Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Electronic Supporting Information for

Effect of Interlayer Anions on [NiFe]-LDH Nanosheet Water Oxidation Activity

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1. X-Ray photoelectron spectroscopy (XPS) data

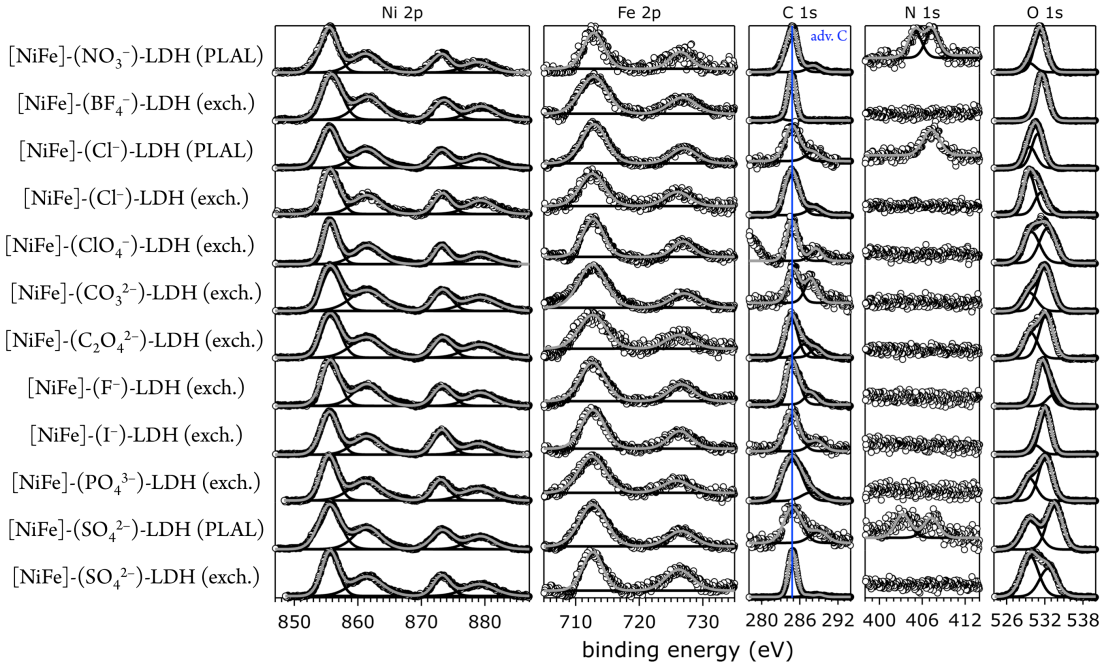

Figure S1: XPS data of [NiFe]-LDH nanosheets with different interlayer anions as synthesized in the Ni 2p, Fe 2p, C 1s, N 1s, and O 1s regions. The materials were prepared by pulsed-laser ablation in liquids (PLAL) or by anion exchange from [NiFe]-(NO_3^-)-LDH (exch.). Open circles, data; black lines, peak fits; grey lines, envelopes. The blue line in the C 1s panel indicates the binding energy of adventitious carbon.

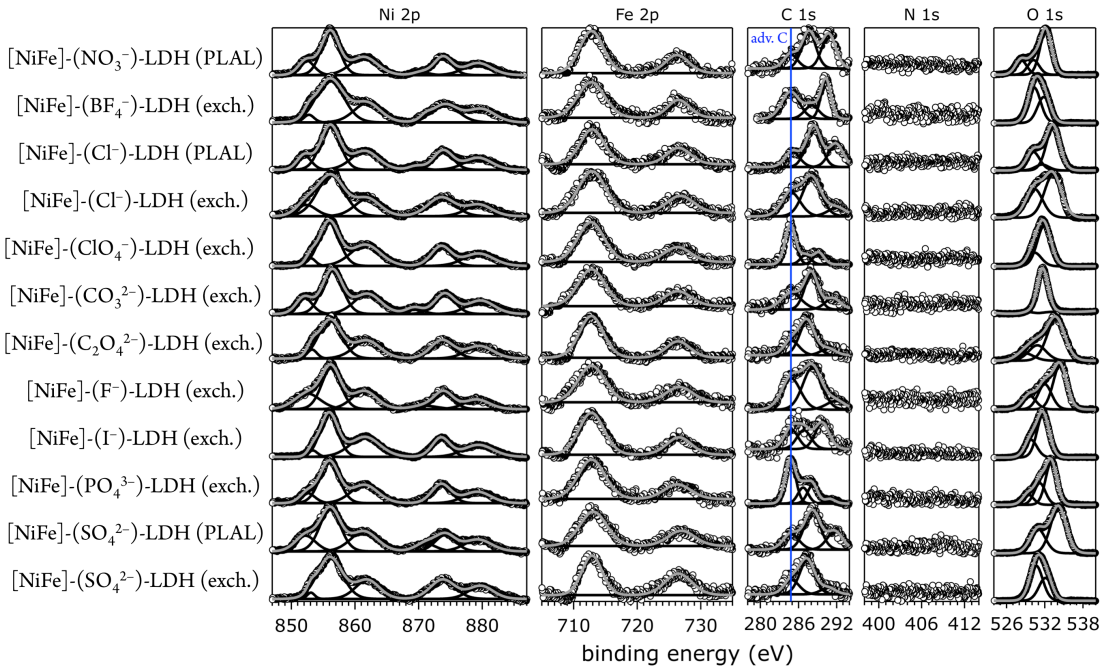

Figure S2: XPS data of [NiFe]-LDH nanosheets with different interlayer anions after suspension in 1.0 M aqueous KOH in ambient air in the Ni 2p, Fe 2p, C 1s, N 1s, and O 1s regions. The materials were prepared by pulsed-laser ablation in liquids (PLAL) or by anion exchange from [NiFe]-(NO_3^-)-LDH (exch.). Open circles, data; black lines, peak fits; grey lines, envelopes. The blue line in the C 1s panel indicates the binding energy of adventitious carbon.

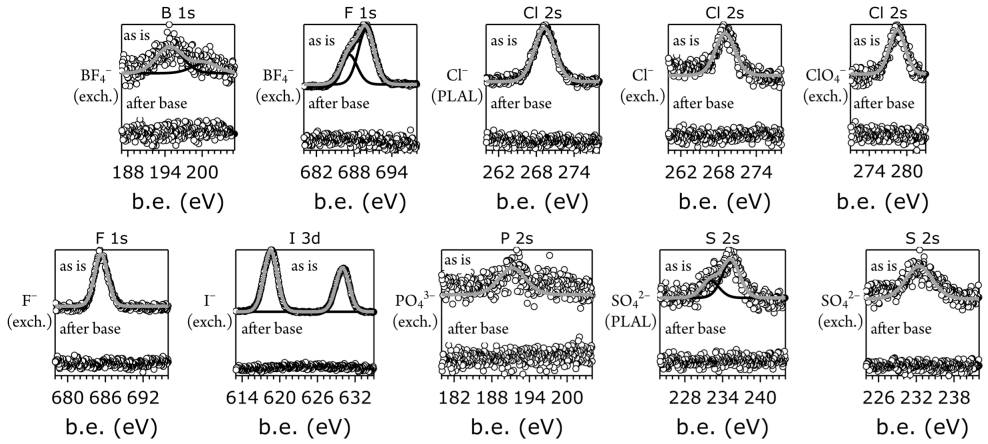

Figure S3: XPS data of [NiFe]-LDH nanosheets with different interlayer anions as synthesized (as is) and after suspension in 1.0 M aqueous KOH in ambient air (after base) in the B 1s, F 1s, Cl 2s, I 3d, P 2s, and S 2s regions, where applicable; b.e., binding energy. Open circles, data; black lines, peak fits; grey lines, envelopes.

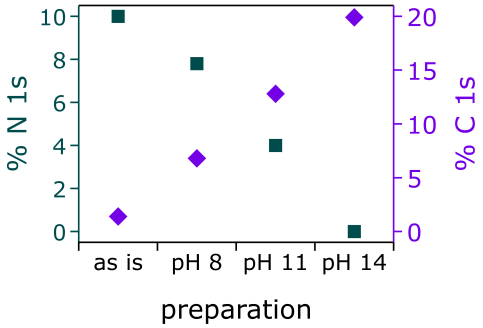

Figure S4: Quantification of the N 1s (teal) and C 1s (purple) regions of [NiFe]-(NO_3^-)-LDH (as is) and exchanged in different pH aqueous KOH solutions in percent with respect to the total metal content.

2. X-Ray diffraction (XRD) data

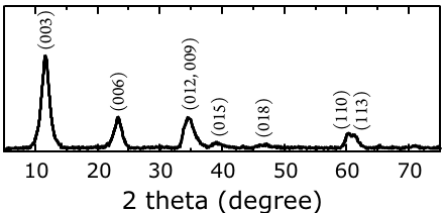

Figure S5: XRD data of [NiFe]-(CO_3)-LDH nanosheets with indices of reflection.

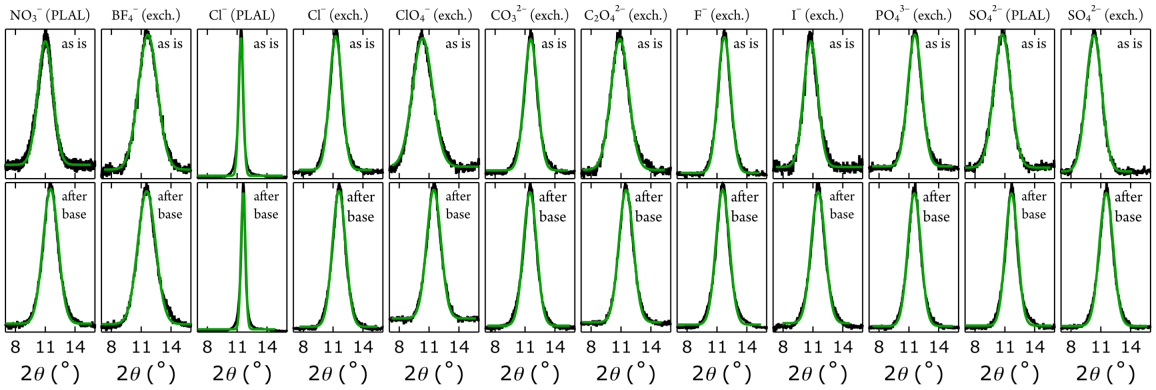

Figure S6: Gaussian fits (green) of the (001) peaks (black) of XRD data of [NiFe]-LDH nanosheets with different interlayer anions.

3. Infrared (IR) data

We attempted to de-carbonate our alkaline aqueous electrolyte with $Ba(OH)_2$ in ambient air. We soaked [NiFe]-(NO_3^-)-LDH for 30 min in electrolytes under different conditions, centrifuged and washed the powders three times with 5 mL water and let them dry in ambient air. We collected IR spectra of the dry powders to identify the interlayer anions.

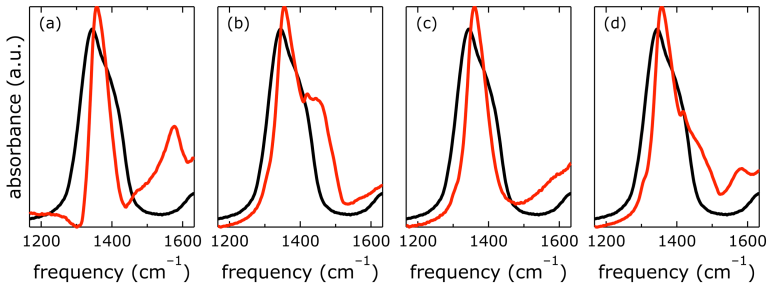

Figure S7: Infrared spectra of [NiFe]-(NO_3^-)-LDH nanosheets as synthesized (black) and after being suspended in 0.1 M aqueous KOH (red). The red spectra were taken using different suspension solution conditions: (a), in ambient air, no $Ba(OH)_2$; (b), in ambient air, with $Ba(OH)_2$; (c), in glove box, no $Ba(OH)_2$; (d), in glove box, with $Ba(OH)_2$.

The IR spectra in Figure S7 clearly show that we could not exclude carbonate using these methods. All "after-suspension" spectra showed bands characteristic for carbonate. Presumably, carbonate adsorbed to the KOH or from ambient CO_2 during the first centrifugation cycle became incorporated into our [NiFe]-(NO_3^-)-LDH nanosheets.

Therefore, we performed all electrochemistry experiments, for which carbonate-free electrolyte was required, in inert atmosphere.

4. Electrochemical Characterization

Electrochemical activity of the nanoparticulate catalysts was assessed in virtually carbonate-free (glove box) electrolyte or 1.0 M aqueous base with dissolved carbonate (ambient air).

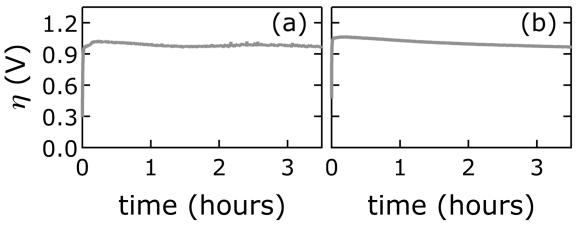

Figure S8: Constant current voltammograms of bare graphite electrodes in carbonate-containing (a) and virtually carbonate-free (b) electrolytes.

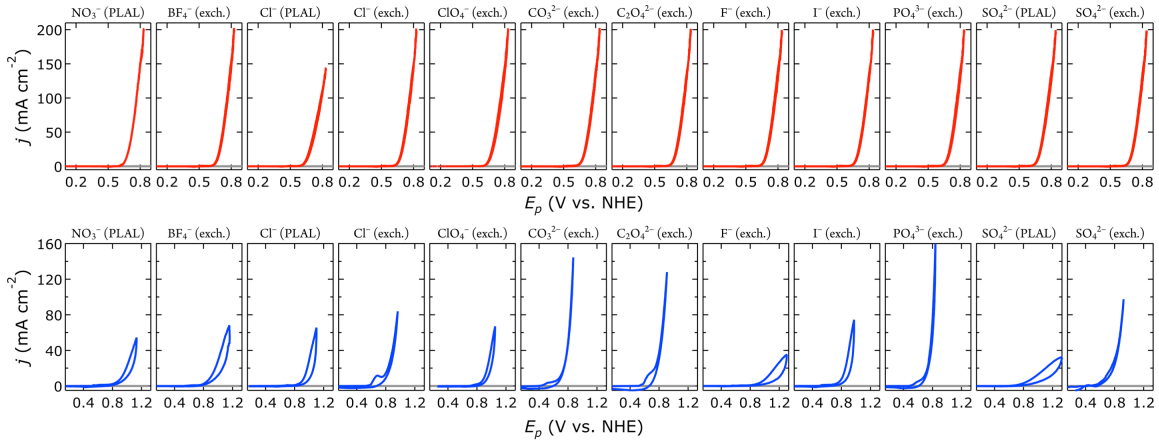

Figure S9: Cyclic voltammograms of [NiFe]-LDH materials with different interlayer anions in virtually carbonate-free electrolyte in a glove box (blue) and after suspension in 1.0 M aqueous KOH in ambient air (red). Cyclic voltammetry data of bare HOPG are shown in grey.

5. Data Correlations

We tried to find correlations of electrochemical data, such as overpotentials and prewave peak positions, with the materials' structural and chemical characteristics, such as basal spacing, intrasheet $[NiFe](OH)_2$ structure, and interlayer anion basicity. Data of unstable materials, such as [NiFe]-(F^-)-LDH (exch.) and [NiFe]-(SO_4^{2-})-LDH (PLAL), were not included into correlations. Only small amounts of the initially deposited [NiFe]-(F^-)-LDH (exch.) and [NiFe]-(SO_4^{2-})-LDH (PLAL) materials were visible on the HOPG electrode after chronopotentiometry experiments.

We derived overpotentials of [NiFe]-LDH materials with different interlayer anions from chronopotentiometry data, which were collected in virtually carbonate-free electrolyte (glove box). They are plotted as a function of the pK_a values of the conjugate acids of the interlayer anions (Table S1) in Figure S10.

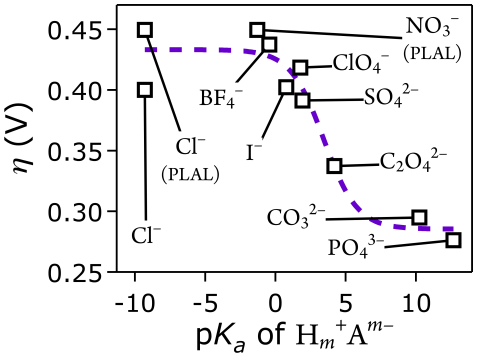

Figure S10: Overpotentials η of [NiFe]-LDH materials with different interlayer anions A^{m-} derived from constant current electrolysis at 1 mA cm^{-2} in virtually carbonate-free electrolyte as a function of anion basicity. Bare anion labels denote materials prepared by exchange from [NiFe]-(NO_3^-)-LDH.

Table S1: Anions, conjugate acids, and pK_a values of conjugate acids of anions with references.

Anion	Conjugate acid	pK_a	Reference
NO_3^-	HNO_3	–1.3	1
BF_4^-	HBF_4	–0.44	2
Cl^-	HCl	–9.3	3
ClO_4^-	$HClO_4$	1.77	4
CO_3^{2-}	HCO_3^-	10.25	4
$C_2O_4^{2-}$	$HC_2O_4^-$	4.19	4
F^-	HF	3.45	4
I^-	HI	0.77	4
PO_4^{3-}	$H_2PO_4^{2-}$	12.67	4
SO_4^{2-}	HSO_4^-	1.92	4

We tried to correlate Ni-based redox features to interlayer anion basicity to assess if more electron-rich anions would lead to electronic changes in the nickel hydroxide layers. We deliberately chose the reduction wave of the cyclic voltammograms for analysis as the oxidation prewave was partly obscured by the catalytic wave, rendering an accurate determination of the peak maximum problematic. This is illustrated in Figure S11 (a). We did not observe a clear correlation of the central polarization potential of the reduction waves of [NiFe]-LDH nanosheets with interlayer anions exhibiting different basicities or overpotential.

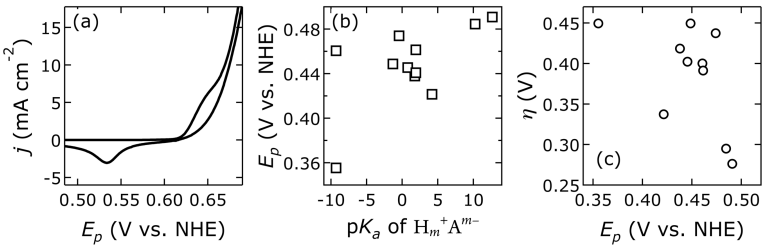

Figure S11: Magnified pre-water-oxidation-wave region of a representative cyclic voltammogram of [NiFe]-LDH nanosheets (a). Central polarization potential E_p of the reduction wave of [NiFe]-LDH nanosheets with different interlayer anions, collected in virtually carbonate-free electrolyte, as a function of anion basicity (b), and overpotential η as a function of E_p (c).

In addition, we investigated if the measured overpotentials depended on the intrasheet [NiFe]$(OH)_2$ structure. To this end, we took far-IR spectra of our [NiFe]-(NO_3^-)-LDH nanosheets that had been soaked in

different pH aqueous KOH solutions and analyzed lines, which are characteristic for OH-deformations; the broad bands centered around 500 cm^{-1} are Ni–O lattice modes[5] (Figure S12 left). The ratios of two such lines as a function of solution pH showed sigmoid behavior with a midpoint of approximately 12 (Figure S12 right).

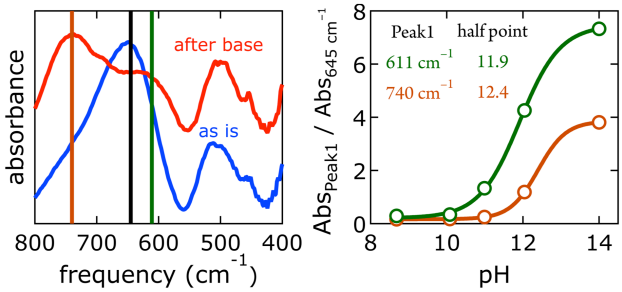

Figure S12: Left: Far-IR spectra of [NiFe]-(NO_3^-)-LDH nanosheets as synthesized (as is) and after suspension in 1.0 M aqueous KOH in ambient air (after base). The vertical lines indicate the peaks that were analyzed. Right: Titration curves as a function of solution pH.

6. Density functional theory calculations

The main purpose of our theoretical analysis was the identification of possible nitrogen species associated with the experimentally observed N 1s XPS peak at 405.1 eV. The other peak was centered at 407.3 eV and was assigned to nitrate based on its agreement with solid-state reference data.[6-11] The XPS binding energy of nitrite (NO_2^-) was reported at 403.5 eV.[8]

Our [NiFe]-LDH materials consisted of nanosheets of edge-shared nickel oxide octahedra, with 22% ferric iron substituting at nickel sites. Hydroxide ligands extended into the interlayer space, which also contained water. As described for other LDH materials,[12] the excess positive charges of Fe^{3+} substituting for Ni^{2+} were balanced by interlayer anions, such as the nitrogen species we focused our calculations on.

Towards this goal, we performed density functional theory (DFT) calculations on cluster models of the [NiFe]-LDH nanosheet material. Technical details concerning the calculation of the N 1s core level binding energies and the choice of the cluster models are described in Section 2 and 6.1. Results obtained with the chosen approach are presented in the main text, while additional details are given in Section 6.2.

6.1. Computational models

Table S2 shows a comparison of N 1s core-level BEs and core-level shifts (CLS) for nitrate and nitrite calculated from orbital energies and STS calculations with the DFT method described above, with and without the COSMO solvation model. The data exhibited excellent agreement of the approximate STS CLS with those from explicit ΔSCF calculations. Experimental BEs from solid-state XPS experiments are 407.3 eV for nitrate and 403.5 eV for nitrite,[8] resulting in an experimental CLS of 3.8 eV between both anions.

Table S2: A small test of various methods to calculate N1s binding energies for nitrate and nitrite; PBE0/SV(P); PBE0(COSMO-80)/SV(P); [eV].

Species	$-\varepsilon$	–STS	ΔSCF	$-\varepsilon$ COSMO	–STS COSMO	ΔSCF COSMO
NO_3^-	391.692	409.134	407.771	397.458	411.940	410.602
NO_2^-	387.323	404.948	403.598	393.545	408.009	406.694
CLS	4.369	4.186	4.173	3.913	3.931	3.908

Effect of basis sets on core level shifts. The standard def2-SV(P) basis set was used in all calculations unless stated otherwise. It is a split-valence double zeta basis set with polarization functions on all non-hydrogen atoms. This basis set is generally known to yield results of qualitative accuracy for chemical reaction energies and structures. One may wonder if this basis set is adequate for core level shift calculations, which involve significant core relaxation (part of the so-called “final state effects” captured via the

STS procedure). We therefore compared the standard SV(P) basis set used throughout this work with more flexible basis sets for the N 1s core level shifts between nitrate and nitrite, which were calculated with the STS method (Table S3). In the following, we use the "U-" prefix to any basis set name to denote a version, in which the basis was uncontracted for the N 1s atom, thereby increasing its flexibility within the exponent range spanned by the primitive Gaussian functions.

The data showed that the N 1s CLS were only minimally affected by the choice of basis set (variation in CLS < 0.2 eV), *i.e.* all basis sets, including the simple SV(P) basis, agreed to within less than 0.2 eV for the N 1s CLS between nitrate and nitrite. This uncertainty was less than 10% of the experimental effects that we aimed to explain; it was also in the same range as the uncertainty of the experimental measurements. We therefore concluded that for CLS calculations the SV(P) basis set were a good compromise between accuracy and computational efficiency.

Table S3: N 1s core ionization energies of NO_3^- and NO_2^- and the resulting CLS (in eV) calculated using the STS method and various basis sets; PBE0/COSMO(ε = 80) level; geometries of nitrate and nitrite were optimized at the B3LYP(COSMO)/TZVP level; the prefix "U-" to a basis set name indicates that the corresponding basis set was uncontracted for the nitrogen atom.

Basis set	NO_3^-	NO_2^-	N 1s CLS
def2-SV(P)	–411.939	–408.009	3.930
U-def2-SV(P)	–410.398	–406.348	4.050
WTBS[a]	–420.944	–415.955	4.989
U-WTBS	–409.965	–406.036	3.929
IGLO3[a]	–410.336	–406.395	3.941
U-IGLO3	–410.331	–406.391	3.940
ANO-TZ[a]	–410.663	–406.883	3.780
U-ANO-TZ	–410.280	–406.382	3.898

[a] Basis set taken from EMSL Basis set exchange, see https://bse.pnl.gov/bse/portal.

Influence of explicit water solvation on calculated core level shifts. The investigated [NiFe]-(NO_3^-)-LDH material contained unknown amounts of water. Hence, defining a suitable reference state for CLS calculations required an estimate of the effect of explicit water molecules in addition to the COSMO continuum solvation model that was used in all calculations. Therefore, we tested the influence of 0-3 explicit water molecules on nitrate and nitrite CLS. The (NO_x^-) · $n H_2O$ (x = 2, 3; n = 0-3) moieties were optimized at the standard PBE0(COSMO-80)/SV(P) level. The water molecules were arranged in the plane spanned by the atoms of the anions in the optimizations. Each water molecule formed a hydrogen bond to one of the anion O atoms. Various H-bridging motifs were considered, the CLS of which were found to be within ± 0.1 eV. Axial coordination to the central N atom was not observed with our level of theory. Note that such static DFT calculations are, in general, not capable of capturing the dynamics of a system, and hence should be considered approximate. Table S4 shows the effect of explicit water molecules on the calculated N 1s BEs. Clearly, the presence of explicit hydrogen bonds had a sizeable effect on absolute N 1s BEs, ranging from 0.4 eV for one water molecule to up to 1 eV for three water molecules.

Table S4: Effect of explicit water molecules on N 1s orbital energies ε and core level binding energies (in eV) calculated by STS for a nitrate or nitrite anion with 0-3 explicit water molecules; PBE0(COSMO-80)/SV(P) level; multiple entries for the same number of water molecules refer to different binding geometries of the O···HOH hydrogen bonds.

Anion	$n H_2O$	ε	STS
NO_3^-	0	–397.458	–411.939
	1	–397.782	–412.342
	2	–398.087	–412.645
	3	–398.423	–412.970
NO_2^-	0	–393.545	–408.009
	1	–393.986	–408.466
	1 (N···HOH)	–394.093	–408.424

The influence of hydrogen bridges is important for the choice of a proper reference configuration in the cluster calculations. The reference configuration of this work is shown in Figure S15.

Cluster models. The exact microscopic structure of the [NiFe]-(NO_3^-)-LDH nanosheet material is hitherto essentially unknown. This required us to make assumptions on the structures for the theoretical modeling of the observed XPS shifts. In this work, we used moieties derived from the experimental $Ni(OH)_2$ structure (American Mineralogist Crystal Structure Database (AMCSD) #0015759)[13] with the sum formula $[Ni_9Fe_1(OH)_{18}]$ as a general basis for our models (Figure S13). Iron incorporation was achieved by replacing one of the Ni centers of the original structure by Fe (Figure S13 and Figure 12 in the main text). The overall charge of this basic fragment was +3, consistent with nine Ni(II) centers and one Fe(III) center (although no means to enforce a specific oxidation state of the individual metal centers was taken).

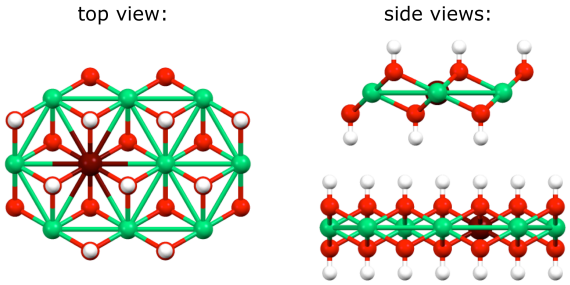

Figure S13: Basic $[Ni_9Fe_1(OH)_{18}]^{3+}$ cluster of our DFT study, depicted here with central Fe; other Fe sites were also explored (Figure 12 in the main text). In the calculations, a nitrate or nitrite anion was bound to various positions of the cluster, resulting in the sum formula $[Ni_9Fe_1(OH)_{18}(NO_x)]^{2+}$ (x = 2, 3). In an extended model (cf. Figure 13 of the main text and Figures S14, S15), two additional hydroxide groups were attached to various positions at the rim of the cluster to neutralize charge, resulting in an overall sum formula of $[Ni_9Fe_1(OH)_{20}(NO_x)]$ (x = 2, 3). Colors: Ni green, Fe maroon, O red, H white.

To model possible binding motifs of nitrate and nitrite anions in the investigated materials, an anion was placed at various sites along the rim of the $[Ni_9Fe_1(OH)_{18}]^{3+}$ fragment, yielding clusters with the overall sum formulae $[Ni_9Fe_1(OH)_{18}(NO_3)]^{2+}$ and $[Ni_9Fe_1(OH)_{18}(NO_2)]^{2+}$. The nitrate anion was assumed to bind via one of its O atoms, whereas for nitrite binding via the O and N atoms was explored. Only anion binding to Fe was considered in this work (with one exception, see below). The Fe was placed at varying positions within the cluster such that the attached anion could bind directly to Fe (see Figure 12 of the main text). Relative energies of the various binding modes were thus not accessible with this approach. In addition to the di-cationic cluster models described above, we also investigated neutral cluster models, in which two additional hydroxide groups were added at various positions at the rim of the clusters; this resulted in structures with the overall sum formulae $[Ni_9Fe_1(OH)_{20}(NO_3)]$ and $[Ni_9Fe_1(OH)_{20}(NO_2)]$ (cf. Figure 13 of the main text and Figures S14, S15). In these more complex models, a multitude of options existed how to place additional hydroxide groups at the cluster. To keep computational efforts within reasonable limits, we chose only two additional hydroxide group binding sites per ($NO_{2\text{ or }3}^-$) binding site.

The purpose of these calculations was to investigate to which extent the N 1s core levels were affected by attached hydroxide groups. We also aimed to avoid possible artifacts arising from the charged clusters, in which the +2 charge of the cluster model may only have partly been screened by the COSMO solvation shell (see above). We found that the arrangement of such "guessed" hydroxide positions did not significantly change the calculated N 1s shifts; this was especially true for all nitrite-binding motifs (Table S6).

The resulting starting structures were subjected to a constrained geometry optimization using the standard convergence criteria of the Turbomole program at the PBE0/COSMO(ε = 80)/SV(P) level. In these optimizations, all atoms except those of the nitrate or nitrite anions and the Fe center were optimized, whereas all other positions (Ni, O, H) were kept fixed at the positions of the original crystal structure moiety. The resulting structures are shown in Figures 13 (main text) and S14; corresponding Cartesian coordinates are enclosed.

Comments on the electronic structure of cluster models. The LDHs of this work belong to the class of so-called strongly correlated systems; a considerable amount of multi-reference character may exist. Hence, the electronic structure of the system poses a significant challenge to present-day density functionals. In this work, we limited our attention to the estimation of N 1s core-level *shifts* of nitrate or nitrite anions

bound to the basic metal hydroxide clusters described above. We tested the sensitivity of the calculated N 1s energies with regard to different electronic configurations of the LDH cluster by imposing different numbers of unpaired electrons in the Kohn-Sham determinant for di-cationic models, *i.e.* by enforcing different S_z in the calculations. In each case, the SCF calculations started from an extended Hückel guess with the appropriate S_z. Fractional occupation numbers with Fermi annealing such that final occupations near zero or one were applied. Constrained geometry optimizations as described above were performed until convergence. Our results obtained for N 1s orbital energies and total energies of the $[Ni_9Fe_1(OH)_{18}(NO_3)]^{2+}$ model cluster are shown in Table S5.

Table S5: N 1s orbital energies ε (α, β spin) and total energies for the $[Ni_9Fe_1(OH)_{18}(NO_3)]^{2+}$ cluster with Slater determinants with 1, 3, 5, 7, 9 unpaired electrons, corresponding to total spin projects numbers S_z = 0.5, 1.5, 2.5, 3.5, 4.5; COSMO solvation (ε = 80), PBE0/SV(P), geometries optimized (with the usual constraints, see text) at the same level for each S_z.

Structure	S_z	ε(N 1s, α) [eV]	ε(N 1s, β) [eV]	E_{total} [a.u.]
"unbound"	0.5	–398.840	–398.840	–16476.846804
	1.5	–398.854	–398.854	–16476.850205
	2.5	–398.851	–398.851	–16476.982457
	3.5	–398.846	–398.846	–16477.005609
	4.5	–398.860	–398.860	–16476.984996
edge (μ_2)	0.5	–399.281	–399.282	–16476.834117
	1.5	–399.286	–399.286	–16476.930302
	2.5	–399.281	–399.282	–16476.977801
	3.5	–399.275	–399.274	–16477.001504
	4.5	–399.277	–399.276	–16477.001668
corner (η^1)	0.5	–399.486	–399.489	–16476.856580
	1.5	–399.496	–399.493	–16476.834383
	2.5	–399.485	–399.488	–16476.927814
	3.5	–399.481	–399.483	–16476.950619
	4.5	–399.477	–399.475	–16476.995283

We found that the calculated N 1s orbital energies were remarkably insensitive of the electronic configuration. Experimental data suggested a non-magnetic ground state of the real material (unreacted ablation target, ferromagnetic Fe powder, could be separated from the formed LDH materials with a strong magnet). In light of the fact that the N 1s core level energies appeared to be essentially unaffected by the precise electronic configuration of the cluster (Table S5), we chose to use a low-spin electronic configuration (S_z = 0.5) for all calculations in this work.

6.2. Results: Anion coordination motifs and N 1s core level shifts

Iron sites within the cluster. We assessed three different Fe atom sites in the basic $[Ni_9Fe_1(OH)_{18}]^{3+}$ cluster fragment (Figure 12 in the main text). In our calculations, we abstained from breaking LDH lattice OH bonds to metal atoms to accommodate anion binding to central Fe because our previous experimental work showed that the [NiFe]-LDH nanosheets were stable for hours during water oxidation catalysis and the LDH crystal structure was retained after turnover.[14] We found *in silico* that nitrate did not bind directly to Fe when located in the center of the intact cluster, presumably for steric reasons. Hydrogen-bridge-bound nitrate perched vertically above the $[Ni_9Fe_1(OH)_{18}]$ sheet was used as reference configuration (see below, Figure S15). Furthermore, our present computational approach did not point to nitrite binding directly (coordinatively) to Fe in the center of the cluster. All attempts undertaken to bind NO_2^- via its N or O atoms to a center-Fe in the intact $[Ni_9Fe_1(OH)_{20}]$ cluster led to structures after geometry optimization, in which the nitrite anion was merely bound via hydrogen bridges to the LDH structure. The calculated CLS of unbound nitrite above the cluster was at (–4.0 ± 0.1) eV, depending on exact configuration and initial-state contributions. Because these results were inconsistent with the experimental data we aimed to explain, we focused in the following on anion binding to edge and corner Fe located at the rim of the $[Ni_9Fe_1(OH)_{20}]$ clusters.

Geometries of model clusters. The basic $[Ni_9Fe_1(OH)_{18}]$ moieties, on which the DFT calculations of this work was based is depicted in Figure 12 and Figure S13. The coordination sites and anion binding motifs of the neutral model clusters $[Ni_9Fe_1(OH)_{20}(NO_3)]$ and $[Ni_9Fe_1(OH)_{20}(NO_2)]$ are shown in Figure 13 (main text) and Figure S14, respectively. The cationic models $[Ni_9Fe_1(OH)_{18}(NO_3)]^{2+}$ and $[Ni_9Fe_1(OH)_{18}(NO_2)]^{2+}$ can be derived from these by omitting the two peripheral hydroxyl groups (not shown).

The structures of the various configurations and associated acronyms, for which the core level binding energies and shifts are listed in Table S6, are shown in Figure S14. Note the different binding sites and coordination motifs of the anions as well as the positions of the extra hydroxide groups at the rim of the clusters. The enclosed xyz coordinate files provide more details.

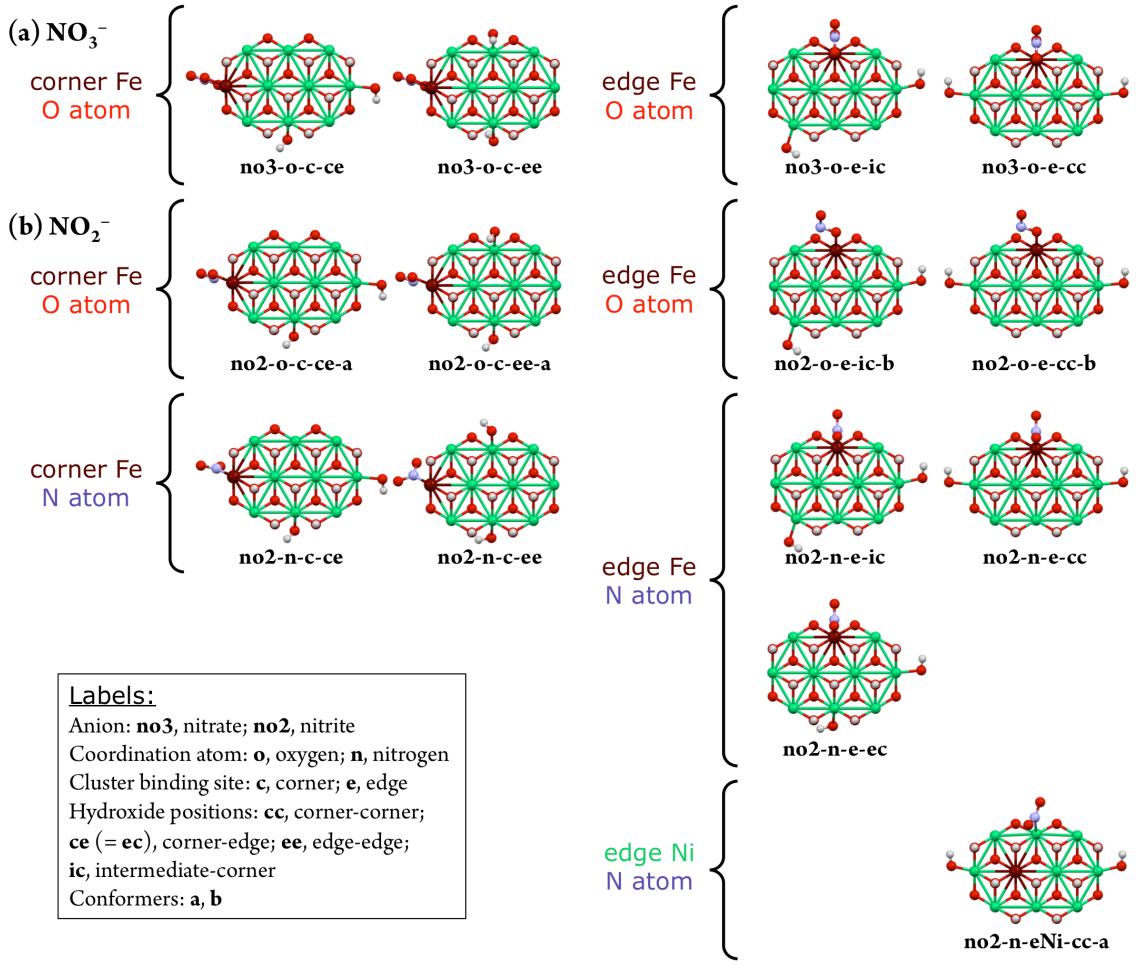

Figure S14: Illustrations of selected geometries of (a) $[Ni_9Fe_1(OH)_{20}(NO_3)]$ and (b) $[Ni_9Fe_1(OH)_{20}(NO_2)]$ model clusters; corresponding N 1s core level shifts are given in Table S6. See enclosed xyz coordinate files for more details. Corner and edge Fe binding sites are also illustrated in Figure 12 (main text). A more detailed view of nitrate and nitrite binding motifs by O- or N-atom coordination can be found in Figure 13 in the main text. The varying positions of attached OH groups to the remaining edges did not significantly change the calculated N 1s core level shifts (Table S6). Colors: Ni green, Fe maroon, N blue, O red, H white.

The configuration of the $[Ni_9Fe_1(OH)_{20}(NO_3)]$ cluster, to which all N 1s core level shifts were referenced, is depicted in Figure S15.

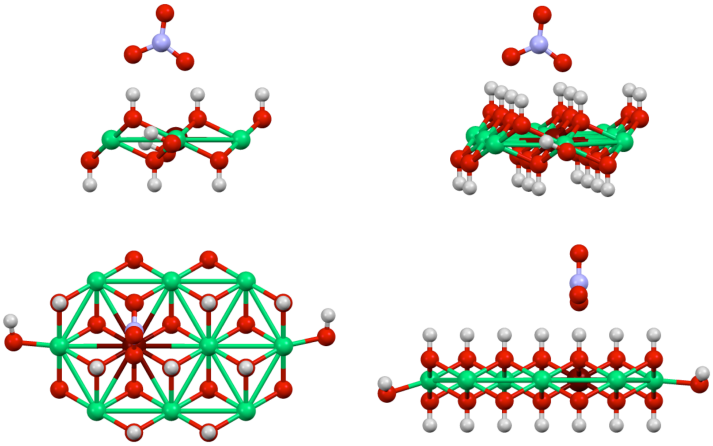

Figure S15: Illustration of the reference configuration of the $[Ni_9Fe_1(OH)_{20}(NO_3)]$ cluster used to calculate all N 1s core level shifts shown in Table S6, *i.e.* the N 1s core level shift of this structure is set to zero for the DFT calculations. Top row: views along the long axis of the cluster; bottom row: top and side views of the same structure. Absolute N 1s orbital energy for this configuration at the present level of theory: –398.40 eV; N 1s binding energy calculated via STS: 413.00 eV. Colors: Ni green, Fe maroon, N blue, O red, H white.

Calculated core level shifts. Table S6 summarizes the N 1s CLS data calculated using the $[Ni_9Fe_1(OH)_{20}(NO_{2\text{ or }3})]$ cluster models described above (Figure S14). The experimental CLS between pristine NO_3^- (407.3 eV) and NO_2^- (403.5 eV) amounted to 3.8 eV.[8] The previously unassigned XPS signal centered at 405.1 eV corresponds to a shift of –2.2 eV with respect to pristine NO_3^- to lower binding energies, or to a shift of +1.6 eV to higher binding energies with respect to NO_2^-. The calculated CLS of Table S6 are given relative to the reference configuration shown in Figure S15.

The data of Table S6 indicated that coordination of NO_3^- to various cluster sites (Figure S14) shifted the N 1s BE only modestly. In contrast, the previously unassigned experimental XPS peak was shifted to lower BE by −2.2 eV with respect to the NO_3^- peak at 407.3 eV. Calculated CLS of *nitrate* binding to Fe sites at the clusters' rims were thus inconsistent with these experimental data.

Next, we consider N 1s shifts due to binding of NO_2^- to the various sites at the cluster. In general, anions are present in LDH materials to balance the excess positive charges of the trivalent metal (here Fe^{3+}) substituting for divalent one (here Ni^{2+}).[12] Nevertheless, as a test we also assessed nitrite binding by its N-atom to edge-site Ni of a $[Ni_9Fe_1(OH)_{20}]$ with center Fe (cf. Figure S14, no2-n-eNi-cc-a, bottom right). We found that the resulting N 1s CLS were too large to explain the experimental data (see Table S6, last line).

The required −2.2 eV shift with respect to free nitrate was best approximated by calculated CLS of NO_2^- coordination to edge-site Fe of the cluster. Specifically, when NO_2^- was bound by its N-atom to edge-site Fe, the calculated CLS amounted to −2.7 eV, which is reasonably close to the experimentally observed shift of −2.2 eV. The corresponding structures are displayed in Figure S14 (structures **no2-n-e-cc**, **no2-n-e-ec**, and **no2-n-e-ic**). Note that the calculated initial state contribution to the core level shifts (is-CLSs) give shifts of –2.1 eV, in very close agreement with the experimental shift of –2.2 eV. These is-CLSs neglect electronic relaxation effects due to formation of the core hole in the cationic final state. On the other hand, the cationic final state is expected to be quite sensitive to solvent screening effects, which are approximated by the COSMO model in this work. Hence, we suggest that both is-CLS and the full CLS should be considered as valid useful approximations for the XPS shifts. Both approaches predict N coordination of NO_2^- to edge-site Fe as the best explanation for the experimentally observed XPS binding energy shift. Furthermore, the real [NiFe]-LDH precatalysts as synthesized by PLAL were nanosheets with a diameter of 13 nm (Table 2 in the main text). Thus, it is expected that edge Fe sites played a predominant role over corner Fe for anion binding.

Table S6: N 1s orbital energies ε, initial-state contributions to core level shifts (is-CLS) calculated from the ε, relaxed core level binding energies calculated via STS (STS-BE) and full core-level shifts (CLS) calculated from the STS-BE from DFT calculations. The structures corresponding to the acronyms are shown in Figure S14. The reference configuration used for the calculation of the is-CLS and CLS is depicted in Figure S15; the N 1s orbital energy ($-\varepsilon_{ref}$ = 398.4 eV) and STS-BE (413.0 eV) thus correspond to the zero in the is-CLS and CLS columns.

Anion	Cluster binding site	($NO_{2\text{ or }3}^-$) binding atom	Acronym	$-\varepsilon$ [eV]	is-CLS [eV]	STS-BE [eV]	CLS [eV]
NO_3^-	edge Fe	O	no3-o-e-ic	399.0	+0.6	413.4	+0.4
			no3-o-e-cc	399.0	+0.6	413.4	+0.4
			no3-o-e-ec	399.0	+0.6	413.4	+0.4
	corner Fe	O	no3-o-c-ce	398.4	+0.0	412.5	–0.5
			no3-o-c-ee	398.3	–0.1	412.5	–0.5
NO_2^-	corner Fe	O	no2-o-c-ce-a	394.6	–3.8	408.5	–4.5
			no2-o-c-ce-b	394.6	–3.8	408.5	–4.5
			no2-o-c-ee-a	394.6	–3.8	408.4	–4.6
			no2-o-c-ee-b	394.5	–3.9	408.3	–4.7
	corner Fe	N	no2-n-c-ee	395.0	–3.4	409.0	–4.0
			no2-n-c-ce	395.0	–3.4	409.1	–3.9
	edge Fe	O	no2-o-e-cc-b	395.3	–3.1	409.6	–3.4
			no2-o-e-ic-a	395.6	–2.8	409.8	–3.2
			no2-o-e-ic-b	395.3	–3.1	409.6	–3.4
	edge Fe	N	no2-n-e-cc	396.3	–2.1	410.3	–2.7
			no2-n-e-ec	396.3	–2.1	410.3	–2.7
			no2-n-e-ic	396.3	–2.1	410.3	–2.7
	edge Ni	N	no2-n-eNi-cc-a	394.9	–3.5	409.2	–3.8

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Cartesian coordinates of cluster models used in the DFT calculations

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54
Energy = -16628.51025415

N	4.6141349	9.1388467	11.4888577
O	4.6303352	7.9813974	11.9686490
O	4.6065662	9.2943327	10.2757484
O	4.6069273	10.1204813	12.2587526
Ni	3.0699991	7.0898580	15.4666657
Ni	1.5349996	9.7485573	15.4666657
Ni	6.1399983	7.0898580	15.4666657
Fe	4.6133376	9.7404004	15.4397088
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
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O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
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H	-0.4725402	8.7224312	15.1919509
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Fe	1.4687197	9.7688473	15.5051178
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no3-o-c-ee

54

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no3-o-e-cc

54

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Ni	7.6749978	9.7485573	15.4666657
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H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
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H	-0.4607993	8.7158933	15.1667398
O	12.6416463	9.5729396	15.6051194
H	12.7386724	8.7129778	15.1689262

no3-o-e-ec

54

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O	6.1256527	7.0199299	12.4258102
Ni	3.0699991	7.0898580	15.4666657
Ni	1.5349996	9.7485573	15.4666657
Fe	6.1464609	7.1014950	15.4485319
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	12.5122573	9.3595208	16.0125965
H	12.5919166	8.4830469	15.6063802
O	6.0401270	13.7119191	17.0280869
H	5.0985677	13.9241120	16.9471708

no3-o-e-ic

54

Energy = -16628.55868222

N	6.1405347	5.8634442	12.8506366
O	6.1436154	4.8928150	12.1228269
O	6.1433817	5.6531483	14.1146589
O	6.1347222	7.0191356	12.4274088
Ni	3.0699991	7.0898580	15.4666657
Ni	1.5349996	9.7485573	15.4666657
Fe	6.1445294	7.0967458	15.4501146
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	12.5100576	9.3640797	16.0117100
H	12.5942264	8.4871109	15.6073343
O	2.5246330	14.1383461	16.0026204
H	3.2492685	14.6164478	15.5701960

no2-n-c-ce

53

Energy = -16553.51213095

N	0.2409911	9.1311614	16.7498042
O	0.5393158	8.9884727	17.9426828
O	-0.9203080	8.9157383	16.3913555
Ni	3.0699991	7.0898580	15.4666657
Fe	1.5209308	9.7490764	15.5443050
Ni	6.1399983	7.0898580	15.4666657
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	6.0837762	13.7682144	16.6597741
H	5.5209406	14.3932942	16.1678560
O	12.6445555	9.9241445	15.3346137
H	12.7309606	10.7850219	15.7713742

no2-n-c-ee

53

Energy = -16553.47431913

N	0.2356863	9.0301970	16.6878549
O	0.4790252	8.1029786	17.4665310
O	-0.9153634	9.4840233	16.6378767
Ni	3.0699991	7.0898580	15.4666657
Fe	1.5246764	9.7460754	15.5462904
Ni	6.1399983	7.0898580	15.4666657
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	6.0678072	13.7066823	17.0339066
H	5.1104494	13.8525141	17.0267777
O	6.0853563	5.7282973	14.2723900
H	5.5103753	5.1097284	14.7584123

no2-n-e-cc

53

Energy = -16553.56003909

N	6.1401284	5.8014258	14.0046591
O	6.1407820	6.2615083	12.8671315
O	6.1395337	4.6070060	14.2133664
Ni	3.0699991	7.0898580	15.4666657
Ni	1.5349996	9.7485573	15.4666657
Fe	6.1399839	7.0779964	15.4483881
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	-0.3626396	9.5752224	15.6011185
H	-0.4581954	8.7138317	15.1673954
O	12.6423691	9.5733820	15.6032866
H	12.7379553	8.7133105	15.1669835

no2-n-e-ec

53

Energy = -16553.52019689

N	6.1437881	5.8028298	14.0037034
O	6.1574492	4.6083378	14.2119045
O	6.1257322	6.2630291	12.8662950
Ni	3.0699991	7.0898580	15.4666657
Ni	1.5349996	9.7485573	15.4666657
Fe	6.1456115	7.0802259	15.4490415
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	12.6453033	9.5670399	15.6015722
H	12.7333140	8.7065990	15.1644661
O	6.0372107	13.7144765	17.0284517
H	5.0970731	13.9289195	16.9377251

no2-n-e-ic

53

Energy = -16553.47197390

N	6.1419724	5.8006113	14.0058652
O	6.1339180	6.2605467	12.8682986
O	6.1466463	4.6063335	14.2149902
Ni	3.0699991	7.0898580	15.4666657
Ni	1.5349996	9.7485573	15.4666657
Fe	6.1440412	7.0796008	15.4480193
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	12.5116304	9.3619850	16.0100616
H	12.5924410	8.4854420	15.6040722
O	2.5233975	14.1360561	16.0061933
H	3.2489755	14.6160766	15.5775060

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53

Energy = -16553.50437074

N	0.1221893	9.4173847	17.8812475
O	0.0319932	9.1322335	16.6441788
O	-0.8349232	9.0854851	18.5564698
Ni	3.0699982	7.0898560	15.4666614
Fe	1.5149402	9.7557011	15.5296528
Ni	6.1399966	7.0898560	15.4666614
Ni	4.6049974	9.7485546	15.4666614
Ni	3.0699982	12.4072530	15.4666614
Ni	9.2099948	7.0898560	15.4666614
Ni	7.6749956	9.7485546	15.4666614
Ni	6.1399966	12.4072530	15.4666614
Ni	10.7449940	9.7485546	15.4666614
Ni	9.2099948	12.4072530	15.4666614
O	4.6049974	6.2036266	16.3173208
O	1.5349992	7.9760856	14.6159918
O	3.0699982	8.8623250	16.3173208
O	1.5349992	11.5210136	16.3173208
O	7.6749956	6.2036266	16.3173208
O	4.6049974	7.9760856	14.6159918
O	6.1399966	8.8623250	16.3173208
O	3.0699982	10.6347840	14.6159918
O	4.6049974	11.5210136	16.3173208
O	7.6749956	7.9760856	14.6159918
O	9.2099948	8.8623250	16.3173208
O	6.1399966	10.6347840	14.6159918
O	7.6749956	11.5210136	16.3173208
O	4.6049974	13.2934826	14.6159918
O	10.7449940	7.9760856	14.6159918
O	9.2099948	10.6347840	14.6159918
O	10.7449940	11.5210136	16.3173208
O	7.6749956	13.2934826	14.6159918
H	4.6049974	6.2036266	17.3173202
H	1.5349992	7.9760856	13.6159924
H	3.0699982	8.8623250	17.3173202
H	1.5349992	11.5210136	17.3173202
H	7.6749956	6.2036266	17.3173202
H	4.6049974	7.9760856	13.6159924
H	6.1399966	8.8623250	17.3173202
H	3.0699982	10.6347840	13.6159924
H	4.6049974	11.5210136	17.3173202
H	7.6749956	7.9760856	13.6159924
H	9.2099948	8.8623250	17.3173202
H	6.1399966	10.6347840	13.6159924
H	7.6749956	11.5210136	17.3173202
H	4.6049974	13.2934826	13.6159924
H	10.7449940	7.9760856	13.6159924
H	9.2099948	10.6347840	13.6159924
H	10.7449940	11.5210136	17.3173202
H	7.6749956	13.2934826	13.6159924
O	6.0834810	13.7682801	16.6597434
H	5.5166835	14.3910397	16.1694126
O	12.6446558	9.9237118	15.3353949
H	12.7312065	10.7845745	15.7721854

no2-o-c-ce-b

53

Energy = -16553.46430354

N	-0.0418445	9.1802228	17.8931074
O	0.9859593	9.5636951	18.4391510
O	-0.0273019	9.1323880	16.6291173
Ni	3.0699982	7.0898560	15.4666614
Fe	1.5101359	9.7479598	15.5472320
Ni	6.1399966	7.0898560	15.4666614
Ni	4.6049974	9.7485546	15.4666614
Ni	3.0699982	12.4072530	15.4666614
Ni	9.2099948	7.0898560	15.4666614
Ni	7.6749956	9.7485546	15.4666614
Ni	6.1399966	12.4072530	15.4666614
Ni	10.7449940	9.7485546	15.4666614
Ni	9.2099948	12.4072530	15.4666614
O	4.6049974	6.2036266	16.3173208
O	1.5349992	7.9760856	14.6159918
O	3.0699982	8.8623250	16.3173208
O	1.5349992	11.5210136	16.3173208
O	7.6749956	6.2036266	16.3173208
O	4.6049974	7.9760856	14.6159918
O	6.1399966	8.8623250	16.3173208
O	3.0699982	10.6347840	14.6159918
O	4.6049974	11.5210136	16.3173208
O	7.6749956	7.9760856	14.6159918
O	9.2099948	8.8623250	16.3173208
O	6.1399966	10.6347840	14.6159918
O	7.6749956	11.5210136	16.3173208
O	4.6049974	13.2934826	14.6159918
O	10.7449940	7.9760856	14.6159918
O	9.2099948	10.6347840	14.6159918
O	10.7449940	11.5210136	16.3173208
O	7.6749956	13.2934826	14.6159918
H	4.6049974	6.2036266	17.3173202
H	1.5349992	7.9760856	13.6159924
H	3.0699982	8.8623250	17.3173202
H	1.5349992	11.5210136	17.3173202
H	7.6749956	6.2036266	17.3173202
H	4.6049974	7.9760856	13.6159924
H	6.1399966	8.8623250	17.3173202
H	3.0699982	10.6347840	13.6159924
H	4.6049974	11.5210136	17.3173202
H	7.6749956	7.9760856	13.6159924
H	9.2099948	8.8623250	17.3173202
H	6.1399966	10.6347840	13.6159924
H	7.6749956	11.5210136	17.3173202
H	4.6049974	13.2934826	13.6159924
H	10.7449940	7.9760856	13.6159924
H	9.2099948	10.6347840	13.6159924
H	10.7449940	11.5210136	17.3173202
H	7.6749956	13.2934826	13.6159924
O	6.0843375	13.7672307	16.6605883
H	5.5111229	14.3875949	16.1748691
O	12.5133078	10.1363681	14.9242132
H	12.5863978	11.0125371	15.3327207

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53

Energy = -16553.44161583

N	0.0832761	9.4406708	17.8602992
O	0.0164720	9.1364492	16.6267508
O	-0.8837173	9.1129407	18.5239893
Ni	3.0699991	7.0898580	15.4666657
Fe	1.5166716	9.7514478	15.5258064
Ni	6.1399983	7.0898580	15.4666657
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	6.0894795	13.7664267	16.6543526
H	5.5138703	14.3885597	16.1736845
O	6.1910420	5.7439566	13.9258094
H	5.8536856	6.2804757	13.1935302

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53

Energy = -16553.46880593

N	-0.0577008	9.1407584	17.8532848
O	0.9763199	9.4954145	18.4076140
O	-0.0460856	9.1268621	16.5889860
Ni	3.0699991	7.0898580	15.4666657
Fe	1.5171041	9.7614368	15.5346143
Ni	6.1399983	7.0898580	15.4666657
Ni	4.6049987	9.7485573	15.4666657
Ni	3.0699991	12.4072565	15.4666657
Ni	9.2099974	7.0898580	15.4666657
Ni	7.6749978	9.7485573	15.4666657
Ni	6.1399983	12.4072565	15.4666657
Ni	10.7449970	9.7485573	15.4666657
Ni	9.2099974	12.4072565	15.4666657
O	4.6049987	6.2036283	16.3173254
O	1.5349996	7.9760878	14.6159959
O	3.0699991	8.8623275	16.3173254
O	1.5349996	11.5210168	16.3173254
O	7.6749978	6.2036283	16.3173254
O	4.6049987	7.9760878	14.6159959
O	6.1399983	8.8623275	16.3173254
O	3.0699991	10.6347870	14.6159959
O	4.6049987	11.5210168	16.3173254
O	7.6749978	7.9760878	14.6159959
O	9.2099974	8.8623275	16.3173254
O	6.1399983	10.6347870	14.6159959
O	7.6749978	11.5210168	16.3173254
O	4.6049987	13.2934863	14.6159959
O	10.7449970	7.9760878	14.6159959
O	9.2099974	10.6347870	14.6159959
O	10.7449970	11.5210168	16.3173254
O	7.6749978	13.2934863	14.6159959
H	4.6049987	6.2036283	17.3173251
H	1.5349996	7.9760878	13.6159962
H	3.0699991	8.8623275	17.3173251
H	1.5349996	11.5210168	17.3173251
H	7.6749978	6.2036283	17.3173251
H	4.6049987	7.9760878	13.6159962
H	6.1399983	8.8623275	17.3173251
H	3.0699991	10.6347870	13.6159962
H	4.6049987	11.5210168	17.3173251
H	7.6749978	7.9760878	13.6159962
H	9.2099974	8.8623275	17.3173251
H	6.1399983	10.6347870	13.6159962
H	7.6749978	11.5210168	17.3173251
H	4.6049987	13.2934863	13.6159962
H	10.7449970	7.9760878	13.6159962
H	9.2099974	10.6347870	13.6159962
H	10.7449970	11.5210168	17.3173251
H	7.6749978	13.2934863	13.6159962
O	6.0687431	13.7072681	17.0342500
H	5.1103751	13.8462940	17.0309147
O	6.0851427	5.7280011	14.2725243
H	5.5076438	5.1115669	14.7582888

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53

Energy = -16553.55541683

N	4.9766729	5.3586010	13.6806839
O	5.0082931	4.4696014	12.8700464
O	6.1398815	5.7323304	14.0949834
Ni	3.0699982	7.0898560	15.4666614
Ni	1.5349992	9.7485546	15.4666614
Fe	6.1264433	7.0821384	15.4529711
Ni	4.6049974	9.7485546	15.4666614
Ni	3.0699982	12.4072530	15.4666614
Ni	9.2099948	7.0898560	15.4666614
Ni	7.6749956	9.7485546	15.4666614
Ni	6.1399966	12.4072530	15.4666614
Ni	10.7449940	9.7485546	15.4666614
Ni	9.2099948	12.4072530	15.4666614
O	4.6049974	6.2036266	16.3173208
O	1.5349992	7.9760856	14.6159918
O	3.0699982	8.8623250	16.3173208
O	1.5349992	11.5210136	16.3173208
O	7.6749956	6.2036266	16.3173208
O	4.6049974	7.9760856	14.6159918
O	6.1399966	8.8623250	16.3173208
O	3.0699982	10.6347840	14.6159918
O	4.6049974	11.5210136	16.3173208
O	7.6749956	7.9760856	14.6159918
O	9.2099948	8.8623250	16.3173208
O	6.1399966	10.6347840	14.6159918
O	7.6749956	11.5210136	16.3173208
O	4.6049974	13.2934826	14.6159918
O	10.7449940	7.9760856	14.6159918
O	9.2099948	10.6347840	14.6159918
O	10.7449940	11.5210136	16.3173208
O	7.6749956	13.2934826	14.6159918
H	4.6049974	6.2036266	17.3173202
H	1.5349992	7.9760856	13.6159924
H	3.0699982	8.8623250	17.3173202
H	1.5349992	11.5210136	17.3173202
H	7.6749956	6.2036266	17.3173202
H	4.6049974	7.9760856	13.6159924
H	6.1399966	8.8623250	17.3173202
H	3.0699982	10.6347840	13.6159924
H	4.6049974	11.5210136	17.3173202
H	7.6749956	7.9760856	13.6159924
H	9.2099948	8.8623250	17.3173202
H	6.1399966	10.6347840	13.6159924
H	7.6749956	11.5210136	17.3173202
H	4.6049974	13.2934826	13.6159924
H	10.7449940	7.9760856	13.6159924
H	9.2099948	10.6347840	13.6159924
H	10.7449940	11.5210136	17.3173202
H	7.6749956	13.2934826	13.6159924
O	-0.3626455	9.5747464	15.6023886
H	-0.4569873	8.7139831	15.1671469
O	12.6424937	9.5739494	15.6026548
H	12.7376499	8.7137212	15.1665635

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53

Energy = -16553.46740846

N	4.9807487	5.3597082	13.6802663
O	5.0127547	4.4713741	12.8692538
O	6.1440132	5.7336573	14.0949364
Ni	3.0699982	7.0898560	15.4666614
Ni	1.5349992	9.7485546	15.4666614
Fe	6.1307354	7.0837596	15.4526060
Ni	4.6049974	9.7485546	15.4666614
Ni	3.0699982	12.4072530	15.4666614
Ni	9.2099948	7.0898560	15.4666614
Ni	7.6749956	9.7485546	15.4666614
Ni	6.1399966	12.4072530	15.4666614
Ni	10.7449940	9.7485546	15.4666614
Ni	9.2099948	12.4072530	15.4666614
O	4.6049974	6.2036266	16.3173208
O	1.5349992	7.9760856	14.6159918
O	3.0699982	8.8623250	16.3173208
O	1.5349992	11.5210136	16.3173208
O	7.6749956	6.2036266	16.3173208
O	4.6049974	7.9760856	14.6159918
O	6.1399966	8.8623250	16.3173208
O	3.0699982	10.6347840	14.6159918
O	4.6049974	11.5210136	16.3173208
O	7.6749956	7.9760856	14.6159918
O	9.2099948	8.8623250	16.3173208
O	6.1399966	10.6347840	14.6159918
O	7.6749956	11.5210136	16.3173208
O	4.6049974	13.2934826	14.6159918
O	10.7449940	7.9760856	14.6159918
O	9.2099948	10.6347840	14.6159918
O	10.7449940	11.5210136	16.3173208
O	7.6749956	13.2934826	14.6159918
H	4.6049974	6.2036266	17.3173202
H	1.5349992	7.9760856	13.6159924
H	3.0699982	8.8623250	17.3173202
H	1.5349992	11.5210136	17.3173202
H	7.6749956	6.2036266	17.3173202
H	4.6049974	7.9760856	13.6159924
H	6.1399966	8.8623250	17.3173202
H	3.0699982	10.6347840	13.6159924
H	4.6049974	11.5210136	17.3173202
H	7.6749956	7.9760856	13.6159924
H	9.2099948	8.8623250	17.3173202
H	6.1399966	10.6347840	13.6159924
H	7.6749956	11.5210136	17.3173202
H	4.6049974	13.2934826	13.6159924
H	10.7449940	7.9760856	13.6159924
H	9.2099948	10.6347840	13.6159924
H	10.7449940	11.5210136	17.3173202
H	7.6749956	13.2934826	13.6159924
O	12.5116921	9.3620398	16.0099796
H	12.5921730	8.4857142	15.6034358
O	2.5238234	14.1358936	16.0068735
H	3.2488810	14.6162746	15.5777245

no2-n-eNi-cc

53

Energy = -16553.45895936

N	6.0336675	5.7283874	13.6671458
O	5.5545224	6.2860392	12.6643187
O	6.4399481	4.5780078	13.5476889
Ni	3.0699982	7.0898560	15.4666614
Ni	1.5349992	9.7485546	15.4666614
Ni	6.1502608	6.9595342	15.3737469
Fe	4.6049974	9.7485546	15.4666614
Ni	3.0699982	12.4072530	15.4666614
Ni	9.2099948	7.0898560	15.4666614
Ni	7.6749956	9.7485546	15.4666614
Ni	6.1399966	12.4072530	15.4666614
Ni	10.7449940	9.7485546	15.4666614
Ni	9.2099948	12.4072530	15.4666614
O	4.6049974	6.2036266	16.3173208
O	1.5349992	7.9760856	14.6159918
O	3.0699982	8.8623250	16.3173208
O	1.5349992	11.5210136	16.3173208
O	7.6749956	6.2036266	16.3173208
O	4.6049974	7.9760856	14.6159918
O	6.1399966	8.8623250	16.3173208
O	3.0699982	10.6347840	14.6159918
O	4.6049974	11.5210136	16.3173208
O	7.6749956	7.9760856	14.6159918
O	9.2099948	8.8623250	16.3173208
O	6.1399966	10.6347840	14.6159918
O	7.6749956	11.5210136	16.3173208
O	4.6049974	13.2934826	14.6159918
O	10.7449940	7.9760856	14.6159918
O	9.2099948	10.6347840	14.6159918
O	10.7449940	11.5210136	16.3173208
O	7.6749956	13.2934826	14.6159918
H	4.6049974	6.2036266	17.3173202
H	1.5349992	7.9760856	13.6159924
H	3.0699982	8.8623250	17.3173202
H	1.5349992	11.5210136	17.3173202
H	7.6749956	6.2036266	17.3173202
H	4.6049974	7.9760856	13.6159924
H	6.1399966	8.8623250	17.3173202
H	3.0699982	10.6347840	13.6159924
H	4.6049974	11.5210136	17.3173202
H	7.6749956	7.9760856	13.6159924
H	9.2099948	8.8623250	17.3173202
H	6.1399966	10.6347840	13.6159924
H	7.6749956	11.5210136	17.3173202
H	4.6049974	13.2934826	13.6159924
H	10.7449940	7.9760856	13.6159924
H	9.2099948	10.6347840	13.6159924
H	10.7449940	11.5210136	17.3173202
H	7.6749956	13.2934826	13.6159924
O	-0.1935283	9.3551282	16.0605408
H	-0.3041805	8.4756834	15.6676121
O	12.5138375	9.3631070	16.0061476
H	12.5860084	8.4878370	15.5954044