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1. Experimental Section

a) Materials

All chemicals were purchased from Sigma-Aldrich, Acros, ABCR, TCI and used without further purification unless otherwise mentioned. Anhydrous solvents (dichloromethane, acetone, *n*-hexane, toluene) were purchased from Carl-Roth GmbH (≥ 99.5% < 50 ppm H_2O) and degassed by freeze-pump-thaw method prior to use. The starting materials $[L^1NiO_2]$[1], $[(C_7H_8)FeL^3]$[2] and $[(C_7H_8)CoL^3]$,[3] were prepared according to literature procedures. All the liquid substrates for reactivity studies were distilled under argon prior to use.

b) Instrumentation and Physical Methods

Preparation and handling of air sensitive materials were performed in a N_2 glove box OMNI-Lab 2 (VAC) with O_2 and moisture concentration less than 1 ppm. ^{1}H NMR spectra were recorded on Bruker Spectrometer APX 200 and chemical shifts are referenced to the ^{1}H NMR signal of tetramethylsilane (TMS). UV-vis spectra were recorded by Agilent 8453 diode array spectrometer connected with a cryostat from Unisoku Scientific Instruments, Japan.

Electron Paramagnetic Resonance (EPR) measurements were performed on a Bruker ESP 300 X-band EPR spectrometer equipped with a fused quartz Dewar for measurements at liquid nitrogen temperature.

Electrospray ionization mass spectrometry experiments were carried out on an Agilent 1200 mass spectrometer using a spray chamber voltage of 4000 V and a gas carrier temperature of 50°C. High-resolution ESI-MS were measured on a Thermo Scientific LTQ orbitrap XL Elemental analyses were performed by the analytical labor in the Institute of Chemistry, Technical University of Berlin, Germany. IR spectra were measured with a FT-IR Spectrometer (PerkinElmer Spectrum 100).

IR Data are recorded using the KBr pellet technique on a PekinElmer Spectrum 100 FT-IR spectromer.

GC-MS experiments were performed on a Varian GC/MS 4000.

Resonance Raman spectra were measured in toluene at -78°C (Bruker cryostat) using 413 nm excitation (Kr^+-laser) with by a Horiba Jobin-Yvon LabRAM HR800 confocal Raman spectrometer. The concentrations of samples were from 3 mM to 8 mM.

X-ray Absorption Spectroscopy data was collected at beamline 2-2 of the Stanford Synchrotron Radiation Lightsource (SLAC National Accelerator Lab, Menlo Park, CA, USA), with the storage ring operating at 3.0 GeV and 500 mA. A Si(111) double crystal monochromator was used for energy selection, and was detuned by ~40% for harmonic rejection. Sample temperatures were maintained at approximately 20 K using a He Displex cryostat. As appropriate, Ni and Co metal foil spectra were recorded simultaneously using a photodiode for internal energy calibration, with the first inflection point of the reference foil edge set to 8333.0 eV for Ni and 7709.0 eV for Co. XAS data were collected as fluorescence spectra using a 13 element solid state germanium detector (Canberra), with the following parameters: 10 eV steps/1 second integration time in the pre-edge region, 0.3 eV steps /2 second integration time in the edge, and 0.05k steps in the EXAFS, with integration time increasing in a k^2-weighted fashion from 2 to 8 seconds over the energy range (k_{max} = 12.5k for Co, 14k for Ni). The total detector counts were typically 5-25 kHz, well within the linear range of the detector electronics. Samples were monitored for photoreduction during data collection, however no photoreduction was observed for any sample based on the absence of any scan-to-scan red-shift in the absorption edge. Tandem Mossbauer/XAS cups with a sample window of ~ 6mm x 10 mm were used as sample cells.

Averaging and normalization of the XAS data was performed using Athena,[4] a graphical implementation of the IFEFFIT package.[5] Pre-edge peak fitting analysis was carried out on normalized XAS spectra using Fityk v. 0.9.8[6] Spectra were fit over a limited energy range around the pre-edge peak (7702-7715 eV for Co, 8326-8339 eV for Ni). The baseline and rising edge was obtained using a pseudo-Voigt function with a fixed 50:50 ratio of Gaussian:Lorentzian character, while the pre-edge peak was modeled using a Gaussian function; this combination accurately reproduced the experimental data. Fits carried out over four different energy ranges within the limits noted above, and the reported pre-edge peak energy, peak height, FWHM, and area values are the average from these four fits for each sample (Table S1).

EXAFS analysis was carried out using Artemis,[4] which incorporates the IFEFFIT fitting engine and FEFF6 for *ab initio* EXAFS phase and amplitude parameters. DFT calculated structures were used as FEFF6 input to identify significant paths. For a given shell in all simulations, the coordination number n was fixed, while r and σ^2 were allowed to float. The amplitude reduction factor S_0^2 was fixed at 0.9, while the edge shift parameter ΔE_0 was allowed to float at a single common value for all shells. The fit was evaluated in k^3-weighted R-space, and fit quality was judged by the reported R-factor. Significant fits are tabulated in Tables S3-1 and S3-2.

Single-Crystal X-ray Structure Determinations: Crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data of compounds **4, 6** and **7** were collected on an Oxford Diffraction SuperNova, Single source at offset, Atlas at 150 K (Cu-Kα radiation, λ = 1.54184 Å). The structures were solved by direct methods and refined on F^2 with the SHELX-97 software package.[5] The positions of the H atoms (except for those attached on the bridging oxygen atoms) were calculated and considered isotropically according to a riding model. CCDC 1477232 (**4**), CCDC 1469429 (**6**), and CCDC 1469430 (**7**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

c) Synthesis, Reactivity and Spectroscopy

Synthesis of 4: A solution of $[L^3Co(C_7H_8)]$ (0.49 g, 0.91 mmol) in toluene (30 ml) was cooled to -78 °C. The N_2 atmosphere in the flask was exchanged to dried oxygen. After stirring for 10 min, the reaction mixture was allowed to warm to room temperature and stirred further for 1h in the oxygen atmosphere. In the course of stirring the colour of the solution changed from brown red to dark blue. Volatiles were removed in *vacuo* to afford **4** as a dark blue powder (0.42 g, 0.46 mmol, 100 %). Dark blue single crystals suitable for X-ray diffraction analysis were growed from n-hexane at -20°C. M.p. 125 °C (decomp.). Elemental analysis (%): calcd for $C_{54}H_{74}N_4Co_2O_2$: C, 69.81; H, 8.03; N, 6.03. Found: C, 69.79; H, 8.15; N, 5.94. μ_{eff} (Evans, C_6D_6, 298 K): 2.55 μB. HR-APCI-MS: *m*/*z* (%): 929.45323 (calc. 929.45485 [M+H]+). IR (KBr, cm^{-1}): ν = 510 (w), 654 (w), 738 (w), 756 (m), 779 (w), 803 (w), 840 (w), 978 (w), 1056 (w), 1094 (w), 1043 (w), 1249 (w), 1305 (s), 1350 (m), 1362 (w), 1383 (w), 1425 (w), 1456 (s), 1509 (m), 1577 (m), 2867 (w), 2927 (w), 2960 (m), 3061 (w).

Synthesis of 6: To a solution of $[L^1Ni^{II}O_2]$ (0.287 g, 0.565 mmol) in diethyl ether (20 mL) was added $[L^3Fe(C_7H_8)]$ (0.303 g, 0.565 mmol) in diethyl ether (15 mL) at – 78 °C. The reaction mixture was allowed to slowly warm to room temperature and stirred further for 2 h. During the course of the reaction, the color of the reaction mixture changed to dark brown green. Volatiles were removed in *vacuum*, and the residue was extracted with n-hexane (40 mL). After concentration of the resulted solution cooling to -20°C for 2 days, **6** crystallized as dark green crystals (0.463 g, 0.486 mmol, 86%). M.p. 238 °C (decomp.). Elemental analysis (%): calcd for $C_{56}H_{78}N_2FeNiO_2$: C, 70.52; H, 8.24; N, 5.87. Found: C, 70.52; H, 8.37; N, 5.67. μ_{eff} (Evans, C_6D_6, 298 K): 4.87 μ_B. IR (KBr, cm^{-1}): ν = 503 (w), 647 (w), 741

(w), 757 (m), 779 (w), 802 (w), 854 (w), 933 (w), 970 (w), 1025 (w), 1057 (w), 1097 (w), 1145 (w), 1187 (w), 1204 (w), 1254 (m), 1302 (s), 1323 (m), 1343 (w), 1362 (w), 1370 (w), 1399 (s), 1449 (s), 1499 (s), 1525 (m), 1556 (w), 1560 (w), 2867 (m), 2925 (m), 2964 (s), 3061 (w), 3644 (m).

Synthesis of 7: To a solution of $[L^1Ni^{II}O_2]$ (0.198 g, 0.389 mmol) in toluene (15 mL) was added $[L^3Co(C_7H_8)]$ (0.221 g, 0.389 mmol) in toluene (15 mL) at – 78 °C. The reaction mixture was allowed to slowly warm to room temperature and stirred further for 2 h. During the course of reaction, the color of the reaction mixture changed to dark brown. Volatiles were removed in *vacuum*, and the brown residue was extracted with diethyl ether (20mL). After concentration of the resulted solution cooling to 4°C for 2 weeks, **7** crystallized as dark red crystals along with a small amount of identical precipitate. The crystals of **7** were isolated by hand from the precipitate in the Glovebox (0.182 g, 0.191 mmol, 49%). M.p. 219 °C (decomp.). Elemental analysis (%): calcd for $C_{56}H_{78}N_4NiCoO_2$: C, 70.29; H, 8.22; N, 5.86. Found: C, 70.87; H, 8.49; N, 5.61. μ_{eff} (Evans, C_6D_6, 298 K): 3.11 μ_B. IR (KBr, cm^{-1}): ν = 512 (w), 634 (w), 730 (w), 758 (m), 753 (m), 780 (w), 801 (w), 846 (m), 932 (w), 968 (w), 981 (w), 1025 (w), 1057 (w), 1101 (w), 1142 (w), 1192 (w), 1205 (w), 1225 (m), 1256 (m), 1301 (s), 1326 (m), 1346 (m), 1361 (w), 1381 (m), 1399 (s), 1439 (s), 1452 (s), 1507 (s), 1552 (m), 1575 (m), 2866 (m), 2928 (m), 2963 (s), 3062 (w), 3658 (m). Self-decay of **2** also led to the formation of **5**, as was confirmed by mass spectrometry, EPR, and IR studies.

Synthesis of 2: A solution of $[L^1Ni^{II}O_2]$ in anhydrous toluene (2 ml; 0.2 mM) was cooled to -78°C. Then one equivalent of $[L^3Co(C_7H_8)]$ in anhydrous toluene (0.1 ml) was added, to yield a brown intermediate **2**. The generation of **2** was monitored by the growth of the 834 nm band in the UV-Vis spectrum.

Synthesis of 3: A solution of $[L^1Ni^{II}O_2]$ in anhydrous toluene (2 ml; 0.2 mM) was cooled to -78°C. Then 0.5 equivalent of $[(L^1Ni)_2(C_7H_8)]$ in anhydrous toluene (0.1 ml) was added, to yield a brown intermediate **3**. The generation of **3** was monitored by the growth of the 853 nm band in the UV-Vis spectrum.

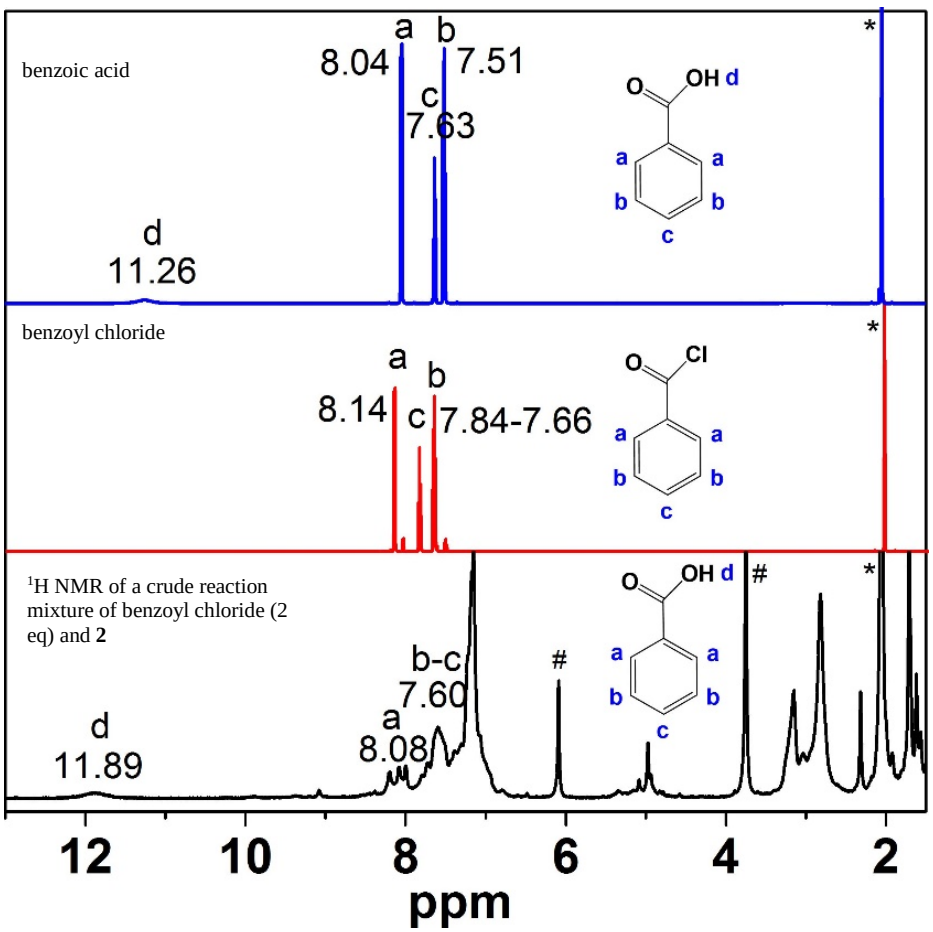
For the determination of the second order rate constant (k_2) values, the concentration of **2** was maintained at 0.2 mM. XAS measurements were performed on samples of 2 having concentrations of 3-5 mM.

Determination of k_2: Reactivity studies of **2-4** were done at -35°C – -85°C, under an inert atmosphere, by injecting the toluene solutions of the substrates (50–400 equivalents) to a preformed solution of **2-4** in toluene. The pseudo-first order decay of the 834 nm, 853 nm or 582 nm band was monitored by

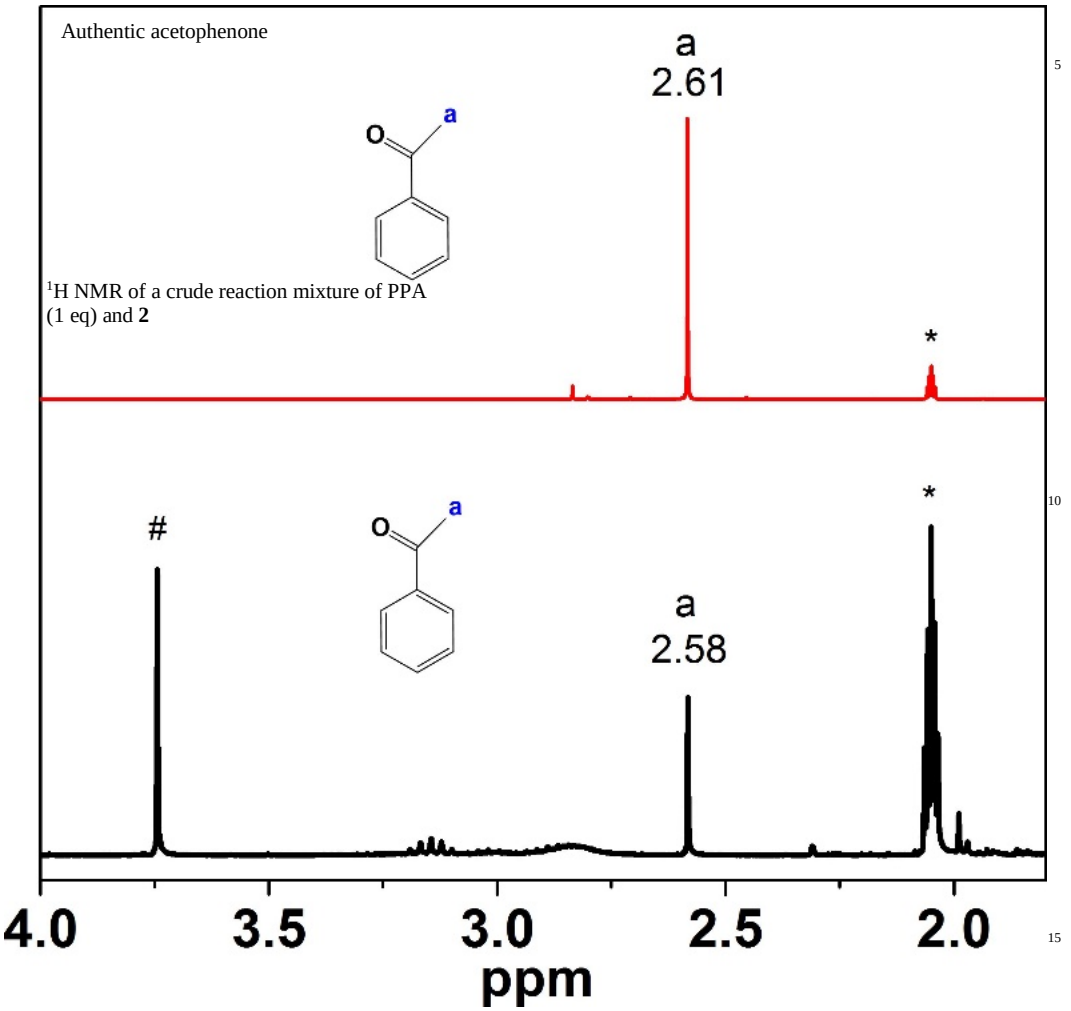
acquiring an UV-Vis spectrum every second. The pseudo-first order fitting of the decay curves yielded the rate constant (k_{obs}), which were found to be linearly increasing with the increment of the substrate concentrations. The slope of the rate constant (k_{obs}) *vs* substrate concentration plot provided the second order rate constant (k_2) values.

Product analysis: A calculated amount of the substrate (1-2 equivalents) in 0.1 ml toluene was added to the preformed solutions of **2-4** in toluene at -78°C and left for 1 hour at -78°C, followed by another hour at -65°C. After adding 0.4 equivalent of 1,3,5-Trimethoxybenzene as an internal standard, the resultant solutions were filtered through silica and diluted with 1 ml ethylacetate. After evaporation of the solvent the residue was dissolved in acetone-d_6 and analyzed for products by ^{1}H-NMR. The chemical shifts are reported in ppm relative to the residual solvent signal. Quantification was performed by comparing the intensity of the product signals relative to that of the standard.

For benzoyl chloride the sole product was characterized to be benzoic acid; the appearance of a new signal at 11.89 ppm (corresponding to the –OH group) in each case confirms the formation of benzoic acid in near stoichiometric amount (in the figure below * represents the solvent signal and # the signal from 1,3,5-Trimethoxybenzene **(-CH$_3$)** , which is used as a standard).

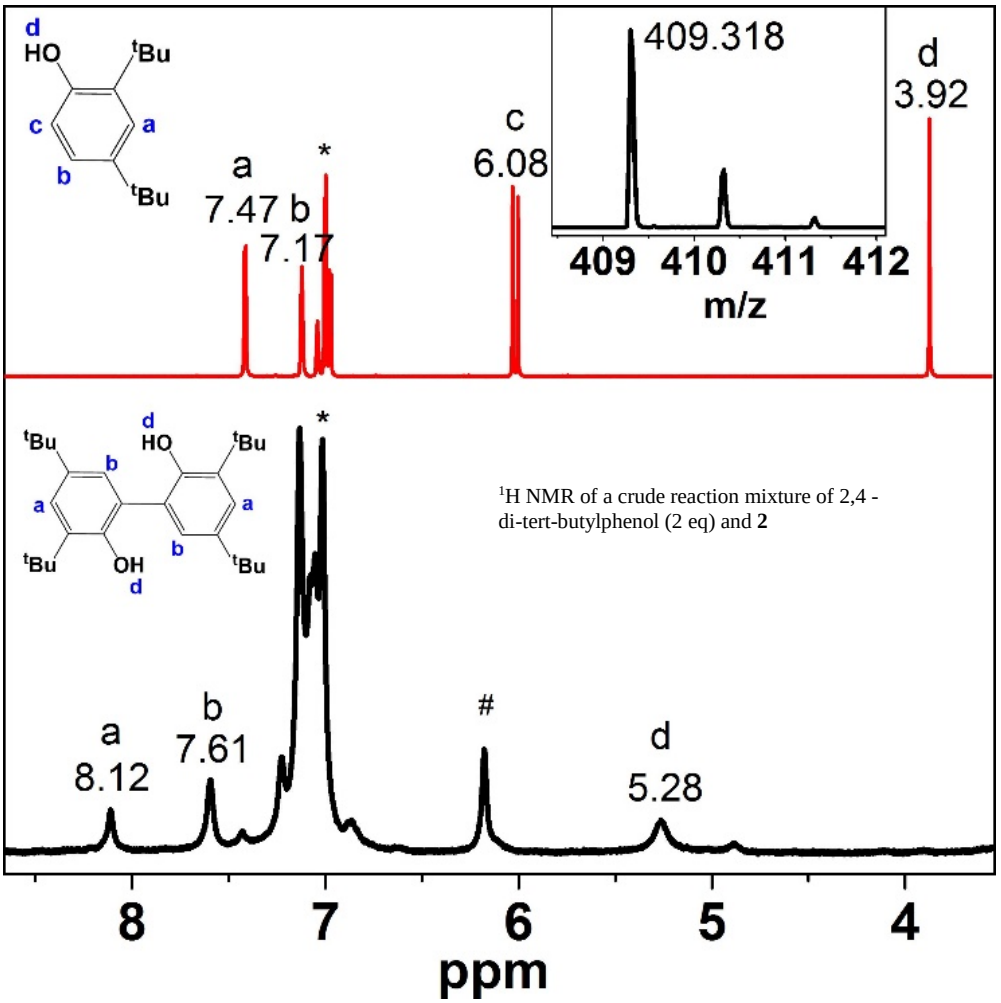


For PPA the product was identified to be acetophenone based on the appearance of a characteristic signal at 2.58 ppm for the $–CH_3$ group (in the figure below * represents the solvent signal and # the signal from 1,3,5-Trimethoxybenzene **$(-CH_3)$** , which is used as a standard). Furthermore, formate analysis was performed by following the previously reported procedure.[7]



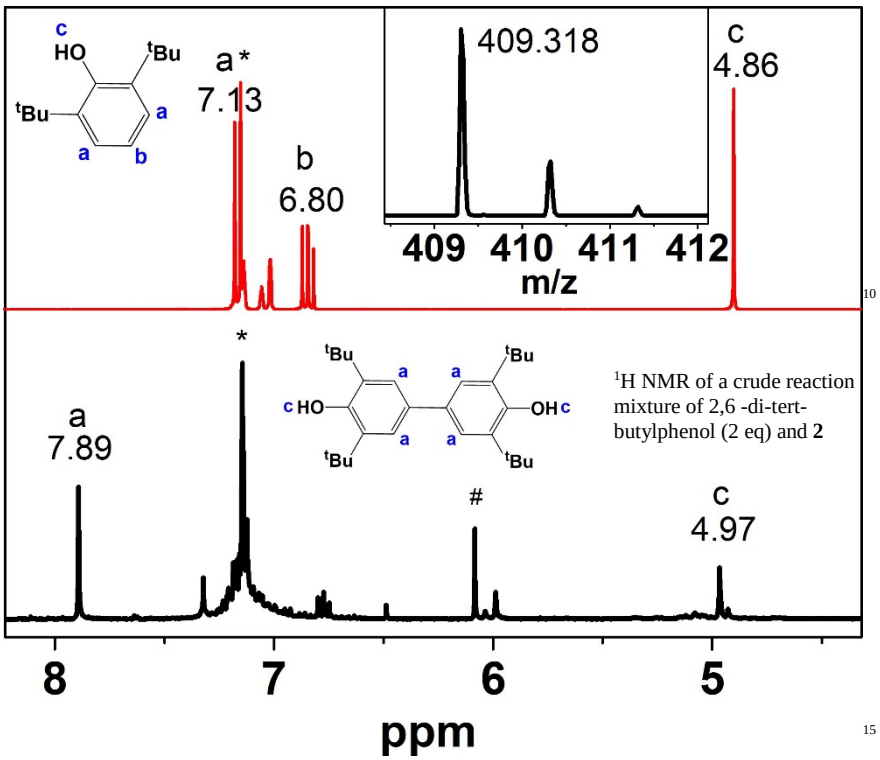
^{1}H NMR of a crude reaction mixture of PPA (1 eq) and **2**

3,3',5,5'-tetra-*tert*-butyl-(1,1'-biphenyl)-2,2'-diol was identified as the product of the oxidation of 2,4-ditertbutyl phenol based on the comparison of the ^{1}H-NMR data of the product with that of the literature known data for 3,3',5,5'-tetra-*tert*-butyl-(1,1'-biphenyl)-2,2'-diol.[8] Electrospray ionization mass spectrum (see the inest of the Figure below) also confirms the formation of the coupled product. * represents the solvent signal and # the signal from 1,3,5-Trimethoxybenzene **(**aromatic **-CH)** , which is used as a standard



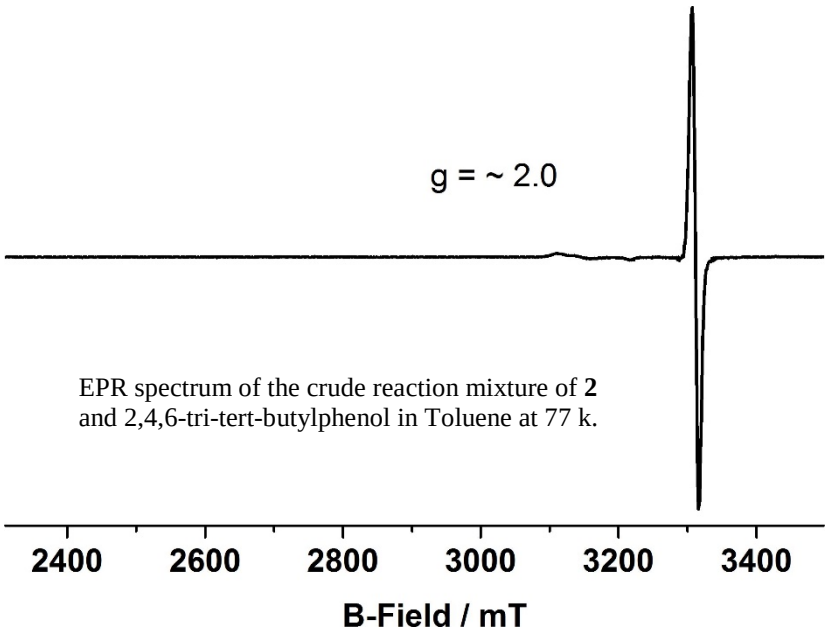
^{1}H NMR of a crude reaction mixture of 2,4 -di-tert-butylphenol (2 eq) and **2**

3,3',5,5'-tetra-*tert*-butyl-(1,1'-biphenyl)-4,4'-diol was identified as the product of the oxidation of 2,6-ditertbutyl phenol based on the comparison of the ^{1}H-NMR data of the product with that of the literature known data for 3,3',5,5'-tetra-*tert*-butyl-(1,1'-biphenyl)-4,4'-diol.[9] * represents the solvent signal and # the signal from 1,3,5-Trimethoxybenzene **(**aromatic **-CH)** , which is used as a standard. Electrospray ionization mass spectrum (see the inest of the Figure below) also confirms the formation of the coupled product.



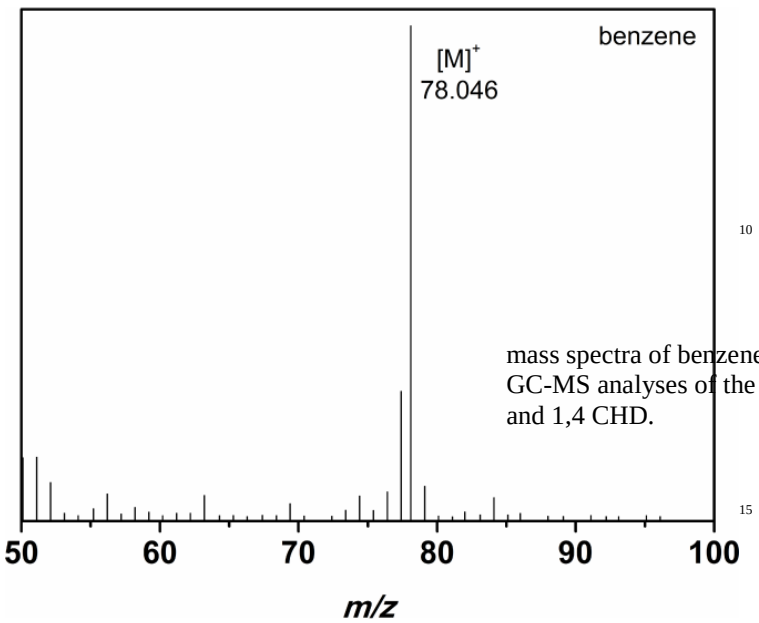
^{1}H NMR of a crude reaction mixture of 2,6 -di-tert-butylphenol (2 eq) and **2**

Formation of 2,4,6-tri-*tert*-butyl phenoxyl radical in the reaction with 2,4,6-tri-*tert*-butyl phenol is confirmed by EPR spectroscopy at 77 K. A calculated amount of the substrate **(50 equivalents)** in 0.1 ml toluene was added to the preformed solutions of **2-4** in toluene at -78°C and left for 1 hour at -78°C, then immediately frozen, and analyzed for phenoxyradicals by EPR. The experimental parameters for EPR spectra were as follows: Microwave frequency = 9.313 GHz, microwave power = 0.5 mW, modulation amplitude = 10 G, gain = 1×10^{4}, modulation frequency = 100 kHz, time constant = 40.96 ms and conversion time = 81.00 ms. For spin quantification, the EPR signal was double integrated to obtain the area under the signal. A strong pitch (0.11% pitch in KCl) external standard was used to quantify the *S = 1/2* signal.



EPR spectrum of the crude reaction mixture of **2** and 2,4,6-tri-tert-butylphenol in Toluene at 77 k.

Benzene was identified as the product of the oxidation of 1,4 cyclohexadiene by GC-MS/FID (Varian GC/MS 4000). The product of the reactivity study was identified by comparing the retention time of the authentic compounds and by MS. Product yields were determined by comparison against standard curves prepared with known authentic samples and using naphthalene as an internal standard. The instrumental setup for product analyses was: Injector temperature: 150 °C; Detector temperature: 300 °C. Column heating set up: temperature: 35 ^{o}C, Hold time: 10 mins; Total time: 10 mins.



mass spectra of benzene product obtained from the GC-MS analyses of the crude reaction mixture of **2** and 1,4 CHD.

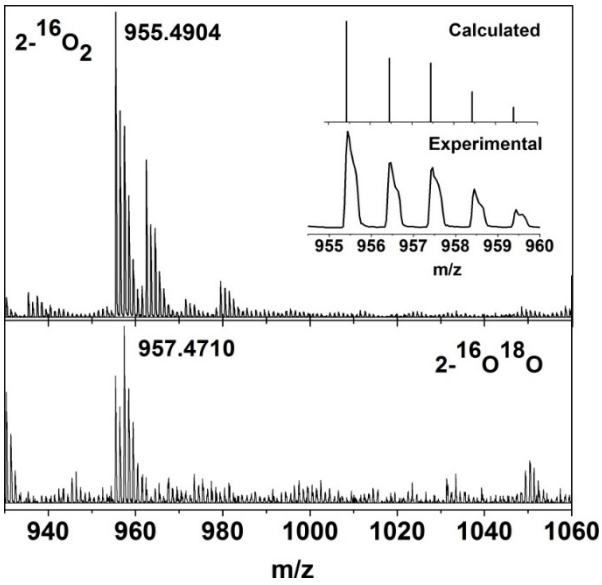


Figure S1. ESI-MS spectra of **2**-$^{16}O_2$ and **2**-$^{16}O^{18}O$ in toluene. Insets show the experimental and calculated mass and isotope distribution pattern of **955.4904** peak, which is consistent with the formulation of **[**$L^1NiO_2CoL^3$] (calculated *m/z* = 955.4913).

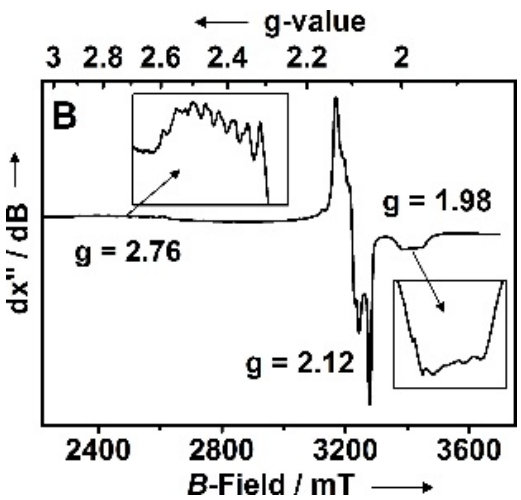


Figure S2. X–band EPR spectrum of **2** in toluene (0.47 mM) at 77 K (frequency: 9.470251 GHz; power: 0.05 mW; modulation: 0.5 mT).

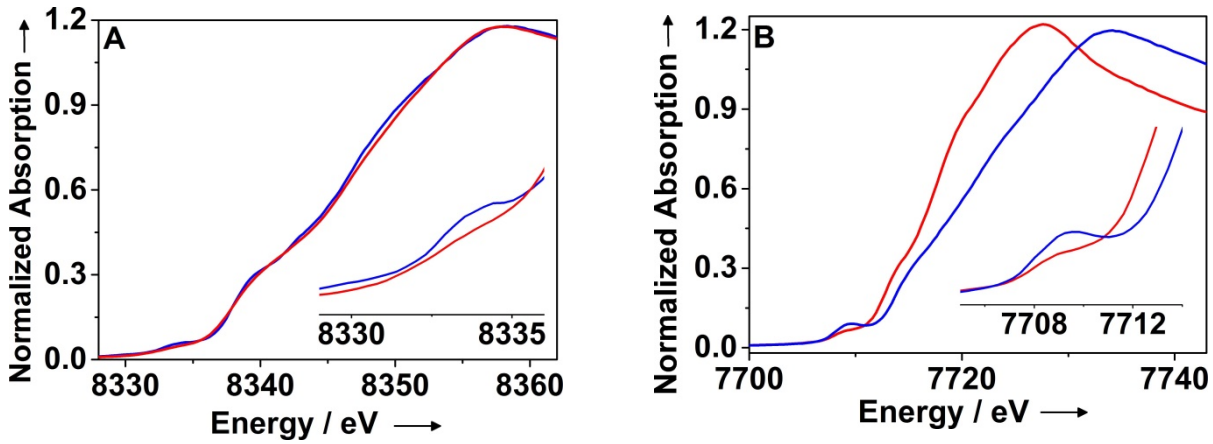


Figure S3. A:Virtually indistinguishable normalized Ni K–edge XANES spectra for **1** (red line), and **2** (blue line). **B**: Normalized Co K–edge XANES spectra for [$L^3Co(C_7H_8)$] (red line) and **2** (blue line). The insets in **A** and **B** show the expansion of the predge regions.

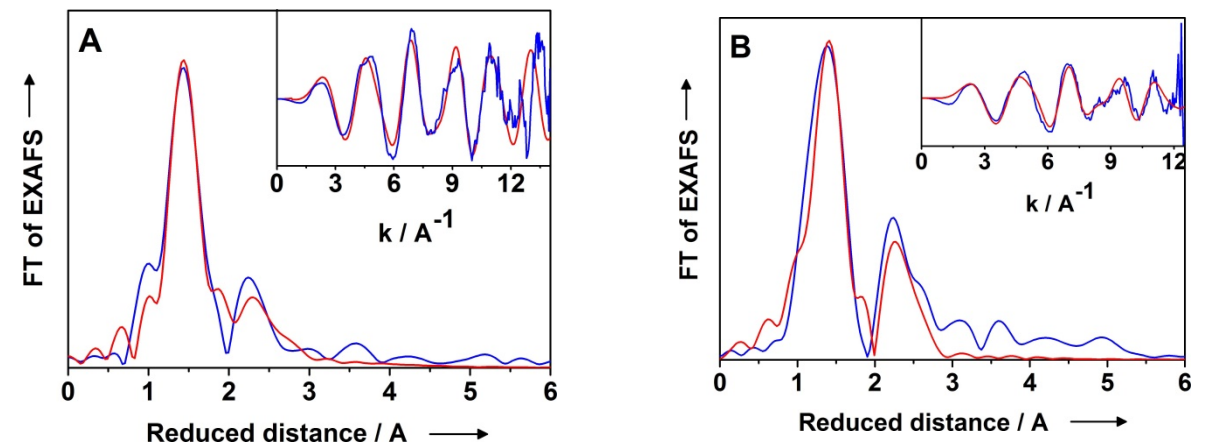


Figure S4. A: Fourier–transformed Ni *K*–edge EXAFS spectra of **2** (Experiment: blue line; simulation: red line). **B**: Fourier–transformed Co *K*–edge EXAFS spectra of **2** (Experiment: blue line; simulation: red line). In the insets are shown the EXAFS data on a wavevector scale before calculation of the Fourier transform.

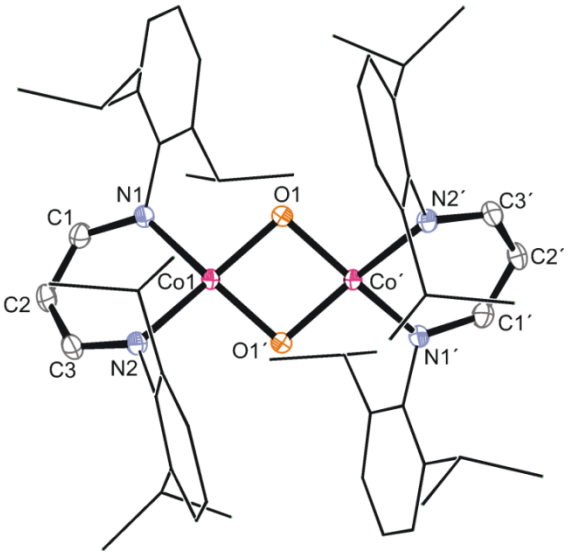


Figure S5. Molecular structure of **4**. Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms are omitted for clarity. Symmetry transformations used to generate equivalent atoms with (´): -x,y,-z+1/2. Selected distances (Å) and angles (°): Co1-O1´ 1.7861), Co1-O1 1.793(1), Co1-N2 1.910(2), Co1-N1 1.912(2), Co1-Co1´ 2.6715(5), O1-Co1´ 1.786(1), N1-C1 1.330(2), C1-C2 1.387(3), N2-C3 1.321(3), C2-C3 1.386(3), O1´-Co1-O1 83.39(6), O1´-Co1-N2 96.90(6), O1-Co1-N2 156.70(7), O1´-Co1-N1 155.36(6), O1-Co1-N1 96.71(6), N2-Co1-N1 92.55(7), O1´-Co1-Co1´ 41.80(4), O1-Co1-Co1´ 41.61(4), N2-Co1-Co1´ 134.67(5), N1-Co1-Co1´ 132.74(5), Co1´-O1-Co1 96.59(6), C1-N1-Co1 123.5(1), N1-C1-C2 126.1(2), C3-N2-Co1 125.0(1).

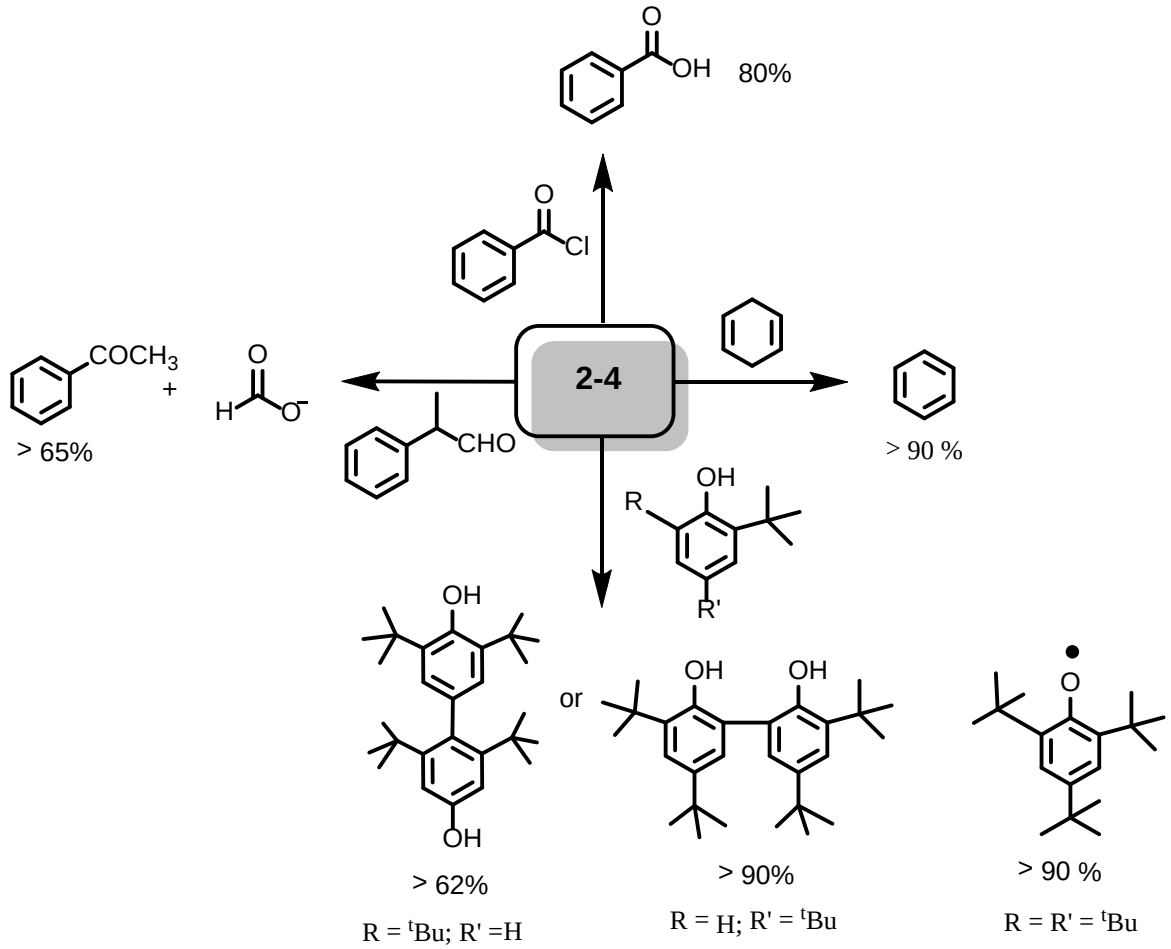


Figure S6. Reactivity of complexes **2**-**4**. Yields are given relative to the metal complexes.

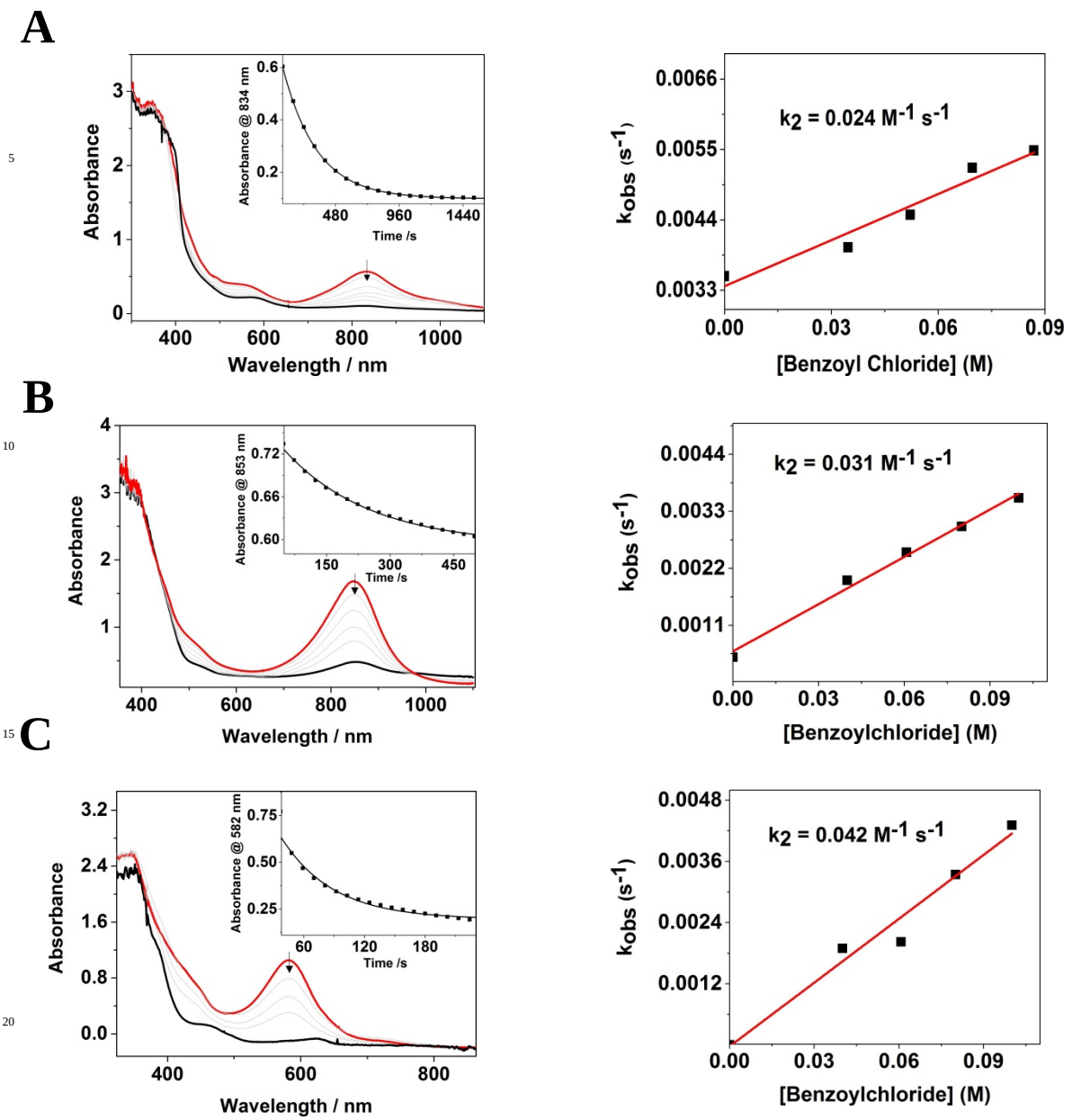


Figure S7. Reactions of **2** (0.2 mM in toluene; A), and **3** (0.2 mM in toluene; B) at -65 ^{o}C and **4** (0.2 mM in toluene; C) at -35 ^{o}C with PhCOCl. On the right are shown the changes in the absorption spectrum upon addition of PhCOCl. The insets show the pseudo-first order decays of the characteristic near IR bands of **2-4**. On the right are shown the linear dependence of k_{obs} on the concentrations of PhCOCl; the slopes of the linear fits correspond to the k_2 values.

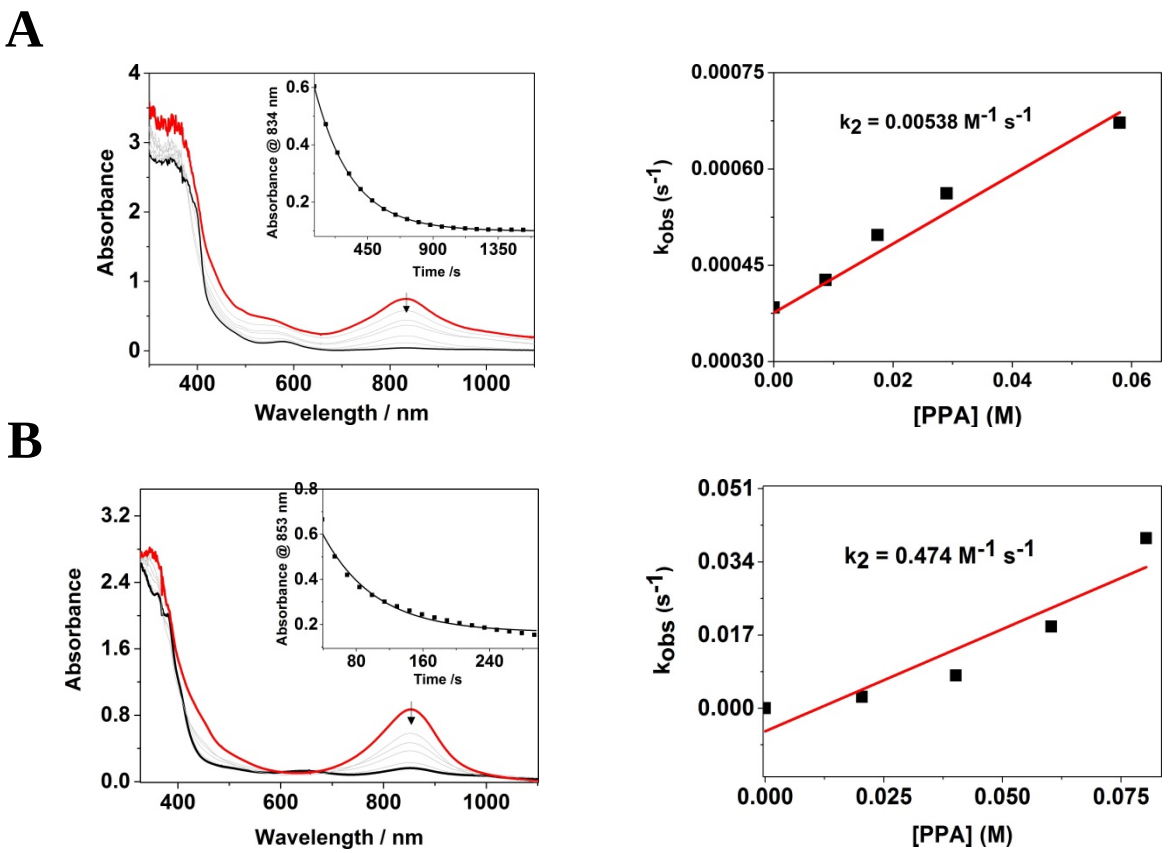
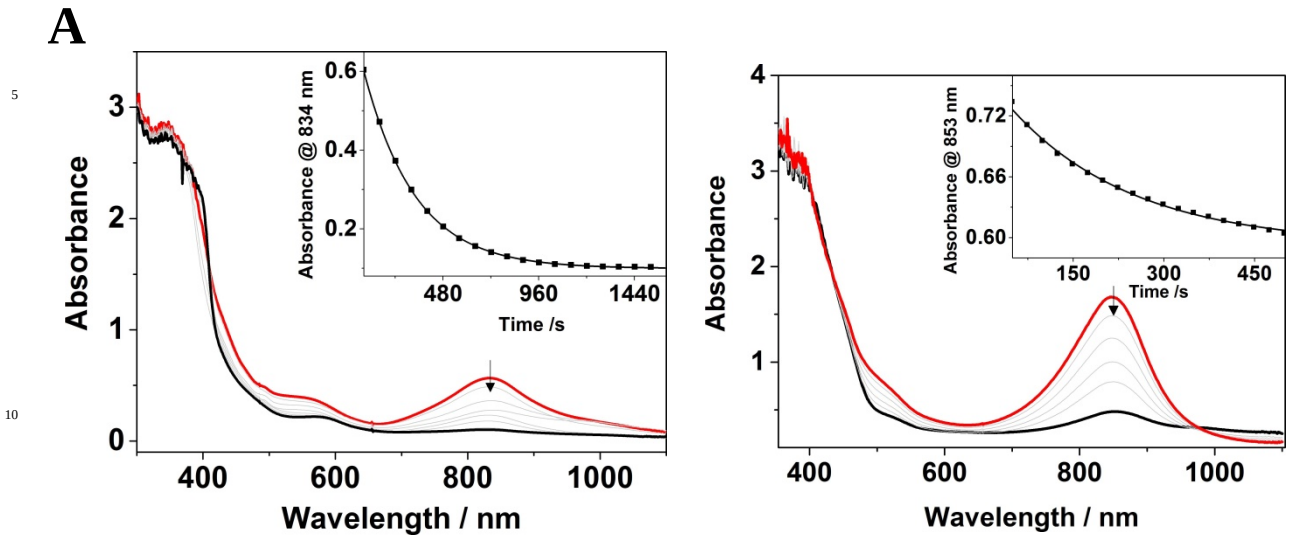
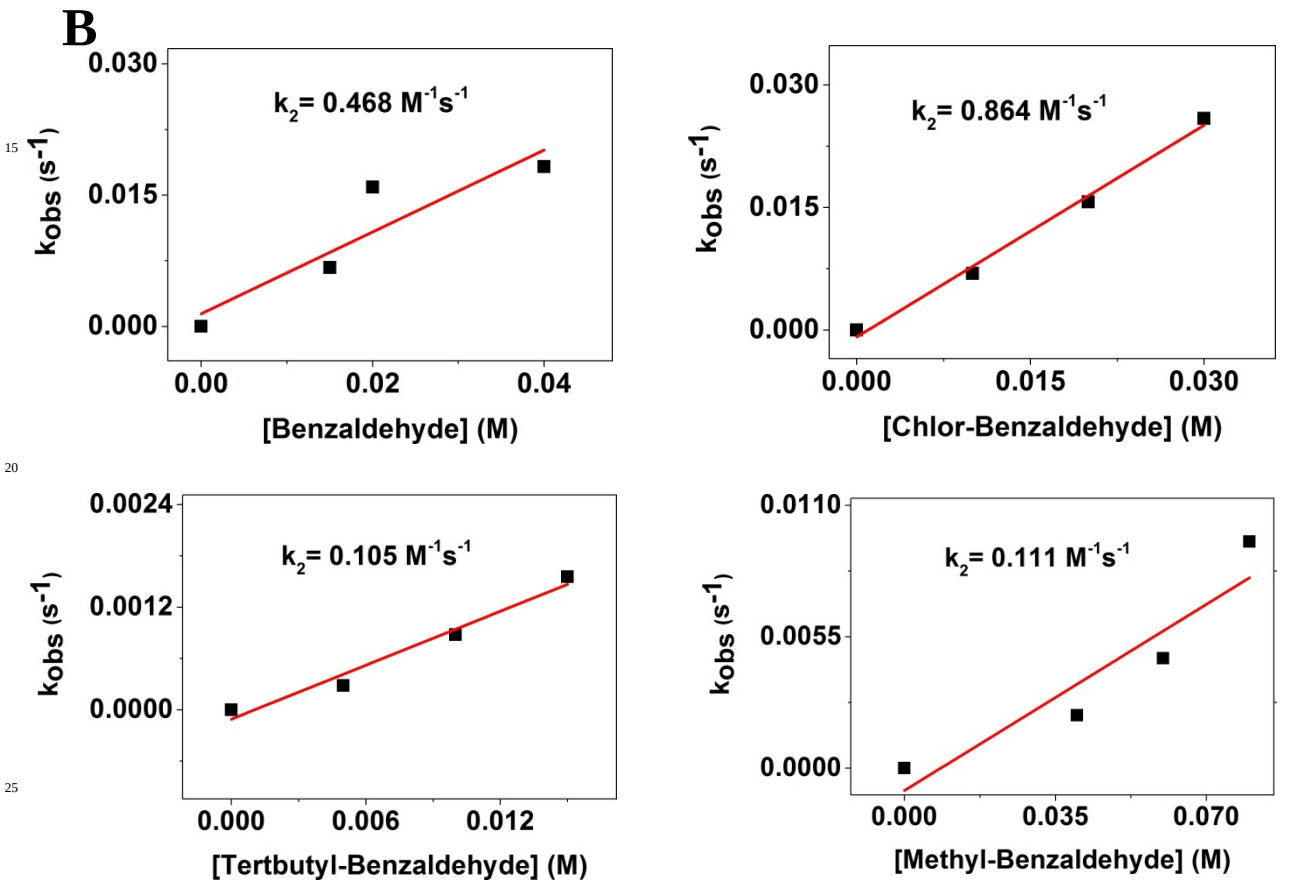


Figure S8. A) Changes in the absorption spectra associated with the reaction of **2** (0.2 mM, A) and **3** (0.2 mM, B) with 2-PPA (100-400 equivalents) at -85°C. The insets show the pseudo-first order decays of the characteristic near IR bands of **2** and **3** (left). Linear dependence of k_{obs} on the substrate concentration (right). B). Reaction of **4** with 2-PPA was found to be too slow for any rate determination.


A
Absorbance
Wavelength / nm
Absorbance @ 834 nm
Time /s
Absorbance @ 853 nm
Time /s


B
k_2= 0.468 $M^{-1}s^{-1}$
k_2= 0.864 $M^{-1}s^{-1}$
k_2= 0.105 $M^{-1}s^{-1}$
k_2= 0.111 $M^{-1}s^{-1}$
kobs (s^{-1})
[Benzaldehyde] (M)
[Chlor-Benzaldehyde] (M)
[Tertbutyl-Benzaldehyde] (M)
[Methyl-Benzaldehyde] (M)

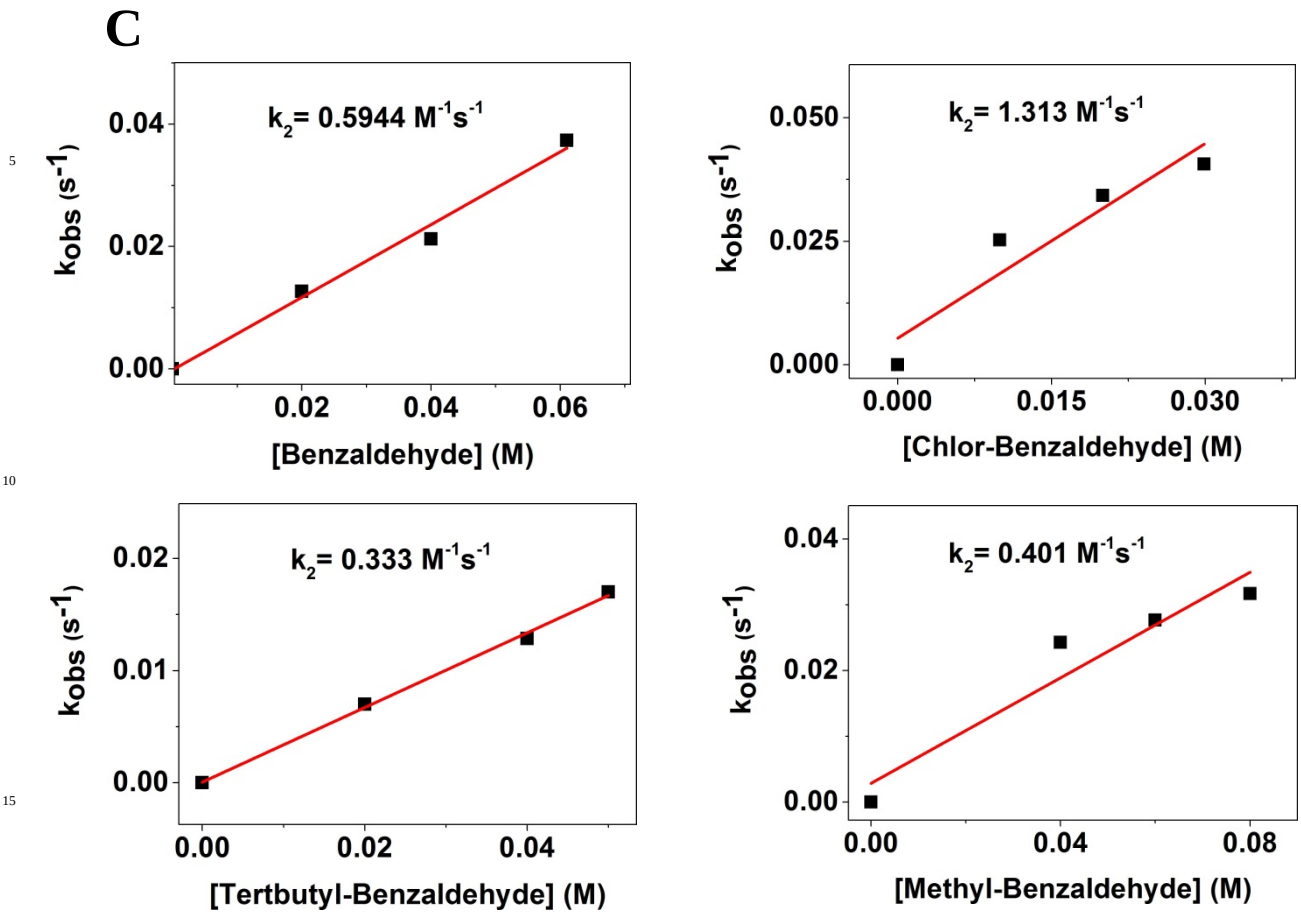


Figure S9. Top: A) Changes in the absorption spectra associated with the reaction of **2** (left) and **3** (right) (0.2 mM) with Benzaldehyde (50-100 equivalents;100-300 equivalents); Chlor-Benzaldehyde (50-150 equivalents); Tertbutyl-Benzaldehyde (25-75 equivalents; 100-250 equivalents) and Methyl-Benzaldehyde (200-400 equivalents) at -85°C in toluene. The insets show the pseudo-first order decays of the characteristic near IR bands of **2** and **3**. B) Linear dependence of k_{obs} on the substrate concentration for **2** at -85°C. C) Linear dependence of k_{obs} on the substrate concentration for **3** at -85°C**.**

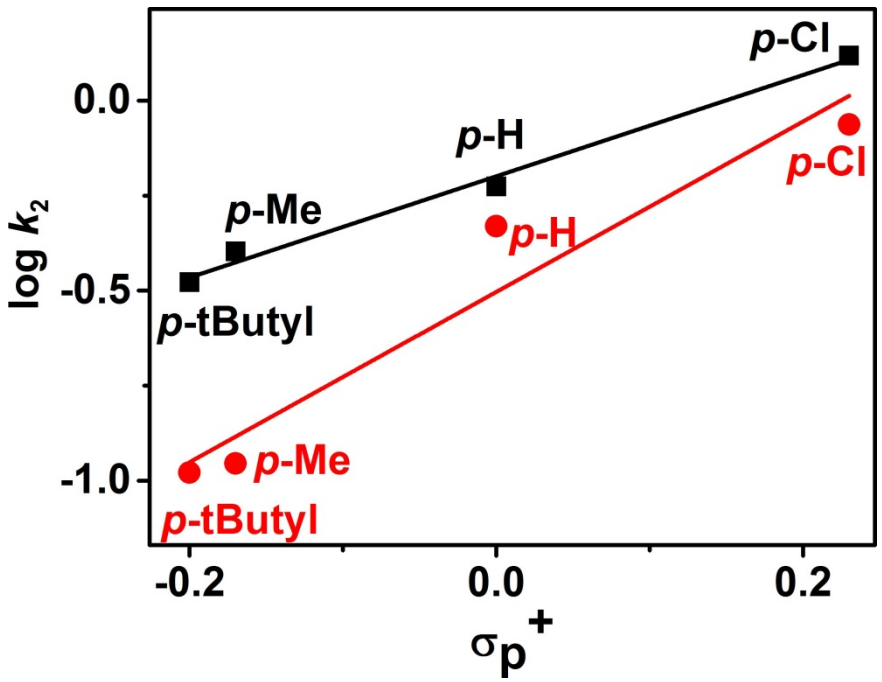


Figure S10. Plot of log k_2 against σ_p^+ for the reaction of **2** (black trace) (ρ value of 1.33) and **3** (red trace) (positive ρ value of 2.26) with p-X substituted benzaldehydes (X = -^{t}Bu, -Me, -H, -Cl) at -85°C.

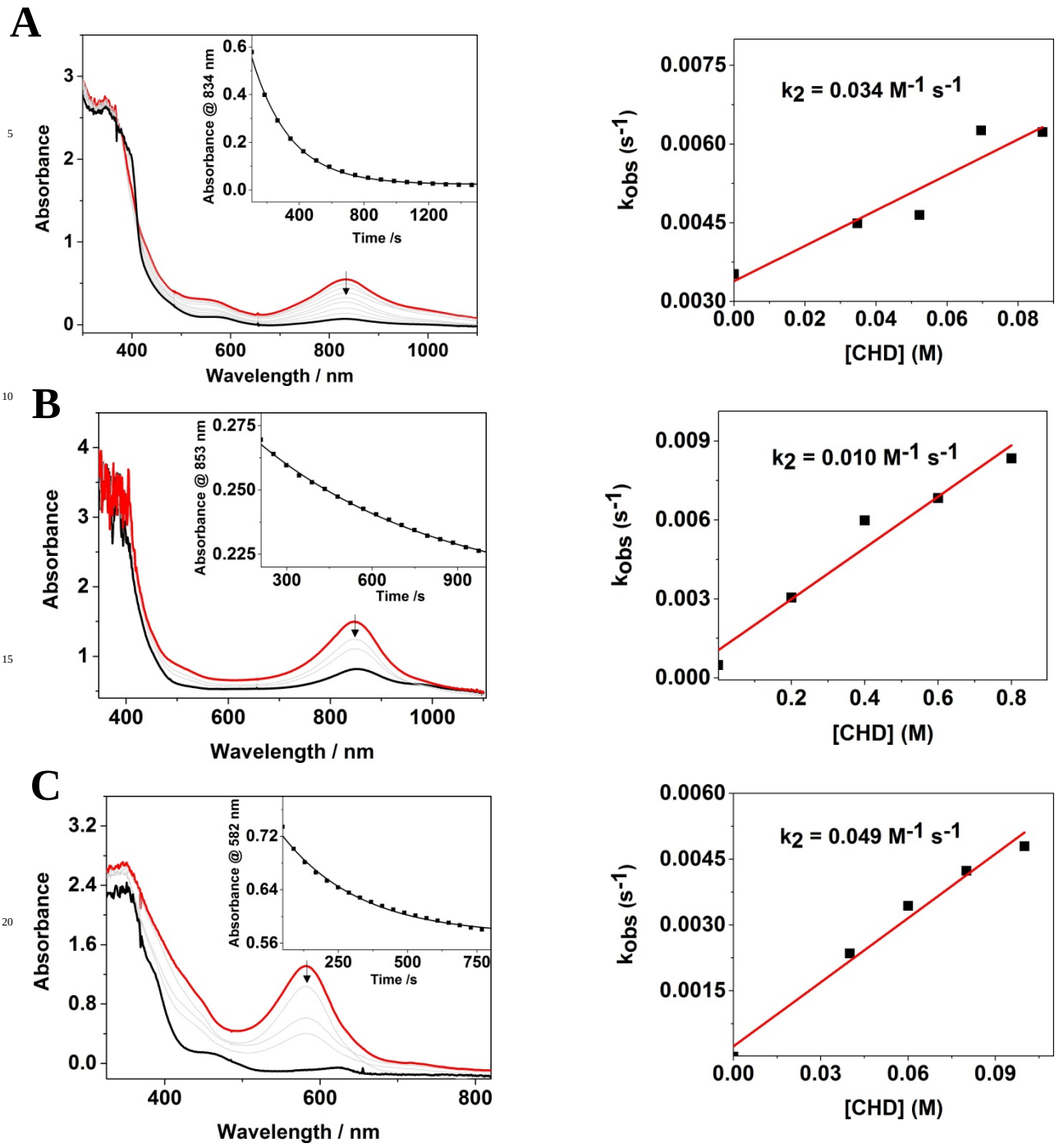


Figure S11. Changes in the absorption spectrum associated with the reactions of **2** (0.2 mM in toluene; A), and **3** (0.2 mM in toluene; B) at -65 ^{o}C and **4** (0.2 mM in toluene; C) at -35 ^{o}C with CHD. The inset shows the time trace of the decay of the characteristic absorption bands upon addition of substrate. On the right are shown the linear dependence of k_{obs} on the substrate concentrations for **2-4**.

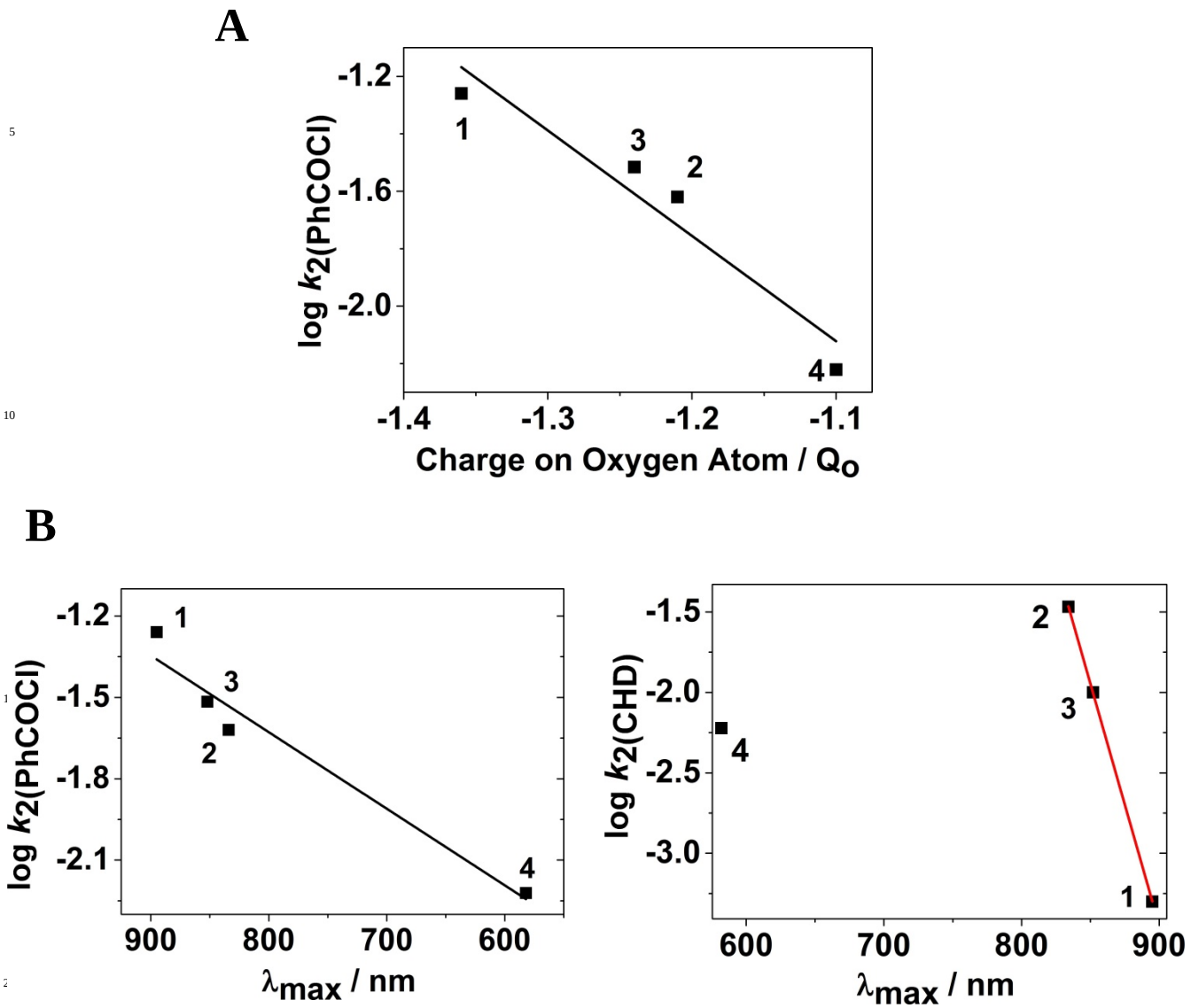


Figure S12. A) The linear correlation observed for the log k_2 values for PhCOCl versus the DFT calculated average charges on the oxygen atoms of the bis(μ-oxo)dimetal cores of **1**-**4**. B) Correlations for log k_2 values for PhCOCl and CHD oxidations versus λ_{max} of **1**-**4**.

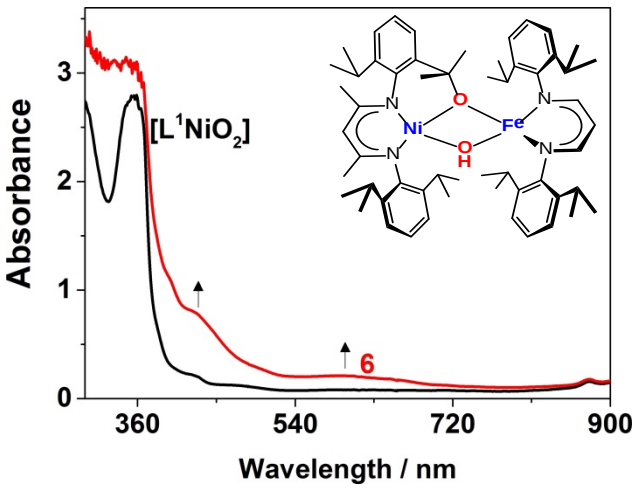


Figure S13. Spectral changes associated with the reaction of [$L^1Ni^{II}O_2$] (0.2 mM) and [$L^3Fe(C_7H_8)$] **(**0.2 mM**)** at -90 ^oC in toluene.

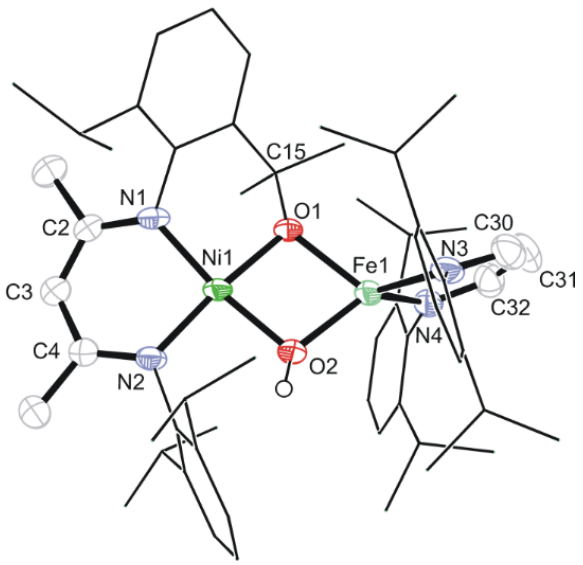


Figure S14. Molecular structure of **6**. Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms (except for that attached to O2) are omitted for clarity. Selected distances (Å) and angles (°):Ni1-N1 1.873(3), Ni1-O1 1.877(3), Ni1-N2 1.886(3), Ni1-O2 1.896(3), Fe1-O2 1.956(3), Fe1-O1 2.016(3), Fe1-N3 2.016(4), Fe1-N4 2.023(4), O1-C15 1.424(5), N1-C2 1.342(6), N2-C4 1.323(6), C2-C3 1.391(6), N3-C30 1.322(6), C3-C4 1.399(6), N4-C32 1.324(6), N1-Ni1-O1 91.6(1), N1-Ni1-N2 94.0(2), O1-Ni1-N2 173.5(1), N1-Ni1-O2 171.4(2), O1-Ni1-O2 79.9(1), N2-Ni1-O2 94.5(1), O2-Fe1-O1 75.2(1), O2-Fe1-N3 122.2(2), O1-Fe1-N3 114.7(1), O2-Fe1-N4 127.7(2), O1-Fe1-N4 125.9(1), N3-Fe1-N4 93.7(2), C15-O1-Ni1 121.9(3), C15-O1-Fe1 128.6(3), Ni1-O1-Fe1 101.6(1), C2-N1-Ni1 122.6(3), C4-N2-Ni1 125.7(3), N1-C2-C3 122.6(4), C30-N3-Fe1 122.2(3), C2-C3-C4 125.9(4), C32-

N4-Fe1 121.3(3), N2-C4-C3 121.9(4).

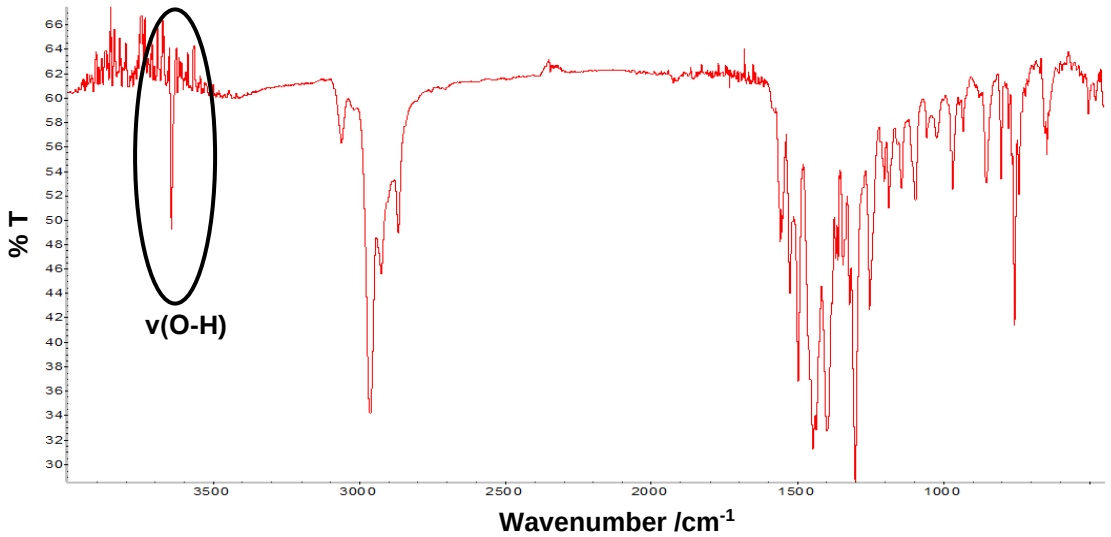


Figure S15. IR Spectra of **6**.

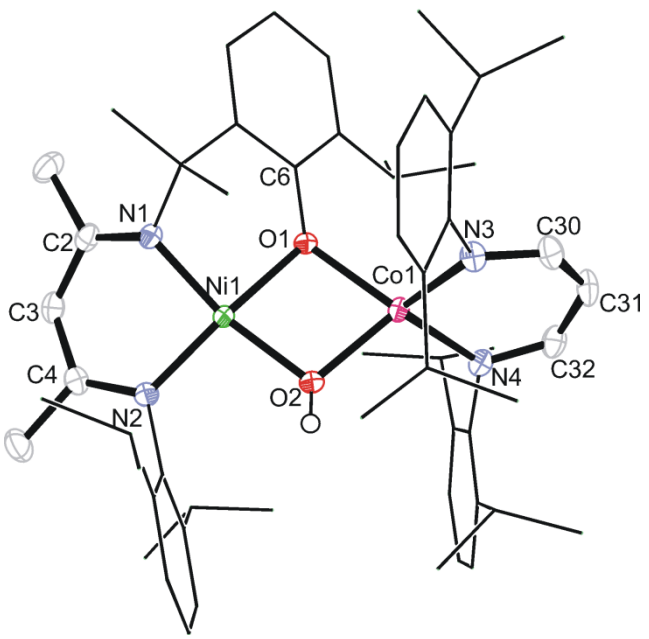


Figure S16. Molecular structure of **7**. Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms (except for that attached to O2) are omitted for clarity. Selected distances (Å) and angles (°):Co1-O2 1.944(1), Co1-N4 1.984(2), Co1-N3 1.993(2), Co1-O1 2.010(1), Co1-Ni1 2.9978(4), Ni1-N1 1.853(1), Ni1-O2 1.878(1), Ni1-N2 1.880(2), Ni1-O1 1.949(1), O1-C6 1.364(2), N1-C2 1.325(2), C1-C2 1.514(3), N2-C4 1.334(2), C2-C3 1.398(3), N3-C30 1.327(2), C3-C4 1.388(3), N4-C32 1.329(2), C30-C31 1.390(3), C31-C32 1.385(3), O2-Co1-N4 107.68(6), O2-Co1-N3 133.82(6), N4-Co1-N3 94.98(6), O2-Co1-O1 76.74(5), N4-Co1-O1 138.90(6), N3-Co1-O1 111.26(6), O2-Co1-Ni1 37.57(4), N4-Co1-Ni1 137.09(5), N3-Co1-Ni1 126.81(4), O1-Co1-Ni1 40.04(3), N1-Ni1-O2 166.31(7), N1-Ni1-

N2 92.92(7), O2-Ni1-N2 97.94(6), N1-Ni1-O1 91.69(6), O2-Ni1-O1 79.77(5), N2-Ni1-O1 165.73(6), N1-Ni1-Co1 129.95(5), O2-Ni1-Co1 39.12(4), N2-Ni1-Co1 136.95(5), O1-Ni1-Co1 41.55(3), C6-O1-Ni1 125.6(1), C6-O1-Co1 134.4(1), Ni1-O1-Co1 98.4(5), C2-N1-Ni1 121.1(1), Ni1-O2-Co1 103.31(7), C4-N2-Ni1 121.6(1), N1-C2-C3 120.3(2), C30-N3-Co1 121.2(1), C33-N3-Co1 123.8(1), C4-C3-C2 125.3(2), C32-N4-Co1 121.1(1), N2-C4-C3 122.9(2), N3-C30-C31 126.8(2), C32-C31-C30 125.7(2), N4-C32-C31 127.0(2).

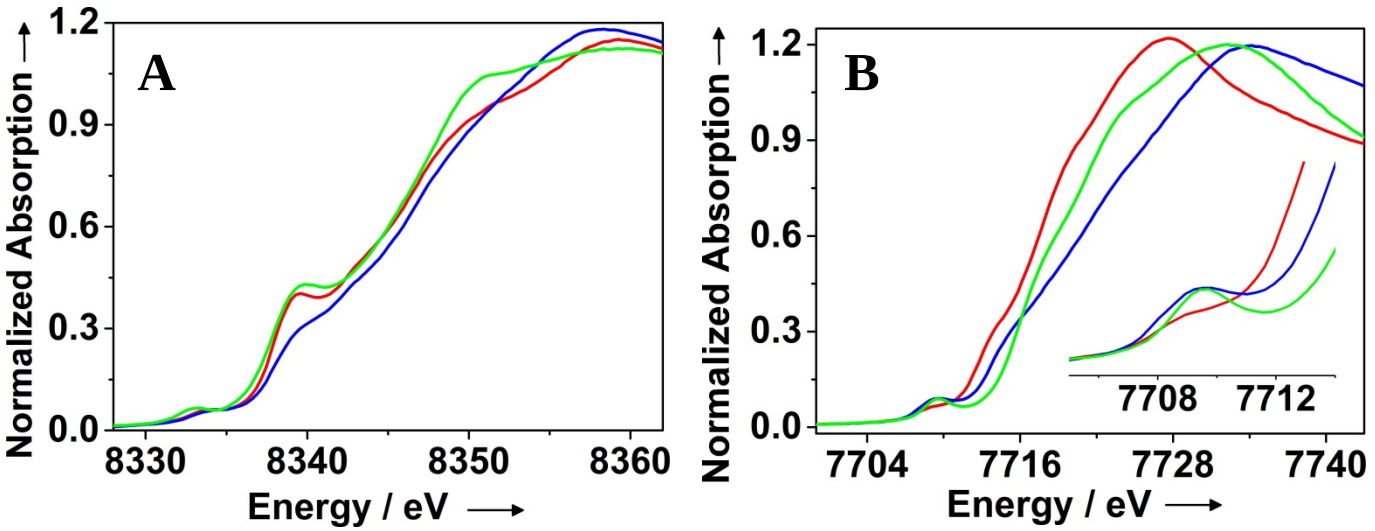


Figure S17. XANES studies: A) Ni K-edges of **7** (green trace), [$L^1Ni^{II}O_2$] (red trace) and **2** (blue trace). B) Co K-edges of **7** (green trace), [$L^3Co(C_7H_8)$] (red trace) and **2** (blue trace). The Inset shows the expansion of the pre-edge region.

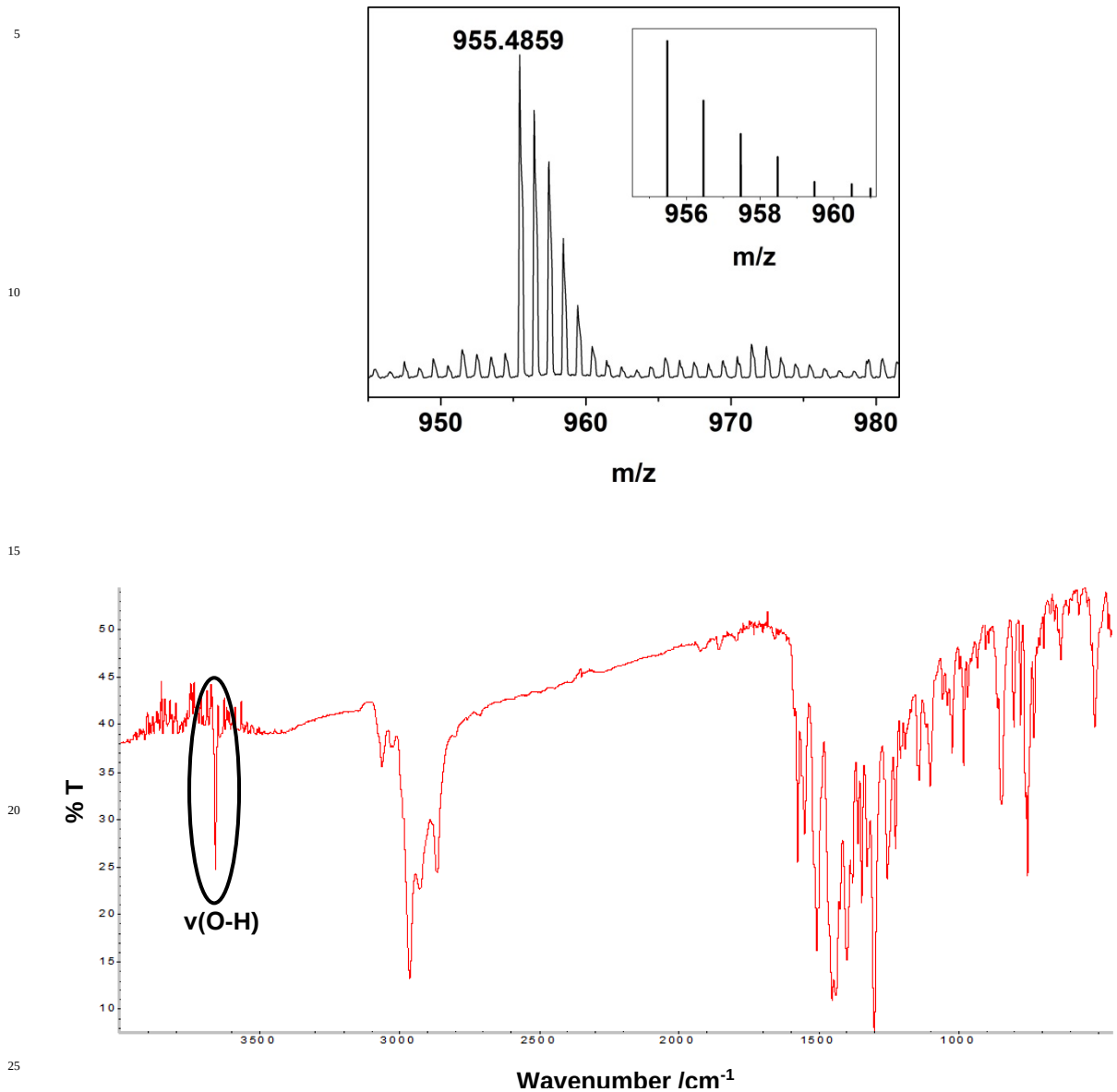


Figure S18. Top: ESI-MS spectra of **7** in toluene. In the inset is the given theoretically calculated isotope distribution pattern of **7**. **Bottom:** IR Spectra of **7**.

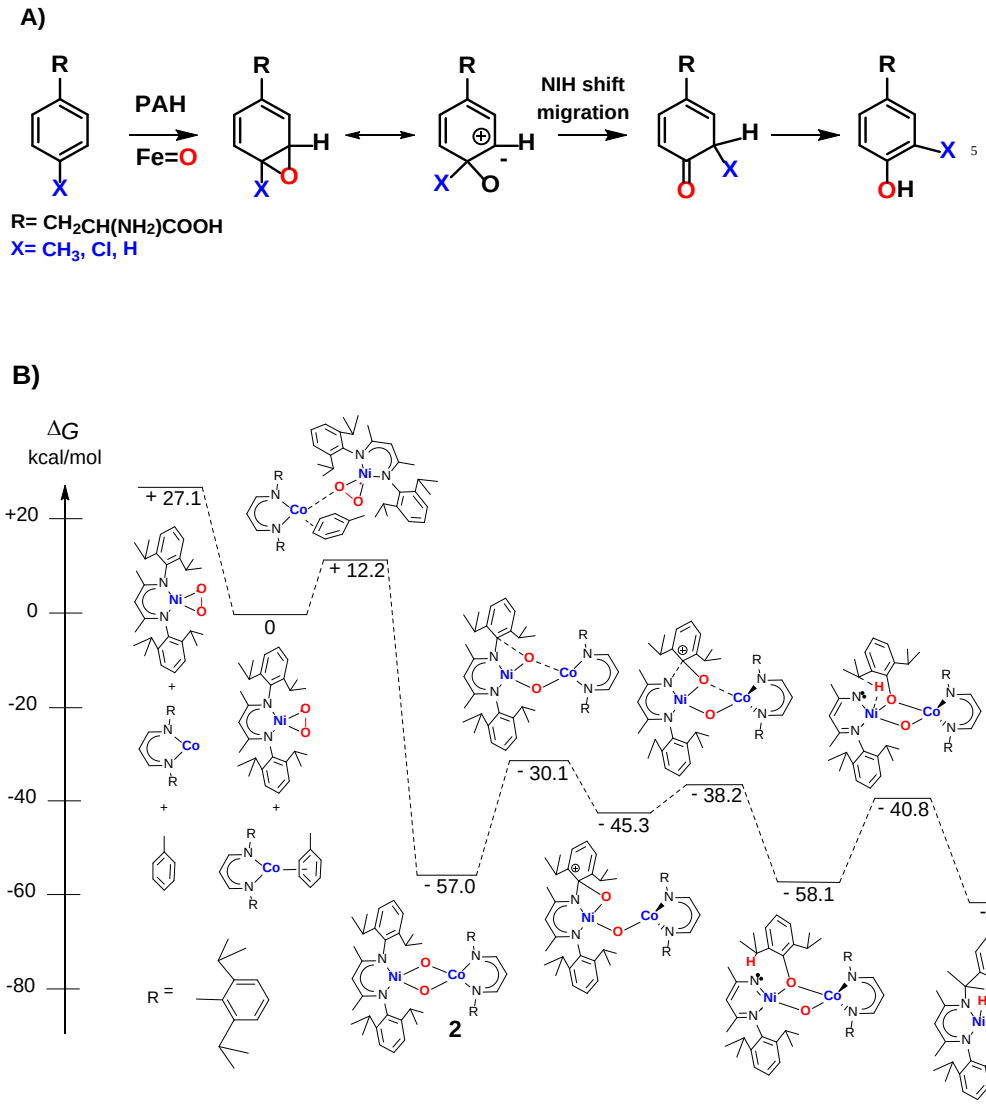


Figure S19. A) Aromatic hydroxylation reaction mediated by an iron-oxo (Fe=O) intermediate in phenylalanine hydroxylases (PAH) by a NIH shift mechanism;B) DFT Calculated reaction mechanism for the formation and decay (by aromatic hydroxylation) of **2**.

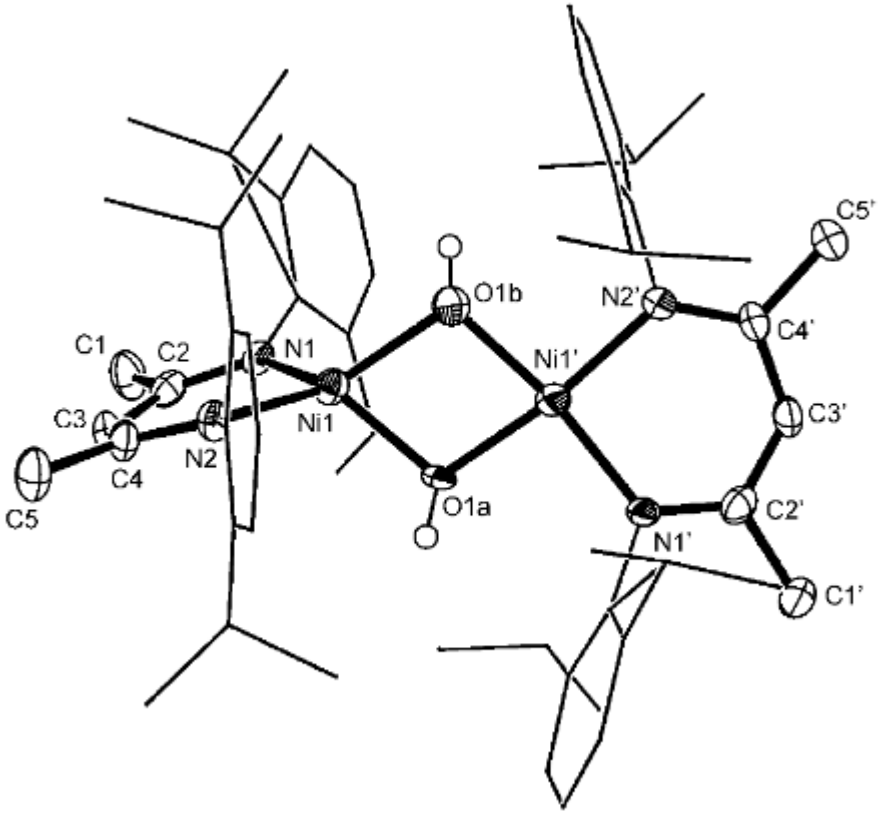


Figure S20: Structure of the bis(hydroxo)dinickel(II) compound, as obtained from the decay of **3.** The X-ray structure was reported previously by some of us.[1]

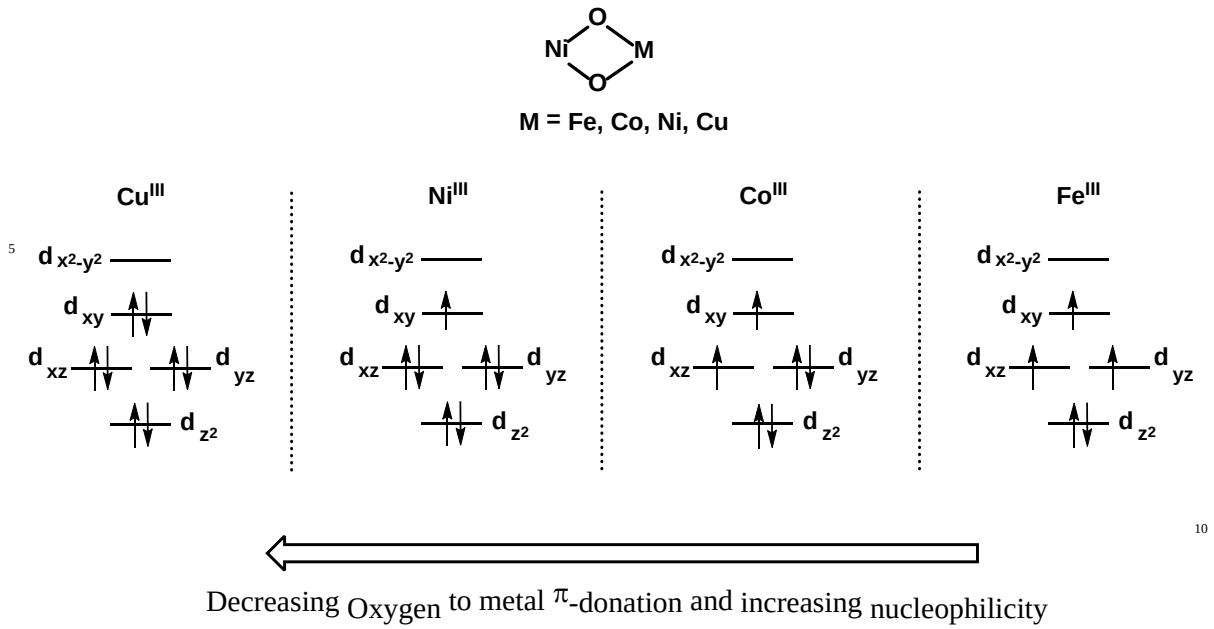


Figure S21. d-orbital splitting of the second metal ion M (in an approximate square planar geometry) in a series of $Ni^{III}(\mu\text{-}O)_2M^{III}$ (M= Fe, Co, Ni and Cu) complexes of betadiketiminate ligands.

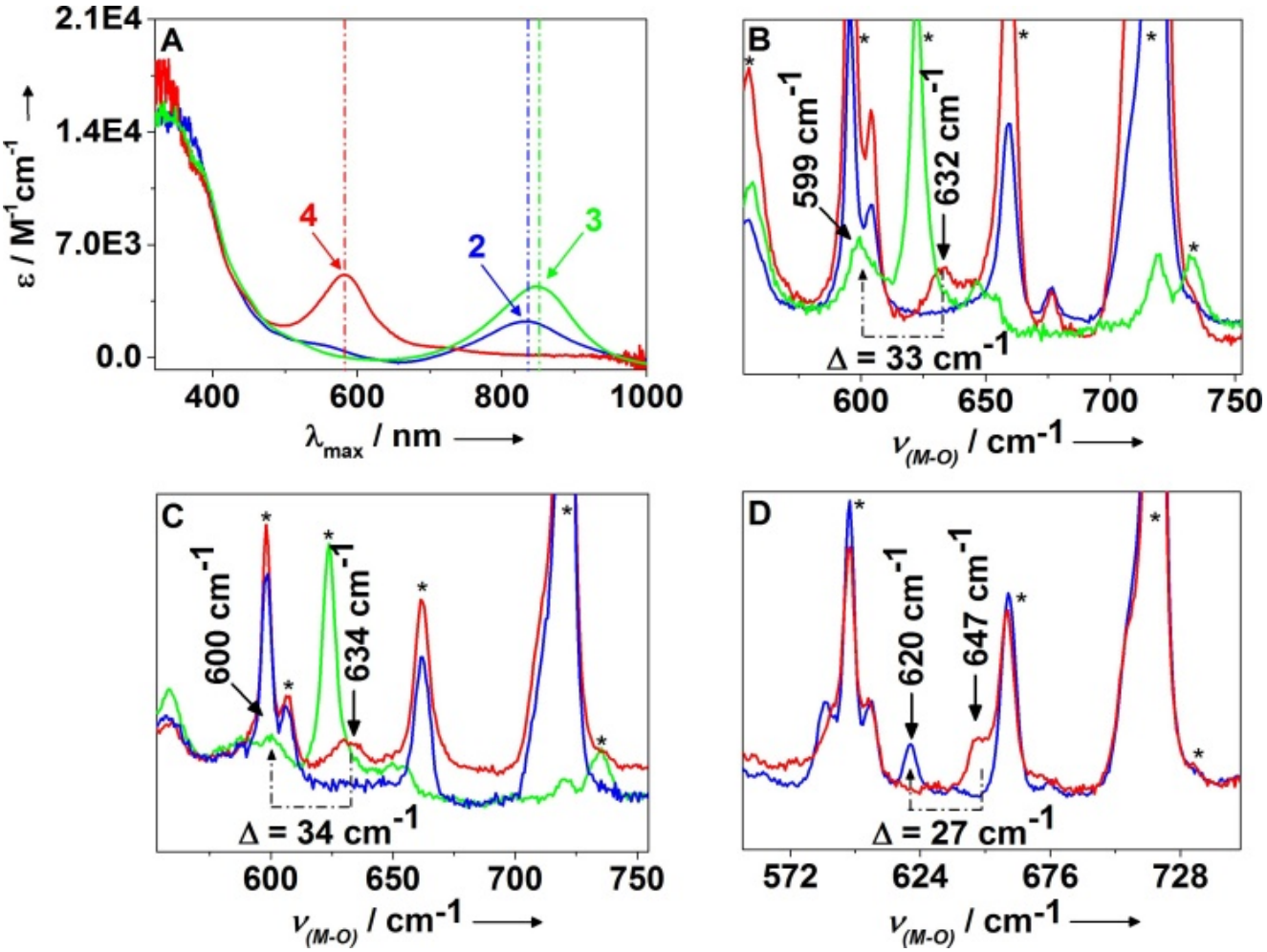


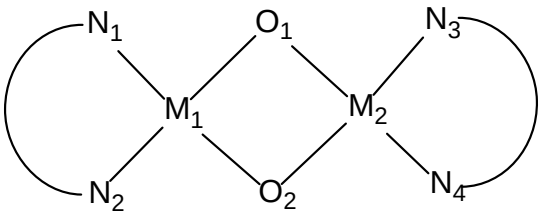
Figure S22. A: Absorption spectra of **2-4** at –78 °C in toluene. **B-D**: rRaman spectra (413 nm excitation) of **2-4** in toluene at -90 °C: **B**. **3-$^{16}O_2$** in d_8-toluene (red trace), **3-$^{18}O_2$** in d_8-toluene (blue trace) and **3-$^{18}O_2$** in toluene (green trace). **C**: **2-$^{16}O_2$** in d_8-toluene (red trace), **2-$^{18}O_2$** in d_8-toluene (blue trace) and **2-$^{18}O_2$** in toluene (green trace). **D**: **4-$^{16}O_2$** in d_8-toluene (red trace) and **4-$^{18}O_2$** in d_8-toluene (blue trace).

Table S1. Pre-edge peak fitting analyses.[a]

Sample	$E_{pre\text{-}edge}$ (eV)	height	FWHM	area
$[L^{1}Ni^{II}O_2]$	8333.3(0)	0.0214(4)	2.24(5)	5.1(2)
2 (Ni)	8333.8(0)	0.0224(9)	2.76(15)	6.6(2)
7 (Ni)	8332.9(0)	0.0302(2)	2.14(4)	6.9(1)
1 (Ni)	8333.6(1)	0.0157(3)	3.23(6)	5.4(1)
$[L^{3}Co(C_7H_8)]$	7709.0(1)	0.0237(3)	2.45(13)	6.2(3)
2 (Co)	7709.8(1)	0.0533(1)	2.98(1)	16.9(1)
7 (Co)	7709.5(0)	0.0519(1)	2.47(1)	13.6(1)

[a] The values in parentheses represent the standard deviation associated with a given parameter, calculated from the four fits conducted on each sample. Areas are multiplied by 100 for convenience.

Table S2. Dihedral angles (°) of **1-5** and **8** in the DFT calculated structures. Dihedral angle (Ø) represents the angle between the $M_1O_1O_2$ and $M_2O_1O_2$ planes. Similarly, Θ represents angle between $O_2M_2O_1$ and $M_2O_1N_3$ planes



	M_1	M_2	Spin state	Ø	Θ
1	Cu	Ni	1/2	177.2	178.8
2	Co	Ni	1/2	178.6	172.0
3	Ni	Ni	0	179.8	172.1
4	Co	Co	2	171.7	143.8
5	Fe	Ni	2	166.7	167.0
8	Cu	Ni	1/2	179.9	172.5

Table S3-1: Summary of the Ni K-edge EXAFS fitting for **2**. Bold line represents the best fit for the system (fit 11). r is in units of Å; σ^2 is in units of 10^{-3} Å; ΔE_0 is in units of eV; R-factor represents the GOF. Fourier transform range: k 1.5-5.0 $Å^{-1}$. The fit was optimized in R space with a k-weight of 3. A comparison to the DFT calculated values is shown below.

					Ni-N/O			Ni-N/O			Ni-Co			Ni••C			Ni••C			Ni••C		
fit	R-factor	red. Chi-sq.	ΔE0	R range	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²
1	0.055	3260.14	-0.543	0.8 - 2				3	1.86	-0.4												
2	**0.043**	**3113.07**	**-0.997**	**0.8 - 2**				**4**	**1.86**	**2.9**												
3	0.107	5429.72	-1.287	0.8 - 2				5	1.87	7.1												
4	0.056	4985.98	2.438	0.8 - 2	2	1.84	-1.1	2	2.01	13.5												
5	0.050	5158.86	0.128	0.8 - 2	1	1.83	-2.9	3	1.90	9.0												
6	0.050	5114.59	2.438	0.8 - 2	3	1.86	1.1	1	2.12	4.3												
7	0.079	1176.72	-0.821	1 - 4				4	1.87	2.7												
8	0.045	1052.89	-1.274	1 - 4				4	1.86	2.5	1	2.80	5.6									
9	0.033	721.55	-0.551	1 - 4				4	1.86	2.9	1	2.79	4.9	4	3.00	28.4						
10	0.031	737.56	-0.558	1 - 4				4	1.86	3.1	1	2.79	5.2	4	2.95	28.2	5	4.14	30.1			
11	**0.019**	**619.21**	**-0.377**	**1 - 4**				**4**	**1.86**	**2.9**	**1**	**2.78**	**3.7**	**4**	**2.99**	**12.2**	**5**	**3.52**	**14.7**	**6**	**4.04**	**14.1**
					DFT			**4**	**1.88**		**1**	**2.77**		**4**	**3.15**							

Table S3-2: Summary of the Co K-edge EXAFS fitting for **2**. Bold line represents the best fit for the system (fit 23). r is in units of Å; σ^2 is in units of 10^{-3} Å; ΔE_0 is in units of eV; R-factor represents the GOF. Fourier transform range: k 1.5-5.0 $Å^{-1}$. The fit was optimized in R space with a k-weight of 3. A comparison to the DFT calculated values is shown below. Note that in the DFT calculated structure the additional interaction @ 2.29 Å (presumably from Toluene solvent) is not taken into account.

					Co-N/O			Co-C/N/O			Co-Ni			Co••C			Co••C			Co••C		
fit	R-factor	red. Chi-sq.	ΔE0	R range	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²
1	0.095	2556.54	-0.298	0.8 - 2.0	2	1.82	1.1															
2	0.027	679.88	-2.183	0.8 - 2.0	3	1.81	5.4															
3	0.054	1761.19	-3.915	0.8 - 2.0	4	1.81	9.9															
4	0.109	3353.97	-5.388	0.8 - 2.0	5	1.80	14.2															
5	0.147	3951.68	-0.031	0.8 - 2.0				2	1.84	-0.4												
6	0.048	968.19	-1.856	0.8 - 2.0				3	1.84	3.3												
7	0.046	1631.17	-3.719	0.8 - 2.0				4	1.83	7.1												
8	0.092	3280.24	-5.372	0.8 - 2.0				5	1.82	10.9												
9	0.04315	1678.67971	-0.51	0.8 - 2.0	1	1.31	57.8	3	1.84	3.45												
10	0.04668	2288.11494	-4.63	0.8 - 2.0	2	1.76	15.6	2	1.84	2.01												
11	0.02672	1085.60005	-0.57	0.8 - 2.0	3	1.82	4.96	1	2.17	25.2												
12	0.02682	1209.37786	-1.79	0.8 - 2.0	1	1.43	27.5	4	1.83	5.88												
13	0.04438	1699.61663	-0.75	0.8 - 2.0	2	1.31	84.4	3	1.84	3.39												
14	0.02611	1052.26663	0.322	0.8 - 2.0	3	1.83	4.97	2	2.17	33.9												
15	**0.01541**	**815.604745**	**-1.78**	**0.8 - 2.0**	**4**	**1.83**	**8.58**	**1**	**2.24**	**3.35**												
16	0.01471	778.20387	-2.29	0.8 - 2.0	1	1.73	-1.7	2	1.88	-0.9												
17	0.01402	801.458516	-2.79	0.8 - 2.0	2	1.77	1.9	1	1.91	-2.3												
18	0.111	906.33	-1.250	0.8 - 4.0	4	1.83	8.7	1	2.24	6.2												
19	0.048	590.17	-3.029	0.8 - 4.0	4	1.82	8.6	1	2.26	6.8	1	2.73	6.0									
20	0.048	598.44	-4.349	0.8 - 4.0	4	1.81	8.9	1	2.25	4.2	1	2.73	5.9	6	2.63	64.6						
21	0.042	517.88	-4.497	0.8 - 4.0	4	1.81	8.9	1	2.26	3.8	1	2.72	5.8	8	3.46	43.9						
22	0.010	175.49	2.848	0.8 - 4.0	4	1.83	8.7	1	1.44	13.9	1	2.73	3.0	6	2.95	7.6	8	3.36	24.4			
22	0.028	461.62	-2.230	0.8 - 4.0	4	1.82	8.5	1*	2.26	7.1	1	2.72	4.8	6	2.96	21.5	8	3.40	20.4			
23	**0.020**	**577.39**	**-2.407**	**0.8 - 4.0**	**4**	**1.82**	**8.5**	**1**	**2.29**	**8.1**	**1**	**2.72**	**3.9**	**6**	**2.95**	**12.6**	**8**	**3.31**	**14.1**	**6**	**3.56**	**20.2**
			DFT		**4**	**1.87**					**1**	**2.77**		**6**	**3.01**							

Table S4. Crystal data and structure refinement for **4.**

Empirical formula	C54 H74 Co2 N4 O2	
Formula weight	929.03	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 15.9699(3) Å	α= 90°.
	b = 15.9767(3) Å	β= 93.716(2)°.
	c = 19.8167(3) Å	γ = 90°.
Volume	5045.53(15) $Å^3$	
Z	4	
Density (calculated)	1.223 Mg/m^3	
Absorption coefficient	5.470 mm^{-1}	
F(000)	1984	
Crystal size	0.59 x 0.38 x 0.29 mm^3	
Theta range for data collection	3.92 to 67.48°.	
Index ranges	-19<=h<=19, -12<=k<=19, -23<=l<=22	
Reflections collected	9163	
Independent reflections	4538 [R(int) = 0.0247]	
Completeness to theta = 67.48°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.70172	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4538 / 0 / 288	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0834	
R indices (all data)	R1 = 0.0415, wR2 = 0.0877	
Largest diff. peak and hole	0.340 and -0.436 $e.Å^{-3}$	

Table S5: Reactions of **1-4** with various electrophilic and nucleophilic substrates. Reactivity done at -65°C unless otherwise mentioned.

Substrate	**3**	**2**	**4[d)]**	**1**
	k_2 [x 10^{-4} $M^{-1}s^{-1}$]	k_2 [x 10^{-4} $M^{-1}s^{-1}$]	k_2 [x 10^{-4} $M^{-1}s^{-1}$]	k_2 [x 10^{-4} $M^{-1}s^{-1}$]
DHA	-	223	-	a)
CHD	97	338	60.87	5
2,4-DTBP	-	-	140	97600
2,6-DTBP	-	270	-	2
PPA	18980[c)]	216[c)]	-	b)
Benzoyl Chloride	305	240	52.5	550
Cyanobenzoyl Chloride	-	44000	-	44000
***para*-Y-C_7H_5O[c)]**				
Y = H	23772	18708		
Y = Cl	52508	34580		
Y = Me	16040	4456		
Y = ^{t}Bu	13320	4204		

[a)] Reaction to slow for any kinetic studies; [b)] Reaction too fast for kinetic studies; [c)] -85°C; [d)] -35°C

(Rates were corrected for difference in temperature by doubling/reducing by half the rate for every 10°C increase/decrease in measurement temperature)

Table S6: Crystal data and structure refinement for **6.**

Empirical formula	C56 H78 Fe N4 Ni O2	
Formula weight	953.78	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.2983(5) Å	α= 76.486(5)°.
	b = 12.0871(8) Å	β= 81.593(4)°.
	c = 22.0117(13) Å	γ = 64.392(5)°.
Volume	2632.2(3) $Å^3$	
Z	2	
Density (calculated)	1.203 Mg/m^3	
Absorption coefficient	2.974 mm^{-1}	
F(000)	1024	
Crystal size	0.19 x 0.14 x 0.05 mm^3	
Theta range for data collection	4.14 to 67.50°.	
Index ranges	-13<=h<=13, -14<=k<=14, -26<=l<=17	
Reflections collected	17398	
Independent reflections	9380 [R(int) = 0.0519]	
Completeness to theta = 67.50°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.37913	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9380 / 0 / 599	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0729, wR2 = 0.1763	
R indices (all data)	R1 = 0.1037, wR2 = 0.1995	
Largest diff. peak and hole	1.252 and -0.652 $e.Å^{-3}$	

Table S7: Crystal data and structure refinement for **7.**

Empirical formula	C56 H78 Co N4 Ni O2	
Formula weight	956.86	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 12.66360(10) Å	α= 90°.
	b = 18.1084(2) Å	β= 91.3300(10)°.
	c = 22.5531(2) Å	γ = 90°.
Volume	5170.43(8) $Å^3$	
Z	4	
Density (calculated)	1.229 Mg/m^3	
Absorption coefficient	3.291 mm^{-1}	
F(000)	2052	
Crystal size	0.34 x 0.19 x 0.13 mm^3	
Theta range for data collection	3.13 to 67.48°.	
Index ranges	-15<=h<=14, -21<=k<=21, -25<=l<=27	
Reflections collected	19395	
Independent reflections	9298 [R(int) = 0.0261]	
Completeness to theta = 67.48°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.74667	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9298 / 0 / 599	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0806	
R indices (all data)	R1 = 0.0430, wR2 = 0.0854	
Largest diff. peak and hole	0.449 and -0.323 $e.Å^{-3}$	

2. ***Theoretical section***

Quantum-chemical Calculations

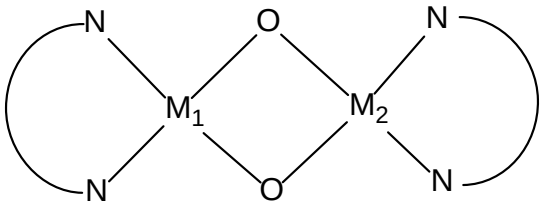
Density Functional Theory (DFT) calculations were carried out by using the GAUSSIAN 09 program.[10] Geometry optimization was performed with the B3LYP functional using ultrafine grid (99, 590).[11-13] For all calculations, aug-cc-pVTZ basis set was used for oxygen and transition metal atoms while 6-31G(d) basis set for all other atoms.[14,15] Electronic structures were analyzed using NBO 6.0 program.[16] Calculation of stationary structures, intermediates and also transition states, were carried out in the low-lying spin states. They were then confirmed by vibrational frequency calculations, intermediates had 0, while transition states had 1 imaginary frequency. Then Intrinsic Reaction Coordinate (IRC) calculations were executed to confirm that transition states connected the anticipated intermediates.

Possible spin-states were carefully checked in every stationary points. For **4** and **5**, we found that high-spin quintet state (S = 2) was the lowest energy state in agreement with experiments. None of our efforts calculating broken-symmetry states yielded lower energy states than the high-spin quintet state. For **1**, **2**, **3**, and **8**, however, low-spin broken-symmetry state (S = ½ for **1**, **2**, and **8**; S = 0 for **3**) showed the lowest energy for all structures.

Table S 8. Calculated energies of different spin states in **1-5** and **8** compounds in Hartree.

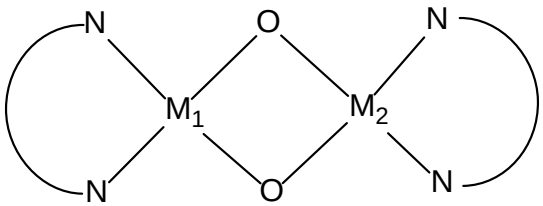
	1	**2**	**3**	**4**	**5**	**8**
S = 0	-	-	-5566.921744	-5315.606540	-5322.113535	-
S = ½	-5138.454877	-5441.261536	-	-	-	-5699.170230
S = 1	-	-	-5566.918310	-5315.619609	-5322.134906	-
S = 3/2	-5138.44128	5441.271149	-	-	-	-5699.155626
S = 2	-	-	-5566.915543	-5315.632959	-5322.159610	-
S = 5/2	-5138.43851	-5441.277735	-	-	-	-5699.143194

Table S9 Calculated important metric parameters of the Metal-Ligand (averaged), Metal-Metal, and O-O distances in [L'$M_1O_2M_2$L''] complexes in the lowest energy spin state and in Å. Notation follows the scheme below:



	M_1	M_2	Spin state	M_1-O	M_1-N	M_2-O	M_2-N	M_1-M_2	O-O
1	Cu	Ni	1/2	1.82	2.10	1.83	1.87	2.85	2.28
2	Co	Ni	1/2	1.78	1.96	1.84	1.92	2.77	2.31
3	Ni	Ni	0	1.81	1.94	1.81	1.93	2.77	2.31
4	Co	Co	2	1.77	1.91	1.77	1.91	2.66	2.35
5	Fe	Ni	2	1.73	1.98	1.92	1.90	2.69	2.44
8	Cu	Ni	1/2	1.84	1.98	1.85	1.92	2.86	2.30

Table S10 Calculated Natural Population Analysis charge, spin density, Mayer Bond Order (MBO) and oxidation state of the transition metal centers and O atoms in the minimum energy spin state of [L'$M_1O_2M_2$L''] complexes. Negative and positive values in the spin density only mean that these are opposite signs in spin density. Notation follows the scheme below:



			charge			Spin			oxidation state		
	M_1	M_2	M_1	M_2	O (Q_o)	M_1	M_2	O	M_1/M_2	O	$MBO_{M_2\text{-}O}$
1	Cu	Ni	1.63	1.29	-1.42	0.02	0.86	0.00	+3/+3	-2	0.26
2	Co	Ni	1.49	1.21	-1.21	-1.95	0.83	0.05	+3/+3	-2	0.42
3	Ni	Ni	1.17	1.17	-1.24	-0.91	0.91	0.02	+3/+3	-2	0.39
4	Co	Co	1.24	1.24	-1.10	1.92	1.92	0.03	+3/+3	-2	0.55
5	Fe	Ni	1.38	1.18	-1.10	2.92	0.89	0.07	+3/+3	-2	0.61
8	Cu	Ni	1.55	1.28	-1.38	0.01	0.75	0.03	+3/+3	-2	0.31

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Table S11. Cartesian geometry of **1** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-3.34728693	-2.84933432	-0.48512068
C	-2.62377493	-2.34172532	0.62659332
C	-3.23047593	-1.53915032	1.61642232
C	-4.59523493	-1.23175832	1.47454732
C	-5.33722793	-1.73805232	0.40407432
C	-4.71740493	-2.54761732	-0.56040868
N	-1.24912493	-2.72940832	0.78432432
C	-1.035491	-3.939779	1.303788
C	0.233191	-4.539158	1.351747
C	1.437007	-3.976139	0.881503
C	2.649779	-4.894129	0.791473
C	-2.45580693	-1.05663432	2.83743332
C	-3.07960493	-1.58910532	4.14823632
C	-2.63674193	-3.71035132	-1.53360568
C	-1.76363993	-2.85335532	-2.48842568
N	1.523697	-2.695506	0.494866
Ni	0.08733	-1.438538	0.295907
O	-1.133551	-0.130454	-0.163311
Cu	-0.036557	1.302045	-0.51287
O	1.156759	-0.019384	-0.050567
C	2.819048	-2.275113	0.032043
C	3.082545	-2.315055	-1.356167
C	4.389364	-2.025301	-1.784247
C	5.383168	-1.654788	-0.87129
C	5.088768	-1.590034	0.497225
C	3.811416	-1.921151	0.98164
C	1.991212	-2.651586	-2.369147
C	1.586434	-1.387582	-3.161833
C	3.495254	-1.950912	2.478275
C	4.741128	-2.133454	3.368766
C	2.712981	-0.693913	2.912991
C	2.401507	-3.796182	-3.320475
C	-2.214208	-4.750718	1.824845
N	-1.477902	2.529174	-1.080842
C	-1.254529	3.658782	-1.749003
C	-0.012089	4.241351	-2.025472
C	1.177547	3.813634	-1.424784
N	1.335933	2.714228	-0.692022
C	2.6018	2.543036	-0.048968
C	2.644749	2.642003	1.369558

C	3.889994	2.520558	2.005454
C	5.059618	2.279695	1.269545
C	4.99969	2.197462	-0.124858
C	3.781076	2.339378	-0.814354
C	1.386638	3.012423	2.155163
C	1.39045	2.580107	3.634263
C	3.788865	2.366728	-2.343761
C	4.465904	3.664327	-2.850545
C	-2.830743	2.32543	-0.647135
C	-3.702372	1.525974	-1.431644
C	-5.027877	1.374324	-0.988441
C	-5.477436	1.996651	0.182759
C	-4.607951	2.799852	0.930077
C	-3.27177	2.984387	0.532993
C	-3.230574	0.935482	-2.761846
C	-3.264963	2.000618	-3.888314
C	-2.355109	3.94093	1.302547
C	-2.579827	3.951143	2.83018
C	-4.063114	-0.273127	-3.229583
C	-2.529543	5.390898	0.782497
C	1.153297	4.540082	2.053778
C	4.482744	1.139515	-2.963521
C	-2.36944893	0.47943568	2.85881132
C	-3.58748793	-4.60538432	-2.35216268
H	0.281747	-5.558311	1.731925
H	5.87158	-1.30227	1.199283
H	6.387784	-1.413293	-1.225265
H	4.621082	-2.070176	-2.849991
H	1.099791	-2.984129	-1.820251
H	3.261756	-3.507354	-3.946953
H	1.563785	-4.043565	-3.993532
H	2.677815	-4.704434	-2.759676
H	1.290801	-0.591227	-2.463219
H	0.740722	-1.61539	-3.831701
H	2.429355	-1.027036	-3.774279
H	2.838878	-2.815414	2.663142
H	3.345986	0.195796	2.797652
H	2.416092	-0.784283	3.972509
H	1.818891	-0.54538	2.293117
H	5.342301	-3.003697	3.057297
H	4.428007	-2.278975	4.415017
H	5.387435	-1.240589	3.336848
H	-5.07522993	-0.59405732	2.21871732

H	-6.39931293	-1.50072132	0.31348532
H	-5.30940693	-2.93990732	-1.38785368
H	-1.94889693	-4.38187832	-0.99705868
H	-4.22364193	-5.22642432	-1.70044068
H	-2.99925793	-5.26960832	-3.00547368
H	-4.24394593	-3.99966132	-2.99830568
H	-2.39566793	-2.36146332	-3.24183868
H	-1.04090293	-3.49968232	-3.01404868
H	-1.21703493	-2.07047732	-1.94625168
H	-1.42820993	-1.44181032	2.77108832
H	-1.89928193	0.83639968	1.93322532
H	-1.77889993	0.81425268	3.72907532
H	-3.37473893	0.92437768	2.92660832
H	-4.10522293	-1.20593732	4.27774332
H	-2.48058993	-1.25907432	5.01330332
H	-3.12467293	-2.69042132	4.15867132
H	-2.143381	4.212638	-2.074176
H	0.006374	5.162008	-2.605649
H	2.053279	4.46505	-1.525752
H	-5.718252	0.757118	-1.562191
H	-6.510074	1.856944	0.511422
H	-4.972244	3.294664	1.831819
H	-1.314367	3.639503	1.116241
H	-3.567799	5.724322	0.947353
H	-1.854651	6.071075	1.328939
H	-2.30685	5.477794	-0.289469
H	-2.491793	2.950576	3.268663
H	-1.830529	4.60708	3.301421
H	-3.572405	4.358201	3.084119
H	-2.189502	0.606069	-2.619551
H	-5.086503	0.033426	-3.505902
H	-3.599477	-0.71052	-4.128084
H	-4.12412	-1.041065	-2.450741
H	-2.58543	2.84113	-3.698831
H	-2.971321	1.5389	-4.846397
H	-4.287935	2.398645	-3.998707
H	5.914491	2.032336	-0.697197
H	6.016832	2.170188	1.784738
H	3.947858	2.608159	3.091041
H	0.52729	2.513547	1.683135
H	1.041512	4.859784	1.0077
H	0.240615	4.824427	2.601491
H	2.007187	5.080852	2.49523

H	2.152946	3.126636	4.214279
H	0.408726	2.810446	4.077921
H	1.577047	1.502405	3.73875
H	2.75119	2.355731	-2.702962
H	3.976333	0.221504	-2.649221
H	4.451839	1.21064	-4.064067
H	5.538999	1.071882	-2.656808
H	5.524746	3.683681	-2.544231
H	4.424071	3.711909	-3.951616
H	3.985513	4.568481	-2.443661
H	3.009379	-4.938075	-0.24908
H	3.488227	-4.520994	1.397823
H	2.390239	-5.908875	1.124376
H	-2.810396	-4.156385	2.533015
H	-2.891619	-5.035892	1.00462
H	-1.860409	-5.663039	2.325698

Table S12. Cartesian geometry of **2** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	3.39257611	-2.77452525	0.53572321
C	2.70215411	-2.27976825	-0.60094279
C	3.33925911	-1.49885725	-1.58746179
C	4.69685211	-1.18123325	-1.40562079
C	5.40520411	-1.66398725	-0.30162679
C	4.75874811	-2.46526625	0.65132921
N	1.32827311	-2.66469925	-0.78752679
C	1.14445407	-3.87466253	-1.33638928
C	-0.11554293	-4.48977953	-1.41786528
C	-1.33417193	-3.96117853	-0.94651028
C	-2.52104693	-4.91478553	-0.87183828
C	2.60062911	-1.04183525	-2.84052779
C	3.31419711	-1.51417825	-4.12833379
C	2.65853211	-3.63346825	1.56906821
C	1.79055911	-2.77070125	2.52077321
N	-1.45222493	-2.69033853	-0.53876528
Ni	-0.04071998	-1.3920438	-0.30056677
O	1.12984717	-0.07032638	0.20658627
Co	-0.00759628	1.26811395	0.49347661
O	-1.17763712	0.00838529	0.03928364
C	-2.76002093	-2.31782253	-0.06767528
C	-3.01852593	-2.38945153	1.31959872
C	-4.33414193	-2.15355453	1.75487772

C	-5.34198293	-1.80263853	0.85038072
C	-5.05268693	-1.70530853	-0.51749028
C	-3.76582893	-1.98353253	-1.00978528
C	-1.91504893	-2.70771053	2.32557372
C	-1.55042293	-1.44770153	3.14367972
C	-3.45367993	-1.97873353	-2.50797028
C	-4.69926193	-2.15982753	-3.39914828
C	-2.68941393	-0.70395953	-2.92154328
C	-2.28655293	-3.88215153	3.25636472
C	2.33956407	-4.66707553	-1.84876228
N	1.37788852	2.54232307	1.04535785
C	1.15360252	3.66777307	1.72904385
C	-0.09866548	4.22357407	2.01302885
C	-1.28328348	3.75415707	1.43346585
N	-1.40137469	2.62941818	0.71984809
C	-2.67831369	2.46487818	0.07469209
C	-2.72962969	2.60375918	-1.33890791
C	-3.97775769	2.47782218	-1.97062491
C	-5.13854069	2.19649018	-1.23605691
C	-5.06912069	2.08474318	0.15583309
C	-3.84913769	2.23530918	0.84183309
C	-1.48351469	3.01600518	-2.12415691
C	-1.48573069	2.61266818	-3.61141791
C	-3.85008069	2.24236618	2.37227609
C	-4.54441269	3.52341118	2.89758309
C	2.75573852	2.38217707	0.64094185
C	3.64556852	1.63036307	1.44787685
C	4.97909052	1.51482707	1.01586585
C	5.41896352	2.13300207	-0.16121215
C	4.53059252	2.89893307	-0.92410915
C	3.18492752	3.04378007	-0.54000315
C	3.18355152	1.03678207	2.78136885
C	3.17398052	2.10837207	3.90243485
C	2.24685052	3.96793107	-1.32390615
C	2.47228052	3.96630207	-2.85117715
C	4.05409752	-0.13919593	3.26430485
C	2.38433652	5.42661607	-0.81761515
C	-1.27435669	4.54511018	-1.99732991
C	-4.52302469	0.99873518	2.98235809
C	2.43098711	0.48775175	-2.84470379
C	3.58832411	-4.54828125	2.39041621
H	-0.14133393	-5.50286353	-1.81610228
H	-5.84729393	-1.43395853	-1.21267628

H	-6.35365593	-1.60227753	1.20986372
H	-4.56157093	-2.22579753	2.82012672
H	-1.01409593	-3.00259253	1.77036872
H	-3.15582493	-3.63309253	3.88716872
H	-1.44077893	-4.11259053	3.92550072
H	-2.53194293	-4.78930853	2.67962672
H	-1.26911293	-0.62639753	2.46797672
H	-0.70433093	-1.66585953	3.81612672
H	-2.40722093	-1.12229453	3.75629572
H	-2.78642393	-2.83070453	-2.71220628
H	-3.32761393	0.17711947	-2.77387328
H	-2.40763593	-0.76545353	-3.98728128
H	-1.78608693	-0.56381253	-2.31344628
H	-5.28872493	-3.04363253	-3.10381128
H	-4.38676893	-2.28065353	-4.44868628
H	-5.35626393	-1.27575053	-3.34774828
H	5.19907711	-0.55338425	-2.14346679
H	6.46222311	-1.41836525	-0.17907779
H	5.32566611	-2.84674125	1.50115821
H	1.96621011	-4.29129625	1.02096021
H	4.22684211	-5.16781925	1.73957421
H	2.98372411	-5.21427125	3.02679621
H	4.24247911	-3.95897925	3.05410721
H	2.42849911	-2.25209925	3.25068121
H	1.08680411	-3.41565725	3.07319121
H	1.22074811	-2.00919025	1.97216621
H	1.59434811	-1.48560025	-2.83220079
H	1.89772811	0.81353075	-1.94187079
H	1.86833511	0.80368675	-3.74009879
H	3.41359611	0.98484275	-2.85419879
H	4.31875511	-1.06725425	-4.20746179
H	2.73464911	-1.20700325	-5.01464579
H	3.42827911	-2.61036725	-4.15142479
H	2.03464052	4.23637007	2.04840985
H	-0.13474648	5.14978607	2.58443085
H	-2.17590248	4.38223507	1.53239585
H	5.68418852	0.92793607	1.60352885
H	6.45838252	2.02186307	-0.47934515
H	4.88501652	3.39615707	-1.82865315
H	1.21363452	3.64289807	-1.13775315
H	3.41457452	5.78396007	-0.98279215
H	1.69402652	6.08561907	-1.37081515
H	2.15838752	5.51676407	0.25386485

H	2.40441652	2.95875907	-3.27729415
H	1.70850652	4.60059707	-3.32956315
H	3.45637252	4.39024407	-3.11078415
H	2.15462552	0.67157707	2.63705985
H	5.06186252	0.20651407	3.55185085
H	3.59627252	-0.59076793	4.15886585
H	4.15473552	-0.90641393	2.48865485
H	2.46133252	2.92013707	3.70917485
H	2.89741852	1.64015207	4.86254385
H	4.17996352	2.54783507	4.01212385
H	-5.97758969	1.89207418	0.72981909
H	-6.09643369	2.08199118	-1.74897991
H	-4.04271569	2.59296818	-3.05339391
H	-0.61431769	2.52304418	-1.66269391
H	-1.16328569	4.85070918	-0.94693591
H	-0.36713169	4.85235318	-2.54223991
H	-2.13734169	5.08126918	-2.42697391
H	-2.26131469	3.15491818	-4.17820991
H	-0.51067469	2.87162618	-4.05436491
H	-1.65133169	1.53391518	-3.73684691
H	-2.81063369	2.24228018	2.72710109
H	-4.00021169	0.09185318	2.66315509
H	-4.49511569	1.06261618	4.08352509
H	-5.57749169	0.91440018	2.67349709
H	-5.60506669	3.52968918	2.59692409
H	-4.49758569	3.55931218	3.99897909
H	-4.08071069	4.43964918	2.49836909
H	-2.87756493	-4.98350553	0.16834872
H	-3.37067393	-4.55775053	-1.47170528
H	-2.23259593	-5.91685953	-1.21894128
H	2.93061907	-4.06293653	-2.55267228
H	3.01530007	-4.93836653	-1.02251028
H	2.00545207	-5.58564553	-2.35153628

Table S13. Cartesian geometry of **3** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-3.42087509	-2.75555757	-0.51301865
C	-2.70458709	-2.26418257	0.61043035
C	-3.31827209	-1.46681957	1.60027635
C	-4.67552109	-1.13626457	1.44105835
C	-5.40788009	-1.61961757	0.35335835
C	-4.78592009	-2.43304457	-0.60595065

N	-1.33491409	-2.65963357	0.78051735
C	-1.14287333	-3.87711172	1.30537962
C	0.11560767	-4.49663772	1.37373162
C	1.32969967	-3.95797972	0.91237862
C	2.51983267	-4.90770572	0.83063962
C	-2.55558609	-1.01125157	2.83926335
C	-3.23483109	-1.50617457	4.13724235
C	-2.71733509	-3.63607557	-1.55136265
C	-1.80669409	-2.80936557	-2.49393365
N	1.45839267	-2.68054972	0.52252062
Ni	0.04037067	-1.37863772	0.30255462
O	-1.13317633	-0.09317745	-0.17651901
Ni	0.00355366	1.27341653	-0.50256948
O	1.17652652	-0.02307282	-0.04706185
C	2.76672267	-2.30408672	0.06281362
C	3.03857567	-2.37201772	-1.32316538
C	4.35633467	-2.13019272	-1.74789838
C	5.35570467	-1.77734972	-0.83453838
C	5.05618567	-1.68687172	0.53161762
C	3.76631267	-1.97095672	1.01288362
C	1.94454967	-2.69747872	-2.33735138
C	1.57068867	-1.44041772	-3.15622838
C	3.44692167	-1.98871572	2.50978762
C	4.69006967	-2.16874872	3.40458362
C	2.66677467	-0.72969672	2.94062062
C	2.33371167	-3.86527572	-3.26936238
C	-2.33531033	-4.67343172	1.82062962
N	-1.37842147	2.52053982	-1.05710793
C	-1.15600234	3.64514853	-1.74738148
C	0.09666966	4.19997953	-2.03529548
C	1.27591866	3.73624653	-1.44233048
N	1.39148901	2.61538347	-0.72025605
C	2.66041901	2.44005247	-0.06891105
C	2.70421001	2.57023947	1.34626395
C	3.94750201	2.43616147	1.98508295
C	5.11186301	2.15594447	1.25565595
C	5.05125501	2.05467747	-0.13741105
C	3.83628701	2.21183147	-0.83049805
C	1.45608501	2.98870747	2.12474195
C	1.44594701	2.58412847	3.61165895
C	3.84955801	2.23620847	-2.36068105
C	4.54736401	3.52445247	-2.86419705
C	-2.74979247	2.35913282	-0.64143793

C	-3.64417847	1.60373082	-1.44142993
C	-4.97753147	1.49706382	-1.00697893
C	-5.41288847	2.12516482	0.16644107
C	-4.52075847	2.89261982	0.92337107
C	-3.17551347	3.03041982	0.53603307
C	-3.18830047	0.99907682	-2.77244593
C	-3.16592547	2.06435782	-3.89962193
C	-2.23491347	3.96134382	1.30849707
C	-2.45837747	3.97722682	2.83605807
C	-4.07371347	-0.16772218	-3.25166393
C	-2.37338947	5.41490782	0.78748707
C	1.26264901	4.52003647	1.99765895
C	4.52976001	1.00241647	-2.98219405
C	-2.40375009	0.51989943	2.85790335
C	-3.68088209	-4.50333357	-2.38550465
H	0.14180467	-5.51515272	1.75669062
H	5.84588067	-1.41875672	1.23367062
H	6.36950567	-1.57256472	-1.18562338
H	4.59365567	-2.20121272	-2.81110338
H	1.04370967	-3.00276072	-1.78793638
H	3.20304367	-3.60532872	-3.89577138
H	1.49364167	-4.10395772	-3.94267038
H	2.58657767	-4.77062272	-2.69322338
H	1.28034367	-0.62072972	-2.48251938
H	0.72799567	-1.66587972	-3.83087838
H	2.42550867	-1.10672972	-3.76718438
H	2.78779667	-2.85054472	2.69767862
H	3.29179767	0.16201728	2.80176762
H	2.38796167	-0.80739972	4.00607462
H	1.75888667	-0.59687772	2.33788662
H	5.28949267	-3.04261872	3.10017862
H	4.37390367	-2.30689172	4.45089862
H	5.33871667	-1.27766672	3.36800862
H	-5.15838909	-0.49935857	2.18420635
H	-6.46461609	-1.36489857	0.24778135
H	-5.37298209	-2.81338257	-1.44241965
H	-2.05649409	-4.32646957	-1.00430865
H	-4.34674909	-5.10258457	-1.74325165
H	-3.10159009	-5.18713057	-3.02639165
H	-4.30806209	-3.88065557	-3.04458365
H	-2.41476909	-2.21846457	-3.19310365
H	-1.16483309	-3.48786757	-3.08080365
H	-1.16704809	-2.11569057	-1.93352165

H	-1.54533509	-1.44391557	2.80331435
H	-1.89329909	0.86554543	1.94914935
H	-1.82578009	0.83294343	3.74444835
H	-3.39084809	1.00686843	2.89364635
H	-4.24414309	-1.07512657	4.24157835
H	-2.64119909	-1.20012857	5.01466935
H	-3.33182209	-2.60402757	4.15017635
H	-2.03717134	4.21137753	-2.07002948
H	0.13459166	5.12054753	-2.61500848
H	2.16915866	4.36321953	-1.53743748
H	-5.68640747	0.90954982	-1.58920193
H	-6.45218047	2.01988082	0.48684907
H	-4.87282747	3.39783282	1.82432707
H	-1.20240347	3.63428182	1.12243407
H	-3.40296947	5.77429282	0.95211507
H	-1.68126647	6.07873982	1.33248407
H	-2.14963847	5.49438282	-0.28511093
H	-2.38560547	2.97598882	3.27576907
H	-1.69742147	4.62103582	3.30575907
H	-3.44391547	4.40022282	3.09143707
H	-2.16326547	0.62305582	-2.62708093
H	-5.07588347	0.19118182	-3.54230693
H	-3.62091247	-0.62843218	-4.14405093
H	-4.18709347	-0.93090818	-2.47374393
H	-2.43963947	2.86530482	-3.71404793
H	-2.90040947	1.58584182	-4.85771493
H	-4.16553147	2.51821682	-4.00849193
H	5.96324401	1.86506947	-0.70659405
H	6.06617001	2.03507747	1.77370095
H	4.00647501	2.54548447	3.06875495
H	0.58561001	2.50447747	1.65758495
H	1.15841401	4.82620047	0.94682595
H	0.35719801	4.83667447	2.53976095
H	2.12989801	5.04654347	2.43044095
H	2.22253501	3.11967047	4.18323095
H	0.47042701	2.85118247	4.04858095
H	1.60174901	1.50398447	3.73777695
H	2.81310301	2.23985147	-2.72382105
H	4.00560301	0.09028347	-2.68110105
H	4.51171801	1.08271847	-4.08243705
H	5.58146601	0.91478147	-2.66513405
H	5.60673101	3.52487647	-2.55897605
H	4.50534201	3.57594247	-3.96513005

H	4.08366701	4.43583347	-2.45419605
H	2.87553367	-4.96870072	-0.21038238
H	3.36960667	-4.55270872	1.43172062
H	2.23424767	-5.91278772	1.17105762
H	-2.91715433	-4.07455072	2.53709562
H	-3.02122433	-4.93529672	0.99996862
H	-1.99789533	-5.59761372	2.31053662

Table S14. Cartesian geometry of **4** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-4.40762271	0.65295936	1.13045228
C	-3.21212516	0.66037668	1.89191301
C	-3.01136383	-0.23723062	2.96460919
C	-4.08883376	-1.05376841	3.34918376
C	-5.3114506	-1.01529202	2.66834043
C	-5.45437502	-0.18656305	1.55006305
N	-2.20711087	1.63950246	1.55039116
C	-2.44095145	2.87334981	2.00094524
C	-1.78490398	4.04226893	1.5904226
C	-0.87902959	4.08414263	0.51385539
N	-0.43741964	3.00931941	-0.12159917
C	0.34710883	3.18366783	-1.3110304
C	-0.26049684	2.89369976	-2.56501466
C	0.52122074	3.05370334	-3.72157058
C	1.86126324	3.46081744	-3.64362771
C	2.43870932	3.72038979	-2.39823589
C	1.69787803	3.58695198	-1.20813408
C	-1.72913245	2.46735806	-2.64910775
C	-2.08496905	1.69551553	-3.93423156
C	2.35809197	3.88425378	0.13384555
C	3.65205881	3.06843122	0.3228321
C	-1.66974486	-0.3532415	3.67654764
C	-1.77096292	0.10380203	5.14852265
C	-4.55570192	1.47043885	-0.15225857
C	-5.74040178	2.45872211	-0.07862725
Co	-0.705731	1.209342	0.45591
O	0.957335	0.675492	0.304986
Co	0.608865	-1.06587762	0.06240854
N	2.22599471	-1.69775559	0.85511004
C	3.25099049	-0.77404751	1.27046289
C	3.16890053	-0.10986597	2.51582872
C	4.29095463	0.61595197	2.95235071

C	5.44696748	0.71449148	2.16844261
C	5.46717115	0.13319663	0.89657714
C	4.36999989	-0.60498566	0.41760917
C	1.92505647	-0.18460878	3.39136893
C	2.2193167	-0.95055793	4.70184178
C	4.39432815	-1.15098132	-1.00972301
C	4.45420936	0.0248956	-2.01470822
N	0.26477685	-2.67637254	-0.90592604
C	0.79627491	-3.87115013	-0.63858291
C	1.76703161	-4.02463419	0.37943641
C	2.47823763	-3.00240608	1.03177115
C	-0.65278609	-2.48822005	-1.99493944
C	-0.18931368	-1.801724	-3.15450032
C	-1.10788544	-1.56850632	-4.19119584
C	-2.44797986	-1.96444362	-4.08204727
C	-2.88236821	-2.62706277	-2.93160914
C	-1.99967874	-2.91183576	-1.87227441
C	1.27528298	-1.37902334	-3.2929414
C	2.1555762	-2.58765878	-3.69659842
C	-2.52940144	-3.66449519	-0.65357928
C	-3.62009929	-2.84974383	0.07196882
C	1.49752102	-0.20816808	-4.26934328
O	-1.04265724	-0.55413674	0.40482981
C	-3.08817267	-5.05239617	-1.05542528
C	-2.66702596	3.69017568	-2.49512869
C	2.62909645	5.40069594	0.28138071
C	1.37185517	1.23033101	3.67927301
C	5.56406114	-2.13244883	-1.24404472
C	-1.12152431	-1.79531079	3.56728754
C	-4.68830237	0.5234577	-1.36843675
H	6.31047437	1.27623427	2.5308885
H	6.3403544	0.25912724	0.25321017
H	5.3701732	0.61936902	-1.86587644
H	6.53559442	-1.63031306	-1.10954583
H	5.52595569	-2.53132128	-2.27083562
H	5.51829958	-2.97813374	-0.54017205
H	-3.26041868	2.97522769	2.7224682
C	3.62558761	-3.45790299	1.93367651
H	-2.07767752	4.98262634	2.054785
H	2.08500287	-5.0455871	0.59437929
H	-0.55223983	5.060348	0.13442063
C	0.4302836	-5.12035119	-1.42857654
H	-3.95856308	-1.73698038	4.19069572

H	4.25237143	1.1112937	3.92450416
H	-6.13728701	-1.65469086	2.98775645
H	-6.38464783	-0.1962021	0.97825313
H	-3.6420268	2.0599305	-0.30039583
H	3.45980545	-1.69557439	-1.19751304
H	-3.81469118	-0.13932567	-1.44766832
H	3.59015188	0.69436069	-1.89102436
H	-4.77120041	1.111105	-2.29724727
H	4.45832687	-0.35824759	-3.04778138
H	-5.58902748	-0.10602771	-1.28017787
H	-6.69417638	1.92506103	0.06376959
H	-5.81059014	3.03951389	-1.01282446
H	-5.61491983	3.1623993	0.75983159
H	-0.95985047	0.30517808	3.16092907
H	1.15343541	-0.73455476	2.83754185
H	-1.81159222	-2.52245181	4.02470085
H	2.12548255	1.86000716	4.17897568
H	-0.15197	-1.87463771	4.08179414
H	0.48975573	1.17105031	4.33469787
H	-0.98307832	-2.05967743	2.50860468
H	1.07980015	1.71625597	2.73695112
H	-2.09449028	1.1551527	5.2128091
H	2.55463313	-1.97881296	4.49193577
H	-0.79329967	0.01069664	5.64873493
H	1.31584093	-1.00205883	5.33037259
H	-2.49965627	-0.5109989	5.70186507
H	3.01037717	-0.44602965	5.28040548
H	3.48398154	4.028786	-2.33700942
H	-3.92503759	-2.93809555	-2.84328773
H	1.67294955	3.57919336	0.93564841
H	-1.70542679	-3.81229275	0.05762289
H	3.31416483	5.75060301	-0.50816923
H	-3.96062538	-4.93475535	-1.71815949
H	3.09270585	5.6132157	1.25881419
H	-3.4180039	-5.59976748	-0.15718333
H	1.69869528	5.98635726	0.20234441
H	-2.34328342	-5.66420947	-1.58432592
H	3.4341176	1.99494817	0.26884328
H	-3.22254333	-1.88484215	0.40448782
H	4.0901597	3.27998792	1.30929452
H	-3.98418759	-3.40094515	0.95240592
H	4.40603897	3.31704326	-0.44213285
H	-4.48050042	-2.66565749	-0.59064176

H	-1.9277679	1.79097214	-1.80298464
H	1.62131145	-1.04067423	-2.30471585
H	-2.49748744	4.40523823	-3.31733588
H	1.83141993	-2.98911059	-4.6709537
H	-2.50211619	4.21261464	-1.54239326
H	2.09433501	-3.39417748	-2.95259566
H	-3.71970463	3.36527237	-2.52942129
H	3.2103682	-2.27882288	-3.78131196
H	0.08367294	2.84698358	-4.69830905
H	-0.77766878	-1.05653646	-5.09482146
H	2.4527458	3.56749651	-4.55564751
H	-3.14757798	-1.75220459	-4.89327418
H	-3.11022738	1.30600548	-3.85181927
H	2.5477582	0.11138798	-4.22097162
H	-1.4105648	0.84242543	-4.08776307
H	0.86911088	0.65494686	-4.00748706
H	-2.04178737	2.34708744	-4.82285704
H	1.28314699	-0.49976471	-5.31101269
H	4.02200704	-2.65263248	2.56415315
H	3.26616242	-4.27452413	2.58076953
H	4.45462812	-3.85839159	1.32760938
H	-0.16902081	-4.89137927	-2.31818451
H	1.34574495	-5.64757332	-1.74136799
H	-0.14714363	-5.80820224	-0.78924527

Table S15. Cartesian geometry of **5** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	0.19005366	-2.12740881	-3.0758429
C	0.69474766	-2.67628481	-1.8684039
C	2.06047266	-3.03178681	-1.7408569
C	2.91780966	-2.78413881	-2.8289099
C	2.44281166	-2.21916281	-4.0179339
C	1.08285666	-1.90541381	-4.1379909
N	-0.20475334	-2.80806881	-0.7549289
C	-0.79116634	-3.98322981	-0.5099849
C	-1.81414834	-4.13281481	0.4490411
C	-2.54708034	-3.08739881	1.0415771
C	-3.75207834	-3.47966781	1.8901031
C	2.62956066	-3.65091481	-0.4693949
C	3.36964666	-4.98057781	-0.7533729
C	-1.28108534	-1.75451381	-3.2299259
C	-1.91612934	-2.37212181	-4.4952709

Ni	-0.65006034	-1.16021081	0.0827861
N	-2.26929834	-1.78456781	0.8473531
C	-3.28336634	-0.85656981	1.2713801
Fe	0.646068	1.163957	0.484722
O	-1.014141	0.66463	0.537906
N	2.21178856	1.65040899	1.60139417
C	2.41552156	2.88442099	2.08423417
C	1.69670856	4.03769299	1.73630217
C	0.78489456	4.10213799	0.66734117
N	0.39249956	3.05611199	-0.05420183
C	-0.44348044	3.26346599	-1.19842983
C	0.11605056	3.00049899	-2.47905483
C	-0.70611544	3.18452699	-3.60256983
C	-2.04187844	3.59009799	-3.46546483
C	-2.57539544	3.81956699	-2.19299183
C	-1.79359544	3.65624299	-1.03363083
C	1.58281056	2.58423699	-2.61639783
C	1.90421656	1.82494799	-3.91724583
C	-2.41763044	3.89758999	0.33775017
C	-3.66757644	3.02105899	0.55007017
C	3.27229356	0.71206299	1.85476217
C	3.11378856	-0.27736801	2.85276617
C	4.23133056	-1.06530001	3.18112017
C	5.44729456	-0.92031501	2.50289017
C	5.54458956	-0.01231801	1.44124517
C	4.46201456	0.81280999	1.09026317
C	1.77441156	-0.54210201	3.53124617
C	1.28054056	-1.96893501	3.19169917
C	4.54802256	1.69848599	-0.15162983
C	5.75584356	2.65827299	-0.11528983
C	2.50712556	3.81744299	-2.47421483
C	-2.74644144	5.39573399	0.53408617
C	4.57727056	0.80514699	-1.41523183
C	1.85199656	-0.32682201	5.05818517
O	1.069173	-0.35922	-0.225436
C	-0.39592634	-5.20289581	-1.3266089
C	3.58681466	-2.66766081	0.2318241
C	-1.44951534	-0.21990981	-3.2245559
H	3.07362166	-1.73037981	0.4757781
H	0.39745056	5.08653599	0.37328117
H	1.95195956	4.96643999	2.24406217
H	3.25189956	3.00384799	2.78538617
H	-0.30412144	2.99545999	-4.59811083

H	-2.66656644	3.71707399	-4.35250583
H	-3.61875344	4.12361099	-2.08648083
H	-1.69485244	3.60335899	1.11028017
H	-1.84620944	6.02430699	0.42940017
H	-3.17660444	5.56391099	1.53547517
H	-3.48088944	5.73245899	-0.21631283
H	1.81980956	1.89883099	-1.78801783
H	2.30896956	4.53611999	-3.28716383
H	3.56381456	3.50865199	-2.53304283
H	2.34968556	4.32844699	-1.51294683
H	1.25207256	0.94879699	-4.03764383
H	2.94500756	1.46970999	-3.88229583
H	1.79952456	2.47615299	-4.80150583
H	6.46996056	0.05499599	0.86535817
H	3.64033256	2.31297399	-0.21307683
H	5.46853756	0.15599399	-1.41079783
H	4.61257256	1.43310899	-2.32055683
H	3.68427356	0.16486699	-1.46283783
H	5.71643456	3.31106299	0.77191717
H	5.76076356	3.29325499	-1.01658983
H	6.70680756	2.10128299	-0.08803183
H	4.44299566	-2.43424981	-0.4215129
H	3.97816566	-3.10940081	1.1607221
H	4.13328256	-1.81640601	3.96762917
H	6.30319856	-1.54311201	2.77224717
H	1.03568356	0.16710799	3.13156817
H	2.57691556	-1.02003001	5.51586617
H	0.86792156	-0.50907501	5.51938117
H	2.16539156	0.70243899	5.29752417
H	2.01696156	-2.72393101	3.51282317
H	1.12106056	-2.07475201	2.10767217
H	0.32982456	-2.17547801	3.70720317
H	-3.71680734	-2.98708281	2.8722741
H	-4.45614044	3.25953499	-0.18269483
H	-4.07962644	3.18630599	1.55755617
H	-3.40599944	1.96034399	0.45714517
H	-2.15427534	-5.14706781	0.6508881
H	-0.56552234	-5.00784281	-2.3981789
H	-0.98515334	-6.08016581	-1.0254609
H	0.67244566	-5.43048681	-1.2100799
H	0.70384166	-1.47741881	-5.0684129
H	3.12657466	-2.02898081	-4.8484709
H	3.97566766	-3.03764881	-2.7337279

H	-1.82419334	-2.15864281	-2.3657849
H	-1.06550534	0.21986119	-2.2928339
H	-2.50912434	0.05898819	-3.3250869
H	-0.89906834	0.22881119	-4.0659879
H	-1.45754234	-1.96881081	-5.4131409
H	-2.99304134	-2.13615681	-4.5252819
H	-1.79775934	-3.46805881	-4.5074009
H	1.79758466	-3.85808281	0.2187901
H	4.27314666	-4.79983281	-1.3585659
H	2.74253266	-5.70334981	-1.2996289
H	3.68797166	-5.44205081	0.1960171
H	-3.78316234	-4.56921381	2.0317841
H	-4.68911434	-3.15599181	1.4118811
C	-4.36668434	-0.59472481	0.3913941
C	-5.48430134	0.09038219	0.8982281
C	-5.50615734	0.56055719	2.2182871
C	-4.37368734	0.40622919	3.0256861
C	-3.23829134	-0.28568381	2.5653651
C	-4.29418434	-1.01510981	-1.0762659
H	-6.33921334	0.27703619	0.2463161
H	-6.38578634	1.08449219	2.5992641
H	-4.36264134	0.82863819	4.0329731
C	-1.99755434	-0.37783881	3.4468481
H	-1.20864934	-0.87001881	2.8644811
C	-1.49907934	1.04068619	3.8105431
C	-2.24533034	-1.20702481	4.7262161
H	-3.22778934	-1.09867681	-1.3227109
C	-4.94347434	-2.39298081	-1.3417709
C	-4.89701234	0.04995219	-2.0182649
H	-1.33563434	-1.22830481	5.3490301
H	-3.05927734	-0.76761281	5.3266071
H	-2.51839434	-2.24674881	4.4871011
H	-0.58038334	0.98017319	4.4148701
H	-1.29071934	1.60941819	2.8929541
H	-2.25554534	1.58642819	4.3986361
H	-4.71895234	-0.24404581	-3.0653499
H	-5.98740834	0.14285219	-1.8833039
H	-4.43639934	1.03479719	-1.8478899
H	-4.90475434	-2.62543981	-2.4195889
H	-4.41846234	-3.19464081	-0.8036139
H	-6.00173934	-2.38988281	-1.0289389

Table S16. Cartesian geometry of **7** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	2.653138	-2.924561	-2.046762
C	2.45964	-2.847309	-0.643794
C	3.562457	-2.666445	0.234511
C	4.859765	-2.658029	-0.3088
C	5.069148	-2.781676	-1.685508
C	3.967619	-2.890058	-2.54376
N	1.143238	-2.948898	-0.067447
C	0.915454	-4.095021	0.595357
C	-0.064335	-4.310111	1.577231
C	-0.85868	-3.313149	2.173551
N	-0.983261	-2.053769	1.747529
C	-1.666153	-1.133073	2.614679
C	-0.881989	-0.318292	3.476159
C	-1.54864	0.589039	4.318605
C	-2.946375	0.685772	4.315196
C	-3.699048	-0.117623	3.451083
C	-3.080643	-1.027009	2.572954
C	0.638252	-0.47095	3.527947
C	1.03457	-1.59104	4.518947
C	-3.909432	-1.856283	1.592781
C	-4.289527	-3.237372	2.179482
C	3.382268	-2.450493	1.737492
C	4.082548	-1.155271	2.207564
C	1.465044	-2.978457	-2.998158
C	1.705224	-3.843955	-4.252769
Co	-0.074667	-1.412303	0.128917
O	0.985672	0.213028	-0.117076
Ni	-0.276581	1.447593	-0.838083
O	-1.334499	-0.209179	-0.934897
C	-2.587908	-0.338856	-1.440561
C	-3.500606	0.762657	-1.393394
C	-4.799973	0.595213	-1.898525
C	-5.226562	-0.629211	-2.429973
C	-4.321326	-1.692868	-2.490771
C	-2.996641	-1.567284	-2.035311
C	-3.035236	2.0865	-0.783875
C	-4.081539	3.230617	-0.860237
C	-2.027601	-2.727243	-2.220634
C	-2.275249	-3.872669	-1.216007
N	0.923434	2.894311	-1.020561

C	0.781016	3.807674	-1.99366
C	1.874889	4.838919	-2.221018
C	1.903468	3.053725	0.009255
C	3.218537	2.547057	-0.16755
C	4.118176	2.640381	0.912981
C	3.748153	3.248793	2.117646
C	2.457415	3.777259	2.260561
C	1.51053	3.676995	1.227313
C	3.696414	1.954018	-1.491135
C	4.070649	0.464188	-1.357272
C	0.118291	4.286944	1.383192
C	-0.534678	3.997095	2.750373
C	-0.34517	3.828708	-2.835694
C	-1.585989	3.223802	-2.519981
N	-1.727285	2.469672	-1.42418
C	-2.723583	3.487262	-3.502732
C	0.180884	5.811143	1.122143
C	4.914157	2.741237	-2.036983
C	-2.787921	1.908029	0.744396
C	-2.048307	-3.273399	-3.665406
C	1.38607	0.832125	3.865461
C	-5.193636	-1.143941	1.120111
C	3.88508	-3.666788	2.546567
C	1.075357	-1.534921	-3.403745
H	1.710722	0.557565	0.432955
H	-2.091491	1.096139	0.977988
H	-3.743057	1.670519	1.233593
H	-2.398584	2.843934	1.168277
H	-1.018992	-2.337578	-2.044172
H	-2.137985	-3.53564	-0.180824
H	-1.569282	-4.699941	-1.396495
H	-3.302601	-4.2608	-1.321158
H	3.202823	-0.140656	-1.068881
H	-1.388933	-3.582959	3.095883
H	-0.110324	-5.305682	2.017742
H	1.612999	-4.922662	0.40537
H	-0.968139	1.22436	4.988605
H	-3.446532	1.395419	4.978186
H	-4.78542	-0.020984	3.438225
H	-3.28753	-2.023617	0.703111
H	-3.406069	-3.845624	2.417518
H	-4.903597	-3.795957	1.453291
H	-4.879068	-3.1077	3.10284

H	0.973456	-0.783111	2.528497
H	0.700155	-1.332743	5.5378
H	2.129748	-1.716491	4.53328
H	0.582096	-2.55358	4.238478
H	1.110865	1.640983	3.176326
H	2.470423	0.669098	3.778703
H	1.180551	1.165799	4.896303
H	5.713453	-2.540149	0.362144
H	2.311667	-2.33654	1.948116
H	5.172672	-1.211829	2.055461
H	3.899247	-0.999866	3.282499
H	3.710708	-0.275695	1.660205
H	3.335771	-4.57847	2.264013
H	3.742402	-3.494432	3.626483
H	4.958382	-3.840195	2.361881
H	-3.007687	-3.765938	-3.893203
H	-1.248585	-4.020046	-3.792815
H	-1.89637	-2.465457	-4.397678
H	4.862403	0.325397	-0.604376
H	4.450194	0.078548	-2.315882
H	4.131014	-2.959067	-3.620207
H	6.083059	-2.77195	-2.091798
H	0.623773	-3.424821	-2.450635
H	2.458168	-3.390973	-4.918308
H	0.769023	-3.930009	-4.826406
H	2.048191	-4.855839	-3.982771
H	1.906205	-1.072076	-3.962946
H	0.869577	-0.908816	-2.523632
H	0.181048	-1.541328	-4.046802
H	-3.415467	2.634236	-3.536705
H	-4.89083	3.02114	-0.144692
H	-4.541172	3.361553	-1.844328
H	-4.635628	-2.645284	-2.923659
H	-6.24848	-0.746027	-2.796213
H	-5.505536	1.425138	-1.851854
H	-5.942854	-1.088816	1.928139
H	-5.633322	-1.707385	0.284433
H	-4.97944	-0.129032	0.7612
H	-0.309298	4.46816	-3.71694
H	2.200321	5.286261	-1.269707
H	1.520735	5.635654	-2.889652
H	2.759164	4.365646	-2.6749
H	2.175128	4.262209	3.196711

H	4.462931	3.317682	2.940655
H	5.127578	2.241455	0.792495
H	-0.526942	3.846329	0.611792
H	-0.653858	2.91694	2.917621
H	-1.535488	4.458683	2.78431
H	0.052245	4.418234	3.583408
H	0.837853	6.304291	1.858566
H	-0.8261	6.254146	1.204718
H	0.570714	6.024206	0.114953
H	2.873695	2.030079	-2.215904
H	5.7928	2.587269	-1.388944
H	4.72212	3.824326	-2.086196
H	5.173004	2.381216	-3.046367
H	-2.293728	3.634196	-4.504761
H	-3.293423	4.395501	-3.250087
H	-3.594013	4.172265	-0.566046

Table S17. Cartesian geometry of **8** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
O	-0.4239697	-1.19868572	-0.1743018
O	0.846796	0.664512	-0.481987
N	-2.60334964	0.11035738	0.71590404
N	-1.05587311	2.36234959	0.43464486
H	-2.24734174	-0.66431432	2.96983188
C	-3.54234337	0.95126028	1.16951997
C	-2.94891662	-1.2727023	0.5095931
C	-2.12278497	3.0198379	0.91130142
C	0.11656628	3.0991164	0.05073991
C	-2.28922222	-1.76301271	2.94450228
C	-4.91336784	0.41464392	1.53717217
C	-3.30112422	2.33931066	1.2863076
C	-2.80094644	-2.19434485	1.57436779
C	-3.37205962	-1.6746609	-0.78182022
C	-2.07803409	4.53237688	1.03096625
C	0.31250937	3.38588264	-1.32356711
C	1.06886169	3.45263926	1.04279407
C	-0.84608833	-2.27843993	3.14770362
C	-3.21262376	-2.22976642	4.09199718
H	-5.56520704	1.21975639	1.90185617
H	-4.82791881	-0.360692	2.31394194
H	-5.38368348	-0.06181603	0.66229961
H	-4.12087454	2.94903831	1.66227736

C	-3.09662713	-3.54550406	1.31954333
C	-3.66047518	-3.03419185	-0.98460743
C	-3.46669404	-0.68669965	-1.94088583
H	-1.28507432	4.84412795	1.72853332
H	-3.04020229	4.9260534	1.38471337
H	-1.83954118	4.98324059	0.05489071
C	1.50006962	4.04028232	-1.69488777
C	-0.72763612	3.02584726	-2.37982817
C	2.24521264	4.08984014	0.61674416
C	0.84056766	3.10768192	2.51318404
H	-0.83190631	-3.38165626	3.16128877
H	-0.43689924	-1.91719014	4.10573877
H	-0.21066791	-1.92783568	2.32308411
H	-4.24663466	-1.87730385	3.94761306
H	-2.8430473	-1.83928537	5.05348551
H	-3.23588142	-3.32889882	4.16114618
H	-2.98800932	-4.2728973	2.12600293
C	-3.52834722	-3.96638126	0.05483524
H	-3.99010262	-3.36544531	-1.9710769
H	-3.32268503	0.32994033	-1.54716942
C	-2.32694622	-0.94906565	-2.95299823
C	-4.84636947	-0.72713335	-2.63489388
H	1.66703331	4.28045603	-2.74665395
C	2.46349811	4.38331956	-0.73901343
H	-1.55861355	2.50186584	-1.88541509
C	-1.30035063	4.29829734	-3.04714608
C	-0.14766606	2.06154707	-3.43718981
H	2.997941	4.37149638	1.35417188
H	-0.24315492	3.02980869	2.68408455
C	1.44554077	1.72238545	2.83821201
C	1.38072191	4.17927524	3.48365635
H	-3.76044113	-5.01855831	-0.12187262
H	-2.42639798	-1.95812652	-3.38711496
H	-1.35287275	-0.87532935	-2.44621428
H	-2.36389076	-0.21486145	-3.77380223
H	-5.02994364	-1.70803384	-3.10156112
H	-4.89191428	0.03746516	-3.42700534
H	-5.65957704	-0.53442098	-1.9168169
H	3.38155369	4.8892796	-1.04479067
H	-1.75137885	4.97212303	-2.30101511
H	-2.07380704	4.02547879	-3.78317323
H	-0.5083034	4.8556935	-3.57235206
H	0.70545553	2.52119888	-3.96297096

H	-0.91640629	1.81519819	-4.18712881
H	0.18958207	1.13635463	-2.94792163
H	2.53810031	1.74283139	2.6978197
H	1.0283656	0.95114203	2.17555676
H	1.23598585	1.44923529	3.8858545
H	2.48179792	4.21732558	3.46886389
H	1.07199184	3.93551402	4.51226083
Ni	-0.85827666	0.52238329	0.18403922
Cu	1.241312	-1.063268	-0.900004
C	3.58711153	-1.45770601	-2.75017149
C	3.53064453	-2.96743201	-2.49295049
H	4.61687153	-1.16619001	-3.02663649
H	2.93147853	-1.21050701	-3.60037449
C	2.11205953	-3.53472501	-2.44756649
H	4.03768253	-3.45249301	-3.34196849
H	4.10137653	-3.25153401	-1.59785749
H	1.56287353	-3.20165901	-3.34254549
H	2.14998753	-4.63947701	-2.46989849
N	3.16143053	-0.59092001	-1.60422949
C	4.14996953	-0.73801401	-0.47886049
C	3.85835953	0.14137699	0.74670451
H	5.15418553	-0.51990201	-0.88963249
H	4.13507753	-1.78474901	-0.15779949
C	4.40792653	-0.52460201	2.02385351
H	4.31988553	1.13421899	0.63483551
H	2.77879953	0.31640899	0.83729051
H	5.49618853	-0.67047101	1.91602451
H	4.25429053	0.15929199	2.88737451
N	1.29257353	-3.13281801	-1.26289249
N	3.80488953	-1.84564401	2.27099251
C	2.40383953	-1.72128901	2.68556051
H	1.99808253	-2.72103501	2.89975651
H	2.28409053	-1.09334201	3.59584651
H	1.80185653	-1.27538501	1.88080851
C	4.56732153	-2.57404201	3.29427551
H	4.57154653	-2.05099401	4.27637051
H	4.12446753	-3.57229601	3.43714051
H	5.60964053	-2.69469901	2.95982151
C	-0.09580247	-3.65334701	-1.48812949
H	-0.72671947	-3.39599001	-0.63290649
H	-0.51350747	-3.18409001	-2.38671049
H	-0.04844547	-4.74908301	-1.62007849
C	1.81569753	-3.75326901	-0.00780149

H	1.10726253	-3.52397001	0.79651351
H	1.89358353	-4.84809301	-0.13793849
H	2.79287753	-3.33514201	0.26354451
H	0.99978361	5.18183279	3.23113101
C	3.18694353	0.82755299	-2.07970049
H	2.84106953	1.49013199	-1.28253349
H	4.21892953	1.08479799	-2.37912049
H	2.51088753	0.93124999	-2.93600349

Table S18. Cartesian geometry of toluene in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-0.91785	0.000358	-0.009802
C	-0.196766	-1.209625	-0.008445
C	1.206389	-1.21309	0.002118
C	1.913716	-0.000276	0.008385
C	1.20704	1.212773	0.00209
C	-0.196265	1.209876	-0.0084
C	-2.434978	0.000218	0.008396
H	-0.743162	-2.156732	-0.018153
H	1.746926	-2.162493	0.0002
H	3.005921	-0.000551	0.012392
H	1.748003	2.161903	0.000134
H	-0.74244	2.157077	-0.018114
H	-2.841105	-0.880719	-0.514511
H	-2.840689	0.905354	-0.471435
H	-2.821177	-0.025244	1.043424

Table S19. Cartesian geometry of L^1NiO_2 in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	3.382522	1.181693	-0.085362
C	2.694589	-0.045104	0.103252
C	3.236395	-1.27859	-0.330342
C	4.496897	-1.266797	-0.954605
C	5.195321	-0.069253	-1.148195
C	4.637285	1.143185	-0.717307
N	1.388294	-0.029655	0.695179
Ni	-0.013837	-0.008281	-0.54802
N	-1.390188	0.035284	0.70006
C	-1.255699	0.054196	2.037241
C	-2.507769	0.116916	2.895777

C	2.485617	-2.594814	-0.147132
C	3.286995	-3.581067	0.733034
C	2.747411	2.507113	0.333063
C	3.765092	3.52318	0.893484
C	-2.697519	0.049574	0.110032
C	-3.242808	1.282071	-0.322956
C	-4.502821	1.267076	-0.94774
C	-5.199624	0.068031	-1.139471
C	-4.64002	-1.142891	-0.706687
C	-3.384535	-1.178207	-0.076081
C	-2.487103	2.597126	-0.153009
C	-2.078525	3.171054	-1.529339
C	-2.744819	-2.501298	0.341737
C	-3.757016	-3.517149	0.91224
C	-0.00137	0.013814	2.670632
C	1.255279	-0.032565	2.025963
C	2.508435	-0.078407	2.88584
C	-1.970808	-3.112553	-0.850968
C	-3.309077	3.626852	0.6544
C	2.140724	-3.2294	-1.51355
C	1.964969	3.116359	-0.854997
H	0.003858	0.020556	3.759145
H	4.92837	-2.2107	-1.294831
H	1.536436	-2.381051	0.365017
H	4.246098	-3.842408	0.256376
H	2.714246	-4.511602	0.88113
H	3.506279	-3.145449	1.721672
H	1.543646	-2.534455	-2.122382
H	1.565449	-4.158768	-1.366647
H	3.058506	-3.477427	-2.072139
H	2.017343	2.301331	1.129375
H	4.362568	3.085216	1.709774
H	3.232461	4.405884	1.282697
H	4.458752	3.872944	0.111652
H	-5.186195	-2.074375	-0.864508
H	-4.935924	2.209511	-1.289929
H	-1.562276	2.392706	0.405436
H	-1.476618	2.439873	-2.089357
H	-1.488754	4.093763	-1.398051
H	-2.971656	3.414277	-2.128758
H	-4.241353	3.888285	0.12741
H	-2.726427	4.552453	0.794223
H	-3.57929	3.231026	1.647246

H	-2.009158	-2.29161	1.131993
H	-4.346798	-3.078574	1.733778
H	-3.220899	-4.399655	1.297205
H	-4.45794	-3.867365	0.137116
H	-2.665786	-3.354952	-1.672012
H	-1.45714	-4.038709	-0.541557
H	-1.221559	-2.405054	-1.236602
H	-6.175995	0.073924	-1.629089
H	5.184428	2.073594	-0.877809
H	6.171542	-0.077086	-1.638056
H	2.651514	3.345284	-1.686881
H	1.4644	4.049899	-0.546526
H	1.20274	2.413679	-1.22325
H	-2.248749	0.16101	3.962671
H	-3.109985	1.000983	2.631531
H	-3.144951	-0.763811	2.715701
H	2.248568	-0.129224	3.952172
H	3.125056	-0.95165	2.619996
H	3.130915	0.813525	2.709676
O	-0.655318	-0.00775	-2.35425
O	0.676176	-0.054028	-2.213305

Table S20. Cartesian geometry of L³Co in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-3.291574	1.336872	-0.253359
C	-2.853536	0.000249	-0.017357
C	-3.723186	-1.1041	-0.22091
C	-5.052477	-0.843669	-0.604989
C	-5.507295	0.4622	-0.811693
C	-4.624693	1.540196	-0.647577
N	-1.498376	-0.209104	0.392924
Co	0.000741	0.181871	-0.649988
N	1.494856	-0.219811	0.394214
C	1.260504	-0.733729	1.621628
C	-0.005297	-0.968389	2.191668
C	-1.269206	-0.722858	1.621385
C	-3.261339	-2.553712	-0.069992
C	-3.959481	-3.24081	1.125971
C	-2.339203	2.514675	-0.037498
C	-2.143492	2.798445	1.470574
C	2.851797	-0.023415	-0.016499
C	3.315335	1.310973	-0.21139

C	4.65057	1.500296	-0.605253
C	5.509991	0.41045	-0.809485
C	5.03	-0.892258	-0.642388
C	3.69778	-1.138005	-0.259076
C	2.389212	2.499557	0.051957
C	2.235706	2.751764	1.570549
C	3.206447	-2.580627	-0.141901
C	3.44118	-3.365554	-1.453569
C	-3.496502	-3.355508	-1.371619
C	-2.746912	3.803588	-0.777185
C	3.876582	-3.302246	1.049844
C	2.805439	3.796889	-0.668508
H	-2.154512	-0.954174	2.227388
H	-0.007009	-1.377045	3.202398
H	2.143743	-0.973448	2.22746
H	-4.983375	2.554404	-0.82623
H	-1.344605	2.21921	-0.430896
H	-3.103077	3.098357	1.924596
H	-1.419306	3.618431	1.613003
H	-1.767795	1.908425	1.993944
H	-2.93221	3.614934	-1.846739
H	-1.942398	4.550536	-0.684723
H	-3.659612	4.24316	-0.341339
H	-2.180188	-2.559325	0.123441
H	-3.750153	-2.707272	2.067145
H	-3.61001	-4.281805	1.228686
H	-5.052407	-3.257388	0.981024
H	5.029081	2.512542	-0.751723
H	5.692568	-1.741867	-0.821332
H	2.122814	-2.566894	0.039284
H	2.95382	-2.862461	-2.303951
H	3.02692	-4.383314	-1.362718
H	4.516402	-3.455581	-1.679048
H	4.970926	-3.335029	0.918273
H	3.507698	-4.338711	1.128165
H	3.663763	-2.782934	1.997892
H	1.381908	2.229984	-0.323664
H	1.85785	1.855725	2.082483
H	1.529181	3.57989	1.749811
H	3.210913	3.024905	2.007905
H	3.737285	4.208755	-0.246417
H	2.018712	4.557477	-0.540084
H	2.960833	3.628737	-1.746327

H	6.546527	0.580382	-1.109008
H	-5.732033	-1.685481	-0.754954
H	-6.541716	0.643483	-1.111844
H	-4.570425	-3.422603	-1.610676
H	-3.108263	-4.381337	-1.258438
H	-2.985313	-2.878426	-2.223044

Table S21. Cartesian geometry of L³Co(toluene) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	3.296651	1.422379	0.094141
C	2.79507	0.145829	0.462679
C	3.574455	-1.027078	0.290688
C	4.885162	-0.893355	-0.203124
C	5.407975	0.363664	-0.536215
C	4.612816	1.509381	-0.393559
N	1.444496	0.040059	0.913738
C	1.247577	0.13444	2.23082
C	-0.000076	0.147212	2.876529
C	-1.247693	0.134354	2.23076
N	-1.444557	0.039967	0.913662
C	-2.795129	0.145793	0.46258
C	-3.574512	-1.027083	0.290473
C	-4.885204	-0.893344	-0.203374
C	-5.408007	0.363687	-0.536419
C	-4.612845	1.509399	-0.393664
C	-3.29671	1.422368	0.094106
C	-2.989933	-2.392771	0.645539
C	-3.495725	-3.532815	-0.264012
C	-2.412706	2.660886	0.229027
C	-2.628617	3.695275	-0.895555
C	2.98984	-2.3927	0.645952
C	3.264917	-2.742262	2.128073
C	2.412614	2.660881	0.228977
C	2.628187	3.694998	-0.895928
Co	0.000015	-0.111426	-0.477585
C	-1.226158	-0.96705	-2.137464
C	-1.229055	0.438222	-2.288447
C	0.000399	1.152763	-2.303178
C	1.22969	0.437937	-2.288661
C	1.22649	-0.967309	-2.137663
C	0.000102	-1.687249	-2.004146

C	-0.000004	-3.186111	-1.79656
C	-3.265105	-2.742546	2.127593
C	-2.602856	3.324289	1.613175
C	3.495583	-3.532962	-0.263369
C	2.602994	3.324548	1.612962
H	-2.138418	0.226845	2.869342
H	-0.000111	0.222722	3.963664
H	2.138274	0.226974	2.869435
H	-5.017191	2.483775	-0.674616
H	-1.36759	2.320059	0.166928
H	-3.647523	3.655473	1.73969
H	-1.94441	4.204341	1.712067
H	-2.362031	2.618805	2.422458
H	-2.535989	3.23277	-1.891584
H	-1.876699	4.497051	-0.810966
H	-3.623278	4.166365	-0.830471
H	-1.897557	-2.317417	0.521432
H	-2.831526	-1.986638	2.798488
H	-2.827236	-3.723547	2.379635
H	-4.351558	-2.789083	2.312471
H	5.017216	2.483741	-0.674494
H	5.502091	-1.783989	-0.336105
H	1.897467	-2.317306	0.521803
H	3.373328	-3.288008	-1.330838
H	2.933401	-4.456802	-0.05032
H	4.562203	-3.746797	-0.085147
H	4.351359	-2.78886	2.313011
H	2.826968	-3.723196	2.380241
H	2.831366	-1.986231	2.798839
H	1.367508	2.319995	0.167157
H	2.362384	2.619136	2.42238
H	1.944489	4.20455	1.711849
H	3.647657	3.655828	1.739254
H	3.62284	4.166157	-0.831289
H	1.876254	4.496761	-0.811354
H	2.535266	3.232177	-1.891781
H	-2.172075	-1.492975	-2.0172
H	-2.175836	0.974427	-2.279076
H	0.00053	2.241703	-2.345279
H	2.176576	0.973956	-2.279403
H	2.172301	-1.493447	-2.017504
H	-0.893593	-3.504278	-1.240045
H	0.893301	-3.504318	-1.239605

H	0.00024	-3.716944	-2.76598
H	6.428035	0.448755	-0.917705
H	-5.50211	-1.78399	-0.336422
H	-6.428046	0.448793	-0.91796
H	-4.562434	-3.74644	-0.086075
H	-2.933791	-4.456807	-0.050939
H	-3.37315	-3.287766	-1.331421

Table S22. Cartesian geometry of transition state (+ 12.2 kcal/mol) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	4.494071	-1.306973	1.538899
C	3.175791	-1.38777	2.068914
C	2.71028	-2.59665	2.660782
C	3.550889	-3.726045	2.60528
C	4.798	-3.695581	1.9685
C	5.271157	-2.476173	1.468416
N	2.353519	-0.209821	2.00131
C	2.431017	0.650915	3.024052
C	1.955688	1.973262	3.021862
C	1.677994	2.725381	1.86256
N	1.69925	2.279661	0.601314
C	1.612179	3.32594	-0.386484
C	2.771949	3.651444	-1.154359
C	2.686901	4.687636	-2.099923
C	1.49713	5.403825	-2.297057
C	0.382048	5.10448	-1.511742
C	0.418204	4.081606	-0.543835
C	4.113732	2.957706	-0.903787
C	4.761625	3.531209	0.382458
C	-0.828123	3.851045	0.310838
C	-2.035163	3.418911	-0.536755
C	1.376437	-2.672802	3.406205
C	0.820444	-4.105814	3.589779
C	5.115261	0.040025	1.172188
C	5.990069	0.523829	2.354041
Co	1.725584	0.326154	0.210526
O	-0.173784	-0.030478	0.138552
Ni	-2.100121	-0.610464	-0.124906
O	-1.18356	0.677741	0.752454
N	-3.759074	-0.540354	0.759347

C	-4.690587	-1.506156	0.704502
C	-5.88077	-1.432061	1.653191
C	-4.067334	0.677	1.446804
C	-4.980005	1.5874	0.834272
C	-5.285403	2.78026	1.510598
C	-4.704896	3.07677	2.754094
C	-3.820027	2.168302	3.344188
C	-3.487559	0.956447	2.710181
C	-5.616867	1.268538	-0.526073
C	-7.010791	1.906252	-0.716109
C	-2.554849	-0.026583	3.416558
C	-1.214948	0.629502	3.817957
C	-4.627965	-2.587953	-0.19659
C	-3.65156	-2.79779	-1.191939
N	-2.516362	-2.081563	-1.253607
C	-1.55494	-2.383729	-2.27599
C	-1.521129	-1.6147	-3.462189
C	-0.521337	-1.908114	-4.407608
C	0.379266	-2.954633	-4.192236
C	0.326129	-3.712153	-3.010805
C	-0.637053	-3.438682	-2.024315
C	-2.507456	-0.479551	-3.707883
C	-3.12579	-0.521699	-5.122784
C	-0.687624	-4.168509	-0.696021
C	0.057754	-3.390433	0.409836
C	-3.899366	-3.892562	-2.219354
C	-3.23448	-0.625083	4.672247
C	-4.68747	1.680444	-1.684152
C	-1.827639	0.884408	-3.461285
C	-0.169165	-5.61992	-0.765238
C	5.135246	3.020582	-2.065646
C	-1.180113	5.110805	1.136268
C	1.482475	-2.070252	4.836143
C	5.932989	0.022257	-0.133229
H	-5.465636	-3.28343	-0.180003
H	1.037946	-4.52751	-2.873081
H	1.146494	-3.172727	-4.93849
H	-0.458211	-1.313018	-5.320257
H	-3.332272	-0.576193	-2.987965
H	-2.371452	-0.313346	-5.898963
H	-3.913441	0.245084	-5.207386
H	-3.571718	-1.507164	-5.334908
H	-1.372518	0.913098	-2.462248

H	-2.563174	1.700838	-3.525194
H	-1.034444	1.064478	-4.205324
H	-1.739519	-4.212967	-0.382881
H	1.146417	-3.56586	0.374608
H	-0.312357	-3.713464	1.392068
H	-0.12267	-2.312926	0.332683
H	-0.677913	-6.196561	-1.555381
H	-0.34138	-6.121961	0.2005
H	0.915351	-5.64697	-0.963129
H	-3.3789	2.390526	4.318031
H	-4.951626	4.012175	3.261796
H	-5.981971	3.491787	1.066024
H	-5.76196	0.183541	-0.605363
H	-7.686262	1.661634	0.119973
H	-7.458924	1.53177	-1.650505
H	-6.948194	3.003964	-0.797255
H	-4.483805	2.762475	-1.668699
H	-5.145332	1.412463	-2.651786
H	-3.732897	1.144284	-1.596587
H	-2.342542	-0.851288	2.720495
H	-0.685915	1.030231	2.947943
H	-0.564889	-0.111254	4.306589
H	-1.38503	1.449452	4.537154
H	-3.457318	0.166332	5.407373
H	-2.562111	-1.356615	5.151783
H	-4.179732	-1.133842	4.425489
H	2.944306	0.302553	3.928788
H	1.968993	2.508848	3.970467
H	1.476192	3.795231	1.999137
H	3.204435	-4.660475	3.047278
H	5.415034	-4.594813	1.911486
H	6.2722	-2.419172	1.036127
H	4.310834	0.775324	1.042942
H	6.787418	-0.208296	2.56463
H	6.456853	1.492911	2.114136
H	5.385902	0.646831	3.266198
H	5.315763	-0.327611	-0.972095
H	6.283107	1.040552	-0.360079
H	6.821512	-0.625289	-0.050143
H	0.642124	-2.072953	2.844442
H	1.414842	-4.649112	4.344551
H	-0.212921	-4.040362	3.962444
H	0.830852	-4.718158	2.672448

H	1.807069	-1.023718	4.831676
H	0.501248	-2.11229	5.33902
H	2.200129	-2.655873	5.435146
H	-0.541509	5.674265	-1.63619
H	1.452677	6.202019	-3.041686
H	3.570483	4.95848	-2.680456
H	3.904204	1.894373	-0.716988
H	4.138923	3.340944	1.26663
H	5.74772	3.066841	0.549892
H	4.907042	4.619104	0.276757
H	5.809844	3.886856	-1.945513
H	5.745362	2.107592	-2.084632
H	4.639033	3.135517	-3.043615
H	-0.637122	3.037619	1.018222
H	-1.825485	2.491057	-1.081496
H	-2.893991	3.236094	0.123046
H	-2.312596	4.202684	-1.262677
H	-1.427553	5.961059	0.479024
H	-2.053076	4.901768	1.776098
H	-0.337623	5.415644	1.779404
H	-3.993633	-3.45031	-3.225766
H	-3.058932	-4.60189	-2.261506
H	-4.822171	-4.443021	-1.988409
H	-5.534044	-1.384953	2.696504
H	-6.48011	-0.525793	1.477636
H	-6.526439	-2.313004	1.530227
C	1.596761	-0.838422	-1.860488
C	1.56356	0.541705	-2.214493
C	2.648572	1.07658	-2.934911
C	3.785248	0.310223	-3.204436
C	3.866918	-1.03851	-2.784152
C	2.763475	-1.593201	-2.118914
H	0.654486	1.121611	-2.100816
H	2.610979	2.111557	-3.259322
H	4.625051	0.769214	-3.731892
C	5.09897	-1.872376	-3.078056
H	2.780571	-2.647321	-1.836591
H	0.695878	-1.335212	-1.518786
H	4.971791	-2.907717	-2.726348
H	5.310852	-1.897741	-4.161007
H	5.994533	-1.45806	-2.585509

Table S23. Cartesian geometry of transition state (- 30.1 kcal/mol) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-3.997075	-2.135669	-1.974393
C	-3.724698	-1.128767	-1.011045
C	-4.135756	0.22184	-1.220004
C	-4.77208	0.539678	-2.43
C	-5.012515	-0.433907	-3.408066
C	-4.642004	-1.758113	-3.167749
N	-3.044288	-1.446113	0.211279
C	-3.706825	-2.177713	1.115105
C	-3.307655	-2.412576	2.440381
C	-2.242753	-1.763426	3.093837
N	-1.343315	-0.959498	2.517864
C	-0.576314	-0.125679	3.403812
C	-1.17373	1.069369	3.875688
C	-0.465928	1.851811	4.804153
C	0.809639	1.476119	5.240002
C	1.408302	0.326509	4.713089
C	0.741654	-0.484876	3.77696
C	-2.533507	1.541798	3.357519
C	-2.394936	2.895256	2.62574
C	1.424427	-1.71104	3.184997
C	2.839613	-1.370116	2.686289
C	-3.999844	1.262398	-0.102672
C	-4.010026	2.722188	-0.589054
C	-3.698535	-3.613746	-1.718832
C	-5.013971	-4.376908	-1.411724
Co	-1.236511	-0.769036	0.579124
O	0.455278	-1.420067	-0.251877
Ni	1.185663	0.196766	-0.948221
O	-0.498074	0.836133	-0.227732
N	2.725218	-0.706505	-1.574022
C	3.394488	-0.335035	-2.687729
C	4.23546	-1.357211	-3.443249
C	3.157055	-1.873616	-0.879353
C	2.240031	-2.929264	-0.610945
C	2.717638	-4.115307	-0.034059
C	4.064793	-4.254355	0.324678
C	4.931568	-3.167795	0.170536
C	4.500634	-1.962431	-0.410321
C	0.744698	-2.688391	-0.871161

C	-0.171379	-3.732222	-0.204242
C	5.46551	-0.77193	-0.438959
C	6.923685	-1.177653	-0.781244
C	0.406747	-2.62781	-2.380774
C	3.348974	0.971289	-3.192691
C	2.633543	2.045176	-2.623398
N	1.706297	1.868188	-1.671587
C	0.94571	2.993334	-1.220962
C	1.260933	3.570958	0.041835
C	0.434606	4.600461	0.528946
C	-0.659517	5.058063	-0.213084
C	-0.940981	4.492957	-1.462725
C	-0.161315	3.452112	-1.993713
C	2.437803	3.058697	0.873728
C	3.286156	4.203601	1.466336
C	-0.529014	2.814038	-3.332956
C	-0.894106	3.867035	-4.402124
C	2.939391	3.450556	-3.125363
C	5.415079	-0.032876	0.924454
C	-3.584616	1.628818	4.489289
C	1.456139	-2.883196	4.188378
C	1.935884	2.111355	1.990927
C	-1.678294	1.788672	-3.162493
C	-5.119968	1.045469	0.948175
C	-2.967395	-4.293889	-2.899635
H	6.14161	0.802535	0.935561
H	5.663286	-0.721783	1.752013
H	7.483347	-0.308633	-1.17042
H	7.465149	-1.54139	0.112032
H	2.083856	3.888513	-3.668582
H	3.814225	3.442114	-3.795054
H	3.145595	4.126127	-2.27634
H	4.409406	0.377658	1.110752
H	0.033084	-3.814367	0.875245
H	-1.216658	-3.4137	-0.340765
H	-1.798454	4.856089	-2.031394
H	-1.297905	5.850526	0.183764
H	0.652778	5.045441	1.501393
H	3.091052	2.471112	0.206517
H	1.239457	2.632656	2.671539
H	2.780727	1.738411	2.597933
H	1.403346	1.240479	1.57395
H	3.640465	4.897011	0.681628

H	4.166871	3.784199	1.985634
H	2.719747	4.794885	2.208734
H	0.342331	2.255392	-3.707147
H	-1.816982	4.415103	-4.13931
H	-1.077556	3.366864	-5.370191
H	-0.090085	4.612726	-4.543596
H	-1.465984	1.089887	-2.339105
H	-1.816138	1.215018	-4.09812
H	-2.633857	2.29436	-2.941637
H	2.797587	-0.548448	1.955908
H	-2.903596	0.808952	2.623294
H	-3.379258	3.242953	2.264093
H	-1.717064	2.815772	1.759153
H	-1.987983	3.672599	3.297721
H	-5.095264	1.563927	-2.614595
H	-5.505204	-0.160382	-4.34394
H	-4.858789	-2.524293	-3.914948
H	-3.049634	-3.69663	-0.832481
H	-5.550497	-3.94284	-0.5494
H	-4.80354	-5.440213	-1.191215
H	-5.696718	-4.335381	-2.279887
H	-3.034292	1.103937	0.406724
H	-3.216522	2.909106	-1.327474
H	-3.837148	3.392332	0.269232
H	-4.981943	3.007495	-1.033225
H	-6.115021	1.147091	0.475664
H	-5.04119	1.800217	1.752165
H	-5.057766	0.046963	1.410988
H	-0.548261	1.771368	0.013983
H	5.130224	-1.684352	-2.892012
H	4.561774	-0.941291	-4.410056
H	3.633517	-2.265544	-3.628821
H	3.963869	1.194311	-4.062849
H	2.030511	-4.938631	0.157627
H	4.420961	-5.187671	0.766206
H	5.9642	-3.244776	0.517259
H	5.138679	-0.041248	-1.192666
H	6.965187	-1.979653	-1.539787
H	-0.056933	-4.728121	-0.667143
H	-0.632404	-2.273029	-2.491189
H	0.500771	-3.626645	-2.846447
H	1.063416	-1.923418	-2.910956
H	-3.564755	-4.250831	-3.827793

H	-2.79575	-5.361505	-2.668505
H	-1.993517	-3.824532	-3.103716
H	-2.190996	-1.871039	4.187979
H	-3.95246	-3.047011	3.04765
H	-4.684554	-2.576297	0.810894
H	-0.923384	2.769619	5.181292
H	1.346468	2.09302	5.964592
H	2.416671	0.050163	5.026463
H	0.845818	-2.028427	2.304412
H	2.027492	-2.610072	5.095357
H	1.941956	-3.766403	3.732251
H	0.437333	-3.171075	4.506632
H	3.292431	-2.240428	2.190106
H	3.50895	-1.06482	3.511816
H	-3.743544	0.642582	4.961477
H	-4.55354	1.980464	4.088732
H	-3.269318	2.334183	5.279578

Table S24. Cartesian geometry of intermediate (- 45.3 kcal/mol) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	2.126595	-0.086658	3.313948
C	2.314269	0.334484	1.893062
C	3.672413	0.119553	1.306164
C	4.66266	-0.487345	2.057988
C	4.415425	-0.942914	3.377392
C	3.153325	-0.730497	3.985107
Ni	0.853595	2.079252	0.922983
N	2.06065	2.140278	2.273583
C	2.349582	3.062997	3.178163
C	3.393932	2.841032	4.258351
O	1.456596	0.238164	1.003124
Co	-0.245479	-0.22348	-0.356473
O	-0.537732	1.502283	-0.095634
C	4.148058	1.102369	0.252343
C	4.524275	0.410055	-1.056193
C	0.760182	0.096593	3.932913
C	0.833468	1.033653	5.151589
N	0.552991	-1.465155	-1.731207
C	-0.035533	-2.619186	-2.091325
C	-1.301475	-3.083568	-1.72344
C	-2.265054	-2.334675	-1.028045

N	-2.062888	-1.156651	-0.446688
C	-3.26179	-0.457936	-0.064571
C	-3.977981	-0.830303	1.104526
C	-5.173761	-0.145052	1.391109
C	-5.669743	0.842085	0.530832
C	-4.982827	1.14026	-0.651431
C	-3.777772	0.496025	-0.975408
C	-3.600225	-2.066584	1.923569
C	-4.578004	-3.226718	1.588233
C	-3.105745	0.768216	-2.318711
C	-2.81879	2.261753	-2.543714
C	1.785348	-1.223091	-2.430191
C	2.914927	-2.043606	-2.166718
C	4.085635	-1.819084	-2.917199
C	4.152317	-0.799549	-3.870666
C	3.02913	0.006064	-4.109633
C	1.825797	-0.194878	-3.411895
C	2.907229	-3.156121	-1.116401
C	2.962516	-4.551149	-1.784093
C	0.552778	0.569275	-3.783902
C	-0.32231	-0.304348	-4.716036
C	-3.613638	-1.864781	3.448177
C	-3.972042	0.168924	-3.451857
C	0.795599	1.93689	-4.448421
C	4.067683	-3.00739	-0.107299
N	0.547505	3.942677	1.115599
C	0.936676	4.679938	2.168289
C	0.609146	6.165151	2.198655
C	-0.084807	4.570104	-0.002324
C	0.742731	4.918624	-1.101017
C	0.129668	5.406507	-2.266852
C	-1.261231	5.569505	-2.331654
C	-2.052307	5.260265	-1.217415
C	-1.487273	4.752766	-0.033344
C	2.26684	4.833761	-1.00156
C	2.87738	3.898998	-2.065764
C	-2.373219	4.449573	1.171083
C	-3.376232	3.321999	0.851494
C	2.893661	6.245559	-1.092751
C	-3.142145	5.709763	1.642214
C	1.634718	4.27907	3.161458
C	5.338187	1.908291	0.79904
C	0.144887	-1.234196	4.366967

H	-2.854598	2.399116	0.565756
H	0.519163	-3.248144	-2.797711
H	-1.585839	-4.077652	-2.065289
H	-3.282939	-2.743006	-0.991
H	3.086581	0.796757	-4.858208
H	5.077266	-0.625541	-4.42431
H	4.958222	-2.448375	-2.732586
H	1.975568	-3.087345	-0.539712
H	2.11306	-4.711675	-2.465642
H	2.946992	-5.341513	-1.015834
H	3.890496	-4.656547	-2.369061
H	-0.019227	0.748401	-2.861402
H	0.231247	-0.537844	-5.64033
H	-1.239647	0.240595	-4.987817
H	-0.610946	-1.248042	-4.232732
H	1.467388	2.562658	-3.850532
H	-0.16375	2.464466	-4.555918
H	1.232546	1.818076	-5.454038
H	-5.385729	1.883926	-1.341219
H	-2.136943	0.254486	-2.334201
H	-3.746403	2.857116	-2.547797
H	-2.318493	2.40658	-3.514772
H	-2.160683	2.63915	-1.753332
H	-4.145041	-0.90664	-3.287729
H	-3.476006	0.2975	-4.426709
H	-4.952399	0.67117	-3.493756
H	-4.028624	3.621965	0.018319
H	-4.016835	3.11271	1.723709
H	-5.740426	-0.42213	2.282492
H	-6.6085	1.349324	0.762544
H	-2.592383	-2.382906	1.619871
H	-5.618112	-2.905198	1.754781
H	-4.373741	-4.097218	2.233289
H	-4.487164	-3.546564	0.539684
H	-4.633487	-1.652465	3.808707
H	-2.963064	-1.034152	3.753729
H	-3.261973	-2.796446	3.927446
H	3.651474	1.785148	4.38569
H	5.041726	-3.190099	-0.590062
H	3.947239	-3.740061	0.706916
H	4.075531	-2.0017	0.330237
H	1.759774	4.953327	4.007262
H	1.289515	6.706554	1.521633

H	0.742996	6.565057	3.213488
H	-0.413763	6.366152	1.861537
H	0.751163	5.671791	-3.124738
H	-1.728681	5.928822	-3.250659
H	-3.133685	5.398304	-1.26669
H	2.527229	4.410028	-0.023013
H	2.510082	2.871865	-1.926086
H	3.976196	3.889797	-1.977468
H	2.616022	4.228971	-3.083767
H	2.705043	6.690891	-2.082976
H	3.984105	6.188631	-0.94173
H	2.469777	6.91958	-0.332381
H	-1.733891	4.10129	1.993809
H	-3.923915	5.97517	0.911947
H	-2.485759	6.585331	1.761408
H	-3.633669	5.509388	2.607836
H	3.030766	3.246787	5.214795
H	4.314379	3.385912	3.988907
H	5.653664	-0.626502	1.618611
H	5.210811	-1.437787	3.937865
H	2.994171	-1.056112	5.01627
H	0.097968	0.547942	3.179897
H	3.331047	1.80449	0.039364
H	-0.171552	1.174307	5.581342
H	1.482022	0.596568	5.927771
H	1.236778	2.018214	4.882062
H	-0.852084	-1.04319	4.788732
H	0.050383	-1.917657	3.510293
H	0.771944	-1.717158	5.134323
H	5.672868	2.647016	0.052261
H	5.065056	2.442422	1.722146
H	6.181586	1.235819	1.024124
H	4.837397	1.15072	-1.809555
H	5.350617	-0.302308	-0.901894
H	3.663422	-0.134222	-1.451008

Table S25. Cartesian geometry of transition state (- 38.2 kcal/mol) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	2.896221	-3.091961	-1.144634
C	1.550467	-2.876907	-1.539924

C	1.2152	-2.507417	-2.876289
C	2.262957	-2.371881	-3.803038
C	3.597162	-2.597249	-3.434785
C	3.903001	-2.956201	-2.119272
N	0.485677	-3.007415	-0.588957
C	0.250886	-4.219531	-0.071808
C	-0.827258	-4.558274	0.763817
C	-1.923167	-3.72854	1.069742
N	-2.040494	-2.440715	0.735505
C	-3.304157	-1.807345	0.973063
C	-3.705253	-1.489722	2.295513
C	-4.967415	-0.898012	2.482782
C	-5.800198	-0.60447	1.396714
C	-5.367318	-0.890472	0.095005
C	-4.119585	-1.493089	-0.14457
C	-2.803329	-1.742407	3.501852
C	-2.468259	-0.423664	4.235066
C	-3.686733	-1.7904	-1.578743
C	-4.686074	-2.732906	-2.286347
C	-0.245831	-2.326315	-3.305906
C	-0.424365	-1.610646	-4.658703
C	3.293049	-3.460749	0.284331
C	4.356815	-2.496042	0.846282
Co	-0.544714	-1.432349	-0.061243
Ni	0.461599	1.38936	0.276497
N	-0.388565	3.068268	-0.002825
C	-1.34023	3.077788	-1.073153
C	-0.855541	2.995218	-2.400228
C	-1.79339	2.923193	-3.44592
C	-3.167089	2.944153	-3.181811
C	-3.625044	3.039519	-1.859247
C	-2.728474	3.105548	-0.779081
C	0.640322	2.958889	-2.708346
C	1.056338	4.089575	-3.674888
C	-3.211739	3.190961	0.669493
C	-4.649827	3.731023	0.808789
O	1.770116	0.01984	0.527914
O	-0.801881	0.259864	-0.358486
N	1.777377	2.077811	1.312538
C	1.939793	3.283101	1.847456
C	1.057166	4.324748	1.494233
C	0.015977	4.227934	0.537351
C	-0.60536	5.528258	0.044281

C	3.102689	3.538489	2.783499
C	1.045557	1.577628	-3.267291
C	-3.093708	1.824576	1.38022
C	-3.434298	-2.765596	4.472912
C	-3.490481	-0.483103	-2.376728
C	-0.989178	-3.683973	-3.350179
C	3.795164	-4.921912	0.35795
H	-2.05469	1.474282	1.391265
H	0.931946	-5.026982	-0.368213
H	-0.882009	-5.592184	1.103248
H	-2.775806	-4.187621	1.588804
H	2.037048	-2.09108	-4.831595
H	4.394052	-2.485519	-4.173398
H	4.942232	-3.123529	-1.829455
H	2.410739	-3.369017	0.930765
H	3.031967	-5.634919	0.005484
H	4.062858	-5.181699	1.3959
H	4.691672	-5.051954	-0.270833
H	-0.748196	-1.696033	-2.55271
H	-0.51605	-4.34617	-4.094668
H	-2.039834	-3.527281	-3.644737
H	-0.978098	-4.189959	-2.375847
H	0.126276	-0.660466	-4.68859
H	-1.493026	-1.399801	-4.81843
H	-0.076757	-2.243636	-5.492589
H	-6.005828	-0.646889	-0.756727
H	-2.71903	-2.310516	-1.549069
H	-4.433938	0.083065	-2.436383
H	-3.165569	-0.712171	-3.405516
H	-2.73557	0.157622	-1.901882
H	-4.800202	-3.679723	-1.733819
H	-4.331463	-2.962466	-3.304952
H	-5.679937	-2.26314	-2.370652
H	-3.699616	1.069912	0.863123
H	-3.457435	1.911	2.417133
H	-5.288938	-0.651867	3.497128
H	-6.77409	-0.138229	1.561747
H	-1.853273	-2.161558	3.145314
H	-4.390674	-2.387827	4.870535
H	-2.75888	-2.953401	5.324322
H	-3.633463	-3.723699	3.965727
H	-3.380959	0.053334	4.628145
H	-1.977544	0.28666	3.553669

H	-1.79422	-0.625123	5.084143
H	3.036541	2.881843	3.664732
H	5.304226	-2.571951	0.287437
H	4.564426	-2.73701	1.901254
H	4.001228	-1.461424	0.789598
H	1.250425	5.307459	1.922189
H	-0.33243	5.687957	-1.012351
H	-0.241673	6.380515	0.63531
H	-1.703749	5.50178	0.08603
H	-1.43642	2.849634	-4.475683
H	-3.884429	2.883127	-4.003397
H	-4.698307	3.056398	-1.667371
H	1.193895	3.108149	-1.771276
H	0.763914	0.778172	-2.56639
H	2.133723	1.530524	-3.437703
H	0.537232	1.396637	-4.228432
H	0.562243	3.977664	-4.65411
H	2.146684	4.064044	-3.838908
H	0.787838	5.078812	-3.269122
H	-2.54643	3.887261	1.203945
H	-5.383481	3.002531	0.425318
H	-4.786842	4.679815	0.264036
H	-4.876985	3.89975	1.87346
H	3.118863	4.588395	3.109368
H	4.051735	3.295392	2.280832
C	2.611843	0.847576	1.334521
C	3.925174	1.13385	0.623285
C	5.125263	0.976364	1.290641
C	5.17787	0.49892	2.625103
C	3.990018	0.145475	3.315756
C	2.743372	0.287442	2.736739
C	3.83857	1.629716	-0.808854
H	6.059911	1.194149	0.766785
H	6.144956	0.372998	3.116148
H	4.070654	-0.263679	4.325945
C	1.453762	-0.133677	3.417059
H	0.628312	0.394946	2.913086
C	1.210054	-1.65125	3.220133
C	1.414229	0.233428	4.91524
H	2.795193	1.520755	-1.131086
C	4.210816	3.128893	-0.907345
C	4.70443	0.777972	-1.762315
H	0.428907	-0.020931	5.337176

H	2.177379	-0.322594	5.484639
H	1.59011	1.310906	5.065842
H	0.261516	-1.950097	3.696189
H	1.167667	-1.888577	2.147545
H	2.028475	-2.234829	3.674583
H	4.109176	3.47456	-1.950335
H	3.551211	3.741386	-0.273801
H	5.254633	3.294674	-0.590903
H	4.591826	1.142585	-2.797509
H	5.772775	0.842213	-1.494503
H	4.394872	-0.276423	-1.729076
H	-3.030956	4.087809	1.586566
H	-4.279793	3.864591	0.335822
H	-3.773839	2.480752	1.348374
H	-1.282609	4.948173	0.083058
H	-0.830799	4.08964	-1.418595
H	-2.405088	4.928019	-1.303834

Table S26. Cartesian geometry of intermediate (- 58.1 kcal/mol) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	1.857343	2.670604	2.114105
C	2.52564	2.280653	0.9301
C	3.787038	1.634271	0.967921
C	4.354506	1.367082	2.225601
C	3.709055	1.74375	3.410659
C	2.473679	2.39905	3.347937
N	1.893473	2.506098	-0.341724
C	2.316084	3.548079	-1.092565
C	1.844888	3.766933	-2.391215
C	0.882082	2.916985	-3.027004
C	0.465428	3.253862	-4.461798
C	4.502009	1.178369	-0.300155
C	5.982521	1.621064	-0.333412
C	0.501348	3.363188	2.079441
C	0.571271	4.784583	2.680495
Ni	0.567359	1.262442	-0.800711
N	0.323161	1.882474	-2.467256
C	-2.351381	0.836362	-1.539283
Co	-0.398338	-1.055785	0.07375
O	-1.316627	0.405844	-0.783065
N	0.340713	-2.815034	-0.572514

C	-0.384556	-3.931709	-0.542181
C	-1.641803	-4.081773	0.077046
C	-2.231425	-3.155684	0.953089
N	-1.806021	-1.911972	1.187331
C	-2.482022	-1.136048	2.186839
C	-1.766157	-0.801119	3.371884
C	-2.410779	-0.001034	4.330333
C	-3.718122	0.462753	4.132157
C	-4.408117	0.117968	2.965656
C	-3.812441	-0.679962	1.970242
C	-0.367349	-1.368963	3.624923
C	0.45408	-0.592472	4.671864
C	-4.615142	-1.048517	0.722748
C	-5.400752	0.137711	0.124214
C	1.737817	-2.996125	-0.871481
C	2.232115	-2.819626	-2.184816
C	3.581796	-3.127066	-2.436371
C	4.428968	-3.573871	-1.416759
C	3.937483	-3.67693	-0.11066
C	2.597023	-3.379843	0.190393
C	1.36252	-2.295304	-3.319063
C	1.913896	-0.947195	-3.837532
C	2.126158	-3.441511	1.641031
C	2.249764	-4.870134	2.214904
C	-0.473224	-2.855753	4.044001
C	-5.609865	-2.198476	1.020378
C	2.90537	-2.418497	2.498909
C	1.250339	-3.32491	-4.465084
O	1.006796	-0.059064	0.486799
C	3.332014	4.516291	-0.508788
C	4.390242	-0.352928	-0.445866
C	-0.561847	2.50962	2.800147
H	3.339496	-0.670459	-0.45258
H	-3.093661	-3.503463	1.533385
H	-2.121558	-5.056385	-0.004846
H	0.065662	-4.83351	-0.982007
H	-1.88232	0.27005	5.244142
H	-4.196438	1.090496	4.887371
H	-5.427833	0.476361	2.814586
H	-3.907162	-1.385685	-0.044899
H	-5.114755	-3.096838	1.418487
H	-6.150048	-2.478381	0.100235
H	-6.350822	-1.867141	1.76683

H	0.195557	-1.322786	2.681738
H	-1.049361	-2.944145	4.980464
H	0.531595	-3.27395	4.213598
H	-0.969972	-3.459581	3.271192
H	0.530885	0.471318	4.411151
H	1.47258	-1.005231	4.712942
H	0.013683	-0.684161	5.679221
H	4.602822	-3.984345	0.698937
H	1.066539	-3.158758	1.680308
H	3.987861	-2.626055	2.470814
H	2.5752	-2.480596	3.547926
H	2.733894	-1.396383	2.132237
H	1.652768	-5.584756	1.625178
H	1.89341	-4.894809	3.257723
H	3.298735	-5.209601	2.203228
H	4.891441	-0.855886	0.396005
H	4.86786	-0.688347	-1.379322
H	3.966593	-3.009059	-3.451562
H	5.472603	-3.812942	-1.633113
H	0.355136	-2.114082	-2.925285
H	2.245308	-3.560537	-4.877219
H	0.630358	-2.923039	-5.282214
H	0.798658	-4.265895	-4.110106
H	2.932935	-1.074011	-4.240039
H	1.942119	-0.200706	-3.030473
H	1.270433	-0.555135	-4.641318
H	-0.291638	2.541309	-4.815748
H	-6.227263	0.444067	0.786769
H	-5.83511	-0.161719	-0.841779
H	-4.751437	1.00221	-0.051211
H	2.239489	4.618104	-2.947713
H	3.005199	4.867641	0.482164
H	3.466439	5.380242	-1.174566
H	4.305054	4.021543	-0.36696
H	1.968841	2.700529	4.268064
H	4.167113	1.52602	4.378091
H	5.314617	0.84983	2.272719
H	0.199167	3.466489	1.029874
H	-0.622556	1.506032	2.35717
H	-1.553337	2.979617	2.735982
H	-0.311318	2.397585	3.866693
H	0.862156	4.748512	3.743422
H	-0.41484	5.273781	2.612174

H	1.306932	5.408288	2.146386
H	4.002222	1.627295	-1.169553
H	6.562918	1.127868	0.463266
H	6.087808	2.710841	-0.20313
H	6.433711	1.340025	-1.299064
H	1.340415	3.219375	-5.132819
H	0.047465	4.27397	-4.501947
C	-2.850836	2.15553	-1.309012
C	-3.90684	2.621246	-2.106258
C	-4.494528	1.813778	-3.088832
C	-4.010393	0.514891	-3.285017
C	-2.936374	0.004077	-2.535764
C	-2.310499	3.041019	-0.191554
H	-4.287321	3.630687	-1.934416
H	-5.323036	2.191126	-3.692044
H	-4.460446	-0.119021	-4.052356
C	-2.399637	-1.381258	-2.871491
H	-1.599151	-1.636324	-2.163928
C	-3.47957	-2.482	-2.770322
C	-1.78414	-1.368897	-4.290183
H	-1.539537	2.476671	0.345182
C	-1.66512	4.329826	-0.746173
C	-3.419695	3.385055	0.831197
H	-1.383103	-2.362349	-4.543553
H	-2.551435	-1.105162	-5.036563
H	-0.971577	-0.630256	-4.351233
H	-3.035124	-3.463294	-3.002875
H	-3.913647	-2.533985	-1.76164
H	-4.295539	-2.297446	-3.488485

Table S27. Cartesian geometry of transition state (- 40.8 kcal/mol) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-2.943707	-0.043415	-2.5294
C	-2.353236	0.807455	-1.551744
C	-2.848968	2.132495	-1.346977
C	-3.905807	2.584408	-2.151028
C	-4.498539	1.758583	-3.115086
C	-4.018583	0.454668	-3.285891
O	-1.31724	0.389178	-0.790659
Co	-0.102634	-0.901585	-0.035904

O	0.946015	0.343581	0.663072
Ni	0.261927	1.694557	-0.479035
N	-0.012791	2.483142	-2.068221
C	0.284617	3.701375	-2.419294
C	-0.094854	4.139605	-3.836938
C	-2.305425	3.039332	-0.248125
C	-3.289139	3.116425	0.944139
C	-2.411688	-1.436256	-2.83966
C	-1.522249	-1.380805	-4.103815
C	0.926567	4.660975	-1.570267
C	1.337665	4.370649	-0.265383
C	2.004046	5.464312	0.553468
N	1.159387	3.150081	0.288626
C	1.728903	2.898961	1.584713
C	0.890543	2.917664	2.723444
C	1.460014	2.629279	3.975842
C	2.818181	2.31294	4.097106
C	3.631478	2.301462	2.956228
C	3.111953	2.602614	1.685524
C	-0.595552	3.234699	2.620017
C	-1.439673	2.03966	3.107018
C	4.020977	2.549738	0.461401
C	4.344056	1.083531	0.107843
C	5.321264	3.3618	0.657745
C	-0.959583	4.521788	3.393347
N	1.130104	-2.289388	-0.820944
C	2.541714	-2.054165	-0.983775
C	3.064055	-1.557294	-2.201081
C	4.460765	-1.457458	-2.336331
C	5.320838	-1.816146	-1.293072
C	4.782124	-2.244131	-0.074794
C	3.393339	-2.35882	0.109474
C	2.170956	-1.114602	-3.351727
C	2.437234	-1.948735	-4.624509
C	2.854243	-2.767911	1.477584
C	3.259808	-1.72567	2.544752
N	-1.302631	-2.255336	0.791292
C	-2.234679	-1.845412	1.801678
C	-1.724058	-1.522778	3.09174
C	-2.628474	-1.070007	4.067117
C	-3.994293	-0.931643	3.786298
C	-4.479031	-1.261237	2.516655
C	-3.6197	-1.719859	1.500005

C	-0.246196	-1.743775	3.423934
C	0.022858	-3.253616	3.637119
C	-4.201524	-2.090929	0.136223
C	-4.872749	-3.486678	0.17844
C	0.734148	-3.545266	-1.019619
C	-0.477295	-4.108462	-0.569836
C	-1.357594	-3.513935	0.349033
C	0.256704	-0.950151	4.645061
C	-5.230036	-1.068217	-0.392041
C	2.362747	0.394447	-3.628548
C	3.324245	-4.186467	1.86782
C	-2.186792	4.503928	-0.723431
C	-3.537497	-2.467755	-3.077135
H	3.42402	0.509692	-0.063181
H	-2.133816	-4.157851	0.778257
H	-0.668351	-5.148365	-0.832431
H	1.442358	-4.220406	-1.52175
H	-2.260519	-0.814254	5.060654
H	-4.677713	-0.569537	4.557737
H	-5.543935	-1.157981	2.300897
H	-3.375262	-2.119519	-0.58539
H	-4.186334	-4.279181	0.512393
H	-5.251495	-3.754031	-0.822548
H	-5.72686	-3.468834	0.875818
H	0.350705	-1.412415	2.562298
H	-0.572863	-3.627372	4.486948
H	1.088626	-3.42043	3.860082
H	-0.236751	-3.840963	2.74478
H	0.063036	0.124518	4.531198
H	1.343011	-1.089107	4.745495
H	-0.21463	-1.303043	5.578103
H	5.445251	-2.487387	0.758128
H	1.757665	-2.781181	1.435624
H	4.356961	-1.637484	2.609979
H	2.88501	-2.036289	3.532905
H	2.841587	-0.738936	2.299895
H	2.990317	-4.930592	1.126385
H	2.915402	-4.466935	2.852342
H	4.424241	-4.23383	1.927923
H	4.895741	0.602805	0.930954
H	4.967095	1.032977	-0.798501
H	4.872037	-1.089369	-3.278698
H	6.402961	-1.736566	-1.419459

H	1.126067	-1.269495	-3.057089
H	3.484502	-1.839141	-4.951112
H	1.787815	-1.610167	-5.447638
H	2.248325	-3.019876	-4.44423
H	3.406658	0.606236	-3.915005
H	2.111385	0.990355	-2.738927
H	1.705737	0.718315	-4.45157
H	-0.598883	3.320478	-4.367281
H	-6.154778	-1.085709	0.20854
H	-5.496079	-1.320456	-1.429896
H	-4.825254	-0.050283	-0.385591
H	1.11552	5.66166	-1.961256
H	1.519367	5.559727	1.537449
H	1.948452	6.426962	0.026179
H	3.061512	5.221584	0.740696
H	0.822479	2.646244	4.862276
H	3.241877	2.075757	5.075615
H	4.689653	2.049476	3.048004
H	-0.832969	3.409506	1.563206
H	-1.19136	1.130445	2.542222
H	-2.513504	2.242024	2.988424
H	-1.25093	1.841267	4.173658
H	-0.754513	4.405157	4.470437
H	-2.032631	4.746187	3.27181
H	-0.379818	5.385146	3.027236
H	3.486932	2.982762	-0.395604
H	5.952236	2.918289	1.445223
H	5.112815	4.407117	0.940107
H	5.904768	3.362788	-0.27752
H	0.805742	4.438434	-4.399822
H	-0.770878	5.010285	-3.792026
H	-4.283304	3.598112	-1.999022
H	-5.327988	2.125639	-3.723365
H	-4.473092	-0.193729	-4.038345
H	-1.84378	-1.803465	-1.974191
H	-1.124568	2.50188	-0.299354
H	-1.117492	-2.378664	-4.33278
H	-2.111552	-1.039508	-4.97074
H	-0.685855	-0.682355	-3.955179
H	-3.099314	-3.459169	-3.276452
H	-4.198581	-2.55612	-2.203279
H	-4.151561	-2.184087	-3.947875
H	-2.920353	3.838318	1.691359

H	-4.285549	3.452885	0.613832
H	-3.395313	2.135714	1.431718
H	-1.791434	5.134783	0.090193
H	-1.511485	4.579918	-1.586062
H	-3.173721	4.901599	-1.013565

Table S28. Cartesian geometry of intermediate (- 61.3 kcal/mol) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	3.707755	-2.372204	0.345108
C	2.620732	-2.734041	-0.493785
C	2.814833	-2.986919	-1.874034
C	4.120893	-2.91274	-2.39008
C	5.211882	-2.607425	-1.566781
C	4.997943	-2.33247	-0.212315
N	1.317143	-2.845009	0.106595
C	1.140662	-3.952547	0.842603
C	0.180576	-4.14572	1.848619
C	-0.644658	-3.147509	2.396467
N	-0.819383	-1.914313	1.914015
C	-1.565792	-1.001434	2.734832
C	-0.84796	-0.100034	3.569932
C	-1.590016	0.788511	4.369629
C	-2.991211	0.784405	4.3532
C	-3.676793	-0.104073	3.517405
C	-2.985015	-1.000076	2.681191
C	0.68171	-0.130841	3.633046
C	1.170924	-1.259204	4.573866
C	-3.744299	-1.924321	1.728519
C	-4.042939	-3.303287	2.365861
C	1.636381	-3.275744	-2.796068
C	1.928071	-4.37128	-3.84367
C	3.518102	-1.980357	1.81011
C	3.939243	-0.51151	2.037153
Co	0.094857	-1.296011	0.273998
O	0.927161	0.300386	-0.0643
Ni	-0.347886	1.30088	-0.95851
O	-1.369598	-0.363927	-0.91898
C	-2.602644	-0.575999	-1.432754
C	-3.575465	0.472811	-1.447973
C	-4.85922	0.200375	-1.947968
C	-5.205838	-1.076363	-2.410382

C	-4.238391	-2.087757	-2.41349
C	-2.926006	-1.856776	-1.967239
C	-3.184737	1.854045	-0.91836
C	-4.295563	2.927835	-1.056827
C	-1.874938	-2.953783	-2.073558
C	-2.026056	-4.015807	-0.963931
N	0.725967	2.866229	-1.165718
C	0.539991	3.693374	-2.206225
C	1.571948	4.77473	-2.485417
C	1.719684	3.111709	-0.169651
C	1.30543	3.759806	1.025719
C	2.261236	3.959424	2.03542
C	3.579934	3.510555	1.881167
C	3.96891	2.88766	0.689333
C	3.058038	2.688519	-0.363264
C	-0.11205	4.311377	1.178044
C	-0.754042	4.00626	2.546624
C	3.537734	2.058489	-1.667094
C	3.923195	0.579605	-1.471435
C	-0.575671	3.603068	-3.057188
C	-1.792326	2.962649	-2.718075
N	-1.90069	2.267849	-1.583532
C	-2.936025	3.125765	-3.714369
C	4.740574	2.83571	-2.256743
C	-0.110127	5.835294	0.906042
C	-2.904004	1.79232	0.612682
C	-1.883646	-3.631834	-3.46115
C	1.315663	1.204721	4.067935
C	-5.070305	-1.324569	1.21479
C	1.198851	-1.962888	-3.488211
C	4.280653	-2.934791	2.755087
H	-2.156724	1.039343	0.888138
H	-3.829847	1.529296	1.141254
H	-2.567932	2.777294	0.964887
H	-0.895851	-2.475989	-1.949211
H	-1.891009	-3.576367	0.031668
H	-1.268884	-4.80757	-1.086137
H	-3.026605	-4.478687	-1.008458
H	3.070785	0.005014	-1.092173
H	-1.159637	-3.390937	3.334571
H	0.175421	-5.115468	2.345392
H	1.866088	-4.764462	0.691032
H	-1.065862	1.492055	5.016926

H	-3.546561	1.481413	4.985133
H	-4.767363	-0.088439	3.495247
H	-3.100731	-2.085605	0.853359
H	-3.127496	-3.84252	2.643677
H	-4.604918	-3.929767	1.652949
H	-4.65811	-3.175418	3.272584
H	1.054294	-0.349206	2.621206
H	0.795604	-1.087825	5.597054
H	2.272887	-1.267912	4.605704
H	0.832267	-2.249774	4.240325
H	0.97135	2.037102	3.442481
H	2.408245	1.140584	3.964712
H	1.090881	1.433308	5.123761
H	5.840713	-2.064981	0.429117
H	2.453172	-2.051717	2.063111
H	4.9961	-0.356922	1.763012
H	3.822944	-0.250599	3.101034
H	3.321038	0.170453	1.436896
H	3.935725	-3.973646	2.627264
H	4.117961	-2.639451	3.804934
H	5.364685	-2.906642	2.554975
H	-2.803908	-4.219005	-3.614576
H	-1.028553	-4.320999	-3.541961
H	-1.814141	-2.887594	-4.269642
H	4.749671	0.488671	-0.750449
H	4.257758	0.14116	-2.424798
H	4.285341	-3.108232	-3.451142
H	6.220478	-2.567367	-1.984506
H	0.80227	-3.628629	-2.17441
H	2.683042	-4.040247	-4.575266
H	1.008223	-4.606548	-4.402678
H	2.295138	-5.293009	-3.364347
H	2.032216	-1.557418	-4.08615
H	0.91282	-1.205187	-2.741377
H	0.339733	-2.138867	-4.154096
H	-3.579757	2.23509	-3.713254
H	-5.090013	2.711579	-0.326701
H	-4.761418	2.971519	-2.045905
H	-4.495017	-3.078655	-2.794505
H	-6.217204	-1.27506	-2.770478
H	-5.614775	0.986461	-1.950272
H	-5.830604	-1.290849	2.013523
H	-5.459095	-1.952053	0.399558

H	-4.928909	-0.312032	0.815989
H	-0.561108	4.195244	-3.971174
H	1.85646	5.294363	-1.558629
H	1.176373	5.506055	-3.20345
H	2.488185	4.328329	-2.900654
H	1.96722	4.46544	2.956742
H	4.304278	3.654176	2.686095
H	4.998828	2.547551	0.566385
H	-0.742235	3.84254	0.410419
H	-0.856751	2.924081	2.709028
H	-1.761015	4.453946	2.59017
H	-0.166453	4.429215	3.377707
H	0.530027	6.357357	1.636934
H	-1.132729	6.241101	0.98864
H	0.270645	6.057266	-0.103125
H	2.71147	2.09588	-2.391552
H	5.615038	2.755687	-1.590662
H	4.522397	3.907154	-2.391355
H	5.022051	2.406464	-3.232418
H	-2.512377	3.258437	-4.720977
H	-3.555843	4.009151	-3.494643
H	-3.866139	3.912932	-0.819898
H	0.528767	0.653371	-1.899616

Table S29. Cartesian geometry of transition state (- 59.2 kcal/mol) in Figure S19B in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	1.495305	3.607691	1.201784
C	1.871829	3.019159	-0.036122
C	3.185959	2.534612	-0.259109
C	4.105248	2.613639	0.801692
C	3.751114	3.177802	2.033682
C	2.459369	3.68671	2.22074
N	0.865545	2.89727	-1.041667
C	0.730875	3.800529	-2.026415
C	-0.365887	3.809584	-2.90489
C	-1.61292	3.186536	-2.649346
C	-2.712747	3.443576	-3.676001
C	3.627492	1.947433	-1.594354
C	4.88283	2.669249	-2.145299
C	0.108898	4.213442	1.415167

C	0.194775	5.758453	1.392469
Ni	-0.275467	1.371415	-0.930411
N	-1.780742	2.42421	-1.566906
C	-3.094962	2.047166	-0.943288
C	-2.850047	1.950004	0.595191
Co	0.078476	-1.244201	0.250933
O	-1.38695	-0.248171	-0.907424
C	-2.613168	-0.414135	-1.448039
C	-3.527605	0.689989	-1.505633
C	-4.803719	0.491148	-2.056409
C	-5.210995	-0.766962	-2.520076
C	-4.316087	-1.839017	-2.449422
C	-3.013127	-1.6908	-1.942024
C	-2.078366	-2.89583	-1.976498
C	-1.850006	-3.35741	-3.435165
N	1.200378	-2.849158	-0.042387
C	0.89339	-4.010739	0.553996
C	-0.131753	-4.228089	1.490393
C	-0.894688	-3.231469	2.128793
N	-0.94851	-1.942179	1.789665
C	-1.650185	-1.049499	2.669539
C	-0.890551	-0.247906	3.568498
C	-1.586987	0.635951	4.413
C	-2.984472	0.730375	4.376497
C	-3.712283	-0.061979	3.482429
C	-3.067044	-0.954962	2.606602
C	0.632219	-0.385537	3.655924
C	1.346045	0.862607	4.211301
C	-3.880125	-1.788506	1.617492
C	-5.129033	-1.06249	1.074905
C	2.526797	-2.787474	-0.597416
C	2.743574	-2.930063	-1.989817
C	4.067351	-2.931811	-2.464376
C	5.153382	-2.790563	-1.592004
C	4.918718	-2.600111	-0.226161
C	3.612287	-2.580249	0.293667
C	1.580692	-2.998564	-2.970286
C	1.394862	-1.613434	-3.634167
C	3.405612	-2.280998	1.776719
C	4.070761	-3.350947	2.670572
C	1.018651	-1.622509	4.503146
C	-4.325522	-3.139161	2.230866
C	3.921822	-0.864518	2.115763

C	1.745867	-4.101963	-4.036953
O	0.936043	0.310913	-0.030221
C	-4.161646	3.165408	-1.081409
C	-2.602187	-4.077781	-1.129447
C	1.798687	4.870156	-2.188964
C	3.914145	0.43837	-1.47013
C	-0.563943	3.727203	2.715298
H	-2.165546	1.140508	0.874257
H	-3.801682	1.754762	1.108935
H	-2.445754	2.904867	0.958822
H	-1.104534	-2.59677	-1.568116
H	-2.672757	-3.812084	-0.06694
H	-1.916184	-4.935908	-1.21776
H	-3.599469	-4.393294	-1.479638
H	3.025152	-0.094382	-1.113985
H	-1.462547	-3.536915	3.017659
H	-0.24368	-5.245235	1.866852
H	1.548992	-4.865916	0.33349
H	-1.029111	1.262966	5.109521
H	-3.502926	1.425857	5.041716
H	-4.800072	0.023377	3.448169
H	-3.229324	-1.997551	0.758782
H	-3.472208	-3.763453	2.530027
H	-4.922959	-3.705088	1.496223
H	-4.950806	-2.960744	3.12214
H	1.015181	-0.543828	2.63647
H	0.641257	-1.508103	5.533766
H	2.115799	-1.721164	4.543457
H	0.607186	-2.550904	4.082062
H	1.078508	1.763465	3.644558
H	2.434241	0.724843	4.131072
H	1.106378	1.024811	5.276149
H	5.759793	-2.449774	0.455534
H	2.329694	-2.293682	1.993412
H	4.995302	-0.769601	1.881331
H	3.789776	-0.666583	3.191587
H	3.3719	-0.100894	1.546371
H	3.659017	-4.351036	2.458191
H	3.89633	-3.119919	3.734753
H	5.159929	-3.384991	2.499923
H	-2.799259	-3.684124	-3.891233
H	-1.147152	-4.205134	-3.461667
H	-1.438309	-2.540809	-4.047643

H	4.734639	0.259571	-0.757419
H	4.217251	0.025524	-2.444854
H	4.24642	-3.045232	-3.535848
H	6.175465	-2.803985	-1.97936
H	0.670984	-3.219665	-2.399878
H	2.604331	-3.89851	-4.698024
H	0.843052	-4.151865	-4.666656
H	1.902017	-5.087033	-3.567156
H	2.30625	-1.32797	-4.186121
H	1.200687	-0.845683	-2.869048
H	0.549136	-1.631249	-4.341378
H	-3.391543	2.581326	-3.737868
H	-4.991327	2.950442	-0.390943
H	-4.585771	3.264935	-2.085266
H	-4.621993	-2.823725	-2.812502
H	-6.215653	-0.90625	-2.925932
H	-5.51144	1.320009	-2.095032
H	-5.901095	-0.955072	1.855816
H	-5.557263	-1.649436	0.248983
H	-4.878899	-0.069059	0.682607
H	-0.305158	4.462466	-3.775595
H	1.951277	5.404118	-1.237757
H	1.504588	5.591802	-2.963716
H	2.763059	4.419872	-2.463969
H	2.190079	4.147487	3.17403
H	4.482559	3.227805	2.844387
H	5.114872	2.223834	0.654333
H	-0.531337	3.905815	0.577266
H	-0.694861	2.635956	2.714931
H	-1.559541	4.190545	2.818636
H	0.029626	4.004851	3.602115
H	0.832759	6.122909	2.215277
H	-0.809429	6.19983	1.511696
H	0.622467	6.11887	0.442866
H	2.80823	2.077185	-2.316385
H	5.756212	2.468733	-1.502866
H	4.751682	3.762488	-2.195646
H	5.116661	2.295296	-3.155838
H	-2.246745	3.601458	-4.660436
H	-3.304195	4.342351	-3.438843
H	-3.70717	4.124886	-0.790611
H	0.282746	0.909765	-2.17113