Supporting information:

Reductive Cleavage of Azoarene as a Key Step in Nickel-Catalyzed Amidation of Esters with Nitroarenes

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Experimental details

Reaction profile of nitrobenzene

In a nitrogen filled glove box, the following were added to an oven dried Schlenk flask: Zn (653 mg, 9.99 mmol), Ni(DME)Cl_2 (41.9 mg, 0.19 mmol), 1,10-phenanthroline (33.6 mg, 0.19 mmol), naphthalene (64.1 mg, 0.500 mmol), 5.0 ml NMP, trimethylsilylchloride (553 mg, 5.09 mmol), methyl decanoate (461 mg, 2.47 mmol) and nitrobenzene (372 mg, 3.02 mmol). The sealed Schlenk flask was brought out of the glove box, where the stopper was replaced with a septum under a nitrogen flow. The Schlenk flask was then submerged in a 90^{0}C oil bath. Three aliquots were taken at the indicated times which were immediately quenched in 0^{0}C by diethyl ether. The aliquot samples were analysed with GC-MS. Quantification was done by comparing the integrals of the analytes to the integral of the internal standard (naphthalene) and averaging over the three measured aliquots for each time point.

Reaction profile of azoxybenzene

In a nitrogen filled glove box, the following were added to an oven dried Schlenk flask: Zn (250 mg, 3.82 mmol), Ni(DME)Cl_2 (40.2 mg, 0.18 mmol), 1,10-phenanthroline (33.5 mg, 0.19 mmol), naphthalene (64.0 mg, 0.499 mmol), azoxybenzene (248 mg, 1.25 mmol), 5.0 ml NMP, trimethylsilylchloride (154 mg, 1.42 mmol) and methyl decanoate (467 mg, 2.51 mmol). The sealed Schlenk flask was brought out of the glove box, where the stopper was replaced with a septum under a nitrogen flow. The Schlenk flask was then submerged in a 90^{0}C oil bath. Three aliquots were taken at the indicated times which were immediately quenched in 0^{0}C by diethyl ether. The aliquot samples were analysed with GC-MS. Quantification was done by comparing the integrals of the analytes to the integral of the internal standard (naphthalene) and averaging over the three measured aliquots for each time point.

General remarks of kinetic measurements

Concentration of methyl decanoate was measured with ATR-IR, using an IN350-T probe on a Brucker Vertex 80 spectrometer. Reactions were set up by mixing zinc (261 mg, 4 mmol), the appropriate amount of (DME)$NiCl_2$ and phenanthroline, 3.2 ml NMP and TMSCl (4.3 mg, 0.04 mmol) in an oven dried 2-neck Schlenk flask for 10-15 minutes in the glove box. During this time, the mixture turned from dark blue to black. Then, the appropriate amount of azoarene and (if required) $ZnCl_2$ were added. The Schlenk flask was taken out of the glove box and connected to a N_2 line. Under a nitrogen flow, a septum pierced with the infrared probe was installed to the main neck and a second septum was installed on the smaller neck (see Figure S1 for setup). The mixture was then submerged in a 90^{0}C oil bath. After stirring for 10-15 minutes at this temperature, the infrared background was measured and the periodic infrared monitoring was started. Within one minute of starting the monitoring, 0.80 ml of a NMP solution of methyldecanoate, which was prepared in the glove box, was added, after which the integral of the peak at 1742 cm^{-1} (see Figure 2 in the main text) was measured periodically. The integral was measured between 1716 and 1759 cm^{-1} with a baseline drawn from the average value between 610 and 628 cm^{-1} to the average value between 1777 and 1821 cm^{-1}. From the integral, the concentration of ester was obtained by multiplying by 0.254. This conversion factor was obtained by a calibration curve ranging from 0.12 to 0.48 M ester in NMP at 90^{0}C.

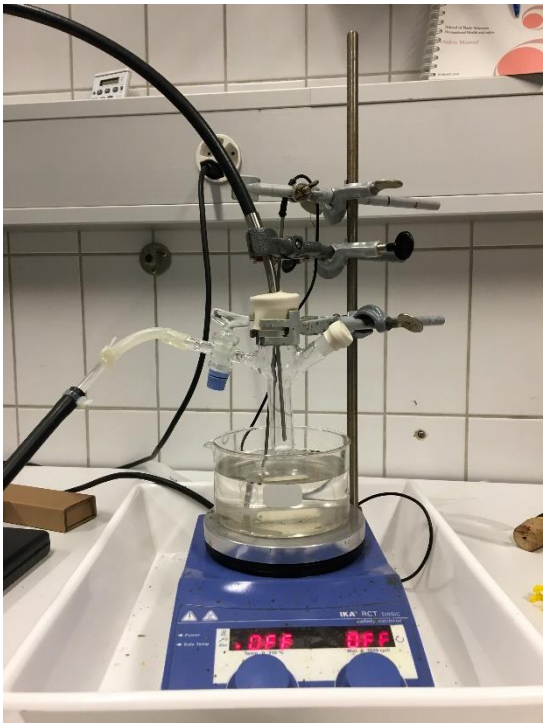


Figure S1. Picture of the setup used for kinetic measurements by IR. On the left side is the nitrogen line. The IR-probe connected to the Vortex 80 spectrometer is at the top and the septum through which the ester solution is added is at the right.

Reaction FTIR traces for [Ni]-dependance rate without additional $ZnCl_2$

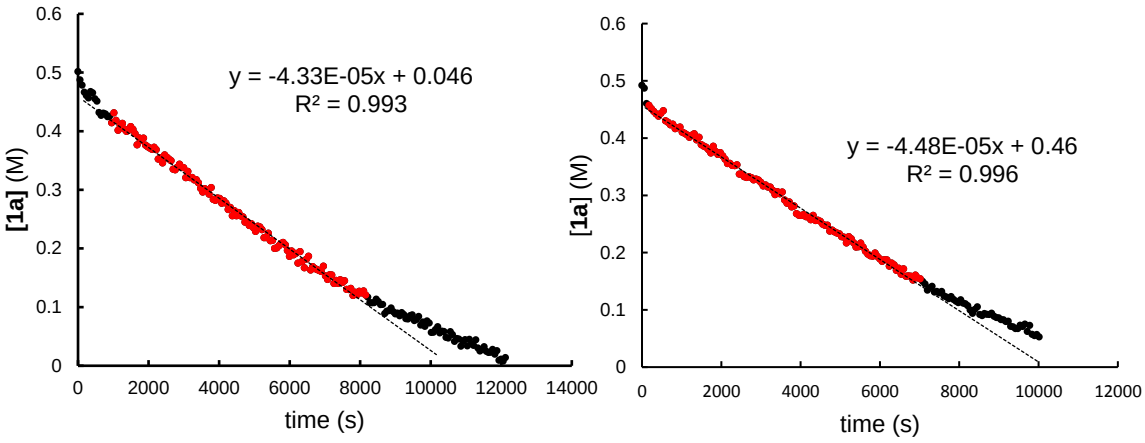


Figure S2. Reaction traces of FTIR-followed azobenzene-ester coupling with 0.037 M Ni-cat. Black points are the whole data set; the red points were used to obtain the slope, which was used as data point for Figure 3B in the main text.

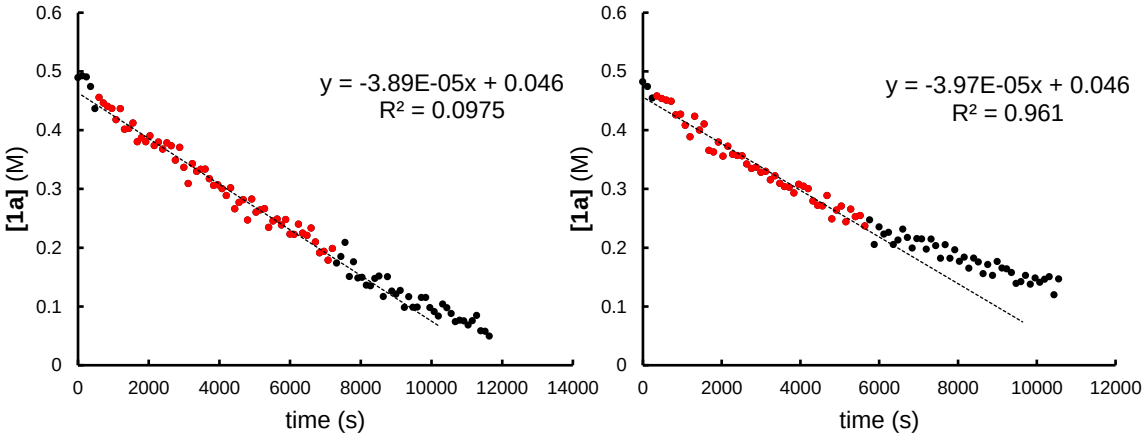


Figure S3. Reaction traces of FTIR-followed azobenzene-ester coupling with 0.035 M Ni cat. Black points are the whole data set; the red points were used to obtain the slope, which was used as data point for Figure 3B in the main text.

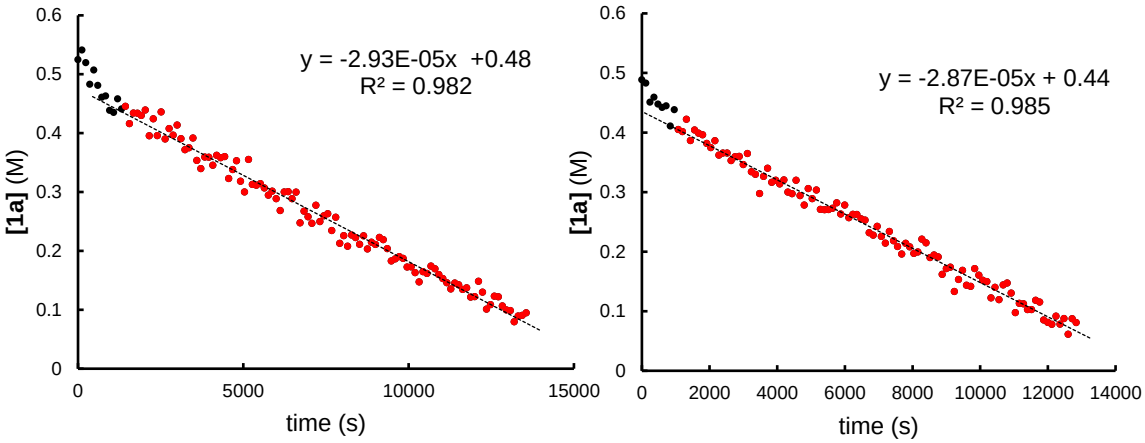


Figure S4. Reaction traces of FTIR-followed azobenzene-ester coupling with 0.029 M Ni cat. Black points are the whole data set; the red points were used to obtain the slope, which was used as data point for Figure 3B in the main text.

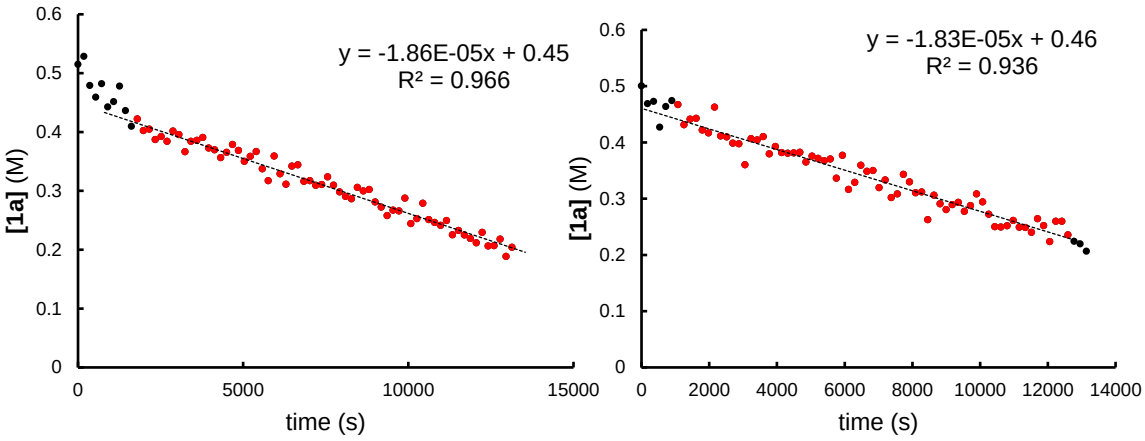


Figure S5. Reaction traces of FTIR-followed azobenzene-ester coupling with 0.025 M Ni cat. Black points are the whole data set; the red points were used to obtain the slope, which was used as data point for Figure 3B in the main text.

Stirring rate influence under conditions without additional $ZnCl_2$

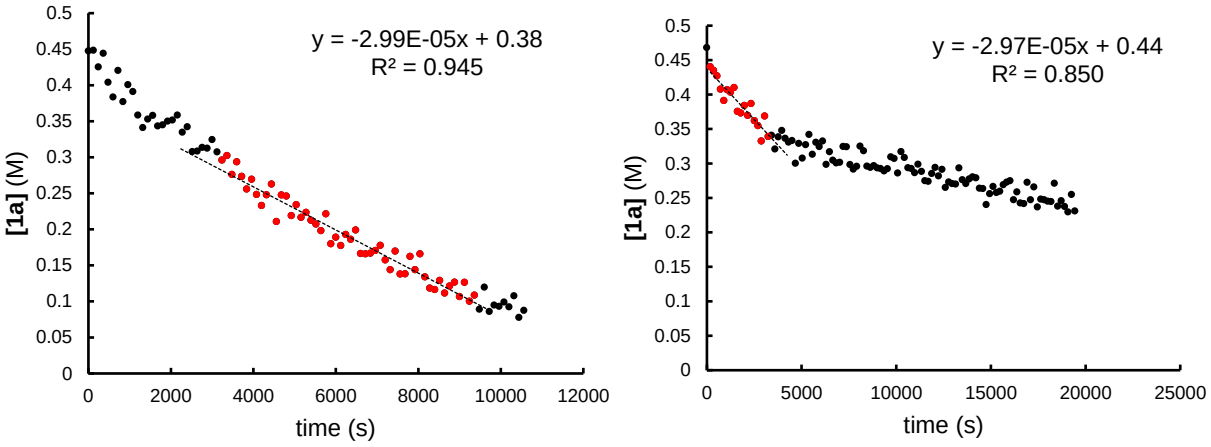


Figure S6. Reaction traces of FTIR-followed azobenzene-ester coupling under standard conditions, but at stirring rate of 350 rpm. For 500 rpm data, the reaction traces of Figure S2 were used. Note that the quality of fitting is not high; moreover, data reproducibility at the same stirring rate is not high. The data shown here are for indication purpose only. The conversion rate of ester at a stirring rate of 500 rpm was 4.41(8) 10^{-5} M s^{-1}, and it decreased to 2.98(1) 10^{-5} M s^{-1} at a stirring rate of 350 rpm. Nevertheless, all data show the dependence of the reaction in stirring rate is significant.

Competition between an aromatic ester and an aliphatic ester

A NMP stock solution was prepared in the glove box in a 1 ml volumetric flask of 1,2-bis(4-fluorophenyl)diazene (**2**^{F} 161 mg, 0.74 mmol), methyldecanoate (231 mg, 1.24 mmol) and methyl benzoate (165 mg, 1.21 mmol). Four (4) reaction mixtures were set up by adding Zn (0.5 mmol), Ni(DME)Cl_2 (0.019 mmol), 1,10-phenanthroline (0.019 mmol), 0.10 ml NMP and 2 µl trimethylsilylchloride to oven dried scintillation vials. After stirring for a few minutes, the mixtures turned black. $ZnCl_2$ (0.23 mmol) was then added to two of the vials. Finally, 0.40 ml of the stock solution was added to all four mixtures and they were set to stir on a 90^{0}C heating plate for 15 hours. After cooling down, 3 ml water and 3 ml ethyl acetate were added to each of the vials. After shaking the mixtures and settling of the resulting emulsion, 0.5 ml of the top layer was transferred to NMR tubes equipped with DMSO-d6 capilarries, to measure Fluorine NMR (figure S7).

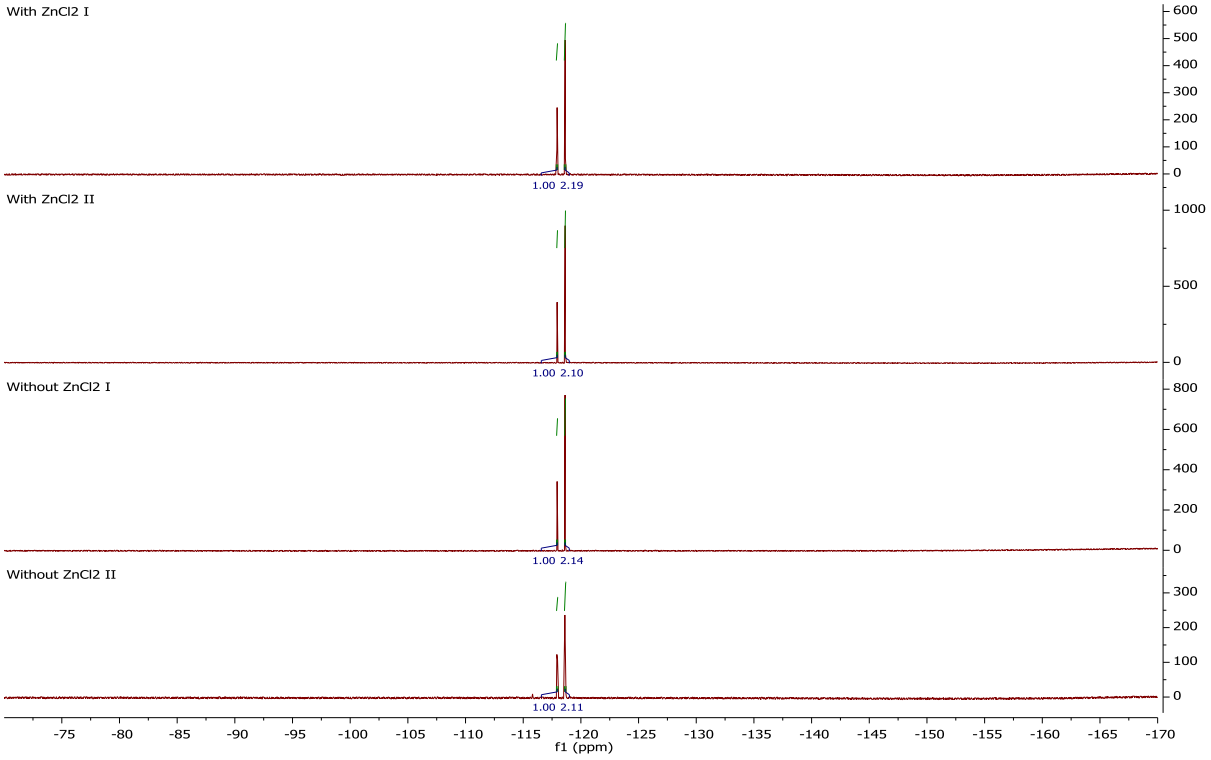


Figure S7. 19F NMR spectra of the crude reaction mixtures for competition methyl decanoate and methyl benzoate in reaction with **2**^{F}

Reaction rate Hammett study

The general procedure for infrared kinetic measurements was followed with 33.0 mg (DME)$NiCl_2$ (0.15 mmol), 27.0 mg phenanthroline (0.15 mmol), 1.2 mmol of the appropriate azoarene, 252 mg $ZnCl_2$ (1.85 mmol). The ester solution was made in a 1 ml volumetric flask with 466 mg methyl decanoate (2.5 mmol). From the resulting reaction trace based on [ester], a straight line was generated by multiplying the time values on the x-axis with [Ni] and with a Riemann sum approximation of the integral of [ester]. The slope of this straight line is taken as the rate constant, which was used for generation of the Hammett plot depicted in Figure 6A. The raw and processed reaction traces are depicted in Figures S8-13.

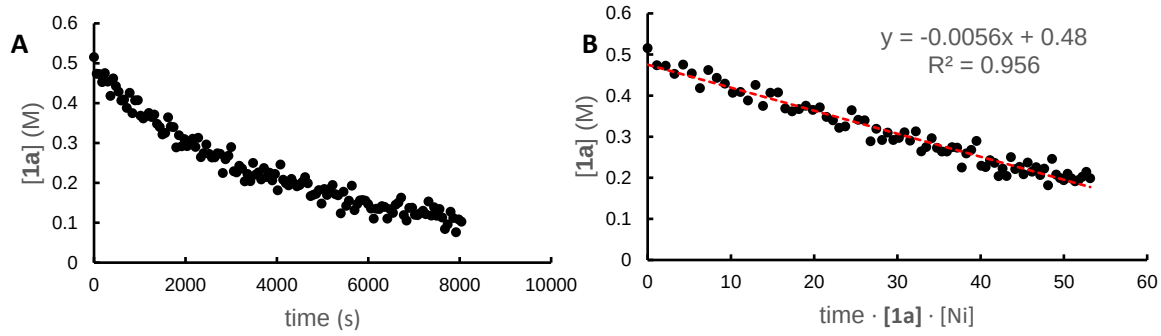


Figure S8. Raw (A) and processed (B) reaction trace for 1,2-bis(4-(dimethylamino)phenyl)diazene.

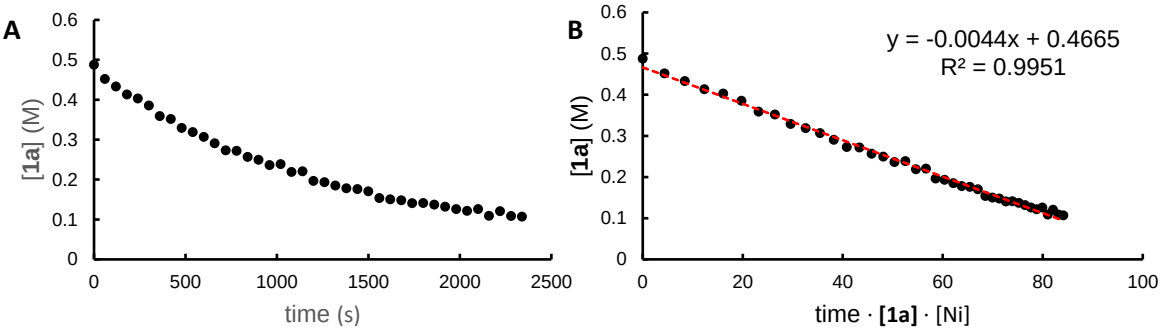


Figure S9. Raw (A) and processed (B) reaction trace for 1,2-bis(4-methoxyphenyl)diazene.

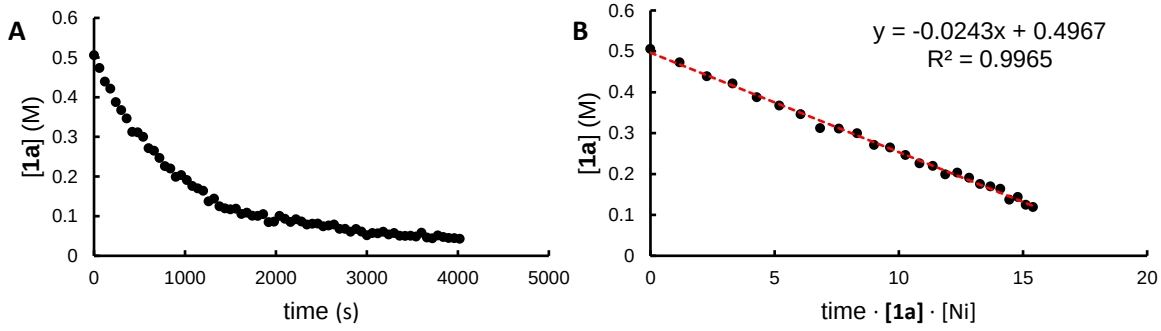


Figure S10. Raw (A) and processed (B) reaction trace for 1,2-bis(4-methyphenyl)diazene.

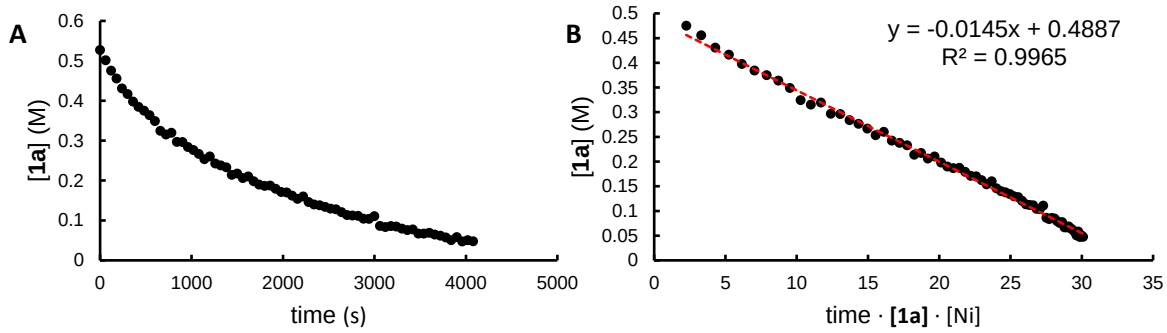


Figure S11. Raw (A) and processed (B) reaction trace for 1,2-bis(4-fluorophenyl)diazene.

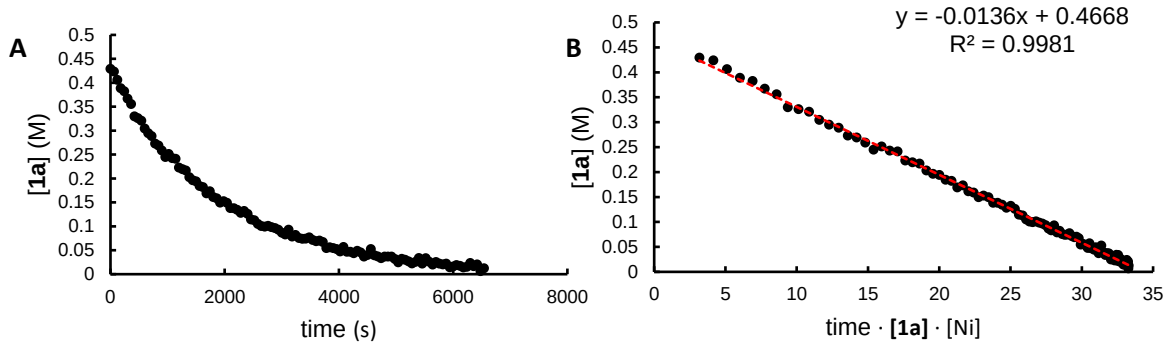


Figure S12. Raw (A) and processed (B) reaction trace for azobenzene.

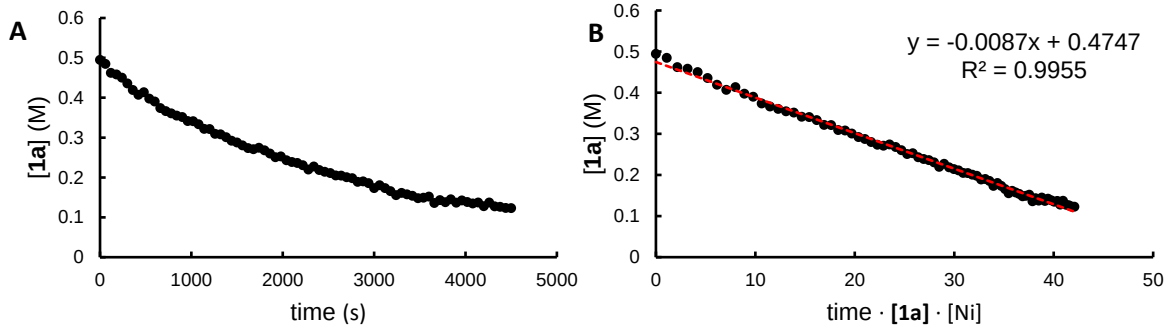


Figure S13. Raw (A) and processed (B) reaction trace for 1,2-bis(4-trifluoromethoxy)phenyl)diazene.

Competition Hammett study

A stock solution of azobenzene (150 mg, 0.823 mmol) and methyl decanoate (316 mg, 1.70 mmol) in NMP was prepared in a 2 ml volumetric flask. Zn (1 mmol), Ni(DME)Cl_2 (0.0375 mmol), 1,10-phenanthroline (0.0375 mmol), 0.40 ml NMP and 2 µl trimethylsilylchloride were added to 3 oven dried scintillation vials in the glove box. Stirred for a few minutes, which turned the mixtures from blue to black. Subsequently, $ZnCl_2$ (0.46 mmol), the appropriate substituted azoarene (0.25 mmol) and 0.60 ml of the azo/ester stock solution were added. The mixture was stirred on a 90^0C on a heating plate for 21 hours. After cooling down, 5 ml water and 5 ml ethyl acetate were added to each vial. The mixtures were shaken and after the emulsion settled down 1 ml of the top layer was added to an NMR tube for each vial. The volatiles were removed in vacuum and NMR was measured after redissolution in $CDCl_3$. The spectra were overlapped with spectra of the isolated amides to ascertain the correct peak intensities were compared. In cases where the crude mixture showed insufficient overlap with the spectra of isolated compounds to ascertain the peak identities, pure amide was added to the crude samples, identifying the grown peaks as the ones of interest.

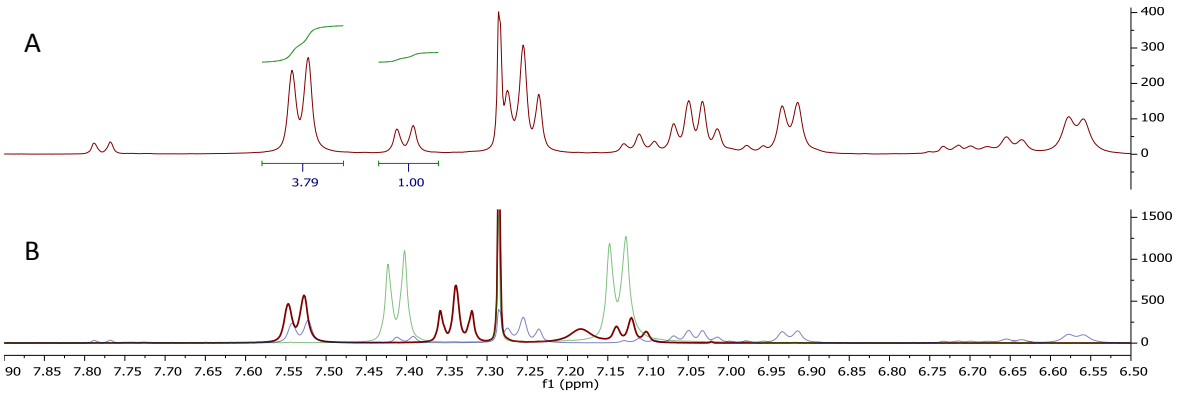


Figure S14. (A) Aromatic region from crude NMR of competition experiment between azobenzene and 1,2-bis(4-methylphenyl)diazene. (B) Overlap of crude NMR from competition (purple) with N-(p-toyl)decanamide (green) and N-phenyldecanamide (red), showing the integrals measured in A are representative of the two different product amides.

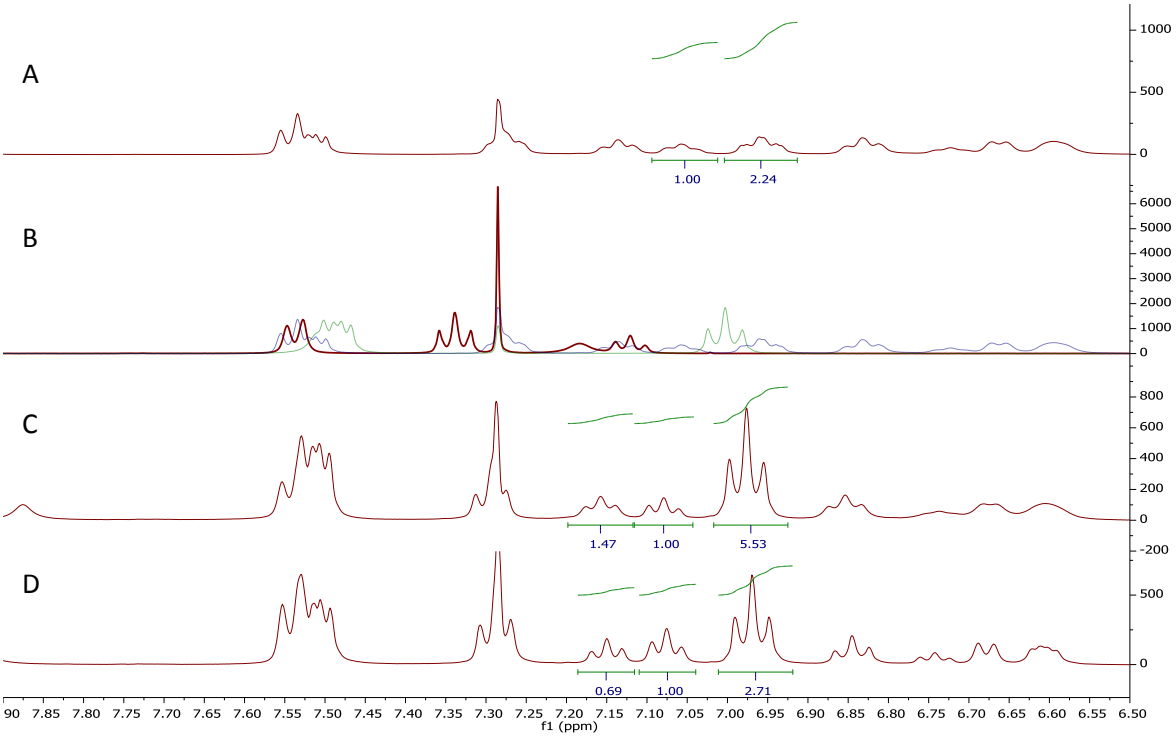


Figure S15. (A)Aromatic region from crude NMR of competition experiment between azobenzene and 1,2-bis(4-fluorophenyl)diazene. (B) Overlap of crude NMR from competition (purple) with N-(4-fluorophenyl)decanamide (green) and N-phenyldecanamide (red), showing it is ambiguous which integrals to measure in order to obtain the product ratio. (C) Crude NMR of competition experiment (A) with additional N-(4-fluorophenyl)decanamide, identifying one of the triplets as part of the added amide, since it has grown compared to the others. (D) Spectrum (C) with additional N-phenyldecanamide, identifying one of the triplets as part of the added amide, since it has grown compared to the others.

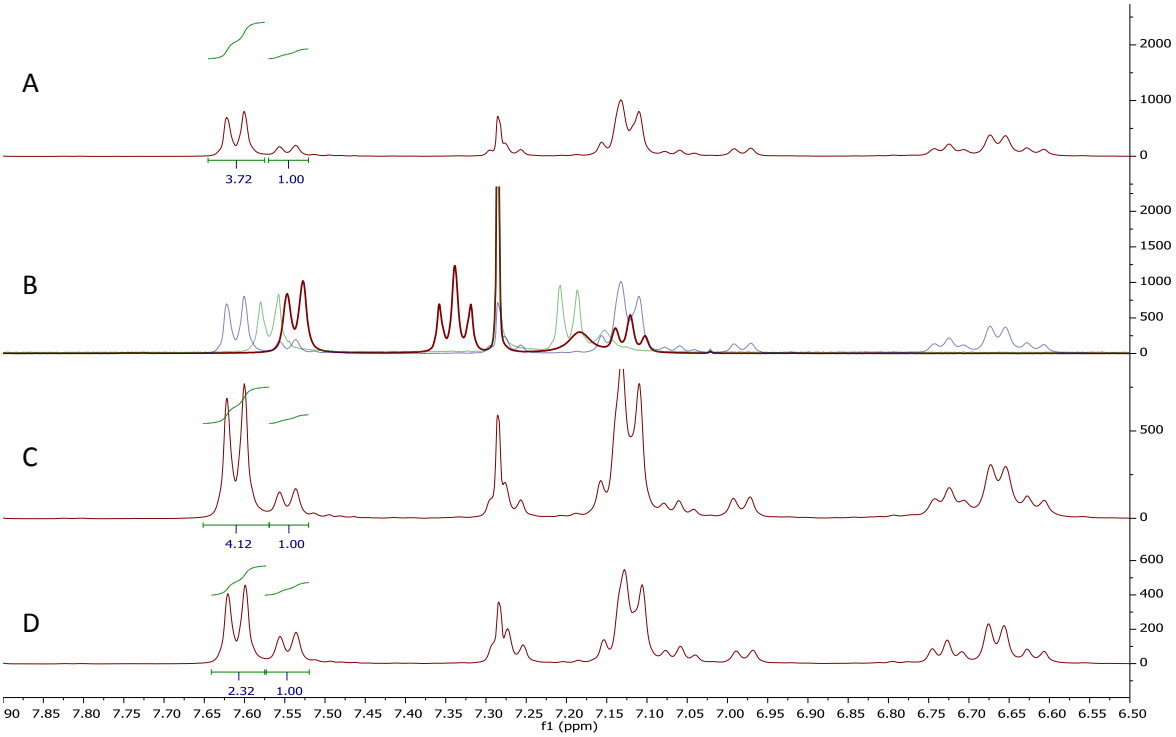


Figure S16. (A)Aromatic region from crude NMR of competition experiment between azobenzene and 1,2-bis(4-(trifluoromethoxy)phenyl)diazene. (B) Overlap of crude NMR from competition (purple) with N-(4-fluorophenyl)decanamide (green) and N-phenyldecanamide (red), showing the two most downfield doublets should belong to the two amide products, but leaving ambiguity regarding which peak belongs to which amide. (C) Crude NMR of competition experiment (A) with additional N-(4-(trifluoromethoxy)phenyl)decanamide, identifying the largest doublet as part of the added amide, since it has grown compared to the other. (D) Spectrum (C) with additional N-phenyldecanamide, confirming the other doublet as part of the added amide, since the ratio has now decreased again.

Synthesis of 3^F

105 mg (Bipy)Ni(0)(COD)[1] (0.325 mmol) was dissolved in 24 ml THF in the glove box. 74.8 mg 1,2-bis(4-fluorophenyl)diazene (**2^F**, 0.343 mmol) was added via a weighing boat and the purple colour of the solution quickly turned darker. After stirring for 4.5 hours, the mixture was filtered over Celite. After washing with copious THF, the filtrate was concentrated to about 10 ml. 50 ml Et_2O was added and the mixture was stirred for 10 minutes. A dark brown residue was then filtered off and washed with Et_2O before drying under vacuum. 94 mg, 67% yield. ^{1}H NMR (400 MHz, DMF-d_7, ppm) δ = 9.13 – 8.86 (m, 1H), 8.40 – 8.25 (m, 1H), 8.18 (td, *J* = 7.8, 1.5 Hz, 1H), 7.70 (ddd, *J* = 7.5, 5.3, 1.3 Hz, 1H), 7.61 (dd, *J* = 9.0, 5.3 Hz, 2H), 6.89 (t, *J* = 8.9 Hz, 2H).^{13}C NMR (101 MHz, DMF-d_7, ppm) δ = 157.29 (d, $J_{C,F}$ = 235.7 Hz), 156.89 (d, $J_{C,F}$ = 2.2 Hz), 154.69, 151.46, 138.51, 128.54, 123.18, 121.11 (d, $J_{C,F}$ = 7.3 Hz), 116.49 (d, $J_{C,F}$ = 21.9 Hz). ^{19}F NMR (376 MHz, NMP with DMSO-*d6* capillary for locking purposes, relative to internal standard fluorobenzene set to -114.51 ppm) δ = -127.06 ppm. The highly air sensitive nature of the compound precluded characterization by HRMS. Elemantal analysis: Calculated for $C_{22}H_{16}F_2N_4Ni$: C, 61.01; H, 3.72; N, 12.94. Found: C, 58.22-58.94; H, 3.64-3.65; N. 12.12-12.36. Note that despite multiple trials we could not obtain perfect elemental analysis. The C content was about 3% lower than expected. The discrepancy might be due to the decomposition of samples during handling as the compound is quite sensitive to air. According to NMR (see below), there are at most trace amounts of unidentified impurities. We think the samples are of sufficient purity for the stoichiometric model amidation reactions.

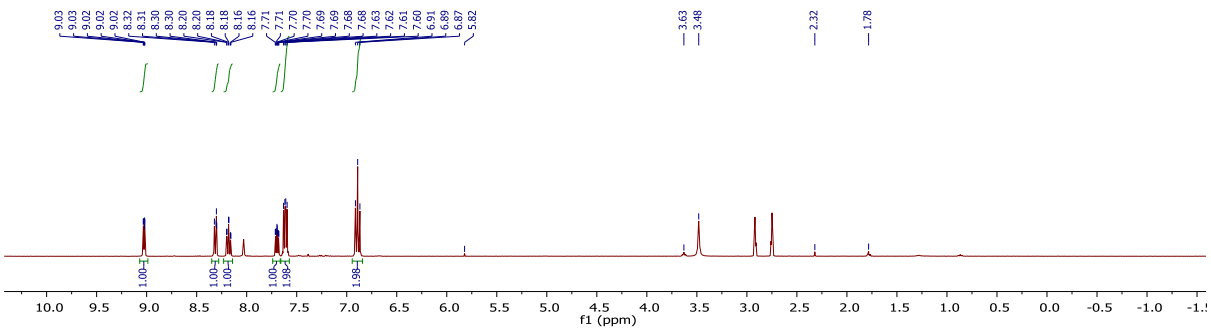


Figure S17. ^{1}H NMR spectrum of ^{3}F in DMF-d7. Residual peaks at 5.82 and 2.32 ppm belong to 1,5-cyclooctadiene (COD); peaks at 3.63 and 1.78 ppm belong to residual THF. Peak at 3.63 ppm belongs to trace water of the NMR solvent. The identity of the trace impurities observed between 7.0 and 7.5 ppm is unknown and their relative intensity varies between batches (although always small).

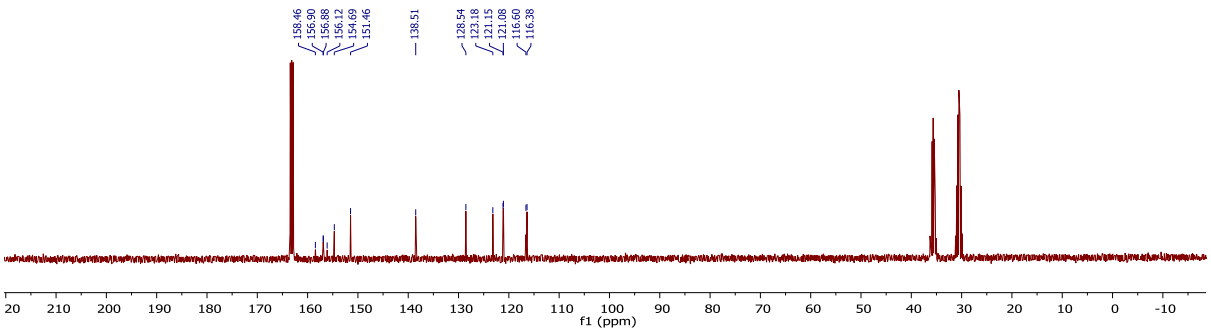


Figure S18. ^{13}C NMR of ^{3}F in DMF-d7.

Reactivity 3^F with ester 1c

10.2 mg **3^F** (0.0236 mmol), 33.6 mg $ZnCl_2$ (0.247 mmol) and 53 µl methyl decanoate (**1c**, 0.25 mmol) and 0.50 ml NMP were added to a scintillation vial in the glove box. The mixture was stirred for 2 hours on a 90^{0}C heating plate. After cooling down, the mixture was opened to air and 3.0 µl fluorobenzene (0.032 mmol), 0.5 ml $CDCl_3$ and 1 ml water were added. After shaking the mixture, the layers were separated by centrifugation. The bottom layer was then transferred to an NMR tube to measure ^{19}F NMR. Yields were determined by comparing the integrals to that of the fluorobenzene internal standard (figure S19).The experiment was performed twice with different batches of **3^F**, giving the same results.

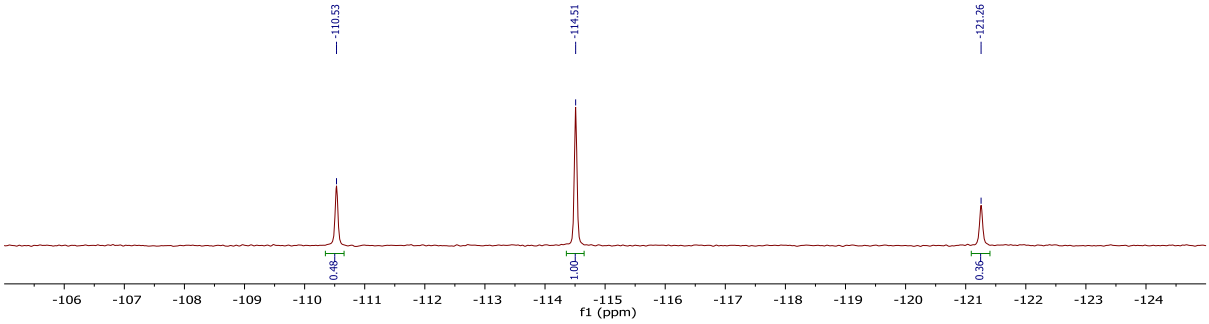


Figure S19. Partial 19F NMR spectrum of the extracted reaction mixture of reaction between 3F and 1c. Peak assignments: -110.53 ppm: 2F; -114.51 ppm: fluorobenzene; -121.26 ppm: N-4-fluorophenyldecanamide.

Computational details

Treatment of solid zinc

In order to calculate the free energy of the solid zinc we made use of the experimental value of the free energy of sublimation which we subtracted from the computed free energy of the zinc atom calculated in the gas phase. The calculation of these values was made at the temperature of 363 K in order to be consistent with the experimental conditions. The sublimation free energy was calculated based on the enthalpy end entropy values provided in NIST WebBook[2] with the following equations and values for gas and solid phase (Table S1).

Table S1. Values used for calculating the sublimation free energy of zinc. The value are from the NIST chemistry WebBook.[2]

Parameter	*Gas phase*	*Solid*
$H°_{298.15}$ (kJ mol^{-1})	130.42	0.00
T (K)	363	
$t = T / 1000$ (K)	0.363	
A	18.20166	25.60123
B	2.313999	−4.405292
C	−0.736547	20.42206
D	0.079950	−7.399697
E	1.073557	−0.045801
F	126.9388	−7.755964
G	184.6977	72.91373
H	130.4203	0.00000

Gas phase:

$\Delta H°_{363}$ = A*t + B*t^2/2 + C*t^3/3 + D*t^4/4 − E/t + F − H + $H°_{298.15}$ = 132.96673 kJ mol^{-1}

= 31.76983 kcal mol^{-1}

$S°_{363}$ = A*ln(t) + B*t + C*t^2/2 + D*t^3/3 − E/(2*t^2) + G = 0.16297 kJ mol^{-1} K^{-1} = 0.03894 kcal mol^{-1} K^{-1}

$\Delta G°_{363}$ = 73.79786 kJ mol^{-1} = 17.63390 kcal mol^{-1} = 0.028101 hartree

Solid phase:

$\Delta H°_{363}$ = A*t + B*t^2/2 + C*t^3/3 + D*t^4/4 − E/t + F − H + $H°_{298.15}$ = −2.38246 kJ mol^{-1}

= −0.56929 kcal mol^{-1}

$S°_{363}$ = A*ln(t) + B*t + C*t^2/2 + D*t^3/3 − E/(2*t^2) + G = 0.046773 kJ mol^{-1} K^{-1}

= 0.01118 kcal mol^{-1} K^{-1}

$\Delta G°_{363}$ = -19.36101 kJ mol^{-1} = -4.63629 kcal mol^{-1} = −0.007372 hartree

Once we obtained the experimental free energy values for the formation of zinc solid and gas the difference between these values provides the ΔG of sublimation:

$\Delta G°_{363}$ (s → g) = $\Delta G°_{363}$ (g) − $\Delta G°_{363}$ (s) = −0.007372 − 0.028101 = 0.035482 hartree

= 22.27 kcal mol^{-1}

This value can then be subtracted from the free energy value of a zinc atom in the gas phase to obtain the free energy for a zinc atom in solid phase.

Coupled cluster

In order to test the quality of the functional TPSSh-D3BJ used to calculate the energy of the complex involved in the reaction mechanism, we carried out some coupled cluster calculations for some steps of the reaction mechanism suggested in the main text. Specifically, we calculated the following relative electronic energies for a simplified model system with a smaller mimic **L'** of the phenanthroline ligand (see details below):

Step a: the energy difference between singlet and triplet for $NiCl_2$ complex **I**:

$$^3L'NiCl_2 \rightarrow {}^1L'NiCl_2$$

Step b: the reduction steps for the formation of **II**:

$$^3L'NiCl_2 + Zn + DMF \rightarrow {}^2L'NiCl + ½\ ZnCl_2(DMF)_2$$

Step c: the reduction steps for the formation of a model of III without explicit solvation at nickel:

$$^3L'NiCl_2 + Zn + \rightarrow {}^1L'Ni(0) + ZnCl_2(DMF)_2$$

Step d: the formation of the Ni-azo complex **V** starting from **III**:

$$^1L'Ni(0) + Azo \rightarrow {}^1L'Ni(Azo)$$

We used the CCSD(T) method[3] including scalar relativistic effects by using the scalar-relativistic Douglass-Kroll-Hess (DKH) Hamiltonian for one-electron integrals,[4] and the appropriate contracted correlation consistent basis set with correlated core electrons **BS2**. We performed single point calculations by taking the optimized structure for the model system obtained at the TPSSh-D3BJ/Def2SVP level of theory in gas phase. The model system is simplified and we also used the highest symmetry possible in order to reduce the computational costs. Therefore, the phenanthroline ligand has been substituted with (E)-N,N-(ethene-1,2-diyl)dimethanimine $(H_2CNCH)_2$ that in this section will be abbreviated with **L'**; the explicit solvent NMP has been replaced by DMF; the azobenzene is modelled with 1,2-dimethyldiazene abbreviated as **Azo**, and the zinc is calculated as an atom in the gas phase. We then compared CCSD(T) electronic energy results with single-point calculations obtained for the same model system with the same structures by using the functionals TPSSh-D3BJ,[5] B3LYP-D3BJ,[6,7] BP86-D3BJ,[6,8] MN15,[9] PBEPBE-D3BJ,[10] and M06L[11] using the same basis set and relativistic Hamiltonian as the *ab initio* calculations. The obtained results are reported in Table S2a/b/c.

Table S2a. Electronic energies obtained at the CCSD(T) and DFT level of theory. The empirical correction D3BJ is applied to all the functionals except for MN15 and M06L.

	PG	CCSD(T)	TPSSh	B3LYP	BP86
^{1}L'NiCl$_2$	C2v	−2707.533975	−2709.789465	−2709.823685	−2710.143168
^{3}L'NiCl$_2$	C2v	−2707.536065	−2709.792702	−2709.833032	−2710.128207
^{2}L'NiCl	C2v	−2246.333352	−2248.086224	−2248.122173	−2248.399725
^{1}L'Ni	C2v	−1785.045298	−1786.296179	−1786.322020	n.c.
^{1}L'NiAzo	C2	−1974.177667	−1975.839288	−1975.852831	−1976.124238
ZnCl$_2$(DMF)$_2$	C2v	−3214.118204	−3216.821503	−3216.899361	−3217.201395
Zn	/	−1795.245770	−1795.862525	−1795.94704	−1796.192508
DMF	/	−248.197918	−248.7363855	−248.7350377	−248.7308431
Azo	/	−189.002452	−189.435526	−189.431795	−189.430383
		CCSD(T)	MN15	PBEPBE	M06L
^{1}L'NiCl$_2$	C2v	−2707.533975	−2710.635077	−2708.837184	−2709.566801
^{3}L'NiCl$_2$	C2v	−2707.536065	−2710.615927	−2708.822480	−2709.573423
^{2}L'NiCl	C2v	−2246.333352	−2248.872372	−2247.330435	−2247.895154
^{1}L'Ni	C2v	−1785.045298	−1787.016496	n.c.	−1786.137756
^{1}L'NiAzo	C2	−1974.177667	−1976.326075	−1975.045326	−1975.621579
ZnCl$_2$(DMF)$_2$	C2v	−3214.118204	−3217.71202	−3215.56229	−3216.56221
Zn	/	−1795.245770	−1797.188362	−1795.64528	−1795.81139
DMF	/	−248.197918	−248.4579837	−248.419764	−248.667612
Azo	/	−189.002452	−189.206201	−189.185824	−189.378161

Table S2b. relative electronic energy in kcal mol^{-1} for the benchmark steps calculated with the electronic energy of Tab S1a.

	Δ*E* CCSD(T)	Δ*E* TPSSh	Δ*E* B3LYP	Δ*E* BP86	Δ*E* MN15	Δ*E* PBEPBE	Δ*E* M06L
Step a	1.31	2.03	5.87	−9.39	−12.02	−9.23	4.16
Step b	−22.33	−22.98	−18.99	−28.31	−37.83	−29.30	−18.53
Step c	8.89	6.47	18.05	/	−5.18	/	12.60
Step d	−81.52	−67.51	−62.13	/	−64.87	/	−66.30

Table S2c. electronic energy deviation in kcal mol^{-1} calculated in respect of the CCSD(T) level of theory from data of Tab. S2a. The color code is green < 3 kcal mol^{-1}; yellow < 5 kcal mol^{-1}; orange < 7 kcal mol^{-1}; red > 7 kcal mol^{-1}.

	Δ*E* CCSD(T)	Δ*E* TPSSh	Δ*E* B3LYP	Δ*E* BP86	Δ*E* MN15	Δ*E* PBEPBE	Δ*E* M06L
Step a	0.00	0.72	4.55	−10.70	−13.33	−10.54	2.84
Step b	0.00	−0.65	3.34	−5.98	−15.50	−6.97	3.80
Step c	0.00	−2.42	9.16	/	−14.07	/	3.70
Step d	0.00	14.01	19.39	/	16.65	/	15.22

From these benchmark results, we see first of all that the TPSSh, and M06L functionals account well for the energy differences in the spin-state change Step a and in the redox Steps b and c. B3LYP also

provides reasonably accurate results for steps a and b, while the error for Step c is somewhat larger. The GGA functionals BP86 and PBE are less accurate, as is the meta-hybrid MN15. For step a, this is a clear case of the known trend whereby GGA functionals underestimate the stability of the high-spin state.[12] The B3LYP functional appears to slightly *over*estimate the stability of the high-spin state. The best results are obtained with TPSSh-D3BJ and this motivates our use of this functional in the present study.

All the tested functionals yield less accurate energies for Step d, coordination of Azo with the Ni(0) species to create the **V**-like complex. This step is highly exothermic, showing the strong interaction between Ni(0) and Azo, confirming, as discussed in the main text, that this complex cannot be understood as involving only ligand to metal coordination. In fact, with the model used in the present benchmarking, this effect is very large, as shown by the change in the Ni-N distances (for N in the L' ligand) between the ^{1}L'Ni(0) and ^{1}L'NiAzo species (respectively 1.83 and 1.90 Å), or by the change in N-N bond length between the free Azo and the complex ^{1}L'NiAzo (respectively 1.24 and 1.37 Å). All of this denotes significant electronic donation from Ni to the Azo π* orbitals. Unfortunately, this seems to create significant multi-reference character in ^{1}L'NiAzo, which shows up in the CCSD(T) calculations by high values of the T_1 and D_1 diagnostics, of 0.051 and 0.34 respectively. It is frequently argued that values exceeding 0.02 or perhaps 0.05 in the case of T_1, and 0.15 in the case of D_1, correlate with poor performance of the CCSD(T) method.[12] Accordingly, we consider that the Step d CCSD(T) benchmark is perhaps not completely reliable, and further work would be needed to obtain a reliable reference. As such extensive benchmarking goes beyond the scope of this work, we have here simply assumed that the good performance of TPSSh-D3BJ for the other steps can be taken as evidence to support its accuracy for the whole reactivity study.

Spin state analysis for $NiCl_2$, Ni-dimer and NiZn-heterodimer

While CCSD(T) benchmarking of the type reported cannot be carried out for the larger species studied in the main text, it is nevertheless instructive to compare energies predicted by different DFT functionals.

In this section we are going to analyze the results of spin state multiplicity for the complexes $LNiCl_2$ **I**, Ni-dimer **VI**, and the Ni,Zn-heterodimer **VII**. The values shown will be electronic and free energy by using the functionals TPSSh-D3BJ, B3LYP-D3BJ and BP86-D3BJ with the basis set **BS2** and relativistic effect.

We started the analysis by calculating the complex $LNiCl_2$ without any explicit solvation to know which spin state corresponds to the ground state. Therefore, we calculated the complex with singlet and triplet multiplicity and the results are reported in Table S3. We found that the triplet spin state is more stable for the hybrid functional TPSSh and B3LYP. The opposite result has been obtained by using BP86 as expected from the previous benchmark with CCSD(T). Therefore, the complex $LNiCl_2$ can be associated to a triplet ground state.

Table S3a. Absolute and relative electronic energy for the complex **I** in the singlet and triplet state.

	Electronic energy (/ hartree)		
	TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
^{3}**I**	−3016.249737	−3016.277747	−3016.566464
^{1}I	−3016.240606	−3016.263346	−3016.575264
Δ_{1-3}	−0.009131	−0.014401	0.0088
Δ_{1-3} kcal mol^{-1}	−5.7	−9.0	5.5

Table S3b. Absolute and relative Gibbs free energy for the complex **I** in the singlet and triplet state.

	Gcorr (363K)	Gibbs free energy (/ hartree)		
		TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
^{3}I	0.124331	−3016.125406	−3016.153416	−3016.442133
^{1}I	0.128204	−3016.112402	−3016.135142	−3016.447060
Δ_{1-3}		−0.013004	−0.018274	0.004927
Δ_{1-3} kcal mol^{-1}		−8.2	−11.5	3.1

We now move on to the analysis of the Ni-dimer VI. This dimetallic Ni(II) species has 3 accessible multiplicities: singlet, triplet and quintet. The singlet can furthermore either correspond to an open-shell situation with antiparallel spins on the two nickel centres, or a closed-shell situation. All four options have been considered. In Table S4 we report the results for electronic and free energy.

Table S4a. Absolute and relative electronic energy for the Ni-dimer **VI** in the singlet, triplet, quintet and open-shell singlet states.

	Electronic energy (/ hartree)		
	TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
^{1}VI	−4758.956120	−4758.949685	−4759.475259
^{3}VI	−4758.948366	−4758.949167	−4759.455085
^{1open}VI	−4758.939921	−4758.939743	−4759.447670
^{5}VI	−4758.936649	−4758.932078	−4759.442074
Δ_{1-1}	0.000000	0.000000	0.000000
Δ_{1-3}	0.007754	0.000519	0.020174
$\Delta_{1-1open}$	0.016199	0.009943	0.027589
Δ_{1-5}	0.019471	0.017608	0.033185
Δ_{1-1} kcal mol^{-1}	0.0	0.0	0.0
Δ_{1-3} kcal mol^{-1}	4.9	0.3	12.7
$\Delta_{1-1open}$ kcal mol^{-1}	10.2	6.2	17.3
Δ_{1-5} kcal mol^{-1}	12.2	11.0	20.8

Table S4b. Absolute and relative Gibbs free energy for the Ni-dimer **VI** in the singlet, triplet, quintet and open-shell singlet states.

	Gcorr (363K)	Gibbs free energy (/ hartree)		
		TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
^{1}VI	0.461872	−4758.494248	−4758.487813	−4759.013387
^{3}VI	0.457954	−4758.490412	−4758.491213	−4758.997131
^{1open}VI	0.457354	−4758.482567	−4758.482389	−4758.990316
^{5}VI	0.454701	−4758.481948	−4758.477377	−4758.987373
Δ_{1-1}		0.000000	0.000000	0.000000
Δ_{1-3}		0.003836	−0.003399	0.016256
$\Delta_{1-1open}$		0.011681	0.005425	0.023071
Δ_{1-5}		0.012300	0.010437	0.026014
Δ_{1-1}		0.0	0.0	0.0

kcal mol^{-1}				
Δ_{1-3} kcal mol^{-1}		2.4	−2.1	10.2
$\Delta_{1-1open}$ kcal mol^{-1}		7.3	3.4	14.5
Δ_{1-5} kcal mol^{-1}		7.7	6.5	16.3

The closed shell singlet form turns out to be the most stable state of dimer **VI** for almost all functionals. The only exception is for the case of free energy differences calculated using B3LYP-D3BJ, which yields a difference of 2.1 kcal mol^{-1} in favor of the triplet. It should however be noted that even with B3LYP, the singlet is slightly more stable than the triplet in terms of the electronic energies. Therefore, assuming that TPSSh is the most accurate functional for the description of the nickel chemistry under study and that B3LYP overstabilizes the higher spin state, we are tempted to conclude that the singlet state is the ground state of species **VI.**

The last structure that will be analyzed in this section is the Ni,Zn-heterodimer **VII**. This complex contains one Ni(II) metal and one Zn(II) center, connected by an amido group and a chloride group. The ground state can therefore be either a singlet or a triplet with the unpaired electrons located on the Ni center. The results are reported in Table S5.

Table S5a. Absolute and relative electronic energy values for the Ni,Zn-heterodimer **VII** in the singlet and triplet state.

	Electronic energy (/ hartree)		
	TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
^{1}VII	−5425.081822	−5425.156945	−5425.715974
^{3}VII	−5425.087202	−5425.169775	−5425.713551
Δ_{3-1}	−0.005380	−0.012830	0.002423
Δ_{3-1} kcal mol^{-1}	−3.4	−8.1	1.5

Table S5b. Absolute and relative Gibbs free energy values for the Ni,Zn-heterodimer **VII** in the singlet and triplet state.

	Gcorr (363K)	Gibbs free energy (/ hartree)		
		TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
^{1}VII	0.339405	−5424.742417	−5424.817540	−5425.376569
^{3}VII	0.337065	−5424.750137	−5424.832710	−5425.376486
Δ_{3-1}		−0.007720	−0.015170	0.000083
Δ_{3-1} kcal mol^{-1}		−4.8	−9.5	0.1

It is clear that a triplet ground state is the preferred one for the dimer **VII** for both TPSSh and B3LYP. However, once again BP86 appears to underestimate the stability of the high spin state as for $LNiCl_2$ complex **I** previously discussed.

Solvation analysis for the complexes $NiCl_2$, NiCl and Ni(0)

In this section we are going to analyze the results of solvation analysis for the complexes $LNiCl_2$ **I**, LNiCl **II** and LNi(0) **III**. The values shown will be electronic and free energy by using the functionals TPSSh-D3BJ, B3LYP-D3BJ and BP86-D3BJ with the basis set **BS2**. We used NMP as explicit solvent in order to know the more stable geometry of the 3 complex under study. For the 3 Ni-complexes we calculated the bis-, mono-, and non- solvated structure and analyzed the final free energy value (Table S6). From these results we can notice the general agreement given by the 3 functionals used. The results allow us to conclude that the complexes $LNiCl_2$ **I** and LNiCl **II** most probably exist in solution without any additional solvent coordination to the nickel center, while the LNi(0) complex **III** appears to prefer bis-solvation. It is also reassuring that for such solvent coordination steps, which involve smaller changes in electronic structure at the metal center than do the redox or spin-state change steps, the different DFT functionals are in quite good agreement.

Table S6a. Absolute Gibbs free energy values for the complexes $LNiCl_2$ **I**, NiCl **II**, and the LNi(0) complex **III** coordinated with 0, 1 and 2 explicit NMP solvent(s).

	Gibbs free energy (/ hartree)		
	TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
NMP	−326.140182	−326.133708	−326.127637
^{3}LNiCl2_0NMP	−3016.125406	−3016.153416	−3016.442133
^{3}LNiCl2_1NMP	−3342.256971	−3342.278711	−3342.558282
^{3}LNiCl2_2NMP	−3668.390131	−3668.405895	−3668.67897
^{2}LNiCl_0NMP	−2554.404373	−2554.42773	−2554.698846
^{2}LNiCl_1NMP	−2880.535251	−2880.550328	−2880.819082
^{2}LNiCl_2NMP	−3206.651933	−3206.661496	−3206.914005
^{1}LNi_0NMP	−2092.598036	−2092.608365	−2092.874358
^{1}LNi_1NMP	−2418.764206	−2418.766379	−2419.030131
^{1}LNi_2NMP	−2744.904563	−2744.900806	−2745.152474

Table S6b. Absolute Gibbs free energy values for the complexes $LNiCl_2$ **I**, NiCl **II**, and the LNi(0) complex **III**. The appropriate number of solvents is already added to have an easier comparison of the Gibbs free energy values.

	Gibbs free energy (/ hartree)		
	TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
^{3}LNiCl2_0NMP	−3668.405771	−3668.420832	−3668.697408
^{3}LNiCl2_1NMP	−3668.397154	−3668.412419	−3668.685919
^{3}LNiCl2_2NMP	−3668.390131	−3668.405895	−3668.678970
^{2}LNiCl_0NMP	−3206.684738	−3206.695145	−3206.954121
^{2}LNiCl_1NMP	−3206.675433	−3206.684036	−3206.946720
^{2}LNiCl_2NMP	−3206.651933	−3206.661496	−3206.914005
^{1}LNi_0NMP	−2744.878401	−2744.875781	−2745.129633
^{1}LNi_1NMP	−2744.904389	−2744.900086	−2745.157768
^{1}LNi_2NMP	−2744.904563	−2744.900806	−2745.152474

Table S6c. Relative Gibbs free energy values for the complexes $LNiCl_2$ **I**, NiCl **II**, and the LNi(0) complex **III**. Showing ^{3}LNiCl2_0NMP, ^{2}LNiCl_0NMP, and ^{1}LNi_2NMP as more stable structures.

	Gibbs free energy (kcal mol^{-1})		
	TPSSh-D3BJ	B3LYP-D3BJ	BP86-D3BJ
^{3}LNiCl2_0NMP	0.0	0.0	0.0
^{3}LNiCl2_1NMP	5.4	5.3	7.2
^{3}LNiCl2_2NMP	9.8	9.4	11.6
^{2}LNiCl_0NMP	0.0	0.0	0.0
^{2}LNiCl_1NMP	5.8	7.0	4.6
^{2}LNiCl_2NMP	20.6	21.1	25.2
^{1}LNi_0NMP	16.4	15.7	14.3
^{1}LNi_1NMP	0.1	0.5	−3.3
^{1}LNi_2NMP	0.0	0.0	0.0

From these results we can notice the general agreement given by the 3 functionals used. The results allow us to conclude that the complexes $LNiCl_2$ **I** and LNiCl **II** most probably exist in solution without any additional solvent coordination to the nickel center, while the LNi(0) complex **III** appears to prefer bis-solvation.

Process of generation of the dicoordinated Ni-dimer **VI_2Zn**

We now switch to an extended version of the mechanistic discussion given in the main text, starting with further details concerning formation of the activated diimide species **VI_2Zn**.

We describe with more details some of the steps that lead to the formation of the bis-Zn(II)-coordinated Ni-dimer **VI_2Zn** that have been left out on the main text. Also we will focus on the electronic structures of complexes involved in these steps. We begin with the formation of the two bis-Zn(II)-coordinated Ni(0)-amido complexes **V_2Zn**, which was only briefly mentioned in the main text. The reaction mechanism we proposed resulting from calculations is shown in Figure 7 in the main text. In this mechanism, the complex **I** $LNiCl_2$ with a triplet ground state undergoes double reduction by solid Zn(0). The first reduction leads to the NiCl complex **II** with a doublet ground state lying 2.9 kcal mol^{-1} below **I**. Next, in a slightly exothermic process the coordination between the complex **II** and the azo-compound **2** generates the Ni(I) complex **IV**. This last complex is able to undergo the second reduction producing **V** with a closed shell singlet ground state. Next, as detailed in the main text, it can coordinate one or two $ZnCl_2$ to form **V_Zn** and **V_2Zn** respectively. However, to undergo N=N splitting (crossing TS1), **V_2Zn** needs to release one $ZnCl_2$, forming **V_Zn**. The splitting has been described in the main text but the description of the complicated electronic structure of **TS1** has been left out. Overall, it has a singlet ground state, with open-shell character. The two nickel centers have different environments. One is tightly associated with the N atoms of the azo molecule undergoing N−N bond splitting (color grey in Fig. 7). This nickel center adopts a near-closed shell singlet structure with spin density very close to 0. The other Ni center (colored in black in Fig. 7) is positioned between one of the N atoms of the azo molecule that is undergoing N–N bond splitting, that bridges the two Ni center, and the spectator second azo moiety. This second nickel center adopts an electronic structure best described as having doublet character, with spin density close to −1.0 (*i.e.* one excess spin-down electron). Since the overall multiplicity is a singlet, there is corresponding spin-up density, which is shared between 3 nitrogen atoms: 0.4 on the N of the azo molecule undergoing splitting that does not bridge with the second nickel center; 0.2 and 0.3 on the N atoms belonging to the pendant azo moiety. The product formed after crossing **TS1** is the intermediate complex **PreVI** that is predicted to be a closed shell singlet. Attempts to calculate an open-shell singlet resulted in the wavefunction collapsing to the closed shell solution.

The subsequent step coming from **PreVI** is the release of the azo moiety by crossing **TS2** that generates the NiNi-dimer **VI_2Zn**. The ground state of both **TS2** and **VI_2Zn** is found to be a closed shell singlet, in fact with the release of the azo-compound the previous non-innocent character of the complex is lost. The analysis of the possible spin state multiplicity for the Ni dimer has been previously described in a different section.

Alternative routes for nucleophilic attack

In the main text, we argued that nucleophilic addition to ester **1c** most likely occurs through the heterobimetallic species **VII_Zn.** In this section we discuss our computational results in which the nucleophile is instead a NiNi-dimer such as VI or VI_Zn. These routes are found to be more energy-demanding than the one proposed in the main text.

The transformation of 2 equivalents of **V** to **VI** is predicted to be somewhat uphill in free energy terms (by 7.0 kcal mol^{-1}, Fig. S20) in the absence of complexation with Zn(II) species. Species **VI** is considerably (33.3 kcal mol^{-1}) more stable than the monomeric amido complex **VII_split**, suggesting that the latter should not be observed under the reaction conditions. In the presence of Lewis-acid activation of the ester **1c** by $ZnCl_2$, the bridged dimer **VI** is able to carry out nucleophilic addition of the amido nitrogen to the carbonyl group, yielding a tetrahedral adduct **VIII** that can then re-arrange to the anionic amide complex **IX** in an overall exothermic step. Subsequent exchange of zinc for nickel yields the deprotonated amide product alongside dinickel monoamide **X** (Fig. 8 in the main text). Another nucleophilic addition of **X** to the ester will then generate another product-Zn complex and regenerate the catalyst.

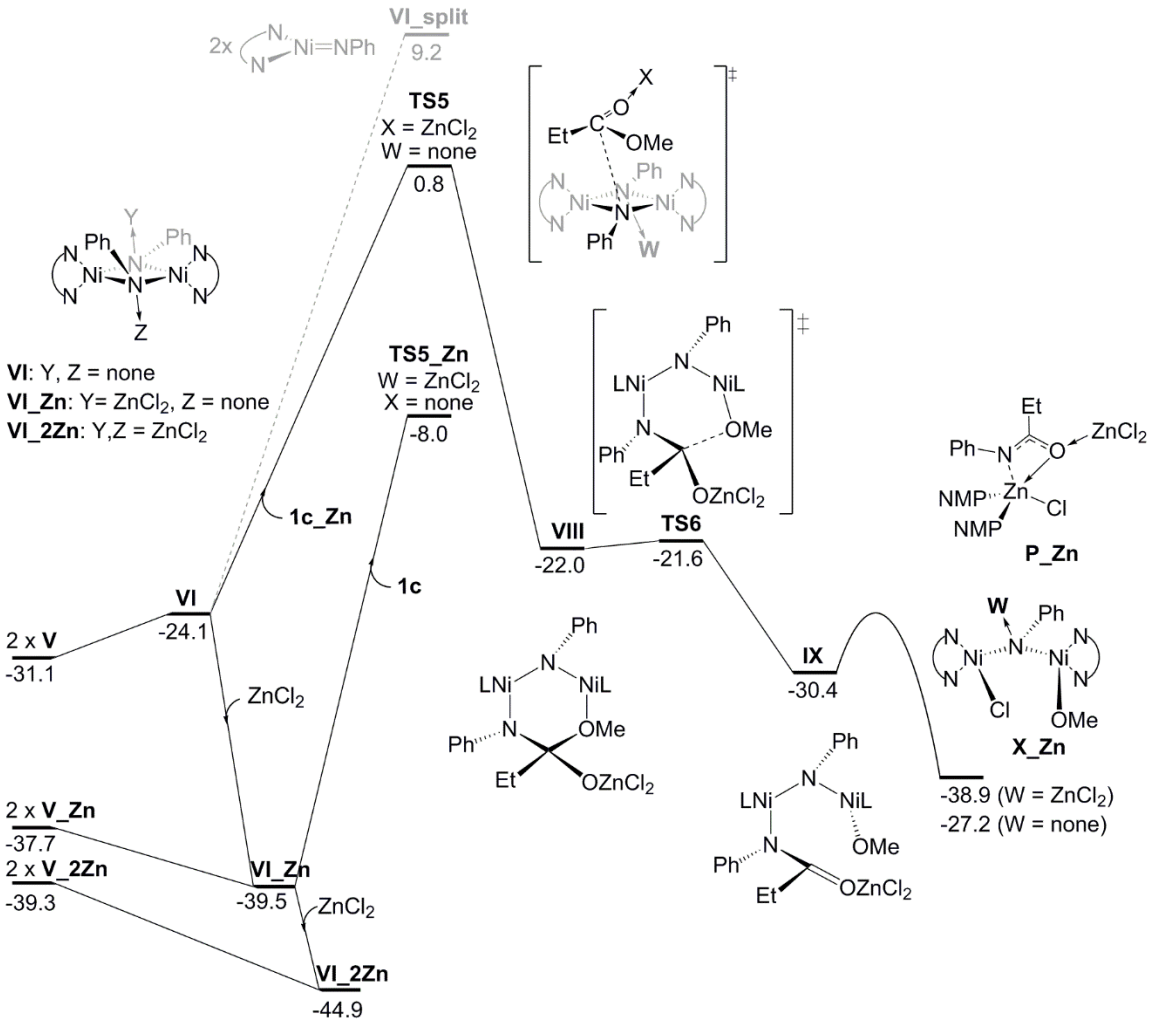


Figure S20. A possible reaction path of nucleophilic addition of nickel dimer to ester and subsequent product release; with relative free energy values at 363 K in kcal mol^{-1}.

A possible variant of this mechanism takes into account the fact that more complicated patterns of $ZnCl_2$ complexation are possible. In Figure S20, we have included $ZnCl_2$ complexation only for the ester in **TS5** and in the subsequent complexes formed. The computations however show that $ZnCl_2$ can complex exothermically with many of the species present in Figure S20, e.g. with the nickel-amido complexes **V** and **VI**. Variants of **TS5** with $ZnCl_2$ complexing to the amido nitrogen *not* involved in nucleophilic addition can also be found (**TS5_Zn**).

As shown in Figure S20, binding of two equivalents of $ZnCl_2$ to **V** to form **V_Zn** and **V_2Zn** is favorable in free energy terms. $ZnCl_2$ binds even more strongly to the dimer **VI**. As a consequence of the stronger binding energy to **VI,** conversion of two equivalents of **V_2Zn** into **VI_2Zn**, with cleavage of the N=N bond in one of the azo moieties, becomes favorable in free energy, by 5.6 kcal mol^{-1}, as was already discussed in the main text. The form of the nickel amide dimer bearing only one complexing $ZnCl_2$ metal, **VI_Zn**, can also behave also as a nucleophile towards the ester, following a similar process to that previously described for **VI**, through **TS5_Zn,** with an activation free energy of 31.5 kcal mol^{-1}.

These two alternative routes are more energetically demanding than the one proposed in the main text where the nucleophile reactant is the NiZn-dimer **VII**. For this reason, a direct involvement of a NiNI-dimer such as **VI** seems to be very unlikely.

Splitting of the Ni-dimer to generate a NiZn-heterodimer

As described in the main text, we argue that the key step with nucleophilic addition to the ester is carried out by the Ni,Zn-heterodimer **VII**. We also stated that this species can be formed from the homodimer **VI**, but gave few details on the proposed mechanism. In this section, we report the calculations we performed to get insight into the mechanism of the process leading to splitting of the Ni-dimer **VI_2Zn** into two equivalents of **VII**.

TS3 in which one of the four Ni-N bonds is being broken. **TS3** is overall a triplet state, with the nickel involved in the bond splitting adopting a triplet state and the other nickel keeping the singlet state. We note that reaching **TS3** from **VI_2Zn** requires a change in spin state. The detailed pathway involved in this spin-state change has not been studied, but we note that **VI** has a relatively low-lying triplet state (see Table S4 for the energetics), and in such cases spin-state change is generally facile.[13] The overall activation free energy barrier for this process is 13.4 kcal mol^{-1} leading to the mixed-spin complex **PreVII** that preserves the same spin state as **TS3**. This step is slightly endothermic with intermediate complex **PreVII** lying 7.2 kcal mol^{-1} higher in free energy than **VI_2Zn**.

In order to obtain two equivalents of the heterodimer **VII**, an additional Ni−N bond in **PreVII** needs to break, and an additional Cl—Ni interaction is formed. This splitting process is complex and *a priori* should involve a relatively small barrier above the energy of the two separated fragments **VII**, since only relatively simple coordination/decoordination steps are involved. Despite several attempts, no saddle-point could be found on the potential energy surface corresponding to a TS for this step. We explored not only the triplet potential energy surface corresponding to the ground state of **PreVII**, but also the quintet potential energy surface that corresponds to combination of the two triplets corresponding to **VII**, and the open-shell singlet potential energy surface that can also be accessed based on two triplet nickel moieties. We provisionally interpret this failure to find a TS as meaning that there may be no barrier above the endothermicity.

The two Ni,Zn-heterodimers **VII** that are formed through the barrierless process just described, are 24.1 kcal mol^{-1} higher in free energy compared with the Ni-dimer **VI_2Zn**. However, after coordination with one equivalent of $ZnCl_2$ each they are stabilized by 21.9 kcal mol^{-1}. As a result, the two equivalents of complex **VII_Zn** that are formed from **VI_2Zn** and two equivalents of $ZnCl_2$ lie rather close in free energy to **VI_2Zn**, lying just 2.2 kcal mol^{-1} higher in free energy compared to the Ni-dimer **VI_2Zn**.

An alternative route from **PreVII** plus two $ZnCl_2$ to form two **VII_Zn** would involve coordination of one $ZnCl_2$ to the nitrogen free lone pair of **PreVII**, followed by Ni—N bond breaking. Some preliminary exploration of this step was performed but again locating TSs was difficult and was not pursued further.

Overall, conversion of **VI_2Zn** and two equivalents of zinc chloride to form two equivalents of **VII_Zn** is slightly endothermic, so **VI_2Zn** should predominate under reaction conditions. A definitive estimate for the barrier of interconversion was not obtained, but it is likely that this barrier is low, so that the interconversion should also be reasonably rapid under the reaction conditions. Note that **VII_Zn** can only be formed in the presence of excess zinc chloride.

Qualitative kinetic analysis

(i) Pathway via **TS5**:

$$2 \times \mathbf{V} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathbf{VI} + \text{azo} \xrightarrow[k_2]{\text{ester}\cdot ZnCl_2} \mathbf{VIII}$$

This reaction may be analysed with the steady state approximation

Rate = k_2 [**VI**][ester·$ZnCl_2$] (1)

d[**VI**]/dt = k_1[**V**]^2 – k_{-1}[**VI**][azo] – k_2[**VI**][ester·$ZnCl_2$] = 0

$$[\mathbf{VI}]_{SS} = \frac{k_1[\boldsymbol{V}]^2}{k_{-1}[azo] + k_2[ester\cdot ZnCl_2]} \quad (2)$$

Insert (2) into (1):

$$\text{Rate} = \frac{k_1 k_2[\boldsymbol{V}]^2[ester\cdot ZnCl_2]}{k_{-1}[azo] + k_2[ester\cdot ZnCl_2]} \quad (3)$$

Equation (3) may simplify under two limiting conditions.

a. The reverse reaction in the first equilibrium is much faster than the forward reaction with ester. The

$$\text{rate} = K_1 \frac{k_2[\boldsymbol{V}]^2[ester\cdot ZnCl_2]}{[azo]} \quad (4)$$

b. The forward reaction rate with ester is much faster than the reverse reaction of the equilibrium, rendering the formation of **VI** irreversible: rate = k_1[**V**]^2 (5)

In equations 3-5, the only nickel species that appears is **V**. Since **V** is the most stable nickel species before the rate limiting transition state by a considerable margin, it is reasonable to consider it as the resting state, i.e., [**V**] ≈ $[Ni]_{total}$. Hence, the pathway via **TS5** would certainly lead to a second order in nickel, which contradicts our experimental results. Furthermore, while equation 5 would correctly predict 0th order in both substrates, it is unclear how $ZnCl_2$ would speed up the reaction, or result in a rate law with 1st order in ester, but 0th order in azobenzene.

(ii) Pathway via **TS5_Zn**:

$$2 \times \mathbf{V\_Zn} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathbf{VI\_Zn} + ZnCl_2 + \text{azo}$$

$$\mathbf{VI\_Zn} \xrightarrow[k_2]{\text{ester}\cdot ZnCl_2} \mathbf{P\_Zn} + \mathbf{X\_Zn}$$

Steady state approximation would again lead to an equation similar to (3), but with [**V**] substituted by [**V_Zn**]. In other words,

$$\text{rate} = \frac{k_1 k_2[\boldsymbol{V\_Zn}]^2[ester\cdot ZnCl_2]}{k_{-1}[azo] + k_2[ester\cdot ZnCl_2]} \quad (6)$$

However, the computations suggest the energies of reactants and products of the first equilibrium are close to one another. As a result, the approximation [**V_Zn**] ≈ $[Ni]_{total}$ is invalid. Rather, we consider

$[Ni]_{total} \approx 2[\mathbf{VI\_Zn}] + [\mathbf{V\_Zn}]$ (7)

$$K_1 = \frac{[\boldsymbol{VI\_Zn}][azo][ZnCl_2]}{[\boldsymbol{V\_Zn}]^2} \quad (8)$$

Rearrangement of (7) followed by insertion into (8) leads to

$2K_1[\mathbf{V\_Zn}]^2 + [azo][ZnCl_2]([\mathbf{V\_Zn}]-[Ni]_{total}) = 0$ (9)

Solution of equation 9 for [**V_Zn**] leads to a non-linear dependence of the rate (eqs. 6 and 10) on $[Ni]_{total}$, [azo], and $[ZnCl_2]$.

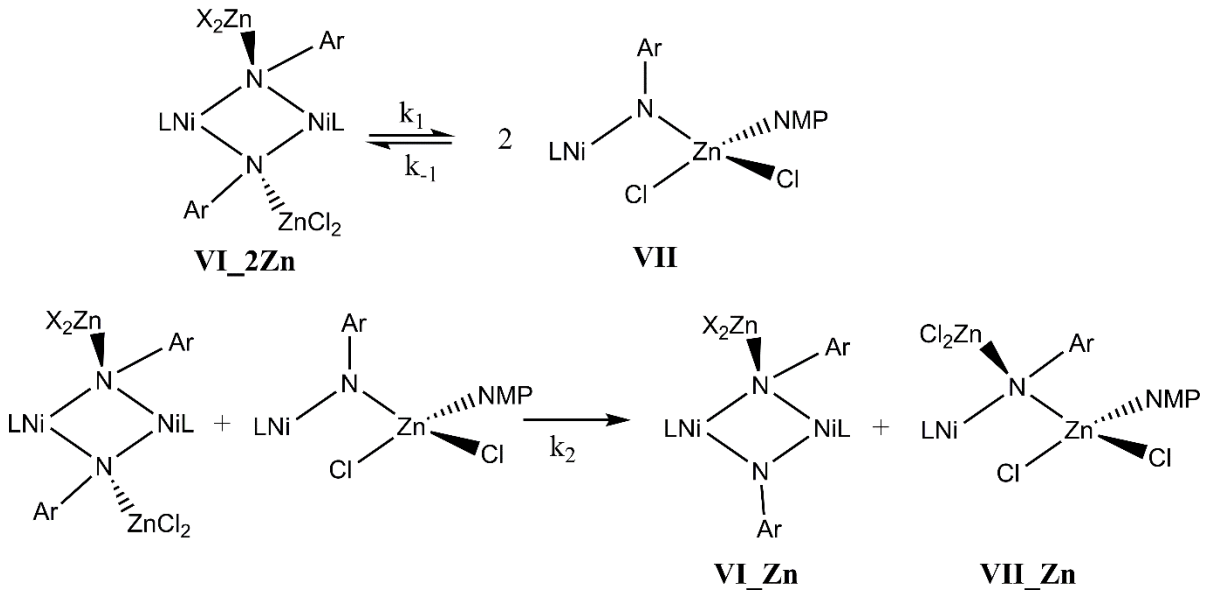
$$[\mathbf{V\_Zn}] \approx \frac{-[azo][ZnCl_2]+\sqrt{([azo][ZnCl_2])^2+8K_1[azo][ZnCl_2][Ni]_{total}}}{4K_1} \quad (10)$$

Note that $[ZnCl_2]$ depends on $[Ni]_{total}$ when no additional amounts are added. As such, the square dependence of the rate on [**V_Zn**] translates into a complicated dependence on nickel catalyst. The measured order of 1.4 does not contradict this. However, the rate also has a dependence on [azo] (eq. 10), which is not observed experimentally.

(iii) Pathway via **TS4**:

It is possible that the formation of **VII_Zn** is rate limiting under low-$[ZnCl_2]$ conditions, with the subsequent reaction with ester being faster than the equilibrium. In this case, a feasible reaction pathway towards the formation of **VII_Zn** is depicted in Scheme S1 (see also Figure S18).

Scheme S1. Formation pathway of **VII_Zn**



Here a reversible uphill splitting of the dimer **VI_2Zn** into two monomeric **VII** is followed by a reaction with VI_2Zn to give **VI_Zn** and **VII_Zn**.

Applying a steady state approximation:

Rate = k_2[**VI_2Zn**][**VII**] (11)

d[**VII**]/dt = k_1[**VI_2Zn**] – k_{-1}[**VII**]^2 – k_2[**VI_2Zn**][**VII**] = 0

$$[\mathbf{VII}]_{SS} = \frac{k_2[\boldsymbol{VI\_2Zn}] - \sqrt{{k_2}^2[\boldsymbol{Ni\_2Zn}]^2 + 4k_1k_{-1}[\boldsymbol{VI\_2Zn}]}}{-2k_{-1}} \quad (12)$$

If **VI_2Zn** is the resting state, [**VI_2Zn**] ≈ 0.5[Ni]$_{total}$. Evaluating equation (12) shows that [**VII**]$_{SS}$ will increase with increasing [Ni]$_{total}$, but not linearly, so [**VII**]$_{SS}$ ∝ ([Ni]$_{total}$)$^{\alpha}$, where $0 < \alpha < 1$. Inserting this relation into equation (11) leads to a relation where rate ∝ ([Ni]$_{total}$)$^{\alpha+1}$, which is in agreement with experiment. Under this model, the rate is 0th order in ester and azobenzene, which agree with experimental results under no additional [$ZnCl_2$].

Upon addition of supplementary $ZnCl_2$, **VII** could directly react with $ZnCl_2$ to give **VII_Zn**.

At sufficiently high [$ZnCl_2$], the formation of **VII_Zn** is fast and **VII_Zn** is the new resting state, i.e. [**VII_Zn**] ≈ [Ni]$_{total}$. Thus,

Rate = k[ester][**VII_Zn**]

So the reaction becomes first order in ester and nickel, and 0th order in azobenzene. This prediction agrees with the experimental results under high [$ZnCl_2$].

Cartesian coordinates

Main path geometries

Name: Zn(0) – gas phase
Opt Eel: -1779.114149
SP Eel TPSSh-D3BJ: -1795.862525
Gcorr (363K): -0.016221
Gsublimation: -0.035482
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0 1
Zn 0.000000 0.000000 0.000000

name: NMP
Opt Eel: -325.760125501
SP Eel TPSSh-D3BJ: -326.245563
Gcorr (363K): 0.102758
ZPE: 0.138357
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0 1
O -0.946999 1.826528 -0.053341
C -0.183293 0.867370 -0.000577
C 1.333859 0.905899 0.147344
C 1.779990 -0.514488 -0.212056
H 1.557321 1.155751 1.199584
H 1.768961 1.695888 -0.480919
C 0.555300 -1.376480 0.134068
H 1.979616 -0.580303 -1.293092
H 2.682724 -0.841947 0.321913
H 0.436539 -2.242854 -0.535503
H 0.592420 -1.755176 1.173416
N -0.554859 -0.447054 -0.029489
C -1.932158 -0.877258 -0.019114
H -2.132113 -1.574064 -0.850007
H -2.183320 -1.384784 0.929011
H -2.564330 0.014375 -0.129243

name: ester
Opt Eel: -307.510381576
SP Eel TPSSh-D3BJ: -307.996055
Gcorr (363K): 0.081894
ZPE: 0.117967
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0 1
C -1.216256 -0.737409 0.000307
H -1.176568 -1.402861 0.879490
H -1.176317 -1.403892 -0.878068
C 0.050828 0.086436 0.000087
O 0.108686 1.299136 0.000339
O 1.143420 -0.699766 -0.000157
C 2.407714 -0.020471 -0.000204
H 3.171375 -0.807583 -0.001292
H 2.510513 0.609215 -0.896527
H 2.511444 0.607561 0.897184
C -2.481137 0.109157 -0.000321
H -2.525630 0.755715 -0.890328
H -3.372821 -0.536255 0.000033
H -2.525736 0.756861 0.888841

name: ZnCl2(NMP)2
Opt Eel: -3351.00716280
SP Eel TPSSh-D3BJ: -3371.867695
Gcorr (363K): 0.221905
ZPE: 0.283655
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Zn -0.000229 0.424298 0.010810
Cl -0.009837 1.655716 1.899305
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C 2.736614 -0.461127 0.044733
C 3.204675 0.972637 0.005156
N 3.792754 -1.278143 0.067172
C 4.690989 0.855230 -0.355171
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H 2.599388 1.548543 -0.710555
C 5.072304 -0.563089 0.097236
C 3.709264 -2.718555 0.194131
H 4.815621 0.940746 -1.445036
H 5.313770 1.622225 0.123199
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H -4.275401 -3.180955 0.723041
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H -2.649041 -3.015198 -0.023845

name: I
Opt Eel: -2999.78475216
SP Eel TPSSh-D3BJ: -3016.249737
Gcorr (363K): 0.124331
ZPE: 0.176270
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C 0.206732 2.658417 -0.088888
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H 1.202435 3.107042 -0.103468
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C -2.284541 -1.428417 0.042745
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C -3.515219 -0.684804 0.019213
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C 0.206910 -2.658331 0.089753
H -4.455413 -1.239716 0.034252
H -3.117659 -3.436035 0.098311
C -0.956946 -3.450799 0.106428
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H -0.861701 -4.537037 0.136916
N 0.148924 1.331017 -0.052289
N 0.149003 -1.330938 0.052982
Cl 2.466663 0.211210 2.069420
Cl 2.466014 -0.211165 -2.069974

name: II
Opt Eel: -3191.20108108
SP Eel TPSSh-D3BJ: -3207.030248
Gcorr (363K): 0.378315
ZPE: 0.452369
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C 1.455223 -2.985176 -2.950098
H 0.458147 -1.107401 -3.398630
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C 2.100004 -4.236798 0.564535
C 1.207959 -2.556475 2.118368
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H 2.397081 -4.781675 -2.132937
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N 0.183033 -0.532482 1.159843
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C -3.069154 1.570332 0.422110
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C 1.942442 2.303803 -0.074188
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H 4.148436 1.289767 -0.839282

name: III
Opt Eel: -2731.03495639
SP Eel TPSSh-D3BJ: -2745.287257
Gcorr (363K): 0.382694
ZPE: 0.451329
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H 0.627160 2.991898 -0.726726
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C 4.153872 -1.425393 0.286210
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H 4.958336 3.405774 -0.650972
C 5.379015 -0.675334 0.121750
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N -3.210557 -2.055646 -0.534555
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H -3.416327 -3.994883 0.254889

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name: IV
Opt Eel: -3112.13155636
SP Eel TPSSh-D3BJ: -3127.812227
Gcorr (363K): 0.301180
ZPE: 0.366926
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 C 2.422680 -0.428001 0.370862
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 C 1.897384 -1.552618 -0.352104
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 H -6.320827 -2.226102 0.783493
 Cl -0.925900 -1.011324 2.202120

name: V
Opt Eel: -2652.01166027
SP Eel TPSSh-D3BJ: -2666.111709
Gcorr (363K): 0.305234
ZPE: 0.365704
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 Ni 0.000000 0.000000 0.209606
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 C 0.000136 2.635233 -1.147290
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 H 0.002271 1.238937 -5.823054
 C -0.004261 -2.844987 -3.560233
 C -0.000136 -2.635233 -1.147290
 H -0.002271 -1.238937 -5.823054
 H -0.005784 -3.450599 -4.468807
 C -0.002215 -3.435743 -2.305380
 H 0.009944 -3.083780 -0.153972
 H -0.001611 -4.521184 -2.195024
 N 0.000000 1.301295 -1.202417
 N 0.000000 -1.301295 -1.202417
 N -0.067293 -0.691676 1.948302
 N 0.067293 0.691676 1.948302
 C -1.101597 1.375669 2.321513
 C -1.087450 2.787529 2.246616
 C -2.258576 0.747387 2.836410
 C -2.204689 3.536886 2.616808
 H -0.171871 3.283841 1.915252
 C -3.369514 1.506855 3.212006
 H -2.260548 -0.339247 2.932234
 C -3.360450 2.903709 3.097025
 H -2.168046 4.627499 2.543964
 H -4.256059 0.999334 3.603841
 H -4.233080 3.491086 3.392874
 C 1.101597 -1.375669 2.321513
 C 1.087450 -2.787529 2.246616
 C 2.258576 -0.747387 2.836410
 C 2.204689 -3.536886 2.616808
 H 0.171871 -3.283841 1.915252
 C 3.369514 -1.506855 3.212006
 H 2.260548 0.339247 2.932234
 C 3.360450 -2.903709 3.097025
 H 2.168046 -4.627499 2.543964
 H 4.256059 -0.999334 3.603841
 H 4.233080 -3.491086 3.392874

name: V_Zn
Opt Eel: -5677.28491455
SP Eel TPSSh-D3BJ: -5711.747353
Gcorr (363K): 0.430002
ZPE: 0.511729
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0 1
 Ni -0.914161 0.101611 0.775845
 C -3.152543 -1.415545 0.343458
 C -1.870420 -2.460845 1.958289
 C -4.115536 -2.450214 0.324246
 C -3.331963 -0.247805 -0.452247
 C -2.774306 -3.538645 2.009214
 H -0.994317 -2.441792 2.604056
 C -3.890852 -3.549508 1.187738
 C -5.252600 -2.304229 -0.544180
 C -4.474764 -0.098813 -1.267714
 H -2.576606 -4.357368 2.702372
 H -4.599291 -4.380134 1.209678
 C -5.425417 -1.177066 -1.306011
 H -5.988648 -3.110361 -0.572873
 C -4.599933 1.125934 -1.970828
 C -2.520786 1.858159 -0.965007
 H -6.301615 -1.073552 -1.949475
 H -5.461025 1.295543 -2.620552
 C -3.628022 2.098911 -1.802847
 H -1.750004 2.612165 -0.820467
 H -3.697704 3.059040 -2.315944
 N -2.036729 -1.425770 1.131749
 N -2.366583 0.705416 -0.314204
 N 0.591855 1.269472 0.785398
 N 0.675716 0.214946 1.693757
 C 1.834899 -0.543855 1.707338
 C 1.815708 -1.845791 2.258753
 C 3.079166 -0.020543 1.287075
 C 2.980532 -2.607050 2.337011
 H 0.874996 -2.255197 2.623656
 C 4.238692 -0.795499 1.364380
 H 3.134687 0.992824 0.887559
 C 4.206179 -2.095141 1.884748
 H 2.930119 -3.615165 2.757721
 H 5.182335 -0.367864 1.013734
 H 5.117126 -2.694715 1.947172
 C 0.279244 2.533635 1.363753
 C 0.142758 3.640509 0.505174
 C 0.145877 2.720488 2.751542
 C -0.160701 4.901488 1.023343
 H 0.283438 3.503522 -0.571646
 C -0.154957 3.986922 3.259442
 H 0.282895 1.864511 3.412967
 C -0.318103 5.083555 2.402953
 H -0.266697 5.748883 0.341057
 H -0.257700 4.118747 4.340007
 H -0.551995 6.071156 2.807427
 Zn 1.397922 1.236057 -1.128014
 Cl 3.519361 1.996857 -1.474676
 Cl 0.057133 2.029731 -2.804786
 H 2.550779 -4.471941 -2.317492
 C 2.855304 -3.871332 -1.442533
 C 4.032482 -2.929228 -1.748988
 N 1.775767 -2.951516 -1.080868
 H 3.055534 -4.557313 -0.606178
 C 3.365283 -1.594673 -2.104341
 H 4.670987 -3.319387 -2.552333
 H 4.649421 -2.806480 -0.847125
 C 2.011315 -1.688527 -1.448374
 C 0.517804 -3.394973 -0.518764
 H 3.893928 -0.692265 -1.766753
 H 3.190592 -1.483613 -3.189146
 O 1.175736 -0.765103 -1.302086
 H -0.034273 -2.508688 -0.185927
 H -0.075499 -3.938201 -1.273438
 H 0.704910 -4.060105 0.335649

name: V_2Zn
Opt Eel: -8702.55373724
SP Eel TPSSh-D3BJ: -8757.377976
Gcorr (363K): 0.553741
ZPE: 0.656513
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0 1
 Ni 0.942443 0.642493 0.236790
 C 3.172344 2.181618 -0.185163
 C 1.812990 2.350231 -2.049378
 C 4.155874 3.041957 -0.723202
 C 3.320175 1.651694 1.130511
 C 2.732897 3.221474 -2.664018
 H 0.872506 2.095345 -2.544710
 C 3.909917 3.562038 -2.016857
 C 5.318835 3.330193 0.072386
 C 4.467968 1.943277 1.900182
 H 2.497762 3.618289 -3.652595
 H 4.637632 4.228985 -2.483776
 C 5.472100 2.798509 1.326835
 H 6.082855 3.987861 -0.347293
 C 4.531403 1.367313 3.192819
 C 2.370273 0.343541 2.792599
 H 6.361066 3.024274 1.919313
 H 5.397402 1.556673 3.830590
 C 3.483635 0.569695 3.625868
 H 1.538481 -0.290286 3.115659
 H 3.498992 0.107854 4.614235
 N 2.040012 1.813464 -0.848393
 N 2.290753 0.874969 1.571841
 N -0.533691 -0.425781 0.750130
 N -0.592719 0.016523 -0.594536
 C -0.427906 -1.004589 -1.578569
 C 0.473298 -0.830410 -2.639580
 C -1.211159 -2.165675 -1.527942
 C 0.588000 -1.803077 -3.632352
 H 1.098039 0.057631 -2.671623
 C -1.079078 -3.147724 -2.515481
 H -1.916991 -2.309991 -0.710686
 C -0.187362 -2.969345 -3.577092
 H 1.300877 -1.654829 -4.447271
 H -1.683774 -4.054828 -2.446845
 H -0.091692 -3.732817 -4.352513
 C -1.525074 0.179444 1.605047
 C -1.297655 1.409522 2.231884
 C -2.722056 -0.515910 1.838311
 C -2.278488 1.957832 3.065235
 H -0.354040 1.929784 2.057773
 C -3.698194 0.035519 2.669684
 H -2.866972 -1.497445 1.380066
 C -3.480298 1.277117 3.281883
 H -2.097755 2.921461 3.547823
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 H -4.630200 -0.507445 2.844191
 H -4.244148 1.707324 3.933905
 Zn -0.107266 -2.349840 1.393994
 Cl -1.220602 -4.296390 0.990866
 Cl 0.084516 -2.110710 3.660206
 H 4.663679 -3.933300 -1.797477
 C 3.648603 -3.656915 -2.132223
 C 2.633001 -4.798233 -1.957198
 N 3.117976 -2.603086 -1.264630
 H 3.714705 -3.288452 -3.166392
 C 1.989810 -4.523521 -0.592608
 H 3.109140 -5.785393 -2.019983
 H 1.868892 -4.733037 -2.745080
 C 2.215990 -3.047786 -0.385077
 C 3.622995 -1.246736 -1.276742
 H 0.919880 -4.762768 -0.514435
 H 2.502770 -5.048514 0.232525
 O 1.703719 -2.318327 0.499133
 H 2.922591 -0.618976 -0.712666
 H 4.620586 -1.194895 -0.809717
 H 3.690424 -0.884004 -2.311720
 Zn -1.485733 1.842000 -1.048125
 Cl -1.680590 1.752745 -3.327825
 Cl -0.594278 3.811524 -0.322330
 O -3.411321 1.985471 -0.409022
 C -4.294156 1.108454 -0.552874
 N -5.508471 1.183825 0.002787
 C -4.201459 -0.144311 -1.385791
 C -6.379236 0.062201 -0.355552
 C -5.968080 2.298061 0.803165
 C -5.395224 -0.979992 -0.912060
 H -3.224546 -0.625615 -1.257056
 H -4.273420 0.158879 -2.443758
 H -7.118156 0.392606 -1.106338
 H -6.924254 -0.285840 0.534220
 H -5.126816 2.984689 0.956867
 H -6.787302 2.826405 0.288790
 H -6.334452 1.936753 1.776149
 H -5.843183 -1.586970 -1.709473
 H -5.077050 -1.655244 -0.103678

name: PreVI
Opt Eel: -10703.0468800
SP Eel TPSSh-D3BJ: -10770.985290
Gcorr (363K): 0.629529
ZPE: 0.741515
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0 3
 Ni 1.628085 -0.573738 -0.046335
 C 4.050325 -1.193671 -1.206059
 C 2.384629 -1.457594 -2.784054
 C 5.066717 -1.615737 -2.094719
 C 4.379650 -0.754189 0.108577
 C 3.321344 -1.906820 -3.732699
 H 1.332849 -1.363842 -3.049097
 C 4.661902 -1.995401 -3.396447
 C 6.427178 -1.613359 -1.629512
 C 5.726759 -0.731348 0.541010
 H 2.970582 -2.170176 -4.731338
 H 5.404750 -2.337415 -4.119945
 C 6.744188 -1.187248 -0.366461
 H 7.208642 -1.949183 -2.314167
 C 5.971842 -0.243997 1.846352
 C 3.595089 0.128588 2.093564
 H 7.782055 -1.177671 -0.027630
 H 6.992757 -0.207631 2.231872
 C 4.901274 0.188719 2.611654
 H 2.753963 0.462818 2.698674
 H 5.047774 0.580199 3.619081
 N 2.731333 -1.132392 -1.538888
 N 3.331576 -0.346184 0.875547
 N 0.554290 -0.245848 1.466273
 N 0.002781 -0.716672 -0.980240
 C -0.360534 -1.976977 -1.458223
 C 0.057894 -3.165444 -0.808606
 C -1.209849 -2.108631 -2.585754
 C -0.376881 -4.416686 -1.241675
 H 0.710420 -3.080162 0.060119
 C -1.636066 -3.364308 -3.017791
 H -1.521883 -1.201212 -3.109991
 C -1.234596 -4.527130 -2.345220
 H -0.047779 -5.313498 -0.710438
 H -2.296529 -3.435479 -3.886094
 H -1.580829 -5.507490 -2.680655
 C 0.776891 -1.074999 2.563787
 C 0.251017 -0.729043 3.835436
 C 1.547906 -2.263103 2.470061
 C 0.473960 -1.538485 4.948189
 H -0.310684 0.202973 3.932082
 C 1.774887 -3.062764 3.589832
 H 1.976965 -2.537827 1.504731
 C 1.232945 -2.712774 4.834000
 H 0.055844 -1.249360 5.915622
 H 2.374273 -3.970823 3.489028
 H 1.404154 -3.345686 5.707644
 Ni -1.172924 -0.362686 0.567492
 N -2.842619 -0.466630 -0.560690
 C -3.486962 -1.661840 -0.492111
 C -3.247348 0.428291 -1.454657
 C -4.570435 -1.997777 -1.340071
 C -3.018734 -2.594850 0.483351
 C -4.332428 0.192734 -2.321617
 H -2.685119 1.355424 -1.528523
 C -4.993457 -1.018628 -2.271986
 C -5.162066 -3.299683 -1.232163
 C -3.629192 -3.872435 0.577436
 N -1.994420 -2.194472 1.288806
 H -4.609338 0.968122 -3.035470
 H -5.826313 -1.237096 -2.943597
 C -4.702384 -4.205581 -0.314941
 H -5.986472 -3.551365 -1.902263
 C -3.138450 -4.756552 1.566109
 C -1.591408 -3.034469 2.238115
 H -5.150066 -5.198231 -0.236489
 H -3.569649 -5.755144 1.662509
 C -2.129034 -4.324733 2.405650
 H -0.807340 -2.687880 2.904413
 H -1.734326 -4.960681 3.198781
 N -0.743139 2.289681 -0.688912
 N -1.213160 1.703191 0.435627
 C -0.671827 3.672726 -0.791429
 C -2.434967 2.086809 1.030196
 C -0.493132 4.219186 -2.083221
 C -0.709604 4.539721 0.327899
 C -2.785148 1.388810 2.206044
 C -3.377278 2.961181 0.452630
 C -0.384115 5.598197 -2.250324
 H -0.472291 3.542265 -2.939284
 C -0.590691 5.914170 0.143737
 H -0.792175 4.128052 1.336096
 C -4.041529 1.549856 2.784296
 H -2.054348 0.711911 2.656171
 C -4.632266 3.122462 1.047067
 H -3.147577 3.492717 -0.470213
 C -0.434757 6.455555 -1.141817
 H -0.258740 6.009252 -3.255215
 H -0.607624 6.572911 1.015785
 C -4.975068 2.425320 2.211648
 H -4.291255 0.990616 3.689189
 H -5.355148 3.796703 0.580803
 H -0.344430 7.536076 -1.276001
 H -5.960535 2.556470 2.664095
 Zn 0.622330 1.758770 1.768146
 Cl 2.362655 2.959341 0.910025
 Cl -0.184877 2.820094 3.632802
 Zn 0.067000 0.963459 -2.108643
 Cl -1.417033 1.228039 -3.907999
 Cl 2.016159 1.748600 -3.013706

name: VI
Opt Eel: -4731.56874605
SP Eel TPSSh-D3BJ: -4758.956120
Gcorr (363K): 0.461872
ZPE: 0.539217
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0 1
 Ni 1.336326 -0.109151 -0.469101
 C 3.857797 -0.824584 0.466295
 C 2.329564 -2.326711 1.329171
 C 4.951627 -1.445461 1.118051
 C 4.057348 0.351011 -0.305370
 C 3.345727 -2.985796 2.040884
 H 1.294924 -2.661681 1.402792
 C 4.666087 -2.569052 1.925430
 C 6.264723 -0.890446 0.919932
 C 5.357019 0.875288 -0.511481
 H 3.076799 -3.836172 2.669556
 H 5.471854 -3.085091 2.451555
 C 6.460899 0.213178 0.131171
 H 7.109885 -1.374718 1.413993
 C 5.465515 2.017373 -1.335513
 C 3.058855 1.973942 -1.621435
 H 7.465071 0.616375 -0.017077
 H 6.443226 2.464265 -1.527072
 C 4.308565 2.547579 -1.898561
 H 2.140048 2.380930 -2.044427
 H 4.352198 3.420352 -2.552180
 N 2.567149 -1.278722 0.528240
 N 2.920775 0.911309 -0.814915
 Ni -1.336335 0.109174 -0.469088
 N -2.567163 1.278689 0.528315
 N -2.920780 -0.911281 -0.814942
 C -3.857810 0.824550 0.466346
 C -2.329585 2.326634 1.329306
 C -4.057355 -0.351010 -0.305372
 C -3.058855 -1.973885 -1.621501
 C -4.951643 1.445392 1.118130
 C -3.345752 2.985679 2.041051
 H -1.294945 2.661588 1.402971
 C -5.357024 -0.875286 -0.511505
 C -4.308562 -2.547517 -1.898651
 H -2.140046 -2.380850 -2.044512
 C -4.666110 2.568943 1.925565
 C -6.264737 0.890381 0.919983
 H -3.076827 3.836013 2.669780
 C -6.460907 -0.213209 0.131173
 C -5.465515 -2.017338 -1.335583
 H -4.352191 -3.420264 -2.552305
 H -5.471880 3.084948 2.451719
 H -7.109902 1.374624 1.414068
 H -7.465077 -0.616405 -0.017090
 H -6.443223 -2.464228 -1.527160
 C 0.253789 2.471810 -0.378546
 C -0.399636 3.576112 -0.998031
 C 1.040657 2.766412 0.773255
 C -0.271631 4.874389 -0.505748
 H -1.018031 3.372146 -1.876682
 C 1.175636 4.070551 1.252898
 H 1.529931 1.934508 1.286676
 C 0.521258 5.139138 0.622461
 H -0.792772 5.694470 -1.009031
 H 1.789492 4.255256 2.139891
 H 0.622702 6.157787 1.004776
 C -0.253787 -2.471773 -0.378631
 C 0.399689 -3.576055 -0.998097
 C -1.040668 -2.766395 0.773155
 C 0.271711 -4.874335 -0.505815
 H 1.018100 -3.372072 -1.876733
 C -1.175627 -4.070538 1.252792
 H -1.529984 -1.934505 1.286559
 C -0.521207 -5.139107 0.622369
 H 0.792886 -5.694402 -1.009086
 H -1.789506 -4.255261 2.139764
 H -0.622637 -6.157760 1.004678
 N -0.095427 -1.211134 -0.907209
 N 0.095418 1.211182 -0.907147

name: VI_Zn
Opt Eel: -7756.86928820
SP Eel TPSSh-D3BJ: -7804.612233
Gcorr (363K): 0.587712
ZPE: 0.685297
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0 1
 Ni -0.932775 0.076950 -0.755885
 C -3.343811 -0.628796 -1.949233
 C -1.785762 -2.243192 -2.497768
 C -4.389020 -1.300767 -2.627911
 C -3.592991 0.610127 -1.295825
 C -2.749232 -2.958826 -3.230116
 H -0.759943 -2.603175 -2.435631
 C -4.059585 -2.508177 -3.285193
 C -5.707153 -0.726877 -2.593393
 C -4.902558 1.148016 -1.245122
 H -2.446147 -3.877412 -3.734576
 H -4.828908 -3.064135 -3.824978
 C -5.955830 0.440542 -1.920772
 H -6.513225 -1.252169 -3.109867
 C -5.081063 2.340191 -0.508533
 C -2.718809 2.297637 0.019697
 H -6.964500 0.857462 -1.886483
 H -6.070291 2.796796 -0.438177
 C -3.982703 2.898341 0.130633
 H -1.856434 2.712714 0.536028
 H -4.079139 3.805911 0.727601
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 N -2.068433 -1.110849 -1.843727
 N -2.508849 1.193204 -0.707206
 Ni 1.735206 0.144036 -0.243027
 N 3.173339 1.258225 -0.976577
 N 3.178905 -0.997533 0.311501
 C 4.398520 0.673057 -0.803815
 C 3.126709 2.374466 -1.711515
 C 4.404996 -0.537975 -0.057444
 C 3.117963 -2.042080 1.144933
 C 5.611543 1.212355 -1.294369
 C 4.275097 2.965315 -2.267855
 H 2.143676 2.822714 -1.858467
 C 5.620197 -1.174534 0.288749
 C 4.274710 -2.722739 1.561716
 H 2.125375 -2.330660 1.501438
 C 5.525032 2.401964 -2.053622
 C 6.837573 0.526838 -0.980274
 H 4.161624 3.878686 -2.853706
 C 6.844121 -0.608509 -0.211963
 C 5.527289 -2.316764 1.117201
 H 4.167232 -3.577509 2.231407
 H 6.429599 2.860109 -2.458899
 H 7.773208 0.943621 -1.359064
 H 7.785211 -1.104550 0.035092
 H 6.431930 -2.851369 1.414372
 C 0.318898 2.601417 -0.311191
 C 0.904256 3.518443 0.600083
 C -0.160844 3.118761 -1.544626
 C 1.001575 4.875495 0.290293
 H 1.275753 3.111603 1.545167
 C -0.075546 4.481425 -1.837676
 H -0.599900 2.422513 -2.263825
 C 0.510153 5.372220 -0.926797
 H 1.462218 5.559527 1.009504
 H -0.457646 4.851103 -2.793705
 H 0.585285 6.436573 -1.162890
 C 0.545863 -2.387844 -0.460136
 C -0.141317 -3.475723 0.131051
 C 1.404228 -2.672665 -1.553966
 C 0.017153 -4.774846 -0.356668
 H -0.768164 -3.272570 0.999144
 C 1.567480 -3.975332 -2.028483
 H 1.927019 -1.838643 -2.029951
 C 0.870696 -5.039030 -1.437335
 H -0.527724 -5.596021 0.118485
 H 2.234977 -4.161141 -2.874810
 H 0.990648 -6.057885 -1.813863
 N 0.350401 -1.091884 -0.002684
 N 0.258444 1.262038 0.022841
 Zn 0.181402 -0.103675 1.843582
 Cl 1.747488 1.108865 3.133840
 Cl 0.031924 -2.060109 3.237016
 O -1.701496 0.614846 2.405302
 C -2.784362 0.008840 2.268967
 C -2.994815 -1.361966 1.675864
 N -3.968935 0.502180 2.671024
 H -2.418363 -1.459307 0.744839
 C -4.514179 -1.472978 1.507898
 H -2.564235 -2.082232 2.391005
 C -5.080037 -0.430748 2.487903
 C -4.119777 1.735378 3.412186
 H -4.801066 -1.209156 0.479513
 H -4.897206 -2.480596 1.716938
 H -5.958434 0.102473 2.093978
 H -5.356143 -0.872550 3.461964
 H -4.924370 2.343964 2.973560
 H -4.370071 1.523634 4.465639
 H -3.172087 2.286262 3.368653

name: VI_2Zn
Opt Eel: -10782.1474377
SP Eel TPSSh-D3BJ: -10850.250448
Gcorr (363K): 0.711757
ZPE: 0.830463
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0 1
 Ni 0.149828 -1.372619 -0.033329
 C -0.383983 -4.069162 -0.182257
 C -2.208350 -2.899790 -0.982600
 C -1.012456 -5.325010 -0.347146
 C 0.931549 -3.984475 0.351578
 C -2.922810 -4.099830 -1.159969
 H -2.671489 -1.941442 -1.206817
 C -2.332404 -5.316824 -0.857736
 C -0.272541 -6.506345 0.006436
 C 1.660263 -5.155624 0.662031
 H -3.942551 -4.047902 -1.543910
 H -2.867613 -6.257385 -1.003624
 C 1.011510 -6.426035 0.480572
 H -0.755803 -7.477223 -0.121543
 C 2.986831 -4.978489 1.122712
 C 2.680985 -2.583606 0.914145
 H 1.567226 -7.332061 0.731247
 H 3.596941 -5.847615 1.377425
 C 3.491785 -3.691530 1.224859
 H 3.075427 -1.571001 0.978068
 H 4.516868 -3.511892 1.552574
 N -0.957422 -2.878654 -0.518949
 N 1.416276 -2.721672 0.511887
 Ni -0.041129 1.473353 -0.016979
 N 0.040862 2.898194 1.327185
 N -0.525584 2.919721 -1.215647
 C -0.349271 4.099801 0.815616
 C 0.131499 2.793800 2.654801
 C -0.595952 4.123855 -0.585941
 C -0.598595 2.905615 -2.547935
 C -0.532517 5.268055 1.592038
 C -0.075886 3.888191 3.514248
 H 0.378832 1.811559 3.056329
 C -0.879487 5.342050 -1.247038
 C -0.833210 4.072644 -3.298097
 H -0.474532 1.941339 -3.039681
 C -0.376221 5.137017 2.991553
 C -0.867857 6.491350 0.913098
 H 0.022734 3.735552 4.589980
 C -1.015169 6.531374 -0.449222
 C -1.007568 5.289273 -2.655129
 H -0.893710 3.995278 -4.384579
 H -0.508808 6.005243 3.640510
 H -0.994637 7.396783 1.510462
 H -1.249790 7.470902 -0.954184
 H -1.225373 6.199293 -3.218221
 C 1.701413 0.217438 1.870686
 C 2.709193 1.190729 2.092529
 C 1.312849 -0.587172 2.967225
 C 3.300324 1.344296 3.344905
 H 3.006359 1.825187 1.254569
 C 1.913602 -0.429756 4.220378
 H 0.507390 -1.309340 2.821666
 C 2.910628 0.533248 4.422299
 H 4.073295 2.105486 3.484677
 H 1.590722 -1.063661 5.051518
 H 3.375878 0.653744 5.403799
 C -1.542411 -0.001015 -1.976862
 C -0.963675 -0.702804 -3.059829
 C -2.708063 0.764061 -2.239403
 C -1.528867 -0.646532 -4.337368
 H -0.045848 -1.267634 -2.883702
 C -3.267011 0.814325 -3.515512
 H -3.156884 1.323691 -1.415285
 C -2.684216 0.108216 -4.578977
 H -1.055333 -1.197428 -5.155506
 H -4.165759 1.414506 -3.684340
 H -3.123059 0.148838 -5.579014
 N 1.105684 0.113271 0.615989
 Zn 2.278885 0.373068 -1.014294
 Cl 2.857565 2.512734 -1.681346
 Cl 2.469952 -1.304093 -2.584077
 O 4.130631 -0.067857 -0.110543
 C 5.279154 -0.099324 -0.594583
 C 5.685620 0.221190 -2.012930
 N 6.373788 -0.408729 0.120520
 H 4.976106 -0.236852 -2.715719
 C 7.122487 -0.307614 -2.103103
 H 5.612300 1.314992 -2.133323
 C 7.614437 -0.298481 -0.647298
 C 6.364777 -0.665637 1.544946
 H 7.113905 -1.341491 -2.480863
 H 7.766665 0.291480 -2.760369
 H 8.283037 -1.138802 -0.408368
 H 8.133198 0.639911 -0.381164
 H 6.824235 -1.643341 1.759330
 H 6.931024 0.115585 2.078261
 H 5.325064 -0.659311 1.894675
 N -0.993768 -0.021092 -0.695294
 Zn -2.277517 0.143115 0.857937
 Cl -3.220852 2.161253 1.438483
 Cl -2.086950 -1.444699 2.517004
 O -4.016700 -0.652701 -0.018949
 C -5.120923 -0.896111 0.507205
 C -5.528196 -0.640628 1.937536
 N -6.162692 -1.414875 -0.164289
 H -4.716377 -0.944564 2.612845
 C -6.832124 -1.432712 2.087407
 H -5.661461 0.448859 2.047056
 C -7.371507 -1.536026 0.651918
 C -6.162076 -1.673250 -1.588425
 H -6.611901 -2.441046 2.470220
 H -7.553915 -0.959496 2.766315
 H -7.874665 -2.491968 0.443552
 H -8.070433 -0.717854 0.401894
 H -6.415222 -2.726555 -1.786594
 H -6.903454 -1.031554 -2.092259
 H -5.163219 -1.450324 -1.983698

name: VII_split
Opt Eel: -2365.72840681
SP Eel TPSSh-D3BJ: -2379.432175
Gcorr (363K): 0.211514
ZPE: 0.267232
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0 3
 Ni -0.510521 -0.016517 -0.563372
 C 2.175835 -0.710219 -0.019973
 C 0.951677 -2.655490 -0.292735
 C 3.377435 -1.411303 0.237649
 C 2.161045 0.724296 -0.010981
 C 2.094678 -3.441617 -0.048847
 H -0.017482 -3.113503 -0.502727
 C 3.308599 -2.826066 0.216382
 C 4.572485 -0.656245 0.503185
 C 3.347906 1.447054 0.255044
 H 2.008148 -4.528941 -0.072262
 H 4.207574 -3.415465 0.409222
 C 4.558343 0.713886 0.511531
 H 5.497285 -1.202242 0.701188
 C 3.249798 2.860175 0.250682
 C 0.896915 2.647033 -0.260596
 H 5.471719 1.276377 0.716244
 H 4.136423 3.465635 0.450784
 C 2.023471 3.453691 -0.007600
 H -0.081742 3.087098 -0.464894
 H 1.914425 4.539187 -0.018035
 N 0.989790 -1.323571 -0.278983
 N 0.962689 1.316131 -0.262263
 N -2.211594 -0.018173 -0.429229
 C -3.496023 -0.014071 -0.075413
 C -3.914889 -0.094224 1.299263
 C -4.556100 0.070531 -1.044940
 C -5.261028 -0.086583 1.656713
 H -3.137254 -0.160339 2.066262
 C -5.896656 0.075391 -0.666129
 H -4.278888 0.132188 -2.101661
 C -6.274511 -0.001983 0.685733
 H -5.529817 -0.148307 2.716635
 H -6.667487 0.141524 -1.441291
 H -7.328392 0.003018 0.974463

name: VIII
Opt Eel: -8064.40119294
SP Eel TPSSh-D3BJ: -8112.605376
Gcorr (363K): 0.694611
ZPE: 0.804040
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0 1 0 3 0 -3
 Ni 1.246640 0.426826 -0.367318
 N 3.225633 -0.046028 -0.203112
 N 2.004400 2.316268 -0.411280
 C 4.002504 1.067257 -0.095675
 C 3.812276 -1.240231 -0.150502
 C 3.345870 2.338220 -0.212451
 C 1.357516 3.464787 -0.580470
 C 5.404344 1.016275 0.103074
 C 5.199757 -1.388330 0.041536
 H 3.167794 -2.111064 -0.265488
 C 4.094056 3.539587 -0.134930
 C 2.013893 4.709609 -0.526585
 H 0.284262 3.399891 -0.769298
 C 5.999058 -0.266331 0.177845
 C 6.138897 2.248045 0.201750
 H 5.623084 -2.393169 0.078044
 C 5.511518 3.459826 0.086639
 C 3.379459 4.751641 -0.293350
 H 1.436484 5.624380 -0.667678
 H 7.076597 -0.355296 0.332057
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H 7.217526 2.194269 0.363625
H 6.080057 4.389630 0.154299
H 3.911712 5.703705 -0.238872
C 0.335116 0.904617 2.408084
C 1.599718 1.377434 2.885068
C -0.752093 0.985523 3.338038
C 1.753575 1.889337 4.172614
H 2.458046 1.314613 2.213263
C -0.583924 1.500254 4.621486
H -1.726042 0.610213 3.016481
C 0.668058 1.963166 5.061059
H 2.742099 2.235572 4.491406
H -1.445164 1.537005 5.296440
H 0.795016 2.365038 6.069159
N 0.186223 0.348477 1.186891
Ni -1.271445 0.222376 -0.006772
H -0.008624 1.345254 -4.314122
C -0.958172 1.808405 -4.049814
C -1.639552 1.390807 -2.867483
C -1.466243 2.829136 -4.857736
C -2.849595 2.083017 -2.563383
N -1.222226 0.405541 -2.015354
C -2.656216 3.495715 -4.537201
H -0.907259 3.116579 -5.754154
C -3.338029 3.106092 -3.372287
H -3.400932 1.779184 -1.672037
C -0.191615 -0.513619 -2.331695
H -3.041887 4.296050 -5.173404
H -4.272906 3.602570 -3.093611
C -0.396524 -1.396630 -3.564015
O 0.006559 -1.246199 -1.153809
O 1.077147 0.302274 -2.462828
H 0.446901 -2.103009 -3.626685
H -0.366249 -0.768198 -4.466316
C -1.710716 -2.171749 -3.517958
C 2.177486 -0.206119 -3.217119
H -2.568945 -1.495517 -3.386369
H -1.852618 -2.730879 -4.456632
H -1.713174 -2.902417 -2.694892
H 3.023722 0.468587 -3.025173
H 2.444605 -1.231923 -2.917031
H 1.951192 -0.182877 -4.295690
H -1.124834 3.277061 0.845481
C -2.153832 2.971409 1.037553
N -2.470101 1.714861 0.738872
C -3.087303 3.873983 1.581521
C -3.732308 1.283749 0.989829
C -4.385829 3.453574 1.823450
H -2.774159 4.895080 1.803999
C -4.015671 -0.088073 0.684534
C -4.745088 2.117044 1.527157
H -5.130150 4.135558 2.240167
N -2.985165 -0.834222 0.208155
C -5.316932 -0.609326 0.891220
C -6.055977 1.564640 1.734715
C -3.204328 -2.110070 -0.098677
C -5.525301 -1.970038 0.559591
C -6.331593 0.259182 1.424050
H -6.832437 2.213365 2.145721
C -4.465710 -2.713755 0.063643
H -2.352530 -2.685254 -0.466928
H -6.511986 -2.416667 0.700486
H -7.332153 -0.149149 1.581856
H -4.583973 -3.765956 -0.199848
Zn 0.562229 -3.121196 -0.955226
Cl 2.318816 -3.748597 -2.269796
Cl -1.026868 -4.758745 -0.771583
O 1.400283 -2.978803 0.888025
C 0.848557 -2.728131 1.987441
C -0.628407 -2.679726 2.266563
C -0.714278 -2.661000 3.798345
H -1.137771 -3.521815 1.778710
H -0.986283 -1.744183 1.803817
C 0.666042 -2.153623 4.251612
H -1.524951 -2.022288 4.172989
H -0.878282 -3.680575 4.178516
H 0.674916 -1.069345 4.449938
H 1.046662 -2.673800 5.143312
N 1.527958 -2.445299 3.103413
C 2.966752 -2.298838 3.167354
H 3.244491 -1.235421 3.249844
H 3.355038 -2.838034 4.044330
H 3.403359 -2.719553 2.254205
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name: IX

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Opt Eel: -8064.40389632
SP Eel TPSSh-D3BJ: -8112.614887
Gcorr (363K): 0.690712
ZPE: 0.802786
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0 1 0 3 0 -3
 Ni 1.312752 0.517914 -0.672956
 N 3.246586 -0.125370 -0.515715
 N 2.229323 2.332889 -0.688165
 C 4.119307 0.913009 -0.421445
 C 3.727395 -1.365890 -0.525972
 C 3.571203 2.236578 -0.514460
 C 1.684961 3.534445 -0.846257
 C 5.516951 0.737895 -0.267839
 C 5.103322 -1.637759 -0.389766
 H 3.006675 -2.174669 -0.649494
 C 4.422841 3.367651 -0.447691
 C 2.448070 4.717110 -0.798347
 H 0.608048 3.564163 -1.023396
 C 5.999970 -0.592832 -0.242360
 C 6.356692 1.900800 -0.171038
 H 5.440146 -2.675440 -0.400060
 C 5.832538 3.163061 -0.257399
 C 3.815648 4.638414 -0.586972
 H 1.950580 5.679575 -0.926397
 H 7.069762 -0.778350 -0.123979
 H 7.430626 1.753301 -0.038372
 H 6.480495 4.039795 -0.194181
 H 4.430318 5.539817 -0.538210
 C 0.659619 1.069519 2.168912
 C 1.983896 1.458413 2.551672
 C -0.350511 1.245412 3.171675
 C 2.261985 1.983616 3.812518
 H 2.790750 1.318422 1.831344
 C -0.058951 1.770648 4.428394
 H -1.369008 0.936322 2.924275
 C 1.249399 2.152419 4.771770
 H 3.292886 2.261898 4.054644
 H -0.867319 1.880467 5.158680
 H 1.473813 2.563103 5.759133
 N 0.380472 0.506834 0.972700
 Ni -1.258630 0.296655 0.106721
 H -0.378768 1.371149 -3.699965
 C -1.445921 1.616950 -3.741532
 C -2.277955 0.977057 -2.800727
 C -1.986370 2.555812 -4.624589
 C -3.642877 1.315189 -2.739312
 N -1.738862 0.094743 -1.857554
 C -3.349874 2.878195 -4.576326
 H -1.335365 3.049686 -5.351794
 C -4.171992 2.257719 -3.626364
 H -4.278044 0.829522 -1.994774
 C -1.076013 -1.006268 -2.101657
 H -3.767514 3.614497 -5.267633
 H -5.234892 2.509008 -3.575128
 C -1.004176 -1.736945 -3.409792
 O -0.543745 -1.546603 -1.034356
 O 1.124327 0.356321 -2.571312
 H 0.020512 -2.125599 -3.501418
 H -1.188858 -1.036853 -4.235898
 C -2.010106 -2.895930 -3.455175
 C 2.197961 0.167298 -3.413611
 H -3.044278 -2.527405 -3.360899
 H -1.922659 -3.436692 -4.410395
 H -1.829003 -3.613504 -2.638982
 H 3.008900 0.928765 -3.296655
 H 2.692360 -0.826661 -3.304424
 H 1.882110 0.232574 -4.481217
 H -0.976560 3.440957 0.334024
 C -1.990493 3.216980 0.667020
 N -2.344450 1.935241 0.677911
 C -2.864919 4.243509 1.070904
 C -3.588692 1.603995 1.108378
 C -4.143350 3.922506 1.499691
 H -2.522965 5.278949 1.039502
 C -3.921637 0.208409 1.115787
 C -4.542386 2.565179 1.528747
 H -4.843337 4.699388 1.814525
 N -2.954837 -0.657844 0.714267
 C -5.216851 -0.209055 1.513117
 C -5.841968 2.114965 1.946383
 C -3.243638 -1.955861 0.649214
 C -5.491979 -1.596455 1.457973
 C -6.166849 0.784680 1.933836
 H -6.570406 2.861878 2.268887
 C -4.504497 -2.462928 1.016733
 H -2.455112 -2.624949 0.297570
 H -6.476206 -1.965299 1.754790
 H -7.159965 0.452776 2.244023
 H -4.680261 -3.537683 0.948945
 Zn 0.301344 -3.299702 -0.713890
 Cl 1.802669 -3.934361 -2.279394
 Cl -1.264317 -4.844453 -0.109001
 O 1.403165 -2.913726 0.929155
 C 1.030328 -2.539167 2.068756
 C -0.384702 -2.374007 2.550523
 C -0.241768 -2.249614 4.072492
 H -1.005548 -3.212758 2.207766
 H -0.756775 -1.449881 2.075739
 C 1.207749 -1.779024 4.277570
 H -0.964204 -1.551103 4.514615
 H -0.382709 -3.234131 4.543821
 H 1.289484 -0.684172 4.374154
 H 1.695112 -2.243363 5.147785
 N 1.878667 -2.211759 3.048037
 C 3.318030 -2.166117 2.901870
 H 3.669628 -1.122895 2.853124
 H 3.792188 -2.662480 3.761721
 H 3.593030 -2.687690 1.978122
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name: X

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Opt Eel: -5020.52617528
SP Eel TPSSh-D3BJ: -5049.270988
Gcorr (363K): 0.406736
ZPE: 0.485863
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0 1 0 3 0 -3
 Ni 1.404321 -0.544536 0.814484
 N 3.101088 0.476863 1.376463
 N 2.672318 -1.230997 -0.628148
 C 4.170147 0.157631 0.599719
 C 3.262622 1.351793 2.366861
 C 3.939227 -0.761680 -0.479991
 C 2.389954 -2.029688 -1.657326
 C 5.458929 0.711895 0.795630
 C 4.506086 1.952157 2.641221
 H 2.375893 1.586779 2.960258
 C 4.997324 -1.109644 -1.354639
 C 3.379438 -2.429543 -2.576719
 H 1.340830 -2.331417 -1.765524
 C 5.606525 1.633767 1.859835
 C 6.522900 0.322633 -0.089655
 H 4.586373 2.662195 3.465685
 C 6.301477 -0.551178 -1.120955
 C 4.683365 -1.983024 -2.424205
 H 3.103361 -3.086737 -3.402906
 H 6.581386 2.087429 2.051393
 H 7.515217 0.748186 0.074085
 H 7.114225 -0.833082 -1.793625
 H 5.466320 -2.283982 -3.123707
 C 0.002587 1.954197 0.225484
 C 1.117260 2.599974 -0.403159
 C -1.104705 2.804505 0.551145
 C 1.118419 3.967855 -0.673080
 H 1.975431 1.981136 -0.679772
 C -1.086980 4.171492 0.279943
 H -1.975654 2.348020 1.029982
 C 0.021108 4.777952 -0.335813
 H 1.993184 4.412987 -1.159021
 H -1.957193 4.778336 0.551616
 H 0.027811 5.849716 -0.549116
 N -0.013919 0.628664 0.495075
 Ni -1.221798 -0.764898 -0.071660
 O 0.023239 -1.936253 1.124077
 C 0.260967 -3.297649 0.912816
 H 0.129507 -3.591106 -0.146356
 H 1.282739 -3.594884 1.230698
 H -0.445802 -3.920531 1.504710
 H -1.333434 1.332408 -2.480538
 C -2.354920 1.290388 -2.095557
 N -2.576465 0.451379 -1.091294
 C -3.377829 2.087311 -2.647086
 C -3.826308 0.353401 -0.581391
 C -4.663867 1.998963 -2.135218
 H -3.145003 2.764892 -3.470083
 C -4.007379 -0.557580 0.514135
 C -4.924349 1.107537 -1.066879
 H -5.474703 2.606163 -2.543804
 N -2.905890 -1.224637 0.943466
 C -5.284495 -0.712157 1.108578
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 C -6.212037 0.928297 -0.452018
 C -3.016079 -2.059149 1.974440
 C -5.381942 -1.617131 2.192604
 C -6.385142 0.054465 0.588925
 H -7.054700 1.509282 -0.833348
 C -4.244845 -2.286077 2.622699
 H -2.090506 -2.545742 2.289524
 H -6.345715 -1.775192 2.681670
 H -7.367555 -0.071899 1.049115
 H -4.286426 -2.984352 3.460265
 Cl -1.203341 -2.246684 -1.923759

name: X_Zn
Opt Eel: -8045.82128132
SP Eel TPSSh-D3BJ: -8094.920281
Gcorr (363K): 0.531690
ZPE: 0.630940
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0 1 0 3 0 -3
 Ni 1.070427 -0.703498 1.413655
 N 2.929252 -0.021008 0.835630
 N 1.915719 -2.488424 0.828817
 C 3.678056 -0.994007 0.255005
 C 3.422186 1.213196 0.898860
 C 3.135245 -2.323084 0.256215
 C 1.353073 -3.694819 0.815189
 C 4.946454 -0.748343 -0.328353
 C 4.676497 1.552903 0.357771
 H 2.795826 1.945257 1.409331
 C 3.853463 -3.383066 -0.351008
 C 1.993686 -4.809625 0.238988
 H 0.341215 -3.775831 1.225322
 C 5.436705 0.578447 -0.268329
 C 5.657273 -1.841455 -0.933382
 H 5.030925 2.581361 0.439040
 C 5.132032 -3.106065 -0.946033
 C 3.242360 -4.660146 -0.342290
 H 1.486132 -5.775454 0.248800
 H 6.408985 0.816137 -0.705431
 H 6.630555 -1.639431 -1.385599
 H 5.677090 -3.930102 -1.411162
 H 3.756077 -5.507804 -0.801145
 C -0.013662 -0.320779 -1.417615
 C 0.697011 -1.387698 -2.036215
 C -0.571649 0.642927 -2.310412
 C 0.857436 -1.469146 -3.422234
 H 1.112647 -2.171683 -1.405430
 C -0.422191 0.551196 -3.693063
 H -1.136692 1.478290 -1.884530
 C 0.302363 -0.503581 -4.272106
 H 1.418881 -2.309596 -3.842521
 H -0.877779 1.315769 -4.330167
 H 0.425191 -0.571039 -5.355888
 N -0.225360 -0.246105 -0.053086
 Ni -1.556891 -1.652320 0.648173
 O -0.480834 -1.482960 2.318798
 C -0.412102 -2.309187 3.435747
 H 0.452095 -3.009589 3.410322
 H -0.309406 -1.714201 4.369042
 H -1.322010 -2.932229 3.524745
 H -1.749166 -3.032554 -2.226732
 C -2.480905 -2.222888 -2.245103
 N -2.676294 -1.577586 -1.101506
 C -3.180017 -1.888727 -3.422225
 C -3.598439 -0.588074 -1.052002
 C -4.121254 -0.871029 -3.390850
 H -2.972180 -2.435952 -4.342942
 C -3.787265 0.061893 0.215250
 C -4.369208 -0.191825 -2.173580
 H -4.678096 -0.593335 -4.288605
 N -2.987578 -0.338563 1.233281
 C -4.771522 1.068695 0.359923
 C -5.344248 0.852235 -2.008543
 C -3.111180 0.239966 2.423585
 C -4.913536 1.644720 1.644395
 C -5.543053 1.450085 -0.791606
 H -5.931633 1.155553 -2.878030
 C -4.083228 1.227808 2.672105
 H -2.404369 -0.091281 3.186599
 H -5.662851 2.422282 1.807919
 H -6.292542 2.236221 -0.676642
 H -4.157229 1.666212 3.668517
 Cl -2.114134 -3.924242 0.947142
 Zn -0.482066 1.591539 0.604180
 Cl -2.002513 3.300107 0.539156
 Cl 0.645661 1.455591 2.717260
 O 1.031704 2.527070 -0.490287
 C 1.571446 3.643856 -0.368954
 C 1.336416 4.661535 0.722062
 N 2.515346 4.104552 -1.206658
 C 1.990535 5.934523 0.171282
 H 1.829309 4.289299 1.636547
 H 0.260770 4.738962 0.932439
 C 3.044486 5.412517 -0.819198
 C 3.040299 3.350314 -2.325191
 H 1.241525 6.531632 -0.370938
 H 2.434306 6.568253 0.950566
 H 3.160248 6.052131 -1.706736
 H 4.038483 5.287512 -0.353917
 H 2.828235 3.872272 -3.272347
 H 4.130076 3.228260 -2.225514
 H 2.559150 2.364105 -2.333918

name: PreVII
Opt Eel: -10782.1408502
SP Eel TPSSh-D3BJ: -10850.234737
Gcorr (363K): 0.707454
ZPE: 0.828335
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0 3
 Ni 0.942979 0.143377 -0.084534
 C 3.170354 1.753638 0.344952
 C 1.400061 2.664961 1.513796
 C 4.081976 2.727971 0.814058
 C 3.613445 0.719896 -0.527417
 C 2.239413 3.651838 2.064385
 H 0.339959 2.637466 1.759438
 C 3.578607 3.698535 1.712085
 C 5.443651 2.667844 0.353912
 C 4.946054 0.691388 -0.998482
 H 1.813236 4.377090 2.758180
 H 4.242301 4.466341 2.114891
 C 5.856229 1.698585 -0.523077
 H 6.145432 3.422183 0.715938
 C 5.277161 -0.336016 -1.914926
 C 3.004283 -1.152401 -1.741293
 H 6.889607 1.673107 -0.875216
 H 6.290186 -0.401638 -2.317064
 C 4.297206 -1.242180 -2.291718
 H 2.220983 -1.870655 -1.982269
 H 4.513497 -2.038169 -3.005050
 N 1.846652 1.733020 0.670532
 N 2.675717 -0.202038 -0.867562
 Ni -2.475163 0.017404 -0.786972
 N -4.525446 -0.211825 -1.261234
 N -3.030014 -1.399072 0.607376
 C -5.161009 -1.041604 -0.394988
 C -5.235523 0.351898 -2.235442
 C -4.359771 -1.665205 0.620110
 C -2.251100 -1.990785 1.506886
 C -6.551736 -1.317285 -0.464280
 C -6.616611 0.130513 -2.394941
 H -4.687654 1.013906 -2.908326
 C -4.963503 -2.534593 1.564173
 C -2.758999 -2.855578 2.494990
 H -1.182863 -1.790460 1.425270
 C -7.281158 -0.698436 -1.506588
 C -7.139926 -2.196449 0.507944
 H -7.144084 0.621067 -3.214359
 C -6.377041 -2.777077 1.485079
 C -4.115367 -3.125196 2.531792
 H -2.055881 -3.314449 3.189758
 H -8.353705 -0.882837 -1.599694
 H -8.212532 -2.392578 0.447572
 H -6.829853 -3.445198 2.220865
 H -4.538888 -3.795411 3.283285
 C -0.555331 -2.001922 -1.147083
 C -1.079654 -3.349135 -1.078406
 C -1.192814 -1.118291 -2.111942
 C -2.123031 -3.758165 -1.883035
 H -0.634033 -4.025068 -0.342846
 C -2.226269 -1.598070 -2.958113
 H -0.640889 -0.218745 -2.402003
 C -2.727480 -2.885574 -2.829716
 H -2.500187 -4.781263 -1.784368
 H -2.636454 -0.915875 -3.708327
 H -3.558029 -3.230274 -3.449758
 C -1.375516 1.052859 1.385669
 C -0.847333 0.564110 2.611774
 C -2.604747 1.774463 1.453705
 C -1.530010 0.749931 3.815017
 H 0.102503 0.020820 2.589050
 C -3.284184 1.940623 2.661201
 H -3.002561 2.209671 0.530757
 C -2.758990 1.426292 3.856346
 H -1.098827 0.348558 4.737312
 H -4.231696 2.487659 2.670400
 H -3.291259 1.558381 4.801353
 N 0.414018 -1.591342 -0.350041
 Zn 1.391467 -2.524272 1.079455
 Cl 0.420002 -4.217038 2.296675
 Cl 2.582660 -1.093650 2.451257
 O 2.757165 -3.659548 0.028950
 C 4.002985 -3.738611 -0.002815
 C 4.983853 -3.235513 1.028515
 N 4.677099 -4.345929 -0.992630
 H 4.687142 -2.240676 1.387049
 C 6.335508 -3.307705 0.309222
 H 4.926591 -3.920913 1.892688
 C 6.124131 -4.374246 -0.777464
 C 4.044353 -5.026720 -2.101351
 H 6.555985 -2.339235 -0.163613
 H 7.169481 -3.559947 0.977286
 H 6.648117 -4.145845 -1.717549
 H 6.430665 -5.383105 -0.448770
 H 4.436688 -4.644298 -3.056329
 H 4.238994 -6.110559 -2.048313
 H 2.963421 -4.846882 -2.046340
 N -0.812092 0.776282 0.155423
 Zn -0.437055 2.189380 -1.191035
 Cl -2.483809 2.009412 -2.365736
 Cl 1.257982 2.384129 -2.693781
 O -0.701845 3.978224 -0.285062
 C 0.016405 4.992454 -0.122789
 C 1.101526 5.502759 -1.037762
 N -0.116829 5.820757 0.919804
 H 1.737459 4.672165 -1.373322
 C 1.807767 6.579608 -0.204471
 H 0.607611 5.912232 -1.935970
 C 0.768233 6.985440 0.853475
 C -1.107087 5.655794 1.963435
 H 2.690322 6.148824 0.289972
 H 2.138531 7.438103 -0.803445
 H 1.207779 7.176738 1.843444
 H 0.183593 7.874299 0.559106
 H -0.617492 5.661800 2.949276
 H -1.842093 6.476183 1.927262
 H -1.618880 4.697604 1.809985

name: VII
Opt Eel: -5391.02615949
SP Eel TPSSh-D3BJ: -5425.087202
Gcorr (363K): 0.337065
ZPE: 0.413092
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0 3
 Ni 0.605826 -0.604706 -1.098124
 N 2.166778 0.670563 -1.366970
 N 1.926142 -1.507197 0.148887
 C 3.209935 0.373592 -0.549560
 C 2.236339 1.752967 -2.137916
 C 3.080677 -0.800530 0.267414
 C 1.759922 -2.605024 0.882957
 C 4.381368 1.165588 -0.474768
 C 3.361522 2.599172 -2.136273
 H 1.370397 1.958825 -2.770910
 C 4.124165 -1.170714 1.149553
 C 2.741550 -3.051917 1.787886
 H 0.818541 -3.140848 0.742970
 C 4.433763 2.310732 -1.306065
 C 5.428084 0.768478 0.427429
 H 3.372624 3.474257 -2.787588
 C 5.305023 -0.351933 1.205943
 C 3.922096 -2.337771 1.926299
 H 2.558301 -3.955953 2.370438
 H 5.315603 2.954612 -1.284699
 H 6.328734 1.383741 0.479353
 H 6.105927 -0.644255 1.888187
 H 4.697104 -2.663596 2.623337
 C -1.159081 1.664589 -0.446202
 C -0.169124 2.443344 0.230883
 C -2.427676 2.296607 -0.640523
 C -0.428122 3.744976 0.660671
 H 0.801160 1.983384 0.429471
 C -2.672506 3.600214 -0.213144
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 H -3.212610 1.716315 -1.136573
 C -1.677531 4.346268 0.441458
 H 0.358370 4.299655 1.182383
 H -3.658521 4.042627 -0.387237
 H -1.875109 5.366323 0.779682
 N -0.927784 0.393505 -0.869332
 Zn -2.296921 -0.993039 -0.982208
 H -0.285677 -1.464812 2.860910
 C -0.691960 -0.516653 2.482655
 C -2.047475 -0.723181 1.851580
 C -0.931503 0.549272 3.559175
 H -0.031923 -0.176177 1.666566
 O -2.351330 -1.627283 1.038301
 N -2.873365 0.252763 2.253117
 C -2.238869 1.237975 3.128995
 H -1.069503 0.069451 4.539632
 H -0.104338 1.266574 3.644230
 C -4.227035 0.420573 1.766984
 H -2.901886 1.475221 3.974341
 H -2.061997 2.164743 2.556859
 H -4.951577 0.228734 2.575347
 H -4.364326 1.450002 1.404459
 H -4.396704 -0.281704 0.939651
 Cl -4.408345 -1.303315 -1.704097
 Cl -0.649375 -2.622161 -1.750962

name: VII_Zn
Opt Eel: -8416.32264566
SP Eel TPSSh-D3BJ: -8470.735283
Gcorr (363K): 0.462100
ZPE: 0.558328
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0 3
 Ni 1.074225 -0.079320 -1.389412
 N 2.312508 1.538864 -1.202187
 N 2.835642 -1.078297 -1.064714
 C 3.549575 1.176160 -0.774262
 C 2.004832 2.832015 -1.264375
 C 3.825956 -0.229811 -0.687877
 C 3.031596 -2.388867 -0.957488
 C 4.536068 2.115951 -0.386705
 C 2.921634 3.838280 -0.904839
 H 0.991714 3.072082 -1.590848
 C 5.076966 -0.676672 -0.195743
 C 4.241072 -2.927155 -0.476225
 H 2.193835 -3.029627 -1.239596
 C 4.186212 3.485093 -0.464695
 C 5.802314 1.637552 0.093982
 H 2.614797 4.883196 -0.966567
 C 6.060680 0.296440 0.190231
 C 5.265880 -2.076653 -0.097184
 H 4.346661 -4.010278 -0.399685
 H 4.912289 4.245269 -0.168523
 H 6.552820 2.371430 0.394824
 H 7.020718 -0.059785 0.569304
 H 6.211065 -2.468359 0.284692
 C 1.460719 -0.130915 1.488609
 C 1.953294 1.133104 1.908995
 C 2.109891 -1.269305 2.035647
 C 3.042411 1.248679 2.774590
 H 1.465449 2.036769 1.532451
 C 3.198971 -1.150270 2.900884
 H 1.748319 -2.263401 1.756242
 C 3.687949 0.109281 3.273703
 H 3.394053 2.245524 3.056711
 H 3.674798 -2.057675 3.284922
 H 4.546413 0.200858 3.943577
 N 0.426282 -0.246434 0.553046
 Cl -0.031462 -2.042935 -2.246337
 Cl 0.416088 -4.172064 0.728894
 Zn -0.742417 1.322318 0.318945
 Cl -0.815123 1.292886 -2.122700
 H -6.551705 1.917338 -0.097080
 C -5.852941 2.500989 0.527562
 C -5.006725 3.486263 -0.292805
 N -4.847700 1.603458 1.102922
 H -6.428425 2.982954 1.331122
 C -3.738866 2.691844 -0.627727
 H -4.744066 4.353670 0.331840
 H -5.539223 3.849757 -1.181366
 C -3.666994 1.665314 0.477203
 C -5.156943 0.686990 2.180364
 H -2.814463 3.283788 -0.655446
 H -3.817429 2.146590 -1.583195
 O -2.691221 0.932760 0.771369
 H -5.448636 1.251121 3.080189
 H -5.990162 0.028906 1.890982
 H -4.265643 0.085498 2.394265
 Cl -0.624810 3.524212 0.917084
 Zn -0.287974 -2.067401 0.185566
 O -2.266682 -2.244926 0.530853
 C -3.290098 -1.955442 -0.129331
 N -4.533092 -2.207859 0.305900
 C -3.355926 -1.354135 -1.510120
 C -5.566030 -1.895715 -0.683746
 C -4.831135 -2.914855 1.533381
 C -4.833896 -0.979206 -1.674968
 H -2.646667 -0.521526 -1.611304
 H -3.035847 -2.134906 -2.220073
 H -5.918958 -2.830959 -1.153232
 H -6.424568 -1.412942 -0.194193
 H -5.603561 -2.375701 2.101014
 H -5.197748 -3.931006 1.311576
 H -3.912013 -2.981443 2.128303
 H -4.993202 0.070991 -1.393349
 H -5.198016 -1.110881 -2.702298

name: P
Opt Eel: -3369.60684188
SP Eel TPSSh-D3BJ: -3389.569942
Gcorr (363K): 0.379951
ZPE: 0.455105
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0 1
 O -0.284450 1.531570 -0.755407
 C -1.440598 1.834258 -1.136109
 C -2.150928 1.229396 -2.323188
 C -3.349772 2.159056 -2.543454
 H -2.450142 0.207990 -2.029207
 H -1.473327 1.139069 -3.183486
 C -3.563602 2.813133 -1.169374
 H -3.091815 2.931091 -3.283984
 H -4.248787 1.635260 -2.894161
 H -3.883958 3.863527 -1.231095
 H -4.292821 2.265064 -0.548124
 N -2.241885 2.725401 -0.546074
 C -1.947584 3.382191 0.709751
 H -1.963416 4.475702 0.577130
 H -2.701974 3.099315 1.459240
 H -0.960300 3.058265 1.062819
 O 2.040262 -0.181388 0.145017
 C 2.974652 0.596432 -0.147342
 C 2.939238 2.106342 -0.157529
 N 4.205931 0.180687 -0.479500
 C 4.225186 2.492934 -0.898078
 H 2.921325 2.434231 0.895349
 H 2.011007 2.464060 -0.622522
 C 5.147479 1.279662 -0.700425
 C 4.622157 -1.205616 -0.472214
 H 4.012739 2.622459 -1.970263
 H 4.678832 3.420588 -0.524765
 H 5.779196 1.065361 -1.575130
 H 5.804189 1.385464 0.181287
 H 5.044547 -1.480288 -1.451473
 H 5.388094 -1.371455 0.303023
 H 3.745294 -1.830206 -0.260288
 Zn 0.165526 0.348643 0.851678
 N -0.858136 -1.366363 0.509935
 C -0.480404 -2.635161 0.063045
 C -0.912534 -3.833245 0.672841
 C 0.425258 -2.726997 -1.016862
 C -0.471949 -5.073569 0.199389
 H -1.577929 -3.787337 1.536985
 C 0.869694 -3.967727 -1.476881
 H 0.775136 -1.801890 -1.477706
 C 0.419250 -5.152254 -0.877198
 H -0.821486 -5.987333 0.688034
 H 1.569926 -4.010910 -2.315858
 H 0.765410 -6.123277 -1.239594
 C -3.331404 -1.827121 0.655473
 H -3.489649 -2.379535 1.598496
 H -3.142399 -2.588891 -0.116972
 C -2.097411 -0.958622 0.837381
 O -2.218557 0.217036 1.268685
 C -4.578417 -1.010276 0.325770
 H -4.475205 -0.499639 -0.644852
 H -5.464173 -1.662806 0.273149
 H -4.753494 -0.243256 1.094032
 Cl 0.794124 1.582787 2.660160

name: P_Zn
Opt Eel: -6394.87553668
SP Eel TPSSh-D3BJ: -6435.205942
Gcorr (363K): 0.505450
ZPE: 0.601101
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0 1
 O 0.221582 1.986452 -0.651485
 C -0.530463 1.718703 -1.619726
 C -0.298157 0.700287 -2.708894
 C -1.293044 1.112848 -3.800505
 H -0.548740 -0.285135 -2.284314
 H 0.753775 0.685685 -3.023055
 C -2.394535 1.854543 -3.028974
 H -0.810752 1.798998 -4.513539
 H -1.693848 0.254367 -4.353997
 H -2.822427 2.703890 -3.581488
 H -3.209713 1.178605 -2.723213
 N -1.695939 2.334841 -1.833745
 C -2.290758 3.287445 -0.920180
 H -2.347014 4.283344 -1.388314
 H -3.307970 2.963461 -0.655451
 H -1.669133 3.337050 -0.018360
 O 2.964587 1.831907 0.635268
 C 3.803514 1.575814 -0.259367
 C 3.514716 1.141989 -1.677751
 N 5.125866 1.700731 -0.095163
 C 4.883198 0.699064 -2.209347
 H 3.112329 2.018505 -2.213564
 H 2.743451 0.359904 -1.697716
 C 5.890679 1.440397 -1.316128
 C 5.748496 2.180740 1.120107
 H 5.000583 -0.384913 -2.068999
 H 5.028659 0.928010 -3.273097
 H 6.781342 0.840722 -1.078044
 H 6.224570 2.397790 -1.753250
 H 6.549557 1.491735 1.426342
 H 6.181659 3.182058 0.960732
 H 4.983303 2.233369 1.904287
 Zn 1.120696 0.945372 0.786772
 N 1.736587 -0.965194 0.531939
 C 3.050292 -1.436462 0.703397
 C 3.759332 -1.022086 1.846800
 C 3.713000 -2.205939 -0.270868
 C 5.100278 -1.371646 2.012287
 H 3.241342 -0.412357 2.590047
 C 5.054475 -2.560634 -0.093626
 H 3.183150 -2.499512 -1.179012
 C 5.756059 -2.142422 1.042842
 H 5.638251 -1.037361 2.902955
 H 5.558064 -3.154061 -0.860968
 H 6.807436 -2.410562 1.170734
 C 0.653640 -3.181876 0.052117
 H -0.162980 -3.527370 0.709732
 H 1.594301 -3.620780 0.411556
 C 0.682473 -1.682648 0.193254
 O -0.400989 -1.017872 0.007930
 C 0.357081 -3.624483 -1.385314
 H 1.139024 -3.279713 -2.080474
 H 0.308069 -4.722802 -1.438790
 H -0.608494 -3.223735 -1.732363
 Cl 0.316116 1.520503 2.801138
 Zn -2.291337 -1.567004 -0.149402
 Cl -3.006089 -1.724827 -2.300565
 Cl -2.894134 -3.206822 1.274738
 O -2.957327 0.159143 0.634381
 C -4.156327 0.456625 0.840788
 C -5.374332 -0.268122 0.323705
 N -4.538018 1.484840 1.606226
 C -6.511602 0.729921 0.573979
 H -5.475211 -1.193510 0.917539
 H -5.232424 -0.565545 -0.724635
 C -5.993596 1.594875 1.733950
 C -3.625227 2.297511 2.385753
 H -6.655923 1.357558 -0.318564
 H -7.468262 0.247587 0.813396
 H -6.300042 2.648665 1.662764
 H -6.303911 1.210115 2.721230
 H -3.699474 3.353995 2.084748
 H -3.879073 2.216203 3.454878
 H -2.601881 1.933948 2.225518

name: NiClOMe
Opt Eel: -2654.70904055
SP Eel TPSSh-D3BJ: -2669.780657
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Gcorr (363K): 0.160994
ZPE: 0.215546
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0 3
 Ni 1.694453 -0.058111 0.032356
 N 0.146311 -1.340220 -0.091824
 N 0.225598 1.318825 -0.005877
 C -1.045838 -0.689250 -0.116347
 C 0.157899 -2.670252 -0.124858
 C -1.002884 0.744266 -0.072799
 C 0.320097 2.645019 0.032521
 C -2.290833 -1.361204 -0.179266
 C -1.029233 -3.425261 -0.183531
 H 1.137691 -3.152799 -0.104622
 C -2.203934 1.493932 -0.097368
 C -0.818099 3.473712 0.013925
 H 1.328354 3.062945 0.076905
 C -2.254102 -2.776068 -0.212852
 C -3.497308 -0.578959 -0.202665
 H -0.968002 -4.514213 -0.207488
 C -3.455737 0.789718 -0.164128
 C -2.080368 2.903354 -0.050990
 H -0.690095 4.556539 0.049284
 H -3.187618 -3.340769 -0.260048
 H -4.453573 -1.103793 -0.251691
 H -4.378161 1.373775 -0.182171
 H -2.977599 3.525702 -0.066775
 O 2.296325 -0.178038 1.768750
 C 1.463438 -0.255034 2.865460
 H 0.793724 0.630795 2.980989
 H 0.795151 -1.149251 2.860768
 H 2.050449 -0.318444 3.809249
 Cl 2.856026 0.109814 -1.889358

name: TS5
Opt Eel: -5039.07762405
Freq: -235.1149
SP Eel TPSSh-D3BJ: -5066.928521
Gcorr (363K): 0.566726
ZPE: 0.656080
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0 1 0 3 0 -3
 Ni 1.190203 0.030281 0.742274
 C 3.991923 0.308511 0.547936
 C 3.531979 -1.267598 2.182774
 C 5.392843 0.193053 0.732892
 C 3.469462 1.247905 -0.396058
 C 4.902680 -1.439708 2.441462
 H 2.771532 -1.837882 2.717566
 C 5.841742 -0.720779 1.713602
 C 6.262875 1.015777 -0.064240
 C 4.343392 2.067748 -1.153623
 H 5.210934 -2.146686 3.213483
 H 6.911813 -0.844871 1.893265
 C 5.760990 1.914678 -0.967869
 H 7.341277 0.914338 0.076135
 C 3.747628 2.996073 -2.038708
 C 1.577097 2.215097 -1.315579
 H 6.432510 2.540670 -1.559571
 H 4.378316 3.648271 -2.646601
 C 2.362683 3.069383 -2.109613
 H 0.487831 2.263038 -1.343330
 H 1.869530 3.782388 -2.772204
 N 3.078755 -0.422265 1.251198
 N 2.114776 1.315588 -0.491464
 Ni -1.195900 -0.483201 0.602016
 N -3.100832 -0.363464 1.279117
 N -2.090664 0.242746 -1.098183
 C -3.983981 0.031978 0.325206
 C -3.558424 -0.672957 2.490788
 C -3.438028 0.352470 -0.961794
 C -1.543587 0.529963 -2.277193
 C -5.377979 0.138098 0.556035
 C -4.925348 -0.593509 2.816052
 H -2.812963 -1.004799 3.216090
 C -4.293660 0.769903 -2.011579
 C -2.310213 0.949294 -3.380976
 H -0.461420 0.421555 -2.351845
 C -5.839555 -0.188806 1.853301
 C -6.225557 0.563955 -0.524673
 H -5.249788 -0.854162 3.824722
 C -5.705444 0.865106 -1.755866
 C -3.685753 1.071601 -3.253693
 H -1.808222 1.172613 -4.323662
 H -6.905262 -0.121668 2.082582
 H -7.299382 0.642166 -0.341551
 H -6.358558 1.186919 -2.569940
 H -4.302454 1.397006 -4.094322
 C -0.519968 2.342090 1.368691
 C -1.830387 2.850190 1.079550
 C 0.480567 3.342667 1.627044
 C -2.101202 4.217240 1.040323
 H -2.628650 2.133809 0.886113
 C 0.193741 4.704283 1.586211
 H 1.494088 2.997698 1.853014
 C -1.099692 5.169973 1.288916
 H -3.120104 4.546496 0.809860
 H 0.996837 5.421603 1.786381
 H -1.318504 6.240031 1.254245
 C 0.597588 -1.850252 -1.479187
 C 1.889569 -1.657860 -2.062918
 C -0.380261 -2.456339 -2.329075
 C 2.172543 -2.029881 -3.375657
 H 2.663155 -1.202537 -1.440900
 C -0.084353 -2.833530 -3.640516
 H -1.390469 -2.596964 -1.940098
 C 1.191283 -2.626451 -4.185583
 H 3.176748 -1.854546 -3.775032
 H -0.870299 -3.286841 -4.253331
 H 1.414991 -2.916648 -5.215128
 N 0.331512 -1.492077 -0.188840
 N -0.219062 1.029481 1.428673
 C -0.857738 -3.877798 0.656050
 H -0.747770 -4.783759 1.281175
 H -0.397328 -4.114416 -0.315501
 C -0.072137 -2.780635 1.362132
 O -0.637853 -1.942292 2.115810
 O 1.191888 -3.139038 1.759560
 C 1.963232 -3.980429 0.909165
 H 2.982301 -3.988593 1.319183
 H 1.580898 -5.014493 0.896598
 H 1.987407 -3.579659 -0.114919
 C -2.333771 -3.551349 0.490191
 H -2.470989 -2.600575 -0.050077
 H -2.843924 -4.344170 -0.079224
 H -2.828921 -3.447935 1.466733

name: TS5_Zn
Opt Eel: -11089.6319551
Freq: -119.9897
SP Eel TPSSh-D3BJ: -11158.216165
Gcorr (363K): 0.822063
ZPE: 0.950551
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 Ni 0.633603 -0.162505 -0.514834
 C 2.584371 1.538374 -1.442344
 C 1.371946 2.633183 0.188374
 C 3.353376 2.682160 -1.755243
 C 2.833440 0.301600 -2.097820
 C 2.067358 3.830847 -0.072100
 H 0.601146 2.596156 0.953809
 C 3.058879 3.867777 -1.038132
 C 4.378222 2.559653 -2.755965
 C 3.865158 0.185531 -3.057116
 H 1.813926 4.718509 0.508619
 H 3.614170 4.784623 -1.245977
 C 4.625107 1.362455 -3.379380
 H 4.969438 3.444063 -3.002502
 C 4.091082 -1.103347 -3.598272
 C 2.311837 -1.947811 -2.187117
 H 5.418498 1.280252 -4.125291
 H 4.873689 -1.251369 -4.345306
 C 3.327089 -2.162745 -3.139970
 H 1.714553 -2.774033 -1.804462
 H 3.496808 -3.177175 -3.502397
 N 1.613792 1.508025 -0.482339
 N 2.043745 -0.734958 -1.703419
 Ni -2.010080 -0.954528 0.155485
 N -3.585896 -1.469879 -0.885209
 N -3.280351 -0.984105 1.665097
 C -4.719806 -1.511562 -0.128599
 C -3.730036 -1.498579 -2.213423
 C -4.543419 -1.306138 1.269339
 C -3.046609 -0.881398 2.976219
 C -6.015757 -1.710894 -0.661255
 C -4.981786 -1.648969 -2.836016
 H -2.821820 -1.402825 -2.808448
 C -5.638138 -1.432121 2.157729
 C -4.061444 -1.032143 3.938758
 H -2.022710 -0.663368 3.278944
 C -6.128129 -1.789236 -2.068377
 C -7.123389 -1.805655 0.251397
 H -5.025291 -1.671241 -3.925861
 C -6.940549 -1.689565 1.604301
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 H -3.804682 -0.928511 4.993972
 H -7.105591 -1.939430 -2.531570
 H -8.120082 -1.976719 -0.161035
 H -7.787148 -1.776160 2.288726
 H -6.173864 -1.370651 4.266373
 C -0.754229 -2.229643 -1.996105
 C -1.370662 -3.506802 -2.070827
 C -0.457799 -1.592127 -3.230933
 C -1.642866 -4.120192 -3.293126
 H -1.677034 -3.988267 -1.142149
 C -0.740206 -2.207435 -4.452909
 H -0.054128 -0.579601 -3.207688
 C -1.323646 -3.480800 -4.500188
 H -2.123079 -5.103053 -3.304969
 H -0.508863 -1.677859 -5.381957
 H -1.538530 -3.960464 -5.458248
 C -0.574301 0.804348 1.920641
 C 0.484313 0.268079 2.693988
 C -1.448044 1.726075 2.555305
 C 0.658407 0.635843 4.030632
 H 1.157681 -0.445385 2.221623
 C -1.260553 2.095165 3.888013
 H -2.284816 2.128360 1.979714
 C -0.207098 1.554106 4.641054
 H 1.484614 0.193580 4.595048
 H -1.950983 2.808122 4.348300
 H -0.065778 1.843448 5.685428
 N -0.514076 -1.652406 -0.761249
 N -0.779155 0.422754 0.597892
 Zn -1.847340 1.593392 -0.638618
 Cl -4.125879 1.873612 -0.302979
 Cl -1.134923 1.879362 -2.800134
 O -1.376156 3.512565 0.087165
 C -1.775130 4.622177 -0.317625
 C -2.577214 4.911712 -1.563127
 N -1.563264 5.771648 0.346825
 H -2.194093 4.318001 -2.404472
 C -2.461711 6.432320 -1.720327
 H -3.607376 4.570412 -1.362953
 C -2.186107 6.930956 -0.293138
 C -0.942208 5.850388 1.651480
 H -1.604400 6.675878 -2.366621
 H -3.358579 6.895114 -2.153283
 H -1.505826 7.794908 -0.257004
 H -3.111527 7.199317 0.247425
 H -0.071226 6.523896 1.622836
 H -1.661581 6.235888 2.392624
 H -0.622686 4.843416 1.947596
 C 0.548362 -2.928740 0.646150
 C -0.542576 -3.030221 1.684524
 O 1.493653 -2.108993 0.853982
 O 0.887521 -3.998169 -0.109460
 H -1.442059 -3.514567 1.279202
 H -0.797868 -1.984504 1.900814
 C -0.062139 -3.716455 2.968489
 Zn 3.409908 -2.146574 1.294955
 C 0.264422 -5.277742 0.035010
 H 0.889613 -3.278440 3.308046
 H -0.815171 -3.585436 3.761794
 H 0.092194 -4.797781 2.827620
 Cl 4.863083 -3.112881 -0.126963
 Cl 3.567993 -2.648126 3.504842
 O 3.653305 -0.147207 1.355269
 H 0.337702 -5.775085 -0.940150
 H 0.815505 -5.864207 0.786697
 H -0.791067 -5.204011 0.326690
 C 4.606773 0.622041 1.102238
 N 4.733822 1.836802 1.650375
 C 5.748966 0.380028 0.146487
 C 3.824164 2.383919 2.636283
 C 5.896129 2.577560 1.156193
 C 6.752552 1.486393 0.492161
 H 6.122376 -0.647813 0.249987
 H 5.354120 0.473152 -0.877136
 H 3.503660 3.391687 2.337350
 H 2.950949 1.724872 2.709604
 H 4.323071 2.446558 3.617409
 H 6.404135 3.078571 1.993109
 H 5.561985 3.350219 0.442265
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 H 7.491220 1.108056 1.214765
 H 7.293991 1.864961 -0.384837

name: TS6
Opt Eel: -8064.39699212
Freq: -237.1708
SP Eel TPSSh-D3BJ: -8112.603116
Gcorr (363K): 0.693050
ZPE: 0.802678
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 Ni 1.253939 0.443475 -0.497423
 N 3.236465 -0.028516 -0.329671
 N 2.020038 2.330656 -0.600518
 C 4.017765 1.084738 -0.270519
 C 3.821983 -1.222056 -0.263005
 C 3.363044 2.353930 -0.416634
 C 1.375219 3.474988 -0.798922
 C 5.423050 1.035395 -0.095339
 C 5.213088 -1.369172 -0.096706
 H 3.173579 -2.094030 -0.343597
 C 4.115687 3.554893 -0.384019
 C 2.034961 4.719334 -0.787544
 H 0.300160 3.407357 -0.978080
 C 6.016733 -0.246209 -0.000333
 C 6.161910 2.267361 -0.040796
 H 5.635335 -2.373872 -0.045869
 C 5.535776 3.477301 -0.179060
 C 3.402932 4.764044 -0.569279
 H 1.458662 5.631430 -0.949417
 H 7.096771 -0.333895 0.136237
 H 7.242817 2.214965 0.105785
 H 6.107555 4.406989 -0.144827
 H 3.938419 5.715625 -0.548078
 C 0.466828 1.036234 2.308570
 C 1.750988 1.508064 2.730765
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 C 1.952344 2.053811 3.997777
 H 2.586701 1.416235 2.034970
 C -0.372531 1.702968 4.534011
 H -1.575449 0.781631 2.991496
 C 0.898053 2.163577 4.919525
 H 2.954506 2.397277 4.274157
 H -1.210644 1.767179 5.235526
 H 1.062528 2.591155 5.911503
 N 0.267864 0.445396 1.110838
Ni -1.266872 0.248078 0.049649
 H -0.193898 1.241890 -4.171725
 C -1.212873 1.593210 -4.011354
 C -1.921256 1.117131 -2.878541
 C -1.786216 2.536356 -4.868662
 C -3.213560 1.651501 -2.644131
 N -1.408807 0.212458 -1.967864
 C -3.067703 3.049507 -4.628102
 H -1.213210 2.886719 -5.732597
 C -3.772065 2.600028 -3.501297
 H -3.772724 1.296743 -1.775933
 C -0.488044 -0.744162 -2.241591
 H -3.507187 3.789931 -5.301030
 H -4.773005 2.987928 -3.290472
 C -0.550170 -1.592354 -3.492058
 O -0.134941 -1.366489 -1.096721
 O 1.073446 0.263191 -2.481995
 H 0.361413 -2.207056 -3.537291
 H -0.567523 -0.945389 -4.379772
 C -1.784527 -2.500406 -3.479071
 C 2.129305 -0.230565 -3.259898
 H -2.711106 -1.912066 -3.387834
 H -1.837446 -3.082985 -4.412580
 H -1.743909 -3.213367 -2.640349
 H 3.018759 0.418952 -3.143638
 H 2.422768 -1.262909 -2.988174
 H 1.865484 -0.223017 -4.336697
 H -1.113258 3.364911 0.613517
 C -2.131784 3.072827 0.871811
 N -2.445497 1.791400 0.704599
 C -3.053892 4.016368 1.363068
 C -3.694085 1.377267 1.040474
 C -4.339150 3.612006 1.689257
 H -2.743011 5.055737 1.477943
 C -3.976951 -0.018429 0.872940
 C -4.695653 2.251618 1.531513
 H -5.075118 4.325133 2.066765
 N -2.959349 -0.799334 0.426288
 C -5.268807 -0.523112 1.163506
 C -5.994707 1.714670 1.833047
 C -3.185948 -2.094124 0.219958
 C -5.482616 -1.906337 0.948992
 C -6.271127 0.385464 1.650702
 H -6.762172 2.394772 2.208610
 C -4.438951 -2.684359 0.472273
 H -2.348392 -2.694442 -0.141568
 H -6.462053 -2.342032 1.158262
 H -7.263543 -0.010799 1.876125
 H -4.563773 -3.753080 0.291034
 Zn 0.533987 -3.195891 -0.807485
 Cl 2.212166 -3.873442 -2.176943
 Cl -1.053645 -4.791542 -0.425962
 O 1.463070 -2.902648 0.963877
 C 0.981051 -2.588219 2.080080
 C -0.475257 -2.506536 2.449291
 C -0.461871 -2.419760 3.980803
 H -1.025758 -3.362201 2.035602
 H -0.851447 -1.586799 1.968881
 C 0.945350 -1.899125 4.319723
 H -1.246108 -1.762336 4.378633
 H -0.601569 -3.421357 4.414911
 H 0.970989 -0.806353 4.462001
 H 1.380481 -2.376046 5.210661
 N 1.731166 -2.255771 3.135481
 C 3.172589 -2.126481 3.104641
 H 3.465551 -1.064197 3.114708
 H 3.607334 -2.624806 3.983960
 H 3.548326 -2.600132 2.190539

name: TS4
Opt Eel: -5698.54108093
Freq: -35.5006
SP Eel TPSSh-D3BJ: -5733.075113
Gcorr (363K): 0.444039
ZPE: 0.531796
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 Ni -1.011636 -0.010479 0.156680
 N -2.283923 1.537260 -0.248788
 N -2.698745 -1.099800 -0.258219
 C -3.543154 1.107293 -0.525023
 C -2.052725 2.844870 -0.182552
 C -3.762428 -0.312987 -0.545766
 C -2.836056 -2.421431 -0.296681
 C -4.620401 1.990508 -0.785885
 C -3.062389 3.799997 -0.411409
 H -1.032672 3.151986 0.055484
 C -5.042780 -0.831714 -0.860180
 C -4.068850 -3.031407 -0.603500
 H -1.937248 -3.012105 -0.091794
 C -4.344724 3.377567 -0.721442
 C -5.912895 1.439813 -1.092825
 H -2.816914 4.860904 -0.345999
 C -6.114783 0.085946 -1.133999
 C -5.173865 -2.241573 -0.879734
 H -4.137267 -4.120235 -0.619014
 H -5.143716 4.097181 -0.912421
 H -6.734107 2.130383 -1.295679
 H -7.099223 -0.321946 -1.372859
 H -6.140962 -2.691051 -1.115759
 C 1.725241 1.091103 0.674775
 C 1.570103 2.180247 -0.241926
 C 2.909296 1.131366 1.478791
 C 2.496043 3.221097 -0.326546
 H 0.700895 2.158118 -0.903926
 C 3.831738 2.173192 1.383420
 H 3.078008 0.317115 2.187513
 C 3.641238 3.237388 0.485720
 H 2.326380 4.029544 -1.045486
 H 4.718231 2.159729 2.026266
 H 4.366170 4.052471 0.419332
 N 0.793974 0.104571 0.800045
 Zn 1.201400 -1.509496 -0.252222
 H 3.360016 -0.670589 -3.496428
 C 3.315210 0.076446 -2.684130
 C 3.776668 -0.612029 -1.423587
 C 4.329336 1.211016 -2.868354
 H 2.267299 0.391921 -2.590835
 O 3.152645 -1.480851 -0.766521
 N 5.017601 -0.211727 -1.126811
 C 5.571207 0.732678 -2.099401
 H 4.553649 1.425959 -3.921336
 H 3.942164 2.127707 -2.400749
 C 5.795569 -0.732162 -0.023276
 H 6.299342 0.210932 -2.745039
 H 6.095301 1.544684 -1.574435
 H 6.658849 -1.304545 -0.400236
 H 6.162698 0.096860 0.600215
 H 5.152180 -1.389200 0.574415
 Cl -0.160640 -0.692630 -2.116954
 Cl 0.677746 -3.694839 0.090142
 C -0.455565 -0.183114 2.844565
 O -1.476043 0.180477 2.227660
 O 0.205794 0.655305 3.641408
 C -0.103969 -1.632200 3.053144
 H -0.789928 -1.984495 3.847666
 H -0.386279 -2.163531 2.132703
 C 1.338394 -1.944081 3.423663
 H 1.652415 -1.400285 4.327245
 H 1.455242 -3.022969 3.609283
 H 2.007143 -1.663577 2.596750
 C -0.108894 2.046409 3.485851
 H 0.644119 2.591509 4.067268
 H -0.053019 2.325395 2.425323
 H -1.116665 2.260356 3.871719

name: TS1
Opt Eel: -11354.5719212
Freq: -407.1214
SP Eel TPSSh-D3BJ: -11423.479076
Gcorr (363K): 0.887467
ZPE: 1.021744
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0 1
 Ni -1.732860 0.313142 -0.254039
 C -1.864414 2.744519 1.016832
 C -0.924096 1.192594 2.454824
 C -1.787566 3.790369 1.962927
 C -2.434711 2.968037 -0.268413
 C -0.829631 2.162781 3.469048
 H -0.574325 0.173402 2.611154
 C -1.248648 3.463485 3.230157
 C -2.262081 5.091274 1.573701
 C -2.898302 4.249848 -0.636833
 H -0.409420 1.875350 4.433161
 H -1.167094 4.230929 4.002431
 C -2.789641 5.312031 0.327097
 H -2.193650 5.905693 2.297755
 C -3.439234 4.379698 -1.939710
 C -3.007693 2.023435 -2.301317
 H -3.144239 6.305635 0.045416
 H -3.810187 5.348069 -2.281716
 C -3.489279 3.264818 -2.761743
 H -3.038612 1.135824 -2.930205
 H -3.900048 3.327172 -3.770240
 N -1.431893 1.473053 1.253056
 N -2.488798 1.877751 -1.083441
 N -2.160539 -1.136838 -1.331504
 N -0.864440 -1.263255 0.115761
 C -1.348133 -2.254990 0.969981
 C -2.260791 -1.966530 2.008200
 C -0.870631 -3.579568 0.844313
 C -2.645134 -2.955140 2.915524
 H -2.657358 -0.955253 2.086714
 C -1.263594 -4.564237 1.749087
 H -0.174384 -3.811288 0.038216
 C -2.144067 -4.257688 2.797731
 H -3.344468 -2.706132 3.718540
 H -0.876976 -5.581234 1.641167
 H -2.443401 -5.031073 3.509333
 C -1.604494 -1.519991 -2.541310
 C -0.402330 -2.257952 -2.657023
 C -2.295073 -1.201049 -3.741762
 C 0.121488 -2.575889 -3.912376
 H 0.122720 -2.555380 -1.750834
 C -1.760774 -1.524974 -4.989135
 H -3.271102 -0.714575 -3.669593
 C -0.536862 -2.199916 -5.089173
 H 1.061004 -3.128473 -3.964755
 H -2.313540 -1.250102 -5.892076
 H -0.115531 -2.450526 -6.065616
 Ni 0.948250 -0.710283 -0.033460
 N 0.790650 0.910118 -1.514738
 C 0.924946 2.107201 -0.883258
 C 0.417800 0.902888 -2.793623
 C 0.598585 3.341846 -1.505761
 C 1.448365 2.100729 0.454776
 C 0.084042 2.076014 -3.495319
 H 0.374509 -0.068681 -3.283131
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C 0.146169 3.296423 -2.845829
C 0.748492 4.563759 -0.768416
C 1.628923 3.327499 1.142007
N 1.763284 0.894829 1.010583
H -0.229721 2.001472 -4.537169
H -0.126552 4.223181 -3.354671
C 1.244615 4.555579 0.506158
H 0.466047 5.500430 -1.252756
C 2.197304 3.276690 2.438084
C 2.308933 0.881346 2.224669
H 1.367681 5.486619 1.062746
H 2.352467 4.203059 2.994804
C 2.552840 2.052216 2.967778
H 2.564797 -0.092314 2.637916
H 3.013464 1.966595 3.951575
N 2.041483 -2.182442 0.712173
N 3.113336 -1.851843 -0.049642
C 2.299747 -2.405985 2.059018
C 3.171978 -2.500047 -1.290803
C 1.282029 -2.204685 3.021651
C 3.542828 -2.926172 2.493555
C 3.854895 -1.894680 -2.367253
C 2.641944 -3.798477 -1.457600
C 1.508771 -2.492589 4.364308
H 0.322753 -1.807091 2.694576
C 3.758563 -3.206514 3.844678
H 4.328410 -3.117303 1.758220
C 4.017070 -2.582705 -3.569178
H 4.260053 -0.891083 -2.235262
C 2.823139 -4.481753 -2.661315
H 2.127672 -4.267840 -0.617575
C 2.750052 -2.992544 4.791132
H 0.708395 -2.319511 5.088650
H 4.728570 -3.602130 4.157510
C 3.514421 -3.883141 -3.723960
H 4.547225 -2.100700 -4.394952
H 2.424553 -5.493996 -2.769183
H 2.923439 -3.216538 5.846261
H 3.654188 -4.421459 -4.664314
Zn -4.093429 -1.490272 -0.971502
Cl -5.535976 -0.386025 -2.395053
Cl -4.718403 -3.607178 -0.448455
H -6.508176 -2.091170 0.801254
C -6.751193 -1.069117 1.126124
C -5.482695 -0.290572 1.368680
C -7.494276 -0.964276 2.463139
H -7.282254 -0.574598 0.294837
O -4.451048 -0.288395 0.658881
N -5.620145 0.452927 2.474494
C -6.939584 0.322189 3.096344
H -8.586128 -0.932607 2.352513
H -7.237545 -1.826199 3.097715
C -4.627899 1.398333 2.940224
H -7.549298 1.211340 2.857111
H -6.835522 0.260083 4.189527
H -3.783949 1.370291 2.243710
H -5.051990 2.414672 2.963198
H -4.284881 1.130683 3.951462
Zn 4.759949 -0.744673 0.588741
Cl 5.434796 0.185785 2.580704
Cl 6.519675 -1.925732 -0.283095
O 4.468971 0.818450 -0.711286
C 4.632146 2.058487 -0.692955
N 4.265986 2.855826 -1.706597
C 5.298876 2.884050 0.378695
C 3.761884 2.361876 -2.971034
C 4.664574 4.251855 -1.518935
C 4.975219 4.330103 -0.015520
H 6.379099 2.662464 0.324941
H 4.962994 2.574608 1.376586
H 3.403780 1.335753 -2.828481
H 2.937143 2.998876 -3.317337
H 4.560381 2.367713 -3.732339
H 3.848769 4.920916 -1.830170
H 5.547105 4.468684 -2.146290
H 4.085615 4.676664 0.529089
H 5.796715 5.026857 0.196541

name: TS2
Opt Eel: -11354.5894623
Freq: -11.6610
SP Eel TPSSh-D3BJ: -11423.491056
Gcorr (363K): 0.888636
ZPE: 1.022566
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0 1
Ni -1.503075 1.089563 -0.132326
C -3.510780 2.707090 0.810396
C -4.087294 0.509129 1.228245
C -4.611145 3.217183 1.538815
C -2.668595 3.576618 0.063300
C -5.214960 0.922112 1.963385
H -3.894886 -0.547040 1.048551
C -5.468592 2.271366 2.150384
C -4.803945 4.640800 1.573136
C -2.915882 4.968246 0.051793
H -5.874893 0.160023 2.380462
H -6.328906 2.610757 2.731237
C -3.988665 5.480690 0.860031
H -5.633687 5.038702 2.161207
C -2.107998 5.757804 -0.802210
C -0.974504 3.732790 -1.492010
H -4.158481 6.559436 0.870525
H -2.257218 6.838541 -0.850224
C -1.161289 5.126785 -1.588182
H -0.221639 3.237084 -2.097559
H -0.540672 5.689965 -2.285389
N -3.228944 1.380374 0.695413
N -1.695496 2.964858 -0.675906
Ni 0.450071 -1.015142 -0.186753
N 1.477371 -1.993592 -1.682921
N 0.846727 -2.651808 0.785985
C 1.789730 -3.263150 -1.294561
C 1.720724 -1.675974 -2.953769
C 1.486464 -3.604953 0.055915
C 0.715424 -2.853610 2.099132
C 2.411160 -4.219500 -2.136881
C 2.300054 -2.566211 -3.878000
H 1.456431 -0.670810 -3.267933
C 1.890565 -4.852229 0.592075
C 1.110806 -4.050104 2.725547
H 0.279184 -2.045988 2.681749
C 2.664976 -3.838634 -3.474530
C 2.761462 -5.502785 -1.593218
H 2.468332 -2.223992 -4.900238
C 2.523432 -5.802971 -0.278663
C 1.666357 -5.068699 1.971953
H 0.962330 -4.153824 3.800570
H 3.138639 -4.541817 -4.162891
H 3.240438 -6.229980 -2.252434
H 2.815940 -6.770662 0.134547
H 1.960907 -6.015843 2.428768
C 0.745403 1.128262 -1.981493
C 2.098933 1.481772 -2.208949
C -0.109408 1.067435 -3.108313
C 2.570308 1.748860 -3.494754
H 2.775276 1.540106 -1.354360
C 0.366179 1.345704 -4.392920
H -1.153543 0.781451 -2.956004
C 1.710113 1.685318 -4.601395
H 3.622731 2.011689 -3.634663
H -0.322327 1.286475 -5.240998
H 2.081795 1.897213 -5.606901
C -1.685052 -1.151785 1.716574
C -1.593270 -0.337883 2.869764
C -2.129710 -2.486883 1.892338
C -1.950780 -0.828984 4.128103
H -1.231433 0.687114 2.753763
C -2.489901 -2.969394 3.150760
H -2.168498 -3.139241 1.018149
C -2.407388 -2.145581 4.282563
H -1.870772 -0.172497 4.999814
H -2.829832 -4.004285 3.250210
H -2.689507 -2.525068 5.267813
N 0.299984 0.827952 -0.690329
Zn 1.196368 1.956985 0.728265
Cl 3.365352 2.183204 1.569291
Cl -0.209163 2.842755 2.380562
O 1.526693 3.709410 -0.399277
C 1.804343 4.883795 -0.096154
C 1.796834 5.515176 1.274487
N 2.185161 5.805934 -1.000131
H 0.934950 5.155539 1.851753
C 1.821170 7.018116 0.974735
H 2.706825 5.164670 1.790816
C 2.492766 7.105580 -0.404832
C 2.431130 5.511785 -2.395193
H 0.790535 7.399457 0.905349
H 2.354346 7.606735 1.733209
H 2.091691 7.914290 -1.033951
H 3.587904 7.235131 -0.334982
H 1.852778 6.192546 -3.039162
H 3.502244 5.630687 -2.629423
H 2.131740 4.473873 -2.587517
N -1.319889 -0.691185 0.451905
Zn -2.191114 -1.525036 -1.153367
Cl -1.544422 -3.601339 -1.917284
Cl -3.352497 -0.215585 -2.695928
O -4.012783 -2.189536 -0.270566
C -4.962740 -2.825706 -0.766488
C -5.102830 -3.300604 -2.192581
N -6.035104 -3.226311 -0.060745
H -4.786754 -2.505243 -2.881242
C -6.578930 -3.702413 -2.295762
H -4.406089 -4.145541 -2.322413
C -6.980460 -4.019895 -0.846696
C -6.179265 -3.044958 1.367853
H -7.171138 -2.849689 -2.661798
H -6.753131 -4.553103 -2.968073
H -8.013261 -3.725957 -0.607100
H -6.861725 -5.090000 -0.598711
H -7.093530 -2.473050 1.593044
H -6.241855 -4.023605 1.871072
H -5.301964 -2.502866 1.742002
N 3.032500 -0.824935 0.604029
N 3.809212 -0.691792 -0.360875
C 3.424981 -1.367718 1.865018
C 5.219981 -0.816847 -0.255999
C 2.842153 -0.815220 3.017305
C 4.189021 -2.544479 1.953900
C 5.954963 -0.142858 0.735810
C 5.876805 -1.525685 -1.275027
C 3.093605 -1.391580 4.263040
H 2.219253 0.073685 2.918609
C 4.405721 -3.131125 3.202119
H 4.589121 -3.007579 1.051108
C 7.348482 -0.217586 0.718752
H 5.423181 0.455239 1.478332
C 7.269708 -1.623372 -1.257824
H 5.284151 -2.007884 -2.055502
C 3.876469 -2.549144 4.360740
H 2.657614 -0.946309 5.160525
H 4.988348 -4.053088 3.268086
C 8.008673 -0.970377 -0.262417
H 7.925439 0.314095 1.479617
H 7.781964 -2.198795 -2.032670
H 4.056131 -3.009267 5.335217
H 9.099381 -1.033924 -0.260714

name: TS3
Opt Eel: -10782.1296753
Freq: -119.5837
SP Eel TPSSh-D3BJ: -10850.2244585
Gcorr (363K): 0.707113
ZPE: 0.827762
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0 3
Ni -0.526995 1.020192 0.013751
C -2.402233 3.067999 -0.078414
C -3.269776 1.347786 1.193113
C -3.573076 3.853179 0.042516
C -1.289575 3.545955 -0.827273
C -4.463616 2.066068 1.393283
H -3.134755 0.358057 1.627571
C -4.629304 3.313953 0.814023
C -3.610814 5.129369 -0.618810
C -1.344671 4.798872 -1.480233
H -5.248908 1.619910 2.003212
H -5.553325 3.880359 0.947046
C -2.544153 5.581621 -1.351249
H -4.515867 5.733331 -0.526221
C -0.201854 5.184921 -2.221360
C 0.850392 3.099254 -1.581421
H -2.587376 6.550675 -1.852818
H -0.190115 6.142838 -2.745448
C 0.886725 4.327903 -2.267891
H 1.701805 2.421382 -1.579175
H 1.785388 4.589658 -2.828383
N -2.252641 1.833850 0.478858
N -0.210187 2.716577 -0.868883
Ni 0.159237 -2.027652 -0.650145
N 1.262585 -3.573210 -1.452697
N 1.552903 -2.457909 0.965825
C 2.205214 -4.102302 -0.631320
C 1.103804 -4.098884 -2.664620
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 C 2.345959 -3.517629 0.674139
 C 1.700163 -1.861345 2.142353
 C 3.033380 -5.190483 -1.009870
 C 1.888259 -5.169410 -3.135713
 H 0.309675 -3.669699 -3.274845
 C 3.297705 -4.044934 1.585090
 C 2.590324 -2.330021 3.127938
 H 1.088083 -0.976550 2.316948
 C 2.855751 -5.717230 -2.311686
 C 3.991492 -5.701433 -0.069178
 H 1.716566 -5.553968 -4.142172
 C 4.114463 -5.154974 1.179866
 C 3.384510 -3.428617 2.856593
 H 2.651256 -1.805142 4.081839
 H 3.475772 -6.551952 -2.646219
 H 4.619544 -6.541208 -0.374359
 H 4.841982 -5.551194 1.891643
 H 4.090799 -3.813297 3.595711
 C 1.533880 -0.171784 -1.418260
 C 2.889609 -0.577982 -1.725362
 C 0.523660 -0.531236 -2.393139
 C 3.201806 -1.173316 -2.930141
 H 3.661816 -0.370132 -0.978983
 C 0.891455 -1.094351 -3.636298
 H -0.461260 -0.062146 -2.302368
 C 2.207627 -1.434386 -3.912416
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 H 2.482487 -1.889858 -4.866441
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 H -0.775515 0.616118 2.671744
 C -1.977618 -3.045175 3.139943
 H -1.919287 -3.184270 0.982646
 C -1.794265 -2.233645 4.271821
 H -1.217389 -0.256437 4.944689
 H -2.304028 -4.082810 3.260178
 H -1.968010 -2.627679 5.276133
 N 1.213949 0.444041 -0.279581
 Zn 2.478021 1.121275 1.061177
 Cl 4.443713 0.092515 1.651198
 Cl 1.379447 2.267562 2.725884
 O 3.425802 2.604366 -0.072331
 C 4.245544 3.453049 0.336078
 C 4.617475 3.745167 1.769563
 N 4.967233 4.240988 -0.476691
 H 3.718670 3.750668 2.402104
 C 5.366240 5.080141 1.682471
 H 5.253214 2.909636 2.109192
 C 5.899159 5.112517 0.241129
 C 4.951669 4.148803 -1.920862
 H 4.661756 5.912369 1.833178
 H 6.172164 5.176067 2.422131
 H 5.893526 6.119366 -0.202225
 H 6.922814 4.705926 0.158458
 H 4.620626 5.101331 -2.364316
 H 5.961516 3.916628 -2.295694
 H 4.262442 3.346382 -2.211580
 N -1.058607 -0.748709 0.359648
 Zn -2.512567 -0.943218 -0.970931
 Cl -1.856889 -3.087747 -1.762482
 Cl -3.108276 0.557766 -2.569059
 O -4.195255 -1.457916 0.030410
 C -5.347152 -0.976302 0.130969
 C -6.168277 -0.337411 -0.960650
 N -6.053049 -1.002375 1.267676
 H -5.544011 0.356961 -1.540252
 C -7.340386 0.304951 -0.207259
 H -6.488394 -1.141501 -1.645991
 C -7.409224 -0.470405 1.119623
 C -5.576476 -1.598071 2.498996
 H -7.118739 1.363449 -0.006763
 H -8.287412 0.254676 -0.760268
 H -7.658374 0.164537 1.982495
 H -8.129672 -1.306249 1.087934
 H -5.631387 -0.864630 3.318025
 H -6.191746 -2.473088 2.764119
 H -4.535457 -1.912592 2.352062
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Coupled-cluster geometries

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Opt Eel: -248.354776829
DMF
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0 1
 O 0.195450 -1.938779 0.000000
 N 0.000000 0.352033 0.000000
 C 0.677190 1.629479 0.000000
 C 0.691748 -0.827820 0.000000
 C -1.450129 0.335592 0.000000
 H 0.414024 2.221921 0.894103
 H -1.848219 0.843101 -0.895581
 H -1.767742 -0.714901 0.000000
 H -1.848219 0.843101 0.895581
 H 1.764350 1.462758 0.000000
 H 0.414024 2.221921 -0.894103
 H 1.795329 -0.655410 0.000000

Opt Eel: -189.151895681
Azo
---------------------------------
0 1
 N -0.369304 0.498315 0.000000
 N 0.369304 -0.498315 0.000000
 C -0.369304 -1.757820 0.000000
 C 0.369304 1.757820 0.000000
 H -0.058173 -2.333951 0.886181
 H -1.460718 -1.601659 0.000000
 H -0.058173 -2.333951 -0.886181
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 H 0.058173 2.333951 0.886181
 H 1.460718 1.601659 0.000000

Opt Eel: -2233.61836503
C2v - L'NiCl
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0 2
 Ni 0.000000 0.000000 0.496471
 C 0.000000 0.676902 -2.170895
 C 0.000000 2.612753 -0.856154
 C 0.000000 -0.676902 -2.170895
 C 0.000000 -2.612753 -0.856154
 N 0.000000 1.313615 -0.924143
 N 0.000000 -1.313615 -0.924143
 H 0.000000 -1.270791 -3.090686
 H 0.000000 1.270791 -3.090686
 H 0.000000 -3.240541 -1.757626
 H 0.000000 -3.083163 0.129760
 H 0.000000 3.083163 0.129760
 H 0.000000 3.240541 -1.757626
 Cl 0.000000 0.000000 2.635207

Opt Eel: -1962.67702562
C2 - L'NiAzo
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0 1
 Ni 0.000000 0.000000 0.163136
 C 0.479692 0.475858 -2.473505
 C 1.857632 1.827043 -1.158606
 C -0.479692 -0.475858 -2.473505
 C -1.857632 -1.827043 -1.158606
 N 0.924610 0.926839 -1.219284
 N -0.924610 -0.926839 -1.219284
 H -0.905020 -0.895375 -3.391084
 H 0.905020 0.895375 -3.391084
 N 0.502249 0.466458 1.889668
 N -0.502249 -0.466458 1.889668
 C 0.000000 1.795582 2.236485
 C 0.000000 -1.795582 2.236485
 H -1.059102 1.951573 1.953357
 H 0.080625 1.953453 3.328753
 H 0.623602 2.561844 1.747202
 H -0.623602 -2.561844 1.747202
 H 1.059102 -1.951573 1.953357
 H -0.080625 -1.953453 3.328753
 H -2.313996 -2.250047 -2.064563
 H -2.199473 -2.160004 -0.176500
 H 2.199473 2.160004 -0.176500
 H 2.313996 2.250047 -2.064563

Opt Eel: -1773.40485961
C2v - L'Ni
---------------------------------
0 1
 Ni 0.000000 0.000000 0.976154
 C 0.000000 0.680307 -1.354474
 C 0.000000 2.746630 -0.259607
 C 0.000000 -0.680307 -1.354474
 C 0.000000 -2.746630 -0.259607
 N 0.000000 1.441825 -0.154485
 N 0.000000 -1.441825 -0.154485
 H 0.000000 -1.221722 -2.311646
 H 0.000000 1.221722 -2.311646
 H 0.000000 -3.249129 -1.237642
 H 0.000000 -3.350653 0.649017
 H 0.000000 3.350653 0.649017
 H 0.000000 3.249129 -1.237642

Opt Eel: -2693.74323968
C2v - L'NiCl2
---------------------------------
0 1
 Ni 0.000000 0.000000 0.284110
 C 0.000000 0.672669 -2.419546
 C 0.000000 2.580677 -1.079588
 C 0.000000 -0.672669 -2.419546
 C 0.000000 -2.580677 -1.079588
 N 0.000000 1.291923 -1.158447
 N 0.000000 -1.291923 -1.158447
 H 0.000000 -1.284198 -3.325598
 H 0.000000 1.284198 -3.325598
 H 0.000000 -3.196335 -1.988876
 H 0.000000 -3.019187 -0.075615
 H 0.000000 3.019187 -0.075615
 H 0.000000 3.196335 -1.988876
 Cl 0.000000 1.551749 1.795087
 Cl 0.000000 -1.551749 1.795087

Opt Eel: -2693.74616364
C2v - L'NiCl2
---------------------------------
0 3
 Ni 0.000000 0.000000 0.572125
 C 0.000000 0.675948 -2.180224
 C 0.000000 2.607230 -0.862550
 C 0.000000 -0.675948 -2.180224
 C 0.000000 -2.607230 -0.862550
 N 0.000000 1.327399 -0.945705
 N 0.000000 -1.327399 -0.945705
 H 0.000000 -1.262531 -3.104585
 H 0.000000 1.262531 -3.104585
 H 0.000000 -3.250166 -1.754892
 H 0.000000 -3.069586 0.128265
 H 0.000000 3.069586 0.128265
 H 0.000000 3.250166 -1.754892
 Cl -2.077299 0.000000 1.270473
 Cl 2.077299 0.000000 1.270473

Opt Eel: -3196.16478694
C2v - ZnCl2(DMF)2
---------------------------------
0 1
 Zn 0.000000 0.000000 0.353537
 Cl -1.973953 0.000000 1.343744
 Cl 1.973953 0.000000 1.343744
 C 0.000000 5.155735 0.208883
 H 0.895583 5.769882 0.020637
 C 0.000000 2.746033 -0.127665
 N 0.000000 3.981445 -0.646835
 C 0.000000 4.179195 -2.088739
 H 0.000000 3.193734 -2.568537
 H -0.896479 4.742315 -2.394140
 H 0.896479 4.742315 -2.394140
 C 0.000000 -5.155735 0.208883
```

C 0.000000 -2.746033 -0.127665
N 0.000000 -3.981445 -0.646835
C 0.000000 -4.179195 -2.088739
H 0.895583 -5.769882 0.020637
H -0.896479 -4.742315 -2.394140
H 0.000000 -3.193734 -2.568537
H 0.896479 -4.742315 -2.394140
O 0.000000 -1.709301 -0.812007
O 0.000000 1.709301 -0.812007
H 0.000000 -4.839584 1.260404
H -0.895583 -5.769882 0.020637
H 0.000000 4.839584 1.260404
H -0.895583 5.769882 0.020637
H 0.000000 -2.712722 0.977469
H 0.000000 2.712722 0.977469

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