Supporting Information for:

The Aldimine Effect in Bis(imino)pyridine Complexes: Non-Planar Nickel(I) Complexes of a Bis(aldimino)pyridine Ligand

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Table of Contents *Page*

1. General methods and procedures

All reactions involving air-sensitive materials were executed in a nitrogen-filled glovebox. L^1 was synthesized as previously described.[1] $NiCl_2$(dme) (dme = dimethoxyethane), $NiBr_2$(dme), and $CoCp^*_2$ (Cp^* = pentamethylcyclopentadienyl) were purchased from Aldrich and used as received. All solvents were purchased from Fisher scientific and were of HPLC grade. The solvents were purified using an MBRAUN solvent purification system and stored over 3-Å molecular sieves. The complexes were characterized by ^{1}H NMR spectroscopy (**4** and **5**), X-ray crystallography (**4**-**7**), elemental analysis (**4**-**7**), EPR spectroscopy (**6** and **7**), Evans method (**4**-**7**), and UV-vis spectroscopy (**6** and **7**).[2] NMR spectra were recorded at the Lumigen Instrument Center (Wayne State University) on a Varian Mercury 400 MHz NMR Spectrometer in C_6D_6 or CD_2Cl_2 at room temperature. Elemental analyses were performed by Midwest Microlab LLC. UV-visible spectra were obtained on a Shimadzu UV-1800 spectrometer. High-frequency EPR spectra were recorded on a home-built spectrometer fitted with a 17 T superconducting magnet (Oxford Instruments) at the EMR facility of NHMFL. This transmission-type spectrometer uses cylindrical lightpipes and microwaves that were generated by a phase-locked oscillator (Virginia Diodes) operating at a frequency of 13 ± 1 GHz and generating its harmonics, of which the 4th, 8th, 16th, 24th and 32nd were available. The spectral simulations were performed using the Spin Count software suite developed by Dr. M. P. Hendrich at CMU that can be downloaded from http://www.chem.cmu.edu/groups/hendrich/facilities/index.html.

2. Synthesis and characterization of compounds

Compound 4 [Ni(L^1)Cl_2]. To a solution of nickel(II) chloride dimethoxyethane complex (48 mg, 0.22 mmol) in 3 mL THF was added a solution of L^1 (100 mg, 0.22 mmol) in THF (2 mL). The reaction was stirred at ambient temperature for 1.5 h. Volatiles were removed *in vacuo*, and the resulting brown solid was washed with ether (10 mL). The solid was dissolved in CH_2Cl_2 (2 mL), covered with ether (20 mL), and allowed to stand for 24 h at −30 °C. The solid was collected, washed with ether, and dried, giving the product as orange crystalline solid (119 mg 0.20 mmol, 93%). ^{1}H NMR (CD_2Cl_2): δ 66.4, 15.2, 14.2, 5.2, 1.7, −4.2 ppm. Anal. Calcd for $C_{31}H_{39}N_3Cl_2Ni$: C, 63.84; H, 6.74; N, 7.20. Found: C, 63.46; H, 6.52; N, 7.09. μ_{eff} (Evans method, CD_3CN, 298 K): 3.12 μ_B. X-ray quality crystals were obtained by vapor diffusion of ether into a saturated THF solution of purified **4**.

Compound 5 [Ni(L^1)Br_2]. To a solution of nickel(II) bromide dimethoxyethane complex (68 mg, 0.22 mmol) in THF (3 mL) was added a solution of L^1 (100 mg, 0.22 mmol) in THF (2 mL). The reaction was stirred at ambient temperature for 1.5 h. Volatiles were removed *in vacuo*, and the resulting brown solid was washed with ether (10 mL). The solid was dissolved in CH_2Cl_2 (2 mL), covered with ether (20 mL), and allowed to stand for 24 h at −30 °C. The solid was collected, washed with ether, and dried, giving the product as brown crystalline solid (127 mg 0.19 mmol, 86%). ^{1}H NMR (CD_2Cl_2): δ 68.9, 13.9, 11.4, 3.8, 1.6, −4.9 ppm. Anal. Calcd for $C_{31}H_{39}N_3Br_2Ni$: C, 55.39; H, 5.85; N, 6.25. Found: C, 55.30; H, 6.16; N, 5.99. μ_{eff} (Evans method, CD_3CN, 298 K): 3.10 μ_B. X-ray quality crystals were obtained by slow diffusion of ether into a saturated CH_2Cl_2 solution of **5**.

Compound 6 [Ni(L^1)Cl]. To the orange solution of compound **4** [Ni(L^1)Cl_2] (100 mg, 0.17 mmol) in THF (3 mL) was added a solution of $CoCp^*_2$ (decamethylcobaltocene, 56 mg, 0.17 mmol) in THF (3 mL). The reaction color turned dark purple. The reaction mixture was stirred at ambient temperature for 2 h, filtered, and evaporated. The resulting black solid was washed with hexanes and ether, and dissolved in THF (ca. 1 mL). Diffusion of ether into the THF solution at −30 °C led to the formation of black crystals. The crystals were dried under vacuum for several hours to give compound **6** in 37% yield (35 mg, 0.06 mmol). Compound **6** is air- and moisture-sensitive. ^{1}H NMR (CD_2Cl_2, selected peaks) δ 48.5, 15.1 ppm. Anal. Calcd for $C_{31}H_{39}N_3ClNi$: C, 67.97; H, 7.18; N, 7.67. Found: C, 67.68; H, 7.05; N, 7.20. μ_{eff} (Evans method, C_6D_6, 298 K): 1.09 μ_B. Absorption Spectrum (toluene): λ_{max} (ε_M) 331 (13429) 465 (2413) 532 (1750) 694 (940) 910 (1028) nm. X-ray quality crystals for the X-ray data collection were obtained by vapor diffusion of ether into a saturated THF solution of purified **6**.

Compound 7 [Ni(L^1)Br] (crystallized as a mixture of different solvate forms 7a/7b). To the orange solution of compound **5** [Ni(L^1)Br_2] (100 mg, 0.15 mmol) in THF (3 mL) was added a solution of $CoCp^*_2$ (49 mg, 0.15 mmol) in THF (3 mL). The reaction color turned dark purple. The reaction mixture was stirred at ambient temperature for 2 h, filtered, and evaporated. The resulting purple-black solid was washed with hexanes and ether, and dissolved in THF (ca. 1 mL). Vapor diffusion of ether into the THF solution at −30 °C led to the formation of dark purple crystals (mixture of **7a**/**7b**). The crystals were dried under vacuum for several hours to give compound **7** in 47% yield (42 mg, 0.07 mmol). Compound **7** is air- and moisture-sensitive. ^{1}H NMR (CD_2Cl_2, selected peaks) δ 49.8, -43.9 ppm. Anal. Calcd for $C_{31}H_{39}N_3BrNi$: C, 62.87; H, 6.64; N, 7.09. Found: C, 63.21; H, 6.61; N, 7.30. μ_{eff} (Evans method, C_6D_6, 298 K): 1.35 μ_B. Absorption Spectrum (toluene): λ_{max} (ε_M) 331 (7979) 534 (1369) 699 (759) 933 (835) nm. X-ray

quality crystals for the X-ray data collection were obtained by vapor diffusion of ether into a saturated THF solution of purified **7**.

Reaction of compound 7 [Ni(L^1)Br] with atmospheric O_2. Black THF solution (2 mL) of compound 7 (31 mg, 0.052 mmol) was exposed to ambient atmosphere. A facile color change to dark orange was observed immediately, and the solution was left to stir for 5 min. After, volatiles were removed *in vacuo*. The ^{1}H NMR of the crude reaction mixture demonstrates the presence of two species: a free ligand and compound **4**. Hexane extraction of the crude reaction mixture leads to the isolation of 9 mg of free ligand (Figure S6, δ 8.49 (s, 2H), 8.25 (d, 2H), 7.21 (t, 1H), 7.10 (m, 6H), 3.09 (sept, 2H), 1.10 (d, 24H) ppm). The material was then washed with diethyl ether (20 mL). THF extraction of the remaining material led to the isolation of 4 mg of compound **2** (Figure S7, δ 68.66, 13.91, 11.17, 3.91, 1.55, -4.93 ppm).

3. X-ray crystallographic details

The structures of **4-7** were confirmed by X-ray analysis. The crystals were mounted on a Bruker APEXII/Kappa three circle goniometer platform diffractometer equipped with an APEX-2 detector. A graphic monochromator was employed for wavelength selection of the Mo Kα radiation (λ = 0.71073 Å). The data were processed and the structure was solved using the APEX-2 software supplied by Bruker-AXS. The structure was refined by standard difference Fourier techniques with SHELXL (6.10 v., Sheldrick G. M., and Siemens Industrial Automation, 2000). Hydrogen atoms were placed in calculated positions using a standard riding model and refined isotropically; all other non-solvent atoms were refined anisotropically. The crystal structure of **2** contained a disordered molecule of CH_2Cl_2 in the asymmetric unit. The disorder was modeled by finding two alternative conformations. The structures of **6** and **7a** contained two

THF molecules per asymmetric unit. In both cases, one of the THF molecules was found to be disordered over two positions. For the disordered solvents, no anisotropic refinement and hydrogens atoms attachment were undertaken. The structure of **7b** contained a disordered ether solvent and THF solvent in the asymmetric unit. The disorder in ether was modeled using two alternative conformations. The structure of **7b** also demonstrates elongated ellipsoids for one of the isopropyl groups indicative of some disorder in its position. We were not able to model this disorder using the two conformations model commonly used for the isopropyl group disorder.

Table S1. Crystal and structure refinement data for **4-7**.

	4	**5**	**6**	**7a**	**7b**
formula	$C_{31}H_{39}Cl_2N_3Ni$	$C_3H_{39}Br_2N_3Ni$• DCM	$C_{31}H_{39}ClN_3Ni$• 2THF	$C_{31}H_{39}BrN_3Ni$• 2THF	$C_{31}H_{39}BrN_3Ni$• THF•OEt_2
Fw, g/mol	583.26	755.09	683.96	728.42	698.41
temperature	100(2)	100(2)	100(2)	100(2)	100(2)
cryst syst	orthorhombic	monoclinic	triclinic	triclinic	triclinic
space group	$P2_12_12_1$	$P2_1$/n	*P*-1	*P*-1	*P*-1
color	orange	brown	black	black	black
Z	4	4	2	2	2
a, Å	13.6222(7)	9.7870(6)	9.7349(5)	9.8908(13)	9.7274(10)
b, Å	14.2676(8)	26.3927(17)	12.3308(7)	12.3807(14)	14.2320(15)
c, Å	15.7854(8)	13.7739(8)	15.6197(8)	15.5767(18)	14.9719(13)
α, deg	90.00	90.00	87.490(3)	86.987(3)	111.974(4)
β, deg	90.00	108.906(3)	75.776(2)	75.727(5)	99.695(3)
γ, deg	90.00	90.00	85.562(3)	85.167(4)	101.376(2)
V, A^3	3068.0(3)	3365.9(4)	1811.45(17)	1841.0(4)	1816.3(3)
d_{calcd}, g/cm^3	1.263	1.490	1.254	1.314	1.277
μ, mm^{-1}	0.830	3.135	0.646	1.648	1.666
2θ, deg	62.72	57.04	57.02	49.00	56.00
R_1[a] (all data)	0.0401	0.0429	0.0542	0.0491	0.0869
wR_2[b] (all data)	0.0782	0.0700	0.1307	0.1019	0.1421
R_1[a] [(I>2σ)]	0.0342	0.0301	0.0470	0.0388	0.0549
wR_2[b] [(I>2σ)]	0.0765	0.0653	0.1257	0.0983	0.1263
GOF (F^2)	1.019	1.022	1.040	1.046	1.024

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = (\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma(w(F_o^2)^2))^{1/2}$. [c] GOF = $(\Sigma\, w(F_o^2 - F_c^2)^2/(n-p))^{1/2}$ where *n* is the number of data and *p* is the number of parameters refined.

4. Crystal structures of 4, 5, 6, 7b

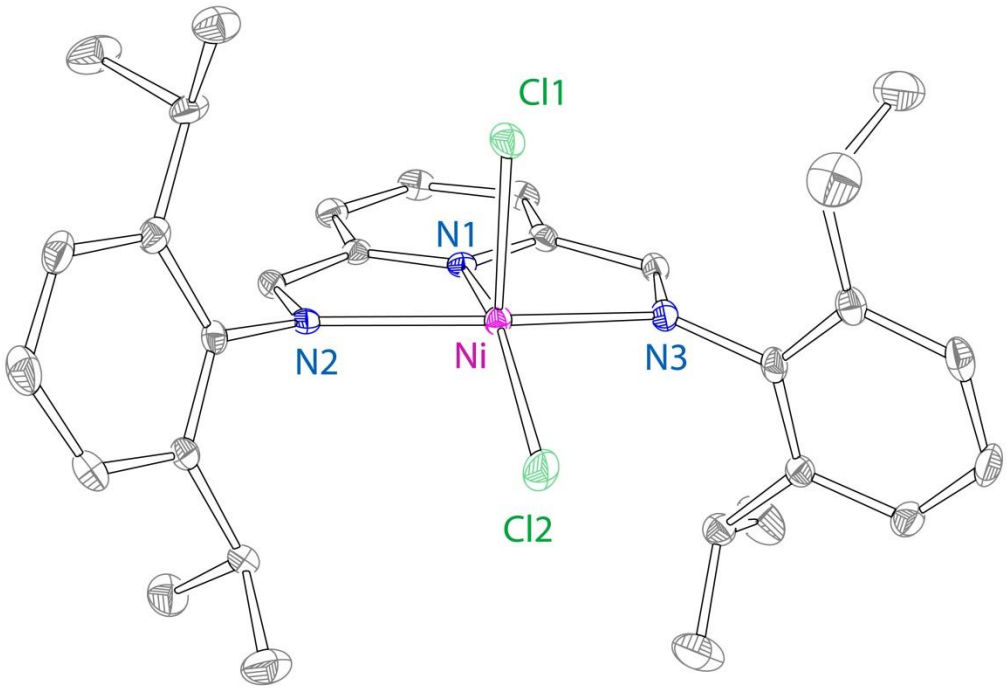

Figure S1. Crystal structure of **4**, 50% probability ellipsoids. H atoms are omitted for clarity.

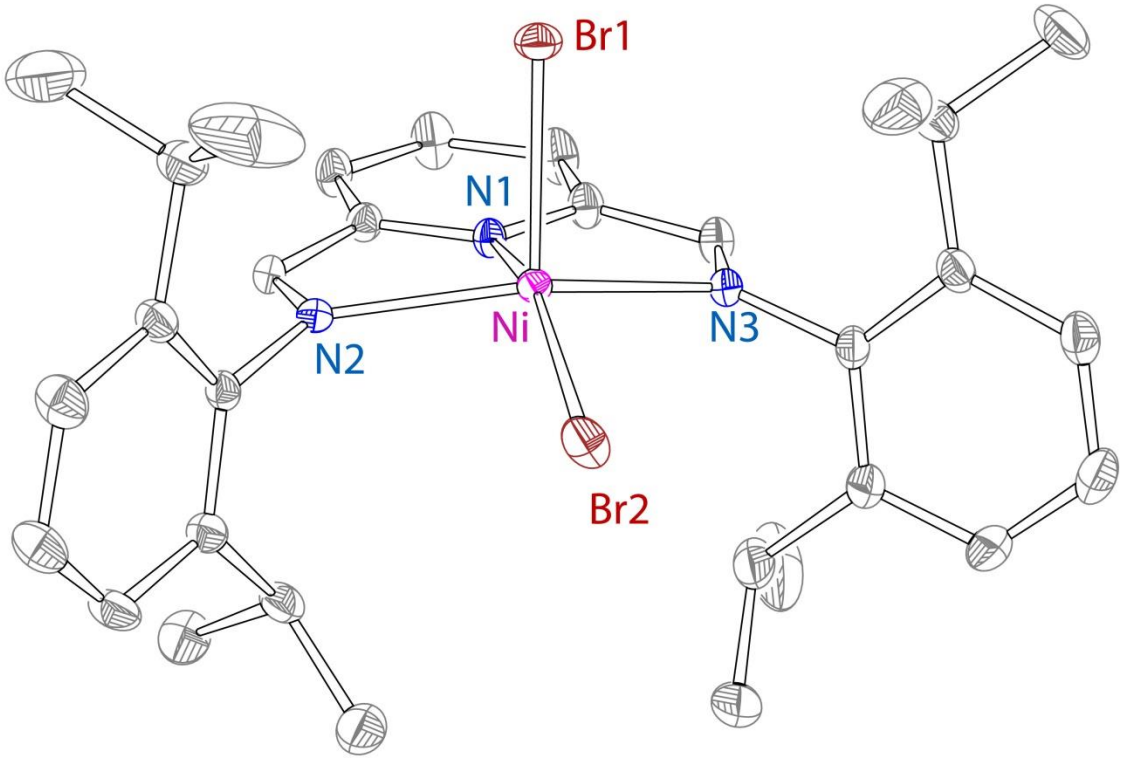

Figure S2. Crystal structure of **5**, 50% probability ellipsoids. H atoms and the disordered solvent molecule are omitted for clarity.

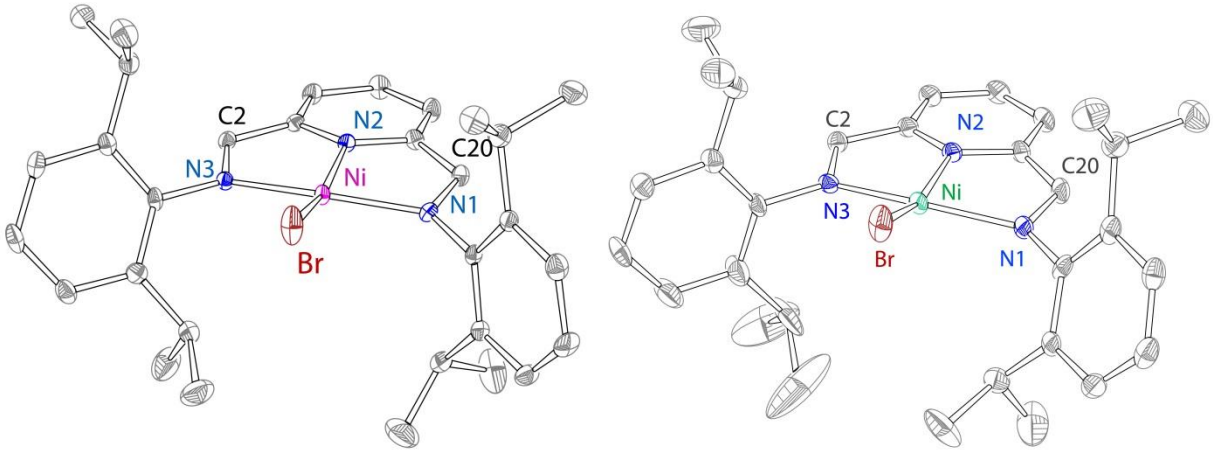

Figure S3. Crystal structure of **7a** (left) and **7b** (right), 50% probability ellipsoids. H atoms and the solvent molecules are omitted for clarity. Selected bond distances for **7a**: Ni Br 2.308(1) Å, Ni N2 1.854(3) Å, Ni N1 1.982(2) Å, Ni N3 2.005(3) Å, N1 C20 1.303(4) Å, N3 C2 1.294(4) Å. Selected bond distances for **7b**: Ni Br 2.321(1) Å, Ni N2 1.865(3) Å, Ni1 N1 2.018(3) Å, Ni N3 2.006(3) Å, N3 C2 1.307(5) Å, N1 C20 1.309(5) Å.

5. ^{1}H NMR spectra

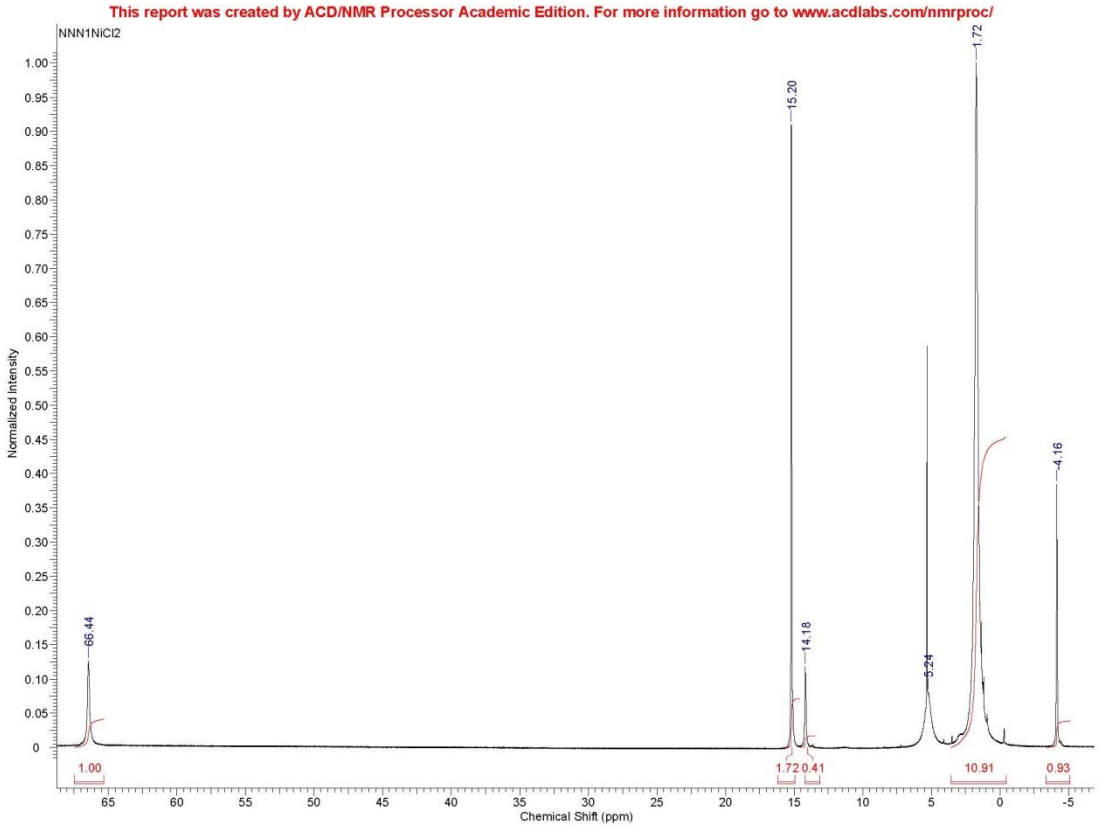

Figure S4. ^{1}H NMR spectrum of compound **4** in CD_2Cl_2**.**

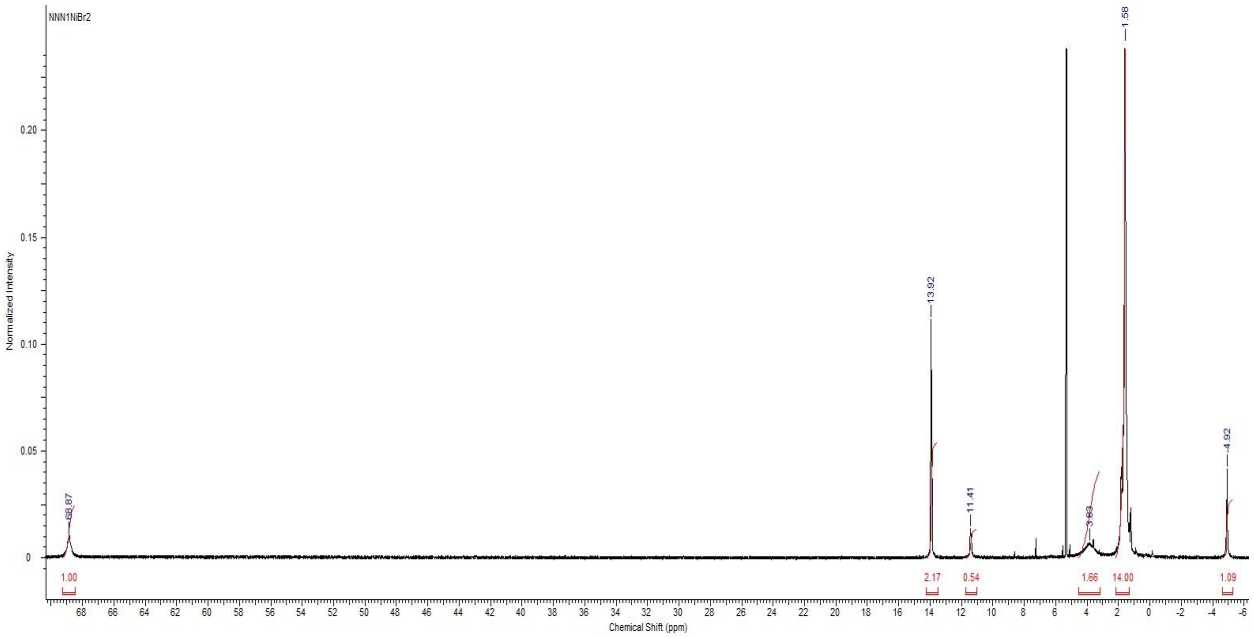

Figure S5. ^{1}H NMR spectrum of compound **5** in CD_2Cl_2.

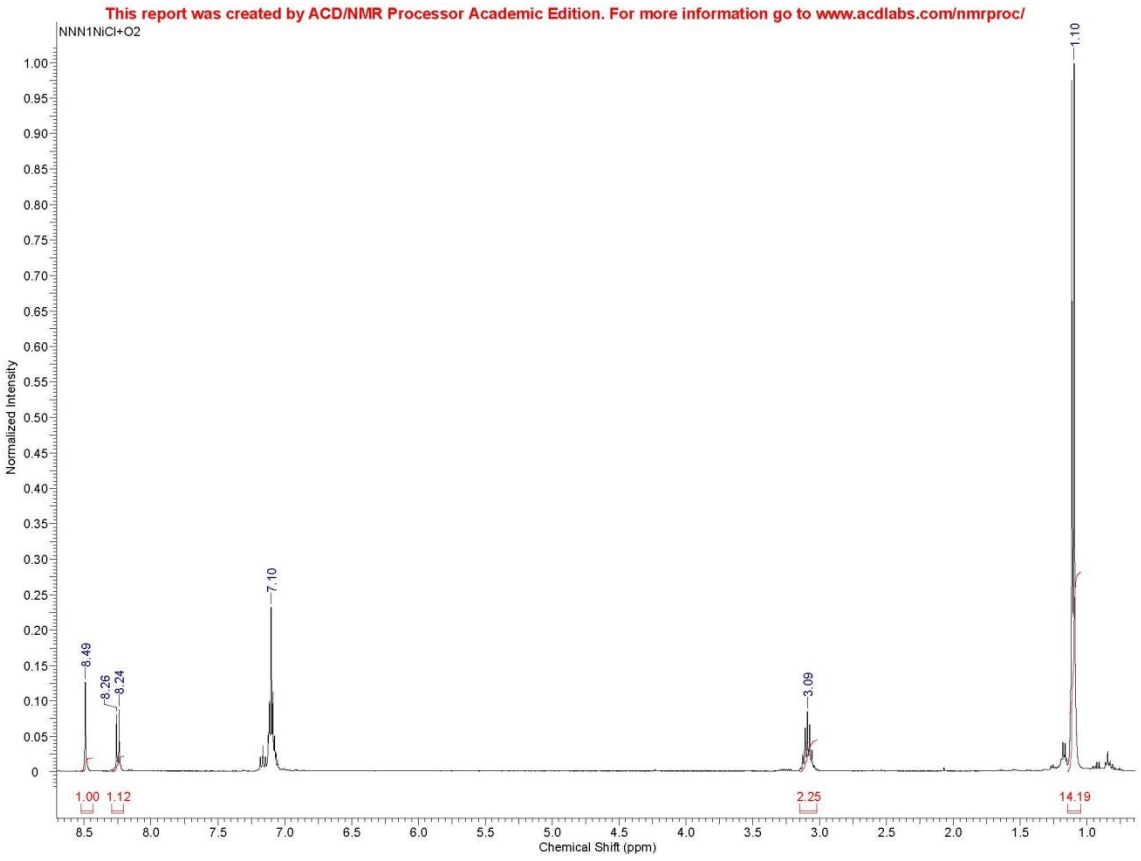

Figure S6. ^{1}H NMR spectrum of the extracted hexane layer of the reaction of compound **7** with O_2.

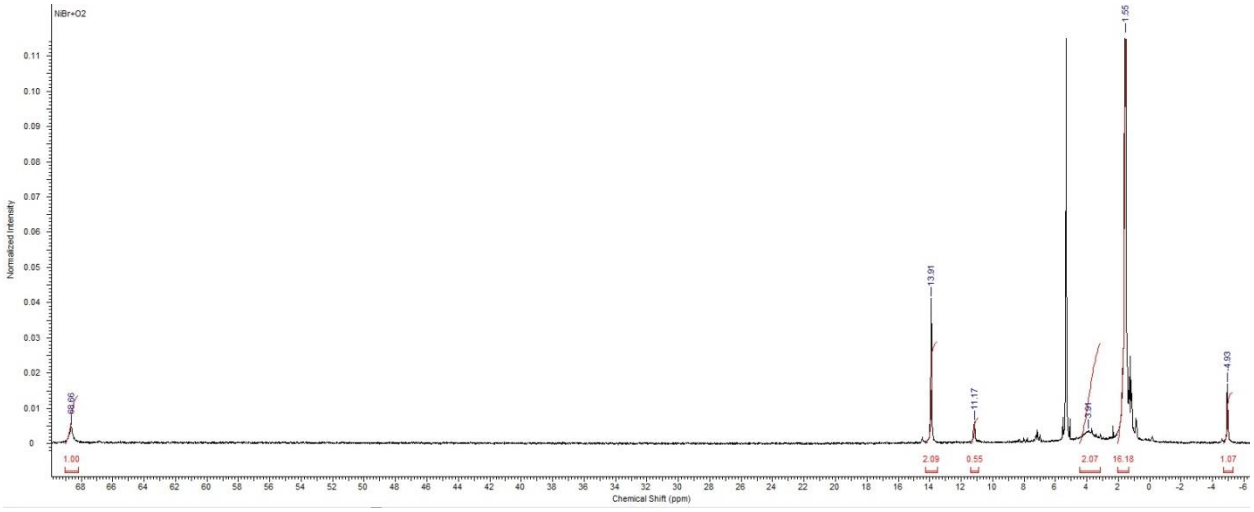

Figure S7. ^{1}H NMR spectrum of the extracted THF layer of the reaction of compound **7** with O_2.

6. UV-vis spectra

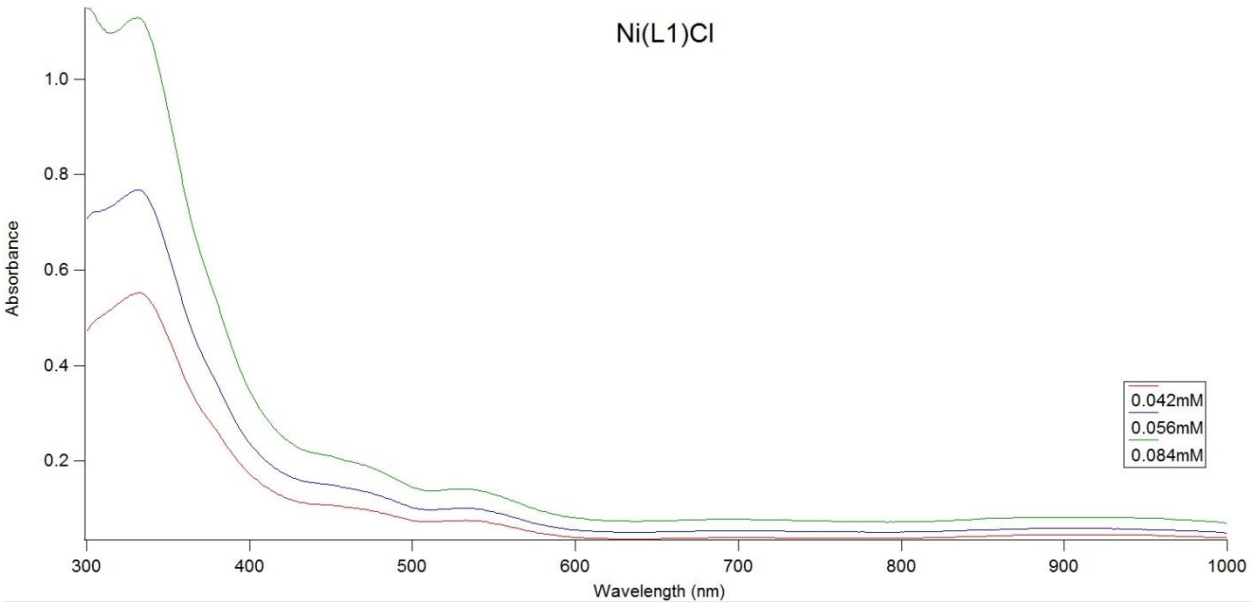

Figure S8. UV-vis spectra of Ni(L^2)Cl (compound **6**) at three concentrations (see legend). The spectra were collected in the range of 300-1000 nm.

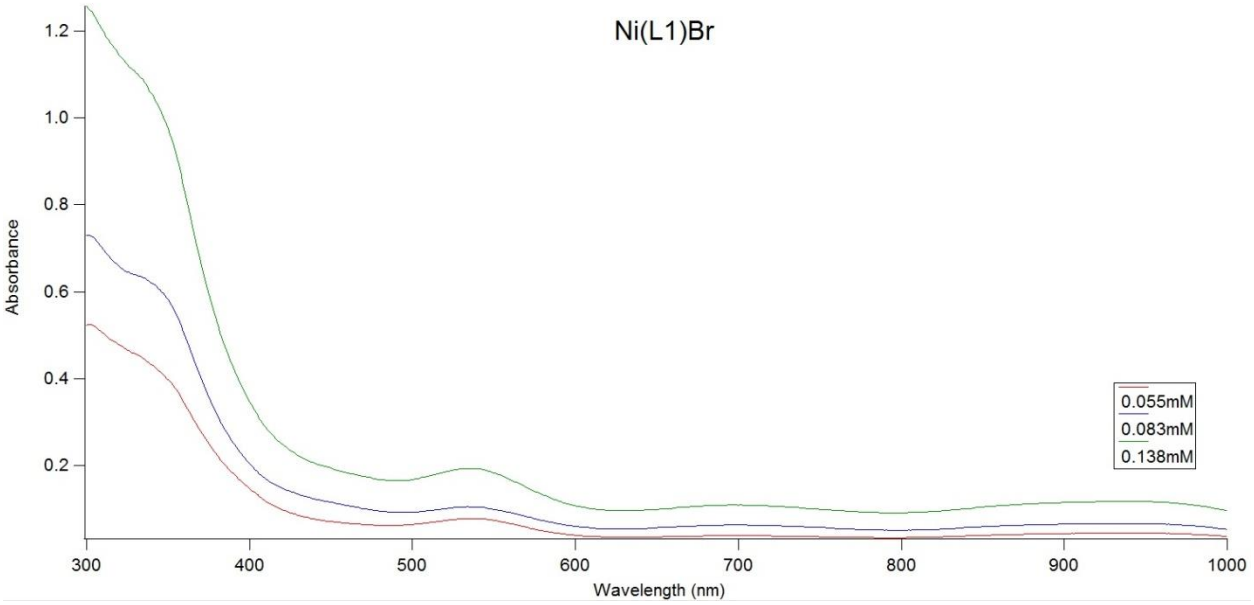

Figure S9. UV-vis spectra of Ni(L1)Br (compound **7**) at three concentrations (see legend). The spectra were collected in the range of 300-1000 nm.

7. Computational Details

Electronic structure calculations were carried out using DFT[2] as implemented in Gaussian09.[3] Geometry optimizations were initially performed at the B3LYP[4-7] level of theory using 6-31G(d,p) for main group atoms and LANL2DZ[8] for nickel, but the bond lengths differed significantly from the experimental X-ray structure for **6** and **7a/7b** (Table S2). Thus, we re-optimized the structures with larger triple-zeta basis sets for all atoms (6-311G(d,p) and def2TZVP[9]) and found similar results for both basis sets that matched the experimental metrics (Table S2) other than the N_{pyr}–Ni–X angle. We chose to use the 6-311G(d,p) basis set for further analysis due to the difference in calculation cost. No symmetry constraints were imposed during geometry optimizations, and multiple starting geometries were found to converge to similar geometries other than trivial differences in the methyl groups of the aryl arms. All optimized structures were confirmed to have stable wavefunctions,[10-11] and to be local minima by analyzing the harmonic frequencies.[12-13] Cartesian coordinates for all species, and frequencies and thermodynamics for fully optimized species with the 6-311G(d,p) basis set, may be found in Tables S6, S7, and S8.

We performed constrained optimizations varying that angle from its optimized value near linearity to a significant bend of 140°. This range covers all of the experimentally observed N_{pyr}–Ni–X angles in the X-ray structures. A summary of the bond length metrics, the deviation of the imino aryl group torsional angle from perpendicular, and spin densities condensed to Ni, X, and the bis-iminopyridine (L) are shown in Tables S3 and 1 for **6** and **7**, respectively. The angle deviation has a small energetic penalty of ~2-4 kcal/mol to reach the experimentally observed angles. It is interesting to note that as the angle varies, there is a strong correlation to the rotation of the bulky imino aryl groups. Is it possible that the ability (or inability) of these aryl groups to rotate due to the C_{im} substituent is responsible for the stark difference in the aldimine and ketimine ligands? We performed analogous constrained optimizations on Rohde's compound **1** and the analogous Br complex (**1-Br**) (Tables S4 and S5). Qualitatively similar results are found, but the energetic penalty for the angle variation is larger (~1.5x) and the variation in the aryl rotation is much smaller (14-18° vs. 22–25°). Based on this computational evidence, we interpret the effect of the aldimine versus ketimine ligand to be largely steric in nature.

Table S2. Comparison of primary coordination sphere metrics (Angstroms, degrees) for computationally optimized (*S* = 1/2 only) and X-ray structures. Average values from the two arms are recorded for the X-ray data, and the computational data only differed in decimal places beyond those reported here.

Metric	$\mathbf{6}_{\text{x-ray}}$	$\mathbf{6}_{\text{calc}}$ 6-31G(d,p)	$\mathbf{6}_{\text{calc}}$ 6-311G(d,p)	$\mathbf{6}_{\text{calc}}$ def2TZVP
$Ni–N_{pyr}$	1.859(2)	1.946	1.826	1.844
$Ni–N_{imine}$	1.988(6)	2.212	1.930	1.968
Ni–X	2.186(1)	2.230	2.181	2.183
$N_{pyr}–C_{pyr}$	1.358(3)	1.356	1.366	1.361
$C_{pyr}–C_{imine}$	1.444(3)	1.459	1.431	1.430
$C_{imine}–N_{imine}$	1.307(3)	1.291	1.320	1.310
$N_{pyr}–Ni–X$	162.3(1)	168.7	177.6	175.4

Metric	$\mathbf{7}_{\text{x-ray}}$	$\mathbf{7}_{\text{calc}}$ 6-31G(d,p)	$\mathbf{7}_{\text{calc}}$ 6-311G(d,p)	$\mathbf{7}_{\text{calc}}$ def2TZVP
$Ni–N_{pyr}$	1.856(3)	1.953	1.835	1.852
$Ni–N_{imine}$	1.993(6)	2.215	1.943	1.983
Ni–X	2.309(1)	2.349	2.324	2.337
$N_{pyr}–C_{pyr}$	1.364(3)	1.355	1.365	1.360
$C_{pyr}–C_{imine}$	1.445(6)	1.460	1.430	1.430
$C_{imine}–N_{imine}$	1.300(5)	1.290	1.319	1.309
$N_{pyr}–Ni–X$	161.4(1)	166.4	176.7	174.1

Table S3. Summary of structural parameters, spin densities, and electronic energy (relative to relaxed minimum) for optimized structures holding N_{py}–Ni–Cl fixed for the aldimine ligand (**6**).

$\mathbf{N_{py}–Ni–Cl}$ (fixed)	$\mathbf{177.6^{o,a}}$	$\mathbf{170^{o}}$	$\mathbf{160^{o}}$	$\mathbf{150^{o}}$	$\mathbf{140^{o}}$
Ni–Cl	2.181	2.187	2.197	2.208	2.219
$Ni–N_{py}$	1.826	1.833	1.842	1.854	1.866
$Ni–N_{im}$	1.930	1.943	1.961	1.981	2.000
$N_{py}–C_{py}$	1.366	1.366	1.365	1.363	1.360
$C_{py}–C_{im}$	1.431	1.432	1.434	1.437	1.440
$C_{im}–N_{im}$	1.320	1.318	1.315	1.313	1.311
$C_{im}–N_{im}–C_{Ar}–C_{Ar,ortho}$	3.5	6.6	13.3	16.4	21.7
Ni spin density	0.04	0.08	0.15	0.22	0.31
Br spin density	0.01	0.00	–0.02	–0.04	–0.05
L spin density	0.95	0.92	0.83	0.82	0.74
Relative E(SCF) kcal/mol	0.00	0.50	2.19	4.66	7.64

[a]Fully optimized minimum
[b]Measures the deviation from perpendicular

Table S4. Summary of structural parameters, spin densities, and electronic energy (relative to relaxed minimum) for optimized structures holding N_{py}–Ni–Br fixed for the aldimine ligand (**7**).

N_{py}–Ni–Br	**176.7°,[a]**	**170°**	**160°**	**150°**	**140°**
Ni–Br	2.324	2.328	2.336	2.342	2.349
Ni–N_{py}	1.835	1.840	1.848	1.858	1.870
Ni–N_{im}	1.943	1.954	1.972	1.992	2.013
N_{py}–C_{py}	1.365	1.365	1.364	1.362	1.359
C_{py}–C_{im}	1.430	1.432	1.434	1.437	1.440
C_{im}–N_{im}	1.319	1.317	1.315	1.313	1.310
C_{im}–N_{im}–C_{Ar}–$C_{Ar,ortho}$	5.8	8.2	17.1	23.6	25.2
Ni spin density	0.06	0.10	0.17	0.26	0.36
Br spin density	0.01	–0.01	–0.03	–0.04	–0.05
L spin density	0.93	0.91	0.84	0.78	0.79
Relative E(SCF) kcal/mol	0.00	0.25	1.68	3.91	6.66

[a]Fully optimized minimum
[b]Measures the deviation from perpendicular

Table S5. Summary of structural parameters, spin densities, and electronic energy (relative to relaxed minimum) for optimized structures holding N_{py}–Ni–Cl fixed for the ketimine ligand (**1**).

N_{py}–Ni–Cl(fixed)	**177.8°,[a]**	**170°**	**160°**	**150°**	**140°**
Ni–Cl	2.191	2.196	2.204	2.214	2.223
Ni–N_{py}	1.820	1.825	1.833	1.845	1.858
Ni–N_{im}	1.941	1.950	1.968	1.989	2.013
N_{py}–C_{py}	1.369	1.369	1.368	1.366	1.363
C_{py}–C_{im}	1.443	1.444	1.447	1.451	1.455
C_{im}–N_{im}	1.326	1.324	1.322	1.319	1.316
C_{im}–N_{im}–C_{Ar}–$C_{Ar,ortho}$[b]	5.7	6.6	10.7	14.1	14.6
Ni spin density	0.06	0.09	0.15	0.22	0.30
Cl spin density	0.00	–0.01	–0.02	–0.04	–0.05
L spin density	0.94	0.92	0.87	0.82	0.75
Relative E(SCF) kcal/mol	0.00	0.67	2.78	6.00	9.73

[a]Fully optimized minimum
[b]Measures the deviation from perpendicular

Table S6. Summary of structural parameters, spin densities, and electronic energy (relative to relaxed minimum) for optimized structures holding N_{py}–Ni–Br fixed for the ketimine ligand.

N_{py}–Ni–Br (fixed)	**177.4°[a]**	**170°**	**160°**	**150°**	**140°**
Ni–Br	2.337	2.341	2.346	2.352	2.354
Ni–N_{py}	1.829	1.833	1.840	1.850	1.865
Ni–N_{im}	1.961	1.966	1.980	2.001	2.035
N_{py}–C_{py}	1.369	1.369	1.368	1.366	1.361
C_{py}–C_{im}	1.443	1.445	1.447	1.451	1.457
C_{im}–N_{im}	1.324	1.323	1.321	1.318	1.314
C_{im}–N_{im}–C_{Ar}–$C_{Ar,ortho}$	3.0	8.9	12.8	18.4	18.8
Ni spin density	0.08	0.11	0.18	0.25	0.37
Br spin density	0.00	–0.01	–0.03	–0.04	–0.05
L spin density	0.92	0.90	0.85	0.79	0.68
Relative E(SCF) kcal/mol	0.00	0.48	2.50	5.59	9.60

[a]Fully optimized minimum
[b]Measures the deviation from perpendicular

Table S7. Cartesian coordinates (Å) for optimized structures.

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6, S=1/2
LANL2DZ/6-31G(d,p)
------------------
    Ni  -0.016765  -0.023168   0.270072
    N   -0.037467   1.922020   0.330559
    C    1.129518   2.611564   0.362782
    C   -1.219332   2.586099   0.358831
    C    1.146625   4.005178   0.441933
    C   -1.267339   3.978767   0.438795
    C   -0.068087   4.697495   0.481248
    H    2.093908   4.534872   0.470778
    H   -2.226099   4.487513   0.465368
    H   -0.080007   5.780544   0.541533
    C   -2.380392   1.704014   0.293406
    C    2.310289   1.755986   0.306931
    N    2.133331   0.486045   0.159357
    N   -2.171448   0.439642   0.144502
    C    3.257638  -0.393234   0.158708
    C    4.007666  -0.600342   1.339736
    C    3.548490  -1.089457  -1.035574
    C    5.099136  -1.475811   1.271646
    C    4.657490  -1.939732  -1.048314
    C    5.435960  -2.128920   0.090791
    H    5.687743  -1.655492   2.166701
    H    4.911481  -2.466192  -1.963750
    H    6.292488  -2.796371   0.061983
    C   -3.276040  -0.466221   0.114149
    C   -3.985701  -0.765524   1.299240
    C   -3.580570  -1.093954  -1.113136
    C   -5.053598  -1.667288   1.206053
    C   -4.666119  -1.973905  -1.149922
    C   -5.405919  -2.255609  -0.004369
    H   -5.611170  -1.919950   2.103283
    H   -4.930811  -2.450830  -2.089303
    H   -6.244019  -2.945034  -0.051802
    C    2.705097  -0.911340  -2.293745
    H    1.840540  -0.295357  -2.026928
    C    3.626446   0.005276   2.689641
    H    2.759794   0.655527   2.546511
    C   -2.768396  -0.824389  -2.375858
    H   -1.926266  -0.183419  -2.096656
    C   -3.568896  -0.237684   2.670701
    H   -2.789649   0.515807   2.530086
    C    2.157106  -2.255420  -2.806505
    H    2.961969  -2.931576  -3.115851
    H    1.568396  -2.750835  -2.029521
    H    1.512286  -2.092484  -3.677589
    C    3.485005  -0.162211  -3.391946
    H    3.836302   0.814032  -3.040303
    H    4.363336  -0.732845  -3.713670
    H    2.852643   0.000567  -4.271868
    C    3.187474  -1.096281   3.675484
    H    2.361827  -1.680735   3.259583
    H    4.010288  -1.783493   3.900189
    H    2.856185  -0.651969   4.621053
    C    4.754916   0.870798   3.281461
    H    5.655022   0.279159   3.479791
    H    5.039225   1.682065   2.602091
    H    4.438319   1.317177   4.230566
    C   -4.727432   0.443644   3.421608
    H   -5.158087   1.265212   2.838681
    H   -5.535465  -0.260191   3.646583
    H   -4.374867   0.851277   4.375314
    C   -2.940902  -1.370786   3.508797
    H   -2.088393  -1.813281   2.984913
    H   -2.595091  -0.985296   4.474974
    H   -3.669008  -2.165462   3.705653
    C   -2.172394  -2.122278  -2.951328
    H   -1.554774  -2.626479  -2.202923
    H   -2.953719  -2.817531  -3.277719
    H   -1.546505  -1.898134  -3.822732
    C   -3.595985  -0.065856  -3.431421
    H   -4.456765  -0.657726  -3.761855
    H   -3.979183   0.881503  -3.036706
    H   -2.985872   0.155679  -4.314230
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Cl	0.006396	-2.222371	0.639297
H	-3.385152	2.128308	0.368071
H	3.303762	2.204521	0.389660

7, S=1/2
LANL2DZ/6-31G(d,p)

Ni	-0.000062	-0.171302	0.186408
N	-0.000084	-1.469572	1.645437
C	-1.173730	-1.930115	2.142233
C	1.173552	-1.930295	2.142096
C	-1.206950	-2.890138	3.155385
C	1.206735	-2.890335	3.155237
C	-0.000115	-3.376241	3.668222
H	-2.160178	-3.246433	3.533700
H	2.159950	-3.246791	3.533433
H	-0.000125	-4.120728	4.457260
C	2.345530	-1.326754	1.515440
C	-2.345692	-1.326457	1.515640
N	-2.155066	-0.391961	0.646892
N	2.154974	-0.392119	0.646808
C	-3.273800	0.188484	-0.025457
C	-3.581866	1.538049	0.253090
C	-3.995818	-0.556437	-0.985752
C	-4.679744	2.109554	-0.396344
C	-5.077228	0.072696	-1.615989
C	-5.430417	1.384759	-1.318546
H	-4.946058	3.140456	-0.181431
H	-5.644821	-0.475302	-2.362650
H	-6.278080	1.847169	-1.816173
C	3.273842	0.188202	-0.025444
C	3.582212	1.537634	0.253380
C	3.995740	-0.556703	-0.985857
C	4.680280	2.109005	-0.395864
C	5.077346	0.072290	-1.615883
C	5.430842	1.384210	-1.318146
H	4.946825	3.139801	-0.180725
H	5.644846	-0.475684	-2.362631
H	6.278665	1.846501	-1.815612
C	-3.589980	-1.960846	-1.428555
H	-2.755155	-2.292939	-0.806261
C	-2.761717	2.361826	1.240652
H	-1.919306	1.744155	1.567685
C	3.589499	-1.960871	-1.429068
H	2.754820	-2.293062	-0.806633
C	2.762148	2.361443	1.240989
H	1.919743	1.743800	1.568083
C	-3.071724	-1.940390	-2.881120
H	-3.857042	-1.632592	-3.580197
H	-2.234050	-1.243969	-2.981311
H	-2.731374	-2.938969	-3.178613
C	-4.726369	-2.984827	-1.249307
H	-5.069708	-3.028854	-0.209698
H	-5.593811	-2.740261	-1.871476
H	-4.387240	-3.985743	-1.538156
C	-2.169130	3.616373	0.572625
H	-1.559743	3.339954	-0.292451
H	-2.953186	4.303981	0.236544
H	-1.535562	4.160564	1.282322
C	-3.580344	2.722161	2.495571
H	-4.441060	3.351704	2.243702
H	-3.962428	1.825613	2.995901
H	-2.963077	3.274557	3.212816
C	3.580820	2.721838	2.495853
H	3.962938	1.825322	2.996213
H	4.441515	3.351393	2.243942
H	2.963564	3.274252	3.213094
C	2.169545	3.615972	0.572915
H	1.560119	3.339512	-0.292119
H	1.536023	4.160218	1.282610
H	2.953616	4.303526	0.236763
C	3.070774	-1.939684	-2.881460
H	2.233196	-1.243063	-2.981080
H	3.855938	-1.631710	-3.580635
H	2.730152	-2.938071	-3.179287
C	4.725716	-2.985177	-1.250617
H	5.592980	-2.740639	-1.873045
H	5.069444	-3.029650	-0.211156
H	4.386218	-3.985906	-1.539679
H	3.343729	-1.675655	1.792617
H	-3.343914	-1.675179	1.792965
Br	0.000139	0.933296	-1.886787

6, S=1/2
6-311G(d,p)

Ni	0.000086	-0.086222	0.345694
N	0.000077	-0.408396	2.142703
C	-1.197150	-0.465947	2.797203
C	1.197239	-0.464876	2.797417
C	-1.216390	-0.641716	4.176854
C	1.216384	-0.640623	4.177074
C	-0.000023	-0.735557	4.865775
H	-2.159710	-0.698910	4.706415
H	2.159657	-0.696978	4.706807
H	-0.000059	-0.870092	5.940090
C	2.271317	-0.307166	1.865724
C	-2.271197	-0.309131	1.865320
N	-1.910548	-0.090197	0.614868
N	1.910713	-0.088603	0.615196
C	-2.950282	0.067409	-0.365985
C	-3.397391	1.364618	-0.676829
C	-3.486927	-1.072976	-0.990610
C	-4.447076	1.493772	-1.588761
C	-4.534388	-0.888946	-1.896831
C	-5.020761	0.378991	-2.187376
H	-4.815634	2.482044	-1.839577
H	-4.968376	-1.751818	-2.389329
H	-5.835540	0.499974	-2.892690
C	2.950447	0.069467	-0.365571
C	3.395455	1.367038	-0.677927
C	3.489102	-1.070791	-0.988713
C	4.445047	1.496833	-1.589861
C	4.536357	-0.886109	-1.895053
C	5.020638	0.382283	-2.187084
H	4.812008	2.485409	-1.841819
H	4.971796	-1.748842	-2.386519
H	5.835287	0.503772	-2.892463
C	-2.935354	-2.471233	-0.736618
H	-2.078394	-2.370747	-0.068031
C	-2.761459	2.602979	-0.057068
H	-1.886541	2.271966	0.505653
C	2.939636	-2.469638	-0.733404
H	2.083224	-2.369966	-0.064002

C	2.757364	2.605025	-0.059677
H	1.882851	2.273162	0.503159
C	-2.413141	-3.109558	-2.036994
H	-3.221165	-3.279561	-2.754607
H	-1.667816	-2.465948	-2.508190
H	-1.950108	-4.077964	-1.823818
C	-3.965994	-3.378897	-0.040711
H	-4.299286	-2.952573	0.909759
H	-4.851808	-3.525782	-0.665712
H	-3.534693	-4.363727	0.162644
C	-2.258323	3.581841	-1.132458
H	-1.572449	3.080188	-1.817812
H	-3.083306	3.999757	-1.716573
H	-1.729284	4.417837	-0.664796
C	-3.716462	3.297303	0.931621
H	-4.620112	3.650618	0.425860
H	-4.028646	2.618833	1.730677
H	-3.231034	4.162737	1.393005
C	3.710964	3.301873	0.928610
H	4.023857	2.624759	1.728545
H	4.614276	3.655982	0.422805
H	3.224048	4.167084	1.388837
C	2.252941	3.581948	-1.136203
H	1.567895	3.078501	-1.821078
H	1.722582	4.417653	-0.669513
H	3.077402	4.000470	-1.720626
C	2.416932	-3.109186	-2.032994
H	1.670160	-2.466834	-2.503623
H	3.224444	-3.278174	-2.751421
H	1.955575	-4.078218	-1.819012
C	3.972111	-3.375685	-0.038137
H	4.857298	-3.522129	-0.664121
H	4.306137	-2.948305	0.911597
H	3.542108	-4.360822	0.166474
Cl	0.000085	0.207198	-1.815509
H	3.316871	-0.359173	2.152024
H	-3.316760	-0.362026	2.151435

7, S=1/2
6-311G(d,p)

Ni	0.000433	0.128864	-0.414121
N	0.001405	0.629089	-2.180047
C	-1.194355	0.735647	-2.830272
C	1.195084	0.698413	-2.839356
C	-1.216108	1.001864	-4.195137
C	1.214256	0.963891	-4.204619
C	-0.001212	1.125927	-4.881680
H	-2.160834	1.101473	-4.715895
H	2.157535	1.034350	-4.732722
H	-0.002149	1.329568	-5.945026
C	2.272207	0.446943	-1.932536
C	-2.271914	0.515112	-1.915447
N	-1.922471	0.172166	-0.691445
N	1.922050	0.116630	-0.704871
C	-2.981175	-0.043983	0.259459
C	-3.489623	-1.345152	0.422736
C	-3.476558	1.047308	0.996162
C	-4.560658	-1.521828	1.301777
C	-4.546859	0.816697	1.863679
C	-5.094629	-0.451729	2.008827
H	-4.977821	-2.512879	1.440000
H	-4.952348	1.640868	2.439458
H	-5.926808	-0.609575	2.685966
C	2.980942	-0.115234	0.241532
C	3.415360	-1.435521	0.459182
C	3.552028	0.977409	0.919183
C	4.486702	-1.635559	1.331923
C	4.619190	0.722586	1.784636
C	5.092690	-0.567789	1.982930
H	4.847958	-2.642046	1.509365
H	5.080235	1.547061	2.316833
H	5.923667	-0.743748	2.657076
C	-2.866949	2.439450	0.875298
H	-1.943505	2.339571	0.301381
C	-2.897510	-2.536599	-0.321444
H	-1.976039	-2.196157	-0.798255
C	3.021755	2.398076	0.756730
H	2.121206	2.344197	0.142110
C	2.749362	-2.618015	-0.233758
H	1.826764	-2.247515	-0.685280
C	-2.476922	3.018793	2.246347
H	-3.353637	3.204470	2.873290
H	-1.812028	2.336300	2.778764
H	-1.958074	3.973306	2.116515
C	-3.794484	3.400991	0.108878
H	-4.019560	3.028863	-0.894522
H	-4.745535	3.532274	0.633668
H	-3.328667	4.385912	0.007221
C	-2.508466	-3.677039	0.635370
H	-1.828195	-3.316454	1.409451
H	-3.383579	-4.114628	1.124374
H	-2.007388	-4.477130	0.082099
C	-3.839449	-3.035814	-1.433165
H	-4.790075	-3.384028	-1.018377
H	-4.063816	-2.244511	-2.154043
H	-3.385130	-3.869681	-1.976944
C	3.631794	-3.177260	-1.365542
H	3.865635	-2.409142	-2.108074
H	4.579937	-3.557839	-0.973859
H	3.125720	-4.000636	-1.878949
C	2.347946	-3.721337	0.759921
H	1.718036	-3.314552	1.553252
H	1.786582	-4.505813	0.243637
H	3.220860	-4.192716	1.220828
C	2.601898	3.005352	2.107802
H	1.872492	2.366389	2.609210
H	3.458449	3.136369	2.775085
H	2.149960	3.989995	1.953788
C	4.030436	3.305512	0.028340
H	4.961445	3.397658	0.595574
H	4.283724	2.912612	-0.960342
H	3.618118	4.310559	-0.102760
H	3.315671	0.521183	-2.222148
H	-3.314891	0.618773	-2.197576
Br	0.000811	-0.376250	1.854263

6, S=1/2
def2TZVP

Ni	0.000156	-0.118237	0.299680
N	-0.000342	-0.644028	2.067169
C	-1.191277	-0.736560	2.718955
C	1.190396	-0.738850	2.718989

C	-1.212494	-1.020154	4.077472
C	1.211027	-1.022515	4.077502
C	-0.000889	-1.174457	4.757220
H	-2.156502	-1.110411	4.598498
H	2.154848	-1.114589	4.598549
H	-0.001114	-1.392327	5.816294
C	2.275184	-0.489305	1.822027
C	-2.275588	-0.485149	1.821933
N	-1.944119	-0.122652	0.607177
N	1.944355	-0.125954	0.607355
C	-2.990104	0.113655	-0.344848
C	-3.427164	1.432308	-0.555247
C	-3.538311	-0.969739	-1.052847
C	-4.468133	1.638687	-1.458036
C	-4.575428	-0.706037	-1.946552
C	-5.045315	0.582120	-2.144775
H	-4.829180	2.644817	-1.630154
H	-5.016628	-1.523796	-2.502460
H	-5.853085	0.764450	-2.842630
C	2.990701	0.109597	-0.344482
C	3.431747	1.427423	-0.551725
C	3.534980	-0.973620	-1.055769
C	4.472117	1.633014	-1.455410
C	4.571833	-0.710738	-1.950001
C	5.045218	0.576539	-2.145657
H	4.835936	2.638531	-1.625361
H	5.010036	-1.528421	-2.508381
H	5.852608	0.758260	-2.844110
C	-3.024487	-2.393907	-0.895576
H	-2.173159	-2.369668	-0.215724
C	-2.804844	2.616967	0.168388
H	-1.947973	2.247322	0.732036
C	3.017505	-2.396742	-0.901110
H	2.167453	-2.371877	-0.219685
C	2.813955	2.612476	0.175191
H	1.961338	2.243258	0.745478
C	-2.509755	-2.956345	-2.229418
H	-3.313915	-3.051749	-2.962161
H	-1.740678	-2.308193	-2.650064
H	-2.079748	-3.949545	-2.079205
C	-4.083166	-3.318246	-0.274732
H	-4.415667	-2.950715	0.698488
H	-4.964446	-3.399239	-0.914819
H	-3.678871	-4.323802	-0.136728
C	-2.270854	3.667368	-0.816315
H	-1.562759	3.217597	-1.512469
H	-3.076416	4.124090	-1.395497
H	-1.760772	4.467236	-0.274391
C	-3.783636	3.243336	1.173816
H	-4.664939	3.646168	0.669350
H	-4.128666	2.510111	1.905927
H	-3.305158	4.063033	1.715147
C	3.799409	3.240795	1.172877
H	4.150311	2.508681	1.903311
H	4.676743	3.643990	0.661852
H	3.323981	4.060637	1.716656
C	2.272474	3.661126	-0.807305
H	1.558755	3.210116	-1.496901
H	1.767075	4.462360	-0.262988
H	3.073736	4.116124	-1.393777
C	2.498921	-2.954422	-2.235449
H	1.730807	-2.303110	-2.652977
H	3.301534	-3.050046	-2.969871
H	2.066561	-3.946872	-2.087024
C	4.074760	-3.325391	-0.284282
H	4.954730	-3.407240	-0.926058
H	4.409892	-2.961011	0.689227
H	3.667994	-4.330176	-0.147949
Cl	0.000565	0.335537	-1.836082
H	3.313098	-0.592208	2.121059
H	-3.313683	-0.586256	2.120951

7, S=1/2
def2TZVP

Ni	0.000000	-0.178214	0.366354
N	0.000005	-0.883435	2.079178
C	-1.188489	-1.026083	2.725306
C	1.188500	-1.026056	2.725312
C	-1.210682	-1.421774	4.055379
C	1.210693	-1.421747	4.055386
C	0.000006	-1.632631	4.720758
H	-2.155379	-1.552905	4.566434
H	2.155389	-1.552856	4.566447
H	0.000007	-1.936384	5.758442
C	2.276862	-0.691319	1.860586
C	-2.276856	-0.691370	1.860574
N	-1.956852	-0.203381	0.688860
N	1.956852	-0.203338	0.688870
C	-3.023120	0.118840	-0.216404
C	-3.470507	1.449131	-0.282678
C	-3.584329	-0.892593	-1.014994
C	-4.538963	1.736853	-1.129228
C	-4.649714	-0.548819	-1.845917
C	-5.132211	0.748891	-1.899396
H	-4.909694	2.752099	-1.190442
H	-5.104503	-1.309589	-2.467837
H	-5.961998	0.993124	-2.550955
C	3.023118	0.118895	-0.216392
C	3.470450	1.449203	-0.282705
C	3.584382	-0.892541	-1.014939
C	4.538905	1.736942	-1.129250
C	4.649770	-0.548751	-1.845854
C	5.132209	0.748978	-1.899372
H	4.909593	2.752202	-1.190492
H	5.104605	-1.309523	-2.467736
H	5.961997	0.993225	-2.550925
C	-3.058936	-2.321164	-1.010740
H	-2.149773	-2.338858	-0.409655
C	-2.832294	2.557157	0.541962
H	-1.931830	2.148264	1.001225
C	3.059059	-2.321137	-1.010643
H	2.149913	-2.338866	-0.409533
C	2.832177	2.557227	0.541892
H	1.931725	2.148309	1.001153
C	-2.662728	-2.788207	-2.419028
H	-3.527627	-2.852566	-3.082708
H	-1.940096	-2.104060	-2.863985
H	-2.210685	-3.781747	-2.371323
C	-4.060157	-3.293607	-0.367704
H	-4.305427	-3.000683	0.655354
H	-4.994323	-3.329487	-0.932817
H	-3.647919	-4.305043	-0.339969
C	-2.389338	3.741133	-0.328696
H	-1.715755	3.409432	-1.119257

H	-3.240197	4.244176	-0.793206
H	-1.864954	4.480274	0.281562
C	-3.758793	3.018826	1.678229
H	-4.683603	3.447066	1.284894
H	-4.032092	2.189517	2.334198
H	-3.268215	3.783065	2.285703
C	3.758640	3.018967	1.678160
H	4.031964	2.189688	2.334157
H	4.683439	3.447234	1.284826
H	3.268022	3.783203	2.285605
C	2.389183	3.741161	-0.328805
H	1.715623	3.409410	-1.119365
H	1.864761	4.480296	0.281426
H	3.240027	4.244227	-0.793318
C	2.662837	-2.788216	-2.418916
H	1.940165	-2.104103	-2.863860
H	3.527725	-2.852539	-3.082613
H	2.210839	-3.781776	-2.371192
C	4.060340	-3.293521	-0.367612
H	4.994491	-3.329380	-0.932749
H	4.305626	-3.000559	0.655431
H	3.648143	-4.304973	-0.339839
H	3.312441	-0.828001	2.154275
H	-3.312433	-0.828069	2.154263
Br	-0.000004	0.486063	-1.873814

1, S=1/2
6-311G(d,p)

Ni	0.000000	-0.157463	0.234979
N	0.000000	-1.129709	1.772934
C	-1.198848	-1.388504	2.381241
C	1.198848	-1.388502	2.381242
C	-1.214080	-2.018884	3.619782
C	1.214081	-2.018882	3.619783
C	0.000000	-2.345162	4.236986
H	-2.153322	-2.249690	4.106049
H	2.153322	-2.249687	4.106050
H	0.000000	-2.832255	5.203839
C	2.300211	-0.920617	1.575349
C	-2.300211	-0.920621	1.575346
N	-1.921708	-0.260632	0.489289
N	1.921709	-0.260628	0.489292
C	-2.919962	0.247211	-0.412952
C	-3.355794	1.577776	-0.262079
C	-3.428094	-0.582813	-1.430536
C	-4.365341	2.039777	-1.109506
C	-4.432109	-0.070190	-2.255870
C	-4.910620	1.223098	-2.091847
H	-4.722031	3.058328	-1.005083
H	-4.839037	-0.691655	-3.045779
H	-5.693213	1.600399	-2.740803
C	2.919962	0.247221	-0.412946
C	3.355782	1.577790	-0.262074
C	3.428108	-0.582801	-1.430525
C	4.365328	2.039799	-1.109498
C	4.432121	-0.070170	-2.255857
C	4.910619	1.223122	-2.091835
H	4.722008	3.058354	-1.005076
H	4.839060	-0.691633	-3.045762
H	5.693211	1.600430	-2.740789
C	-2.879877	-1.982047	-1.689608
H	-2.118075	-2.184948	-0.934158
C	-2.744238	2.514176	0.773804
H	-1.906427	1.987765	1.234905
C	2.879907	-1.982041	-1.689596
H	2.118107	-2.184951	-0.934146
C	2.744213	2.514187	0.773804
H	1.906408	1.987768	1.234907
C	3.725641	-1.198350	1.954409
H	3.854058	-1.137726	3.036994
H	4.018799	-2.207124	1.644391
H	4.407685	-0.495013	1.480650
C	-3.725641	-1.198358	1.954403
H	-4.018799	-2.207127	1.644371
H	-3.854057	-1.137750	3.036989
H	-4.407685	-0.495014	1.480655
C	-2.181475	-2.049333	-3.061603
H	-2.894920	-1.895986	-3.876756
H	-1.408154	-1.283335	-3.139349
H	-1.717878	-3.030462	-3.204681
C	-3.961092	-3.071386	-1.569063
H	-4.457110	-3.045476	-0.595116
H	-4.733379	-2.953925	-2.334734
H	-3.518446	-4.063704	-1.697167
C	-2.169395	3.781244	0.115258
H	-1.454629	3.516020	-0.665688
H	-2.956007	4.395774	-0.332449
H	-1.656096	4.394984	0.861829
C	-3.743043	2.871000	1.890593
H	-4.607826	3.409330	1.491439
H	-4.115440	1.977929	2.399915
H	-3.268184	3.512073	2.639629
C	3.743012	2.871028	1.890592
H	4.115422	1.977964	2.399917
H	4.607788	3.409371	1.491438
H	3.268143	3.512096	2.639627
C	2.169354	3.781244	0.115252
H	1.454591	3.516008	-0.665692
H	1.656047	4.394982	0.861820
H	2.955959	4.395782	-0.332459
C	2.181503	-2.049333	-3.061591
H	1.408176	-1.283342	-3.139335
H	2.894945	-1.895979	-3.876745
H	1.717915	-3.030466	-3.204668
C	3.961132	-3.071368	-1.569053
H	4.733418	-2.953900	-2.334725
H	4.457151	-3.045455	-0.595106
H	3.518497	-4.063691	-1.697157
Cl	-0.000002	0.939695	-1.661344

1-Br, S=1/2
6-311G(d,p)

Ni	0.000044	0.367900	0.018602
N	-0.000005	2.195458	0.091926
C	-1.195571	2.851954	-0.024853
C	1.195587	2.852005	-0.024298
C	-1.212538	4.235770	-0.149761
C	1.212559	4.235829	-0.149109
C	0.000008	4.934558	-0.198034
H	-2.153338	4.766924	-0.220537
H	2.153378	4.767021	-0.219371
H	0.000009	6.012169	-0.301668

C	2.303747	1.927461	-0.012349
C	-2.303729	1.927395	-0.012765
N	-1.938753	0.654815	-0.034612
N	1.938764	0.654886	-0.034822
C	-2.952137	-0.366541	-0.001707
C	-3.423721	-0.893481	-1.219512
C	-3.439693	-0.824482	1.237595
C	-4.448445	-1.841379	-1.172607
C	-4.460809	-1.777886	1.229147
C	-4.974212	-2.274388	0.038070
H	-4.833816	-2.253761	-2.098254
H	-4.854310	-2.142071	2.171619
H	-5.769682	-3.011219	0.053520
C	2.952092	-0.366558	-0.003593
C	3.421356	-0.893424	-1.222365
C	3.441849	-0.824747	1.234715
C	4.445845	-1.841638	-1.177530
C	4.462607	-1.778549	1.224199
C	4.973637	-2.275067	0.032131
H	4.829412	-2.253939	-2.103960
H	4.857745	-2.142958	2.165895
H	5.768858	-3.012197	0.046022
C	-2.863989	-0.344387	2.565930
H	-2.044124	0.340894	2.341536
C	-2.834936	-0.470336	-2.560741
H	-1.965643	0.155615	-2.350140
C	2.869024	-0.344752	2.564339
H	2.050576	0.342892	2.341991
C	2.830388	-0.469485	-2.562387
H	1.960674	0.155231	-2.349884
C	-2.264102	-1.514072	3.368663
H	-3.037102	-2.223267	3.678810
H	-1.526113	-2.053286	2.772584
H	-1.775184	-1.140049	4.273549
C	-3.901122	0.422510	3.407409
H	-4.314483	1.275769	2.863593
H	-4.736982	-0.223844	3.690965
H	-3.444683	0.797087	4.328593
C	-2.329121	-1.679987	-3.367073
H	-1.620076	-2.265671	-2.779233
H	-3.149671	-2.337126	-3.670103
H	-1.826318	-1.340809	-4.278006
C	-3.826984	0.370306	-3.386309
H	-4.720786	-0.207924	-3.639226
H	-4.152353	1.260789	-2.841815
H	-3.365770	0.697516	-4.323140
C	3.820505	0.373303	-3.388107
H	4.145434	1.263551	-2.842970
H	4.714702	-0.203613	-3.642648
H	3.357856	0.701036	-4.324048
C	2.324935	-1.678617	-3.369665
H	1.617304	-2.265900	-2.781717
H	1.820554	-1.338757	-4.279468
H	3.145812	-2.334399	-3.674723
C	2.267285	-1.514067	3.366290
H	1.527284	-2.050731	2.770407
H	3.039027	-2.225524	3.674389
H	1.780433	-1.140132	4.272327
C	3.909202	0.418400	3.405479
H	4.743787	-0.230445	3.687078
H	4.324012	1.271349	2.862265
H	3.454919	0.792870	4.327770
Br	0.000003	-1.968705	0.029106
C	3.721728	2.420984	0.032901
H	3.881284	3.189162	-0.728429
H	3.940582	2.875260	1.004550
H	4.432181	1.614967	-0.133521
C	-3.721708	2.420953	0.032240
H	-3.940596	2.875738	1.003640
H	-3.881203	3.188723	-0.729513
H	-4.432184	1.614876	-0.133786

6, S=1/2, a=170
6-311G(d,p)

Ni	0.006393	-0.103181	0.328722
N	-0.001950	-0.500548	2.117875
C	-1.200000	-0.548311	2.771626
C	1.190986	-0.557895	2.780293
C	-1.225931	-0.744496	4.148363
C	1.205281	-0.753812	4.157285
C	-0.013239	-0.857324	4.840585
H	-2.171787	-0.800133	4.673694
H	2.146839	-0.816783	4.689461
H	-0.017745	-1.006170	5.912989
C	2.273581	-0.374545	1.861064
C	-2.274334	-0.353351	1.844894
N	-1.916481	-0.073949	0.607968
N	1.927142	-0.095026	0.620763
C	-2.956049	0.105690	-0.368668
C	-3.376102	1.414054	-0.671335
C	-3.517693	-1.019694	-0.999198
C	-4.424221	1.571540	-1.580329
C	-4.561954	-0.807043	-1.903065
C	-5.021849	0.472539	-2.185037
H	-4.773720	2.568558	-1.823374
H	-5.013872	-1.657295	-2.401305
H	-5.834733	0.615012	-2.888509
C	2.973779	0.061194	-0.351695
C	3.368423	1.362935	-0.711558
C	3.565809	-1.079314	-0.926002
C	4.424199	1.501841	-1.614405
C	4.615737	-0.884898	-1.827589
C	5.052769	0.390112	-2.161580
H	4.753885	2.494597	-1.899394
H	5.089367	-1.746640	-2.284270
H	5.871022	0.518086	-2.861604
C	-2.996211	-2.431855	-0.756704
H	-2.129080	-2.354673	-0.098496
C	-2.718020	2.631305	-0.033427
H	-1.826299	2.279251	0.489426
C	3.062877	-2.490466	-0.641082
H	2.208371	-2.408883	0.032692
C	2.669749	2.595206	-0.150618
H	1.812090	2.245684	0.427468
C	-2.503831	-3.079084	-2.064402
H	-3.322485	-3.223053	-2.775544
H	-1.742978	-2.455334	-2.536982
H	-2.067601	-4.061335	-1.858063
C	-4.040963	-3.316950	-0.052543
H	-4.352783	-2.887858	0.903988
H	-4.937441	-3.438639	-0.667690
H	-3.631834	-4.313171	0.140796
C	-2.248646	3.649329	-1.087007
H	-1.592519	3.174302	-1.818934

H	-3.090592	4.096399	-1.623240
H	-1.696465	4.462677	-0.606624
C	-3.639068	3.290143	1.010256
H	-4.557867	3.660816	0.545981
H	-3.926234	2.582955	1.793427
H	-3.138183	4.138240	1.487162
C	3.584465	3.382415	0.805862
H	3.925800	2.758264	1.636540
H	4.471817	3.756399	0.286405
H	3.053941	4.243140	1.224201
C	2.121035	3.494343	-1.272157
H	1.458217	2.928414	-1.929746
H	1.555454	4.328316	-0.845395
H	2.926117	3.918314	-1.879205
C	2.549482	-3.165043	-1.927262
H	1.774881	-2.555668	-2.396671
H	3.355384	-3.313293	-2.652028
H	2.125753	-4.147255	-1.695922
C	4.127404	-3.354798	0.058602
H	5.009467	-3.490198	-0.574064
H	4.460420	-2.901328	0.996541
H	3.726278	-4.347066	0.285928
Cl	0.016822	-0.006943	-1.856164
H	3.315853	-0.458318	2.153073
H	-3.319379	-0.428339	2.129280

6, S=1/2, a=160
6-311G(d,p)

Ni	-0.000003	-0.125063	0.297681
N	0.000123	-0.583077	2.082319
C	-1.193208	-0.645791	2.741642
C	1.193444	-0.644623	2.741769
C	-1.214637	-0.874346	4.113662
C	1.214955	-0.873163	4.113788
C	0.000184	-0.999523	4.799307
H	-2.158794	-0.944201	4.640520
H	2.159123	-0.942105	4.640746
H	0.000212	-1.172097	5.868168
C	2.277475	-0.423328	1.828892
C	-2.277360	-0.425600	1.828644
N	-1.936278	-0.082856	0.605477
N	1.936187	-0.080892	0.605698
C	-2.982905	0.097816	-0.361375
C	-3.344472	1.411270	-0.715407
C	-3.606427	-1.024949	-0.938839
C	-4.398438	1.582346	-1.614520
C	-4.653048	-0.797855	-1.836818
C	-5.057276	0.489434	-2.164392
H	-4.704890	2.584221	-1.893012
H	-5.150068	-1.644651	-2.296446
H	-5.873742	0.641657	-2.861623
C	2.982799	0.100999	-0.360954
C	3.343288	1.414872	-0.714514
C	3.607386	-1.021047	-0.938658
C	4.397285	1.587132	-1.613368
C	4.653983	-0.792780	-1.836366
C	5.057176	0.494962	-2.163448
H	4.702918	2.589364	-1.891479
H	5.151827	-1.639005	-2.296156
H	5.873651	0.648109	-2.860468
C	-3.145165	-2.451934	-0.660053
H	-2.266676	-2.397799	-0.015223
C	-2.620959	2.619507	-0.134160
H	-1.738778	2.244963	0.389519
C	3.147304	-2.448492	-0.660301
H	2.268492	-2.395232	-0.015837
C	2.618546	2.622330	-0.133173
H	1.736911	2.246850	0.390752
C	-2.696426	-3.155586	-1.954574
H	-3.527663	-3.278753	-2.654787
H	-1.910191	-2.580721	-2.446879
H	-2.305274	-4.151677	-1.725303
C	-4.219668	-3.270745	0.078804
H	-4.505468	-2.800799	1.024333
H	-5.126208	-3.374101	-0.524804
H	-3.850356	-4.276841	0.299076
C	-2.123266	3.576222	-1.230653
H	-1.494875	3.048144	-1.950773
H	-2.952653	4.036269	-1.775284
H	-1.533621	4.384317	-0.787466
C	-3.492947	3.356862	0.899270
H	-4.401094	3.753942	0.435906
H	-3.799227	2.691322	1.711080
H	-2.944881	4.196449	1.337619
C	3.489907	3.360811	0.899979
H	3.797203	2.695696	1.711754
H	4.397455	3.758991	0.436387
H	2.940915	4.199749	1.338412
C	2.119506	3.578327	-1.229689
H	1.491418	3.049457	-1.949495
H	1.529186	4.385913	-0.786467
H	2.948255	4.039093	-1.774690
C	2.699759	-3.152365	-1.955105
H	1.913300	-2.578074	-2.447722
H	3.531434	-3.274806	-2.654920
H	2.309286	-4.148789	-1.726129
C	4.222242	-3.266423	0.078903
H	5.129163	-3.368798	-0.524303
H	4.507155	-2.796383	1.024653
H	3.853786	-4.272912	0.298817
Cl	0.000207	-0.339729	-1.889267
H	3.318439	-0.531434	2.119031
H	-3.318246	-0.534762	2.118668

6, S=1/2, a=150
6-311G(d,p)

Ni	-0.000067	-0.176941	0.240353
N	0.000100	-0.626246	2.038711
C	-1.190923	-0.696624	2.696759
C	1.191150	-0.695389	2.696840
C	-1.214005	-0.937041	4.067170
C	1.214389	-0.935789	4.067251
C	0.000237	-1.067369	4.752066
H	-2.158457	-1.012211	4.592914
H	2.158883	-1.009993	4.593058
H	0.000295	-1.247986	5.819645
C	2.280989	-0.462780	1.789204
C	-2.280945	-0.465200	1.789039
N	-1.950919	-0.092916	0.574002
N	1.950655	-0.090823	0.574152
C	-3.000916	0.103577	-0.384208
C	-3.318451	1.425490	-0.753380

C	-3.671150	-1.003599	-0.941568
C	-4.369265	1.623866	-1.649977
C	-4.712036	-0.748052	-1.839057
C	-5.069263	0.548410	-2.183499
H	-4.642744	2.632429	-1.937511
H	-5.243914	-1.581420	-2.283760
H	-5.882494	0.721133	-2.879720
C	3.000568	0.106977	-0.383901
C	3.317148	1.429335	-0.752285
C	3.671713	-0.999383	-0.941790
C	4.367872	1.629000	-1.648704
C	4.712461	-0.742550	-1.839070
C	5.068711	0.554374	-2.182787
H	4.640622	2.637935	-1.935617
H	5.245027	-1.575269	-2.284168
H	5.881852	0.728102	-2.878864
C	-3.278649	-2.445778	-0.634226
H	-2.377643	-2.422927	-0.019655
C	-2.560960	2.612927	-0.171729
H	-1.655448	2.217498	0.294799
C	3.280397	-2.442025	-0.635125
H	2.378921	-2.420218	-0.021206
C	2.558814	2.615888	-0.169920
H	1.653618	2.219543	0.296449
C	-2.913246	-3.218294	-1.914996
H	-3.770297	-3.315039	-2.587523
H	-2.105543	-2.712308	-2.445627
H	-2.577380	-4.228062	-1.659681
C	-4.374895	-3.177756	0.162987
H	-4.605183	-2.664374	1.101061
H	-5.304170	-3.246512	-0.410390
H	-4.056550	-4.196336	0.404317
C	-2.116565	3.613930	-1.250901
H	-1.538269	3.117331	-2.032861
H	-2.968935	4.109692	-1.723773
H	-1.491700	4.394040	-0.806222
C	-3.378301	3.311608	0.931475
H	-4.305881	3.728006	0.527036
H	-3.647694	2.615375	1.730238
H	-2.806103	4.132010	1.375370
C	3.375722	3.314548	0.933624
H	3.645779	2.618042	1.731924
H	4.302916	3.731954	0.529336
H	2.802911	4.134208	1.378096
C	2.113619	3.617202	-1.248481
H	1.535551	3.120671	-2.030651
H	1.488297	4.396654	-0.803287
H	2.965600	4.113792	-1.721187
C	2.916736	-3.214632	-1.916324
H	2.108997	-2.709301	-2.447517
H	3.774410	-3.310512	-2.588184
H	2.581578	-4.224744	-1.661446
C	4.376813	-3.173091	0.162698
H	5.306576	-3.240708	-0.410023
H	4.605877	-2.659746	1.101090
H	4.059349	-4.192072	0.403501
Cl	0.000313	-0.784440	-1.882150
H	3.318906	-0.584883	2.085872
H	-3.318753	-0.588428	2.085629

6, S=1/2, a=140
6-311G(d,p)

Ni	-0.009913	-0.236249	0.190925
N	0.002932	-0.685273	2.001599
C	-1.181698	-0.780212	2.662120
C	1.195480	-0.758014	2.650273
C	-1.197491	-1.045541	4.028606
C	1.229839	-1.023102	4.016600
C	0.020977	-1.176778	4.705004
H	-2.138754	-1.138532	4.557308
H	2.177858	-1.098323	4.535993
H	0.028095	-1.375638	5.769388
C	2.283708	-0.494629	1.744554
C	-2.283693	-0.539162	1.766847
N	-1.971986	-0.131117	0.560781
N	1.953706	-0.089675	0.542096
C	-3.027526	0.079206	-0.384344
C	-3.277906	1.403004	-0.799380
C	-3.770783	-1.008014	-0.890005
C	-4.331881	1.629067	-1.685118
C	-4.810888	-0.724190	-1.780154
C	-5.101563	0.576933	-2.166441
H	-4.553996	2.640929	-2.003710
H	-5.396829	-1.540985	-2.185750
H	-5.916892	0.770116	-2.854768
C	3.000639	0.145543	-0.408696
C	3.266812	1.483198	-0.768937
C	3.718925	-0.930279	-0.968805
C	4.303886	1.729471	-1.668680
C	4.745335	-0.625593	-1.868574
C	5.044935	0.685424	-2.210567
H	4.536479	2.749084	-1.951393
H	5.312896	-1.433610	-2.315570
H	5.846976	0.894766	-2.909713
C	-3.459294	-2.461765	-0.543812
H	-2.546730	-2.477690	0.053481
C	-2.448459	2.568390	-0.273402
H	-1.571508	2.141507	0.219370
C	3.403791	-2.390480	-0.655867
H	2.484074	-2.416727	-0.069959
C	2.476085	2.629866	-0.149959
H	1.526047	2.210945	0.193608
C	-3.164107	-3.294490	-1.804879
H	-4.036431	-3.361153	-2.461388
H	-2.335074	-2.856965	-2.362318
H	-2.885112	-4.313780	-1.520894
C	-4.583927	-3.102811	0.291846
H	-4.771221	-2.549188	1.216654
H	-5.524219	-3.135233	-0.266490
H	-4.321320	-4.130348	0.560640
C	-1.940410	3.480811	-1.401831
H	-1.386139	2.908525	-2.148996
H	-2.760397	3.995116	-1.910744
H	-1.275351	4.248468	-0.996097
C	-3.222437	3.372215	0.788383
H	-4.119777	3.827856	0.358917
H	-3.538733	2.734762	1.618339
H	-2.599362	4.174625	1.195198
C	3.200393	3.193412	1.088572
H	3.381982	2.415338	1.834315
H	4.168720	3.620394	0.810545
H	2.605408	3.981586	1.560254
C	2.150398	3.750811	-1.148727
H	1.656214	3.358136	-2.040021

H	1.483671	4.483197	-0.684928
H	3.047896	4.288352	-1.467636
C	3.125775	-3.203818	-1.932740
H	2.307031	-2.756088	-2.496862
H	4.008129	-3.267110	-2.576253
H	2.837599	-4.225296	-1.666720
C	4.520962	-3.043530	0.181115
H	5.467321	-3.061905	-0.367699
H	4.695957	-2.506704	1.118043
H	4.258785	-4.076701	0.427930
Cl	-0.022528	-1.211374	-1.801973
H	3.321436	-0.620123	2.041200
H	-3.316203	-0.682094	2.073692

7, S=1/2, a=170

6-311G(d,p)

Ni	0.000018	-0.170734	0.394072
N	0.000009	-1.035047	2.018398
C	-1.193674	-1.246780	2.646460
C	1.193680	-1.246782	2.646482
C	-1.214799	-1.780966	3.930415
C	1.214773	-1.780979	3.930438
C	-0.000018	-2.058722	4.569828
H	-2.159101	-1.968434	4.427310
H	2.159066	-1.968460	4.427347
H	-0.000030	-2.469946	5.571363
C	2.274616	-0.829608	1.805489
C	-2.274598	-0.829677	1.805409
N	-1.931786	-0.233020	0.682315
N	1.931817	-0.232891	0.682423
C	-2.995112	0.153394	-0.207158
C	-3.445018	1.485911	-0.181633
C	-3.552699	-0.803655	-1.075816
C	-4.521664	1.828946	-1.002149
C	-4.626527	-0.408222	-1.877549
C	-5.117539	0.890372	-1.835359
H	-4.895611	2.846481	-0.992789
H	-5.079197	-1.126143	-2.552258
H	-5.953582	1.175436	-2.464436
C	2.995120	0.153721	-0.206969
C	3.444573	1.486399	-0.181572
C	3.553158	-0.803252	-1.075424
C	4.521189	1.829704	-1.002006
C	4.626951	-0.407547	-1.877077
C	5.117500	0.891222	-1.835012
H	4.894782	2.847368	-0.992732
H	5.079957	-1.125401	-2.551634
H	5.953518	1.176492	-2.464030
C	-2.999237	-2.220425	-1.182667
H	-2.085919	-2.261875	-0.586501
C	-2.790174	2.534537	0.709240
H	-1.890098	2.083387	1.132007
C	3.000158	-2.220198	-1.182322
H	2.087130	-2.262150	-0.585747
C	2.789313	2.534872	0.709178
H	1.889191	2.083541	1.131657
C	-2.596955	-2.563674	-2.628352
H	-3.464214	-2.594276	-3.294392
H	-1.891149	-1.826029	-3.014795
H	-2.120253	-3.548089	-2.662380
C	-3.979593	-3.262345	-0.613140
H	-4.223380	-3.055956	0.432935
H	-4.918147	-3.270392	-1.175275
H	-3.548283	-4.266448	-0.668053
C	-2.339927	3.768359	-0.091739
H	-1.679626	3.477822	-0.911224
H	-3.191107	4.310660	-0.513579
H	-1.797833	4.462384	0.557781
C	-3.705919	2.931786	1.882022
H	-4.630688	3.392563	1.521915
H	-3.982521	2.062795	2.485601
H	-3.204523	3.652417	2.535184
C	3.704693	2.932142	1.882243
H	3.981235	2.063140	2.485833
H	4.629504	3.393047	1.522403
H	3.203040	3.652668	2.535324
C	2.339099	3.768704	-0.091789
H	1.679089	3.478151	-0.911502
H	1.796690	4.462554	0.557655
H	3.190303	4.311219	-0.513305
C	2.597349	-2.563171	-2.627933
H	1.891082	-1.825682	-3.013832
H	3.464335	-2.593179	-3.294356
H	2.121045	-3.547775	-2.662065
C	3.981121	-3.261943	-0.613522
H	4.919385	-3.269634	-1.176145
H	4.225397	-3.055695	0.432467
H	3.550064	-4.266154	-0.668419
H	3.316176	-0.993040	2.064705
H	-3.316158	-0.993147	2.064600
Br	0.000017	0.549437	-1.820020

7, S=1/2, a=160

6-311G(d,p)

Ni	-0.000056	0.237755	0.330103
N	-0.000193	1.471218	1.706487
C	1.191296	1.826356	2.267889
C	-1.191711	1.825649	2.268282
C	1.213753	2.655817	3.384435
C	-1.214276	2.655088	3.384853
C	-0.000299	3.081878	3.937049
H	2.158518	2.956761	3.821165
H	-2.159071	2.955461	3.821909
H	-0.000343	3.723606	4.809076
C	-2.278374	1.211759	1.562022
C	2.278083	1.212992	1.561346
N	1.945714	0.344671	0.631585
N	-1.945842	0.343639	0.632114
C	3.006169	-0.248384	-0.133990
C	3.324513	-1.598354	0.109518
C	3.689036	0.512330	-1.103060
C	4.396777	-2.156195	-0.587382
C	4.752932	-0.096155	-1.775578
C	5.115669	-1.410321	-1.514375
H	4.671453	-3.188889	-0.407312
H	5.297624	0.466578	-2.525376
H	5.946248	-1.860471	-2.046752
C	-3.006159	-0.249630	-0.133433
C	-3.323018	-1.600196	0.108870
C	-3.690290	0.511355	-1.101384
C	-4.395084	-2.158407	-0.588007
C	-4.753972	-0.097518	-1.773917

C	-5.115247	-1.412296	-1.513844
H	-4.668609	-3.191564	-0.408891
H	-5.299625	0.465417	-2.522867
H	-5.945657	-1.862746	-2.046230
C	3.272982	1.932238	-1.474622
H	2.365040	2.170239	-0.917980
C	2.538679	-2.421364	1.121991
H	1.603797	-1.886987	1.306656
C	-3.275664	1.931895	-1.472157
H	-2.368284	2.170776	-0.914977
C	-2.535790	-2.423231	1.120236
H	-1.600375	-1.889129	1.303049
C	2.909150	2.037263	-2.967451
H	3.774884	1.849703	-3.609110
H	2.128327	1.318468	-3.222145
H	2.540394	3.042316	-3.194312
C	4.345684	2.967444	-1.088637
H	4.573159	2.933974	-0.019271
H	5.280455	2.791650	-1.629144
H	4.006605	3.979188	-1.330564
C	2.163626	-3.812967	0.588363
H	1.639108	-3.735437	-0.366083
H	3.043225	-4.447403	0.446102
H	1.507079	-4.322479	1.299693
C	3.289237	-2.521408	2.463439
H	4.244030	-3.041141	2.338501
H	3.501611	-1.531959	2.877382
H	2.696802	-3.075535	3.198037
C	-3.284094	-2.522362	2.463018
H	-3.495379	-1.532645	2.876866
H	-4.239297	-3.041786	2.339916
H	-2.690624	-3.076373	3.196869
C	-2.162175	-3.815221	0.586690
H	-1.639470	-3.738414	-0.368807
H	-1.504371	-4.324459	1.297045
H	-3.042188	-4.449564	0.446552
C	-2.911179	2.037688	-2.964797
H	-2.129500	1.319748	-3.219292
H	-3.776427	1.849323	-3.606873
H	-2.543384	3.043185	-3.191258
C	-4.349652	2.965830	-1.086402
H	-5.283961	2.789319	-1.627471
H	-4.577660	2.931746	-0.017167
H	-4.011475	3.978004	-1.327789
H	-3.317254	1.445456	1.775732
H	3.316904	1.447201	1.774780
Br	-0.000060	-0.632412	-1.838219

7, S=1/2, a=150
6-311G(d,p)

Ni	-0.000042	0.228645	0.296822
N	0.000090	1.526005	1.627090
C	1.189538	1.914217	2.165110
C	-1.189336	1.914811	2.164736
C	1.213648	2.809322	3.230602
C	-1.213346	2.809942	3.230198
C	0.000185	3.267576	3.756851
H	2.158565	3.136119	3.648206
H	-2.158234	3.137234	3.647479
H	0.000223	3.959455	4.589731
C	-2.282413	1.260839	1.499557
C	2.282507	1.259877	1.500135
N	1.960968	0.326204	0.635016
N	-1.960989	0.326969	0.634628
C	3.017274	-0.311070	-0.093439
C	3.239574	-1.683816	0.142753
C	3.787964	0.413409	-1.025546
C	4.299412	-2.303034	-0.518722
C	4.835701	-0.258156	-1.663588
C	5.101867	-1.595214	-1.406741
H	4.499604	-3.353064	-0.343605
H	5.444378	0.274869	-2.385325
H	5.921607	-2.093067	-1.912781
C	-3.017316	-0.310511	-0.093628
C	-3.240058	-1.683000	0.143529
C	-3.787630	0.413542	-1.026371
C	-4.299946	-2.302399	-0.517719
C	-4.835381	-0.258196	-1.664194
C	-5.101975	-1.595006	-1.406452
H	-4.500514	-3.352231	-0.341820
H	-5.443763	0.274482	-2.386437
H	-5.921741	-2.092988	-1.912322
C	3.486197	1.859437	-1.410142
H	2.581457	2.167445	-0.884189
C	2.364004	-2.456609	1.120753
H	1.411312	-1.922530	1.177098
C	-3.485501	1.859297	-1.411695
H	-2.580761	2.167362	-0.885775
C	-2.365002	-2.455397	1.122309
H	-1.412615	-1.920886	1.179605
C	3.178376	1.984934	-2.914430
H	4.047634	1.730552	-3.527836
H	2.353474	1.326483	-3.191608
H	2.893215	3.013937	-3.154081
C	4.620026	2.815387	-0.994886
H	4.812593	2.773846	0.081102
H	5.555418	2.567367	-1.504876
H	4.364148	3.847353	-1.252782
C	2.053124	-3.886152	0.653501
H	1.631368	-3.887564	-0.353770
H	2.943236	-4.521805	0.652987
H	1.326934	-4.348938	1.327391
C	2.976568	-2.457600	2.534493
H	3.940171	-2.976218	2.538285
H	3.143132	-1.441003	2.899395
H	2.315560	-2.966830	3.242639
C	-2.978875	-2.456720	2.535473
H	-3.146210	-1.440190	2.900230
H	-3.942269	-2.975732	2.538393
H	-2.318301	-2.965676	3.244219
C	-2.053037	-3.884750	0.655176
H	-1.630119	-3.885798	-0.351607
H	-1.327460	-4.347397	1.329827
H	-2.942909	-4.520732	0.653479
C	-3.177489	1.983993	-2.916008
H	-2.352642	1.325296	-3.192760
H	-4.046716	1.729431	-3.529385
H	-2.892158	3.012836	-3.156139
C	-4.619190	2.815675	-0.997037
H	-5.554569	2.567578	-1.507013
H	-4.811890	2.774701	0.078949
H	-4.363086	3.847466	-1.255409
H	-3.317993	1.519654	1.701501
H	3.318129	1.518362	1.702283

Br	0.000162	-0.349236	-1.973111

7, S=1/2, a=140
6-311G(d,p)

Ni	0.000012	-0.171459	0.271225
N	0.000082	-1.284458	1.773674
C	-1.186688	-1.609205	2.350553
C	1.186860	-1.608569	2.350898
C	-1.212728	-2.372973	3.514509
C	1.212956	-2.372301	3.514890
C	0.000139	-2.764649	4.091932
H	-2.157996	-2.648428	3.966985
H	2.158236	-2.647227	3.967663
H	0.000160	-3.352997	5.001005
C	2.286002	-1.032729	1.619760
C	-2.285920	-1.033754	1.619209
N	-1.974958	-0.196459	0.660366
N	1.974961	-0.195638	0.660732
C	-3.035605	0.359086	-0.124442
C	-3.236049	1.754301	-0.050907
C	-3.834634	-0.459747	-0.950232
C	-4.294804	2.308108	-0.769845
C	-4.880017	0.149752	-1.651399
C	-5.120401	1.512699	-1.556436
H	-4.477606	3.374480	-0.718307
H	-5.508428	-0.455927	-2.294269
H	-5.939153	1.959930	-2.109170
C	3.035618	0.359617	-0.124256
C	3.235674	1.754965	-0.051794
C	3.834973	-0.459611	-0.949340
C	4.294436	2.308479	-0.770922
C	4.880377	0.149612	-1.650734
C	5.120435	1.512667	-1.556705
H	4.476934	3.374939	-0.720230
H	5.509006	-0.456391	-2.293084
H	5.939194	1.959694	-2.109591
C	-3.576671	-1.951432	-1.148444
H	-2.646118	-2.203529	-0.638011
C	-2.346530	2.623252	0.829804
H	-1.395046	2.094066	0.936333
C	3.577225	-1.951433	-1.146834
H	2.646765	-2.203446	-0.636194
C	2.345597	2.624310	0.827954
H	1.393791	2.095479	0.933435
C	-3.361127	-2.298154	-2.633368
H	-4.260509	-2.115498	-3.228602
H	-2.540455	-1.710664	-3.046928
H	-3.107415	-3.357731	-2.734796
C	-4.701133	-2.813163	-0.542507
H	-4.839167	-2.614791	0.524265
H	-5.657745	-2.620500	-1.037089
H	-4.473388	-3.876616	-0.661607
C	-2.039514	3.996695	0.215117
H	-1.634362	3.898396	-0.794292
H	-2.928455	4.631833	0.164644
H	-1.302674	4.523314	0.827600
C	-2.944946	2.775589	2.241850
H	-3.908918	3.291775	2.199761
H	-3.107128	1.804010	2.714920
H	-2.277114	3.357326	2.884695
C	2.942554	2.776468	2.240639
H	3.103838	1.804867	2.713955
H	3.906768	3.292282	2.199522
H	2.274268	3.358516	2.882727
C	2.039730	3.997880	0.212993
H	1.635723	3.899802	-0.796897
H	1.302327	4.524665	0.824648
H	2.928911	4.632775	0.163625
C	3.361542	-2.298814	-2.631589
H	2.540736	-1.711615	-3.045299
H	4.260822	-2.116272	-3.227010
H	3.107976	-3.358474	-2.732539
C	4.701865	-2.812761	-0.540665
H	5.658395	-2.620196	-1.035441
H	4.840009	-2.613930	0.526007
H	4.474241	-3.876293	-0.659293
H	3.318603	-1.275032	1.855590
H	-3.318485	-1.276398	1.854854
Br	0.000207	-0.313559	-2.073127

1, S=1/2, a=170
6-311G(d,p)

Ni	0.000002	-0.159692	0.222487
N	0.000002	-1.188598	1.729481
C	-1.197084	-1.439676	2.345139
C	1.197089	-1.439670	2.345142
C	-1.213237	-2.081100	3.577956
C	1.213241	-2.081095	3.577960
C	0.000002	-2.417629	4.190803
H	-2.152804	-2.309900	4.064627
H	2.152807	-2.309890	4.064633
H	0.000002	-2.913106	5.153376
C	2.302185	-0.947807	1.555850
C	-2.302181	-0.947818	1.555843
N	-1.929659	-0.256862	0.489372
N	1.929661	-0.256850	0.489379
C	-2.929051	0.258799	-0.407010
C	-3.332717	1.600217	-0.265593
C	-3.467245	-0.569413	-1.411576
C	-4.340562	2.078029	-1.106115
C	-4.467493	-0.040294	-2.231109
C	-4.914712	1.265090	-2.074824
H	-4.673249	3.105137	-1.006646
H	-4.896038	-0.659307	-3.011371
H	-5.695205	1.654097	-2.719362
C	2.929053	0.258818	-0.407000
C	3.332706	1.600241	-0.265592
C	3.467258	-0.569397	-1.411556
C	4.340548	2.078056	-1.106115
C	4.467503	-0.040275	-2.231091
C	4.914709	1.265115	-2.074816
H	4.673223	3.105168	-1.006655
H	4.896056	-0.659291	-3.011347
H	5.695200	1.654124	-2.719354
C	-2.958223	-1.984733	-1.666245
H	-2.187433	-2.199969	-0.923582
C	-2.689369	2.529772	0.756733
H	-1.853342	1.990052	1.205879
C	2.958248	-1.984724	-1.666213
H	2.187466	-2.199961	-0.923542
C	2.689343	2.529803	0.756719
H	1.853309	1.990087	1.205857

C	3.725128	-1.229714	1.941869
H	3.849981	-1.149073	3.023910
H	4.011861	-2.246430	1.653856
H	4.412890	-0.539131	1.457929
C	-3.725124	-1.229731	1.941862
H	-4.011848	-2.246452	1.653861
H	-3.849979	-1.149077	3.023902
H	-4.412889	-0.539158	1.457913
C	-2.288286	-2.086653	-3.050508
H	-3.013033	-1.923511	-3.853761
H	-1.494799	-1.344660	-3.151134
H	-1.855956	-3.082597	-3.189686
C	-4.065126	-3.044953	-1.516484
H	-4.547424	-2.996250	-0.536740
H	-4.844625	-2.916550	-2.273049
H	-3.649135	-4.049325	-1.639718
C	-2.105789	3.785652	0.085149
H	-1.411509	3.508954	-0.710484
H	-2.890127	4.412953	-0.348419
H	-1.567283	4.391965	0.819811
C	-3.664015	2.903992	1.888902
H	-4.528394	3.451654	1.501793
H	-4.039085	2.017042	2.406918
H	-3.168592	3.541313	2.627753
C	3.663973	2.904029	1.888899
H	4.039032	2.017083	2.406928
H	4.528360	3.451685	1.501798
H	3.168541	3.541359	2.627737
C	2.105775	3.785679	0.085118
H	1.411503	3.508977	-0.710520
H	1.567264	4.392000	0.819769
H	2.890121	4.412972	-0.348447
C	2.288298	-2.086658	-3.050469
H	1.494803	-1.344673	-3.151092
H	3.013036	-1.923512	-3.853730
H	1.855977	-3.082607	-3.189638
C	4.065161	-3.044933	-1.516454
H	4.844653	-2.916529	-2.273026
H	4.547466	-2.996220	-0.536714
H	3.649177	-4.049309	-1.639678
Cl	0.000002	0.744648	-1.778171

1, S=1/2, a=160
6-311G(d,p)

Ni	0.000338	-0.177564	0.177890
N	0.000040	-1.239302	1.672335
C	-1.194467	-1.491390	2.290650
C	1.194364	-1.492078	2.290728
C	-1.212538	-2.145015	3.517172
C	1.211919	-2.145705	3.517266
C	-0.000435	-2.490152	4.126737
H	-2.152978	-2.374527	4.002095
H	2.152150	-2.375855	4.002276
H	-0.000607	-2.994166	5.084882
C	2.306070	-0.982762	1.517199
C	-2.305857	-0.981338	1.517176
N	-1.943618	-0.260350	0.470446
N	1.944241	-0.261942	0.470204
C	-2.942061	0.274758	-0.414726
C	-3.276194	1.637758	-0.292907
C	-3.542845	-0.544322	-1.392575
C	-4.271985	2.152276	-1.125223
C	-4.527416	0.023063	-2.206012
C	-4.902832	1.352723	-2.069564
H	-4.552147	3.195786	-1.037509
H	-5.000712	-0.587454	-2.966691
H	-5.672366	1.769828	-2.709660
C	2.943054	0.272183	-0.415112
C	3.275596	1.635790	-0.295808
C	3.545684	-0.548223	-1.390751
C	4.271930	2.149601	-1.127901
C	4.530602	0.018527	-2.204212
C	4.904682	1.348778	-2.069883
H	4.550933	3.193569	-1.041968
H	5.005230	-0.592966	-2.963272
H	5.674593	1.765335	-2.709883
C	-3.126245	-1.993353	-1.628347
H	-2.351139	-2.242974	-0.901174
C	-2.581930	2.542003	0.718540
H	-1.726736	1.987945	1.111082
C	3.130073	-1.997799	-1.624941
H	2.356724	-2.247943	-0.896079
C	2.578760	2.541503	0.712540
H	1.723748	1.987196	1.105100
C	3.723456	-1.270874	1.921081
H	3.854511	-1.091908	2.991417
H	3.977577	-2.318635	1.732866
H	4.428001	-0.647387	1.375086
C	-3.723352	-1.268959	1.921151
H	-3.975814	-2.318106	1.738593
H	-3.855691	-1.084207	2.990390
H	-4.428125	-0.649346	1.371115
C	-2.501507	-2.167808	-3.026408
H	-3.235239	-1.974381	-3.814741
H	-1.663688	-1.482573	-3.160470
H	-2.139891	-3.193207	-3.152917
C	-4.294359	-2.978055	-1.429127
H	-4.751886	-2.877652	-0.441748
H	-5.080122	-2.817715	-2.172956
H	-3.944541	-4.009028	-1.537703
C	-2.031729	3.820856	0.064611
H	-1.379428	3.578070	-0.776489
H	-2.834370	4.466846	-0.302740
H	-1.454103	4.398170	0.792573
C	-3.503367	2.878215	1.906319
H	-4.386262	3.432188	1.573383
H	-3.851718	1.974203	2.413170
H	-2.977019	3.495460	2.640905
C	3.497950	2.881730	1.900888
H	3.846495	1.979360	2.410541
H	4.380748	3.435889	1.568011
H	2.969731	3.500180	2.633106
C	2.027742	3.817939	0.054568
H	1.377178	3.571975	-0.786964
H	1.448072	4.396207	0.780136
H	2.830047	4.464171	-0.313082
C	2.502535	-2.173036	-3.021688
H	1.663952	-1.488437	-3.154259
H	3.234555	-1.979012	-3.811465
H	2.141516	-3.198754	-3.147354
C	4.299330	-2.981566	-1.427960
H	5.083175	-2.821384	-2.173835
H	4.759292	-2.880218	-0.441800
H	3.949861	-4.012818	-1.534964

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    Cl   0.000844   0.407351  -1.946645

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1, S=1/2, a=150
6-311G(d,p)
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    Ni  -0.000024  -0.233115   0.088648
    N   -0.000280  -1.264889   1.618198
    C   -1.192286  -1.513492   2.238021
    C    1.191563  -1.513766   2.238226
    C   -1.211811  -2.159930   3.469047
    C    1.210735  -2.160228   3.469242
    C   -0.000630  -2.501947   4.080643
    H   -2.152111  -2.386592   3.955409
    H    2.150902  -2.387123   3.955753
    H   -0.000769  -3.000000   5.041953
    C    2.310272  -0.999475   1.471428
    C   -2.310751  -0.999032   1.470985
    N   -1.959763  -0.278441   0.423749
    N    1.959604  -0.278741   0.424191
    C   -2.957006   0.281201  -0.444532
    C   -3.192093   1.669594  -0.354820
    C   -3.647001  -0.520824  -1.377556
    C   -4.172666   2.231087  -1.173207
    C   -4.612205   0.095450  -2.179815
    C   -4.886361   1.451532  -2.075268
    H   -4.376664   3.293268  -1.110925
    H   -5.151560  -0.500778  -2.906919
    H   -5.642219   1.904620  -2.707135
    C    2.957091   0.281029  -0.443727
    C    3.192340   1.669366  -0.353585
    C    3.647172  -0.520840  -1.376813
    C    4.173109   2.230963  -1.171671
    C    4.612585   0.095529  -2.178743
    C    4.886864   1.451561  -2.073814
    H    4.377222   3.293106  -1.109068
    H    5.152016  -0.500574  -2.905892
    H    5.642874   1.904724  -2.705446
    C   -3.358863  -2.006465  -1.580180
    H   -2.583783  -2.300777  -0.869926
    C   -2.412278   2.535197   0.628211
    H   -1.493751   1.992475   0.866918
    C    3.358959  -2.006420  -1.579747
    H    2.583591  -2.300734  -0.869806
    C    2.412502   2.534848   0.629539
    H    1.494062   1.992033   0.868352
    C    3.723175  -1.270834   1.903133
    H    3.829391  -1.093890   2.976492
    H    3.997049  -2.313496   1.716419
    H    4.429530  -0.633708   1.375023
    C   -3.723783  -1.270096   1.902452
    H   -3.997914  -2.312652   1.715529
    H   -3.830094  -1.093301   2.975825
    H   -4.429898  -0.632698   1.374347
    C   -2.798254  -2.279370  -2.989858
    H   -3.532730  -2.032520  -3.762479
    H   -1.897808  -1.690819  -3.165198
    H   -2.548981  -3.340050  -3.095058
    C   -4.601310  -2.881105  -1.320442
    H   -5.029349  -2.709265  -0.330009
    H   -5.385852  -2.681338  -2.055796
    H   -4.341180  -3.940929  -1.398378
    C   -1.998483   3.890919   0.035133
    H   -1.467919   3.761668  -0.910407
    H   -2.859996   4.540525  -0.143218
    H   -1.336492   4.415939   0.729353
    C   -3.189433   2.727666   1.944870
    H   -4.128517   3.260363   1.766412
    H   -3.433729   1.769975   2.411104
    H   -2.601078   3.310466   2.660398
    C    3.189782   2.727398   1.946107
    H    3.434243   1.769721   2.412286
    H    4.128789   3.260203   1.767563
    H    2.601442   3.310115   2.661714
    C    1.998497   3.890516   0.036480
    H    1.467758   3.761178  -0.908949
    H    1.336609   4.415530   0.730808
    H    2.859932   4.540164  -0.142087
    C    2.798851  -2.279117  -2.989662
    H    1.898550  -1.690433  -3.165294
    H    3.533659  -2.032304  -3.761980
    H    2.549473  -3.339752  -3.095052
    C    4.601231  -2.881201  -1.319644
    H    5.386085  -2.681373  -2.054650
    H    5.028877  -2.709549  -0.329008
    H    4.341051  -3.940992  -1.397851
    Cl   0.000208  -0.078557  -2.120153

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1, S=1/2, a=140
6-311G(d,p)
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    Ni  -0.000061  -0.291482   0.010427
    N    0.000297  -1.274133   1.587217
    C   -1.188743  -1.524570   2.203787
    C    1.189664  -1.524958   2.202995
    C   -1.209891  -2.166216   3.438232
    C    1.211430  -2.166621   3.437420
    C    0.000919  -2.504332   4.051154
    H   -2.150087  -2.392347   3.925000
    H    2.151880  -2.393058   3.923553
    H    0.001159  -2.998307   5.014670
    C    2.315891  -1.011719   1.438133
    C   -2.315315  -1.011042   1.439625
    N   -1.976663  -0.293369   0.390078
    N    1.976767  -0.293892   0.388846
    C   -2.976972   0.282283  -0.463486
    C   -3.174358   1.678088  -0.372101
    C   -3.705203  -0.501824  -1.384319
    C   -4.145066   2.267350  -1.182348
    C   -4.660150   0.143563  -2.176783
    C   -4.890440   1.507607  -2.075706
    H   -4.318344   3.334760  -1.119292
    H   -5.228723  -0.438520  -2.892971
    H   -5.638632   1.981516  -2.701379
    C    2.976703   0.281655  -0.465239
    C    3.174659   1.677355  -0.373550
    C    3.704067  -0.502439  -1.386770
    C    4.145058   2.266518  -1.184241
    C    4.658719   0.142853  -2.179667
    C    4.889564   1.506786  -2.078330
    H    4.318789   3.333841  -1.120929
    H    5.226625  -0.439220  -2.896389
    H    5.637523   1.980614  -2.704340
    C   -3.486256  -2.001121  -1.575511
    H   -2.680090  -2.312505  -0.908483
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C	-2.370146	2.520008	0.612780
H	-1.447959	1.969595	0.820051
C	3.484523	-2.001617	-1.578217
H	2.678565	-2.312887	-0.910886
C	2.371497	2.519270	0.612187
H	1.449543	1.968864	0.820477
C	3.722563	-1.274111	1.896582
H	3.820028	-1.040365	2.960260
H	3.987142	-2.327717	1.769581
H	4.439748	-0.671294	1.343841
C	-3.721771	-1.273048	1.898955
H	-3.986789	-2.326543	1.771950
H	-3.818462	-1.039448	2.962735
H	-4.439123	-0.669903	1.346784
C	-3.030077	-2.330021	-3.010234
H	-3.800674	-2.069104	-3.741917
H	-2.113911	-1.794173	-3.254786
H	-2.836659	-3.403448	-3.101936
C	-4.747930	-2.817206	-1.226504
H	-5.115147	-2.609024	-0.219488
H	-5.561814	-2.598167	-1.923680
H	-4.535759	-3.888235	-1.295955
C	-1.970000	3.892255	0.049681
H	-1.461184	3.795169	-0.911716
H	-2.835658	4.546042	-0.088640
H	-1.292965	4.397353	0.743828
C	-3.118514	2.681447	1.950617
H	-4.059934	3.219746	1.804457
H	-3.354895	1.713683	2.399056
H	-2.513702	3.245960	2.667089
C	3.121334	2.680736	1.949195
H	3.358287	1.712970	2.397336
H	4.062556	3.219100	1.802007
H	2.517279	3.245189	2.666353
C	1.970715	3.891483	0.049443
H	1.460786	3.794304	-0.911355
H	1.294486	4.396649	0.744329
H	2.836213	4.545250	-0.089951
C	3.027562	-2.330049	-3.012800
H	2.111455	-1.793854	-3.256806
H	3.797903	-2.069244	-3.744793
H	2.833738	-3.403392	-3.104638
C	4.746091	-2.818198	-1.229988
H	5.559737	-2.599218	-1.927461
H	5.113806	-2.610412	-0.223071
H	4.533552	-3.889141	-1.299642
Cl	-0.000796	-0.603439	-2.190232

1-Br, S=1/2, a=170
6-311G(d,p)

Ni	0.000019	0.338890	0.126610
N	0.000028	2.070047	0.728873
C	1.194920	2.635551	1.084726
C	-1.194875	2.635503	1.084805
C	1.212050	3.878870	1.705704
C	-1.211994	3.878824	1.705807
C	0.000020	4.513267	2.002503
H	2.152022	4.348049	1.966950
H	-2.151965	4.347954	1.967148
H	0.000021	5.479656	2.490448
C	-2.304647	1.775552	0.744928
C	2.304716	1.775582	0.744885
N	1.942674	0.584228	0.297637
N	-1.942592	0.584217	0.297585
C	2.955484	-0.356958	-0.098682
C	3.311632	-1.374064	0.809104
C	3.552355	-0.263274	-1.371214
C	4.330640	-2.255811	0.444788
C	4.560263	-1.177421	-1.689845
C	4.960297	-2.155848	-0.789756
H	4.628415	-3.038727	1.132498
H	5.033142	-1.125945	-2.664118
H	5.747936	-2.851690	-1.056858
C	-2.955437	-0.356815	-0.099023
C	-3.312084	-1.373831	0.808656
C	-3.551922	-0.262992	-1.371736
C	-4.331176	-2.255363	0.444023
C	-4.559937	-1.176907	-1.690667
C	-4.960443	-2.155260	-0.790702
H	-4.629346	-3.038206	1.131648
H	-5.032532	-1.125315	-2.665072
H	-5.748159	-2.850925	-1.058038
C	3.101445	0.750765	-2.418647
H	2.330748	1.378740	-1.966962
C	2.612363	-1.516123	2.156121
H	1.708366	-0.904975	2.110845
C	-3.100528	0.750997	-2.419008
H	-2.329603	1.378592	-1.967188
C	-2.613310	-1.516070	2.155913
H	-1.709483	-0.904630	2.111221
C	2.454443	0.041769	-3.624758
H	3.183889	-0.577811	-4.155060
H	1.633922	-0.601039	-3.301952
H	2.064626	0.778965	-4.333667
C	4.247582	1.670312	-2.880330
H	4.722554	2.184500	-2.040958
H	5.025080	1.105376	-3.402183
H	3.871192	2.428459	-3.573650
C	2.163555	-2.960862	2.432068
H	1.551749	-3.340735	1.611915
H	3.015243	-3.633980	2.566965
H	1.569806	-2.999178	3.350263
C	3.484014	-0.980114	3.307920
H	4.410278	-1.555992	3.397590
H	3.758100	0.066884	3.153948
H	2.950496	-1.051657	4.260734
C	-3.485592	-0.980727	3.307541
H	-3.760018	0.066214	3.153776
H	-4.411672	-1.556976	3.396711
H	-2.952398	-1.052354	4.260531
C	-2.164173	-2.960778	2.431544
H	-1.551859	-3.340152	1.611539
H	-1.570859	-2.999261	3.350014
H	-3.015726	-3.634202	2.565758
C	-2.453758	0.041904	-3.625187
H	-1.633571	-0.601352	-3.302423
H	-3.183451	-0.577231	-4.155670
H	-2.063518	0.779034	-4.333931
C	-4.246273	1.671065	-2.880623
H	-5.023982	1.106500	-3.402564
H	-4.721061	2.185342	-2.041201
H	-3.869559	2.429149	-3.573838
Br	0.000045	-1.704974	-1.014842
C	-3.723336	2.243505	0.897744

H	-3.843195	2.795524	1.832723
H	-3.998262	2.919281	0.081453
H	-4.421381	1.409001	0.892318
C	3.723396	2.243561	0.897691
H	3.998328	2.919234	0.081318
H	3.843229	2.795700	1.832601
H	4.421447	1.409060	0.892384

1-Br, S=1/2, a=160
6-311G(d,p)

Ni	0.000013	0.298726	0.164581
N	0.000066	1.984123	0.903375
C	1.192405	2.514429	1.314252
C	-1.192296	2.514618	1.313941
C	1.211099	3.702669	2.035603
C	-1.210998	3.702863	2.035283
C	0.000053	4.313006	2.381127
H	2.151567	4.145956	2.337433
H	-2.151479	4.146294	2.336861
H	0.000052	5.236167	2.946658
C	-2.307696	1.681108	0.919775
C	2.307779	1.680762	0.920332
N	1.954955	0.525456	0.386035
N	-1.954908	0.525722	0.385619
C	2.968250	-0.377668	-0.086782
C	3.270517	-1.504304	0.704025
C	3.619431	-0.146148	-1.316205
C	4.283134	-2.363048	0.273346
C	4.618513	-1.042884	-1.704853
C	4.961370	-2.133076	-0.916943
H	4.539732	-3.228662	0.872966
H	5.130777	-0.887779	-2.647685
H	5.743243	-2.812394	-1.238039
C	-2.968259	-0.377277	-0.087347
C	-3.271405	-1.503435	0.703795
C	-3.618680	-0.146034	-1.317225
C	-4.284168	-2.361939	0.272965
C	-4.617952	-1.042502	-1.705989
C	-4.961694	-2.132196	-0.917769
H	-4.541450	-3.227182	0.872835
H	-5.129665	-0.887586	-2.649152
H	-5.743705	-2.811310	-1.238961
C	3.246468	1.000333	-2.253051
H	2.457247	1.584032	-1.775037
C	2.523851	-1.782406	2.003083
H	1.631726	-1.151790	1.998268
C	-3.244758	0.999938	-2.254314
H	-2.454974	1.582972	-1.776420
C	-2.525514	-1.781359	2.003340
H	-1.633496	-1.150591	1.999095
C	2.667708	0.467949	-3.578653
H	3.417207	-0.101493	-4.136517
H	1.811232	-0.181003	-3.393072
H	2.344353	1.301193	-4.210658
C	4.434218	1.942934	-2.528198
H	4.873457	2.333386	-1.607166
H	5.227989	1.429167	-3.077984
H	4.110677	2.792553	-3.136764
C	2.045950	-3.240353	2.101351
H	1.458552	-3.516567	1.223643
H	2.882867	-3.939456	2.186594
H	1.420283	-3.371701	2.988984
C	3.363939	-1.391291	3.233803
H	4.275572	-1.993834	3.291293
H	3.662649	-0.340138	3.200490
H	2.796401	-1.551427	4.155713
C	-3.366433	-1.390442	3.233550
H	-3.665385	-0.339362	3.200066
H	-4.277959	-1.993198	3.290519
H	-2.799406	-1.550443	4.155796
C	-2.047417	-3.239234	2.101847
H	-1.459256	-3.515249	1.224588
H	-1.422454	-3.370569	2.989980
H	-2.884283	-3.938494	2.186310
C	-2.666580	0.466883	-3.579895
H	-1.810647	-0.182778	-3.394305
H	-3.416613	-0.101928	-4.137683
H	-2.342528	1.299784	-4.211996
C	-4.431705	1.943535	-2.529522
H	-5.226004	1.430309	-3.079054
H	-4.870475	2.334627	-1.608542
H	-4.107494	2.792709	-3.138353
Br	0.000137	-1.398282	-1.455387
C	-3.721479	2.136175	1.143439
H	-3.830842	2.540222	2.152978
H	-3.991398	2.932231	0.443022
H	-4.428118	1.318878	1.017540
C	3.721578	2.135621	1.144307
H	3.991980	2.931188	0.443520
H	3.830642	2.540236	2.153647
H	4.428070	1.318079	1.019154

1-Br, S=1/2, a=150
6-311G(d,p)

Ni	0.000059	0.259844	-0.165207
N	0.000010	1.913564	-0.994060
C	-1.189988	2.425899	-1.427430
C	1.189973	2.426194	-1.427143
C	-1.210212	3.583552	-2.198083
C	1.210140	3.583849	-2.197741
C	-0.000076	4.179316	-2.568663
H	-2.150679	4.013738	-2.518109
H	2.150588	4.014285	-2.517484
H	-0.000104	5.078179	-3.172173
C	2.312829	1.608345	-1.008585
C	-2.312737	1.607965	-1.008894
N	-1.971303	0.472635	-0.432254
N	1.971448	0.472997	-0.432062
C	-2.977873	-0.418309	0.070046
C	-3.161700	-1.640163	-0.613552
C	-3.724364	-0.106026	1.226495
C	-4.146049	-2.515826	-0.155788
C	-4.690692	-1.025566	1.646640
C	-4.913937	-2.210489	0.961484
H	-4.308892	-3.454460	-0.670695
H	-5.272147	-0.810743	2.535958
H	-5.671511	-2.904985	1.307358
C	2.977891	-0.418419	0.069593
C	3.161011	-1.640016	-0.614597
C	3.724976	-0.106873	1.225861
C	4.145279	-2.516212	-0.157674
C	4.691170	-1.026921	1.645182

C	4.913738	-2.211627	0.959401
H	4.307602	-3.454638	-0.673148
H	5.273088	-0.812667	2.534334
H	5.671250	-2.906507	1.304635
C	-3.492304	1.147687	2.067805
H	-2.738281	1.759767	1.569209
C	-2.313746	-1.983439	-1.832404
H	-1.363529	-1.455322	-1.707969
C	3.493682	1.146567	2.067795
H	2.739672	1.759120	1.569759
C	2.312550	-1.982523	-1.833296
H	1.363674	-1.451783	-1.709951
C	-2.928434	0.789255	3.457245
H	-3.647439	0.198393	4.032649
H	-2.006196	0.214878	3.365351
H	-2.718184	1.702110	4.023721
C	-4.770309	1.997031	2.216792
H	-5.215931	2.249685	1.251921
H	-5.530075	1.469788	2.800429
H	-4.544754	2.929822	2.742104
C	-1.988937	-3.479911	-1.944075
H	-1.546998	-3.858100	-1.019902
H	-2.876856	-4.077591	-2.169531
H	-1.275704	-3.645935	-2.755812
C	-2.960253	-1.467739	-3.132503
H	-3.923884	-1.956560	-3.306304
H	-3.134337	-0.389987	-3.095413
H	-2.316447	-1.674569	-3.992989
C	2.960833	-1.469968	-3.133732
H	3.137571	-0.392588	-3.097708
H	3.923343	-1.961288	-3.306690
H	2.316830	-1.676125	-3.994233
C	1.983861	-3.478304	-1.942918
H	1.540080	-3.853675	-1.018475
H	1.270906	-3.643762	-2.755022
H	2.870366	-4.078773	-2.166509
C	2.930238	0.787702	3.457298
H	2.007789	0.213651	3.365502
H	3.649285	0.196361	4.032158
H	2.720489	1.700371	4.024259
C	4.772026	1.995412	2.216648
H	5.531916	1.467602	2.799612
H	5.217248	2.248478	1.251701
H	4.547018	2.927975	2.742598
Br	0.000244	-1.034264	1.798876
C	3.721284	2.055671	-1.279202
H	3.809072	2.412310	-2.308578
H	4.005831	2.882694	-0.622198
H	4.430906	1.244326	-1.131960
C	-3.721228	2.055206	-1.279503
H	-4.005848	2.882197	-0.622492
H	-3.809030	2.411857	-2.308875
H	-4.430806	1.243817	-1.132298

1-Br, S=1/2, a=140
6-311G(d,p)

Ni	0.000085	0.252199	0.256845
N	0.000193	2.115136	0.345015
C	-1.186017	2.778129	0.263716
C	1.186446	2.778000	0.263294
C	-1.208746	4.169401	0.228292
C	1.209332	4.169262	0.227927
C	0.000329	4.870691	0.229516
H	-2.149328	4.703822	0.190472
H	2.149965	4.703573	0.189820
H	0.000385	5.953025	0.198489
C	2.320531	1.867764	0.178837
C	-2.320254	1.868025	0.180056
N	-1.995685	0.599718	0.068249
N	1.995698	0.599564	0.066809
C	-3.007217	-0.414443	-0.016284
C	-3.155234	-1.067731	-1.261376
C	-3.796646	-0.777429	1.097685
C	-4.127001	-2.060983	-1.382027
C	-4.748339	-1.787343	0.920144
C	-4.923889	-2.418899	-0.301489
H	-4.262136	-2.567496	-2.329706
H	-5.359495	-2.088405	1.763258
H	-5.670874	-3.197400	-0.410044
C	3.006944	-0.414727	-0.019602
C	3.154029	-1.066346	-1.265671
C	3.797022	-0.779331	1.093358
C	4.125420	-2.059734	-1.388249
C	4.748339	-1.789254	0.913868
C	4.922896	-2.419298	-0.308693
H	4.259810	-2.565018	-2.336699
H	5.359973	-2.091538	1.756194
H	5.669583	-3.197873	-0.418749
C	-3.651126	-0.154605	2.485256
H	-2.855600	0.591802	2.441928
C	-2.298852	-0.667306	-2.457305
H	-1.365995	-0.260900	-2.055109
C	3.652634	-0.158197	2.481806
H	2.856593	0.587761	2.440201
C	2.297199	-0.663954	-2.460632
H	1.365256	-0.256431	-2.057474
C	-3.226158	-1.198346	3.536016
H	-3.990726	-1.971460	3.658645
H	-2.288991	-1.674227	3.250437
H	-3.086177	-0.713587	4.507348
C	-4.947739	0.545046	2.943538
H	-5.309080	1.277299	2.218854
H	-5.750133	-0.181069	3.102284
H	-4.781480	1.060738	3.894031
C	-1.931818	-1.848249	-3.366875
H	-1.476349	-2.661876	-2.798189
H	-2.803341	-2.246298	-3.893745
H	-1.217912	-1.524279	-4.128271
C	-2.971516	0.455096	-3.272032
H	-3.919357	0.109572	-3.695989
H	-3.182313	1.330132	-2.653139
H	-2.327891	0.774438	-4.097664
C	2.970829	0.457970	-3.275215
H	3.183328	1.332338	-2.655954
H	3.917872	0.111383	-3.700089
H	2.327027	0.778696	-4.100172
C	1.927802	-1.843875	-3.370577
H	1.471502	-2.657112	-2.802003
H	1.213884	-1.518438	-4.131349
H	2.798385	-2.242962	-3.898211
C	3.229503	-1.203411	3.531841
H	2.292308	-1.679537	3.246775
H	3.994703	-1.976171	3.652777
H	3.090271	-0.719840	4.503870

C	4.949356	0.541668	2.939461
H	5.752467	-0.184138	3.096008
H	5.309221	1.275302	2.215447
H	4.783984	1.055780	3.890964
Br	0.000481	-1.620729	1.683101
C	3.719389	2.416547	0.161832
H	3.790267	3.233242	-0.561633
H	3.996236	2.821953	1.138950
H	4.443254	1.651540	-0.110066
C	-3.719044	2.417006	0.163705
H	-3.995445	2.822417	1.140947
H	-3.790107	3.233731	-0.559706
H	-4.443135	1.652105	-0.107904

6, S=3/2
6-311G(d,p)

Ni	0.000019	-0.026839	0.063837
N	-0.000044	1.895492	-0.136356
C	1.191385	2.559430	-0.168594
C	-1.191489	2.559370	-0.168779
C	1.214147	3.944476	-0.282399
C	-1.214328	3.944402	-0.282589
C	-0.000097	4.642292	-0.350081
H	2.159974	4.472914	-0.312542
H	-2.160181	4.472785	-0.312878
H	-0.000121	5.721120	-0.441090
C	-2.320791	1.674460	-0.042821
C	2.320700	1.674587	-0.042485
N	2.075896	0.397594	0.101527
N	-2.075946	0.397499	0.101241
C	3.173365	-0.510987	0.235416
C	3.562993	-0.916913	1.527345
C	3.804182	-1.015494	-0.918220
C	4.648007	-1.787763	1.644993
C	4.884924	-1.884386	-0.745359
C	5.314329	-2.260351	0.520711
H	4.974109	-2.105377	2.628935
H	5.390950	-2.281487	-1.618184
H	6.155885	-2.935120	0.631356
C	-3.173382	-0.511138	0.235033
C	-3.563078	-0.917049	1.526940
C	-3.804087	-1.015705	-0.918642
C	-4.648081	-1.787922	1.644533
C	-4.884806	-1.884634	-0.745835
C	-5.314302	-2.260567	0.520215
H	-4.974259	-2.105503	2.628460
H	-5.390742	-2.281791	-1.618687
H	-6.155849	-2.935355	0.630816
C	3.323739	-0.662281	-2.321588
H	2.400241	-0.089865	-2.217427
C	2.829851	-0.417994	2.767562
H	1.897353	0.038875	2.425372
C	-3.323525	-0.662575	-2.321990
H	-2.400088	-0.090068	-2.217797
C	-2.830037	-0.418068	2.767194
H	-1.897630	0.039009	2.425031
C	2.974191	-1.921552	-3.134931
H	3.854390	-2.546191	-3.312218
H	2.225119	-2.519098	-2.612100
H	2.567739	-1.638689	-4.110790
C	4.340352	0.223046	-3.066272
H	4.546177	1.146840	-2.517894
H	5.292700	-0.297589	-3.204063
H	3.961486	0.493977	-4.056371
C	2.446427	-1.558775	3.725224
H	1.873647	-2.331594	3.208007
H	3.327081	-2.031430	4.168585
H	1.836326	-1.171500	4.546736
C	3.634610	0.672900	3.498862
H	4.589346	0.277583	3.858431
H	3.853230	1.517857	2.840400
H	3.079200	1.050339	4.362907
C	-3.634997	0.672621	3.498571
H	-3.853783	1.517576	2.840160
H	-4.589654	0.277105	3.858127
H	-3.079650	1.050113	4.362633
C	-2.446380	-1.558858	3.724755
H	-1.873490	-2.331535	3.207448
H	-1.836313	-1.171545	4.546274
H	-3.326939	-2.031699	4.168106
C	-2.973784	-1.921902	-3.135169
H	-2.224717	-2.519334	-2.612202
H	-3.853917	-2.546629	-3.312479
H	-2.567257	-1.639107	-4.111018
C	-4.340135	0.222583	-3.066877
H	-5.292418	-0.298156	-3.204735
H	-4.546116	1.146410	-2.518614
H	-3.961175	0.493453	-4.056957
Cl	0.000031	-2.166493	-0.484086
H	-3.336892	2.063930	-0.058770
H	3.336786	2.064098	-0.058286

7, S=3/2
6-311G(d,p)

Ni	-0.000181	-0.070577	-0.215828
N	-0.000157	1.872324	-0.286520
C	1.186391	2.542482	-0.241634
C	-1.186841	2.542322	-0.241489
C	1.211037	3.932639	-0.286353
C	-1.211576	3.932532	-0.286244
C	-0.000342	4.634720	-0.334027
H	2.157691	4.460007	-0.261447
H	-2.158282	4.459806	-0.261265
H	-0.000399	5.716717	-0.368208
C	-2.307867	1.659988	-0.077209
C	2.307608	1.660250	-0.077470
N	2.056023	0.380949	0.057159
N	-2.056047	0.380633	0.057321
C	3.152743	-0.524363	0.227943
C	3.525916	-0.903417	1.532068
C	3.806972	-1.041349	-0.908013
C	4.613573	-1.767052	1.679734
C	4.889058	-1.901204	-0.704776
C	5.299009	-2.255205	0.574349
H	4.926136	-2.066336	2.673801
H	5.412966	-2.308393	-1.562060
H	6.141745	-2.924093	0.709150
C	-3.152630	-0.524831	0.228204
C	-3.525837	-0.903742	1.532359
C	-3.806732	-1.042087	-0.907710
C	-4.613370	-1.767530	1.680095
C	-4.888684	-1.902097	-0.704410

C	-5.298652	-2.255971	0.574746
H	-4.925953	-2.066702	2.674189
H	-5.412487	-2.309490	-1.561659
H	-6.141287	-2.924977	0.709598
C	3.356233	-0.696791	-2.323649
H	2.392699	-0.188700	-2.243878
C	2.775363	-0.390385	2.756024
H	1.863883	0.093286	2.396808
C	-3.356014	-0.697580	-2.323364
H	-2.392516	-0.189423	-2.243592
C	-2.775472	-0.390391	2.756295
H	-1.864135	0.093535	2.397063
C	3.123262	-1.953709	-3.179620
H	4.052369	-2.502123	-3.358399
H	2.413458	-2.625045	-2.693010
H	2.715759	-1.672406	-4.155368
C	4.337427	0.271196	-3.011451
H	4.456363	1.196963	-2.441606
H	5.328025	-0.181604	-3.115100
H	3.981999	0.533232	-4.012625
C	2.342209	-1.529564	3.694824
H	1.757278	-2.279507	3.158160
H	3.201441	-2.031690	4.148026
H	1.727986	-1.133834	4.509213
C	3.592391	0.672851	3.514229
H	4.527812	0.251333	3.894254
H	3.848658	1.516754	2.867791
H	3.026396	1.058700	4.367590
C	-3.592824	0.672662	3.514413
H	-3.849325	1.516441	2.867905
H	-4.528126	0.250896	3.894453
H	-3.026956	1.058743	4.367754
C	-2.341996	-1.529370	3.695197
H	-1.756848	-2.279193	3.158604
H	-1.727897	-1.133398	4.509564
H	-3.201096	-2.031696	4.148423
C	-3.122950	-1.954487	-3.179323
H	-2.413163	-2.625807	-2.692667
H	-4.052029	-2.502919	-3.358186
H	-2.715381	-1.673168	-4.155040
C	-4.337258	0.270333	-3.011207
H	-5.327826	-0.182536	-3.114858
H	-4.456257	1.196107	-2.441390
H	-3.981828	0.532366	-4.012382
H	-3.325152	2.045292	-0.054060
H	3.324833	2.045747	-0.054485
Br	0.000082	-2.402457	-0.486731

Table S7. Frequencies (cm^{-1}) for fully optimized structures at the B3LYP/6-311G(d,p) level of theory. Some small imaginary frequencies (< 30 cm^{-1}) corresponding to methyl rotation on the aryl groups were ignored.

6, S=1/2

6-311G(d,p)

4.9838	14.3919	26.1062
28.9980	32.6049	33.9222
37.4625	38.6254	43.0244
47.9034	58.1739	65.0020
85.5969	94.2523	126.2008
127.3038	129.1566	130.4259
131.6655	160.3969	174.5485
195.0611	217.2948	218.6275
225.0184	225.4881	229.4255
234.8227	238.2070	244.2056
244.3329	250.2481	252.4085
258.8923	270.1156	272.1327
280.2675	289.5070	301.1332
307.0541	319.5319	320.7644
356.4337	360.2107	381.5224
392.4597	403.2363	440.9535
441.0781	446.0925	455.8609
458.2922	471.7233	485.8420
492.0705	550.0483	550.3338
552.8653	586.9664	593.2118
594.0344	603.0062	609.7862
613.4153	642.8014	643.4088
646.9738	661.7539	693.8328
714.0460	727.0939	773.4388
774.1799	782.5459	808.8202
812.7895	813.5893	831.5754
834.9711	867.5244	875.9804
878.7611	888.3890	892.4732
922.2831	922.4585	922.8811
923.7788	932.2543	933.1325
936.4414	937.5946	948.5673
948.9231	962.1247	962.6216
963.7129	964.3132	965.1691
984.5529	984.7492	1004.3244
1048.4152	1066.0817	1067.0427
1077.5671	1079.1294	1089.8616
1117.9641	1121.4592	1122.1693
1123.7406	1124.2405	1127.0384
1143.8985	1173.4752	1173.8556
1187.5629	1188.1017	1200.6407
1201.4595	1202.2107	1202.5537
1206.8523	1264.0892	1264.6417
1266.2766	1278.7212	1278.9622
1282.3655	1293.9294	1294.3139
1343.5447	1343.7907	1349.8365
1350.2202	1351.5078	1354.5512
1364.1638	1364.7839	1385.5044
1386.1547	1390.2616	1396.8872
1397.8783	1399.3432	1400.1042
1416.2603	1418.5493	1419.8173
1420.4066	1421.8056	1475.3090
1478.2369	1487.7873	1488.4872
1489.3304	1490.6233	1491.1112
1491.9357	1492.1977	1493.6930
1494.8886	1495.7681	1496.6173
1502.7745	1504.3881	1504.4676
1506.6743	1511.0212	1513.1247
1514.8265	1516.6742	1540.2996
1555.4234	1624.6252	1624.7325
1629.1236	1631.1565	1635.6150

```
 3017.9043  3018.0503  3018.6509
 3018.8710  3023.0664  3023.5914
 3024.9992  3025.8174  3059.1785
 3059.2518  3061.5806  3061.7662
 3078.6845  3079.0325  3079.5491
 3079.8346  3083.3072  3083.6107
 3083.7717  3083.9881  3091.0676
 3091.7616  3092.7570  3093.2891
 3107.8552  3108.4961  3109.1390
 3109.2964  3160.7005  3160.7209
 3169.4632  3169.9605  3173.5550
 3173.5778  3183.3291  3185.4038
 3185.5157  3192.2249  3203.5177

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7, S=1/2
6-311G(d,p)
------------------
   -7.7901    14.2787    29.4504
   29.7855    33.7130    41.9795
   43.1770    47.5294    51.2773
   51.9959    58.7775    61.7414
   79.0144   103.5996   122.9877
  126.7443   129.0138   129.9529
  131.7066   138.5526   166.5004
  188.2074   197.1127   216.6417
  219.3521   223.3890   231.5162
  236.1712   238.9168   243.0369
  246.4658   251.6309   255.3176
  257.8053   264.8939   275.3423
  280.8545   284.6984   293.8119
  305.6594   318.7620   321.4601
  352.1883   359.1322   369.9612
  370.1791   402.1690   440.4384
  441.2234   443.2919   453.4435
  456.3454   471.0650   484.1307
  490.7041   548.3883   549.7736
  552.2061   583.8306   591.5460
  594.0540   603.1269   607.2071
  613.7661   640.9872   641.5303
  646.9011   658.6276   696.5918
  713.1207   726.4627   772.9485
  774.4441   782.4605   809.0217
  812.2338   813.0689   828.9082
  832.3027   872.1813   877.9426
  880.8568   889.6584   893.5368
  920.3480   922.0928   922.2772
  924.0273   932.0585   933.3248
  933.9357   934.9419   948.7994
  949.2051   962.6346   963.1985
  963.9196   964.0745   964.2844
  984.4532   984.8027  1012.7434
 1046.4633  1065.4455  1066.5719
 1077.2078  1078.5852  1086.5092
 1116.8785  1119.9469  1122.4593
 1123.1205  1123.8484  1126.2836
 1143.1991  1172.5985  1173.1112
 1187.3118  1187.8327  1199.4755
 1200.1230  1202.5531  1202.7759
 1207.5082  1263.5686  1264.0776
 1264.9101  1278.1354  1278.3745
 1282.1399  1293.1228  1293.5475
 1341.2042  1341.4502  1345.4493
 1347.9200  1351.1622  1355.0174
 1364.5417  1366.4042  1383.7475
 1385.3370  1389.4683  1399.0854
 1399.3288  1399.6755  1400.1158
 1415.7504  1420.3891  1420.8842
 1421.1837  1422.2158  1474.5365
 1477.0050  1487.7935  1488.9459
 1489.4414  1490.6604  1490.9492
 1492.0534  1492.4508  1493.6861
 1495.3392  1496.0788  1496.5937
 1503.1612  1504.8384  1505.9519
 1506.3073  1511.8721  1513.5774
 1513.8996  1515.8024  1537.8578
 1556.2457  1624.2267  1624.3861
 1628.6825  1630.7270  1635.1964
 3017.7953  3018.0038  3018.3846
 3018.8434  3025.2096  3025.8885
 3026.3012  3026.7761  3057.9903
 3058.3857  3058.6451  3059.9061
 3078.9375  3079.2890  3079.7438
 3080.2876  3083.2398  3083.9377
 3084.6849  3085.3873  3091.1100
 3091.7594  3092.0618  3092.8791
 3107.8102  3110.7336  3110.9840
 3111.7027  3161.1070  3161.2402
 3167.9736  3168.4787  3174.1032
 3174.3906  3183.2463  3185.9331
 3186.1651  3191.7989  3203.5092

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1, S=1/2
6-311G(d,p)
------------------
    8.3088    20.2289    29.9863
   36.8247    45.1613    47.9413
   50.1285    50.8512    56.7056
   68.5431    71.6633    86.5953
   97.3661   104.0991   106.7062
  109.4191   117.7564   121.7262
  126.4378   129.8932   132.6765
  134.1152   159.5728   182.2240
  185.4821   220.2910   220.5026
  224.1177   225.6301   229.3309
  229.7171   238.1291   240.2587
  250.9732   253.0836   255.6847
  261.5762   266.5179   277.3183
  278.0771   278.8608   281.1615
  311.0973   315.9210   316.7490
  318.7945   319.5680   327.7088
  355.4140   373.4023   396.1118
  407.4971   435.3376   438.0025
  443.6156   445.5228   464.8323
  470.2225   476.7514   520.2341
  536.5391   541.1401   549.6403
  558.6227   570.3552   588.2680
  592.1255   611.7048   615.5125
  640.7452   647.3620   647.4474
  651.4146   667.9644   690.4140
  714.5524   718.7036   740.1600
  776.3051   777.1156   794.3505
  811.9307   814.1386   814.4789
  829.7037   852.2249   870.6379
  871.4110   888.7395   891.8738
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  914.5791   922.6685   922.6991
  932.8116   933.8629   935.1258
  937.0391   941.8948   948.5978
  948.6936   954.1218   962.5451
  962.9010   963.2157   963.7661
  984.1461   984.1643   996.9755
 1040.7254  1040.8469  1054.2105
 1065.2434  1066.9032  1077.4567
 1079.1176  1094.0910  1103.1502
 1115.0338  1118.1304  1119.0787
 1122.3595  1122.3912  1126.5495
 1134.6791  1171.3684  1174.4364
 1178.7538  1187.4990  1188.3331
 1202.6196  1203.0614  1212.0408
 1226.2740  1250.6490  1265.4664
 1267.8252  1278.2679  1278.5826
 1289.8747  1290.1480  1344.9233
 1345.5252  1349.4776  1349.6664
 1356.0946  1356.6170  1369.1002
 1375.1706  1382.6747  1383.3168
 1390.3767  1398.6316  1399.5479
 1400.0890  1400.8707  1405.3367
 1410.4044  1420.6506  1422.3496
 1422.4952  1424.0749  1429.1475
 1465.3800  1470.5519  1476.7060
 1477.0388  1486.3446  1488.5373
 1489.4065  1490.0041  1491.1971
 1491.5322  1492.3225  1493.0167
 1493.6711  1495.7477  1496.0507
 1497.1100  1503.2859  1505.2992
 1505.6573  1508.0892  1511.6913
 1514.5530  1515.8198  1518.0166
 1519.5798  1526.9763  1544.3915
 1622.6021  1622.6636  1623.9421
 1631.3814  1631.8573  3018.8738
 3019.2235  3019.7006  3020.6307
 3023.6187  3024.0855  3024.4358
 3024.8334  3029.9716  3030.1398
 3058.3721  3058.3875  3058.7464
 3059.2187  3077.9088  3078.5320
 3078.5618  3079.1324  3084.4301
 3085.0232  3086.8037  3087.2371
 3089.7707  3089.8732  3091.9690
 3092.5591  3092.8896  3093.3097
 3111.3058  3111.8089  3113.1981
 3113.8629  3141.4371  3141.4696
 3159.7148  3159.7373  3171.6189
 3171.6433  3184.4766  3184.5866
 3185.5959  3198.0316  3206.5927

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1-Br, S=1/2
6-311G(d,p)
------------------
   15.2091    17.2272    23.9191
   29.9179    44.1087    48.0850
   49.4752    59.2551    59.7138
   60.1654    60.6247    68.7654
   84.0265   101.4800   101.5606
  114.3788   114.4220   118.5958
  122.3192   123.3301   134.8184
  135.5932   136.8875   167.0796
  188.4434   191.9974   217.6923
  219.5356   222.5391   226.4570
  230.8456   235.2807   241.2675
  244.9354   249.7101   255.2905
  255.4719   259.6367   274.5990
  275.2819   279.6283   280.8125
  302.4970   309.4897   311.3569
  312.9122   320.1331   321.8738
  340.0428   373.1563   386.5175
  406.7209   422.5166   438.4628
  439.9159   446.5624   462.0067
  467.5443   474.9330   521.0438
  537.9537   540.2359   551.1549
  557.1208   569.9252   586.8554
  589.5251   610.2298   615.8280
  641.7888   646.1139   647.1742
  652.5277   665.7349   694.4488
  713.1149   715.4477   737.9842
  773.7977   779.0417   792.3576
  807.0103   812.4797   812.5221
  828.0190   853.0787   867.8219
  873.4986   887.0152   889.5014
  916.4738   917.1752   917.2240
  930.8036   931.7413   932.4767
  933.7232   938.5739   946.3976
  946.9244   956.4185   961.3901
  962.0233   962.3813   962.8364
  980.5177   980.5542   991.5993
 1041.3745  1041.6298  1051.8600
 1064.7255  1065.9237  1077.0287
 1078.5141  1092.4665  1106.8675
 1115.2861  1119.6804  1120.5915
 1121.0129  1121.4941  1125.4611
 1132.9868  1169.5769  1172.9841
 1177.7541  1186.8720  1187.3877
 1201.4402  1201.7963  1210.0539
 1225.6699  1256.9183  1263.8797
 1266.9523  1275.0841  1275.1701
 1287.8973  1288.2873  1345.5259
 1346.2382  1346.7917  1347.2865
 1353.3646  1353.7702  1367.8462
 1374.9962  1379.2050  1379.7576
 1390.1718  1396.2207  1396.4855
 1397.9788  1398.5712  1404.0298
 1410.3308  1419.1425  1420.1305
 1420.3166  1421.8769  1429.7924
 1466.0366  1470.1523  1475.6655
 1476.8760  1485.8153  1486.8626
 1489.8252  1490.2914  1490.5852
 1490.6707  1491.3770  1492.8030
 1493.5387  1494.9424  1495.2601
 1496.7488  1502.4012  1504.3349
 1504.6018  1506.4406  1512.0800
 1514.6339  1516.5792  1516.8939
 1518.9948  1527.6142  1546.2633
 1622.3960  1622.4421  1623.9605
 1630.2629  1630.7867  3018.4583
 3018.7078  3020.0030  3020.2378
 3022.8370  3023.4345  3024.7987
 3025.6451  3031.4152  3031.5197
 3056.7185  3057.0734  3058.1897
 3058.4217  3076.1652  3076.7314
 3078.3951  3078.8046  3080.2742
 3080.2918  3085.9888  3086.5889
```

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 3088.3808  3089.1190  3091.1282
 3091.5136  3093.0312  3093.3439
 3111.3106  3112.3587  3114.6667
 3115.6942  3152.4732  3152.5039
 3158.1484  3158.1758  3168.5349
 3168.5610  3183.1484  3183.2515
 3185.6528  3197.6584  3206.5122

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6, S=3/2
6-311G(d,p)
------------------
  -27.8321   -19.9255     9.9860
   13.5338    27.1896    28.2575
   36.5116    39.4547    46.2381
   47.9378    53.4969    57.4621
   77.8062   106.7569   116.7112
  126.8331   127.4272   129.6465
  130.3433   134.9659   152.5007
  178.9475   180.9937   206.0109
  217.0129   222.6822   230.3163
  241.8564   242.3206   253.2564
  253.5181   255.4021   256.8619
  259.1529   267.4100   268.6305
  273.9468   281.5637   286.9323
  295.6898   304.5668   314.5788
  322.5596   339.1736   346.0821
  355.4732   394.6660   414.4925
  439.7085   440.5911   442.2930
  452.7223   465.7745   479.3508
  490.5619   542.3526   546.1259
  549.1800   575.8145   582.5871
  587.8785   594.6848   603.0932
  624.3966   639.1840   639.7163
  647.7372   649.9352   704.5006
  714.4966   722.3961   771.5829
  777.1132   780.7877   804.4612
  812.2135   813.2912   827.6295
  830.7135   857.7249   888.5933
  889.5814   891.8534   900.9816
  913.2104   922.5740   922.6578
  929.2583   930.3852   933.5464
  937.7890   938.1882   950.2605
  950.3435   961.6236   963.1868
  963.4067   963.7458   964.0956
  968.0914   983.0194   983.1018
 1035.3804  1065.0799  1065.8504
 1077.2088  1078.3243  1080.6218
 1109.1181  1118.5206  1118.7196
 1123.1258  1123.5127  1126.9437
 1127.7423  1172.0054  1172.4714
 1187.5902  1187.8630  1198.2129
 1202.1476  1202.7867  1203.0219
 1204.4655  1260.5583  1261.7815
 1268.4765  1277.6148  1277.9431
 1280.8003  1290.4921  1290.7738
 1338.8100  1340.6687  1346.3254
 1347.8317  1348.8026  1351.4988
 1362.2449  1372.0418  1379.4739
 1380.0127  1392.6706  1397.6770
 1398.1327  1401.1993  1401.4278
 1420.8193  1422.0767  1423.4540
 1423.8980  1429.1553  1473.2483
 1475.4214  1486.6052  1488.6797
 1489.5025  1490.3609  1491.3964
 1492.1327  1493.8864  1494.1402
 1495.4137  1496.1829  1505.0999
 1506.7045  1507.4659  1507.8781
 1508.4052  1511.1779  1512.7196
 1513.8103  1515.6649  1557.6129
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 1621.8420  1631.3145  1632.1803
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 3079.3427  3079.4844  3080.6837
 3080.8958  3082.3506  3082.5699
 3086.8510  3087.5909  3090.0177
 3090.5473  3092.2665  3092.5066
 3103.2408  3104.0170  3111.4649
 3111.8014  3132.0433  3132.6557
 3160.7504  3160.7697  3172.5531
 3172.5701  3179.3273  3185.4032
 3185.5101  3185.8241  3201.4097

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7, S=3/2
6-311G(d,p)
------------------
  -12.9857   -12.0620    -7.2979
    7.0014    16.0624    30.8872
   35.4626    39.9600    44.4431
   49.4871    52.1063    55.8013
   62.4467    92.6885   104.7604
  119.8596   121.6998   128.5458
  130.9157   135.4233   174.0317
  176.8288   181.8039   194.6874
  216.4029   218.3077   231.1028
  231.7160   234.8865   241.4003
  250.0298   250.2003   252.9780
  253.9316   263.7755   273.7989
  281.7430   282.1519   288.1018
  289.4832   305.0456   312.1570
  321.2596   329.4834   332.2083
  345.4949   397.6095   403.9132
  439.2312   439.5762   442.2226
  443.1043   464.8715   484.5455
  493.0794   544.4071   545.1932
  545.8503   575.1911   581.2268
  591.6015   593.7808   601.5728
  619.3335   638.9083   639.2967
  647.8916   647.9758   703.3109
  710.7082   722.7110   771.2475
  779.0595   780.6886   805.6761
  811.3775   812.2620   826.5894
  830.1651   854.4217   888.0664
  888.3730   893.4724   902.2876
  912.3809   921.9904   922.0951
  929.8823   931.5390   932.1718
  934.1690   934.7082   949.0165
  949.4795   959.6519   962.1190
  963.0720   964.2404   964.7962
  966.3660   983.6492   983.6830
 1036.5236  1064.6914  1065.6081
 1076.8635  1077.6732  1080.9414
```

1110.5059	1119.7448	1120.2099
1123.5635	1124.0746	1126.7227
1127.7893	1171.9563	1172.4152
1187.4888	1187.7063	1198.5335
1199.8591	1202.4689	1202.8942
1203.1080	1260.3152	1261.6817
1268.2072	1278.2131	1278.4850
1278.6354	1289.2601	1289.2799
1338.1559	1340.0788	1346.8034
1346.8711	1350.2754	1352.8803
1362.6267	1369.8280	1379.8732
1380.1856	1394.7772	1398.1067
1398.2800	1399.4648	1400.2623
1420.3194	1420.8717	1421.0142
1421.9319	1427.1359	1472.6135
1474.9640	1487.1690	1488.2413
1488.4858	1490.3993	1490.9593
1491.3251	1492.5695	1493.6045
1495.5298	1495.8560	1503.3113
1504.7750	1505.2921	1505.4639
1506.0115	1511.5612	1512.3693
1513.5971	1514.4941	1555.8571
1568.7471	1621.5906	1621.6835
1624.0912	1631.1868	1632.8392
3017.7405	3017.8661	3018.4032
3018.4654	3025.2975	3025.7353
3027.3792	3027.6050	3048.1663
3048.8819	3054.2078	3054.5888
3079.5717	3079.8798	3080.7081
3080.7765	3083.8077	3084.0415
3084.9336	3085.4049	3089.0860
3089.8602	3091.3530	3091.6634
3104.1374	3104.7290	3112.2419
3112.2990	3135.8474	3136.4722
3161.3260	3161.3464	3173.5447
3173.5606	3179.2136	3185.2571
3185.9298	3186.0329	3202.1475

Table S8. Thermodynamics (E_h) for optimized structures at the B3LYP/6-311G(d,p) level of theory.

	E(SCF)	**H(gas)**	**G(gas)**
6, *S*=1/2	-3338.003734	-3337.333756	-3337.447912
6 (170^o), *S*=1/2	-3338.002933	-	-
6 (160^o), *S*=1/2	-3338.000248	-	-
6 (150^o), *S*=1/2	-3337.996306	-	-
6 (140^o), *S*=1/2	-3337.991552	-	-
7, *S*=1/2	-5451.926470	-5451.257607	-5451.367029
7 (170^o), *S*=1/2	-5451.926073	-	-
7 (160^o), *S*=1/2	-5451.923795	-	-
7 (150^o), *S*=1/2	-5451.920244	-	-
7 (140^o), *S*=1/2	-5451.915849	-	-
1, *S*=1/2	-3416.660868	-3415.932331	-3416.049505
1 (170^o), *S*=1/2	-3416.659802	-	-
1 (160^o), *S*=1/2	-3416.656431	-	-
1 (150^o), *S*=1/2	-3416.651305	-	-
1 (140^o), *S*=1/2	-3416.645358	-	-
1-Br, *S*=1/2	-5530.582713	-5529.854678	-5529.973250
1-Br (170^o), *S*=1/2	-5530.581941	-	-
1-Br (160^o), *S*=1/2	-5530.578725	-	-
1-Br (150^o), *S*=1/2	-5530.573799	-	-
1-Br (140^o), *S*=1/2	-5530.567408	-	-
6, *S*=3/2	-3337.986575	-3337.319408	-3337.429637
7, *S*=3/2	-5451.906250	-5451.240234	-5451.348668

8. EPR Spectroscopy

We have recorded a series of high-frequency EPR spectra on a sample ground polycrystalline **7**. Figure S9 and S10 show a series of frequency-dependent spectra recorded at 10 and 150 K, respectively. Inspection of these spectra shows that they account for two very similar species that are characterized by slightly different g-values $g_{x,y,z}$ = 2.236(5), 2.144(4), 2.048(6) for the dominant component and $g_{x,y,z}$ = 2.263(3), 2.140(3), 2.071(2) for the minor fraction. The fits of the resonance field vs. frequency dependence go through zero and show a strict linear relationship. These observations demonstrate that we observe a genuine Kramers doublet that is free of weak exchange interactions.

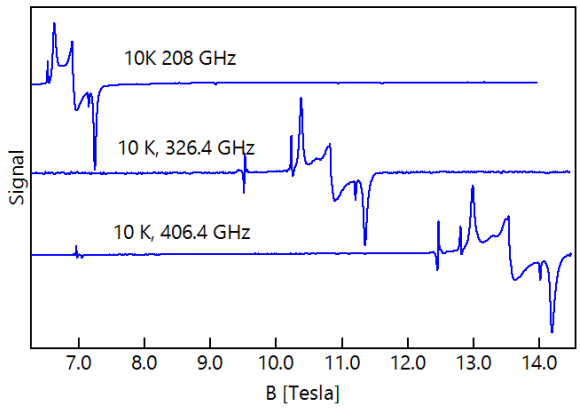

Figure S9. Frequency dependence of the signal observed for $Ni^{I}(L^{2})Br$ (**7**) recorded at 10 K.

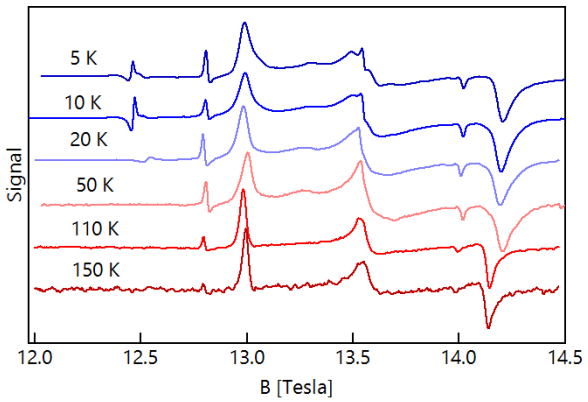

Figure S10. Temperature dependence of the spectra (of compound **7**) recorded at 406.4 GHz. The spectra are normalized and color coded from deep blue for the spectrum recorded at 5 K to deep red for the 150 K.

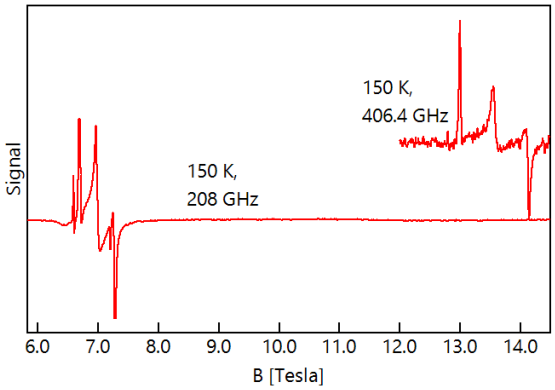

Figure S11. Frequency dependence of the spectra (of compound **7**) recorded at 150 K.

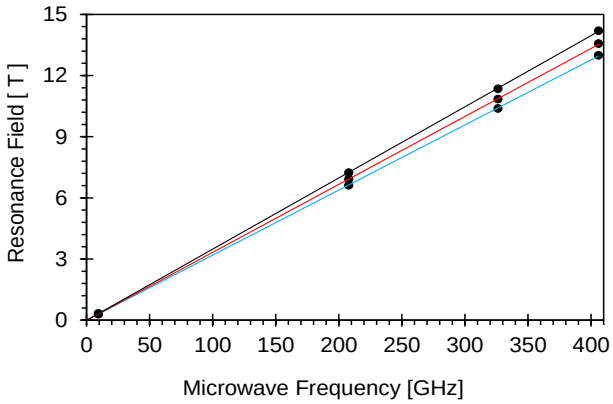

Figure S12. Frequency dependence of the resonance field determined from the analysis of 10 K spectra. The solid lines are linear fits. The fact that the fits go through zero demonstrate that we are observing a genuine Kramers doublet that is, a doublet that is strictly degenerate in zero-field. The slopes of these dependencies are in fact the actual g values.

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