471
C	3.258423	6.107501	12.864859
Ni	0.586352	3.342681	9.501630
C	3.132710	10.503078	13.191975
N	-1.074900	4.074458	8.599774
N	-0.230922	1.557452	9.878147
O	1.293045	5.255079	9.055351
O	2.156837	2.599419	10.523992
C	-0.917455	5.356087	8.182438
C	-2.247518	3.439436	8.419170
C	-1.467556	1.128844	9.564767
C	0.681323	0.726909	10.436028
C	0.381882	6.016749	8.613236
C	2.035802	1.344198	10.826548
C	-1.920017	6.051755	7.500558
C	-3.289779	4.071367	7.704220
C	-2.585130	2.126055	9.172361
C	-1.818288	-0.221491	9.779732
C	0.393124	-0.620503	10.677655
O	0.438997	7.290015	8.583310
O	2.866051	0.621921	11.383564
C	-3.117013	5.376290	7.228464
O	-3.607591	1.423446	8.457487
C	-3.224822	2.580622	10.506444
C	-0.874942	-1.102185	10.327217
H	2.532794	12.161526	11.098574
H	0.673786	13.691322	10.365771
H	-3.931990	5.879449	6.686617
H	-1.755686	7.105540	7.239445
H	-2.836596	-0.555102	9.537324
H	-1.142656	-2.157024	10.495269
H	1.178370	-1.235138	11.140788
H	-1.549475	12.634587	9.595799
H	4.289136	8.015662	12.618736
H	1.974274	4.318621	12.789391
H	2.557824	8.561367	9.085453
H	4.171956	8.558783	9.894327
H	3.504375	10.100881	9.233649
H	4.090051	5.626924	13.402319
H	-4.241333	3.539321	7.568407
C	-3.251356	0.917788	7.177793
H	-4.095737	3.233002	10.301517
H	-2.472927	3.148611	11.090603
H	-3.558458	1.695099	11.081740
C	-4.426176	0.198649	6.548991
H	-2.383256	0.219783	7.255486
H	-2.923228	1.750508	6.507476
C	-4.224500	-0.500134	5.343642
C	-5.284702	-1.168741	4.705012
C	-6.555368	-1.112878	5.317765
C	-6.792233	-0.427199	6.525214
C	-5.702428	0.230140	7.133395
C	-5.103965	-1.951874	3.387241
C	-3.654580	-1.894940	2.868983
H	-2.938583	-2.337991	3.590809
H	-3.331552	-0.855795	2.655006
H	-3.570360	-2.469517	1.924345
C	-5.476067	-3.435985	3.619007
H	-5.357055	-4.016363	2.680290
H	-6.526045	-3.552212	3.954022
H	-4.824353	-3.894134	4.390628
C	-6.029775	-1.351779	2.302282
H	-5.919074	-1.907107	1.347562
H	-5.782160	-0.287742	2.111294
H	-7.097227	-1.400666	2.596041
C	-8.210065	-0.414834	7.135358
C	-9.193264	0.232302	6.130828
H	-8.898573	1.276686	5.901901
H	-10.220796	0.250000	6.550389
H	-9.232450	-0.323837	5.172850
C	-8.654887	-1.867493	7.428823
H	-8.675824	-2.488558	6.510928
H	-9.675519	-1.879407	7.865097
H	-7.968464	-2.355872	8.150189
C	-8.270060	0.383204	8.451373
H	-7.986556	1.445137	8.305769
H	-7.605052	-0.046053	9.227795
H	-9.303473	0.367730	8.853424
H	-7.396574	-1.631411	4.831848
H	-3.215159	-0.517550	4.906011
H	-5.823547	0.775729	8.077060
C	4.099572	11.513654	13.772454
H	3.095388	9.599675	13.846927
H	2.101047	10.927564	13.196850
C	5.245633	11.920520	13.070792
C	6.140913	12.857042	13.629057
C	5.844853	13.367531	14.907854
C	4.702190	12.980322	15.641367
C	3.835835	12.042976	15.050116
H	2.932633	11.710150	15.582745
H	6.534436	14.099009	15.356713
H	5.422870	11.486604	12.079311
C	7.416041	13.322987	12.894103
C	7.557270	12.674421	11.504218
H	6.704450	12.925365	10.841483
H	7.629444	11.569829	11.567028
H	8.480842	13.040447	11.011517
C	7.373713	14.858747	12.709920
H	6.494158	15.164072	12.107190
H	8.287043	15.211563	12.186797
H	7.318002	15.391956	13.680074
C	8.656699	12.939819	13.736400
H	8.714178	11.841840	13.881681
H	8.636682	13.411012	14.739409
H	9.587927	13.268574	13.229302

C	4.444841	13.586130	17.037469
C	3.155177	13.042296	17.680080
H	2.257693	13.279396	17.073322
H	3.009773	13.501295	18.678999
H	3.194340	11.943297	17.823069
C	5.632060	13.245756	17.969837
H	6.589649	13.650133	17.585331
H	5.750171	12.148494	18.079389
H	5.467818	13.676202	18.979717
C	4.312201	15.122903	16.912231
H	3.464800	15.396246	16.251016
H	5.228350	15.585220	16.493451
H	4.131474	15.578921	17.908048
N	1.525230	2.713414	7.733883
C	2.866447	2.860953	7.687886
C	0.881330	2.247721	6.646848
C	3.608953	2.548452	6.541613
C	2.941156	2.064220	5.407584
C	1.548100	1.908194	5.462860
H	0.978502	1.529207	4.601716
H	-0.212680	2.144905	6.732483
H	3.334553	3.215915	8.619066
H	3.498296	1.808970	4.493143
H	4.700404	2.682579	6.548660

$1d_2(py)_2$, 2 · S = 1

Ni	0.065556	8.269445	10.928387
N	0.885754	10.067966	10.610836
N	1.731993	7.505883	11.795420
O	-1.512777	9.062575	9.943081
O	-0.650969	6.365695	11.326182
C	-0.029772	10.924070	10.098625
C	2.123681	10.483605	10.937918
C	2.909349	8.129094	11.987810
C	1.570953	6.209830	12.163060
C	-1.388462	10.327175	9.690187
C	0.257123	5.568589	11.734774
C	0.256768	12.281436	9.917948
C	2.473122	11.842633	10.783774
C	3.242428	9.468128	11.279483
C	3.956069	7.467315	12.666830
C	2.579195	5.484609	12.806604
O	-2.217639	11.076024	9.165792
O	0.183374	4.308392	11.735150
C	1.526601	12.747381	10.282716
C	3.863634	9.062301	9.921451
O	4.277108	10.142370	12.005771
C	3.781141	6.144563	13.092730
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C	3.942122	10.597976	13.309666
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N	0.171444	1.804544	10.076329
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C	0.800157	6.303918	8.952418
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C	-8.823933	0.278686	6.517793
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C	5.953940	12.737733	15.755356
C	4.906871	12.028044	15.139861
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C	8.882597	11.397362	11.885297
H	8.169459	11.794176	11.134787
H	8.661121	10.321059	12.033071
H	9.899433	11.471052	11.448753
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H	8.429463	14.112891	12.220019
H	10.171774	13.737122	12.434753
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H	9.659609	10.528618	14.400391
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H	10.892096	11.639285	13.714302
C	5.781954	13.485531	17.094554
C	4.359861	13.337668	17.667734
H	3.591901	13.751560	16.983049
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H	4.104131	12.278483	17.874550
C	6.782378	12.919306	18.130446
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H	6.604481	11.838778	18.305827
H	6.676314	13.447409	19.101041
C	6.061637	14.992041	16.877897
H	5.353796	15.426767	16.143032
H	7.088582	15.172436	16.502108
H	5.950929	15.548513	17.832036
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C	3.977743	2.928936	6.733887
C	3.297655	2.489742	5.588783
C	1.906425	2.322419	5.655560
H	1.327481	1.978118	4.786059
H	0.161657	2.493739	6.958337
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C	-0.849416	9.550844	15.031364
C	-2.240594	9.383109	15.098191
C	-2.920552	8.943333	13.953231
C	-2.191419	8.684714	12.785103
H	0.895405	9.379638	13.728616
H	-0.270582	9.895610	15.900757
H	-0.532052	12.915820	9.488753
H	1.792985	13.809149	10.162718
H	-4.011108	8.801662	13.955269
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$1d_2(py)_3$, 2 · S = 1

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O	-1.499353	3.519732	9.833011
C	-1.509269	8.254054	10.376150
C	0.814770	7.894617	10.394472
C	1.983847	5.474614	10.345276
C	0.832133	3.423302	10.330381
C	-2.901537	7.638794	10.148184
C	-0.524925	2.747515	10.131039
C	-1.360490	9.608347	10.694149
C	1.030123	9.254786	10.706821
C	2.055512	7.007934	10.104467
C	3.196377	4.797413	10.601277
C	1.993656	2.694907	10.616593
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O	-0.619381	1.504798	10.279848
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C	3.195195	3.405563	10.745280
Ni	0.249233	-0.360658	9.547527
C	3.109484	7.467598	12.253692
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N	-1.024188	-1.139091	10.924785
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C	-2.488300	-0.573086	8.223081
C	-2.332183	-1.414507	10.777549
C	-0.455788	-1.136404	12.155875
C	0.680800	1.046106	7.135717
C	1.012562	-0.690292	12.249492
C	-1.617625	0.879024	6.017373
C	-3.395712	-0.254924	7.188028
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C	-3.137422	-2.882764	8.925108
O	-4.400214	-0.991654	9.617471
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C	5.220514	8.880727	12.085646
H	5.062710	8.909857	10.998413
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C	5.802597	8.671476	16.413151
C	7.312027	10.315370	11.778483
C	4.725252	7.842448	17.137417
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H	4.708787	6.789294	16.790267
C	7.180618	8.025491	16.693953
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H	8.009446	8.604248	16.239694
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C	5.779329	10.106719	16.991788
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H	9.055782	10.218311	13.130147
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H	6.089910	12.149239	11.732961
H	5.737566	11.017979	10.390587
H	7.238805	11.993443	10.362022
C	7.942109	9.340792	10.754982
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C	-6.589536	3.217770	8.582117
C	-7.746080	2.511826	8.204254
C	-7.889248	1.116559	8.395898
C	-6.826572	0.422422	8.999448
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H	-8.574166	3.063369	7.737736
H	-4.601628	2.983925	9.459901
C	-6.430696	4.739199	8.381219
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H	-8.582537	5.231569	8.264595
H	-7.811878	4.942893	6.667146
C	-5.176986	5.013233	7.515777
H	-5.262871	4.518927	6.525574
H	-4.248594	4.662275	8.005552
H	-5.060295	6.104479	7.353994
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C	-9.374080	0.609946	6.420853
H	-9.435243	1.681630	6.145251
H	-10.308665	0.119504	6.075947
H	-8.526688	0.166606	5.858861
C	-10.394293	1.038969	8.690502
H	-10.490223	2.124235	8.487328
H	-10.292421	0.910731	9.787415
H	-11.341092	0.552881	8.373989
C	-9.169618	-1.094869	8.240136
H	-8.342113	-1.609634	7.711040
H	-10.119563	-1.557140	7.902270
H	-9.064187	-1.302406	9.324192

S2 NMR Spectroscopic Studies of CISSS

Dichloromethane-d_2 was dried over CaH_2 and pyridine-d_5 over 4 Å molecular sieves and were each distilled prior to use. Samples were prepared in an M. Braun Labmaster 130 Glovebox under Ar. In the so-called Evans NMR susceptibility measurements, a regular NMR tube contained the complex at a constant concentration (2.92 mmol·L^{-1}) in dichloromethane-d_2 with 1 % tetramethylsilane and a varying concentration of pyridine. An inserted coaxial tube of smaller diameter containing everything but the complex served as the reference. Due to the difference in the volume susceptibility of the solutions, two resonance lines are obtained for TMS, with the signal for the more paramagnetic solution lying at higher frequencies.[8] The difference of the resonance frequencies Δf between the TMS signals of the sample and the reference was determined at different temperatures (250, 260, 270, 280, 290, 300 K).

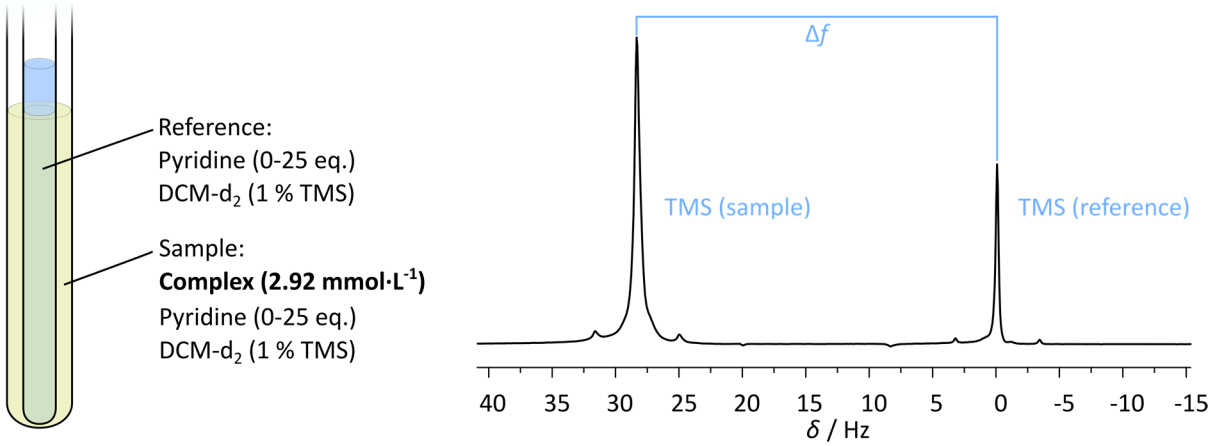

Figure S8. Experimental setup for an Evans NMR susceptibility measurement (left). The inner tube contains the reference with pyridine, TMS, and DCM. The outer tube additionally contains the complex **1d**. This results in two TMS signals in the ^{1}H NMR spectrum whose difference is determined (right).

From these values the mass magnetic susceptibility χ^g_{para} / cm^3·g^{-1} of the complex was calculated.

$$\chi^g_{para} = \frac{3 \cdot \Delta f}{4\pi \cdot f \cdot \rho_{Ni}} - \chi^g_{dia} \qquad \text{(S3)}$$

where $3/4\pi$ is the demagnetization factor for a cylindric sample parallel to the high field of a cryomagnet[9], Δf is difference in the resonance frequencies in Hz, f is the spectrometer frequency ($4 \cdot 10^8$ Hz), ρ_{Ni} is the mass concentration of the complex ($1.6 \cdot 10^{-3}$ g·cm^{-1}), and χ^g_{dia} is the diamagnetic correction for the complex susceptibility which has been calculated from Pascal's constants[10] ($-6.02 \cdot 10^{-7}$ cm^3·g^{-1}). The latter term is not found in the original paper as only completely paramagnetic samples were examined where the paramagnetic susceptibility exceeds the diamagnetic susceptibility in magnitude, thus the latter only has a negligible impact on the measured total susceptibility.[8] Where only partially paramagnetic samples are investigated, it is necessary to take the diamagnetic susceptibility into account.

In the original paper, the equation included two terms for a solvent correction. Grant proved that the mutual omission of these interrelated terms is appropriate for dilute solutions as these terms usually cancel themselves out, thus the error being very small for dilute solutions. The results were more inaccurate if only one term was neglected as had been suggested earlier.[11]

S2.1 Magnetic measurements

The molar magnetic susceptibility χ^m / $cm^3 \cdot mol^{-1}$ is calculated from the mass magnetic susceptibility χ^g_{para} / $cm^3 \cdot g^{-1}$ by multiplication with the molar mass M.

$$\chi^m = \chi^g_{para} \cdot M \tag{S4}$$

In pure pyridine-d_5, complex **1d** is expected to exist as its octahedral bispyridine adduct **1d**(py-d_5)$_2$. Therefore, χ^g_{para} was calculated using $\rho_{Ni} = 2.09 \cdot 10^{-3}$ $g^3 \cdot cm^{-1}$, $\chi^g_{dia} = -6.00 \cdot 10^{-7}$ $cm^3 \cdot g^{-1}$ and χ^m with $M = 715.53$ $g \cdot mol^{-1}$. The effective magnetic moment was calculated from χ^m and varies with temperature (Table S7), thus indicating a deviation from Curie behavior.

$$\mu_{eff} = 2.828 \sqrt{\chi^m \cdot T} \iff \chi^m = \frac{\mu_{eff}^2}{2.828^2} \cdot \frac{1}{T} \tag{S5}$$

Table S7. Results of the Evans NMR measurements of complex **1d** (2.92 $mmol \cdot L^{-1}$) in pyridine-d^5 at different temperatures and conversion into the mass and molar susceptibilities as well as the effective magnetic moment.

T / K	T^{-1} / K^{-1}	Δf / Hz	χ^g_{para} / 10^{-6} $cm^3 \cdot g^{-1}$	χ^m / 10^{-3} $cm^3 \cdot mol^{-1}$	μ_{eff} / μ_B
300	$3.33 \cdot 10^{-3}$	17.68	5.64	4.04	3.11
290	$3.45 \cdot 10^{-3}$	18.51	5.88	4.21	3.12
280	$3.57 \cdot 10^{-3}$	19.25	6.09	4.36	3.12
270	$3.70 \cdot 10^{-3}$	20.35	6.40	4.58	3.15
260	$3.85 \cdot 10^{-3}$	21.43	6.71	4.80	3.16
250	$4.00 \cdot 10^{-3}$	22.54	7.03	5.03	3.17

The linear dependence of the molar susceptibility from the reciprocal temperature in accordance to eq. (S5) was plotted (Figure S9).

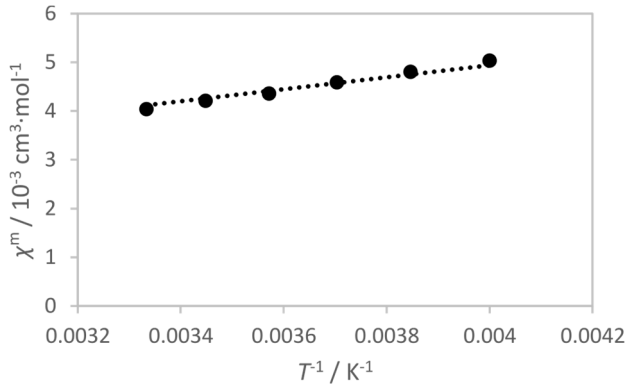

Figure S9. Plot of the molar magnetic susceptibility of complex **1d** (2.92 $mmol \cdot L^{-1}$) in pyridine-d^5 as a function of the reciprocal temperature.

The formula for the fitted straight line is:

$$\chi^m = 1234.4 \cdot \frac{1}{T} \tag{S6}$$

The effective magnetic moment μ_{eff} was calculated from the slope to be 3.14 μ_B.

S2.2 Titration Curves

A quantity of approximately 0.8 mg of complex **1d** was weighed precisely. The respective equivalents of pyridine-d_5 were added and as much DCM-d_2 (1 % TMS) so that always the same complex concentration of 2.92 mmol·L^{-1} was obtained (a total volume of approximately 0.5 mL). The insert was provided with a solution of same equivalents of pyridine-d_5 in DCM-d_2 (1 % TMS).

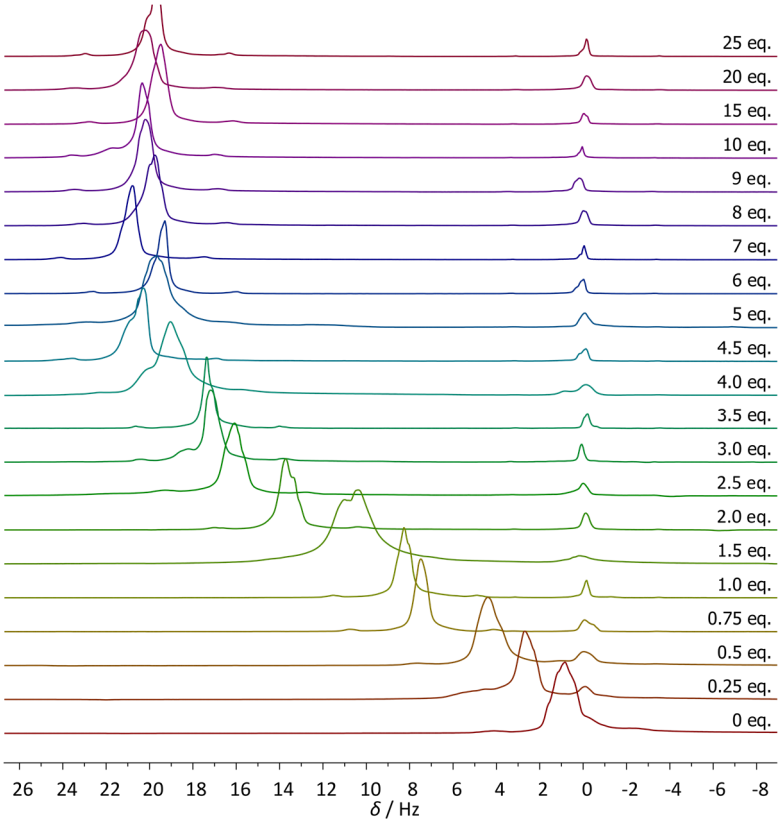

Figure S10. ^{1}H NMR spectra for complex **1d** in DCM-d_2 with different equivalents of pyridine at 300 K.

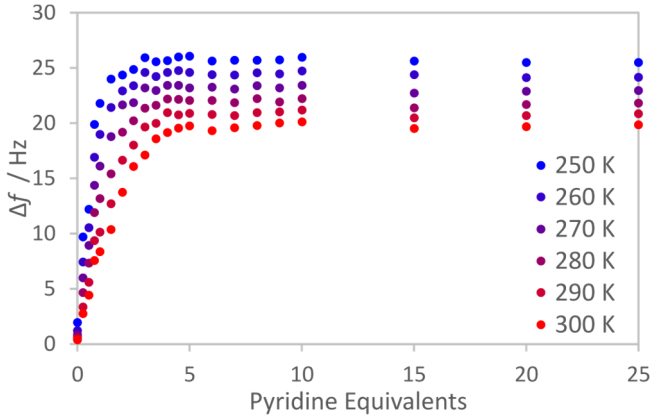

Figure S11. Titration curves for complex **1d** in DCM-d_2 with pyridine at different temperatures.

Table S8. Measured differences of resonance frequencies Δ*f* and mole fraction x_{para} of paramagnetic species for the titration of complex **1d** in DCM-d_2 with pyridine.

eq. Py	Δ*f* / Hz						x_{para}					
	300 K	290 K	280 K	270 K	260 K	250 K	300 K	290 K	280 K	270 K	260 K	250 K
0	0.37	0.50	0.66	0.86	1.23	1.94	0.09	0.09	0.10	0.10	0.11	0.13
0.25	2.77	3.35	4.65	5.98	7.43	9.70	0.20	0.22	0.26	0.30	0.34	0.41
0.5	4.42	5.61	7.34	8.94	10.53	12.20	0.28	0.32	0.38	0.42	0.46	0.50
0.75	7.55	9.37	11.89	14.37	16.92	19.88	0.42	0.48	0.57	0.64	0.70	0.78
1	8.38	10.14	13.18	16.10	19.00	21.80	0.46	0.52	0.62	0.71	0.78	0.85
1.5	10.36	12.71	15.40	18.79	21.42	24.00	0.55	0.63	0.71	0.81	0.87	0.93
2	13.75	16.66	19.17	21.66	22.93	24.37	0.71	0.80	0.87	0.93	0.93	0.94
2.5	16.07	18.01	20.22	21.84	23.40	24.87	0.81	0.86	0.92	0.94	0.95	0.96
3	17.10	19.64	21.37	23.18	24.58	25.94	0.86	0.93	0.96	0.99	0.99	1.00
3.5	18.58	19.99	21.63	22.97	24.24	25.56	0.93	0.95	0.97	0.98	0.98	0.99
4	19.16	20.95	22.19	23.41	24.61	25.65	0.96	0.99	1.00	1.00	1.00	0.99
4.5	19.56	20.76	22.17	23.41	24.76	26.00	0.97	0.98	1.00	1.00	1.00	1.00
5	19.75	20.89	22.06	23.18	24.61	26.05	0.98	0.99	0.99	0.99	1.00	1.00
6	19.31	20.78	22.07	23.25	24.38	25.64	0.96	0.98	0.99	0.99	0.99	0.99
7	19.57	20.69	21.84	23.09	24.37	25.71	0.98	0.98	0.98	0.99	0.99	0.99
8	19.77	20.97	22.22	23.40	24.56	25.68	0.98	0.99	1.00	1.00	0.99	0.99
9	20.01	21.02	21.93	23.19	24.46	25.74	1.00	0.99	0.99	0.99	0.99	0.99
10	20.11	21.18	22.24	23.44	24.73	25.97	1.00	1.00	1.00	1.00	1.00	1.00
15	19.52	20.48	21.40	22.74	24.38	25.64	0.97	0.97	0.96	0.97	0.99	0.99
20	19.70	20.69	21.68	22.89	24.13	25.51	0.98	0.98	0.98	0.98	0.98	0.98
25	19.85	20.84	21.83	22.95	24.17	25.50	0.99	0.99	0.98	0.98	0.98	0.98

S2.3 Dilution Experiments

A solution of the complex already exhibited modest paramagnetism. It was presumed that a dimerization in analogy to a solid state structure (see chapter S3.3) is the reason. This assumption was supported by DFT calculations (see chapter S1.8). A dilution series of the complex **1d** in DCM-d_2 was conducted to investigate the equilibrium. The shift difference increased with rising complex concentration and lowering the temperature. At some measurements at 300 K, sample and reference signals could not be distinguished anymore.

Table S9. Measured differences of resonance frequencies Δf and mass susceptibilities for a dilution series of complex **1d** in DCM-d_2.

c / mmol·L^{-1}	Δf / Hz						χ^g_{para} / 10^{-6} cm^3·g^{-1}					
	300 K	290 K	280 K	270 K	260 K	250 K	300 K	290 K	280 K	270 K	260 K	250 K
1.46	-	0.25	0.37	0.51	0.63	0.93	-	0.79	0.88	0.98	1.07	1.30
2.19	-	0.30	0.47	0.75	0.92	2.02	-	0.75	0.84	0.97	1.06	1.61
2.92	-	0.49	0.73	1.06	1.42	4.50	-	0.78	0.87	1.00	1.13	2.28
3.65	0.49	0.62	0.8	1.17	1.70	5.66	0.75	0.79	0.84	0.95	1.11	2.29
4.39	0.49	0.62	0.79	1.17	1.80	6.69	0.72	0.76	0.80	0.89	1.05	2.26
5.12	-	0.93	1.20	1.57	3.08	9.43	-	0.80	0.86	0.94	1.26	2.61
5.85	0.90	1.07	1.16	1.91	4.36	11.06	0.77	0.80	0.82	0.96	1.41	2.66

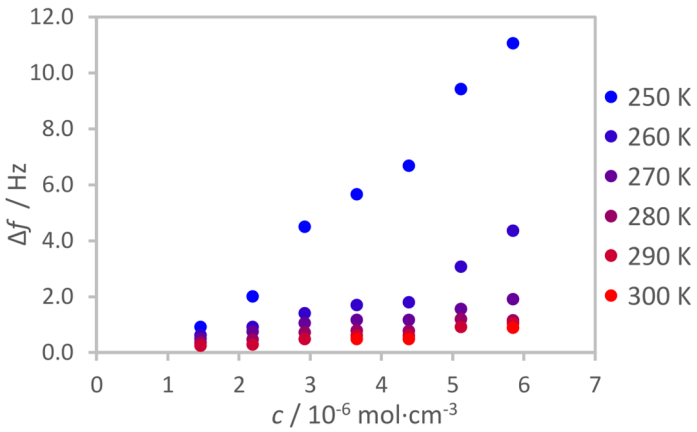

Figure S12. Shift difference as a function of the mass concentration of complex **1d** in DCM-d_2.

S2.4 Evaluation of Equilibria

The Equilibria Speciation Tool (EST) is an Excel utility intended for the calculation of chemical equilibria.[13] It was used to determine the concentration for the occurring species from the titration curves at each titration step (Ni, Ni(py), $Ni(py)_2$ or Ni_2, $Ni_2(py)$, $Ni(py)_2$) and thereof the association constants (K_{1S}, K_2). The equilibria were defined by the stoichiometric coefficients of the contribution species. Furthermore, the initial concentrations of the complex and pyridine ($[Ni]_0$ = 2.92 mmol·L^{-1} or $[Ni_2]_0$ = 1.46 mmol·L^{-1}, $[Py]_0$ here given as equivalents) as well as the measured values ($\chi^g_{para,exp}$) were specified. Considering the contribution of each species to the susceptibility, the program applies nonlinear fitting based on the Newton-Raphson method to calculate susceptibility values ($\chi^g_{para,calc}$) by varying the concentrations of the different species, minimizing the mean square error between measured and calculated values.

Note that equilibrium constants are dimensionless values as they are defined by activities, which are dimensionless as well. To use concentrations instead of activities, the values are formally divided by the standard concentration of 1 mol·L^{-1}.[14]

The change in enthalpy and entropy for the reactions were determined from the temperature-dependent association constants using the van't Hoff equation which is derived from two definitions of the change in the Gibbs free energy.

$$\Delta G = \Delta H - T \cdot \Delta S = -RT \ln K \quad \Leftrightarrow \quad \ln K = -\frac{\Delta H}{R} \cdot \frac{1}{T} + \frac{\Delta S}{R} \tag{S7}$$

S2.4.1 Solvent Coordination Model

Here it is assumed that the intrinsic paramagnetism of the solution is induced by solvent coordination to the square-planar complex Ni. Data evaluation is thus based on the formula

$$\chi^g_{para} = \frac{[Ni] \cdot \chi^g_{para,0} + \left([Ni(py)] + [Ni(py)_2]\right) \cdot \chi^g_{para,max}}{[Ni]_0} \tag{S8}$$

where $\chi^g_{para,0}$ is the susceptibility in the absence of pyridine and $\chi^g_{para,max}$ the highest measured susceptibility.

Table S10. Results for Evans NMR titration experiments of complex **1d** in DCM-d_2 (2.92 mmol·L^{-1}) with pyridine at 300 K and comparison with the values obtained by nonlinear fitting with EST for the solvent coordination model. The mean square error is $0.026 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δf / Hz	$\chi^g_{para,exp}$ / 10^{-6} cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^{-6} cm^3·g^{-1}	[Ni] / mol·L^{-1}	[Ni(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.37	0.740	0.740	$2.92 \cdot 10^{-3}$	0	0
0.25	2.77	1.634	1.541	$2.61 \cdot 10^{-3}$	$2.39 \cdot 10^{-4}$	$7.95 \cdot 10^{-5}$
0.5	4.42	2.250	2.300	$2.30 \cdot 10^{-3}$	$3.86 \cdot 10^{-4}$	$2.34 \cdot 10^{-4}$
0.75	7.55	3.417	3.015	$2.02 \cdot 10^{-3}$	$4.83 \cdot 10^{-4}$	$4.20 \cdot 10^{-4}$
1	8.38	3.726	3.683	$1.75 \cdot 10^{-3}$	$5.48 \cdot 10^{-4}$	$6.21 \cdot 10^{-4}$
1.5	10.36	4.465	4.868	$1.28 \cdot 10^{-3}$	$6.05 \cdot 10^{-4}$	$1.03 \cdot 10^{-3}$
2	13.75	5.729	5.831	$9.01 \cdot 10^{-4}$	$5.95 \cdot 10^{-4}$	$1.43 \cdot 10^{-3}$
2.5	16.07	6.594	6.557	$6.13 \cdot 10^{-4}$	$5.46 \cdot 10^{-4}$	$1.76 \cdot 10^{-3}$
3	17.10	6.978	7.062	$4.12 \cdot 10^{-4}$	$4.80 \cdot 10^{-4}$	$2.03 \cdot 10^{-3}$
3.5	18.58	7.528	7.393	$2.81 \cdot 10^{-4}$	$4.15 \cdot 10^{-4}$	$2.23 \cdot 10^{-3}$
4	19.16	7.746	7.604	$1.97 \cdot 10^{-4}$	$3.59 \cdot 10^{-4}$	$2.37 \cdot 10^{-3}$
4.5	19.56	7.894	7.740	$1.43 \cdot 10^{-4}$	$3.12 \cdot 10^{-4}$	$2.47 \cdot 10^{-3}$
5	19.75	7.966	7.830	$1.08 \cdot 10^{-4}$	$2.75 \cdot 10^{-4}$	$2.54 \cdot 10^{-3}$
6	19.31	7.802	7.934	$6.60 \cdot 10^{-5}$	$2.19 \cdot 10^{-4}$	$2.64 \cdot 10^{-3}$
7	19.57	7.899	7.989	$4.42 \cdot 10^{-5}$	$1.81 \cdot 10^{-4}$	$2.70 \cdot 10^{-3}$
8	19.77	7.974	8.021	$3.15 \cdot 10^{-5}$	$1.54 \cdot 10^{-4}$	$2.74 \cdot 10^{-3}$
9	20.01	8.063	8.041	$2.36 \cdot 10^{-5}$	$1.34 \cdot 10^{-4}$	$2.77 \cdot 10^{-3}$
10	20.11	8.101	8.055	$1.83 \cdot 10^{-5}$	$1.18 \cdot 10^{-4}$	$2.79 \cdot 10^{-3}$
15	19.52	7.881	8.083	$7.11 \cdot 10^{-6}$	$7.46 \cdot 10^{-5}$	$2.84 \cdot 10^{-3}$
20	19.70	7.946	8.091	$3.75 \cdot 10^{-6}$	$5.44 \cdot 10^{-5}$	$2.87 \cdot 10^{-3}$
25	19.85	8.004	8.095	$2.31 \cdot 10^{-6}$	$4.28 \cdot 10^{-5}$	$2.88 \cdot 10^{-3}$

Table S11. Results for Evans NMR titration experiments of complex **1d** in DCM-d_2 (2.92 mmol·L^{-1}) with pyridine at 290 K and comparison with the values obtained by nonlinear fitting with EST for the solvent coordination model. The mean square error is $0.028 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δf / Hz	$\chi^g_{para,exp}$ / 10^{-6} cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^{-6} cm^3·g^{-1}	[Ni] / mol·L^{-1}	[Ni(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.50	0.788	0.788	$2.92 \cdot 10^{-3}$	0	0
0.25	3.35	1.851	1.854	$2.52 \cdot 10^{-3}$	$3.24 \cdot 10^{-4}$	$8.04 \cdot 10^{-5}$
0.5	5.61	2.694	2.794	$2.16 \cdot 10^{-3}$	$5.20 \cdot 10^{-4}$	$2.41 \cdot 10^{-4}$
0.75	9.37	4.096	3.645	$1.84 \cdot 10^{-3}$	$6.46 \cdot 10^{-4}$	$4.37 \cdot 10^{-4}$
1	10.14	4.383	4.417	$1.55 \cdot 10^{-3}$	$7.23 \cdot 10^{-4}$	$6.53 \cdot 10^{-4}$
1.5	12.71	5.341	5.731	$1.05 \cdot 10^{-3}$	$7.73 \cdot 10^{-4}$	$1.10 \cdot 10^{-3}$
2	16.66	6.814	6.725	$6.73 \cdot 10^{-4}$	$7.28 \cdot 10^{-4}$	$1.52 \cdot 10^{-3}$
2.5	18.01	7.317	7.404	$4.15 \cdot 10^{-4}$	$6.35 \cdot 10^{-4}$	$1.87 \cdot 10^{-3}$
3	19.64	7.925	7.822	$2.57 \cdot 10^{-4}$	$5.33 \cdot 10^{-4}$	$2.13 \cdot 10^{-3}$
3.5	19.99	8.056	8.064	$1.65 \cdot 10^{-4}$	$4.45 \cdot 10^{-4}$	$2.31 \cdot 10^{-3}$
4	20.95	8.414	8.206	$1.11 \cdot 10^{-4}$	$3.75 \cdot 10^{-4}$	$2.44 \cdot 10^{-3}$
4.5	20.76	8.341	8.291	$7.91 \cdot 10^{-5}$	$3.21 \cdot 10^{-4}$	$2.52 \cdot 10^{-3}$
5	20.89	8.391	8.346	$5.85 \cdot 10^{-5}$	$2.80 \cdot 10^{-4}$	$2.59 \cdot 10^{-3}$
6	20.78	8.350	8.407	$3.53 \cdot 10^{-5}$	$2.21 \cdot 10^{-4}$	$2.67 \cdot 10^{-3}$
7	20.69	8.315	8.438	$2.34 \cdot 10^{-5}$	$1.82 \cdot 10^{-4}$	$2.72 \cdot 10^{-3}$
8	20.97	8.421	8.456	$1.66 \cdot 10^{-5}$	$1.54 \cdot 10^{-4}$	$2.75 \cdot 10^{-3}$
9	21.02	8.440	8.467	$1.24 \cdot 10^{-5}$	$1.34 \cdot 10^{-4}$	$2.78 \cdot 10^{-3}$
10	21.18	8.500	8.475	$9.60 \cdot 10^{-6}$	$1.18 \cdot 10^{-4}$	$2.80 \cdot 10^{-3}$
15	20.48	8.239	8.490	$3.73 \cdot 10^{-6}$	$7.41 \cdot 10^{-5}$	$2.85 \cdot 10^{-3}$
20	20.69	8.315	8.495	$1.96 \cdot 10^{-6}$	$5.40 \cdot 10^{-5}$	$2.87 \cdot 10^{-3}$
25	20.84	8.373	8.497	$1.21 \cdot 10^{-6}$	$4.25 \cdot 10^{-5}$	$2.88 \cdot 10^{-3}$

Table S12. Results for Evans NMR titration experiments of complex **1d** in DCM-d_2 (2.92 mmol·L^{-1}) with pyridine at 280 K and comparison with the values obtained by nonlinear fitting with EST for the solvent coordination model. The mean square error is $0.034 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δf / Hz	$\chi^g_{para,exp}$ / 10^{-6} cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^{-6} cm^3·g^{-1}	[Ni] / mol·L^{-1}	[Ni(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.50	0.848	0.848	$2.92 \cdot 10^{-3}$	0	0
0.25	3.35	2.340	2.299	$2.40 \cdot 10^{-3}$	$4.81 \cdot 10^{-4}$	$4.65 \cdot 10^{-5}$
0.5	5.61	3.340	3.527	$1.95 \cdot 10^{-3}$	$8.11 \cdot 10^{-4}$	$1.63 \cdot 10^{-4}$
0.75	9.37	5.040	4.574	$1.57 \cdot 10^{-3}$	$1.03 \cdot 10^{-3}$	$3.25 \cdot 10^{-4}$
1	10.14	5.520	5.462	$1.25 \cdot 10^{-3}$	$1.16 \cdot 10^{-3}$	$5.19 \cdot 10^{-4}$
1.5	12.71	6.340	6.817	$7.54 \cdot 10^{-4}$	$1.22 \cdot 10^{-3}$	$9.51 \cdot 10^{-4}$
2	16.66	7.750	7.685	$4.38 \cdot 10^{-4}$	$1.12 \cdot 10^{-3}$	$1.37 \cdot 10^{-3}$
2.5	18.01	8.140	8.189	$2.55 \cdot 10^{-4}$	$9.52 \cdot 10^{-4}$	$1.72 \cdot 10^{-3}$
3	19.64	8.570	8.465	$1.54 \cdot 10^{-4}$	$7.95 \cdot 10^{-4}$	$1.97 \cdot 10^{-3}$
3.5	19.99	8.670	8.617	$9.93 \cdot 10^{-5}$	$6.66 \cdot 10^{-4}$	$2.16 \cdot 10^{-3}$
4	20.95	8.880	8.704	$6.77 \cdot 10^{-5}$	$5.67 \cdot 10^{-4}$	$2.29 \cdot 10^{-3}$
4.5	20.76	8.870	8.757	$4.85 \cdot 10^{-5}$	$4.90 \cdot 10^{-4}$	$2.39 \cdot 10^{-3}$
5	20.89	8.830	8.790	$3.62 \cdot 10^{-5}$	$4.30 \cdot 10^{-4}$	$2.46 \cdot 10^{-3}$
6	20.78	8.830	8.829	$2.22 \cdot 10^{-5}$	$3.43 \cdot 10^{-4}$	$2.56 \cdot 10^{-3}$
7	20.69	8.750	8.849	$1.49 \cdot 10^{-5}$	$2.85 \cdot 10^{-4}$	$2.62 \cdot 10^{-3}$
8	20.97	8.890	8.861	$1.07 \cdot 10^{-5}$	$2.43 \cdot 10^{-4}$	$2.67 \cdot 10^{-3}$
9	21.02	8.780	8.868	$8.01 \cdot 10^{-6}$	$2.12 \cdot 10^{-4}$	$2.70 \cdot 10^{-3}$
10	21.18	8.890	8.873	$6.22 \cdot 10^{-6}$	$1.88 \cdot 10^{-4}$	$2.73 \cdot 10^{-3}$
15	20.48	8.580	8.883	$2.44 \cdot 10^{-6}$	$1.19 \cdot 10^{-4}$	$2.80 \cdot 10^{-3}$
20	20.69	8.690	8.886	$1.29 \cdot 10^{-6}$	$8.72 \cdot 10^{-5}$	$2.84 \cdot 10^{-3}$
25	20.84	8.740	8.888	$7.99 \cdot 10^{-7}$	$6.88 \cdot 10^{-5}$	$2.85 \cdot 10^{-3}$

Table S13. Results for Evans NMR titration experiments of complex **1d** in DCM-d_2 (2.92 mmol·L^{-1}) with pyridine at 270 K and comparison with the values obtained by nonlinear fitting with EST for the solvent coordination model. The mean square error is $0.029 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δf / Hz	$\chi^g_{para,exp}$ / 10^{-6} cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^{-6} cm^3·g^{-1}	[Ni] / mol·L^{-1}	[Ni(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.50	0.922	0.922	$2.92 \cdot 10^{-3}$	0	0
0.25	3.35	2.830	2.703	$2.31 \cdot 10^{-3}$	$6.00 \cdot 10^{-4}$	1.90E-05
0.5	5.61	3.940	4.265	$1.76 \cdot 10^{-3}$	$1.08 \cdot 10^{-3}$	8.06E-05
0.75	9.37	5.960	5.568	$1.31 \cdot 10^{-3}$	$1.42 \cdot 10^{-3}$	$1.89 \cdot 10^{-4}$
1	10.14	6.610	6.595	$9.53 \cdot 10^{-4}$	$1.63 \cdot 10^{-3}$	$3.39 \cdot 10^{-4}$
1.5	12.71	7.610	7.913	$4.95 \cdot 10^{-4}$	$1.71 \cdot 10^{-3}$	$7.18 \cdot 10^{-4}$
2	16.66	8.680	8.571	$2.67 \cdot 10^{-4}$	$1.56 \cdot 10^{-3}$	$1.10 \cdot 10^{-3}$
2.5	18.01	8.750	8.894	$1.55 \cdot 10^{-4}$	$1.35 \cdot 10^{-3}$	$1.42 \cdot 10^{-3}$
3	19.64	9.250	9.061	$9.70 \cdot 10^{-5}$	$1.15 \cdot 10^{-3}$	$1.67 \cdot 10^{-3}$
3.5	19.99	9.170	9.153	$6.49 \cdot 10^{-5}$	$9.97 \cdot 10^{-4}$	$1.86 \cdot 10^{-3}$
4	20.95	9.330	9.208	$4.59 \cdot 10^{-5}$	$8.70 \cdot 10^{-4}$	$2.01 \cdot 10^{-3}$
4.5	20.76	9.330	9.242	$3.39 \cdot 10^{-5}$	$7.69 \cdot 10^{-4}$	$2.12 \cdot 10^{-3}$
5	20.89	9.250	9.265	$2.59 \cdot 10^{-5}$	$6.86 \cdot 10^{-4}$	$2.21 \cdot 10^{-3}$
6	20.78	9.270	9.293	$1.64 \cdot 10^{-5}$	$5.63 \cdot 10^{-4}$	$2.34 \cdot 10^{-3}$
7	20.69	9.210	9.307	$1.13 \cdot 10^{-5}$	$4.76 \cdot 10^{-4}$	$2.44 \cdot 10^{-3}$
8	20.97	9.330	9.316	$8.22 \cdot 10^{-6}$	$4.11 \cdot 10^{-4}$	$2.50 \cdot 10^{-3}$
9	21.02	9.250	9.322	$6.23 \cdot 10^{-6}$	$3.62 \cdot 10^{-4}$	$2.56 \cdot 10^{-3}$
10	21.18	9.340	9.326	$4.89 \cdot 10^{-6}$	$3.23 \cdot 10^{-4}$	$2.60 \cdot 10^{-3}$
15	20.48	9.080	9.334	$1.97 \cdot 10^{-6}$	$2.09 \cdot 10^{-4}$	$2.71 \cdot 10^{-3}$
20	20.69	9.140	9.337	$1.05 \cdot 10^{-6}$	$1.55 \cdot 10^{-4}$	$2.77 \cdot 10^{-3}$
25	20.84	9.160	9.338	$6.54 \cdot 10^{-7}$	$1.23 \cdot 10^{-4}$	$2.80 \cdot 10^{-3}$

Table S14. Results for Evans NMR titration experiments of complex **1d** in DCM-d_2 (2.92 mmol·L^{-1}) with pyridine at 260 K and comparison with the values obtained by nonlinear fitting with EST for the solvent coordination model. The mean square error is $0.034 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δf / Hz	$\chi^g_{para,exp}$ / 10^{-6} cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^{-6} cm^3·g^{-1}	[Ni] / mol·L^{-1}	[Ni(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.50	1.060	1.060	$2.92 \cdot 10^{-3}$	0	0
0.25	3.35	3.370	3.055	$2.26 \cdot 10^{-3}$	$6.64 \cdot 10^{-4}$	$2.22 \cdot 10^{-6}$
0.5	5.61	4.530	4.908	$1.64 \cdot 10^{-3}$	$1.27 \cdot 10^{-3}$	$1.13 \cdot 10^{-5}$
0.75	9.37	6.910	6.500	$1.11 \cdot 10^{-3}$	$1.78 \cdot 10^{-3}$	$3.27 \cdot 10^{-5}$
1	10.14	7.690	7.681	$7.14 \cdot 10^{-4}$	$2.14 \cdot 10^{-3}$	$7.30 \cdot 10^{-5}$
1.5	12.71	8.590	8.849	$3.24 \cdot 10^{-4}$	$2.40 \cdot 10^{-3}$	$2.02 \cdot 10^{-4}$
2	16.66	9.150	9.265	$1.85 \cdot 10^{-4}$	$2.39 \cdot 10^{-3}$	$3.51 \cdot 10^{-4}$
2.5	18.01	9.330	9.451	$1.23 \cdot 10^{-4}$	$2.31 \cdot 10^{-3}$	$4.94 \cdot 10^{-4}$
3	19.64	9.770	9.553	$8.90 \cdot 10^{-5}$	$2.21 \cdot 10^{-3}$	$6.25 \cdot 10^{-4}$
3.5	19.99	9.640	9.616	$6.81 \cdot 10^{-5}$	$2.11 \cdot 10^{-3}$	$7.46 \cdot 10^{-4}$
4	20.95	9.780	9.658	$5.41 \cdot 10^{-5}$	$2.01 \cdot 10^{-3}$	$8.56 \cdot 10^{-4}$
4.5	20.76	9.830	9.688	$4.42 \cdot 10^{-5}$	$1.92 \cdot 10^{-3}$	$9.56 \cdot 10^{-4}$
5	20.89	9.780	9.710	$3.69 \cdot 10^{-5}$	$1.84 \cdot 10^{-3}$	$1.05 \cdot 10^{-3}$
6	20.78	9.690	9.739	$2.69 \cdot 10^{-5}$	$1.69 \cdot 10^{-3}$	$1.21 \cdot 10^{-3}$
7	20.69	9.690	9.758	$2.06 \cdot 10^{-5}$	$1.56 \cdot 10^{-3}$	$1.35 \cdot 10^{-3}$
8	20.97	9.760	9.771	$1.63 \cdot 10^{-5}$	$1.44 \cdot 10^{-3}$	$1.46 \cdot 10^{-3}$
9	21.02	9.720	9.780	$1.32 \cdot 10^{-5}$	$1.34 \cdot 10^{-3}$	$1.57 \cdot 10^{-3}$
10	21.18	9.820	9.787	$1.09 \cdot 10^{-5}$	$1.26 \cdot 10^{-3}$	$1.65 \cdot 10^{-3}$
15	20.48	9.690	9.804	$5.21 \cdot 10^{-6}$	$9.48 \cdot 10^{-4}$	$1.97 \cdot 10^{-3}$
20	20.69	9.600	9.811	$3.04 \cdot 10^{-6}$	$7.59 \cdot 10^{-4}$	$2.16 \cdot 10^{-3}$
25	20.84	9.610	9.814	$2.00 \cdot 10^{-6}$	$6.33 \cdot 10^{-4}$	$2.29 \cdot 10^{-3}$

Table S15. Results for Evans NMR titration experiments of complex **1d** in DCM-d_2 (2.92 mmol·L^{-1}) with pyridine at 250 K and comparison with the values obtained by nonlinear fitting with EST for the solvent coordination model. The mean square error is $0.067 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δf / Hz	$\chi^g_{para,exp}$ / 10^{-6} cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^{-6} cm^3·g^{-1}	[Ni] / mol·L^{-1}	[Ni(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.50	1.320	1.320	$2.92 \cdot 10^{-3}$	0	0
0.25	3.35	4.220	3.469	$2.22 \cdot 10^{-3}$	$7.00 \cdot 10^{-4}$	$9.29 \cdot 10^{-13}$
0.5	5.61	5.150	5.539	$1.55 \cdot 10^{-3}$	$1.37 \cdot 10^{-3}$	$5.14 \cdot 10^{-12}$
0.75	9.37	8.010	7.411	$9.41 \cdot 10^{-4}$	$1.98 \cdot 10^{-3}$	$1.77 \cdot 10^{-12}$
1	10.14	8.730	8.790	$4.92 \cdot 10^{-4}$	$2.43 \cdot 10^{-3}$	$5.08 \cdot 10^{-11}$
1.5	12.71	9.550	9.784	$1.68 \cdot 10^{-4}$	$2.76 \cdot 10^{-3}$	$1.91 \cdot 10^{-10}$
2	16.66	9.690	10.013	$9.33 \cdot 10^{-5}$	$2.83 \cdot 10^{-3}$	$3.63 \cdot 10^{-10}$
2.5	18.01	9.880	10.104	$6.39 \cdot 10^{-5}$	$2.86 \cdot 10^{-3}$	$5.40 \cdot 10^{-10}$
3	19.64	10.300	10.151	$4.85 \cdot 10^{-5}$	$2.88 \cdot 10^{-3}$	$7.20 \cdot 10^{-10}$
3.5	19.99	10.100	10.180	$3.90 \cdot 10^{-5}$	$2.88 \cdot 10^{-3}$	$9.00 \cdot 10^{-9}$
4	20.95	10.200	10.200	$3.27 \cdot 10^{-5}$	$2.89 \cdot 10^{-3}$	$1.08 \cdot 10^{-9}$
4.5	20.76	10.300	10.214	$2.81 \cdot 10^{-5}$	$2.90 \cdot 10^{-3}$	$1.26 \cdot 10^{-9}$
5	20.89	10.300	10.224	$2.46 \cdot 10^{-5}$	$2.90 \cdot 10^{-3}$	$1.44 \cdot 10^{-9}$
6	20.78	10.200	10.239	$1.97 \cdot 10^{-5}$	$2.90 \cdot 10^{-3}$	$1.81 \cdot 10^{-9}$
7	20.69	10.200	10.249	$1.65 \cdot 10^{-5}$	$2.91 \cdot 10^{-3}$	$2.17 \cdot 10^{-9}$
8	20.97	10.200	10.257	$1.41 \cdot 10^{-5}$	$2.91 \cdot 10^{-3}$	$2.53 \cdot 10^{-9}$
9	21.02	10.200	10.262	$1.24 \cdot 10^{-5}$	$2.91 \cdot 10^{-3}$	$2.89 \cdot 10^{-9}$
10	21.18	10.300	10.266	$1.10 \cdot 10^{-5}$	$2.91 \cdot 10^{-3}$	$3.26 \cdot 10^{-9}$
15	20.48	10.200	10.278	$7.08 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$	$5.07 \cdot 10^{-9}$
20	20.69	10.100	10.284	$5.22 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$	$6.88 \cdot 10^{-9}$
25	20.84	10.100	10.287	$4.14 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$	$8.70 \cdot 10^{-9}$

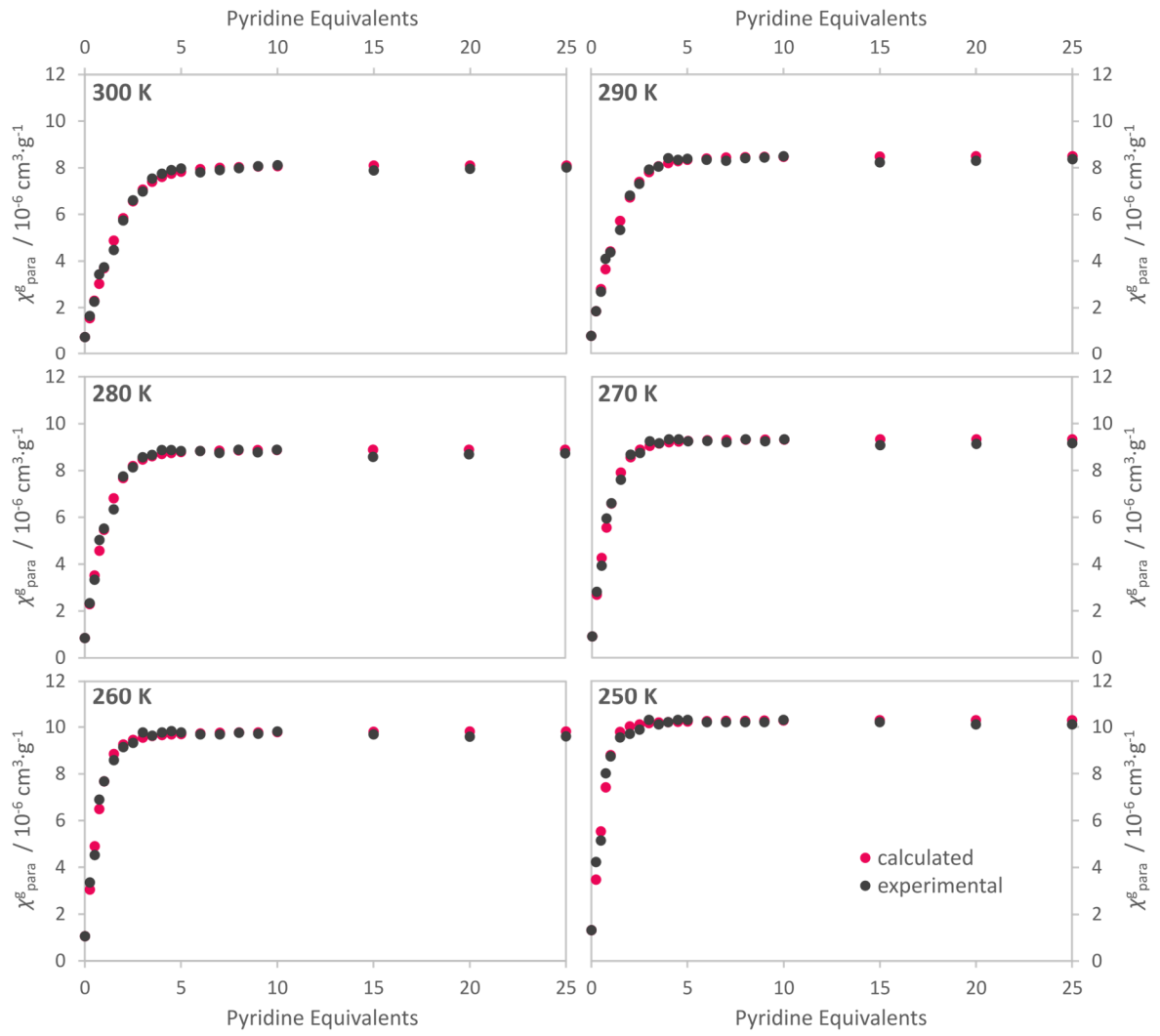

Figure S13. Experimental (black) and calculated pyridine titration curves (red) of **1d** in DCM-d_2 at different temperatures for the evaluation with the solvent coordination model.

Table S16. Association constants K_{1S} and K_2 for the coordination for the first and second pyridine to complex **1d** in dichloromethane-d_2 at different temperatures for the evaluation with the solvent coordination model.

T / K	K_{1S}	K_2
300	275	1000
290	522	1008
280	1279	617
270	2785	339
260	4672	53
250	10057	$4 \cdot 10^{-5}$

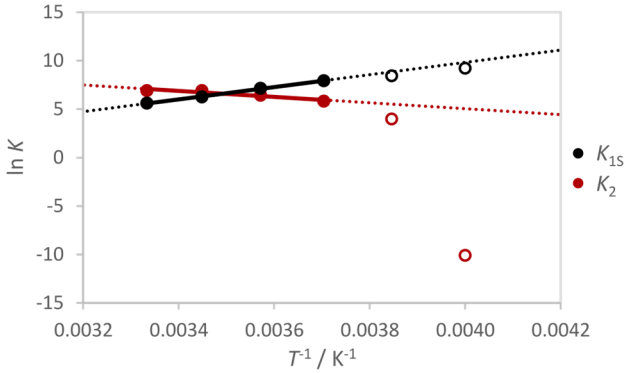

Figure S14. Van't Hoff plots of ln K as a function of the reciprocal temperature for association constants K_{1S} (red) and K_2 (black) determined by the solvent coordination model. The values for 250 K and 260 K (open circles) were not considered.

Fitted straight lines from van't Hoff plots:

$$\ln K_{1S} = -3058.86 \cdot \frac{1}{T} + 17.27 \qquad \text{(S9)}$$

$$\ln K_2 = 6351.28 \cdot \frac{1}{T} - 15.58 \qquad \text{(S10)}$$

Table S17. Binding enthalpies and entropies for the coordination of one or two pyridine ligands to **1d** when considering the solvent model. Association constants from 300-270 K were taken into account for the evaluation.

	1S	2
ΔH / kcal·mol^{-1}	-13	+6
ΔS / cal·mol^{-1}·K^{-1}	-31	+34

S2.4.2 Dimer Model

Here it is assumed that the intrinsic paramagnetism of the solution is induced by dimer formation. Data evaluation is thus based on the formula

$$\chi^{g}_{para} = \frac{[Ni_2] \cdot \chi^{g}_{para,0} + [Ni_2(py)] \cdot \chi^{g}_{para,int} + \frac{1}{2} \cdot [Ni(py)_2] \cdot \chi^{g}_{para,max}}{[Ni_2]_0} \quad (1)$$

where $\chi^{g}_{para,0}$ is the susceptibility in the absence of pyridine and $\chi^{g}_{para,max}$ the highest measured susceptibility. Since it was assumed that the intermediary susceptibility of $Ni_2(py)$ is $\chi^{g}_{para,int} = \chi^{g}_{para,max}$, the formula is simplified to

$$\chi^{g}_{para} = \frac{[Ni_2] \cdot \chi^{g}_{para,0} + \left([Ni_2(py)] + \frac{1}{2} \cdot [Ni(py)_2]\right) \cdot \chi^{g}_{para,max}}{[Ni_2]_0} \quad (S11)$$

Table S18. Results for Evans NMR titration experiments of complex **1d$_2$** in DCM-d_2 (1.46 mmol·L^{-1}) with pyridine at 300 K and comparison with the values obtained by nonlinear fitting with EST for the dimer model. The mean square error is $0.022 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δ*f* / Hz	$\chi^{g}_{para,exp}$ / 10^6 cm^3·g^{-1}	$\chi^{g}_{para,calc}$ / 10^6 cm^3·g^{-1}	[Ni_2] / mol·L^{-1}	[Ni_2(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.37	0.740	0.740	$1.46 \cdot 10^{-3}$	0	0
0.25	2.77	1.634	1.625	$1.29 \cdot 10^{-3}$	$1.48 \cdot 10^{-4}$	$5.58 \cdot 10^{-5}$
0.5	4.42	2.250	2.394	$1.13 \cdot 10^{-3}$	$2.40 \cdot 10^{-4}$	$1.77 \cdot 10^{-4}$
0.75	7.55	3.417	3.082	$9.97 \cdot 10^{-4}$	$2.99 \cdot 10^{-4}$	$3.33 \cdot 10^{-4}$
1	8.38	3.726	3.707	$8.73 \cdot 10^{-4}$	$3.34 \cdot 10^{-4}$	$5.10 \cdot 10^{-4}$
1.5	10.36	4.465	4.798	$6.56 \cdot 10^{-4}$	$3.58 \cdot 10^{-4}$	$8.97 \cdot 10^{-4}$
2	13.75	5.729	5.708	$4.75 \cdot 10^{-4}$	$3.38 \cdot 10^{-4}$	$1.30 \cdot 10^{-3}$
2.5	16.07	6.594	6.452	$3.27 \cdot 10^{-4}$	$2.91 \cdot 10^{-4}$	$1.69 \cdot 10^{-3}$
3	17.10	6.978	7.032	$2.12 \cdot 10^{-4}$	$2.31 \cdot 10^{-4}$	$2.04 \cdot 10^{-3}$
3.5	18.58	7.528	7.453	$1.29 \cdot 10^{-4}$	$1.70 \cdot 10^{-4}$	$2.33 \cdot 10^{-3}$
4	19.16	7.746	7.728	$7.39 \cdot 10^{-5}$	$1.17 \cdot 10^{-4}$	$2.54 \cdot 10^{-3}$
4.5	19.56	7.894	7.892	$4.15 \cdot 10^{-5}$	$7.81 \cdot 10^{-5}$	$2.68 \cdot 10^{-3}$
5	19.75	7.966	7.982	$2.36 \cdot 10^{-5}$	$5.20 \cdot 10^{-5}$	$2.77 \cdot 10^{-3}$
6	19.31	7.802	8.057	$8.56 \cdot 10^{-6}$	$2.47 \cdot 10^{-5}$	$2.86 \cdot 10^{-3}$
7	19.57	7.899	8.082	$3.67 \cdot 10^{-6}$	$1.31 \cdot 10^{-5}$	$2.89 \cdot 10^{-3}$
8	19.77	7.974	8.091	$1.80 \cdot 10^{-6}$	$7.72 \cdot 10^{-6}$	$2.90 \cdot 10^{-3}$
9	20.01	8.063	8.096	$9.80 \cdot 10^{-7}$	$4.90 \cdot 10^{-6}$	$2.91 \cdot 10^{-3}$
10	20.11	8.101	8.098	$5.77 \cdot 10^{-7}$	$3.30 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
15	19.52	7.881	8.100	$8.32 \cdot 10^{-8}$	$7.72 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
20	19.70	7.946	8.100	$2.27 \cdot 10^{-8}$	$2.91 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
25	19.85	8.004	8.101	$8.50 \cdot 10^{-9}$	$1.40 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$

Table S19. Results for Evans NMR titration experiments of complex **1d$_2$** in DCM-d$_2$ (1.46 mmol·L^{-1}) with pyridine at 290 K and comparison with the values obtained by nonlinear fitting with EST for the dimer model. The mean square error is $0.026 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δ*f* / Hz	$\chi^g_{para,exp}$ / 10^6 cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^6 cm^3·g^{-1}	[Ni$_2$] / mol·L^{-1}	[Ni$_2$(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.50	0.788	0.788	$1.46 \cdot 10^{-3}$	0	0
0.25	3.35	1.851	1.958	$1.24 \cdot 10^{-3}$	$1.84 \cdot 10^{-4}$	$7.50 \cdot 10^{-5}$
0.5	5.61	2.694	2.899	$1.06 \cdot 10^{-3}$	$2.86 \cdot 10^{-4}$	$2.28 \cdot 10^{-4}$
0.75	9.37	4.096	3.707	$9.08 \cdot 10^{-4}$	$3.44 \cdot 10^{-4}$	$4.18 \cdot 10^{-4}$
1	10.14	4.383	4.420	$7.73 \cdot 10^{-4}$	$3.74 \cdot 10^{-4}$	$6.29 \cdot 10^{-4}$
1.5	12.71	5.341	5.626	$5.45 \cdot 10^{-4}$	$3.77 \cdot 10^{-4}$	$1.08 \cdot 10^{-3}$
2	16.66	6.814	6.589	$3.62 \cdot 10^{-4}$	$3.31 \cdot 10^{-4}$	$1.54 \cdot 10^{-3}$
2.5	18.01	7.317	7.332	$2.21 \cdot 10^{-4}$	$2.59 \cdot 10^{-4}$	$1.96 \cdot 10^{-3}$
3	19.64	7.925	7.860	$1.21 \cdot 10^{-4}$	$1.79 \cdot 10^{-4}$	$2.32 \cdot 10^{-3}$
3.5	19.99	8.056	8.183	$6.00 \cdot 10^{-5}$	$1.12 \cdot 10^{-4}$	$2.58 \cdot 10^{-3}$
4	20.95	8.414	8.350	$2.84 \cdot 10^{-5}$	$6.55 \cdot 10^{-5}$	$2.74 \cdot 10^{-3}$
4.5	20.76	8.341	8.427	$1.38 \cdot 10^{-5}$	$3.88 \cdot 10^{-5}$	$2.82 \cdot 10^{-3}$
5	20.89	8.391	8.462	$7.21 \cdot 10^{-6}$	$2.40 \cdot 10^{-5}$	$2.86 \cdot 10^{-3}$
6	20.78	8.350	8.487	$2.42 \cdot 10^{-6}$	$1.06 \cdot 10^{-5}$	$2.90 \cdot 10^{-3}$
7	20.69	8.315	8.494	$1.01 \cdot 10^{-6}$	$5.52 \cdot 10^{-6}$	$2.91 \cdot 10^{-3}$
8	20.97	8.421	8.497	$4.89 \cdot 10^{-7}$	$3.21 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
9	21.02	8.440	8.498	$2.65 \cdot 10^{-7}$	$2.03 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
10	21.18	8.500	8.499	$1.55 \cdot 10^{-7}$	$1.36 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
15	20.48	8.239	8.499	$2.23 \cdot 10^{-8}$	$3.18 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
20	20.69	8.315	8.500	$6.08 \cdot 10^{-9}$	$1.20 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
25	20.84	8.373	8.500	$2.28 \cdot 10^{-9}$	$5.74 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$

Table S20. Results for Evans NMR titration experiments of complex **1d$_2$** in DCM-d$_2$ (1.46 mmol·L^{-1}) with pyridine at 280 K and comparison with the values obtained by nonlinear fitting with EST for the dimer model. The mean square error is $0.032 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δ*f* / Hz	$\chi^g_{para,exp}$ / 10^6 cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^6 cm^3·g^{-1}	[Ni$_2$] / mol·L^{-1}	[Ni$_2$(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.66	0.848	0.848	$1.46 \cdot 10^{-3}$	0	0
0.25	4.65	2.336	2.495	$1.16 \cdot 10^{-3}$	$2.59 \cdot 10^{-4}$	$8.11 \cdot 10^{-5}$
0.5	7.34	3.339	3.680	$9.47 \cdot 10^{-4}$	$3.90 \cdot 10^{-4}$	$2.50 \cdot 10^{-4}$
0.75	11.89	5.035	4.621	$7.76 \cdot 10^{-4}$	$4.56 \cdot 10^{-4}$	$4.60 \cdot 10^{-4}$
1	13.18	5.516	5.402	$6.34 \cdot 10^{-4}$	$4.81 \cdot 10^{-4}$	$6.94 \cdot 10^{-4}$
1.5	15.40	6.344	6.634	$4.10 \cdot 10^{-4}$	$4.55 \cdot 10^{-4}$	$1.19 \cdot 10^{-3}$
2	19.17	7.750	7.539	$2.46 \cdot 10^{-4}$	$3.69 \cdot 10^{-4}$	$1.69 \cdot 10^{-3}$
2.5	20.22	8.142	8.174	$1.30E \cdot 10^{-4}$	$2.58 \cdot 10^{-4}$	$2.15 \cdot 10^{-3}$
3	21.37	8.570	8.565	$5.91 \cdot 10^{-5}$	$1.54 \cdot 10^{-4}$	$2.50 \cdot 10^{-3}$
3.5	21.63	8.665	8.758	$2.40 \cdot 10^{-5}$	$8.17 \cdot 10^{-5}$	$2.71 \cdot 10^{-3}$
4	22.19	8.876	8.836	$9.89 \cdot 10^{-6}$	$4.28 \cdot 10^{-5}$	$2.82 \cdot 10^{-3}$
4.5	22.17	8.869	8.865	$4.47 \cdot 10^{-6}$	$2.38 \cdot 10^{-5}$	$2.87 \cdot 10^{-3}$
5	22.06	8.828	8.878	$2.25 \cdot 10^{-6}$	$1.43 \cdot 10^{-5}$	$2.89 \cdot 10^{-3}$
6	22.07	8.831	8.886	$7.33 \cdot 10^{-7}$	$6.17 \cdot 10^{-6}$	$2.91 \cdot 10^{-3}$
7	21.84	8.746	8.888	$3.03 \cdot 10^{-7}$	$3.19 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
8	22.22	8.887	8.889	$1.47 \cdot 10^{-7}$	$1.85 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
9	21.93	8.779	8.890	$7.93 \cdot 10^{-8}$	$1.17 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
10	22.24	8.895	8.890	$4.65 \cdot 10^{-8}$	$7.82 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
15	21.40	8.582	8.890	$6.68 \cdot 10^{-9}$	$1.82 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
20	21.68	8.686	8.890	$1.82 \cdot 10^{-9}$	$6.88 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$
25	21.83	8.742	8.890	$6.82 \cdot 10^{-10}$	$3.30 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$

Table S21. Results for Evans NMR titration experiments of complex **1d$_2$** in DCM-d$_2$ (1.46 mmol·L^{-1}) with pyridine at 270 K and comparison with the values obtained by nonlinear fitting with EST for the dimer model. The mean square error is $0.042 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δ*f* / Hz	$\chi^g_{para,exp}$ / 10^6 cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^6 cm^3·g^{-1}	[Ni$_2$] / mol·L^{-1}	[Ni$_2$(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	0.86	0.922	0.922	$1.46 \cdot 10^{-3}$	0	0
0.25	5.98	2.831	3.073	$1.09 \cdot 10^{-3}$	$3.27 \cdot 10^{-4}$	$9.29 \cdot 10^{-5}$
0.5	8.94	3.935	4.490	$8.42 \cdot 10^{-4}$	$4.75 \cdot 10^{-4}$	$2.88 \cdot 10^{-4}$
0.75	14.37	5.960	5.547	$6.59 \cdot 10^{-4}$	$5.37 \cdot 10^{-4}$	$5.32 \cdot 10^{-4}$
1	16.10	6.605	6.382	$5.14 \cdot 10^{-4}$	$5.47 \cdot 10^{-4}$	$8.02 \cdot 10^{-4}$
1.5	18.79	7.608	7.624	$2.98 \cdot 10^{-4}$	$4.76 \cdot 10^{-4}$	$1.37 \cdot 10^{-3}$
2	21.66	8.679	8.466	$1.52 \cdot 10^{-4}$	$3.41 \cdot 10^{-4}$	$1.94 \cdot 10^{-3}$
2.5	21.84	8.746	8.988	$6.11 \cdot 10^{-5}$	$1.92 \cdot 10^{-4}$	$2.42 \cdot 10^{-3}$
3	23.18	9.245	9.232	$1.88 \cdot 10^{-5}$	$8.43 \cdot 10^{-5}$	$2.72 \cdot 10^{-3}$
3.5	22.97	9.167	9.308	$5.56 \cdot 10^{-6}$	$3.46 \cdot 10^{-5}$	$2.84 \cdot 10^{-3}$
4	23.41	9.331	9.329	$1.96 \cdot 10^{-6}$	$1.59 \cdot 10^{-5}$	$2.89 \cdot 10^{-3}$
4.5	23.41	9.331	9.335	$8.29 \cdot 10^{-7}$	$8.39 \cdot 10^{-6}$	$2.91 \cdot 10^{-3}$
5	23.18	9.245	9.338	$4.05 \cdot 10^{-7}$	$4.91 \cdot 10^{-6}$	$2.91 \cdot 10^{-3}$
6	23.25	9.271	9.339	$1.29 \cdot 10^{-7}$	$2.09 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
7	23.09	9.212	9.340	$5.32 \cdot 10^{-8}$	$1.07 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
8	23.40	9.327	9.340	$2.57 \cdot 10^{-8}$	$6.21 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
9	23.19	9.249	9.340	$1.39 \cdot 10^{-8}$	$3.91 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
10	23.44	9.342	9.340	$8.13 \cdot 10^{-9}$	$2.62 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
15	22.74	9.081	9.340	$1.17 \cdot 10^{-9}$	$6.11 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$
20	22.89	9.135	9.340	$3.17 \cdot 10^{-10}$	$2.30 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$
25	22.95	9.160	9.340	$1.19 \cdot 10^{-10}$	$1.10 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$

Table S22. Results for Evans NMR titration experiments of complex **1d$_2$** in DCM-d$_2$ (1.46 mmol·L^{-1}) with pyridine at 260 K and comparison with the values obtained by nonlinear fitting with EST for the dimer model. The mean square error is $0.064 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δ*f* / Hz	$\chi^g_{para,exp}$ / 10^6 cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^6 cm^3·g^{-1}	[Ni$_2$] / mol·L^{-1}	[Ni$_2$(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	1.23	1.060	1.060	$1.46 \cdot 10^{-3}$	0	0
0.25	7.43	3.372	3.664	$1.03 \cdot 10^{-3}$	$4.00 \cdot 10^{-4}$	$6.98 \cdot 10^{-5}$
0.5	10.53	4.528	5.320	$7.51 \cdot 10^{-4}$	$5.89 \cdot 10^{-4}$	$2.43 \cdot 10^{-4}$
0.75	16.92	6.911	6.453	$5.62 \cdot 10^{-4}$	$6.63 \cdot 10^{-4}$	$4.74 \cdot 10^{-4}$
1	19.00	7.687	7.281	$4.24 \cdot 10^{-4}$	$6.69 \cdot 10^{-4}$	$7.38 \cdot 10^{-4}$
1.5	21.42	8.589	8.409	$2.35 \cdot 10^{-4}$	$5.73 \cdot 10^{-4}$	$1.31 \cdot 10^{-3}$
2	22.93	9.152	9.110	$1.19 \cdot 10^{-4}$	$4.09 \cdot 10^{-4}$	$1.87 \cdot 10^{-3}$
2.5	23.40	9.327	9.524	$4.95 \cdot 10^{-5}$	$2.38 \cdot 10^{-4}$	$2.35 \cdot 10^{-3}$
3	24.58	9.767	9.721	$1.66 \cdot 10^{-5}$	$1.12 \cdot 10^{-4}$	$2.67 \cdot 10^{-3}$
3.5	24.24	9.641	9.788	$5.26 \cdot 10^{-6}$	$4.86 \cdot 10^{-5}$	$2.82 \cdot 10^{-3}$
4	24.61	9.779	9.809	$1.91 \cdot 10^{-6}$	$2.30 \cdot 10^{-5}$	$2.87 \cdot 10^{-3}$
4.5	24.76	9.833	9.815	$8.21 \cdot 10^{-7}$	$1.22 \cdot 10^{-5}$	$2.90 \cdot 10^{-3}$
5	24.61	9.779	9.818	$4.03 \cdot 10^{-7}$	$7.20 \cdot 10^{-6}$	$2.91 \cdot 10^{-3}$
6	24.38	9.693	9.819	$1.29 \cdot 10^{-7}$	$3.07 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
7	24.37	9.689	9.820	$5.32 \cdot 10^{-8}$	$1.58 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
8	24.56	9.760	9.820	$2.57 \cdot 10^{-8}$	$9.15 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
9	24.46	9.723	9.820	$1.39 \cdot 10^{-8}$	$5.76 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
10	24.73	9.823	9.820	$8.14 \cdot 10^{-9}$	$3.86 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
15	24.38	9.693	9.820	$1.17 \cdot 10^{-9}$	$9.01 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$
20	24.13	9.598	9.820	$3.18 \cdot 10^{-10}$	$3.39 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$
25	24.17	9.615	9.820	$1.19 \cdot 10^{-10}$	$1.63 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$

Table S23. Results for Evans NMR titration experiments of complex **1d$_2$** in DCM-d$_2$ (1.46 mmol·L^{-1}) with pyridine at 250 K and comparison with the values obtained by nonlinear fitting with EST for the dimer model. The mean square error is $0.102 \cdot 10^{-6}$ cm^3·g^{-1}. The concentrations of all species at every titration step are given.

eq. Py	Δf / Hz	$\chi^g_{para,exp}$ / 10^6 cm^3·g^{-1}	$\chi^g_{para,calc}$ / 10^6 cm^3·g^{-1}	[Ni$_2$] / mol·L^{-1}	[Ni$_2$(py)] / mol·L^{-1}	[Ni(py)$_2$] / mol·L^{-1}
0	1.94	1.325	1.320	$1.46 \cdot 10^{-3}$	0	0
0.25	9.70	4.219	4.355	$9.68 \cdot 10^{-4}$	$4.69 \cdot 10^{-4}$	$5.05 \cdot 10^{-5}$
0.5	12.20	5.151	6.257	$6.58 \cdot 10^{-4}$	$7.03 \cdot 10^{-4}$	$2.02 \cdot 10^{-4}$
0.75	19.88	8.015	7.441	$4.65 \cdot 10^{-4}$	$7.85 \cdot 10^{-4}$	$4.24 \cdot 10^{-4}$
1	21.80	8.731	8.230	$3.37 \cdot 10^{-4}$	$7.83 \cdot 10^{-4}$	$6.84 \cdot 10^{-4}$
1.5	24.00	9.551	9.203	$1.79 \cdot 10^{-4}$	$6.57 \cdot 10^{-4}$	$1.25 \cdot 10^{-3}$
2	24.37	9.689	9.756	$8.85 \cdot 10^{-5}$	$4.67 \cdot 10^{-4}$	$1.81 \cdot 10^{-3}$
2.5	24.87	9.876	10.068	$3.77 \cdot 10^{-5}$	$2.77 \cdot 10^{-4}$	$2.29 \cdot 10^{-3}$
3	25.94	10.275	10.218	$1.34 \cdot 10^{-5}$	$1.37 \cdot 10^{-4}$	$2.62 \cdot 10^{-3}$
3.5	25.56	10.133	10.272	$4.50 \cdot 10^{-6}$	$6.21 \cdot 10^{-5}$	$2.79 \cdot 10^{-3}$
4	25.65	10.166	10.290	$1.68 \cdot 10^{-6}$	$3.00 \cdot 10^{-5}$	$2.86 \cdot 10^{-3}$
4.5	26.00	10.297	10.296	$7.29 \cdot 10^{-7}$	$1.61 \cdot 10^{-5}$	$2.89 \cdot 10^{-3}$
5	26.05	10.316	10.298	$3.60 \cdot 10^{-7}$	$9.53 \cdot 10^{-6}$	$2.90 \cdot 10^{-3}$
6	25.64	10.163	10.299	$1.16 \cdot 10^{-7}$	$4.08 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
7	25.71	10.187	10.300	$4.78 \cdot 10^{-8}$	$2.10 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
8	25.68	10.178	10.300	$2.31 \cdot 10^{-8}$	$1.22 \cdot 10^{-6}$	$2.92 \cdot 10^{-3}$
9	25.74	10.200	10.300	$1.25 \cdot 10^{-8}$	$7.68 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
10	25.97	10.286	10.300	$7.32 \cdot 10^{-9}$	$5.14 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
15	25.64	10.163	10.300	$1.05 \cdot 10^{-9}$	$1.20 \cdot 10^{-7}$	$2.92 \cdot 10^{-3}$
20	25.51	10.112	10.300	$2.86 \cdot 10^{-10}$	$4.52 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$
25	25.50	10.110	10.300	$1.07 \cdot 10^{-10}$	$2.17 \cdot 10^{-8}$	$2.92 \cdot 10^{-3}$

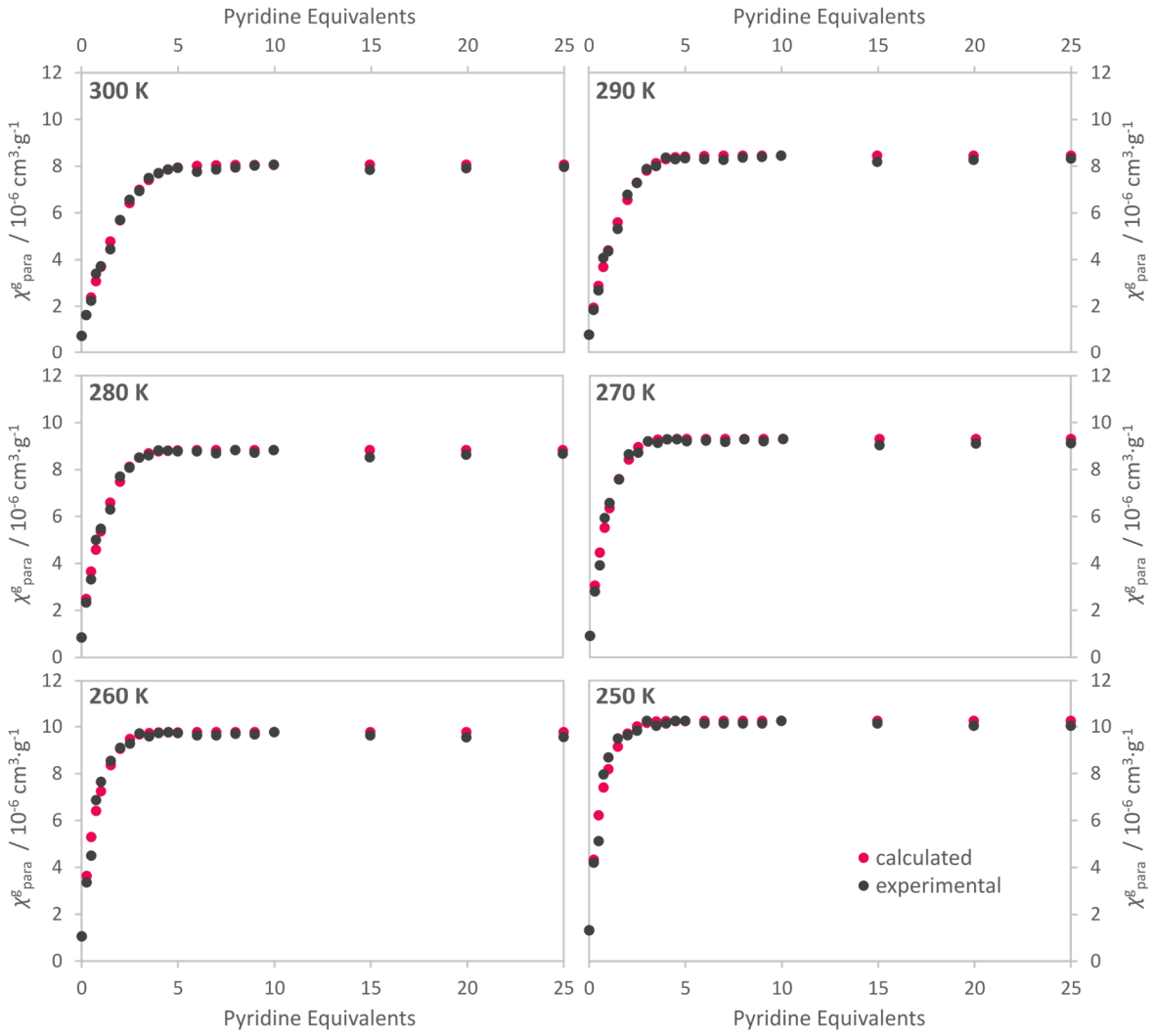

Figure S15. Experimental (black) and calculated pyridine titration curves (red) of **1d** in DCM-d_2 at different temperatures for the evaluation with the dimer model.

Fitted straight lines from van't Hoff Plots:

$$\ln K_{1S} = 940.20 \cdot \frac{1}{T} + 0.26 \qquad \text{(S12)}$$

$$\ln K_2 = 4743.62 \cdot \frac{1}{T} - 10.36 \qquad \text{(S13)}$$

S3 Selected Crystal Data

Table S24. Selected crystal data and details of the structure refinements.

	1a	**1a**$(py)_2$	**1a**$_2(EtOH)_3$
Formula	$C_{15}H_{12}N_2NiO_5$	$C_{32.50}H_{29.50}N_{5.50}NiO_5$	$C_{42}H_{60}N_4Ni_2O_{16}$
M / g·mol^{-1}	358.98	635.82	994.36
Crystal system	monoclinic	monoclinic	triclinic
Space group	$C2/c$	$P2_1/n$	P-1
a / Å	21.7637(9)	11.4677(2)	13.5292(9)
b / Å	6.8956(3)	16.1148(4)	13.8175(11)
c / Å	18.7940(7)	15.6428(4)	14.1756(11)
α / °	90	90	92.609(7)
β / °	101.478(3)	90.183(2)	100.302(6)
γ / °	90	90	116.725(6)
V / Å^3	2764.1(2)	2890.77(11)	2304.7(3)
T / K	170	170	170
Z	8	4	2
D_{calc} / mg·m^3	1.725	1.461	1.433
μ / mm^{-1}	1.433	0.724	0.890
θ_{max} / °	26.005	27.899	26.004
min/max. trans.	0.7360/0.8440	0.8554/0.9375	0.8064/0.9093
Refl. collected	11650	35572	17517
Unique refl.	2717	6890	8835
R_{int}	0.0526	0.0317	0.0347
Refl. [$F_0>4\sigma(F_0)$]	2151	6048	6489
Parameters	210	399	609
R_1 [$F_0>4\sigma(F_0)$]	0.0559	0.0356	0.0500
wR_2	0.1121	0.0829	0.1201
GOF	1.073	1.041	1.039
$\Delta\rho_{max/min}$ / e·Å^{-3}	0.556/ -0.452	0.492/-0.413	0.346/ -0.501

S3.1 [6,6'-(1-methoxy1,1-ethyanediyl)bis(2-pyridinecarboxylato-N,O)]nickel(II) (1a)

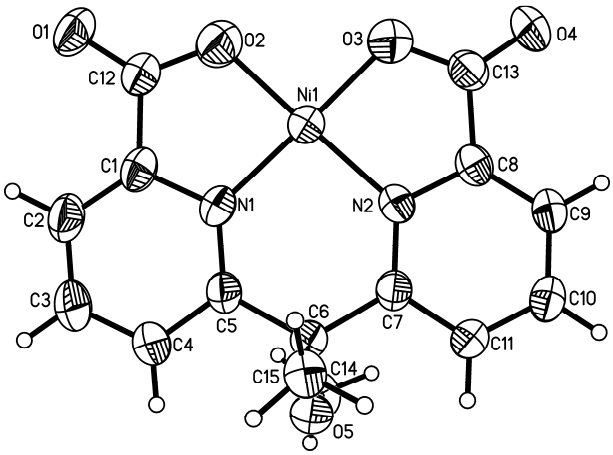

Figure S16. ORTEP plot of **1a** with labeling and displacement ellipsoids drawn at the 50 % probability level.

Table S25. Selected bond lengths [Å] and angles [°] for **1a**.

Ni(1)-O(3)	1.850(3)	Ni(1)-N(1)	1.863(4)
Ni(1)-O(2)	1.853(3)	Ni(1)-N(2)	1.865(4)
O(3)-Ni(1)-O(2)	92.07(16)	O(3)-Ni(1)-N(2)	85.89(15)
O(3)-Ni(1)-N(1)	176.70(16)	O(2)-Ni(1)-N(2)	177.31(16)
O(2)-Ni(1)-N(1)	85.51(15)	N(1)-Ni(1)-N(2)	96.46(15)

S3.2 [6,6'-(1-methoxy-1,1-ethanediyl)bis(2-pyridinecarboxylato-N,O)]di(pyridine)nickel(II) (1a(py)$_2$)

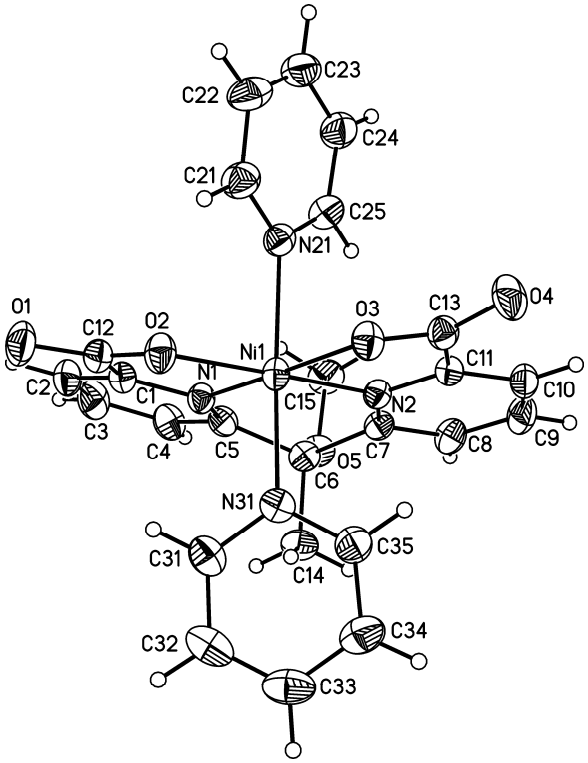

Figure S17. ORTEP plot of **1a**(py)$_2$ with labeling and displacement ellipsoids drawn at the 50% probability level.

Table S26. Selected bond lengths [Å] and angles [°] for **1a**(py)$_2$.

Ni(1)-O(2)	2.0308(12)	Ni(1)-O(3)	2.0330(11)
Ni(1)-N(1)	2.0322(13)	Ni(1)-N(31)	2.1422(14)
Ni(1)-N(2)	2.0322(13)	Ni(1)-N(21)	2.2075(14)
O(2)-Ni(1)-N(1)	82.01(5)	N(2)-Ni(1)-N(31)	90.81(5)
O(2)-Ni(1)-N(2)	173.37(5)	O(3)-Ni(1)-N(31)	90.64(5)
N(1)-Ni(1)-N(2)	91.48(5)	O(2)-Ni(1)-N(21)	88.73(5)
O(2)-Ni(1)-O(3)	104.15(5)	N(1)-Ni(1)-N(21)	91.59(5)
N(1)-Ni(1)-O(3)	172.43(5)	N(2)-Ni(1)-N(21)	90.22(5)
N(2)-Ni(1)-O(3)	82.25(5)	O(3)-Ni(1)-N(21)	84.22(5)
O(2)-Ni(1)-N(31)	90.85(5)	N(31)-Ni(1)-N(21)	174.58(5)
N(1)-Ni(1)-N(31)	93.70(5)	C(25)-N(21)-Ni(1)	123.81(11)
C(5)-N(1)-Ni(1)	128.52(11)	C(21)-N(21)-Ni(1)	118.73(12)
C(1)-N(1)-Ni(1)	110.96(10)	C(35)-N(31)-Ni(1)	119.95(12)
C(7)-N(2)-Ni(1)	128.86(11)	C(31)-N(31)-Ni(1)	122.71(12)
C(11)-N(2)-Ni(1)	111.06(10)	C(13)-O(3)-Ni(1)	113.60(10)
C(12)-O(2)-Ni(1)	114.38(10		

S3.3 (Di{ethanol}{6-[1-methoxy-1-(2-carboxylato-6-pyridyl-N,O)-1-ethyl][μ^2-2-pyridinecarboxylato-N,O,O']}nickel(II))(ethanol)[6,6'-(1-methoxy-1,1-ethanediyl)bis(2-pyridinecarboxylato-N,O)]nickel(II) ($\mathbf{1a}_2(EtOH)_3$)

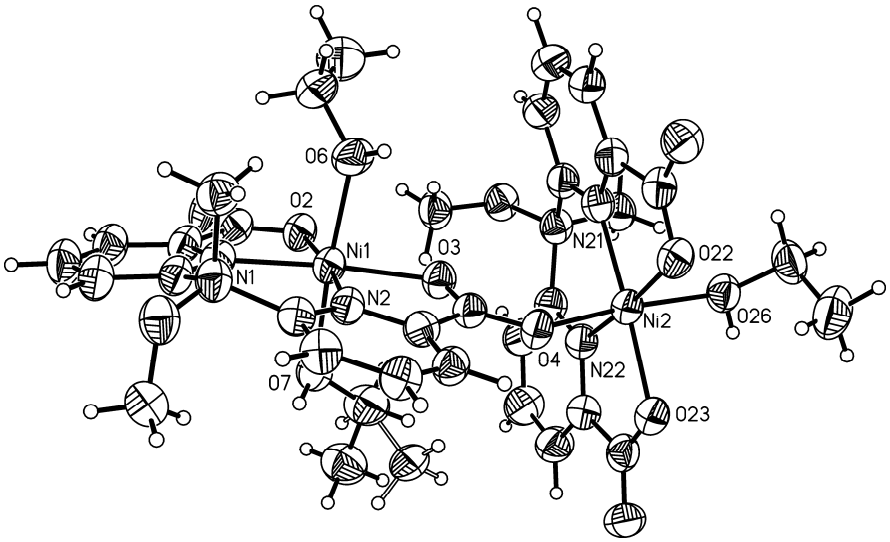

Figure S18. ORTEP plot of $\mathbf{1a}_2(EtOH)_3$ with labeling and displacement ellipsoids drawn at the 50% probability level. Please note that only selected atoms are labeled and that disordering is shown as full and open bonds.

Table S27. Selected bond lengths [Å] and angles [°] for $\mathbf{1a}_2(EtOH)_3$.

Ni(1)-N(2)	2.015(3)	Ni(2)-N(21)	2.020(3)
Ni(1)-O(2)	2.031(3)	Ni(2)-N(22)	2.028(3)
Ni(1)-O(3)	2.035(2)	Ni(2)-O(23)	2.048(2)
Ni(1)-N(1)	2.036(3)	Ni(2)-O(22)	2.049(2)
Ni(1)-O(6)	2.091(2)	Ni(2)-O(26)	2.127(2)
Ni(1)-O(7)	2.136(2)	O(4)-Ni(2)	2.055(2)
N(2)-Ni(1)-O(2)	172.76(11)	N(21)-Ni(2)-N(22)	92.44(11)
N(2)-Ni(1)-O(3)	83.07(10)	N(21)-Ni(2)-O(23)	174.39(11)
O(2)-Ni(1)-O(3)	103.48(10)	N(22)-Ni(2)-O(23)	81.95(11)
N(2)-Ni(1)-N(1)	91.30(12)	N(21)-Ni(2)-O(22)	82.04(10)
O(2)-Ni(1)-N(1)	82.02(11)	N(22)-Ni(2)-O(22)	174.38(10)
O(3)-Ni(1)-N(1)	173.87(11)	O(23)-Ni(2)-O(22)	103.57(10)
N(2)-Ni(1)-O(6)	90.78(11)	N(21)-Ni(2)-O(4)	94.86(10)
O(2)-Ni(1)-O(6)	92.63(10)	N(22)-Ni(2)-O(4)	95.87(11)
O(3)-Ni(1)-O(6)	86.89(10)	O(23)-Ni(2)-O(4)	85.56(9)
N(1)-Ni(1)-O(6)	95.64(11)	O(22)-Ni(2)-O(4)	85.68(10)
N(2)-Ni(1)-O(7)	90.37(10)	N(21)-Ni(2)-O(26)	90.79(10)
O(2)-Ni(1)-O(7)	86.74(10)	N(22)-Ni(2)-O(26)	88.05(11)
O(3)-Ni(1)-O(7)	88.81(9)	O(23)-Ni(2)-O(26)	89.22(10)
N(1)-Ni(1)-O(7)	88.81(10)	O(22)-Ni(2)-O(26)	90.97(10)
O(6)-Ni(1)-O(7)	175.38(11)	O(4)-Ni(2)-O(26)	172.97(10)

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