Rearranging spin electrons by axial-ligand-induced hybridization state transition to boost the activity of nickel single-atom-catalyst for electrochemical CO_2 reduction

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1. Experimental section

1.1 Catalyst synthesis: Ni-N-C for CO_2RR

The catalyst precursors were synthesized through dry ball-milling of the Zn(II) zeolitic imidazolate framework ZIF-8 (Basolite Z1200 from BASF, labeled ZIF-8), nickel acetate, and 1,10-phenanthroline. Specifically, 200 mg of 1,10-phenanthroline, 800 mg of ZIF-8, and the appropriate amount of nickel acetate to achieve a 0.5 wt % transition metal content in the precursor were combined in a ZrO_2 crucible along with 100 zirconium-oxide balls (5 mm diameter). This assembly was sealed under air and subjected to four cycles of 30 minutes of milling at 400 rpm using a planetary ball miller. Subsequently, the catalyst precursors from the milling process underwent pyrolysis at 1050 °C in an N_2 atmosphere for one hour. The resulting catalysts were denoted as Ni-N-C.

1.2 IrOx/Ti-mesh anode

Catalysts based on iridium supported on freestanding titanium substrates were fabricated using a dip coating and thermal decomposition technique. The titanium mesh was etched in boiling 0.5 M oxalic acid (≥98%, Sigma-Aldrich) for 60 minutes. Subsequently, the mesh was dipped into a 10 mL solution of isopropanol (ACS reagent, Fisher Chemicals) with 10% volume of concentrated HCl (ACS reagent, Sigma Aldrich) containing 30 mg of dissolved $IrCl_3 \cdot xH_2O$ (99.8%, Alfa Aesar). The mesh was dried at 100°C for 10 minutes and calcined at 500°C for 10 minutes in an air environment. This process was reiterated to achieve a catalyst loading of 1 mg/cm^2, and the resultant materials were labeled as IrOx/Ti-mesh.

1.3 NiPc for CO_2RR

A total of 196 mg of nickel phthalocyanine (NiPc) and 796 mg of Vulcan with a 2 wt% Ni composition were subjected to ball milling for 30 minutes utilizing a planetary ball miller. This operation occurred within a 50 mL ZrO_2 crucible housing 100 zirconium-oxide balls measuring 5 mm in diameter, rotating at 100 rpm. After milling, the mixture underwent heat treatment at 300°C under a N_2 atmosphere for one hour, with a temperature ramping rate of 15°C per minute.

1.4 Characterization

The morphologies of as-prepared catalysts were observed by SEM (Hitachi S-4800), TEM (Talos F200X), and Aberration-corrected HAADF-STEM (HD2700CS). X-ray diffraction (XRD) patterns were obtained using a PANanalytical X'Pert Pro powder X-ray diffractometer with Cu Kα radiation. Raman spectra were acquired using a Thermo Fisher DXR spectrometer with a length of 532 nm. The pore structures of these catalysts were analyzed with a Micromeritics ASAP 2020 instrument. The acquisition of the X-ray photoelectron spectroscopy (XPS) spectra was performed on a Kratos Axis DLD Supra X-ray photoelectron spectrometer using an Al Kα source monochromatic operating at 300 W. Metal K-edge X-ray absorption spectroscopy (XAS) was performed at room temperature at the SAMBA beamline (Synchrotron SOLEIL). The detailed analysis method for the extended X-ray absorption fine structure (EXAFS) data is available elsewhere[1].

1.5 Flow cell testing and product analysis

The electrochemical tests were all conducted within a commercial flow cell with Sustainion RT anion exchange membrane, and commercial Ag/AgCl reference. The reference electrode, if used, was placed at the cathode side to measure the cathode potential. The cathode potentials reported were measured with a three-electrode mode, and iR was corrected according to the high-frequency resistance. Current densities reported were normalized based on the geometric surface area of 1 cm^2. A self-fabricated IrOx/Ti-mesh was employed as the anode, while the cathode utilized Ni-N-C or NiPc catalysts. The cathode electrolyte utilized 1M $KHCO_3$ as the main supporting electrolyte, with varying concentrations of KCl (0, 10, 100 mM). The flow cell experiments were carried out with a potentiostat (Biologic SP-150) under galvanostatic control(10，15，20，25，30，40，50，60mA /cm^2) for approximately 30 minutes at each designated current level throughout the catalytic assessments, with the current ranging from low to high values.

The change of potential scale versus RHE was done according to the following equation：

$$E\ (V\ vs\ RHE) = E\ (V\ vsAg/AgCl) + E\ (V\ of\ Ag/AgClvs\ NHE) + 0.059\ pH + iR \quad （1）$$

where E (V of Ag/AgCl vs NHE) = 0.199 V.

The catholyte and anolyte were circulated individually through their designated compartments at a flow rate of 10 mL/min each. The CO_2 feed with 99.999% purity was introduced at a flow rate of 20 mL/min to the back of the cathode Gas Diffusion Electrode (GDE).

1.6 CO_2RR product analysis

Gaseous products were analyzed using a gas chromatograph (Shimadzu, GC-2014) with Ar as a carrier gas, which was equipped with a flame ionization detector (FlD) and a thermal conductivity detector (TCD) detector. Gas samples were injected through a sampling loop and analyzed 10 min after the start of the electrolysis and thereafter every 15 min. The Faradaic efficiency (FE) for the gaseous products was calculated with the following equation:

$$FE = \frac{gas\ flow\ through\ the\ cell \times product\ concentration}{electric\ current\ at\ sampling\ time/nF} \times 100\% \quad （2）$$

In the above equations, n is the number of electrons transferred and F is the Faraday constant. Partial current density of CO was calculated with the following equation:

$$J\ （CO）= I\ （total）\times \mathrm{FE}\ (\mathrm{CO})\ \quad （3）$$

1.7 H-cell electrochemical measurement

pH-dependent experiment was measured in a regular three-electrode H-cell divided by a Sustainion RT anion exchange membrane. The working electrode was the catalyst-coated carbon paper mentioned above, and a Pt mesh was deployed as the counter electrodes. A leak-free Ag/AgCl

electrode was used as the reference. The current density was normalized to the working electrode's geometrical area (1.76 cm^2). All the electrochemical experiments were performed in a CO_2-purged electrolyte (CO_2 flow rate, 30mL/min). The pH value of each is presented in Supplementary Table S8.

2. Computational Methods

2.1 DFT calculations

All the DFT calculations were executed in the Vienna ab initio Simulation Package (VASP)[2]. The projector augmented ware pseudopotential (PAW)[3,4] was used to treat nuclear-electron interactions, and the Perdew-Burke-Ernzerhof functional (PBE)[5] was used to establish the exchange and correlation energies. All the DFT calculations considered polarized spin due to the magnetic properties of Ni element. The weak interaction were considered by DFT-D3 dispersion-corrected method[6]. The Gaussian electron smearing σ was set to 0.05 eV and the energy cutoff was set to 500 eV. The convergence conditions of DFT calculations is that the force and energy are less than 0.01 eV/Å and 10^{-6} eV/atom, respectively.

For the NiN_4 model, a 9.8 Å × 12.8 Å × 20.0 Å orthorhombic box was built, which contains 42 C atoms, 4 N atoms, and 1 Ni atom. On the basis of the NiN_4 model, removing 8 C atoms to obtain the NiN_{2+2} model. As for NiPc, we constructed a 20.0 Å × 20.0 Å × 20.0 Å cubical box, which contains 32 C atoms, 8 N atoms, 16 H atoms, and 1 Ni atom. To avoid periodic interaction, a 20 Å vacuum layer was adopted in the *z* direction for each structure. Especially, a 7 Å vacuum layer was adopted in the *x* and *y* direction to avoid periodic interaction in *xy* plane due to the molecular NiPc. The configurations of NiPc, NiN_4, and NiN_{2+2} were shown in Figures 1a-c in the main text. All axial ligands were connected to Ni atoms. The 3 × 3 × 1 Gamma K-point grid was constructed for NiN_4 and NiN_{2+2} models, the 1 × 1 × 1 Gamma K-point grid was constructed for NiPc model.

The Gibbs free energy was given by

$$G = E + E_{ZPE} + \int C_p dT - TS \quad (4)$$

where E is the total energy of calculated system, E_{ZPE} is the zero-point energy, C_p is the heat capacity, TS is the contribution of entropy to free energy (T = 298.15 K). According to the computational hydrogen electrode (CHE) model[7], The free energy of $H^+ + e^-$ was considered to be equal to the free energy of 1/2 H_2.

We supplied the structural coordinate files and input files for DFT calculations in the supporting information (page 31-97).

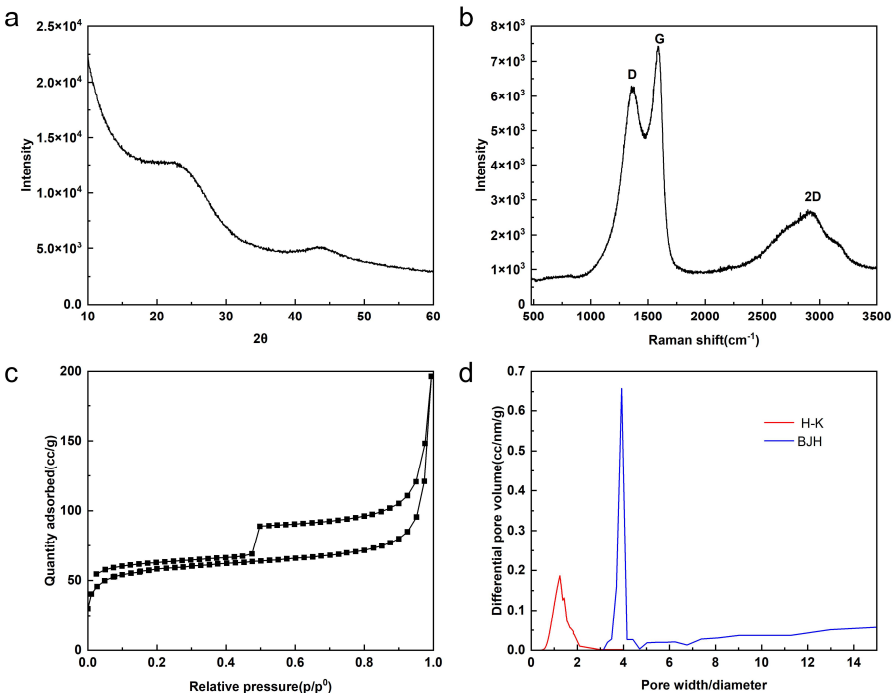

Figure S1. (a) XRD pattern, (b) Raman spectrum, (c) N_2 physisorption isotherms, and (d) pore size distribution of Ni-N-C.

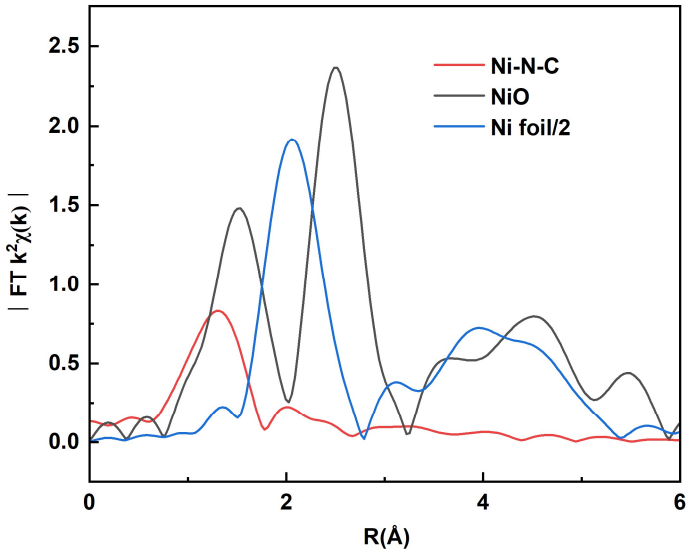

Figure S2. FT-EXAFS spectra in R space of Ni-N-C, nickel foils and nickel oxide powders.

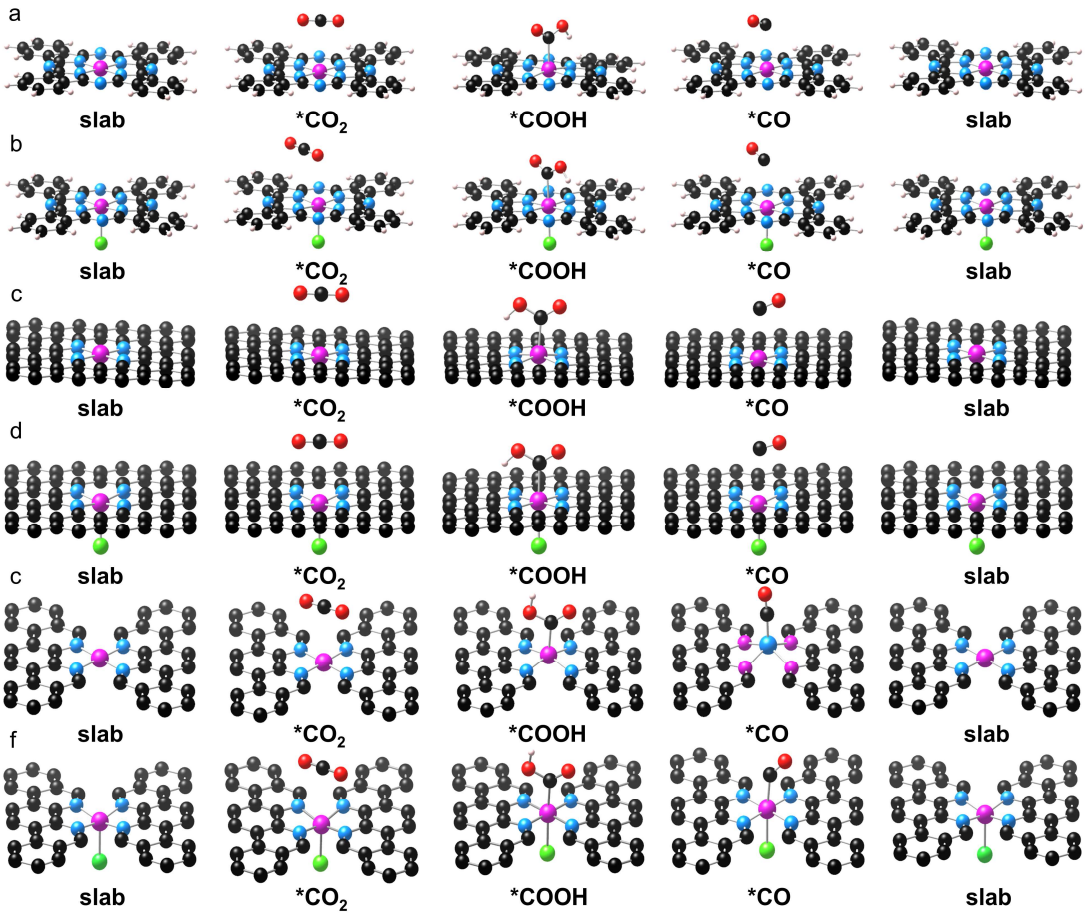

Figure S3. The simulated configurations of four elementary steps on (a) NiPc, (b) NiPc-Cl, (c) NiN_4, (d) NiN_4-Cl, (e) NiN_{2+2}, and (f) NiN_{2+2}-Cl models. The black, blue, purple, green, red and white balls represent C, N, Ni, Cl, O and H atoms, respectively.

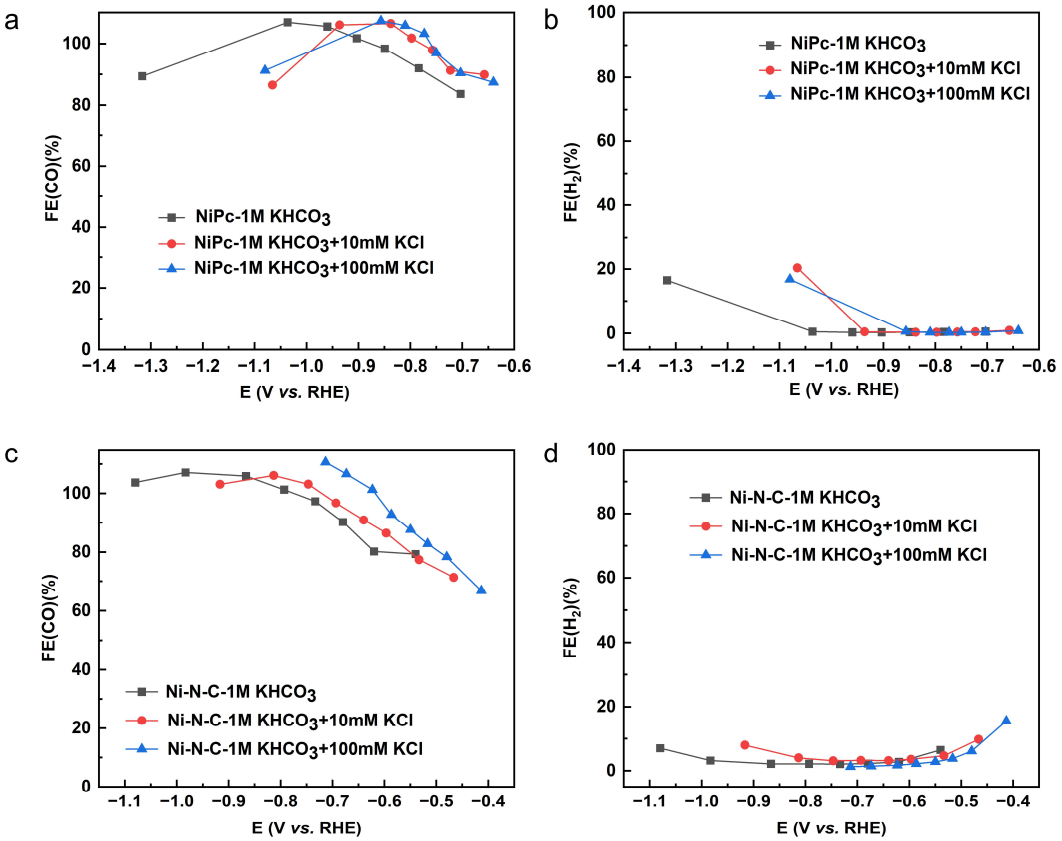

Figure S4. (a) CO and(b) H_2 FEs of NiPc in 1 M $KHCO_3$ electrolyte with different concentrations of KCl (0, 10mM, 100mM). (c) CO and (d) H_2 FEs of of Ni-N-C in 1 M $KHCO_3$ electrolyte with different concentrations of KCl (0, 10mM, 100mM).

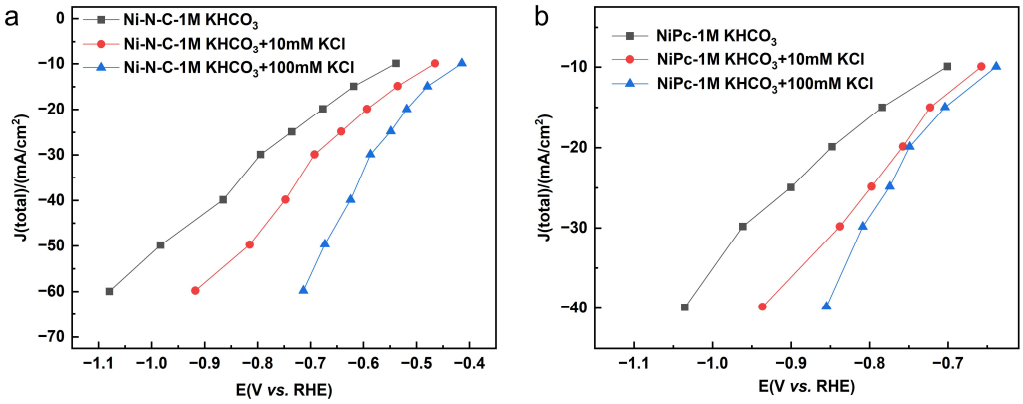

Figure S5. Total current densities measured at different potentials (iR-corrected) for (a) Ni-N-C (b) NiPc in 1 M $KHCO_3$ with 0, 10 and 100mM KCl.

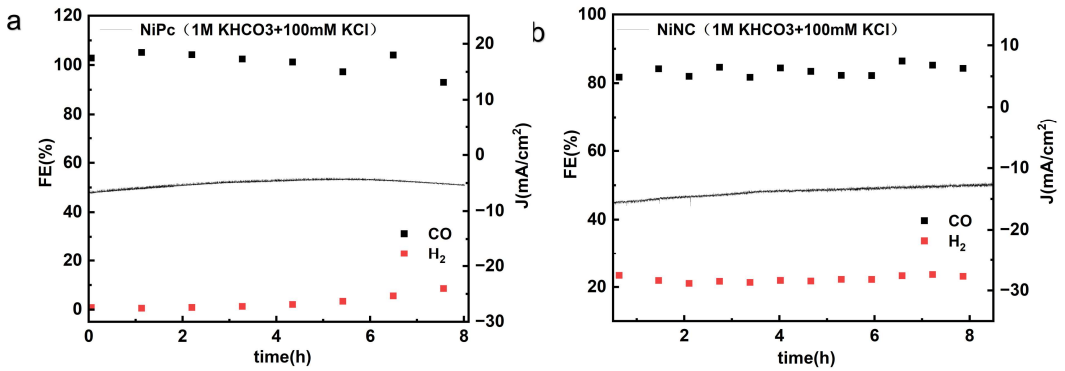

Figure S6. Stability of the current density and Faradaic efficiency of NiPc (a) and NiNC (b) during a 8 h continuous test at −0.7 V(vs. RHE).The above electrochemical characterizations are measured in 1 M KHCO3 electrolyte with 100mM KCl.

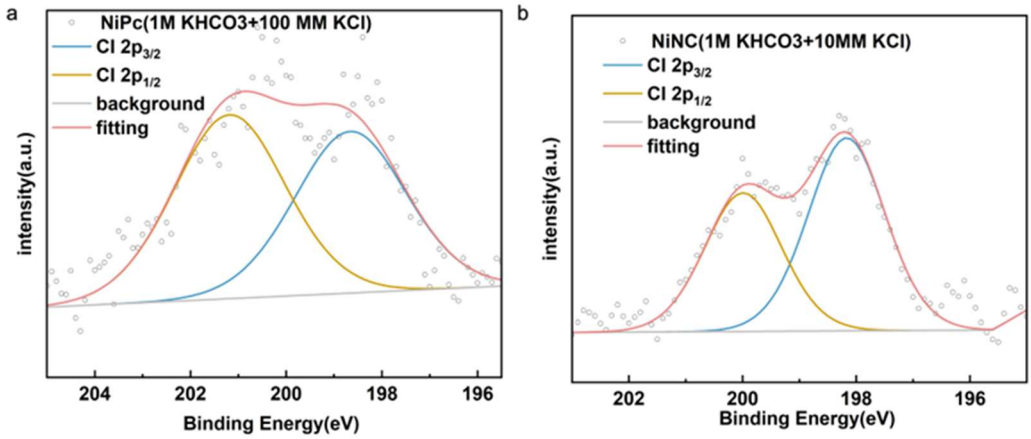

Figure S7. Cl 2p XPS spectrum of (a) NiPc and (b) Ni-N-C after the eCO_2RR stability tests in 1 M $KHCO_3$ electrolyte with 100 mM KCl.

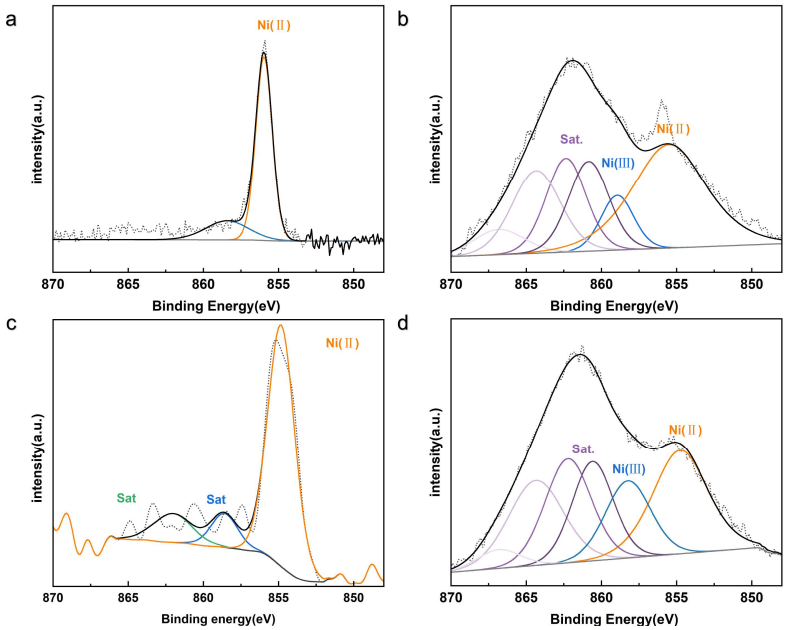

Figure S8. The Ni 2p XPS spectra of NiPc (a) before and (b) after the eCO_2RR stability tests in 1 M $KHCO_3$ electrolyte with 100 mM KCl. The Ni 2p XPS spectra of Ni-N-C (a) before and (b) after the eCO_2RR stability tests in 1 M $KHCO_3$ electrolyte with 100 mM KCl.

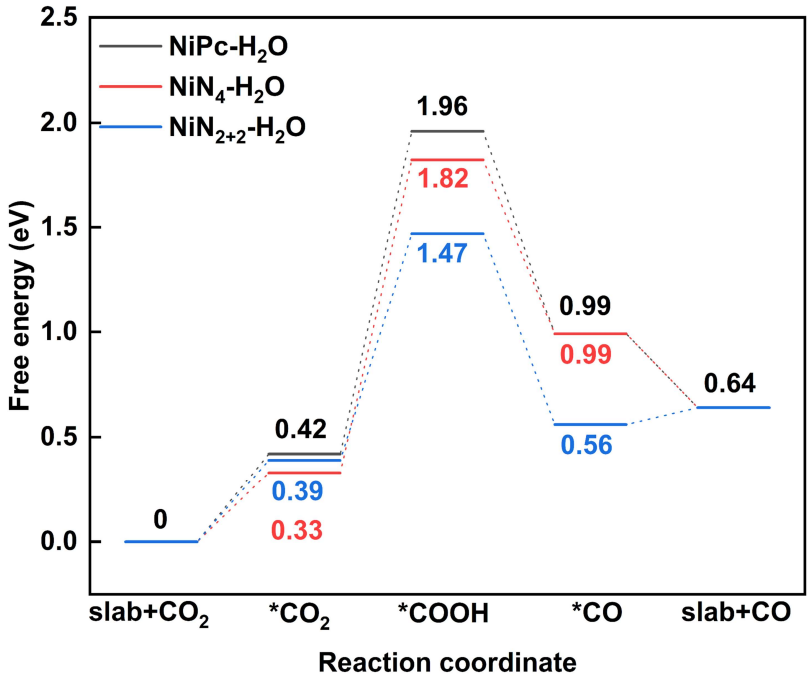

Figure S9. The free energy diagram for CO_2RR to CO on NiPc-H_2O, NiN_4-H_2O, and NiN_{2+2}-H_2O models.

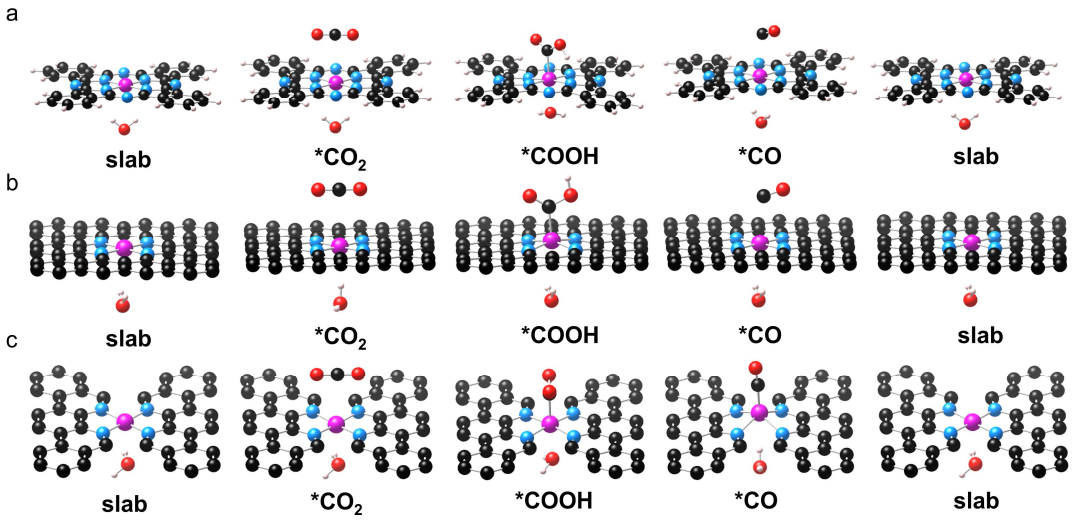

Figure S10. The simulated configurations of four elementary steps on (a) NiPc-H_2O, (b) NiN_4-H_2O, and (c) NiN_{2+2}-H_2O models. The black, blue, purple, red, and white balls represent C, N, Ni, O, and H atoms, respectively.

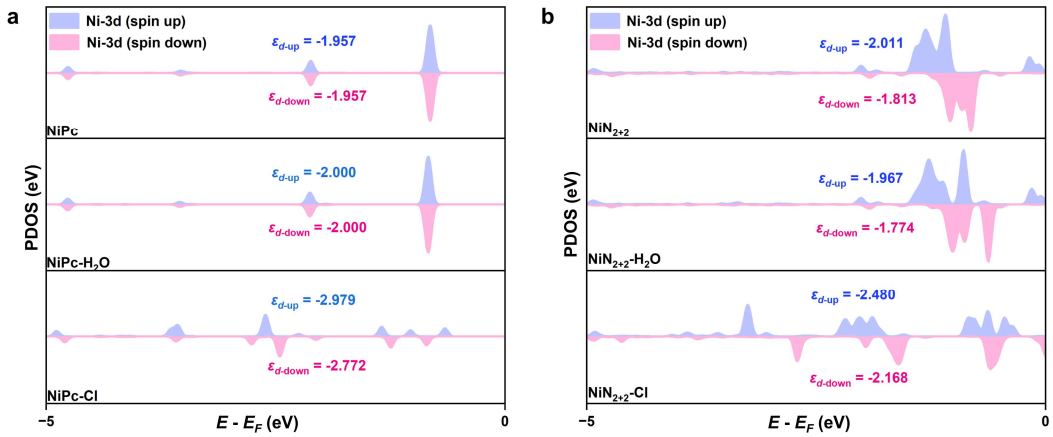

Figure S11. (a) The partial density of states (PDOS) and d-band center of Ni atoms in NiPc, NiPc-Cl, and NiPc-H_2O. (b)The partial density of states (PDOS) and d-band center of Ni atoms in NiN_{2+2}, NiN_{2+2}-Cl, and NiN_{2+2}-H_2O.

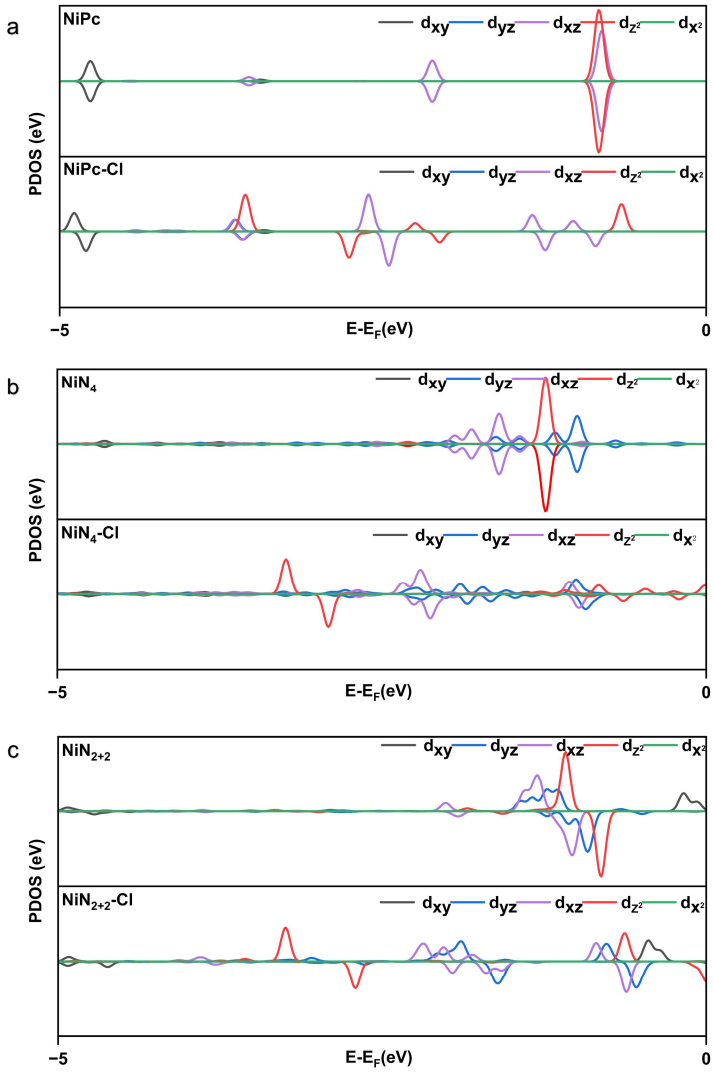

Figure S12 The partial density of states of Ni atoms in (a)NiPc, and NiPc-Cl. (b)NiN_4, and NiN_4-Cl. (c)NiN_{2+2}, and NiN_{2+2}-Cl.

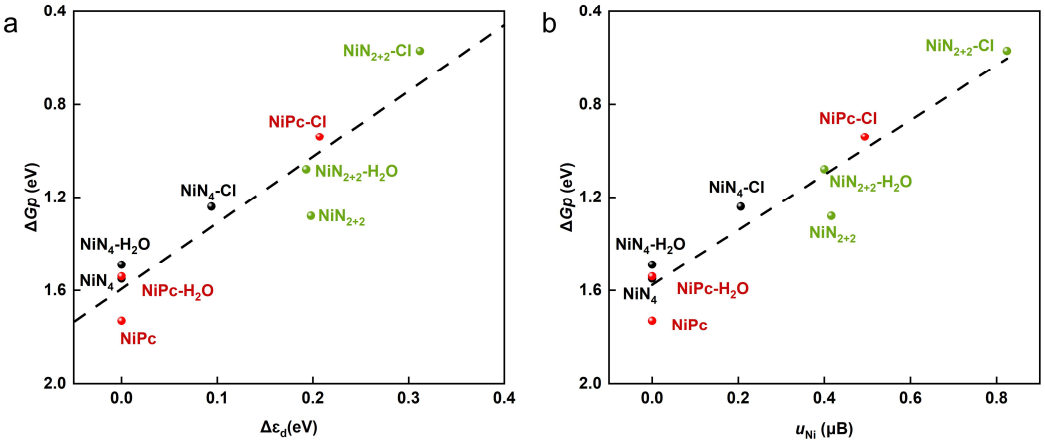

Figure S13. (a) The relationship between the energy barrier of PDS (ΔGp) and d-band center between down and up spin ($\Delta\varepsilon_d$, $\varepsilon_{\text{d-spin down}}$ - $\varepsilon_{\text{d-spin up}}$). (b) The relationship between the ΔGp and the magnetic moment of Ni atoms (u_{Ni}).

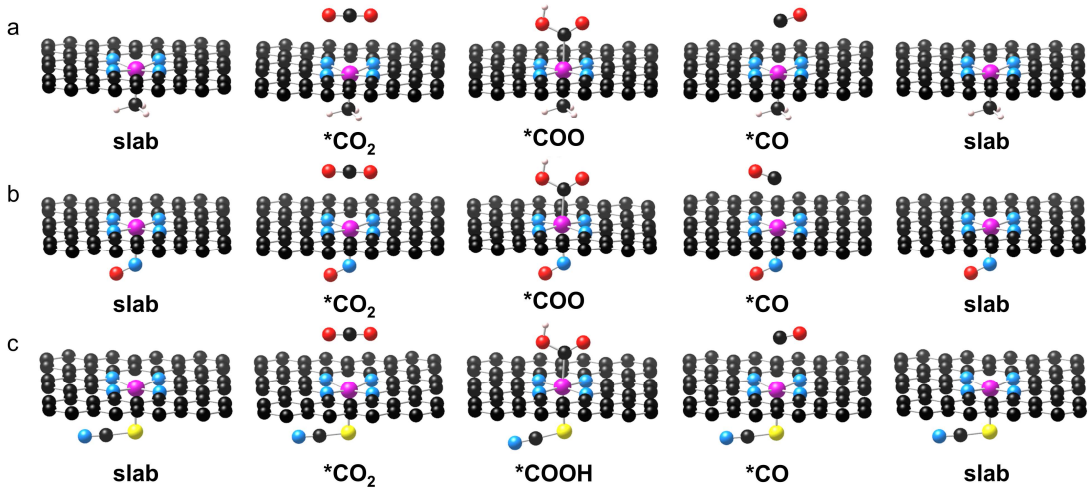

Figure S14. The simulated configurations of all elementary steps on (a) NiN_4-CH_3, (b) NiN_4-NO, and (c) NiN_4-SCN models. The black, blue, purple, red, yellow, and white balls represent C, N, Ni, O, S, and H atoms, respectively.

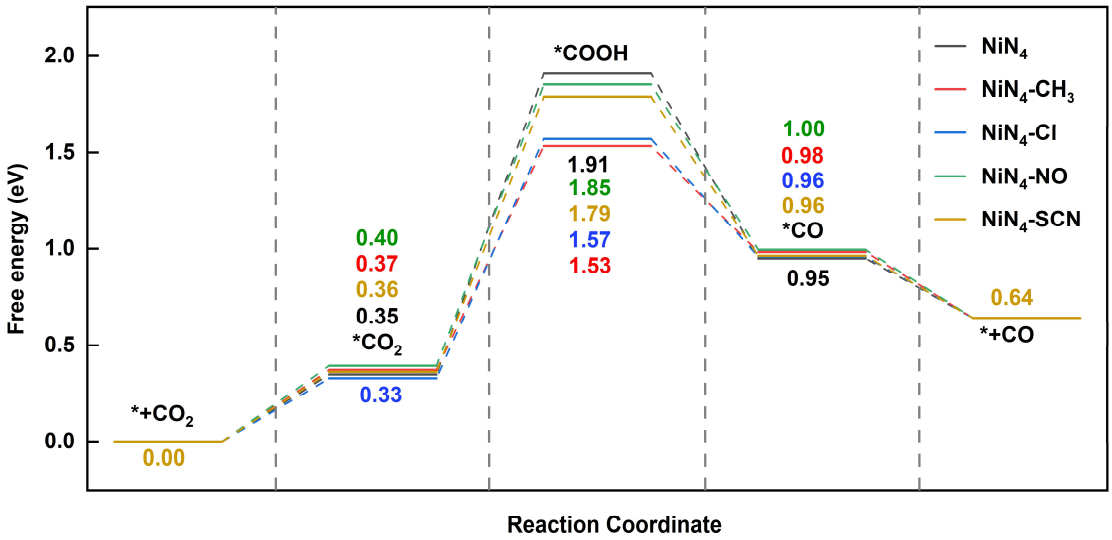

Figure S15.The free energy diagram for CO_2RR to CO on NiN_4 model with and without axial ligands.

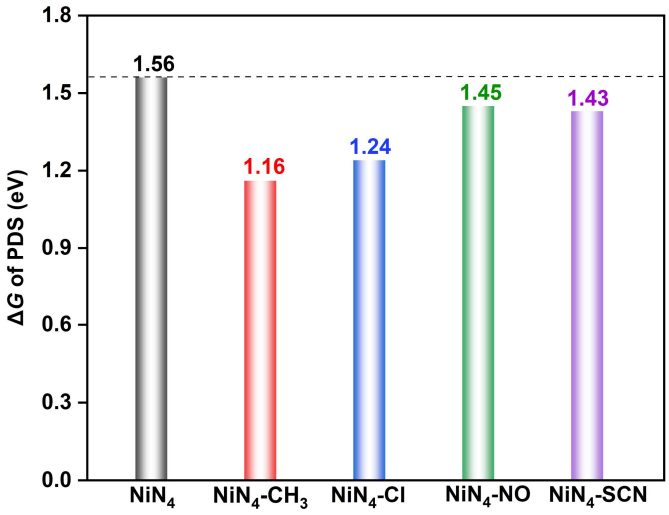

Figure S16. Δ*G* of PDS for CO_2RR to CO on NiN_4 model with and without axial ligand.

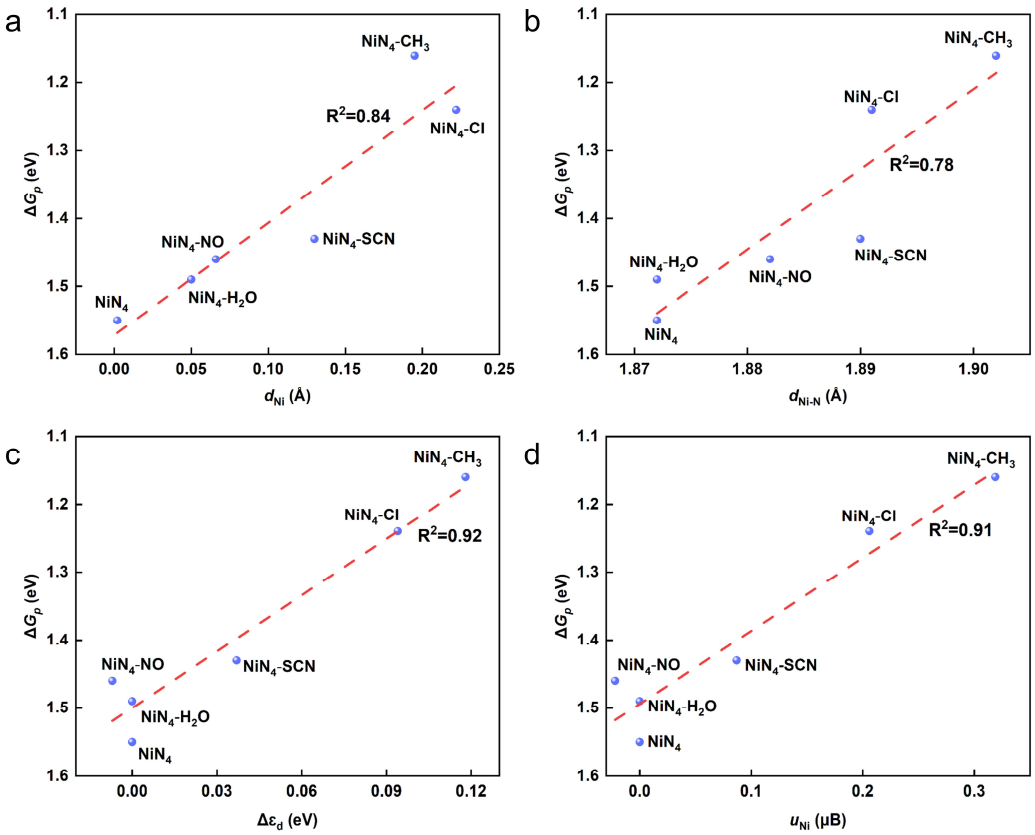

Figure S17. The relationship between ΔGp and (a) d_{Ni}, (b) $d_{Ni\text{-}N}$, (c) $\Delta\varepsilon_d$, (d) u_{Ni} of NiN_4 with various axial ligands.

Table S1. Surface area and pore volume of Ni-N-C catalysts based on N_2 physisorption isotherm analysis.

BET Surface Area ($m^2 \cdot g^{-1}$)	Pore Volume ($cm^3 \cdot g^{-1}$)
223	0.306

Table S2. Elemental composition according to XPS analysis in atomic percentage.

C	N	O	Zn	Ni
90.5%	4.1%	5.3%	0.32%	0.22%

Table S3. Relative content (in % of the N_{1s} signal) of various N functionalities in Ni-N-C catalysts derived from the fitting of N_{1s} XPS spectrum.

N-pyridinic	N_x-M	N-pyrrolic or N-H	N-graphitic	N-oxide
31.8	16.1	26.7	12.0	13.5

Table S4. Structural parameters of Ni-N_x moieties obtained from the best-fit of nickel K-edge EXAFS spectrum.

R_{M-N}(Å)	σ^2(Å^2)	CN
1.92(1)	0.007(1)	4.3(3)

R_{M-N} is the metal−nitrogen bond distance, σ^2 the Debye−Waller factor, and CN the coordination number, obtained from EXAFS fitting. Errors are given in brackets, for example, 1.92(1) means 1.91−1.93.

Table S5. DFT calculated free energy change (ΔG) for the four elementary steps of CO_2RR to CO on NiPc, NiPc-Cl, NiN_4, NiN_4-Cl, NiN_{2+2}, and NiN_{2+2}-Cl.

Reaction Step	ΔG, eV					
	NiPc	NiPc-Cl	NiN_4	NiN_4-Cl	NiN_{2+2}	NiN_{2+2}-Cl
1: slab + CO_2 = *CO_2	0.40	0.39	0.35	0.34	0.27	0.37
2: *CO_2 + H^+ + e^- = *COOH	1.73	0.94	1.55	1.24	1.28	0.57
3: *COOH + H^+ + e^- = *CO + H_2O	-1.10	-0.32	-0.95	-0.61	-1.01	0.07
4: *CO = slab + CO	-0.38	-0.37	-0.31	-0.33	0.11	-0.36
potential-determining step (PDS)	2 1.73	2 0.94	2 1.55	2 1.24	2 1.28	2 0.57

* represents the surface of catalyst

Table S6. DFT calculated Δ*G* for the elementary steps of CO_2RR to CO on NiPc-H_2O, NiN_4-H_2O, and NiN_{2+2}-H_2O.

Reaction Step	Δ*G*, eV		
	NiPc-H_2O	NiN_4-H_2O	NiN_{2+2}-H_2O
1: slab + CO_2 = *CO_2	0.42	0.33	0.39
2: *CO_2 + H^+ + e^- = *COOH	1.54	1.49	1.08
3: *COOH + H^+ + e^- = *CO + H_2O	-0.97	-0.83	-0.91
4: *CO = slab + CO	-0.35	-0.35	0.08
potential-determining step (PDS)	2 1.54	2 1.49	2 1.08

Table S7. DFT calculated ΔG, the distance of Ni atom from the carbon plane (d_{Ni}), the Ni-N bond distance ($d_{Ni\text{-}N}$), the difference in d-band center between down and up spin ($\Delta\varepsilon_d$), and the magnetic moment of Ni atoms (u_{Ni}).

	ΔG (eV)	d_{Ni} (Å)	$d_{Ni\text{-}N}$ (Å)	$\Delta\varepsilon_d$ (eV)	u_{Ni} (μB)
NiPc	1.73	0.001	1.913	0.000	0.000
NiPc-Cl	0.94	0.103	1.927	0.207	0.494
NiPc-H_2O	1.54	0.084	1.913	0.000	0.000
NiN_4	1.55	0.002	1.872	0.000	0.000
NiN_4-Cl	1.24	0.222	1.891	0.094	0.206
NiN_4-H_2O	1.49	0.050	1.872	0.000	0.000
NiN_4-SCN	1.43	0.130	1.890	0.037	0.087
NiN_4-NO	1.46	0.066	1.882	-0.007	-0.022
NiN_4-CH_3	1.16	0.195	1.902	0.118	0.319
NiN_{2+2}	1.28	0.016	1.886	0.198	0.416
NiN_{2+2}-Cl	0.57	0.326	1.903	0.312	0.824
NiN_{2+2}-H_2O	1.08	0.024	1.883	0.193	0.400

Table S8: Details about the pH and electrolyte

Electrolyte	pH
CO_2 saturated 0.5 M $KHCO_3$	7.3
CO_2 saturated 0.1 M $KHCO_3$	6.8
CO_2 saturated 0.05 M K_3PO_4 + 0.05 M H_3PO_4	6.4
CO_2 saturated 0.05 M KH_2PO_4 + 0.05 M H_3PO_4	2.25

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0.5002223811724344	0.2294197607787130	0.0009618499785081
0.6234957473125406	0.0565380518917742	0.0023059557360123
0.7485681896794445	0.1122700449426033	0.0018412998812692
0.8757806318832024	0.2774115549857682	0.9990536966890208
0.7492846403369102	0.2248705038034227	0.0003221416226194
0.8739183015000762	0.0557856167897543	0.0025858962966942
0.0002116743430048	0.4446202932320619	0.9965961301312356
0.1234820880183777	0.6109936408095666	0.9980295056726919
0.0002460008240242	0.5549712516370693	0.9967555169954819
0.1234513432892605	0.3886273605330530	0.9977585129946894
0.2462404585006240	0.4438786467909490	0.9983601275207374
0.2462570993941122	0.5557215289889429	0.9985116114036777
0.7542419253460946	0.4438572481353427	0.9975531186035499
0.8770176582890116	0.6110154482965672	0.9976482257970292
0.7542801011381677	0.5557270317105691	0.9977348439081581
0.8769991295074692	0.3885696623749155	0.9972714680160046
0.0002818465879669	0.7781056617063805	0.0007322149017953
0.1264985305546732	0.9438082992520924	0.0028752498270264
0.0002374131184813	0.8893407255050351	0.0024854809957417
0.1247414655256120	0.7221596890030964	0.9999173532500429
0.2512085295077964	0.7747199251606749	0.0012232617540543
0.3768815241941780	0.9431521567831359	0.0025602661353059
0.2518889582654948	0.8873535493628746	0.0023619977642117
0.3743688799812799	0.7141882547765429	0.0009461375626907
0.5003256986633423	0.7702393414370353	0.0014971274547587
0.6235445940048447	0.9431621859137502	0.0024871257007724

0.5002475236832382 0.8843840202250839 0.0022780875955259
0.6262726487019522 0.7142039614474620 0.0005000028196599
0.7493714212762503 0.7747657300773750 0.0008169199882487
0.8739647398495957 0.9438064755470981 0.0027900793152903
0.7485861785317274 0.8873852958708812 0.0021833202862480
0.8758293241480650 0.7221723321248751 0.9996325425871315
0.3689565830100094 0.6057829191661630 -0.0000098918067114
0.3689367180986196 0.3938246172849130 -0.0003567516697593
0.6315954817378179 0.6057959978302223 -0.0006686782954655
0.6315387703462475 0.3938302156145718 -0.0009386595634627
0.5002663089619618 0.4998173797452976 -0.0001148358047634

NiN4-CO2

1.00000000000000

9.8380002975000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 12.7799997330000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Ni O

43 4 1 2

Direct

0.0005560189041444 0.1102353746291213 -0.0029951767229281
0.1250410426339980 0.2774209735009829 -0.0021581350725271
0.0005676599582302 0.2214680456862448 -0.0023065829789725
0.1268396132056824 0.0557871750989144 -0.0032687120351300
0.2522577493095713 0.1122462196595670 -0.0032148087165586
0.3746487934013903 0.2854800130535697 -0.0033539792837589
0.2515795643344916 0.2248917959060340 -0.0028219781755235
0.3772594774074394 0.0565024263179514 -0.0036003041458999
0.5005693599111224 0.1153521212623459 0.9962704397383040
0.6265345366573528 0.2855024710635065 -0.0036430094536608
0.5006124926994425 0.2295354354450190 0.9962673628075592
0.6238322141207165 0.0564974305479537 -0.0037223704766001
0.7488731293948067 0.1122540836524031 -0.0034471808224332
0.8760878153977434 0.2774261718194297 -0.0023636069451470
0.7496226408907697 0.2249027391789835 -0.0031168306655433
0.8742517886916361 0.0557806566733435 -0.0033803473394090
0.0005515402813325 0.4446075228973189 -0.0016790839264986
0.1237230799908088 0.6109904354132100 -0.0019314654281437
0.0005262187108616 0.5549792639047610 -0.0016896793050286
0.1237415991766746 0.3886099358788108 -0.0018948034276795
0.2464362147634775 0.4439028306875714 -0.0026030724595279
0.2464056324537644 0.5556847597002827 -0.0026267649007171
0.7547276611303216 0.4439093305399534 -0.0030360509688442
0.8773344822518118 0.6110099300556965 -0.0021312397576103

0.7547061926380191 0.5556880889236105 -0.0030376707842423
0.8773875721896068 0.3886106512829632 -0.0021490314724544
0.0005441621239533 0.7781325338395928 -0.0022725046921759
0.1268212166690768 0.9438279964245208 -0.0032742622473227
0.0005453951760358 0.8893597973723767 -0.0029943289427966
0.1250125106807684 0.7221730212063855 -0.0021733981401497
0.2515043454182206 0.7747192066689234 -0.0028892800677481
0.3772222846656158 0.9430785575226863 -0.0036196942597160
0.2522078908678873 0.8873519219906036 -0.0032583888874626
0.3745657865378794 0.7140637811324354 -0.0034564306850819
0.5005292051713710 0.7699966984909584 0.9961965746358525
0.6237665934107830 0.9430778434606412 -0.0037395576501342
0.5005033538675984 0.8841996284778719 0.9962198559998939
0.6264780953117995 0.7140748828925773 -0.0036676177923252
0.7495634583815716 0.7747120242565593 -0.0031086892003284
0.8742394678763545 0.9438078259691135 -0.0033539005268448
0.7488202685650979 0.8873417572588136 -0.0034350795372831
0.8760522719106991 0.7221993808355450 -0.0023209112833091
0.5004727229146870 0.5007357965156148 0.1596187978883126
0.3691643562014842 0.6056849107660898 -0.0035323463515448
0.3692028268674938 0.3938831798568920 -0.0034545929610129
0.6319555283733316 0.6056899205617013 -0.0038434584327070
0.6319894889576017 0.3938886742803218 -0.0038380444398036
0.5005901172184645 0.4997814399832552 -0.0042765533254815
0.3808518840474043 0.5020913351890504 0.1611052699419262
0.6201326082795989 0.4995018882679416 0.1594825886762320

NiN4-COOH
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
43 4 1 2 1
Direct
0.0002326932876121 0.1102025418150702 0.0022303952889555
0.1244545211203310 0.2773170354982276 -0.0009801275268433
0.0002409742121195 0.2213348119841741 0.0000053550472124
0.1262312612433316 0.0555733322184217 0.0028034880923517
0.2516614730400291 0.1120118340147718 0.0022729163443318
0.3735856345458325 0.2843060401746869 0.0010650956244467
0.2508190190874330 0.2240360876388563 0.0008895275643829
0.3767612260817805 0.0563526467458785 0.0027362004034162
0.5002289172759692 0.1150902554593990 0.0025041721228755

0.6270910884560394 0.2844574420477231 0.0004816078070005
0.5002893601249201 0.2289689347005659 0.0016627665168842
0.6236897342753094 0.0563595185911489 0.0026803591112572
0.7488166292249571 0.1119946501184863 0.0021179488559081
0.8759558507841613 0.2773669215817565 -0.0012114628621821
0.7497306194747819 0.2240488866095502 0.0005810806720401
0.8742105516958123 0.0555852966514508 0.0027407768378535
0.0000775643655855 0.4444682212128087 -0.0046119296968681
0.1230137654812935 0.6113871722001195 -0.0032423715799001
0.0001004169150460 0.5551795715535104 -0.0045331543730578
0.1229869027496129 0.3882320885425337 -0.0033765949205359
0.2463414105205509 0.4436250988999337 -0.0029449044527043
0.2463632313432004 0.5559801449094401 -0.0029248763500417
0.7538687148089340 0.4436107251134352 -0.0035962652994554
0.8771103391771372 0.6113940593530304 -0.0035925576607683
0.7538971802632692 0.5560396116581567 -0.0035905885201316
0.8770930533026033 0.3882534808715898 -0.0036904000380839
0.0002737324050339 0.7782407875734864 0.0002353668817035
0.1262156021400742 0.9440298508291574 0.0028534592387535
0.0002441773921062 0.8893725212801877 0.0023890421215259
0.1244999070596207 0.7222763154014467 -0.0007393087211752
0.2508494898770507 0.7755718867925346 0.0010159180736929
0.3767731420473834 0.9432783228649581 0.0027405493595133
0.2516618645739008 0.8876169960917084 0.0022953703340552
0.3736229028718734 0.7152955227259454 0.0010735863372363
0.5003344011241092 0.7706671389357421 0.0016486544058639
0.6236978053884527 0.9432810475457938 0.0026782930469949
0.5002474321089340 0.8845474272370650 0.0025045768617473
0.6271362755403541 0.7151723720593780 0.0004283375323330
0.7497394636992907 0.7755782649678563 0.0006158079018600
0.8742233282473645 0.9440241697860260 0.0028103699177484
0.7488104933960039 0.8876375272699156 0.0021708160554006
0.8759722690639140 0.7222481113708179 -0.0010719158303470
0.5101048556948673 0.4999676442295689 0.1102431705843001
0.3679561405592592 0.6071844106518094 -0.0004818299865557
0.3679252644157388 0.3924168594514267 -0.0004564579338295
0.6328634476606937 0.6072821013728782 -0.0017259254060860
0.6328433900634334 0.3923521147544186 -0.0016706723832407
0.5005761268556566 0.4998104899184367 0.0123201856802406
0.3897205444338461 0.5000593098424713 0.1436645062505971
0.6175733158464493 0.4999973119307750 0.1393398172229054
0.3150223116769262 0.5000849869515024 0.1112617784464277

NiN4-CO

1.00000000000000

9.8380002975000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 12.7799997330000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Ni O

43 4 1 1

Direct

0.0003270841228048 0.1102001018257391 -0.0010908727904287

0.1247507453820802 0.2774065144844707 0.9982541064767620

0.0002862179040882 0.2214502146727817 0.9986643631787379

0.1266212761052653 0.0557433400417441 -0.0011427463507425

0.2519727003253184 0.1122036949677710 -0.0013599549232466

0.3743112239666597 0.2853755314699032 0.9977083401873675

0.2512082488365407 0.2247972449763516 0.9982401992988872

0.3770490804233186 0.0564555439231242 -0.0013184975576857

0.5003075789868081 0.1152345185155989 -0.0013863526419212

0.6262210974872493 0.2853482206604206 0.9978956854544250

0.5002771704814549 0.2293727216259058 -0.0018650999960177

0.6235712320981697 0.0564668397440188 -0.0011377531277182

0.7486696256198104 0.1122224280932016 -0.0010523645751971

0.8758391384231955 0.2773933560046922 0.9984061159061228

0.7493585254882371 0.2248189885949293 0.9984748863305047

0.8740526594658293 0.0557480070182775 -0.0009456599436134

0.0002449410524604 0.4445914930973961 0.9978015545528950

0.1234877645034577 0.6109903835903584 0.9978759195947727

0.0002534991028064 0.5549666419256940 0.9977637149308388

0.1234637883445877 0.3885830407501951 0.9978542135288181

0.2462451928847305 0.4438416902654968 0.9973566917744847

0.2462668919368691 0.5557282680456902 0.9973648216348575

0.7543076320092467 0.4438627377896471 0.9973087195550363

0.8770612196950495 0.6109898759139695 0.9978187391478517

0.7543010615290997 0.5557151543006895 0.9972735593890016

0.8770636584653594 0.3885865359184590 0.9978676880219358

0.0002790600283757 0.7781099320445419 0.9986431869449697

0.1266548179601767 0.9437823977266834 -0.0011565389036249

0.0003549589549270 0.8893440319048428 -0.0011116987730764

0.1247571646933524 0.7221553035193927 0.9983079595053665

0.2512183331896246 0.7747454180493385 0.9982674264407796

0.3770786164284209 0.9431267332530712 -0.0013455464320063

0.2520066882852449 0.8873535931165346 -0.0013510026221148

0.3743445141320296 0.7141880415462544 0.9976828727249192

0.5003003353226495 0.7702106587633534 -0.0020179974499485

0.6236053976944607 0.9431189895853195 -0.0012314783087382

0.5003573469656347 0.8843620504396739 -0.0015177399239027

0.6262277146049240 0.7142072919467997 0.9977712030040780
0.7493670280008445 0.7747496447571502 0.9983535585744984
0.8740745080785184 0.9437914168541052 -0.0009983426819886
0.7486771020253652 0.8873582842145914 -0.0011641537001767
0.8758283262504171 0.7221696162436730 0.9983235650527937
0.5091176253371381 0.4990939639759833 0.1354478804621139
0.3687778146504747 0.6059067110129666 0.9971314615824209
0.3687555371302643 0.3936464437402125 0.9971029702390634
0.6316939301628069 0.6058671640373604 0.9972098531001931
0.6317060367753254 0.3936930153768724 0.9972940666125139
0.5002126287261062 0.4997647418138512 -0.0017176568627176
0.6179253559624456 0.5024214168608959 0.1562860193578711

NiN4-Cl
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni Cl
42 4 1 1
Direct
0.9999856864214465 0.1102906010745599 0.9972033043436213
0.1244452347659220 0.2774761978301967 0.9990954535546734
0.0000042982376698 0.2214179883214911 0.9986229486245435
0.1261703569176689 0.0556975927838366 0.9967119457108851
0.2515824457726481 0.1121988712567088 0.9968386976180099
0.3737401198354036 0.2852931775935659 0.9970653422735936
0.2508667064304930 0.2246806223502773 0.9977136956680326
0.3765407058412862 0.0564443163842014 0.9961883384983423
0.4999964785414619 0.1155546040273165 0.9959834223836168
0.6262753732404747 0.2852913945469950 0.9971685640177199
0.5000067689271432 0.2293387698088623 0.9961549568067412
0.6234529084799831 0.0564449470622250 0.9962086172232176
0.7484169112089205 0.1122108191744218 0.9969016560870472
0.8755650061886726 0.2774804051070348 0.9992370306457659
0.7491570623332038 0.2246864087842795 0.9978345871760936
0.8738242736106798 0.0557005447733090 0.9967378521757624
0.0000061767719757 0.4445404557092303 0.0011875736919009
0.1231975477002862 0.6111509667666439 0.0005724360361796
0.9999986526715716 0.5550575793753083 0.0012360664652249
0.1231985039963135 0.3884739063007672 0.0004973327027074
0.2464499769400916 0.4437575847466633 0.0002664690546084
0.2464654966071151 0.5558752296999074 0.0003135415204056
0.7535388924267821 0.4437631027102498 0.0004225882423512

0.8767895910503967 0.6111471151189320 0.0006542064528006
0.7535224121590218 0.5558764741647479 0.0004221371481066
0.8768004768499651 0.3884831877363766 0.0006405035544219
0.9999939618873341 0.7781752881250270 0.9985986499046575
0.1261652674713787 0.9439049538026367 0.9966782973838235
0.9999984858640616 0.8892939525776029 0.9971164256198719
0.1244276824500403 0.7221228311810748 0.9991637163610463
0.2508364758596286 0.7749273019075247 0.9977779972438725
0.3765494458487524 0.9431786800971977 0.9962348875807479
0.2515853502751284 0.8874144021469519 0.9968429079911942
0.3737331613394161 0.7143187153450370 0.9971456458631138
0.4999900564360900 0.7702618142998503 0.9962646716100920
0.6234453667385793 0.9431789364668361 0.9962452970743882
0.4999976467249283 0.8840603004209768 0.9960740975848879
0.6262560564703605 0.7143206616171724 0.9971984685137016
0.7491530165293057 0.7749195619406635 0.9978234564583204
0.8738265418584561 0.9439084628108603 0.9966992116124089
0.7484210135161291 0.8874122517904297 0.9968800657752368
0.8755559549090535 0.7221166887074730 0.9992114695310192
0.3680926833036864 0.6063558504140900 0.9986698282122219
0.3680803064031082 0.3932635790904300 0.9986137469981173
0.6319032664786235 0.6063599887702296 0.9987592846991049
0.6319186435264825 0.3932577057959179 0.9987624465014164
0.5000238223262485 0.4998052807694151 0.9888856044741559
0.5007578158566162 0.4999001257144826 0.8708143793302199

NiN4-Cl-CO2
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni Cl O
43 4 1 1 2
Direct
0.0003959138990535 0.1102182239100115 -0.0033508945279869
0.1247869812508699 0.2773645952408079 -0.0021858662210309
0.0003628253861423 0.2213112942154341 -0.0024285065097811
0.1265709671567371 0.0556106783613520 -0.0036938309670930
0.2519580812622611 0.1120895734240810 -0.0037198324236532
0.3740404926705087 0.2851549826598072 -0.0040409674593016
0.2511928467579904 0.2245703501501683 -0.0032011001045421
0.3768974839013658 0.0563237911623753 0.9958468814304262
0.5003878681275166 0.1154477343471012 0.9955843811434600
0.6267472517574091 0.2851703612771755 -0.0041397689526113

0.5004070409977400 0.2291903528711506 0.9954028921131833
0.6238861707948885 0.0563121360982311 -0.0042074463173104
0.7488215796969981 0.1121040833009411 -0.0037541765394535
0.8759261783745712 0.2773750975528291 -0.0022728976317956
0.7495971286140218 0.2245928037436535 -0.0033096807947067
0.8742029174870624 0.0556291622014789 -0.0036689565997835
0.0003896014423589 0.4444110084170843 -0.0009146612769963
0.1235852294782584 0.6110391135279720 -0.0012167796752968
0.0003651299945148 0.5549507886802592 -0.0008637584557773
0.1235738720934302 0.3883379140914003 -0.0013333083676955
0.2468537522806503 0.4436000278795711 -0.0017767989459665
0.2468462762706064 0.5557588609564780 -0.0017094088529285
0.7539585363515799 0.4436222233192772 -0.0020976562161116
0.8772187475208144 0.6110260854027222 -0.0014233938105391
0.7539778803984827 0.5557584402566186 -0.0020642508183489
0.8772004772219026 0.3883612829123979 -0.0015110307376617
0.0004228882259609 0.7781184876241307 -0.0022889736403690
0.1265666893341764 0.9438440629038946 -0.0036294834548170
0.0003933197572163 0.8892248319183074 -0.0032128900143595
0.1248666462920590 0.7220461527941537 -0.0020333646140503
0.2512563421815315 0.7748311592860437 -0.0031200088531461
0.3769102632696218 0.9430927428839169 0.9958381364490327
0.2519610409087040 0.8873359741805606 -0.0036551133108844
0.3740787593407029 0.7142076737166733 -0.0039875167853320
0.5004536880848872 0.7701715035842897 0.9953240910551517
0.6238776278416092 0.9430857190333659 -0.0041953464107765
0.5003956762493944 0.8839151123877368 0.9955393706306611
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0.7496393425448971 0.7748261630092084 -0.0032927255665897
0.8742012849303242 0.9438531126745003 -0.0035829714700756
0.7488564450592179 0.8873357787488717 -0.0036937972436693
0.8759865754983244 0.7220270144009676 -0.0021491897023148
0.5001006744327299 0.5000844353476515 0.1537630826522517
0.3684308703170597 0.6062122795204142 -0.0031656338478662
0.3684300830820940 0.3931531929323046 -0.0032498539256511
0.6324205861306411 0.6062254942728995 -0.0034284214365462
0.6323915448242392 0.3931641872130231 -0.0034210978516374
0.5003924148004866 0.4996926047342406 0.9864251654739468
0.5003939573340863 0.4999313399426014 0.8684577737903888
0.3805041786706344 0.4992648497058917 0.1538135622915363
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NiN4-Cl-COOH
1.00000000000000

9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni Cl O H
43 4 1 1 2 1
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0.0000966238157160 0.2214179500520527 -0.0025981208452952
0.1262082908615040 0.0557327494106157 -0.0027757374563390
0.2516779376484711 0.1120381057114568 -0.0021112430625798
0.3741371866954851 0.2846110344165258 -0.0012796346308319
0.2507743881458892 0.2244107857941666 -0.0019184921352389
0.3767973631914140 0.0564150521961565 0.9983457526898497
0.5000988967351309 0.1150877789610453 0.9985017320353559
0.6263044798019920 0.2846810963832347 -0.0021097810391430
0.5000904991986613 0.2288387563797417 0.9984910338846099
0.6234537018790891 0.0564085522456004 -0.0018176944585611
0.7485320783527298 0.1120097440832525 -0.0022422164427775
0.8755720233372741 0.2773935700398714 -0.0027498232678358
0.7494884126756981 0.2244319963301701 -0.0023282719430584
0.8738993154813437 0.0557230799142073 -0.0028165252958426
-0.0000737934718576 0.4446060371855042 -0.0037197099741982
0.1228189911106347 0.6111351574380740 -0.0029278782712844
-0.0000903090382512 0.5550104974354084 -0.0037620279650819
0.1228592863591374 0.3884879078032237 -0.0029993715564625
0.2460100477557067 0.4437718369621034 -0.0026483946761135
0.2459873086218645 0.5558538977773261 -0.0026126018972809
0.7538886397672584 0.4436672957946117 -0.0032581316572788
0.8767508952275357 0.6110994094091159 -0.0034289952100175
0.7538620398495451 0.5558610745152796 -0.0031453871145512
0.8768229662905651 0.3884674623877183 -0.0033416860152296
0.0000109062758465 0.7781755380027885 -0.0026855459270230
0.1261689268122053 0.9438803569173104 -0.0027711883208956
0.0000354448659116 0.8893535459176546 -0.0028740645722930
0.1244227315402263 0.7223419258452959 -0.0024353720874193
0.2507077142629388 0.7752597836290990 -0.0018695097120244
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0.2516410679729732 0.8876378308717641 -0.0020662093051954
0.3740572123821360 0.7150308092222899 -0.0012418329085207
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0.6333970761062451 0.6075658229159537 -0.0017956802417779
0.6334724493261973 0.3919160789940252 -0.0026262203231821
0.5002716305589127 0.4997235762509059 0.9993868159816625
0.4978876146792668 0.4998965312784888 0.8795973180073835
0.3889085529324124 0.5000143273331497 0.1323572050529287
0.6161052985915788 0.4966790448682938 0.1287149193503513
0.3133331095206020 0.5018755575547771 0.1002977116495873

NiN4-Cl-CO
1.00000000000000
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0.0000000000000000 12.7799997330000004 0.0000000000000000
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C N Ni Cl O
43 4 1 1 1
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-0.0000840905461774 0.2213447581053901 0.9975068231667943
0.1261248347695124 0.0556519483236380 0.9961645080647921
0.2515121966240293 0.1121329816475945 0.9960301739400834
0.3735499137514435 0.2852147015204396 0.9957863580839968
0.2507182955707863 0.2246005417712751 0.9965880752800179
0.3764712400918940 0.0563419141452853 0.9955423533081834
0.4999372899784914 0.1155083549896226 0.9952443101445527
0.6262323766113810 0.2851902214167512 0.9956358830511640
0.4999069123212276 0.2292095700587166 0.9951768915297481
0.6234139506155921 0.0563622515100462 0.9954139725941579
0.7483650743095174 0.1121364708534018 0.9959306150561943
0.8754622768155665 0.2774040283989540 0.9976375583357043
0.7490884758185256 0.2246150599003224 0.9964623201904452
0.8737451024140187 0.0556618241257286 0.9961147296929551
-0.0000960893596976 0.4444644476768611 0.9992496568481408
0.1230930508411195 0.6110977198287734 0.9988753525887395
-0.0001138060618539 0.5550015180005046 0.9993037082223920
0.1231309247415323 0.3883851880798828 0.9987943528642413
0.2463916865928013 0.4436338306438215 0.9983164221840568

0.2463570187919447 0.5558110252733154 0.9983769550851481
0.7534283609504516 0.4436331830353040 0.9978816561103894
0.8766914595254072 0.6110957971133306 0.9986362307937706
0.7534316600163400 0.5558107441110157 0.9979020762538708
0.8767040222157739 0.3883788223400975 0.9985559362924539
-0.0001179931251835 0.7781995754748734 0.9976719720105689
0.1261151219269189 0.9439037499323556 0.9962654491125261
-0.0000886460518517 0.8893043140387094 0.9966938239682694
0.1243174454129879 0.7220953278266183 0.9979214756919531
0.2506936181035169 0.7748991620962938 0.9967747317506424
0.3764893859947803 0.9431216867317753 0.9956273340272555
0.2514850246551967 0.8873968861986923 0.9962113262558321
0.3734961832698600 0.7142512003218158 0.9958972557754137
0.4998961777181453 0.7702131117696650 0.9952584826692084
0.6233936479109418 0.9431406086106977 0.9954806294188342
0.4999503443646592 0.8839313808425009 0.9953640965924062
0.6262419531614702 0.7142699324658759 0.9957270858677786
0.7490657687219524 0.7748957229733848 0.9965798345504483
0.8737380204411587 0.9439131630299358 0.9961878503477287
0.7483431548934516 0.8874037718954301 0.9960450582495107
0.8754484199095635 0.7221199063001595 0.9977900922225317
0.5090836495921339 0.4996141979999292 0.1384403424629419
0.3677870649388183 0.6063731377008484 0.9966764088350073
0.3678410395586471 0.3931014185103804 0.9965884796912334
0.6319134700056237 0.6063452250164150 0.9964122125068713
0.6318983993863945 0.3931232639443911 0.9963484111905796
0.4997577445196916 0.4997545051910168 0.9869940532490402
0.4995359798080543 0.4999462384995639 0.8690128874856737
0.6214048627326805 0.4985402672367912 0.1537871446491473

NiN4-H2O
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
42 4 1 1 2
Direct
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0.1246432709550407 0.2792257380553952 0.0010534004213387
0.0002272163148197 0.2232101790299330 0.0013933592795702
0.1264740664776382 0.0575232666235353 0.0025550035981953
0.2518745304258698 0.1139601395363007 0.0025472975369070
0.3742276694288516 0.2871751897238775 0.0026082178761367

0.2510925234626072	0.2265970183894738	0.0021168213000169
0.3769540553757179	0.0582462965558009	0.0027201149010437
0.5002484038822854	0.1170515945503837	0.0029821491256678
0.6261811124441501	0.2871448848408273	0.0025295264886284
0.5002241956606128	0.2312518733279186	0.0030484359136244
0.6235063321999795	0.0581826126847860	0.0027554589783115
0.7485800622314805	0.1139177605228611	0.0025299188567307
0.8757683091670978	0.2791777731801125	0.0010126802441514
0.7493021725031921	0.2265590891365546	0.0020782814292426
0.8739843924996065	0.0574985342121788	0.0025712378355042
0.0001697844590941	0.4463787492946488	0.9989184123027802
0.1233300380327509	0.6127245297089893	0.9990894104200082
0.0001107104879836	0.5567405300426155	0.9985129845573133
0.1234212887488770	0.3903854353062333	0.9998755549950311
0.2461307273795943	0.4457045660235988	0.0004593062260327
0.2460464171268683	0.5574593518848369	0.0000074600212672
0.7542503656706474	0.4457249156343543	0.0004452532604044
0.8769491720089565	0.6127440822009431	0.9991059719579873
0.7542254208308671	0.5574842106067986	0.0000778167423070
0.8769244958403691	0.3903528895589378	0.9998306122340307
0.0001847545407168	0.7798208805581448	0.0004430865353915
0.1264533482355203	0.9455613410410006	0.0021963852081259
0.0001750283557084	0.8910692293958586	0.0017071556269486
0.1246019501578689	0.7239108469891824	0.0000106395362498
0.2510760616214254	0.7765425128323978	0.0010600964003522
0.3769423534703780	0.9448484901223302	0.0023344696372668
0.2518756902757119	0.8891383443383294	0.0019045254772479
0.3742231234398897	0.7160046086384378	0.0013895409776978
0.5001649008540311	0.7718355213799124	0.0017453358064216
0.6234671034792700	0.9447762999227942	0.0023528759828706
0.5001660760054824	0.8859983513958530	0.0021011305130461
0.6261582602862980	0.7159686867018615	0.0014445985283241
0.7492956479292138	0.7764984434501606	0.0010252435301986
0.8739083536897684	0.9455372581996909	0.0022082304926230
0.7485304639324895	0.8890824746495439	0.0018739260785995
0.8757630649392452	0.7239027866390876	0.0000109148266518
0.3687986647375391	0.6075537450350759	0.0011850045569484
0.3688276912051067	0.3956127668712578	0.0020957500025899
0.6315461107852687	0.6075669453977105	0.0014277744606815
0.6315465363164829	0.3956101159018955	0.0019265491174112
0.5001902737399214	0.5016423410797298	0.0024935400385644
0.4943157003601533	0.4951590866688969	0.8389916025966029
0.4826753027453017	0.5572088440265965	0.8666826254056113
0.5058949647304334	0.4396553382480066	0.8719191239265548

NiN4-H2O-CO2

1.00000000000000

9.8380002975000007 0.0000000000000000 0.0000000000000000

0.0000000000000000 12.7799997330000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Ni O H

43 4 1 3 2

Direct

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0.1263802186342235 0.0571344452378050 -0.0038687082164794

0.2517646790361010 0.1136049489167226 -0.0038875625119082

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0.8755917328945427 0.2788484218932799 -0.0029880845071746

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0.2459518057602633 0.5570841361430113 -0.0031092967300148

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0.7491461280458733 0.7760828512027746 -0.0033409445234784
0.8738378552386761 0.9451300808974774 -0.0038206637268160
0.7484610576881052 0.8886635681863272 -0.0037793374503497
0.8756145832503887 0.7235254189694993 -0.0026558876365515
0.4990585190089789 0.5020589970049977 0.1598397241510635
0.3686892644163668 0.6071776418155492 -0.0037738813597503
0.3687039489038436 0.3952637055575361 -0.0039403034617468
0.6314786470254841 0.6071678882550650 -0.0038318721838307
0.6314756881636446 0.3952488380479476 -0.0037100709681989
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0.5016470808653045 0.5355128445078454 0.8299903044010964
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0.6186746752760970 0.5030344156223205 0.1607181082611397
0.4803398642796564 0.4615660715987289 0.8253797401183287
0.5057291425996994 0.5459449182412461 0.8784495302412626

NiN4-H2O-COOH
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
43 4 1 3 3
Direct
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0.1245811426209619 0.2792863993306547 -0.0006765938894446
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0.1262566738591356 0.0574671661825255 0.0026098630309312
0.2516653963445418 0.1138287055475328 0.0025198101487526
0.3733709364551185 0.2862779368805610 0.0014126726532500
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0.7499312638878466 0.7773426135945731 0.0015689914286299
0.8743597235962043 0.9458908611032208 0.0026200916005386
0.7489912251441554 0.8894375722259557 0.0027368356512476
0.8761411226875396 0.7239897895900705 -0.0008068567982239
0.4846403367539526 0.5020245151182657 0.1115060438613055
0.3678305308494511 0.6091310308256623 -0.0017211217754549
0.3677399112667915 0.3942521305510970 -0.0012287843828646
0.6329190127762593 0.6089652309183750 0.0013490125932142
0.6327945154496640 0.3944835828159525 0.0014643747221566
0.4996990198414636 0.5018714200308013 0.0146627244168321
0.4960418377541839 0.4929268022010030 0.8465783501264229
0.3777748184406247 0.4989564464307619 0.1418581427942251
0.6085610015837595 0.5056595302948340 0.1421146416372113
0.4767950042071455 0.5549222751920228 0.8732565451918647
0.5037053054121812 0.4377986926900729 0.8800133486204971
0.5920750290074625 0.5047787486127487 0.1906935656667120

NiN4-H2O-CO
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9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
43 4 1 2 2

Direct

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0.1233749579672962	0.2795812869330241	-0.0002342365759625
0.9989190744645006	0.2236059659985597	-0.0000538924914816
0.1251851744515879	0.0579278520605371	0.0007360916911960
0.2506187368223655	0.1143087777901971	0.0011616148965565
0.3728644010289714	0.2875013001966801	0.0010332241813054
0.2497804912582653	0.2269188517864905	0.0007811693831057
0.3758022556939806	0.0586549177813028	0.0014933153799104
0.4990581258840628	0.1174723915534119	0.0015761539497884
0.6249275410351008	0.2874613146004735	0.0005579391731329
0.4989553879973833	0.2316346416791190	0.0014302657560332
0.6223151070635736	0.0586158867975685	0.0012004334004393
0.7474201704051024	0.1143077553248902	0.0008588733745581
0.8745148419059522	0.2795676508135944	0.9994696035221040
0.7481027012204658	0.2268994462204823	0.0003477892416527
0.8727317460313820	0.0578916122875289	0.0005728424554390
0.9990161145596911	0.4467288647812662	0.9973582148914328
0.1221941674461097	0.6131077566985975	0.9974656708284967
0.9989886543687534	0.5570813938786490	0.9968077566945831
0.1222110052862590	0.3907028869869857	0.9985339359352189
0.2449347297127565	0.4460439179003353	0.9989822553445088
0.2449267155577960	0.5578528550732533	0.9983775821551728
0.7531067865592042	0.4460392231005482	0.9981755689161931
0.8758395548429764	0.6130888538864392	0.9970781025271241
0.7530855970898130	0.5578084072945234	0.9977765682680427
0.8757800738850626	0.3907245362994503	0.9981172427859454
0.9990004589235695	0.7802212965169449	0.9983624523902670
0.1252141735172444	0.9460006430271692	0.0002044797415941
0.9989809257626702	0.8914693611401415	-0.0004891076441858
0.1234330510271664	0.7243078566636583	0.9981727409035961
0.2498573969443715	0.7769967674949043	-0.0006456430287604
0.3758325116458253	0.9452738072137173	0.0010884714957532
0.2506894060373994	0.8895951677410708	0.0002631527608904
0.3729801060329835	0.7164553134289174	-0.0002957229802010
0.4990618290558323	0.7722651789864369	0.0003531853912924
0.6223433856746931	0.9452224657987771	0.0008141131732957
0.4991066114229123	0.8863936022834610	0.0008987282154672
0.6249984707680833	0.7163948073929750	0.9995356855530880
0.7481541175895907	0.7769162620939030	0.9990797504490148
0.8727384909783399	0.9459810273324555	0.0000269138743462
0.7474051057320616	0.8895188098107173	-0.0000192797723749
0.8746066910197078	0.7242384617815992	0.9979556757140623
0.5178477925670062	0.5032166773214446	0.1381355900437395

0.3674613974244750 0.6081079687542823 0.9992121046490372
0.3673927141096954 0.3957997519035670 0.0003792105659671
0.6305226552950008 0.6080357659943334 0.9991313775077860
0.6304545232671657 0.3958528686546327 0.9995159871672779
0.4989487752933792 0.5020002904869965 0.0016811590948368
0.4914518062727085 0.4976242637180260 0.8385666897127151
0.6281868803306250 0.5036925942426083 0.1570289550147039
0.4748221605366290 0.5569997098728050 0.8679997148807829
0.5101303490159906 0.4408721042870310 0.8697766508366372

NiN2+2
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni
34 4 1
Direct
0.0001658106355757 0.1110652048632302 0.0013014024158516
0.1279111746627039 0.2777080217303309 0.9993240121691350
0.0002541092928556 0.2219278247303257 0.9999605968632866
0.1299988526056619 0.0571776521873969 0.0016477546332469
0.2503730767268873 0.1146750487488421 0.0014170692517635
0.3823019563579624 0.2909245892451179 0.0001636040399658
0.2598657996398236 0.2243001333394933 0.0003606783466081
0.6182707982602302 0.2909231294944526 -0.0001384670888737
0.7499539498653897 0.1146326360087393 0.0013494113182207
0.8725845885158759 0.2776572187389877 0.9991370953176757
0.7406613697710815 0.2242571380086724 0.0001617402271840
0.8702960980765545 0.0571539282921108 0.0016073942264022
0.0002599207427739 0.4449594003108495 0.9969430899485882
0.1243219191676061 0.6118541362345353 0.9978072682246937
0.0002614340582486 0.5554082711658708 0.9968849746436734
0.1243176725561338 0.3885176409893090 0.9979293901862614
0.2462667640130216 0.4444972037074244 0.9983642654690226
0.2462601241535148 0.5558540537264985 0.9983107394312650
0.7542949683077724 0.4444679076774488 0.9974337909651322
0.8761978515565282 0.6118523197865201 0.9973620293329867
0.7542849348751479 0.5558334357571005 0.9973576185396177
0.8762232420032890 0.3884656314842196 0.9975079530923285
0.0002494661963573 0.7783660235779657 0.9997337935828464
0.1300632976543852 0.9430465702614715 0.0015666361442809
0.0002345885012714 0.8891777343372225 0.0011566701537137
0.1279331325650040 0.7226630660639496 0.9990911721536342

0.2598942236092580 0.7760676078838310 0.0001437024088633
0.2505002759767128 0.8856785536277960 0.0012871526515658
0.3823110307283567 0.7094153071170675 -0.0000230171119626
0.6182283781886968 0.7093933956833235 -0.0003505893832883
0.7406141159375215 0.7760509409110870 0.0000109686256938
0.8703221614083044 0.9430257871221345 0.0016068784879173
0.7499213641143047 0.8856653837018804 0.0013186051511637
0.8725399818954777 0.7226388545418557 0.9989480342821863
0.3689404134090657 0.6076809119022598 -0.0006734304338938
0.3689492613770693 0.3926662825681632 -0.0005706744887434
0.6315848947492207 0.6076627682343020 -0.0014496562277572
0.6316054662903771 0.3926487382479334 -0.0013120367921718
0.5002713895539794 0.5001595449902724 -0.0007875257580805

NiN2+2-CO2
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O
35 4 1 2
Direct
0.0000573500874027 0.1101991272075534 -0.0041221301967443
0.1278925137193992 0.2768068633425706 -0.0040949286319010
0.0000383393395848 0.2210398569688909 -0.0040568971458947
0.1300319702690809 0.0563576884718857 -0.0042175096345118
0.2503547175800790 0.1139187604542984 -0.0042838059984906
0.3826447324164796 0.2901864553119268 -0.0046169220199235
0.2602582055552231 0.2235102325080328 -0.0042445211697758
0.6174731849276829 0.2902071524083814 -0.0046351359630357
0.7497508050717435 0.1138964889038679 -0.0042444190013388
0.8721463061185677 0.2767852258763682 -0.0041200066431791
0.7398114893774799 0.2234806450570846 -0.0042241669557647
0.8700840558444671 0.0563529037380183 -0.0041889193619618
-0.0000138077912273 0.4441381629435763 -0.0039478563173804
0.1241097170452887 0.6110836885607279 -0.0041397791392099
0.0000065249868261 0.5546285408662002 -0.0039422288748866
0.1240586724426167 0.3876014016912883 -0.0040655120110502
0.2458471595029500 0.4437361872791204 -0.0045413881451757
0.2458754914442380 0.5549248551196944 -0.0046710607085752
0.7541404674228319 0.4436677318500546 -0.0046089293674346
0.8758940043692249 0.6110778019430287 -0.0041358763364078
0.7541461071089648 0.5548627189289599 -0.0045744599951489
0.8759410195304386 0.3875681777365300 -0.0041096651044143

0.0000050425839618 0.7775189530078023 -0.0040967194087348
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0.0000036850126854 0.8883613880338233 -0.0041871847996526
0.1279501585398344 0.7218224543036583 -0.0041542493451141
0.2603444914894377 0.7751088170680004 -0.0043633139562371
0.2503601953510175 0.8847007385475386 -0.0042529811215476
0.3825944922637501 0.7082676306751798 -0.0048467312269339
0.6173234561245683 0.7083380326361214 -0.0046734259491189
0.7396559062507533 0.7751287343338110 -0.0043381011753413
0.8700390671501317 0.9421928361858309 -0.0042200347928879
0.7496014382395497 0.8847463539979473 -0.0042632818890185
0.8720580245073345 0.7218258783506178 -0.0041393718694832
0.5039696005358304 0.5097237133940491 0.1573788628635796
0.3687693570214227 0.6065322763311042 -0.0052996615807326
0.3687850691074892 0.3920285086533231 -0.0048840474703055
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0.6312680427564192 0.3919793612051852 -0.0050881827880756
0.4999978362378317 0.4992184860279050 -0.0058632899217524
0.4012498187786970 0.5569787239251028 0.1570805098767482
0.6067282166056793 0.4625236833828251 0.1586165661072526

NiN2+2-COOH
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
35 4 1 2 1
Direct
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0.1281466528692702 0.2777315449285069 -0.0014533357197241
0.0001529543092629 0.2220340996788150 -0.0007602351808739
0.1297873389268005 0.0571812007293984 0.0015690610873649
0.2500474628812396 0.1145502654807654 0.0013141831273259
0.3826070471214598 0.2905574570652186 0.0012853104869714
0.2604446000214448 0.2239018769011784 0.0002618160704363
0.6178817486473119 0.2905295591281629 0.0002713204915028
0.7502183558043189 0.1145624800709356 0.0012621169516901
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0.1245644031277981 0.6118748712424882 -0.0037412934175442
0.0002824840556486 0.5554239105988795 -0.0049955013222021

0.1245147250646922 0.3884901271008859 -0.0035067337343986
0.2466157306265379 0.4445386184769586 -0.0021041296957344
0.2466483095951947 0.5558320506207942 -0.0022667127473175
0.7539528439730659 0.4444797452983996 -0.0038960869110440
0.8760479485101025 0.6118937281948579 -0.0043611299813060
0.7539872214912279 0.5558403399970092 -0.0039535150926335
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0.0001840540135274 0.8891094769172802 0.0009392529463804
0.1282189646362574 0.7226267668187065 -0.0018031805176944
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0.4038606386950456 0.5011225242024122 0.1908990840655213

NiN2+2-CO
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O
35 4 1 1
Direct
-0.0015025354511269 0.1116150054564207 0.9948508610942902
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0.8686653161376944 0.0577100545381750 0.9951941216949252
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-0.0011540376712245 0.5556973653045985 0.9911942934039083
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0.2462504242135108 0.4447210887126049 0.9950288057110220
0.2462470372114613 0.5560430557180192 0.9950718843937855
0.7512581926195675 0.4447990001079095 0.9961378321069849
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0.8739881156176501 0.3891063965915294 0.9928036371793304
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-0.0013779398299891 0.8892927950090872 0.9951374129094861
0.1269155231079143 0.7226683885969850 0.9943193249870156
0.2593221689634791 0.7760187184343379 0.9960675679503916
0.2478160196178823 0.8852589167608941 0.9960451299696608
0.3815422320469999 0.7093805442992238 0.9993338777348051
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0.7382928335189828 0.7758276649980202 0.9963422354579556
0.8687353176594608 0.9432227986109840 0.9952831963384433
0.7494816718958199 0.8850981029700813 0.9960032834131567
0.8707384343436559 0.7225807306132435 0.9946665870751651
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0.6295502282272492 0.6082513207399139 0.0019676024369101
0.6294351251039504 0.3926216921309574 0.0018096741725358
0.4980877424642567 0.5004648682524031 0.0328626110142540
0.4756339820310988 0.5024548463990397 0.1804305601679206

NiN2+2-Cl
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni Cl
34 4 1 1
Direct
0.0015747512723649 0.1132004141193192 0.9962150105223344

0.1294731054486107 0.2799538901468281 0.9971093263704986
0.0014027668999148 0.2241103829644047 0.9967185850828386
0.1313480554632847 0.0594082369981379 0.9962376916273357
0.2498601952139552 0.1180828718938471 0.9966703683236204
0.3851372626935756 0.2933890569115221 0.9965976888756103
0.2626230225502795 0.2270499178342860 0.9968150225995913
0.6175971291072528 0.2933114841228459 0.9963715240637683
0.7532393273546774 0.1180935452617859 0.9964936052778341
0.8732601937383109 0.2799389365319698 0.9969142312244372
0.7402357936252670 0.2270026612712996 0.9966683227850197
0.8717784568813585 0.0594482436062265 0.9961409381562447
0.0012760554152678 0.4469089597956071 0.9974223001119853
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0.0012663709724094 0.5573812917239422 0.9971989023317036
0.1256445231673169 0.3906034046466758 0.9977652039595526
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0.2477548166487367 0.5577183978439422 0.9978174518307270
0.7548046844762553 0.4466307997382728 0.9969476374146780
0.8769762622064121 0.6137606913459166 0.9967928366991572
0.7548259282126821 0.5577932541967812 0.9967390559062892
0.8769313506416978 0.3905786295291875 0.9972447733757974
0.0013016609794789 0.7801822734671120 0.9962752266975272
0.1312535527178156 0.9448767774461189 0.9961050481956946
0.0014049763213322 0.8910557581067025 0.9960455036530504
0.1293169923381043 0.7243036118161399 0.9965675864727075
0.2623354230613373 0.7772034374841539 0.9964143825529703
0.2496760030576723 0.8861161020494990 0.9963295825589427
0.3848152528438789 0.7110404604534750 0.9961238827151675
0.6177303750668273 0.7111396241253232 0.9957126929232487
0.7402598861413239 0.7773110832228625 0.9961242356957172
0.8716790446479479 0.9449178233865609 0.9960439959405178
0.7531224508490553 0.8862287597645064 0.9962084984850321
0.8732330228689094 0.7244186046690473 0.9963072140224796
0.3701716216817985 0.6098237514976432 0.9967215637516915
0.3702663134313724 0.3945766764844478 0.9970516631370359
0.6324065889722021 0.6098999954289539 0.9958269592755471
0.6323692677559265 0.3945348367272317 0.9962481794054412
0.5011645808354430 0.5022147632318337 0.9836826035360531
0.4983743067616544 0.5014497682276158 0.8689522497090820

NiN2+2-Cl-CO2
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Ni Cl O

35 4 1 1 2

Direct

0.0001720871897128 0.1111351284889214 -0.0041817502975470
0.1282614650056882 0.2780389560897065 -0.0041154497722941
0.0001499278949517 0.2220961149659525 -0.0040599103976797
0.1300498071852140 0.0574746553840632 -0.0042446731471428
0.2477571925815745 0.1168107915378961 -0.0043525545259632
0.3844771851446655 0.2915166491462989 0.9942776165772335
0.2617866202300965 0.2255893801046560 -0.0045371776937674
0.6158437477102703 0.2915460459546868 0.9939517401688509
0.7525444639163448 0.1168060382185492 -0.0044117175728242
0.8720042452803243 0.2780061361665626 -0.0041747222621646
0.7384837245241191 0.2255689335912865 -0.0046357475541626
0.8703028634034814 0.0574829765470167 -0.0042460456967917
0.0000999245042235 0.4448543302173734 -0.0038118212723263
0.1245567825514771 0.6115164372086300 -0.0040497096238469
0.0001137673755933 0.5552656624379873 -0.0038083670962120
0.1245692211862907 0.3886407478847525 -0.0039692963458577
0.2467565734383508 0.4446204959731410 -0.0046064149448315
0.2467600955715545 0.5555953267051743 -0.0048095756369595
0.7534610671696527 0.4445481630750518 -0.0047450073484721
0.8756737024829804 0.6115057468434622 -0.0039383099103055
0.7534574612654048 0.5555363014217349 -0.0045642239492498
0.8756730431423373 0.3886054153379599 -0.0040005770819885
0.0001298590519722 0.7780343365681036 -0.0040537052848499
0.1300061747490085 0.9426444083939121 -0.0042377671012583
0.0001502034315377 0.8889934473709258 -0.0041839325873032
0.1282282359767470 0.7221027065659534 -0.0041932061660382
0.2617189642396007 0.7745147556387649 -0.0046248414785528
0.2476973457025838 0.8832755174159392 -0.0043520830755446
0.3843325051104418 0.7085552304093131 0.9939689513582757
0.6157691223263272 0.7086524833026281 0.9942797284977801
0.7384574500676594 0.7745297149607707 -0.0045559455646992
0.8702648212831013 0.9426429781856206 -0.0042404895514506
0.7525201783755388 0.8832991798852537 -0.0043600853303187
0.8720124043257138 0.7221022525860216 -0.0041094022580330
0.5004953317698135 0.4992719732276056 0.1524176947013173
0.3695620251050754 0.6072251146681875 0.9933334833695532
0.3696840664107693 0.3929735154059724 0.9939922628791182
0.6305507372409902 0.6071906877044057 0.9940322954880225
0.6306797988921689 0.3928847900657942 0.9933953956231215
0.5001543762255372 0.5000620786618057 0.9791106707021574

0.5006209122056983 0.4998933347694989 0.8644085996387600
0.4002912824291312 0.5495637277652486 0.1526240420249358
0.6006592463262882 0.4489272191474189 0.1528220544993313

NiN2+2-Cl-COOH
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni Cl O H
35 4 1 1 2 1
Direct
0.0015907942274611 0.1132141285108848 -0.0044408676902073
0.1287952697666329 0.2797581003408722 -0.0041282003687763
0.0014594963454895 0.2240010058841738 -0.0045589043682229
0.1308498726978966 0.0592441280265426 -0.0042688743892797
0.2494291911025283 0.1174050297495637 -0.0036869195093636
0.3819537274383171 0.2925180032770122 -0.0014045100107226
0.2602906779285608 0.2264114673024709 -0.0033076317121149
0.6211145551699218 0.2924126961325362 0.9969458157892372
0.7537453588793117 0.1174168563011974 -0.0039719170287700
0.8740264802237716 0.2797764648466513 -0.0047980407207916
0.7426984941640991 0.2263335971528136 -0.0040528898557996
0.8723272670628259 0.0592410533173600 -0.0043899325643122
0.0013093126459248 0.4469269814523910 -0.0055049858669298
0.1250459528341435 0.6137044396075687 -0.0047573988283166
0.0013122698216436 0.5573215172141560 -0.0055534370981486
0.1251780959078276 0.3905773804737186 -0.0043638597281037
0.2469744562991974 0.4464374835771933 -0.0026871217632164
0.2469388431168875 0.5579780193974094 -0.0032833240902701
0.7555803964793405 0.4463349202120190 -0.0052121791099774
0.8775434944310571 0.6137284522302930 -0.0056272884796295
0.7556361664887176 0.5579493820607634 -0.0052531302901145
0.8774915760629101 0.3905484091662189 -0.0055946274280678
0.0013410541913947 0.7803610275093973 -0.0049408024902917
0.1307826547171888 0.9450214232764071 -0.0044287041178804
0.0015001080558265 0.8910476535081655 -0.0047327983263322
0.1285913615501316 0.7245540592207139 -0.0046800010650740
0.2600035735733267 0.7778627567612038 -0.0040513937676628
0.2493019452601600 0.8867824389716842 -0.0041005484275302
0.3816030930450691 0.7118975133903506 0.9972034581635069
0.6210784447727203 0.7120355276138175 0.9960982509894053
0.7426977130877886 0.7779626966047085 -0.0047875398577337
0.8722876462551460 0.9450448105409447 -0.0045955609392891

0.7537120598039589 0.8868817362272683 -0.0045311587319924
0.8740409683019122 0.7245627089844872 -0.0051501125762272
0.5137879684729726 0.5034711417117570 0.0950457100721863
0.3668151554204434 0.6118904778133102 0.9981361952219091
0.3669729839936840 0.3926403749920575 -0.0004080208416523
0.6358700946721328 0.6119849923371853 0.9961457088182620
0.6358238004634276 0.3923498157965553 0.9962114988943338
0.5013690026052244 0.5023701796308425 0.9978870059241799
0.4961952624204173 0.5014488884107394 0.8834856879326177
0.3916597584168641 0.5196437526032911 0.1255819058124165
0.6186584238011371 0.4917330083513805 0.1261565694737500
0.4089051810246108 0.5186533785099294 0.1740148929510138

NiN2+2-Cl-CO
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni Cl O
35 4 1 1 1
Direct
0.0017556879206480 0.1130996451842528 0.9950806587453058
0.1294294652593163 0.2794398776142835 0.9949122080777597
0.0016981197190126 0.2238494514005472 0.9947712308026561
0.1310724145658625 0.0590216664919439 0.9952835584448512
0.2509567790228138 0.1162809845629711 0.9956253381258054
0.3829510183648108 0.2918192942918609 0.9967006516945198
0.2609835389811211 0.2253717526602169 0.9955853663396458
0.6203575250976857 0.2918500105679464 0.9969477345877252
0.7525357828398139 0.1164441095664395 0.9954797863206570
0.8739854232447175 0.2794842164553350 0.9946991610960981
0.7424524930287733 0.2255408226272746 0.9954794163507329
0.8723287619861579 0.0590778566440817 0.9951683223300527
0.0016655562000040 0.4467694388844221 0.9938866250695738
0.1256056736780659 0.6137159842468607 0.9945307898696163
0.0016960578244022 0.5572742578298995 0.9939367101060168
0.1255710431875903 0.3902838948131647 0.9946082258342401
0.2475693154073806 0.4460897533081063 0.9957393896025698
0.2475735826783154 0.5578525982218450 0.9955926054090589
0.7558757161747177 0.4461484378913928 0.9953719027698015
0.8778021074529669 0.6137640993830753 0.9942541552012752
0.7559072799472274 0.5578996311727792 0.9952709496602817
0.8777485665717594 0.3902768292283361 0.9941708663583004
0.0016688379228754 0.7802632269653070 0.9946813026732141

0.1310286817630573 0.9450858822196851 0.9951527891386609
0.0016697799326256 0.8909757837880066 0.9949259776470634
0.1293958142514693 0.7246144950650808 0.9947311896403741
0.2608651351424269 0.7787380665017687 0.9951619316807686
0.2509398464040204 0.8878562806900316 0.9953461863676694
0.3827841402467260 0.7122054917847551 0.9959962484130107
0.6203872432107189 0.7122712780597753 0.9961757823628932
0.7424559465282998 0.7785815733691576 0.9951207806659634
0.8723187750360257 0.9450975835081795 0.9950787449455673
0.7525492039913352 0.8877139489923830 0.9952830205283142
0.8740039190515811 0.7246489157186804 0.9946475625367364
0.5161946098935420 0.5019273443208763 0.1015901409270799
0.3677786989879386 0.6119502521925356 0.9967050371684696
0.3678144920318821 0.3920751094821326 0.9971942270368320
0.6354942553312596 0.6117713569998791 0.9970179304702204
0.6354555911326525 0.3923342208471639 0.9974714631891116
0.5016169483965787 0.5020647438301775 0.9980933762567372
0.5025813207043314 0.5011538644139938 0.8802997941758470
0.5991847648874740 0.4984259052033911 0.1423306183789353

NiN2+2-H2O
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
34 4 1 1 2
Direct
0.0006281805693504 0.1098397507296909 0.0017546370858241
0.1285905963912839 0.2763285230209220 0.0015251507241061
0.0006630455746262 0.2206382846962285 0.0016191645678845
0.1304593630159374 0.0560278298212395 0.0016744008268716
0.2510334091539903 0.1133591905929023 0.0015626713979700
0.3833356654317797 0.2898145802362961 0.0011434487502839
0.2609908010146569 0.2229475929267792 0.0014851061112466
0.6180409519437617 0.2899162711355743 0.0009481911673745
0.7502584396878049 0.1134790218776303 0.0012932566810235
0.8727397148322495 0.2763464172609744 0.0012879568240223
0.7403500102790730 0.2230295009143433 0.0012313437334228
0.8707032444119491 0.0560938397383239 0.0014648983835457
0.0006147079244840 0.4435103783435395 0.0009436033847123
0.1246459273416107 0.6105243035346177 0.0005328382590477
0.0006051867371681 0.5539946357063883 0.0005497302974646
0.1247709822514338 0.3870814828244775 0.0012783702557826

0.2467050425122537 0.4431924839431360 0.0010866474612428
0.2465414723302217 0.5543836083552023 0.0007576448826896
0.7545829179198194 0.4431872174786875 0.0005739598302696
0.8765509250574368 0.6104882618990572 0.0002608899694962
0.7547095289390029 0.5543071133897115 0.0003124523676945
0.8765180397016579 0.3871058680883337 0.0009359370474513
0.0006014143816415 0.7771477956355710 0.0005781163287111
0.1304069852882819 0.9419131459018999 0.0013589430145018
0.0005462470840030 0.8880075061036763 0.0010669087139092
0.1283135279907412 0.7213752628120744 0.0005167248722628
0.2604451608925444 0.7748109776845169 0.0006207589485570
0.2508261272918020 0.8844399148018454 0.0010027263025378
0.3826051530943744 0.7079889163890911 0.0002986109076417
0.6187198059664638 0.7079054132194287 0.0000452948080891
0.7407731042379240 0.7747378171837767 0.0002299559625314
0.8706682302961966 0.9419448675803181 0.0010940951716520
0.7503800527407876 0.8843719192874104 0.0005813958693892
0.8728919743546726 0.7213089293792834 0.0002371209669008
0.3693767988081120 0.6061249491891729 0.0004520403413295
0.3696598810021499 0.3916235421143526 0.0009601486024380
0.6319682817811838 0.6060931842211161 0.0001878363206842
0.6317052471488793 0.3916410665048247 0.0006769592537239
0.5006624131529165 0.4988964317031446 0.9987972858621532
0.5222641359498752 0.5262252075115086 0.8531180450837397
0.4447739648452398 0.5045621087487788 0.8263020899250009
0.5074032676706537 0.6003147725141602 0.8617025927348152

NiN2+2-H2O-CO2
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
35 4 1 3 2
Direct
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0.1288383235014123 0.2760658250128888 -0.0033722720852385
0.0011086987795994 0.2203787448974799 -0.0031956277390961
0.1312200593186821 0.0556511188044148 -0.0038508101824559
0.2515810508070710 0.1131155160821128 -0.0038522781149960
0.3832698047033518 0.2894177934475502 -0.0042527979218471
0.2608314125705007 0.2227536565528636 -0.0036939205303096
0.6189023012380314 0.2893319573039806 -0.0038328403465793
0.7511114506431866 0.1131821494179886 -0.0033613207383581

0.8733311351828793 0.2761180235877995 -0.0030845245795649
0.7414046939790432 0.2227788826227410 -0.0033233044449602
0.8713340857088916 0.0556395085654249 -0.0035146393798014
0.0010411362605579 0.4433454147314294 -0.0030972436767757
0.1251590399222447 0.6102421007617408 -0.0033783793668020
0.0010706106236206 0.5537996305030434 -0.0030981667845638
0.1251625515643573 0.3868882597663717 -0.0033821372036301
0.2470274502309489 0.4428719133893376 -0.0039253678223074
0.2469655426783529 0.5541867504213865 -0.0039137615783433
0.7550147417864578 0.4428994383313232 -0.0033672539689641
0.8770021219132336 0.6102816547414598 -0.0029706373922730
0.7551518480790422 0.5542338883661881 -0.0032558251638831
0.8769162059352050 0.3869467792666333 -0.0030536715901317
0.0011822337604917 0.7768027708967468 -0.0034440015551108
0.1313304292308504 0.9415111488647108 -0.0039702845058175
0.0013794837245353 0.8876825069834589 -0.0037682347512477
0.1287954024660317 0.7210616537282367 -0.0034811897689833
0.2606798903652338 0.7744554648404696 -0.0038076498916053
0.2518135602191758 0.8841577046922965 -0.0040438694691873
0.3828731025449975 0.7077851320149520 -0.0042004821653878
0.6194160004521005 0.7078610062630372 -0.0036198274506679
0.7417368790081670 0.7744403293611094 -0.0034112126206449
0.8714188658975485 0.9415104377462101 -0.0036847531576227
0.7511148285621723 0.8840637225057296 -0.0036401452385526
0.8735262462721174 0.7210663190479211 -0.0031678743400966
0.4992870705897025 0.5000019502752165 0.1541251336545231
0.3696522393518539 0.6060235849869244 -0.0044230133053811
0.3698150021935870 0.3911420759863136 -0.0046142184609946
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0.5011789119009610 0.4985652063524999 0.9925210532106107
0.5222034202882205 0.5303018232831760 0.8532229923861403
0.3796372493820331 0.5000437522182168 0.1531519585331916
0.6188254580244728 0.4999963216733199 0.1566914371155928
0.4484845395877032 0.5014133048860665 0.8266023685338520
0.5011565765305120 0.6044551884093166 0.8573588386707653

NiN2+2-H2O-COOH
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
35 4 1 3 2

Direct

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0.1312200593186821	0.0556511188044148	-0.0038508101824559
0.2515810508070710	0.1131155160821128	-0.0038522781149960
0.3832698047033518	0.2894177934475502	-0.0042527979218471
0.2608314125705007	0.2227536565528636	-0.0036939205303096
0.6189023012380314	0.2893319573039806	-0.0038328403465793
0.7511114506431866	0.1131821494179886	-0.0033613207383581
0.8733311351828793	0.2761180235877995	-0.0030845245795649
0.7414046939790432	0.2227788826227410	-0.0033233044449602
0.8713340857088916	0.0556395085654249	-0.0035146393798014
0.0010411362605579	0.4433454147314294	-0.0030972436767757
0.1251590399222447	0.6102421007617408	-0.0033783793668020
0.0010706106236206	0.5537996305030434	-0.0030981667845638
0.1251625515643573	0.3868882597663717	-0.0033821372036301
0.2470274502309489	0.4428719133893376	-0.0039253678223074
0.2469655426783529	0.5541867504213865	-0.0039137615783433
0.7550147417864578	0.4428994383313232	-0.0033672539689641
0.8770021219132336	0.6102816547414598	-0.0029706373922730
0.7551518480790422	0.5542338883661881	-0.0032558251638831
0.8769162059352050	0.3869467792666333	-0.0030536715901317
0.0011822337604917	0.7768027708967468	-0.0034440015551108
0.1313304292308504	0.9415111488647108	-0.0039702845058175
0.0013794837245353	0.8876825069834589	-0.0037682347512477
0.1287954024660317	0.7210616537282367	-0.0034811897689833
0.2606798903652338	0.7744554648404696	-0.0038076498916053
0.2518135602191758	0.8841577046922965	-0.0040438694691873
0.3828731025449975	0.7077851320149520	-0.0042004821653878
0.6194160004521005	0.7078610062630372	-0.0036198274506679
0.7417368790081670	0.7744403293611094	-0.0034112126206449
0.8714188658975485	0.9415104377462101	-0.0036847531576227
0.7511148285621723	0.8840637225057296	-0.0036401452385526
0.8735262462721174	0.7210663190479211	-0.0031678743400966
0.4992870705897025	0.5000019502752165	0.1541251336545231
0.3696522393518539	0.6060235849869244	-0.0044230133053811
0.3698150021935870	0.3911420759863136	-0.0046142184609946
0.6325947249070626	0.6061424930385112	-0.0036335497645590
0.6323664286624292	0.3910447215508289	-0.0039566816618675
0.5011789119009610	0.4985652063524999	0.9925210532106107
0.5222034202882205	0.5303018232831760	0.8532229923861403
0.3796372493820331	0.5000437522182168	0.1531519585331916
0.6188254580244728	0.4999963216733199	0.1566914371155928

0.4484845395877032 0.5014133048860665 0.8266023685338520
0.5011565765305120 0.6044551884093166 0.8573588386707653

NiN2+2-H2O-CO
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
35 4 1 2 2
Direct
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NiPc-COOH
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NiPc-CO
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0.7294317069144757 0.7822605376850489 0.9893059078325666
0.8165242145235793 0.6945515859812030 0.9902854340498709
0.5082633802483862 0.4752472587991943 -0.0013950888249332
0.4596966381101382 0.4355579742154415 0.1633923050215384

NiPc-Cl
1.00000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N H Ni Cl
32 8 16 1 1
Direct
0.2543241684323050 0.2676032528156043 0.9985962348097175
0.3724265390735297 0.2360398642486601 0.0007559982684597
0.3048781152409461 0.2185035251049072 0.9999577450354167
0.6476980884276813 0.2391672628822690 0.9978299767493795
0.7649676085017774 0.2738476411108977 0.9957348808818836
0.7156579937407059 0.2234476600144575 0.9955902093111106
0.2699073432154577 0.3356217025216139 0.9980012698566938
0.3375302609384931 0.3531138182473086 0.9987248472927419
0.3713778499236895 0.4174368138971900 0.9984142388179436
0.3878720093233525 0.3041125989097182 0.0000325636226108
0.4512530615210650 0.3395687119443807 0.0003121603605720
0.5663520768408290 0.3407682043774329 0.0009814686809975
0.6443087029431354 0.4203922678526411 0.0021347050031224
0.6305620369279197 0.3068136821406284 0.9999897972277978
0.6797114106794524 0.3569910807809862 0.0005453223355971

0.7477277647810610	0.3414135649032701	0.9984272791955746
0.2669216080211712	0.6120584150457375	0.9944163540734152
0.3841351275342362	0.6461247368138174	0.9963044138894830
0.3348787818901968	0.5960203859558746	0.9957340944458437
0.3701300736544013	0.5324638773085013	0.9971312099957146
0.4482045554587728	0.6119638134755618	0.9980482917214886
0.6265244399666230	0.6485468838313295	0.0019072943143854
0.5631347075876079	0.6130808407922643	0.0008901468662614
0.6428989446529911	0.5352948854724033	0.0033381768748910
0.7444529942164877	0.6166976879025228	0.0042088612688644
0.6767607236466731	0.5995220193587230	0.0036391262477409
0.2499560843103126	0.6797698214207273	0.9935694033383555
0.2994174688381221	0.7299826717274271	0.9939391999823428
0.3673095163434752	0.7138944384814252	0.9954554557314879
0.6421412841955672	0.7166215734844172	0.0006525880028718
0.7097444396613000	0.7339225220449777	0.0010330513882195
0.7601745893382272	0.6846582291816148	0.0028517555698357
0.4398793183838876	0.4077656767375046	0.0002284433706308
0.5091474286646900	0.3079290850298690	0.0004316123170227
0.5760667911965314	0.4091941624746411	0.0025205610155581
0.4383519317770634	0.5435670600449924	0.9992078715385730
0.5053735051442416	0.6448144095192916	0.9988107322968105
0.5744006653228197	0.5449117284491933	0.0024765015803041
0.3384635060774954	0.4745850480374827	0.9968716961959672
0.6759487005107943	0.4782415472358892	0.0030255392357361
0.2020757871358612	0.2519560450632312	0.9978447781088917
0.4119236269975488	0.1984967907080630	0.0016693816424791
0.2907258530867054	0.1658221065978225	0.0002801884177330
0.6091824762498348	0.2006092547642879	0.9973962060520307
0.8175623579580531	0.2595513755409016	0.9935926369013686
0.7311386986460420	0.1711859186396012	0.9934631085426560
0.2311946995368288	0.3739737355896153	0.9968332006224827
0.7853868800150963	0.3808054466471447	0.9984113603789382
0.2289924411191677	0.5729262350808071	0.9939306396682426
0.7830154917590733	0.5782078345617663	0.0052871371238012
0.1973925859520307	0.6942967041038557	0.9923675470061966
0.2841352249926885	0.7823431371011651	0.9930621558905131
0.4060285231014120	0.7522463849434970	0.9958065668731990
0.6027723182996851	0.7542749974120682	0.9990353447294211
0.7240839022811301	0.7865388695254083	0.9997581355786025
0.8124535206619115	0.7002193523461742	0.0029366842885565
0.5072794230104094	0.4763230243750201	0.9948709843771297
0.5098838662914318	0.4759096374214451	0.8771430370863627

NiPc-Cl-CO2

1.00000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N H Ni Cl O

33 8 16 1 1 2

Direct

0.2537503388707014 0.2678646210351204 0.9999909098504243

0.3716544569733663 0.2356792035087491 0.9988829203662027

0.3040380526527227 0.2184691874910741 0.0003485001318416

0.6468227674227107 0.2375949202859708 0.9992802606435108

0.7641974873879569 0.2716426629741758 0.0009120738547547

0.7146899055214287 0.2214427171701077 0.0010208545918507

0.2696546035504644 0.3357786360988791 0.9980676607884278

0.3373595498492373 0.3528953269778581 0.9964641783780697

0.3715346885613345 0.4170300364986715 0.9948408889042590

0.3874566130867598 0.3036581044715038 0.9968813659507978

0.4509975729687730 0.3388130445785857 0.9956270665050102

0.5660067903483813 0.3396488271594710 0.9958280939851517

0.6443170064472445 0.4189575353814574 0.9956702341417988

0.6299968418170890 0.3053397377626427 0.9972803973960986

0.6793390231681947 0.3553116404267415 0.9971030524482425

0.7472414541515557 0.3393200941464050 0.9990731967892781

0.2677117937524178 0.6119816054105615 0.9957932078447759

0.3850775541729449 0.6457021285962936 0.9945953009427704

0.3356268770037151 0.5957864979854974 0.9945069014461340

0.3706154667738374 0.5321371984246722 0.9938319336694716

0.4490473773265654 0.6114238038787538 0.9937745808864955

0.6275895283109280 0.6473047367278235 0.9956326542068794

0.5641036399844717 0.6120742530049388 0.9941241568256809

0.6435713902477693 0.5339280856661801 0.9954116072344670

0.7453388188345080 0.6151289319017845 0.9995108083380995

0.6776858681310108 0.5980686037232107 0.9966418905113985

0.2509299865850267 0.6797008114462654 0.9969284339052575

0.3005935113981288 0.7297608570545497 0.9971625687364890

0.3684345186518921 0.7134918279675274 0.9960568428665848

0.6432270701304494 0.7153253763249645 0.9970697790391547

0.7107979131042483 0.7324692792364490 0.9999186960642644

0.7611195708685077 0.6830893530657636 0.0012184208232459

0.4556362785756970 0.5223558298406145 0.1533131360283090

0.4399822404298994 0.4070566066416166 0.9950764487348475

0.5087340324172792 0.3069501460107197 0.9958523972774412

0.5760603049806694 0.4080249711009309 0.9954395067493860

0.4389847031253395 0.5429841600302516 0.9941934414396731
0.5063856062749947 0.6440114008504950 0.9937058062809085
0.5751465327058669 0.5438553320065144 0.9946272767435284
0.3388128628129428 0.4743374287674650 0.9941615183179284
0.6762772479826791 0.4766541929872175 0.9957274841785061
0.2014224547844078 0.2525162467658325 0.0012240738892093
0.4109801452524678 0.1979469078324068 0.9992563407817491
0.2896465385035847 0.1658796597968865 0.0018794246400479
0.6080991227981459 0.1992455999529198 0.9994284640307323
0.8167533356332103 0.2571054461038451 0.0023728217804363
0.7299200802825636 0.1690878690185044 0.0025241737789888
0.2311372704915965 0.3743375979414060 0.9977939994552284
0.7851431799736427 0.3784854691902044 0.9991147040416321
0.2297052354103482 0.5729237420957952 0.9958983103533605
0.7838637908904968 0.5765933629468906 0.0004979742435849
0.1984124775328457 0.6944141807187755 0.9979415168101410
0.2854827368702160 0.7821649489948693 0.9983321242056430
0.4072496627211855 0.7517522190656349 0.9963369908535246
0.6039118905356339 0.7530560870655709 0.9962647542843058
0.7252288115951696 0.7850600621351502 0.0012459021313234
0.8133862980219395 0.6985432477606669 0.0035264506001979
0.5076467037489156 0.4753894062203805 0.9881650302460306
0.5081579284046158 0.4749333700843733 0.8705820492167262
0.5017863278775661 0.4866078148215420 0.1455380069413220
0.4095381113117407 0.5580169868698657 0.1609705148984158

NiPc-Cl-COOH
1.00000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N H Ni Cl O
33 8 17 1 1 2
Direct
0.2537843608340258 0.2677972613875590 -0.0020365938058586
0.3717337637914123 0.2359043444771393 0.0008016674493872
0.3041389217354017 0.2185398057198740 -0.0005259534868225
0.6478689929647753 0.2387892101131718 -0.0033173088717595
0.7651281167657824 0.2735602458916042 -0.0051217390123882
0.7157621256307917 0.2231230232672671 -0.0050019512632035
0.2695693923637649 0.3357964374256738 -0.0023599730283904
0.3372016400548378 0.3530641914221853 -0.0008706367686837
0.3711137212141946 0.4174335834461870 -0.0006651351234291
0.3874248040427081 0.3039154451958379 0.0007385255475425

0.4509835834280171 0.3391841272033930 0.0019475707727854
0.5663912765801117 0.3399627635670995 0.0013030267035521
0.6450605362821528 0.4203087820774932 0.0019204194153344
0.6305993302877281 0.3065205589434362 -0.0015645705957465
0.6798804537452858 0.3568456356322643 -0.0014885986780578
0.7479549487606658 0.3410872231734979 -0.0034266355492713
0.2668824496404935 0.6120742647176635 -0.0068364676361760
0.3839960769756894 0.6463988009982096 -0.0054827412379645
0.3348156813957544 0.5962821890899666 -0.0065160041783839
0.3701446157787026 0.5325820302480038 -0.0054926797615972
0.4482686738491750 0.6122808928584137 -0.0040607077986328
0.6267366323360918 0.6490168212720790 0.0024680201436694
0.5632452819577081 0.6136305276606561 0.0021195916878846
0.6431570037637675 0.5355993605401289 0.0045958429797887
0.7446360574748101 0.6169618439750023 0.0041316158669207
0.6769602459593489 0.5999203181428366 0.0041706320594829
0.2497921219538208 0.6798149506082248 -0.0061657947672127
0.2991450681993155 0.7300351559354881 -0.0053209492385740
0.3671388188160694 0.7140670971773057 -0.0048897236000408
0.6423868197061195 0.7170219000740834 0.0004871742405036
0.7100449349194302 0.7342114232274833 0.0006967348332356
0.7603935205451080 0.6849276453948664 0.0025329645311491
0.4998621801139984 0.4818820073667331 0.1028063513080289
0.4392140677361956 0.4072311885809465 0.0022195699263517
0.5089408787245046 0.3075581461277611 0.0015034088837649
0.5766368018550542 0.4085529978611439 0.0050994667212859
0.4379591133532620 0.5442642576183653 -0.0049648908426064
0.5053495396322282 0.6451527892468587 -0.0010832251067763
0.5748634094429299 0.5457730618371809 0.0045032002531811
0.3384553710398429 0.4747412358067270 -0.0036903799367582
0.6761739949979151 0.4784360176558345 0.0033571879149470
0.2014883035518869 0.2523206413309330 -0.0030419449288646
0.4110776163572137 0.1982008646810108 0.0018427985759285
0.2898618487938304 0.1658952636032733 -0.0004087308185353
0.6093636622489179 0.2002201516327854 -0.0033536964429006
0.8177219912826587 0.2591988758154627 -0.0066228340157264
0.7312697985936120 0.1708528547203099 -0.0063975704047037
0.2310040390454283 0.3742758910312734 -0.0037180901150698
0.7856325929867305 0.3804577399347263 -0.0034170050828401
0.2290491114276005 0.5728583505540848 -0.0072774222844191
0.7831661773770257 0.5784404102496481 0.0051864066769334
0.1971942012390400 0.6942522843685375 -0.0062736402798161
0.2837681850387875 0.7823654540435696 -0.0048277564964285
0.4057627038189254 0.7524975383602012 -0.0039612252075082

0.6030522291759878 0.7546972906607052 -0.0013475260957574
0.7244527919781645 0.7868022715307299 -0.0008906674089092
0.8126934091182991 0.7004194657139817 0.0024495536427269
0.5688607045503017 0.4179928387041746 0.0994852621231448
0.5067678699253836 0.4768179184662834 0.0010061820506755
0.5129415259712032 0.4732196005230327 0.8837649922298958
0.4602132473221757 0.5178218311516477 0.1298888875578160
0.5432826365478549 0.4420828759579840 0.1343137407738872

NiPc-Cl-CO
1.00000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N H Ni Cl O
33 8 16 1 1 1
Direct
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0.3725987995980032 0.2358940759721075 0.0006765837203406
0.3050229082013484 0.2184134417795829 0.0005687499063821
0.6478893537970668 0.2389598805977260 0.9962907222766006
0.7651864348850687 0.2735004336003928 0.9954169018945102
0.7158493606067076 0.2231336348182055 0.9956705545183291
0.2701882503742339 0.3355351463853529 0.9975175016018016
0.3378371935848982 0.3529436629781250 0.9974720910019184
0.3717528909871659 0.4172241315412137 0.9959911937026245
0.3881501203608762 0.3039322760668430 -0.0010297185558725
0.4515545576474081 0.3393401981047570 -0.0018741365571892
0.5666089375749983 0.3406682138843319 -0.0028934226316101
0.6446223584851789 0.4202777968015105 -0.0031914252866995
0.6308076412808837 0.3066497755512275 0.9963694365746308
0.6799550704272315 0.3568172534727154 -0.0038971840998259
0.7479894581013871 0.3411380563476168 0.9957389739346747
0.2671637843424767 0.6117394281543261 0.9932222884103120
0.3843718369385113 0.6460120103601801 0.9946404093286547
0.3351601802089220 0.5958569602598142 0.9936577159311675
0.3704826758725702 0.5323350169613577 0.9941635612698034
0.4485307839264729 0.6119468737510906 0.9955791496693348
0.6268806262746517 0.6485418578410983 0.0000993594330467
0.5635343871964131 0.6130661125239237 -0.0018067453070101
0.6433853371292667 0.5352243310092892 -0.0010844355237083
0.7448174680651654 0.6168245159969538 0.0033608852549374
0.6771870577217426 0.5995226169841383 0.0009903549596466
0.2500477020230652 0.6793981731548763 0.9936763837529852

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0.3673880626362377 0.7137388820380617 0.9950737465401924
0.6423591478744222 0.7166389852698994 0.0007626986696880
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0.7604206775565129 0.6848385732393788 0.0041948265533048
0.4930722199813869 0.4867142197121830 0.1411472446557230
0.4402287302426828 0.4075083989571130 -0.0028440797417610
0.5094605633956927 0.3077339270285743 -0.0020563467965899
0.5764376051485165 0.4090539881128079 -0.0025460940596888
0.4386919754638868 0.5435405277380614 0.9957293766259253
0.5057112675299335 0.6447719618863907 0.9969608441436527
0.5749083236207150 0.5449075594450409 -0.0017382789279140
0.3388724981173105 0.4744085131090910 0.9943965349109000
0.6763375519901715 0.4781128639680512 -0.0020880329634975
0.2022292224750229 0.2519669233720827 0.9988860743332177
0.4120590269128659 0.1983170507780509 0.0018053725019899
0.2908581487312585 0.1657480756706150 0.0017192387882703
0.6093530348486652 0.2004265370598115 0.9965576337149746
0.8177986411776956 0.2590954671996178 0.9949693184133765
0.7313154982690681 0.1708230464292928 0.9953864321149336
0.2315453662156733 0.3739449244117518 0.9962344488838650
0.7857287339555994 0.3804541839312992 0.9956717936753772
0.2293533257292434 0.5724852046085883 0.9925711280225318
0.7834622582718090 0.5783997864795420 0.0042725316303228
0.1974508415492281 0.6938555881837385 0.9932613024768737
0.2840667312388597 0.7820230550333700 0.9945949276013386
0.4060147267231342 0.7521759590997231 0.9957725068539147
0.6029274986031626 0.7542451851283249 0.9997237208135580
0.7241379713021577 0.7866823830882704 0.0030075606553142
0.8126460666111619 0.7005044503988026 0.0058816895875093
0.5076834106277797 0.4762189315665596 -0.0087097246934557
0.5090390496757282 0.4766073601308570 0.8735752000048265
0.4532720597950786 0.5197497742693208 0.1655431349104566

NiPc-H2O
1.00000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N H Ni O
32 8 18 1 1
Direct
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0.3714207209771914 0.2359022658547190 0.0009710137042234

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0.6461119124569308	0.2371605540018038	0.0011086969022500
0.7636092487038226	0.2707057499033851	0.9996888778484703
0.7139413424436043	0.2206744541796226	0.9996814258088023
0.2695062063119877	0.3360036041190355	0.0007082829773211
0.3371996052550514	0.3531529051229612	0.0019181808589224
0.3714494170131246	0.4172873940912538	0.0029576346250551
0.3872267801302272	0.3039086054302018	0.0020613412227348
0.4507317001928115	0.3390924788221881	0.0032320508561128
0.5656552146709117	0.3395399466551225	0.0036669203976061
0.6440628410296299	0.4185162815916712	0.0040032976947444
0.6295239559816963	0.3049955284195747	0.0026519819426056
0.6790041359705725	0.3547894975675092	0.0028589310233613
0.7468538893325061	0.3384805727116387	0.0012552712230445
0.2680964152287970	0.6125750153138512	0.0006924797337220
0.3855453643810449	0.6459342787824340	0.0018087555046193
0.3359604315101166	0.5961303374255849	0.0018158153138046
0.3708162110243833	0.5323676943003619	0.0026993670558184
0.4493595923329110	0.6114031295261881	0.0026128845731321
0.6278810756209694	0.6468963646836627	0.0027854584448761
0.5643396341684337	0.6118188514212051	0.0030612739131826
0.6435858288575389	0.5335024453217514	0.0038820609754140
0.7455953289265764	0.6144508259101826	0.0022781043480791
0.6778491636977719	0.5975349688782501	0.0032642092317232
0.2515519410680085	0.6803944923502172	0.9996636028836789
0.3013205850929808	0.7303229167951883	0.9996874586143107
0.3691381741483895	0.7138078524684346	0.0007670026805116
0.6438278801475334	0.7148858591265679	0.0015982392368841
0.7114674133111691	0.7318902846702002	0.0005352180221720
0.7616504381224800	0.6823622561517553	0.0008582743724830
0.4401233040769554	0.4075540139657008	0.0038161951826794
0.5083282205080621	0.3069756239998611	0.0033273013976185
0.5755195091778731	0.4081192081341456	0.0044471430178703
0.4394366120709918	0.5427238463206407	0.0030346099240077
0.5067318865383967	0.6439002927113791	0.0026370152370845
0.5748763826211842	0.5432445602164861	0.0035922831176265
0.3387962192943021	0.4746366215487257	0.0025901998931772
0.6761972145556641	0.4761390234726903	0.0039675665073631
0.2012096231139751	0.2527484317435835	0.9985770801879710
0.4107375774730855	0.1981559106404589	0.0010592940287637
0.2894128765009611	0.1660426337570229	0.9988467866078992
0.6072280583822760	0.1989775540958902	0.0009079910697665
0.8161303465194578	0.2560246357025022	0.9983280895594220
0.7289406098152824	0.1682361510071644	0.9983721353018353

0.2309759894689662 0.3745509625960892 0.0004901494031770
0.7849476320416002 0.3774521303553939 0.0010915856508475
0.2299196156358292 0.5736796811706739 0.0006378693538949
0.7840068018324828 0.5757834039654099 0.0024309998343668
0.1990599145269840 0.6952239895269088 0.9987370582063448
0.2863662940922467 0.7827793672945305 0.9987922966967417
0.4080795174444134 0.7519342648650635 0.0006966388169261
0.6046155371959543 0.7527365413310605 0.0011867352097212
0.7260396957248503 0.7844448980947263 0.9993306487726841
0.8140306615079496 0.6975865762854738 0.9998500208430130
0.5422938126661592 0.5044717783270229 0.8710460866246947
0.4660092539258756 0.5000838820589379 0.8718396599293072
0.5074786834686336 0.4753184505751022 0.0042114799234483
0.5044693951878259 0.4915606303456883 0.8432492649713410

NiPc-H2O-CO2
1.00000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N H Ni O
33 8 18 1 3
Direct
0.2537167148172958 0.2678791286205502 -0.0000293258493452
0.3715564589991490 0.2357284225339714 -0.0008816959002331
0.3039481459728305 0.2184795708277565 -0.0001266826316642
0.6464212025919187 0.2371837976022218 -0.0008677430488707
0.7638568348532143 0.2710500415303581 0.0000628513889069
0.7142976711594531 0.2209146541209125 0.0001605928397823
0.2696292496262989 0.3358251777547572 -0.0007359851322459
0.3373264152688413 0.3529827882985264 -0.0014498921241778
0.3715931057126617 0.4170754200371239 -0.0021184692127165
0.3873611127102687 0.3037276881044135 -0.0014737959234048
0.4508626606597684 0.3388761658077019 -0.0022466560534252
0.5657596442971814 0.3394300243990708 -0.0028376088260009
0.6440596385676794 0.4185192632273949 -0.0034103265199288
0.6296765516561159 0.3049851580779515 -0.0021328232153252
0.6790620315876817 0.3548687337313708 -0.0024245736556996
0.7469626969757480 0.3387780637579397 -0.0012232897013006
0.2681600259348256 0.6121196641523486 -0.0000124359970321
0.3855649999397619 0.6455537103235780 -0.0021920309836613
0.3360301285983814 0.5957460925856020 -0.0016070768715174
0.3708972620338284 0.5320314871058740 -0.0025946485129413
0.4493597952450759 0.6110706271916526 -0.0037254100452089

0.6277545185730792 0.6467673770601408 -0.0040681397227169
0.5643026854157608 0.6116212751481491 -0.0049163633504728
0.6436321996650501 0.5334347619008297 -0.0040828925030002
0.7454924416977903 0.6147127926106436 -0.0010659714708837
0.6778179829910340 0.5975269270718675 -0.0033124812149559
0.2515779439280431 0.6799046841598692 0.0011585377282198
0.3013400955231112 0.7298412256679462 0.0007523036600513
0.3691474336160519 0.7134189610635981 -0.0009382074919081
0.6434100653690413 0.7148146202223586 -0.0030695744257629
0.7109614475313688 0.7320541119179631 -0.0006806075772337
0.7612818334700707 0.6826771736042168 0.0003818701923637
0.5056650490268575 0.4775409055160590 0.1597424487796541
0.4402779228665974 0.4073477716914070 -0.0026720815997491
0.5084736945336129 0.3067892375752557 -0.0022647959504214
0.5755373272574695 0.4080271204674897 -0.0036028019310483
0.4395088134725348 0.5423954630396276 -0.0039907006956182
0.5066743290777077 0.6436595500340977 -0.0043816324450420
0.5748971937028562 0.5430687476897407 -0.0051272619872773
0.3388919732214342 0.4743531482587113 -0.0021171893030622
0.6762210827719358 0.4761063729780786 -0.0035904448855943
0.2013723936880933 0.2525386721837367 0.0005614415928489
0.4108920198487721 0.1979969543069488 -0.0010824265513835
0.2895344240026242 0.1658710356949372 0.0003425207066262
0.6076391601456910 0.1988881099805337 -0.0006953546256450
0.8164037917695072 0.2564325356858671 0.0010163598110547
0.7294606671423838 0.1685247001005725 0.0011551862508887
0.2310754391018789 0.3743511045622777 -0.0007464175328069
0.7849338688746595 0.3778760175666448 -0.0012843034923934
0.2300655596678461 0.5731424464830028 0.0003284379401947
0.7840682868667916 0.5762188570627722 -0.0002765882621200
0.1990955916826619 0.6947285993307466 0.0024441812004359
0.2863328432263731 0.7822740797287665 0.0017670688693698
0.4080680941753638 0.7515696074163880 -0.0012998382442994
0.6040403510402969 0.7524917061770203 -0.0037350451515184
0.7253614795858965 0.7846604796170127 0.0004096164284980
0.8135673135967977 0.6981160269286502 0.0023711051677904
0.5427435591128733 0.5053088851100805 0.8640254698028706
0.4663503652938683 0.5027796845505541 0.8651202882908238
0.5075501954168873 0.4750978561246156 -0.0041517706755580
0.5044700583278265 0.4939655224462121 0.8361613656792517
0.4468072116366476 0.4774558829034917 0.1608604744357431
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NiPc-H2O-COOH

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0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N H Ni O
33 8 19 1 3
Direct
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0.3716073707256577 0.2358259478577567 0.0073240329412258
0.3040783748018449 0.2185030155975380 0.0035619325885152
0.6490749958384735 0.2347932493574166 -0.0048617733759403
0.7663020583732517 0.2684303536646405 0.9869302157283770
0.7165949640724412 0.2184944148644693 0.9883093790846216
0.2699757362290400 0.3358104372692474 0.0011335123111137
0.3374820608667132 0.3531328163817665 0.0052535199976041
0.3714969764000620 0.4176260578394176 0.0052549102921005
0.3876448006131219 0.3037583263750656 0.0082424845884499
0.4515364405285363 0.3386964076853409 0.0107414103109749
0.5686111161072412 0.3365667916786785 0.0092970110576427
0.6477662135919092 0.4162493510796156 0.0076768504167434
0.6324009909107725 0.3023588345429480 0.0010972077836558
0.6823135143202522 0.3525287238831639 -0.0000981024090441
0.7497955551456938 0.3360154513522954 -0.0075080017452311
0.2657116261420528 0.6146405684340536 0.0006598243910394
0.3832008918396758 0.6482379007834803 -0.0005598795261365
0.3334826252988956 0.5981583638833801 -0.0014173898522841
0.3688853166917561 0.5342306412723030 -0.0036131024373329
0.4473304631124247 0.6134154260991410 -0.0026921508506163
0.6277893483306418 0.6472414971670798 0.0054134648109863
0.5640180457160471 0.6122554491386204 0.0055292030636340
0.6443371486853648 0.5333353903549334 0.0085436901992328
0.7457341206727777 0.6153382106361290 0.0049344136336691
0.6781170933105554 0.5978560200192130 0.0063127909562778
0.2489416385210916 0.6824505654307232 0.0032318218729649
0.2985976433239520 0.7323354163159365 0.0042480879059481
0.3664660369188409 0.7158665414327259 0.0026249609255346
0.6435982798624020 0.7152136772676482 0.0031117302017632
0.7111752247620649 0.7325719770172169 0.0019626083225873
0.7615585039447541 0.6832694008047698 0.0027879162777396
0.4989926184668297 0.4850670857345557 0.1072109483667928
0.4397349720305541 0.4069453085658947 0.0097188353091568
0.5095963013393884 0.3063838776788582 0.0103494541766027
0.5800958398616421 0.4043942917443923 0.0149617216581525
0.4364280930125440 0.5457973982132476 -0.0074421010733539

0.5059378325505768 0.6441672858599931 0.0013891339820290
0.5757827129367574 0.5440850296710499 0.0084566783988081
0.3387908995988470 0.4751940239383857 0.0000929281036286
0.6773789017570687 0.4756118423013021 0.0073098717496453
0.2016412070757387 0.2525806714725482 0.9975890993913687
0.4108744782469498 0.1980675077904428 0.0092054217756110
0.2897356895855547 0.1658819579423806 0.0026458305401299
0.6102760909906370 0.1965042634646788 -0.0040536894603738
0.8185817227155936 0.2538082997897596 0.9815354613044267
0.7313587623420355 0.1661664543564496 0.9838463517256939
0.2315684493331648 0.3744119581892232 -0.0014594925640718
0.7879440296396788 0.3749517148833376 -0.0084253075232090
0.2275353249355514 0.5757255563473944 0.0003815789331016
0.7843858933275172 0.5769021866433878 0.0055452842019231
0.1964355533912549 0.6972007741886964 0.0046667527262290
0.2836128163576755 0.7847433027422507 0.0065418697031987
0.4052809894059798 0.7541321819994162 0.0038081143032603
0.6041835083037296 0.7528589251266513 0.0022787105069691
0.7255068827331289 0.7851850958732077 0.0005313285101380
0.8138679483058511 0.6987310311642344 0.0017652426929891
0.5557542825955016 0.4894047361807424 0.8802259984370592
0.4793908475318570 0.5015187566606274 0.8830973765827334
0.5664044828933503 0.4205912986420466 0.1023969441908765
0.5068484537979400 0.4762580173914974 0.0098448534907594
0.5137475563869014 0.4683488128109499 0.8931043695357723
0.4600020689378899 0.5224157264969174 0.1334092617153763
0.5420222925199866 0.4449966766530617 0.1385734871218916

NiPc-H2O-CO
1.00000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N H Ni O
33 8 18 1 2
Direct
0.2524837459703195 0.2688081616161176 0.0039851104283354
0.3702645162703940 0.2362005094570819 0.0005372898195826
0.3025787639432964 0.2192297171838548 0.0022112403946198
0.6457804012105340 0.2379315003316515 0.9959108063761467
0.7631871400958247 0.2721129711903064 0.9975050932629863
0.7137002921558158 0.2219012117146268 0.9963658161317256
0.2687107874380839 0.3366941121630428 0.0039884801132903
0.3364701501467279 0.3534796434124856 0.0023662269165796

0.3707651042364303	0.4175006071475503	0.0016942814920803
0.3863865742937527	0.3041417249665349	0.0007723661399762
0.4499401214782895	0.3392618334987246	0.9996182208625219
0.5648386639220850	0.3399315868308538	0.9970827204657201
0.6430586394110815	0.4191833626941665	0.9977323073954897
0.6288352528744670	0.3056797284549616	0.9963970974537567
0.6781361640551397	0.3556719531187773	0.9970283832203363
0.7461197304346587	0.3397725053836061	0.9977537883797660
0.2669130404114718	0.6121419169328114	0.9976809109881942
0.3842455741688999	0.6459706088176006	0.9984064611393225
0.3348593830665401	0.5960249275301941	0.9987352700628402
0.3699514275717157	0.5324042201187200	0.0001067007001230
0.4481955340789593	0.6115810575105728	0.9996301486948548
0.6266556151844536	0.6473364571681141	0.0022944408745058
0.5631175242474804	0.6121724138764953	0.0013452293096179
0.6423364999270550	0.5340142458901664	0.0002667168240704
0.7444197165810973	0.6149757352087524	0.0013406211662383
0.6766354546474315	0.5980563730567722	0.0013553877006133
0.2500679283298588	0.6798698012666781	0.9961414882112866
0.2996734631957559	0.7299630189692106	0.9957378820588770
0.3675340877430608	0.7137757771535091	0.9968705776241817
0.6425565963837152	0.7153218401279877	0.0038048676907753
0.7102373400109910	0.7323636925488092	0.0041175020183439
0.7604626691019880	0.6828891371631980	0.0027459094822788
0.5166799674973367	0.4640352079262918	0.1473433217587098
0.4393715433363007	0.4077638436157852	0.0004112691844964
0.5075762655155867	0.3072286670069782	0.9979961657406630
0.5745093897683395	0.4086202603378942	0.9975466295343507
0.4384730460051943	0.5429509905349695	-0.0000914646671856
0.5054836415058762	0.6442442274808260	0.0006746408834089
0.5736982496730254	0.5437096288388411	0.0006115736728689
0.3379914233560096	0.4747445632278894	0.0014813060797777
0.6750817597171653	0.4768088584038387	0.9990821290955363
0.2001042053801648	0.2536329030985101	0.0053613267134928
0.4093806151184846	0.1982691347307245	0.9991817361763226
0.2879720222159611	0.1666753641129980	0.0021717936618176
0.6071369075835676	0.1995065343948567	0.9954127554259483
0.8157565863202569	0.2575733600474912	0.9981995181285472
0.7290095425533774	0.1695472888150014	0.9961697316316415
0.2304116058541338	0.3754533890184761	0.0052796238716447
0.7839252841345401	0.3790217305563853	0.9986330518280320
0.2289375068867245	0.5730466258682517	0.9980090133657303
0.7828418569472549	0.5763322652014827	0.0003798439995787
0.1975324875778816	0.6945205634805545	0.9952979732660725

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0.5298529275126526 0.4547080884617405 0.8677748750055704
0.4849361335380268 0.5165315574379161 0.8680786016990286
0.5064861555728062 0.4757635700084960 0.0005566528753009
0.5089252148236894 0.4868954928519028 0.8378012274946629
0.5558546404256526 0.4262824628381799 0.1652607813638360

NiN4-CH3
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0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni H
43 4 1 3
Direct
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0.0007366497575228 0.2216116372833427 0.0012507926813110
0.1268979977296574 0.0558469973632146 -0.0010111710868582
0.2522660063142078 0.1123519123604961 -0.0011364824581555
0.3741048533528422 0.2849532575124360 -0.0002106613639790
0.2514098744633276 0.2245019846059008 -0.0000717961889478
0.3773283152265949 0.0566052408470473 -0.0018042107745304
0.5007361370215702 0.1153854251575129 -0.0016713892545338
0.6273792039192111 0.2849637033918795 0.0001873668019356
0.5007237463851908 0.2293755748396058 -0.0009417174989968
0.6241658138880998 0.0565834323070195 -0.0015867306121785
0.7492571026003827 0.1122878046167097 -0.0006960916913839
0.8764189565214560 0.2775628669526977 0.0022213583099886
0.7500528078550558 0.2244194694898856 0.0004546440776246
0.8747751666629248 0.0558391071028362 -0.0006778291657733
0.0006476196083103 0.4447065527153360 0.0052849621394753
0.1236587337943460 0.6115497687715976 0.0041434580710549
0.0006456254458569 0.5553535679673955 0.0052887534309686
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0.2468080285669376 0.4440133267735207 0.0037820385738758
0.2467856142452734 0.5561148995836599 0.0038709688198358
0.7546287277777286 0.4439859401060713 0.0043816478926971
0.8776627078433025 0.6115909652541988 0.0044802748439877
0.7546230033329665 0.5560638910941657 0.0044778486698919

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0.0008041387589881 0.8896348935123850 -0.0002859544902071
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0.3772995688544043 0.9434643294888790 -0.0017625919373133
0.2522233523867520 0.8877564436575648 -0.0010551194653512
0.3740553038385493 0.7151749763618735 -0.0000229595300317
0.5006789669643341 0.7707206073647666 -0.0007872750413314
0.6241639645394587 0.9434594395471122 -0.0015768616386049
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0.7500478615321957 0.7756492149017291 0.0005178120960247
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0.3683761328647464 0.6070616193147960 0.0018759664778672
0.3684498636558947 0.3930977528132510 0.0015821184428803
0.6330244570632072 0.6070063474484064 0.0024646557148053
0.6329790871669019 0.3931101873746091 0.0021119143245564
0.5008202751558032 0.5001654449268337 -0.0097440068814189
0.3914070450926508 0.4961946462462071 0.8749607004363886
0.5419117465937456 0.5784703341880347 0.8744781561500342
0.5592208042695306 0.4369076770943817 0.8725681344519004

NiN4-CH3-CO2
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9.8380002975000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni H O
44 4 1 3 2
Direct
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0.0008190960472454 0.2228956044037598 -0.0008181443489531
0.1268437209016727 0.0570804853159698 0.9968090388756513
0.2522512769313318 0.1135949156325450 0.9965621202368912
0.3741071361766022 0.2861998100560540 0.9968585459251094
0.2514421634806751 0.2257429706527403 0.9976402453863908
0.3773109096609654 0.0578881809055256 0.9957804212296161
0.5007894173084121 0.1167043134075372 0.9955426027061204

0.6274388664801848 0.2862084281938596 0.9967597461898879
0.5007885368803312 0.2306980140011408 0.9958702971083586
0.6243091568151604 0.0578970968399588 0.9957456183997849
0.7493583058803742 0.1135971448341591 0.9966578434516427
0.8765283765486471 0.2789431111426270 -0.0000317084592398
0.7501754867005894 0.2257839514108120 0.9976631629197090
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0.1237947161049114 0.3898046859253179 0.0026069539783875
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0.2469307100083702 0.5573286568060268 0.0020593472624855
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0.1268447515496399 0.9454554846103943 0.9971610595051622
0.0007875882461386 0.8907918212537217 0.9979991870372046
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NiN4-CH3-COOH
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NiN4-CH3-CO
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C N Ni H O
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0.4998399559300070 0.1165431408148370 0.9957568690239228
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NiN4-NO
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0.0000000000000000 12.7799997330000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Ni O

42 5 1 1

Direct

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NiN4-NO-CO2
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0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O
42 5 1 1
Direct
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NiN4-NO-COOH
1.00000000000000
9.8380002975000007 0.0000000000000000 0.0000000000000000
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0.0000000000000000 0.0000000000000000 20.0000000000000000
C N Ni O H
43 5 1 3 1
Direct
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0.4957854121150683 0.2306940535729633 0.0002092399672070
0.6192858032972844 0.0580603499383561 -0.0005428506269230
0.7444976701856759 0.1136082383815223 -0.0012961016565135

0.8716170377064867 0.2790921842402684 -0.0030016371613980
0.7454737498776198 0.2258631125711056 -0.0017931313741036
0.8698671701066011 0.0572693762457147 -0.0016512677910336
0.9958603741854788 0.4460984548897829 0.9948274841551464
0.1187508448888425 0.6127805152924120 0.9952932140235523
0.9957917748892693 0.5565997660564657 0.9946219564534088
0.1188965711120428 0.3899959653098566 0.9959196331634522
0.2420334822778808 0.4453363469133129 0.9965115380042082
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0.7495717076417602 0.4452044723976566 0.9957428854326065
0.8727358237906574 0.6127290116510111 0.9952965832328496
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0.8728210069672339 0.3900320599356318 0.9955554053497168
0.9957123453352219 0.7798182250517036 -0.0029769912091596
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0.3690420942765099 0.7166471473443563 0.9987943504240266
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0.3628257318123413 0.3940471533377295 0.9998085677512842
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0.6289119287746956 0.3936735875227853 0.9977577092867803
0.5093712373328053 0.4998879952296533 0.8904484022928747
0.4965030842162830 0.5015976931129996 0.0050734384559937
0.4039459994066182 0.4975978819049124 0.8616097425150824
0.6092649873415039 0.4979820836317721 0.1379607379435593
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NiN4-NO-CO
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0.2544392668698723 0.1130969728856773 0.0003774386357515
0.3768691512795456 0.2859313670812111 -0.0005582380469314
0.2536754198174304 0.2254589337405691 -0.0001495085860344
0.3795004864787906 0.0572951158319623 0.0002676231733838
0.5028323982602493 0.1159953741004616 -0.0001835403142107
0.6289357727769277 0.2860096658654873 -0.0012288516734517
0.5028478054675513 0.2300891490439688 -0.0007569178372311
0.6261835703945474 0.0572525428991485 -0.0000039094463213
0.7512091668612823 0.1130149388048434 0.0000885852919552
0.8784095634846543 0.2782727272463823 0.9991560979967978
0.7519454939163116 0.2254232458303961 -0.0005571161876718
0.8767222412077963 0.0564969818362336 0.0005251434221369
0.0028553303534042 0.4453949884801634 0.9978354861424095
0.1259198866408660 0.6119332174694894 0.9983344745788432
0.0028461419067110 0.5558452200612236 0.9977584295452198
0.1259739545002062 0.3893738982315591 0.9985420162128620
0.2489475007684126 0.4447907999577616 0.9988763396538048
0.2489324801831957 0.5564971868577951 0.9987274300484767
0.7568350634891624 0.4447523532283245 0.9977982700109099
0.8796809946133318 0.6119406290994663 0.9980734205441270
0.7568486994538391 0.5564634086249803 0.9977533971326307
0.8797021289462339 0.3892409471109604 0.9981875017203017
0.0028437050296438 0.7789418773366220 0.9997244463433105
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0.0029276780137750 0.8901791743883831 0.0005347303959447
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0.2544943953034832 0.8881954104119559 0.0004312570942302
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0.5028861918598022 0.7711971679625450 -0.0007769243181109
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0.6346752886072902 0.3940765889106267 -0.0018811634658620
0.4914147074086990 0.4995214518360694 0.8839304329741604
0.5027402598948906 0.5006322019817999 -0.0055144126737010
0.3814284626589014 0.4976786094965919 0.8594470486511221
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NiN4-SCN
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0.0000000000000000 0.0000000000000000 20.0000000000000000
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43 5 1 1
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0.1274640251927555 0.0552817020267840 0.0024691159593006
0.2528226916290764 0.1118107069661498 0.0020483204285578
0.3749739553341629 0.2848141399288158 0.0020372417042723
0.2521469395329999 0.2243065066073005 0.0026651394871000
0.3777322873046788 0.0560060939643778 0.0011042458452229
0.5011296881395684 0.1150664772697479 0.0006366032675180
0.6276887471087887 0.2848960266300924 0.0011219572041791
0.5012292400313737 0.2288727366621492 0.0008673452687598
0.6246169691021261 0.0560154754417292 0.0006001253426505
0.7496814352522446 0.1118124590339165 0.0013539429486491
0.8770240600496322 0.2770395456027078 0.0030131212004239
0.7505862136957487 0.2242676793846405 0.0017610293246914
0.8750818795947276 0.0553026455447274 0.0019885504059361
0.0015308370792832 0.4441997822628905 0.0050412117319934
0.1245241437129626 0.6108348959886870 0.0047849641243143
0.0015038478526838 0.5546908297041081 0.0049521106264905
0.1244498991511972 0.3879156881599676 0.0050104717302371
0.2475650076422223 0.4432205720334179 0.0048324387688258
0.2475888861001023 0.5554887138300483 0.0046483780160956
0.7552931045455237 0.4434333422854921 0.0033961847620373

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0.7552903733335417 0.5555228123427451 0.0032948028860145
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0.0013090844916444 0.8889445422859462 0.0026808236541718
0.1257969947187286 0.7216621825186039 0.0035912416550029
0.2521354210641699 0.7745367045361846 0.0024321366599318
0.3777580999096029 0.9427903583721580 0.0010534281462147
0.2528104171985386 0.8870323788025365 0.0020088885113159
0.3749687375386807 0.7139940837405665 0.0016061664110885
0.5012417655710115 0.7699700192357000 0.0004321825361679
0.6246296348047140 0.9428353473065564 0.0004551616961641
0.5011818904847635 0.8837459554543471 0.0003737709274240
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0.5012028106448845 0.4993374159616020 -0.0064926650720887
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NiN4-SCN-CO2
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C N Ni S O
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0.3744705227135920 0.2861149584388474 -0.0007548788926318
0.2517098385058495 0.2255929156414829 0.0005011081309942
0.3774662860941856 0.0573139350202962 -0.0017076931913921

0.5008849540485157 0.1164193422378663 -0.0027468317469932
0.6272902437955049 0.2861154288485996 -0.0022408403251956
0.5008191443104983 0.2302077690597278 -0.0026639794961857
0.6243446149395162 0.0572828901257584 -0.0025695522978557
0.7493897496243345 0.1130292788918975 -0.0014141955531609
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0.7501953527602677 0.2254940333771189 -0.0008783618034804
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NiN4-SCN-COOH
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C N Ni S O H
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0.3724508558890489 0.0580261665624004 0.0014462273271295
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0.6225154345313529 0.2861625890232862 0.0004112140520181
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0.6294883717131249 0.3933759244858001 -0.0015154247154559
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NiN4-SCN-CO
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C N Ni S O
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0.1264876268732802 0.0567828821624954 0.0022750168427714
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0.0004303028593595	0.5560481368419019	0.0042939438555298
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