

Supplementary Information for Molecular Oxidation-Reduction Junctions for Artificial Photosynthetic Overall Reaction

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This PDF file includes:

Supplementary text
Figures S1 to S30
Tables S1 to S7

Supplementary Information Text

All starting materials, reagents and solvents used in experiments were commercially available, high-grade purity materials and used without further purification. Nickel(II) nitrate hexahydrate ($\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, 99.0%), phosphomolybdic acid hydrate ($\text{H}_3\text{PMo}_{12}\text{O}_{40} \cdot \text{H}_2\text{O}$, 96%, **PMo₁₂** for short), acetone (CH_3COCH_3 , 99.5%) were purchased from Sinopharm Chemical Reagent Co. Ltd. Benzotriazole (Hbzt for short, 98%) was purchased from TCI Shanghai Co. Ltd. Pyrazine ($\text{C}_4\text{H}_4\text{N}_2$, 99%) was purchased from Shanghai Adamas reagent Co. Ltd. Ethanol ($\text{CH}_3\text{CH}_2\text{OH}$, 99.7%) was purchased from Wuxi City Yasheng Chemical Co. Ltd.

Preparation of Ni₅ ($\text{Ni}_5(\text{bzt})_6(\text{NO}_3)_4(\text{H}_2\text{O})_4$): A solution of $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (165 mmol, 48 g), Hbzt (100 mmol, 12 g) and 500 mL acetone was charged in a 500 mL glass beaker and left for slow evaporation. Light-blue crystals were collected after 3 days, and dried in air (85% based on Hbzt).

Preparation of d-OR: 100 mg **Ni₅**, 50 mg **PMo₁₂** and 5 mg pyrazine in 4 mL water and 1 mL ethanol were ultrasonically dispersed in a 12 mL Pyrex vial and heat at 85 °C for 72 h. After cooling down to room temperature, light-yellow crystals were obtained (65% based on **Ni₅**).

Preparation of a-OR: 30 mg **Ni₅**, 100 mg **PMo₁₂** and 5 mg pyrazine in 5 mL water and 0.5 mL ethanol were ultrasonically dispersed in a 12 mL Pyrex vial and heat at 85 °C for 72 h. After cooling down to room temperature, light-green crystals were obtained (40% based on **Ni₅**).

Preparation of s-OR: 50 mg **Ni₅**, 50 mg **PMo₁₂** and 20 mg pyrazine in 4 mL water and 1 mL ethanol were ultrasonically dispersed in a 12 mL Pyrex vial and heat at 85 °C for 72 h. After cooling down to room temperature, light-yellow crystals were obtained (50% based on **Ni₅**).

Single-Crystal X-ray Analyses

The diffraction data of **a-OR** was collected on a Bruker AXS Apex II CCD diffractometer (Mo $K\alpha$, $\lambda = 0.71069 \text{ \AA}$) at 293 K. The diffraction data of **d-OR** and **s-OR** were measured on a Bruker D8 Venture Photon II detectors at 190 K with a radiation source of Ga ($K\alpha$) ($\lambda = 1.34139 \text{ \AA}$). The crystal structures were solved and refined by full matrix least-squares methods against F^2 using the SHELXL-2018 program package (1-2) and Olex-2 software (3). All non-hydrogen atoms were refined with anisotropic displacement parameters and hydrogen positions were fixed at calculated positions and refined isotropically. The solvent molecules in these structures are highly disordered and not able to be refined by using conventional discrete-atom models; thus, the contribution of partial solvent electron densities was removed by the SQUEEZE routine in PLATON program (4). The crystallographic data and structure refinement for the four compounds are summarized in *SI Appendix*, Table 1. The selected bond lengths and angles are listed in *SI Appendix*, Table 2~4. CCDC 2052395 (for **d-OR**), 2052396 (for **a-OR**) and 2052397 (for **s-OR**) contain the *SI Appendix*, crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre (www.ccdc.cam.ac.uk/conts/retrieving.html).

Photocatalysis activity test

All the artificial photosynthesis experiments were performed in a gas-solid system with a home-made quartzose reactor. 10 mg of the photocatalysts (**d-OR**, **a-OR** and **s-OR**) were ground and spread evenly over the bottom of a quartz crucible. Then the quartz crucible was placed in the reactor and 300 μL distill water was added around it (ensure that the photocatalysts can not contact with liquid water). After sealed, the reactor was purged by high-purity CO_2 (99.999%) for 30 min to remove all the air. A 300W xenon arc lamp (CEL-HXF300, 300-1100 nm) was utilized as an irradiation source. The gases were detected by GC (GC-7900, CEAULIGHT, China) equipped with a flame ionization detector (FID) and a nickel reformer to analyze CO/CO_2 and a thermal conductivity (TCD) to analyze H_2/O_2 . The isotope-labeled experiments were performed using $^{13}\text{CO}_2$ instead of $^{12}\text{CO}_2$ or H_2^{18}O instead of H_2^{16}O , and the products were analyzed using gas chromatography mass spectrometry (GC-MS, 7890B and 5977B, Agilent). CO , CH_4 and O_2 were analyzed using a HP-MOLESIEVE, C_2H_6 and CH_3CHO were analyzed using a GS-CARBONPLOT.

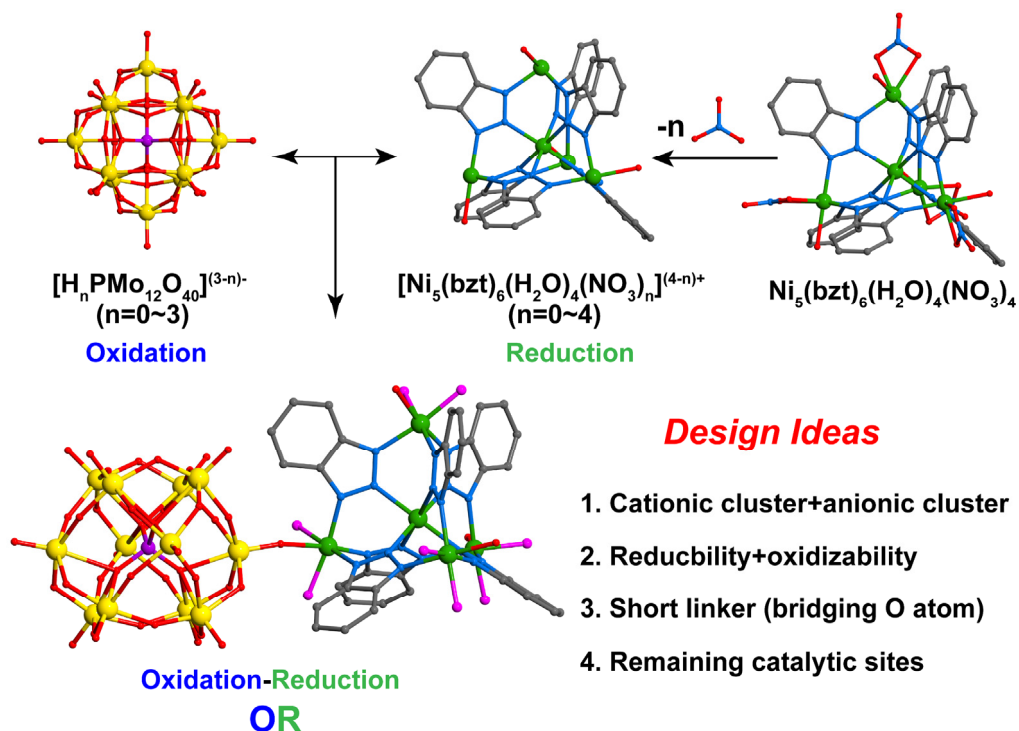


Fig. S1. The design ideas of constructing OR photocatalysts by Ni_5 and PMo_{12} clusters. PMo_{12} is a kind of classical polyanion with strong oxidative capacity. Ni_5 can be regarded as a cationic unit when the NO_3^- ions leave. The Ni sites can coordinate with the terminal O atom of PMo_{12} and remain the active site with reductive capacity (pink ball). All hydrogen atoms are omitted for clarity. Ni, green; Mo, yellow; P, purple; C, gray; N, blue; O, red; solvent molecule, pink.

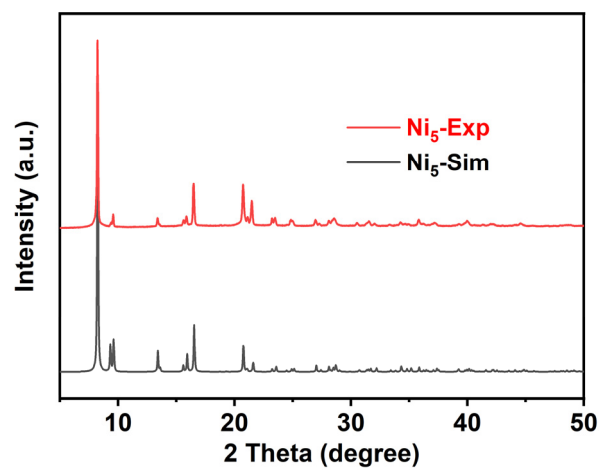


Fig. S2. The experimental and simulated PXRD patterns of Ni_5 . The well-match curves indicate the purity of obtained Ni_5 .

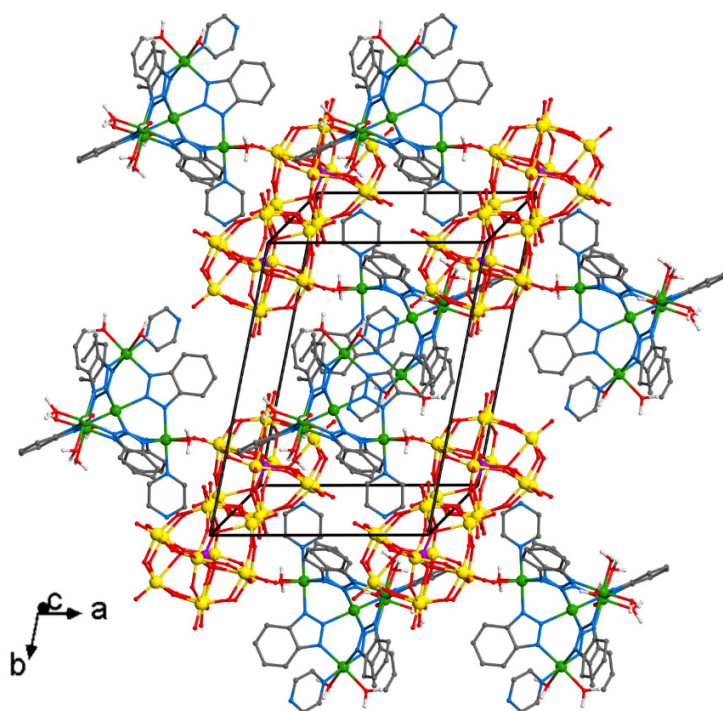


Fig. S3. Packing diagram of **d-OR** along *c* axis. Ni, green; Mo, yellow; P, purple; C, gray; N, blue; O, red.

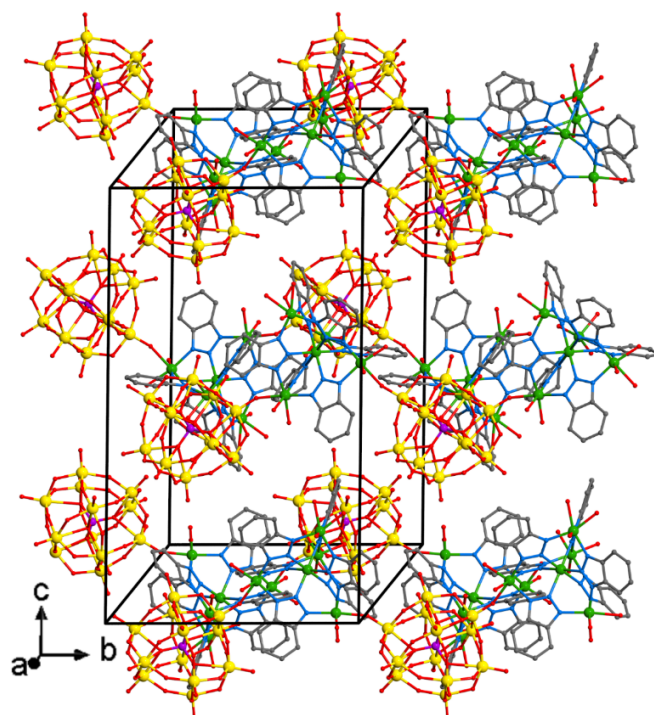


Fig. S4. Packing diagram of **d-OR**. Ni, green; Mo, yellow; P, purple; C, gray; N, blue; O, red.

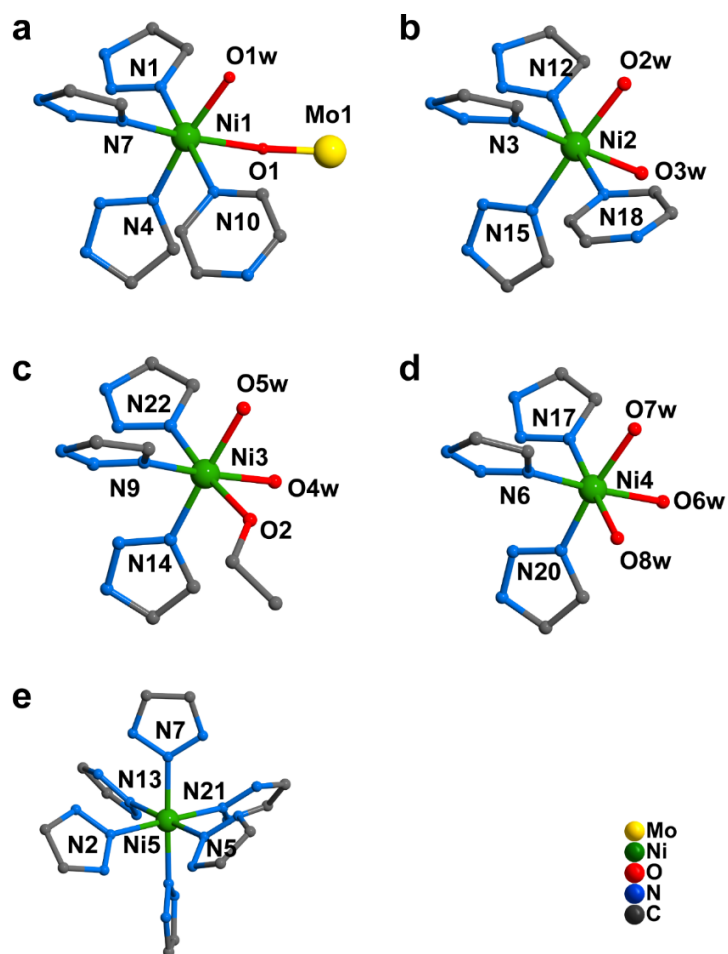


Fig. S5. The coordination environment of Ni ions in *d-OR*. Ni1, Ni2, Ni3 and Ni4 can be catalytic sites to reduce CO₂ due to the coordinated solvent molecules. All hydrogen atoms are omitted for clarity. Ni, green; Mo, yellow; C, gray; N, blue; O, red.

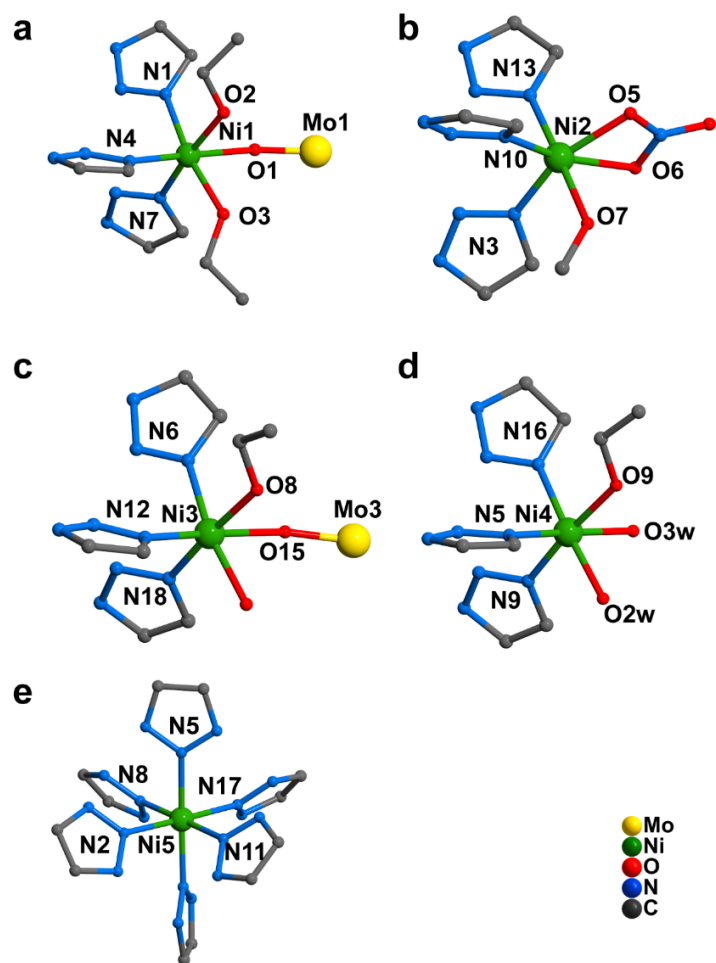


Fig. S6. The coordination environment of Ni ions in **a-OR**. It can be found that Ni1, Ni2, Ni3 and Ni4 can be catalytic sites of CO₂RR. Ni, green; Mo, yellow; C, gray; N, blue; O, red.

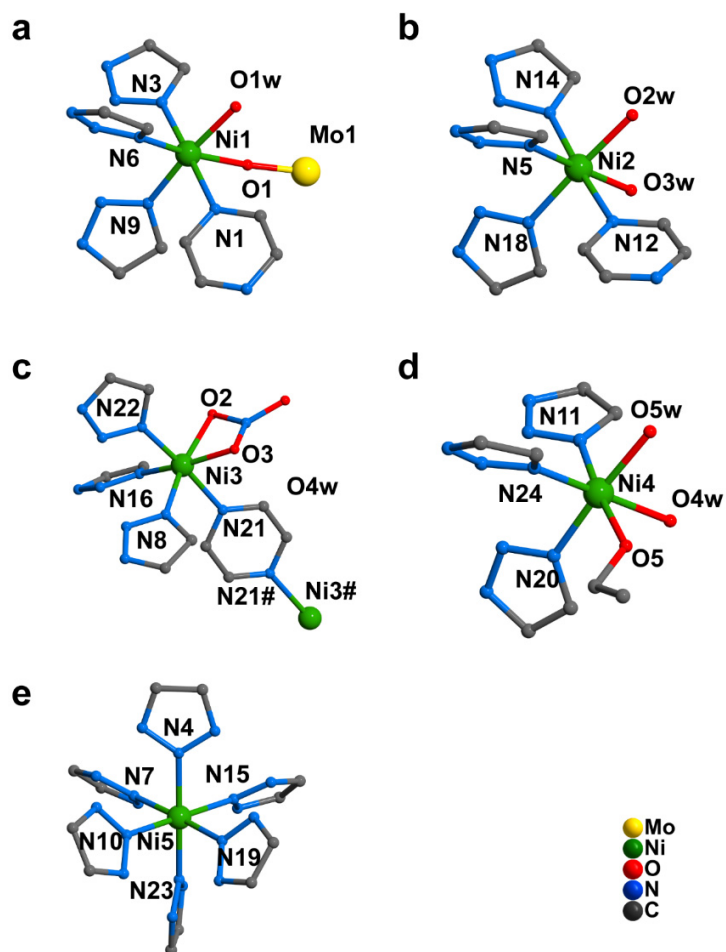


Fig. S7. The coordination environment of Ni ions in *s-OR*. It can be found that only Ni1, Ni2 and Ni4 can be catalytic sites of CO₂RR while Ni3 are six-coordinated without any solvent molecule. Ni, green; Mo, yellow; C, gray; N, blue; O, red

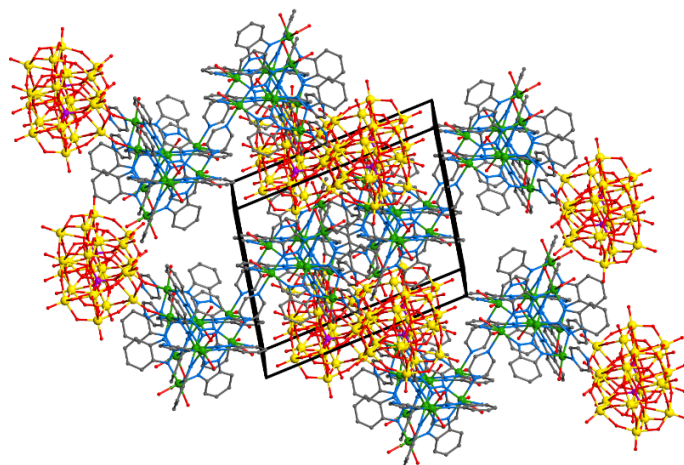


Fig. S8. Packing diagram of **s-OR**. Ni, green; Mo, yellow; P, purple; C, gray; N, blue; O, red.

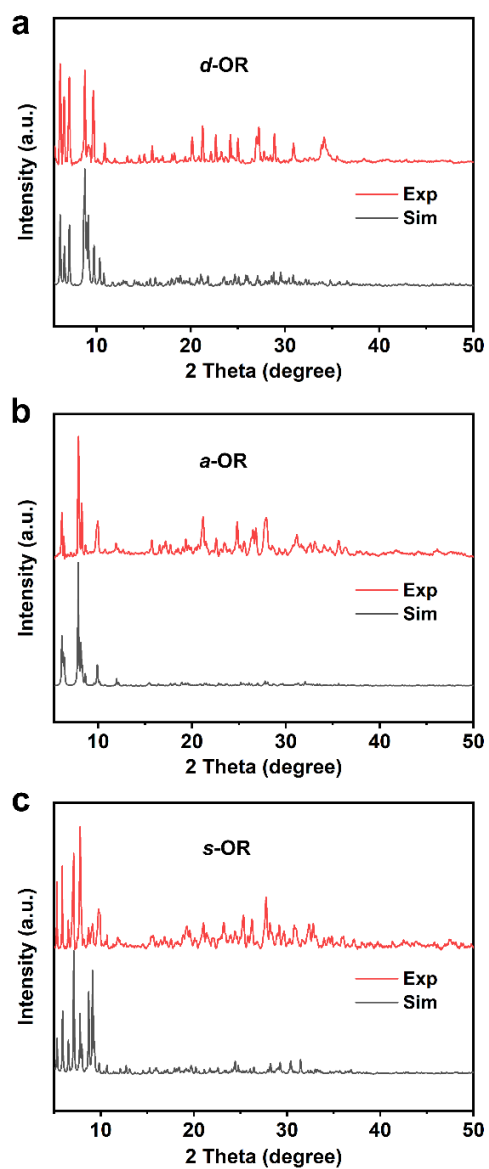


Fig. S9. The experimental and simulated PXRD patterns of **d-OR**, **a-OR** and **s-OR**. The well-matched curves suggest the purity of the samples, which provides the premise for the accuracy of subsequent characterization and performance tests.

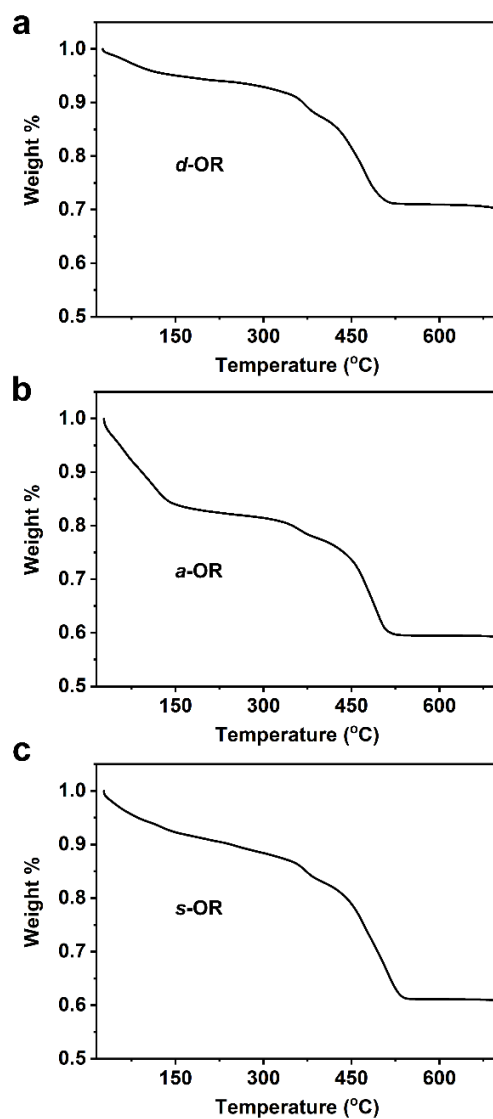


Fig. S10. Thermogravimetry curves of **a** *d*-OR; **b** *a*-OR and **c** *s*-OR measured in N₂/O₂ from room temperature to 700 °C at the heating rate of 20 °C·min⁻¹, respectively.

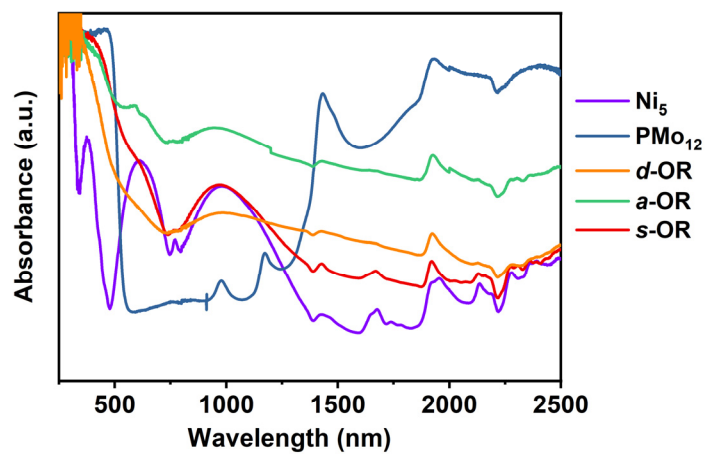


Fig. S11. The ultraviolet-visible-near infrared (Uv-Vis-NIR) absorption spectra of Ni_5 (purple), PMo_{12} (blue), $d\text{-OR}$ (yellow), $a\text{-OR}$ (green) and $s\text{-OR}$ (red) of the ranges from 250-2500 nm.

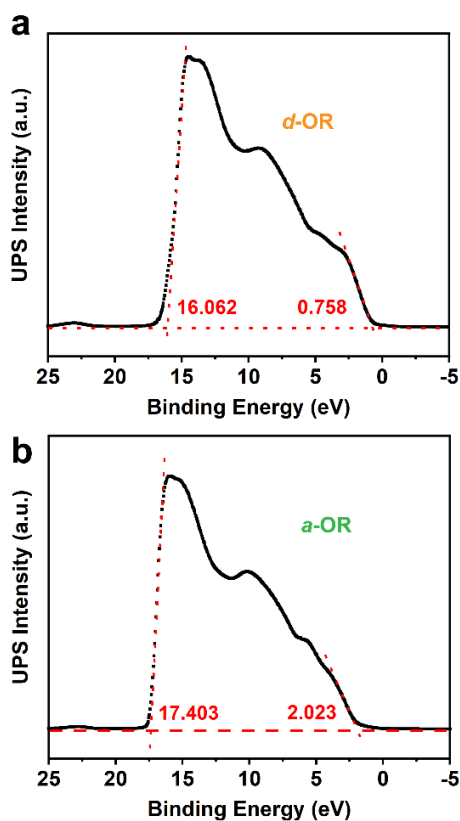


Fig. S12. The UPS spectra of **a. d-OR** and **b. a-OR**. In each figure, the horizontal red dotted line is the baseline. The other two red dotted lines are the tangent of the curve. The edges of the UPS spectrum are determined to be the intersection values of the tangents with the baseline. Then the width of the He I UPS spectra is calculated by the different of the two intersection values. The ionization potential (equivalent to the HOMO energy) is calculated by subtracting the width of the He I UPS spectra from the excitation energy (21.22 eV). Hereby, the HOMO of **d-OR** and **a-OR** are calculated to be -5.916 eV and -5.84 eV vs. Ev (vacuum level), related to 1.066 V and 0.99 V vs. normal hydrogen electrode (NHE, pH=7).

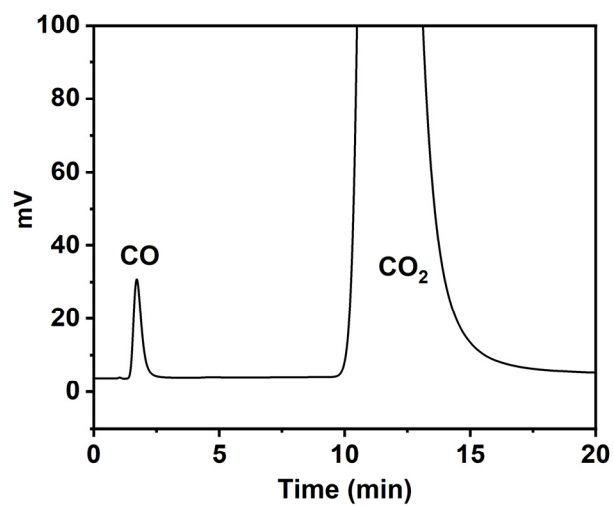


Fig. S13. GC analysis of the gaseous reaction products by using the FID (at the second run). Only CO was detected as the product.

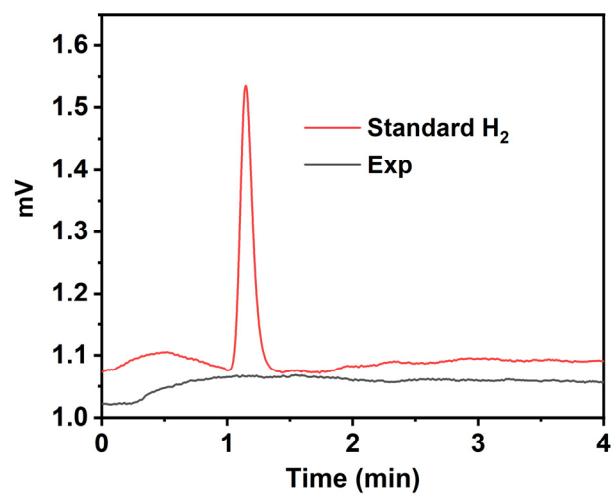


Fig. S14. GC analysis of the gaseous reaction products by using the TCD. There was no H₂ detected.

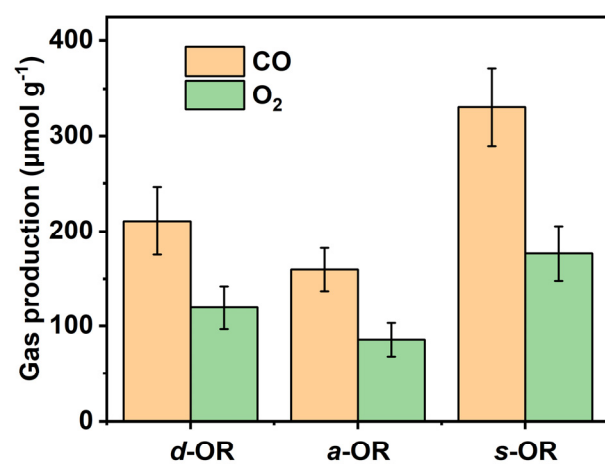


Fig. S15. The yields of CO and O₂ catalyzed by **d-OR**, **a-OR** and **s-OR** and detected on an online system.

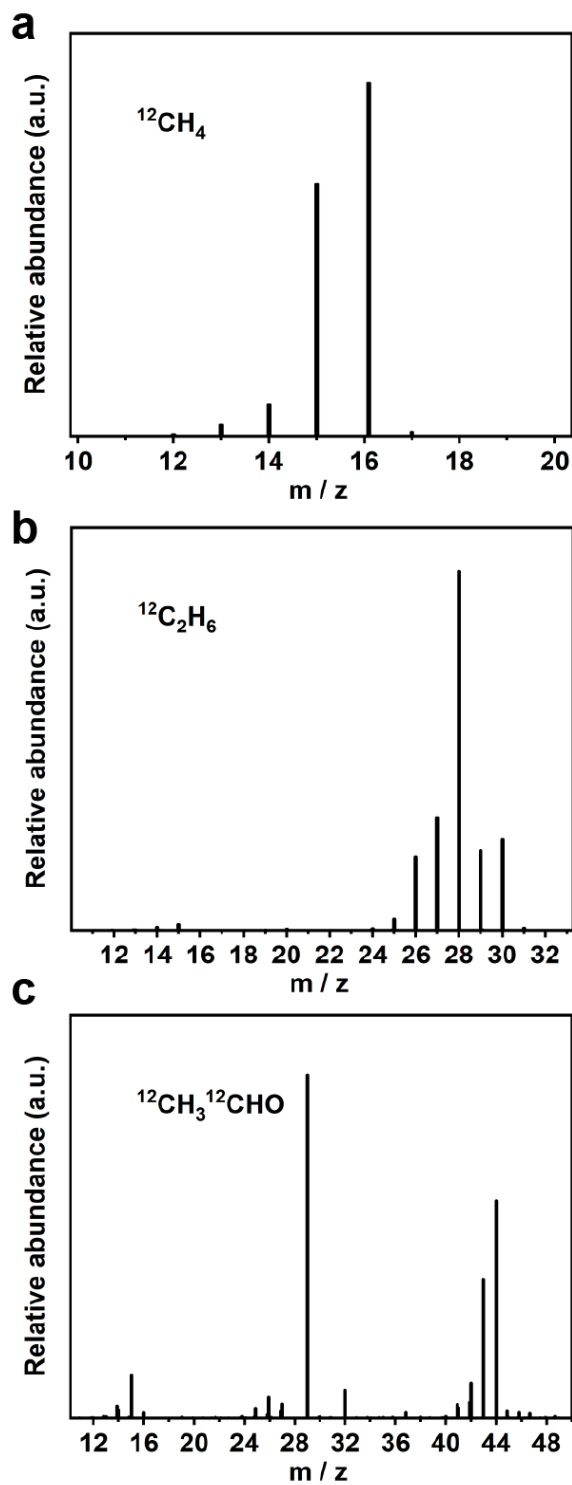


Fig. S16. Mass spectra extracted from GC-MS analysis of **a.** CH_4 ; **b.** C_2H_6 and **c.** CH_3CHO products from $^{13}\text{CO}_2$ reduction. Neither the produced CH_4 , C_2H_6 nor CH_3CHO is converted from CO_2 .

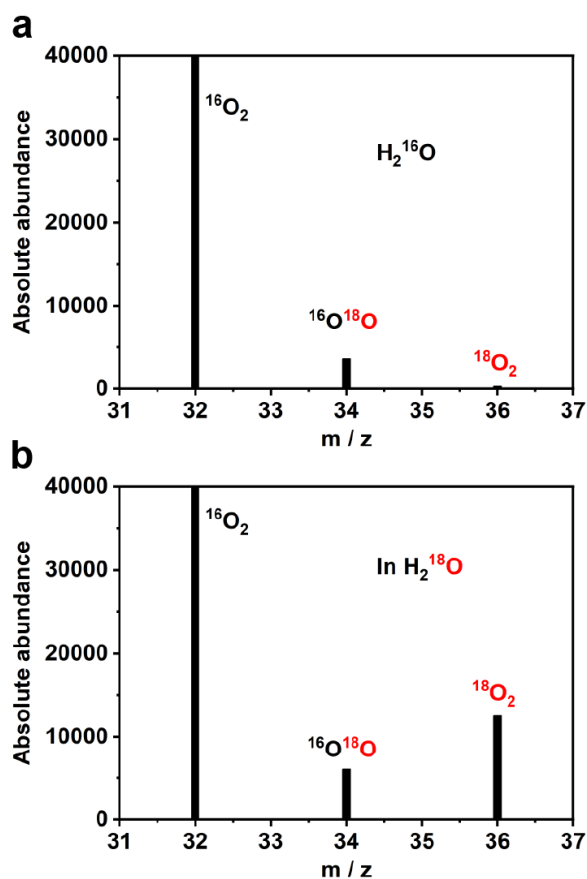


Fig. S17. Mass spectra extracted from GC-MS analysis of O₂ product from the photocatalytic reaction using **a.** H₂¹⁶O and **b.** H₂¹⁸O. When using H₂¹⁶O in reaction system, two weak signals at m/z 34 and 36 corresponding to ¹⁶O¹⁸O and ¹⁸O₂ could be observed because of the natural existence of isotopic ¹⁸O. When the reaction was performed using H₂¹⁸O, the signals at m/z 34 and 36 were obviously enhanced. The abundance of ¹⁸O₂ using H₂¹⁸O as reactant was near 50 times than that of using H₂¹⁶O, which proved that the O₂ product was indeed convert from H₂O.

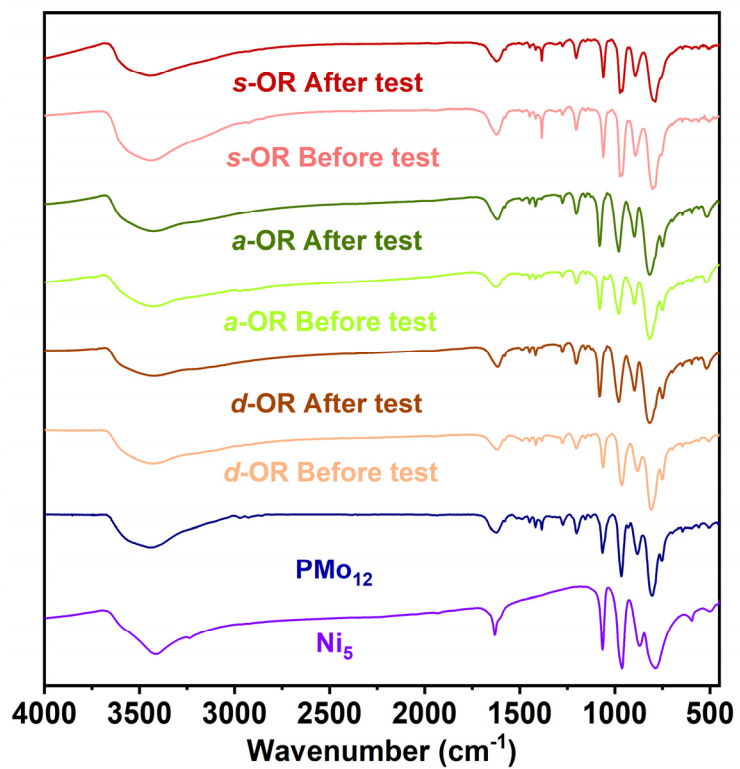


Fig. S18. The FTIR spectra for Ni₅ (purple), PMo₁₂ (blue) and FTIR spectra for *d*-OR, *a*-OR and *s*-OR before and after catalysis.

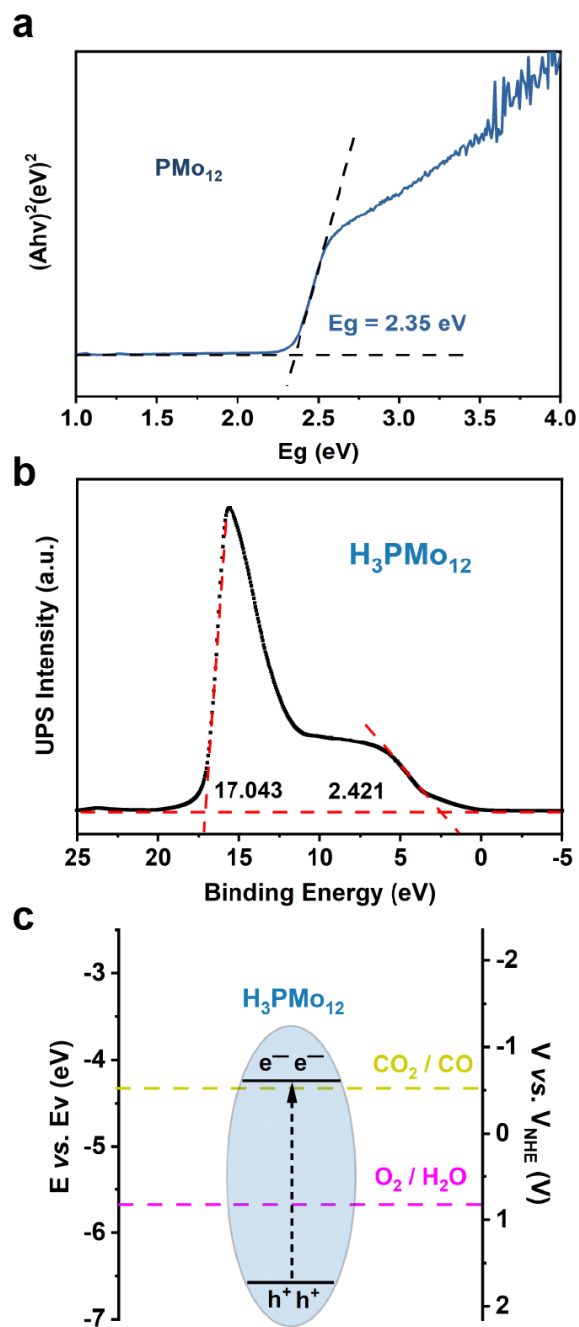


Fig. S19. a. band gap b. UPS spectrum and c. band structure of PMo_{12} .

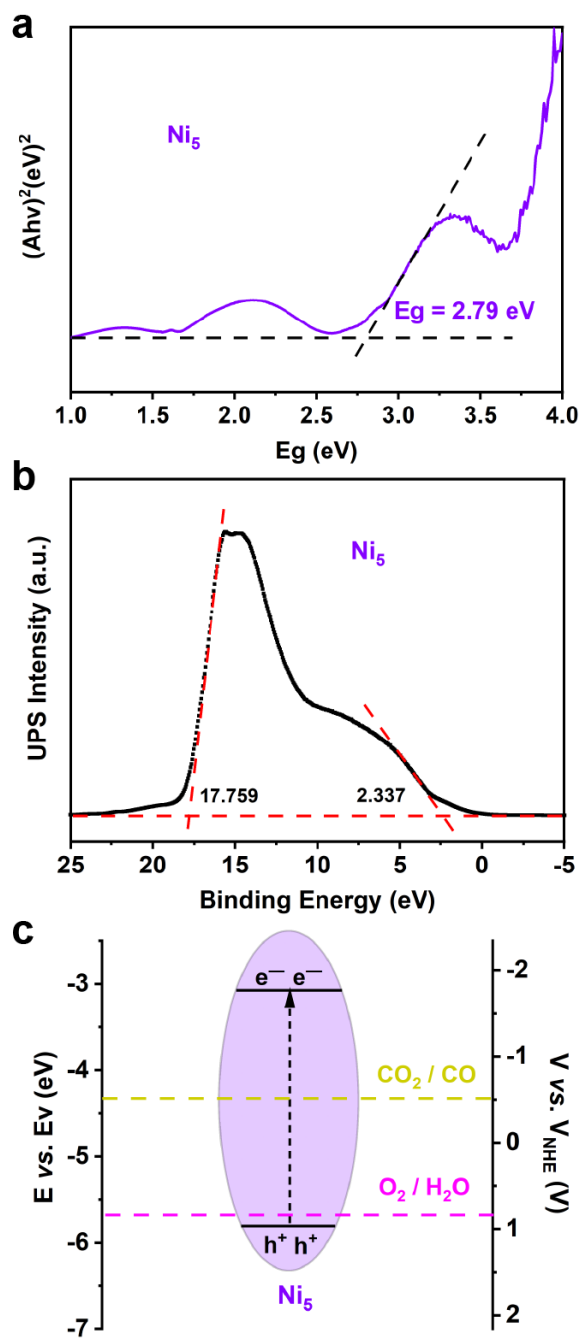


Fig. S20. a. band gap b. UPS spectrum and c. band structure of Ni_5 .

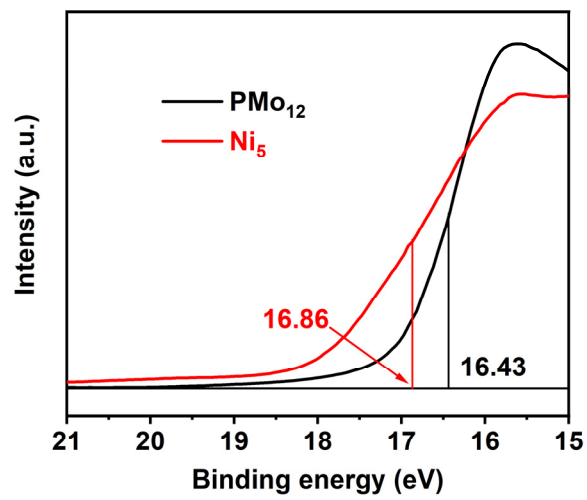


Fig. S21. Photoemission cutoff of PMo_{12} and Ni_5 obtained from UPS. The Fermi level for PMo_{12} and Ni_5 is calculated to be 4.36 eV and 4.79 eV respectively.

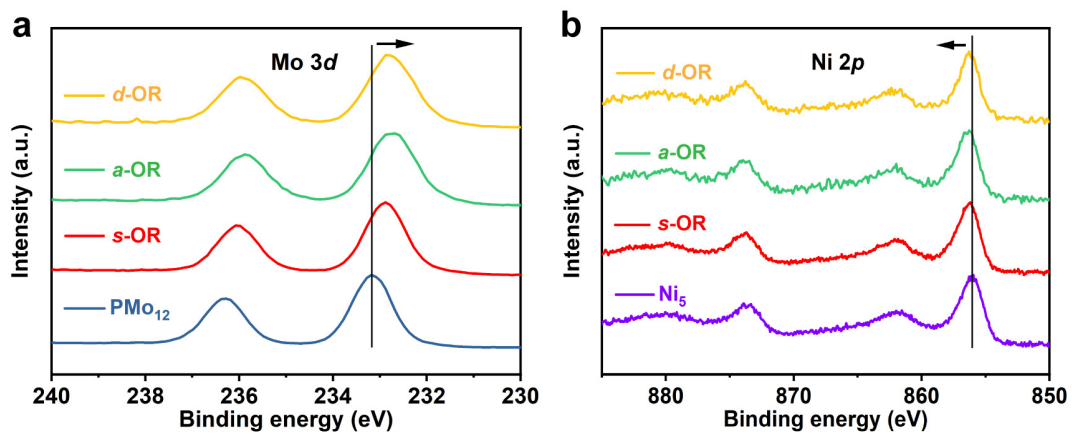


Fig. S22. High-resolution a. Mo 3d and b. Ni 2p XPS spectra of **d-OR**, **a-OR**, **s-OR**, **P_{Mo}₁₂** and **Ni₅**. The positive shift in Mo 3d and the negative shift in Ni 2p of **d-OR**, **a-OR** and **s-OR** reveal that electrons of **Ni₅** transfer to **P_{Mo}₁₂** when they connect together through a bridging O atom.

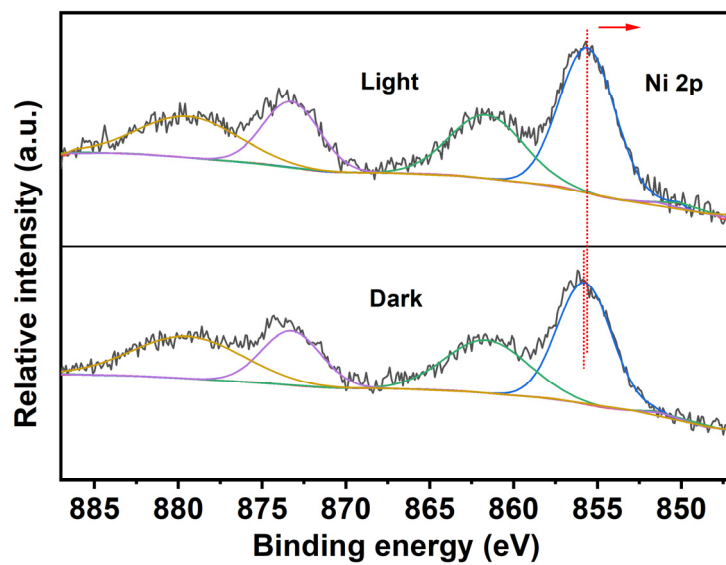


Fig. S23. High-resolution in-situ XPS for Ni 2p of *d*-OR in the dark and under light irradiation.

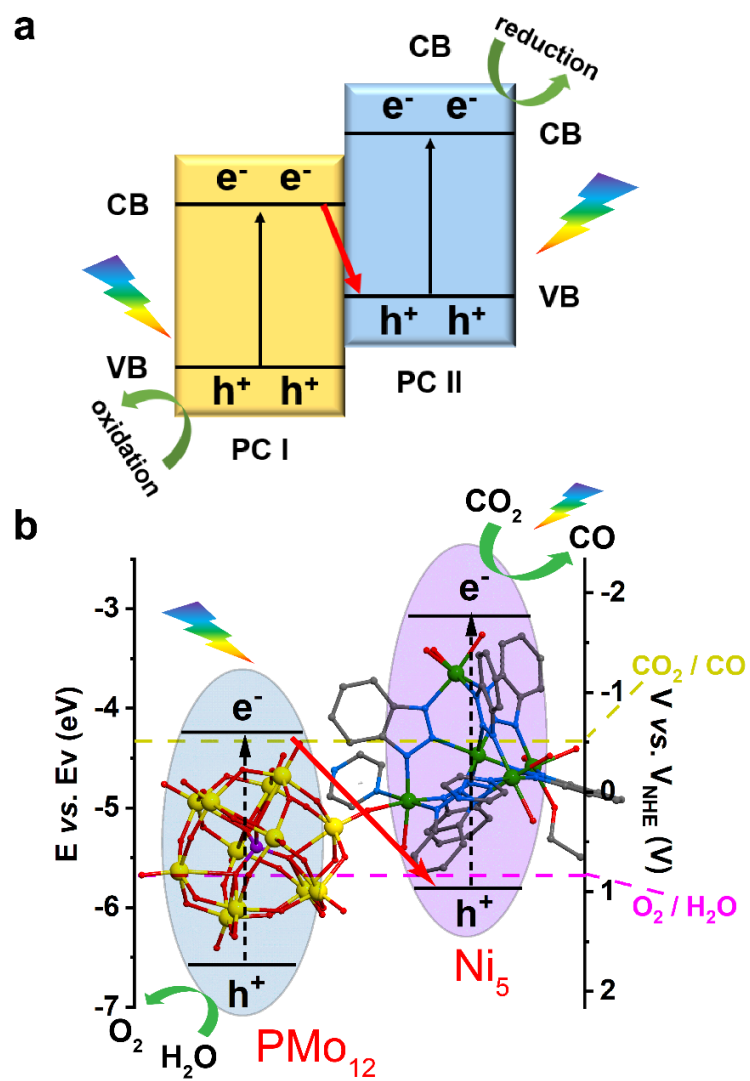


Fig. S24. Schematic diagram of electron transfer in **a.** Z-scheme heterojunction and **b.** OR molecule junction.

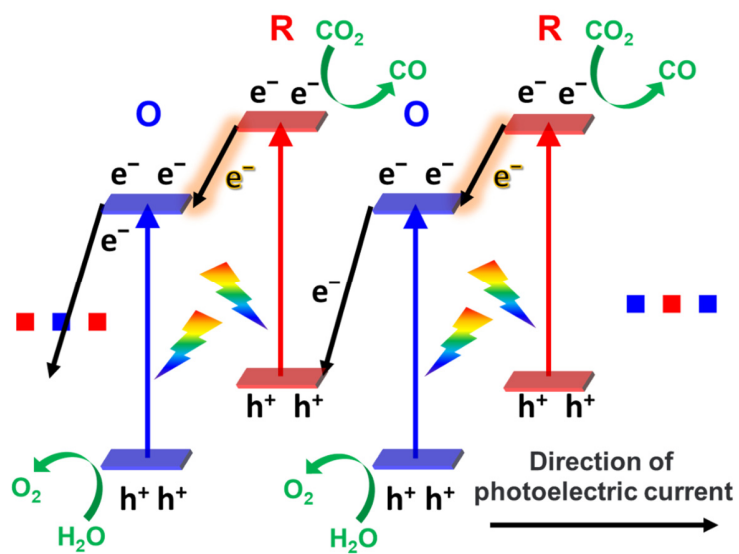


Fig. S25. Proposed charge transfer in a-OR photocatalyst.

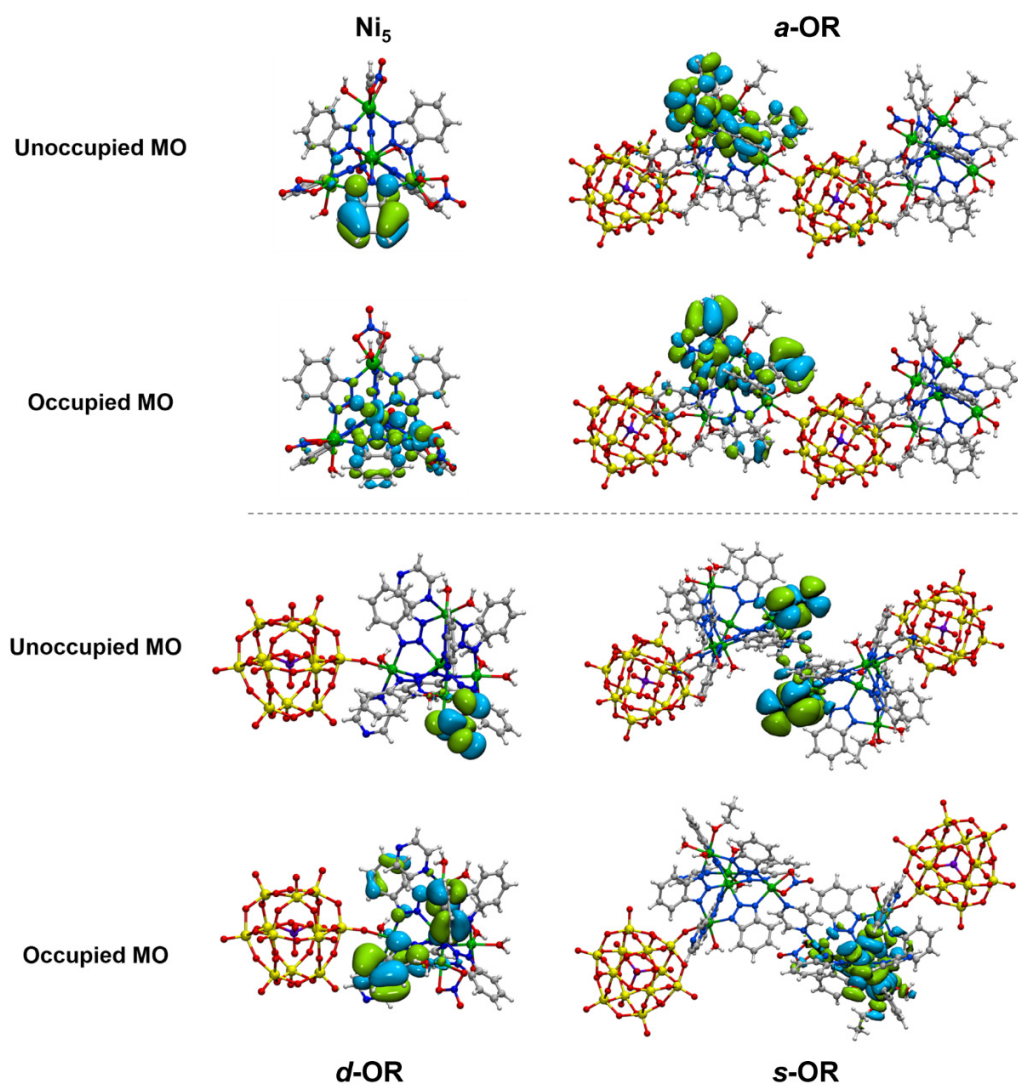


Fig. S26. Frontier molecular orbitals of Ni-cluster moieties of **Ni₅**, **d-OR**, **a-OR**, and **s-OR** marked in **Fig. 4e**.

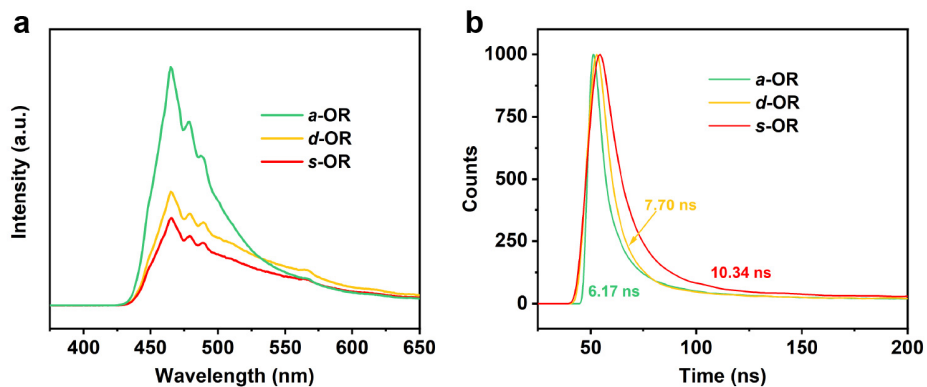


Fig. S27. **a.** PL emissions of **d-OR**, **a-OR** and **s-OR** under excitation at 365 nm. The PL intensity of **s-OR** is weaker than **d-OR** and much weaker than **a-OR**, which indicates that **s-OR** has the weakest efficiency of electron-hole recombination. **b.** Decay curves of **d-OR**, **a-OR** and **s-OR** by using 365 nm laser irradiation.

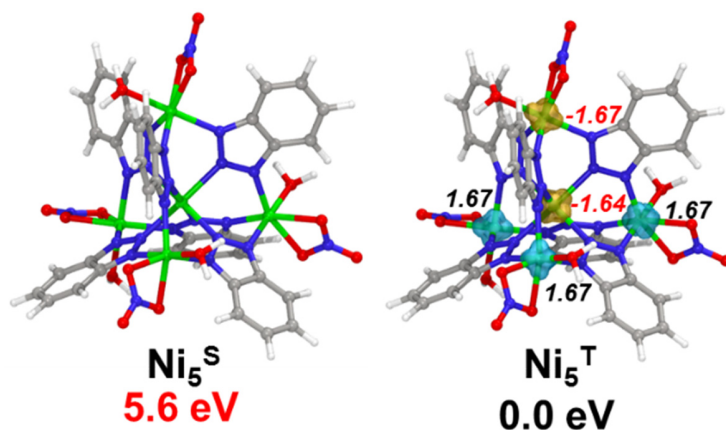


Fig. S28. Structures of triplet and singlet Ni_5 complexes. The Gibbs free energies relative to the most stable Ni_5^{T} conformation are given in eV. White, gray, purple, red and green spheres represent H, C, N, O and Ni atoms, respectively. To identify the stable catalytic activity species, we investigated the different spin states of the Ni_5 complex using unrestricted open-shell DFT at the same level, respectively. The triplet state Ni_5^{T} is proved more stable, which is consistent with the previous experimental reports. (The Ni_5 mentioned in this paper corresponded triplet Ni_5^{T})

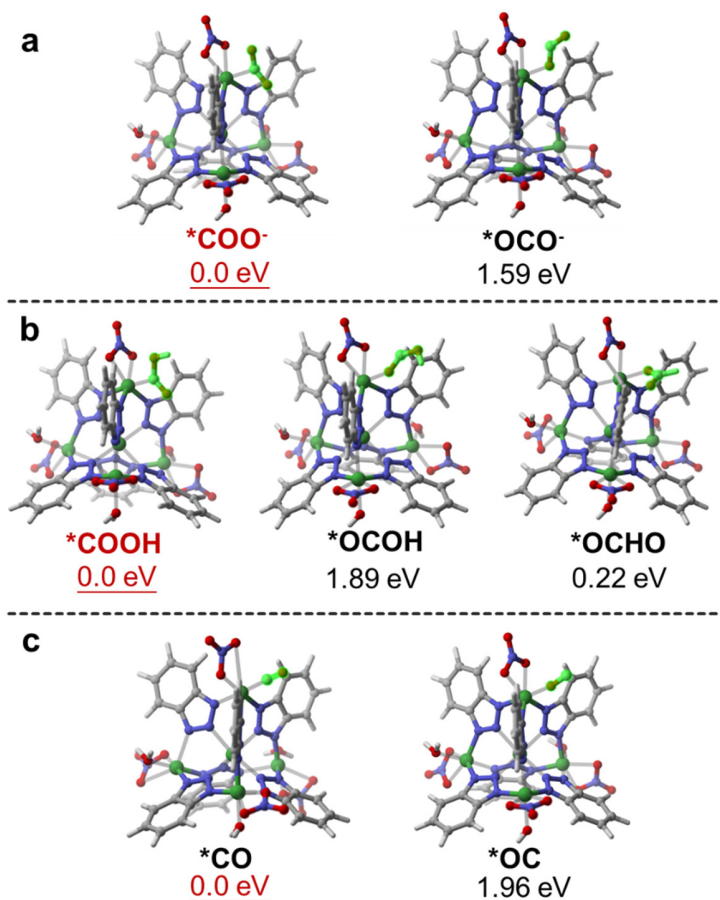


Figure S29. Evaluations of adsorption possibilities of active species. The Gibbs free energies are given in eV. White, gray, purple, red and green spheres represent H, C, N, O and Ni atoms, respectively. The results show that the intermediates *COO⁻, *COOH and *CO are more stable.

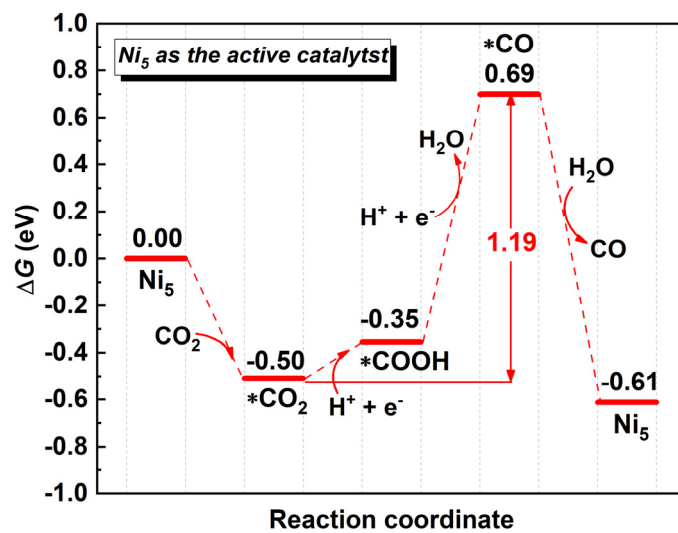


Fig. S30. Gibbs energy profile for the CO_2 reduction process to CO production with the natural Ni_5 as the catalytic center.

Table S1. Crystal data and structure refinement of **d-OR**, **a-OR** and **s-OR**.

	d-OR	a-OR	s-OR
Empirical formula	C ₄₈ H ₇₃ Mo ₁₂ N ₂₃ Ni ₅ O ₆₀ P	C ₁₀₀ H ₁₄₇ Mo ₂₄ N ₃₈ Ni ₁₀ O ₁₁₀ P ₂	C ₁₀₀ H ₁₁₂ Mo ₂₄ N ₄₈ Ni ₁₀ O ₁₀₀ P ₂
Formula weight	3408.09	6593.15	6537.97
Crystal system	triclinic	monoclinic	triclinic
Space group	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1
a (Å)	15.2675(4)	22.668(5)	15.4976(6)
b (Å)	19.4380(5)	17.901(4)	19.5345(7)
c (Å)	19.8495(5)	30.223(8)	21.2881(8)
α (°)	114.2540(10)	90	66.957(2)
β (°)	105.7230(10)	107.304(4)	74.645(2)
γ (°)	94.1390(10)	90	85.217(2)
V (Å³)	5055.6(2)	11709(5)	5717.3(4)
Z	2	2	1
D_{calc}(g·cm⁻³)	2.239	1.870	1.899
Abs.coeff. (mm⁻¹)	13.630	2.119	11.992
F(000)	3322.0	6422.0	3166.0
Reflns collected	51291	106272	88520
Data/restraints /parameters	20287/12/1365	26837/46/1308	25110/21/1287
GO_Fon F²	1.047	1.011	0.985
R_{int}	0.0416	0.0469	0.0780
R₁^a	0.1235	0.0924	0.0825
wR₂(all data)^b	0.2016	0.1323	0.1623

$$^a R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|} \quad ^b wR_2 = \frac{\sum w(|F_o|^2 - |F_c|^2)}{\sum w(F_o^2)^{1/2}}$$

Table S2. Selected bond distance (Å) of **d-OR**.

Atom1	Atom2	Distance (Å)	Atom1	Atom2	Distance (Å)
Mo1	O1	1.696(8)	Ni3	O2	2.123(11)
Mo1	O3	1.839(8)	Ni3	O4w	2.078(11)
Mo1	O13	1.980(9)	Ni3	O5w	2.079(11)
Mo1	O20	1.823(9)	Ni3	N9	2.063(11)
Mo1	O27	2.004(9)	Ni3	N14	2.034(11)
Mo1	O40	2.380(8)	Ni3	N22	2.035(11)
Ni1	O1	2.250(8)	Ni4	O6w	2.063(9)
Ni1	O1w	2.075(9)	Ni4	O7w	2.100(9)
Ni1	N1	2.042(10)	Ni4	O8w	2.109(8)
Ni1	N4	2.035(10)	Ni4	N6	2.050(10)
Ni1	N7	2.037(11)	Ni4	N17	2.067(10)
Ni1	N10	2.147(10)	Ni4	N20	2.016(12)
Ni2	O2W	2.124(10)	Ni5	N2	2.160(9)
Ni2	O3W	2.128(10)	Ni5	N5	2.120(10)
Ni2	N3	2.057(9)	Ni5	N8	2.103(11)
Ni2	N12	2.062(11)	Ni5	N13	2.129(10)
Ni2	N15	2.058(10)	Ni5	N16	2.125(10)
Ni2	N18	2.107(13)	Ni5	N21	2.123(10)

Table S3. Selected bond distance (Å) of **a-OR**.

Atom1	Atom2	Distance (Å)	Atom1	Atom2	Distance (Å)
Mo1	O1	1.702(4)	Ni3	O1w	2.084(4)
Mo1	O12	1.887(4)	Ni3	O8	2.115(4)
Mo1	O22	1.936(4)	Ni3	O15 ¹	2.198(4)
Mo1	O23	1.898(4)	Ni3	N6	2.040(5)
Mo1	O35	1.900(4)	Ni3	N12	2.021(5)
Mo1	O48	2.396(4)	Ni3	N18	2.045(5)
Ni1	O1	2.177(4)	Ni4	O2w	2.102(4)
Ni1	O2	2.106(4)	Ni4	O3w	2.106(4)
Ni1	O3	2.116(4)	Ni4	O9	2.132(4)
Ni1	N1	2.045(5)	Ni4	N9	2.049(5)
Ni1	N4	2.030(5)	Ni4	N15	2.054(5)
Ni1	N7	2.039(4)	Ni4	N16	2.067(5)
Ni2	O5	2.138(5)	Ni5	N2	2.111(5)
Ni2	O6	2.116(5)	Ni5	N5	2.144(4)
Ni2	O7	2.167(4)	Ni5	N8	2.129(4)
Ni2	N3	2.008(5)	Ni5	N11	2.125(5)
Ni2	N10	2.003(5)	Ni5	N14	2.148(5)
Ni2	N13	2.051(5)	Ni5	N17	2.102(4)

¹+X, -1+Y, +Z

Table S4. Selected bond distance (Å) of **s-OR**.

Atom1	Atom2	Distance (Å)	Atom1	Atom2	Distance (Å)
Mo1	O1	1.703(4)	Ni3	O2	2.123(7)
Mo1	O6	1.846(4)	Ni3	O3	2.084(6)
Mo1	O16	1.954(4)	Ni3	N8	2.034(5)
Mo1	O22	1.827(5)	Ni3	N16	2.014(6)
Mo1	O29	1.998(4)	Ni3	N17	2.430(13)
Mo1	O42	2.395(4)	Ni3	N21	2.207(6)
Ni1	O1	2.207(5)	Ni3	N22	2.064(5)
Ni1	O1w	2.067(4)	Ni4	O4w	2.115(5)
Ni1	N1	2.154(5)	Ni4	O5	2.096(4)
Ni1	N3	2.053(5)	Ni4	O5w	2.101(5)
Ni1	N6	2.049(6)	Ni4	N20	2.065(5)
Ni1	N9	2.053(5)	Ni4	N24	2.039(6)
Ni2	O2w	2.078(5)	Ni5	N4	2.125(5)
Ni2	O3w	2.120(6)	Ni5	N7	2.103(5)
Ni2	N5	2.083(5)	Ni5	N10	2.123(5)
Ni2	N12	2.109(6)	Ni5	N15	2.105(5)
Ni2	N14	2.038(6)	Ni5	N19	2.110(5)
Ni2	N18	2.059(5)	Ni5	N23	2.143(5)

Table S5. The CO yield under different experimental conditions catalyzed by **d-OR**, **a-OR** and **s-OR**.

entry	d-OR ($\mu\text{mol/g}$)	a-OR ($\mu\text{mol/g}$)	s-OR ($\mu\text{mol/g}$)
1	202.88	150.12	291.25
2	152.70	112.19	238.68
3	49.45	28.75	46.19
4	n.d. ^(a)	n.d.	n.d.
5	47.18	29.43	49.11
6	n.d.	n.d.	n.d.
7	n.d.	n.d.	n.d.
8	n.d.		
9	2447.13	1703.69	3779.15

1. 10 mg photocatalysts, CO₂ (1 atm), H₂O (0.3 mL), 10 hours, under irradiation. (The CO yield in the first run)

2. 10 mg photocatalysts, CO₂ (1 atm), H₂O (0.3 mL), 10 hours, under irradiation. (The average CO yield in the next four runs)

3. 10 mg photocatalysts, Ar (1 atm), H₂O (0.3 mL), 10 hours, under irradiation. (The CO yield in the first run)

4. 10 mg photocatalysts, Ar (1 atm), H₂O (0.3 mL), 10 hours, under irradiation. (The CO yield in the second run)

5. 10 mg photocatalysts, CO₂ (1 atm), without H₂O, 10 hours, under irradiation. (The CO yield in the first run)

6. 10 mg photocatalysts, CO₂ (1 atm), without H₂O, 10 hours, under irradiation. (The CO yield in the second run)

7. 10 mg photocatalysts, CO₂ (1 atm), H₂O (0.3 mL), 10 hours, in dark.

8. no photocatalyst, CO₂ (1 atm), H₂O (0.3 mL), 10 hours, under irradiation.

9. 10 mg photocatalysts, CO₂ (1 atm), H₂O (0.3 mL), 200 hours, under irradiation. (The photocatalysts were pretreated by irradiating for 10 h)

^(a) n.d. = Not detectable

Table S6. Fitted lifetimes of the fluorescence decay profiles of **d-OR**, **a-OR** and **s-OR**.

	A1 %	T1 / ns	A2 %	T2 / ns
d-OR	80.14	6.80	19.68	109.66
a-OR	75.11	6.05	24.89	50.36
s-OR	82.15	9.84	17.85	119.59

Table S7. XYZ structure files for the structures mentioned in **Fig. S29**.

Ni₅^S			
Ni	-0.0112173	-0.0228114	-0.0192959
Ni	2.7383127	0.4543346	-2.3589689
O	3.5521707	1.7976566	-3.9165749
O	4.8112057	0.9681006	-2.3848599
O	5.6919077	2.1906096	-3.9546829
O	3.2485817	-1.0565774	-3.7605299
N	2.1938387	1.9452466	-1.0397549
N	1.2909447	1.6918086	-0.1068089
N	1.0704077	2.7411336	0.6555961
N	-0.1952013	0.1320926	-2.1097489
N	0.8227477	0.2369786	-2.9378329
N	4.7194977	1.6663286	-3.4461589
C	2.5904697	3.2442276	-0.8913569
C	3.5009497	4.0662496	-1.5969819
H	4.0455387	3.7298426	-2.4743569
C	3.6570807	5.3660886	-1.1482959
H	4.3504287	6.0286316	-1.6727469
C	2.9321577	5.8750486	-0.0346719
H	3.0881057	6.9135896	0.2681781
C	2.0271227	5.0917596	0.6570581
H	1.4427047	5.4814386	1.4898621
C	1.8664277	3.7577946	0.2128961
C	0.3261337	0.3131236	-4.2061229
C	0.9502757	0.4461046	-5.4666499
H	2.0343847	0.5059916	-5.5522409
C	0.1129267	0.4952786	-6.5675329
H	0.5460647	0.5989166	-7.5657829
Ni	-3.1414013	-0.1776414	-1.8722199
Ni	-0.1166803	2.7717626	2.3129181
Ni	0.4907307	-3.1078234	1.8490741
O	-4.2077333	-1.3124684	-3.4110379
O	-1.2175473	3.5342526	4.0202561
O	1.8149177	-4.2871424	3.1943391
O	-5.2253083	-0.7131414	-1.6152249
O	-0.6320623	4.8763516	2.4461391
O	0.9899757	-5.1261934	1.3949251
O	-1.6040403	5.6663926	4.2258351
O	2.1940207	-6.3743654	2.7061711
O	-6.3308813	-1.7344124	-3.1864189
O	-3.8699273	1.4904006	-2.9695879
O	1.5855797	3.3129366	3.4698621
O	-0.9931323	-3.9058344	3.1356351
N	-2.4008033	-1.8283864	-0.8852969

N	-1.7941153	2.2143906	1.2520101
N	1.9561097	-2.3556604	0.6199391
N	1.6930947	-1.3207154	-0.1613719
N	-1.3354643	-1.6991414	-0.1097719
N	-1.6920933	1.2781396	0.3234411
N	2.7331827	-0.9850784	-0.8934879
N	-2.8449643	1.0524466	-0.2697649
N	-1.0225873	-2.8293294	0.4847241
N	0.1816307	-0.1794134	2.0921011
N	-1.3444113	0.1331306	-2.7505959
N	0.1952657	0.8562456	2.9038461
N	0.3257317	-1.3118644	2.7504971
N	-5.2938963	-1.2639104	-2.7580609
N	-1.1606953	4.7280976	3.5916911
N	1.6804877	-5.3030774	2.4476491
C	-3.0960893	2.6286746	1.2813061
C	3.2555577	-2.7178864	0.4022891
C	-2.8090793	-3.1301134	-0.8088479
C	-3.7979663	3.5749616	2.0652511
C	4.0920247	-3.7127764	0.9614581
C	-3.8540333	-3.8564274	-1.4283489
H	-3.3316873	4.1470166	2.8625771
H	3.7689067	-4.3738974	1.7614471
H	-4.5295983	-3.4169054	-2.1567279
C	-5.1477243	3.7343456	1.8019191
C	5.3874267	-3.7900784	0.4792281
C	-3.9701943	-5.1960474	-1.1002279
H	-5.7212973	4.4540556	2.3916071
H	6.0626897	-4.5442354	0.8913231
H	-4.7631703	-5.7887434	-1.5636579
C	-5.8181643	2.9837016	0.7951721
C	5.8758807	-2.9084034	-0.5261279
C	-3.0831853	-5.8323684	-0.1862349
H	-6.8867843	3.1488536	0.6358281
H	6.9101027	-3.0131934	-0.8640209
H	-3.2237343	-6.8938154	0.0338961
C	-5.1507733	2.0463566	0.0285701
C	5.0786117	-1.9170264	-1.0675149
C	-2.0478693	-5.1422664	0.4154661
H	-5.6548273	1.4484326	-0.7299579
H	5.4493817	-1.2177604	-1.8171999
H	-1.3536683	-5.6143384	1.1082661
C	-3.7726103	1.8784136	0.2885361
C	3.7529947	-1.8330204	-0.5857519
C	-1.9201293	-3.7740864	0.0864021
C	-1.0814513	0.2428356	-4.0833379

C	0.3557097	0.3912436	4.1763951
C	0.4505017	-1.0157054	4.0749591
C	-1.9270763	0.2888406	-5.2140639
C	0.6488557	-1.8250834	5.2150581
C	0.4334947	1.0490516	5.4234841
H	-3.0092293	0.2302686	-5.1048529
H	0.7502287	-2.9068914	5.1326621
H	0.3543677	2.1335796	5.4887931
C	-1.3053763	0.4152916	-6.4436729
C	0.7276587	-1.1710094	6.4324881
C	0.6165517	0.2462046	6.5358101
H	-1.9134153	0.4570976	-7.3511789
H	0.6844307	0.7071416	7.5246521
H	0.8844147	-1.7530694	7.3443441
H	1.8247497	4.2546686	3.4596691
H	2.3900707	2.8505946	3.1805561
H	4.1856677	-1.3121364	-3.7832859
H	2.7686027	-1.8874604	-3.6058049
H	-1.6565853	-3.2493024	3.4066421
H	-0.6692373	-4.2932534	3.9651861
H	-3.4151903	2.3209506	-2.7515549
H	-4.8156843	1.6967866	-2.8887209

Ni₅T

Ni	-0.0084909	0.0106254	0.0096076
Ni	2.7957891	-0.2906446	2.2968356
O	3.5906171	-1.5702266	3.8360276
O	4.8813011	-0.7919316	2.3242466
O	5.7124471	-1.9606406	3.9388116
O	3.3213491	1.2708384	3.6335586
N	2.2519431	-1.8596496	1.0603306
N	1.3157621	-1.6694706	0.1526926
N	1.0970591	-2.7507016	-0.5561884
N	-0.1501439	-0.0509436	2.1324966
N	0.8868771	-0.1058836	2.9348936
N	4.7631251	-1.4534986	3.3911976
C	2.6731571	-3.1510246	0.9504906
C	3.6255881	-3.9223676	1.6520766
H	4.2068011	-3.5365976	2.4886166
C	3.7871341	-5.2322946	1.2564586
H	4.5137961	-5.8591086	1.7814926
C	3.0325151	-5.8011716	0.1983866
H	3.1989531	-6.8498336	-0.0649154
C	2.0927901	-5.0683076	-0.4907054
H	1.4916401	-5.5037416	-1.2926674
C	1.9250301	-3.7246486	-0.0984794
C	0.4246661	-0.1332596	4.2127776
C	1.0824771	-0.2013526	5.4578356
H	2.1711101	-0.2478376	5.5241436
C	0.2804271	-0.2063476	6.5779746
H	0.7433091	-0.2592896	7.5678756
Ni	-3.0834999	0.2007994	1.9307416
Ni	-0.1135679	-2.8757366	-2.1822564
Ni	0.3691881	3.0077884	-1.9996034
O	-4.0747659	1.3952794	3.4224896
O	-1.2439119	-3.7230966	-3.8054184
O	1.6675411	4.0089194	-3.3882324
O	-5.1619829	0.7105854	1.7174406
O	-0.6323959	-4.9594776	-2.1757574
O	0.8649311	5.0875674	-1.7298074
O	-1.6612409	-5.8413576	-3.8573954
O	2.0615551	6.1241614	-3.1982474
O	-6.1922959	1.7928394	3.2769536
O	-3.7832429	-1.4254146	3.0977966
O	1.5615931	-3.4629666	-3.3401864
O	-1.1680009	3.7050314	-3.2814524
N	-2.3800809	1.8300564	0.8653316
N	-1.7900049	-2.2785006	-1.1270604
N	1.8905311	2.3502444	-0.7591054

N	1.6695041	1.3451344	0.0618786
N	-1.3498609	1.6802634	0.0575266
N	-1.6764149	-1.3135026	-0.2385934
N	2.7269781	1.0656364	0.7868896
N	-2.8134939	-1.0740706	0.3706966
N	-1.0697969	2.7877294	-0.5863544
N	0.1374611	0.0681884	-2.1152104
N	-1.2789359	-0.0382406	2.8011326
N	0.1518091	-0.9992686	-2.8769804
N	0.2445801	1.1682874	-2.8202464
N	-5.1811489	1.3102584	2.8262366
N	-1.1886129	-4.8774786	-3.3042294
N	1.5414261	5.1136944	-2.7898904
C	-3.0845259	-2.7033426	-1.1093644
C	3.1775661	2.7569284	-0.5743854
C	-2.8029319	3.1205284	0.7553016
C	-3.7936509	-3.6823706	-1.8392044
C	3.9712341	3.7584604	-1.1753994
C	-3.8299239	3.8574564	1.3851696
H	-3.3411559	-4.2903536	-2.6217564
H	3.6144141	4.3976464	-1.9829074
H	-4.4800629	3.4368314	2.1515226
C	-5.1311559	-3.8379076	-1.5464634
C	5.2666181	3.8870154	-0.7233504
C	-3.9695719	5.1780234	1.0183816
H	-5.7102759	-4.5863956	-2.0950834
H	5.9111061	4.6501664	-1.1692904
H	-4.7521419	5.7799364	1.4895366
C	-5.7867739	-3.0507496	-0.5652004
C	5.7991691	3.0510354	0.2918576
C	-3.1230999	5.7879994	0.0566876
H	-6.8530799	-3.2129996	-0.3828384
H	6.8380741	3.1941224	0.6030576
H	-3.2807499	6.8414104	-0.1928564
C	-5.1150559	-2.0837286	0.1483516
C	5.0449981	2.0598824	0.8789906
C	-2.1081809	5.0898294	-0.5576864
H	-5.6191819	-1.4570276	0.8873786
H	5.4565511	1.3958924	1.6428666
H	-1.4462469	5.5531994	-1.2915784
C	-3.7441259	-1.9227146	-0.1371004
C	3.7154531	1.9257274	0.4302646
C	-1.9571849	3.7371484	-0.1902724
C	-0.9809659	-0.0840916	4.1262806
C	0.2701211	-0.5893116	-4.1673254
C	0.3368141	0.8180164	-4.1296244

C	-1.7912629	-0.0817926	5.2801306
C	0.4824381	1.5806694	-5.3062344
C	0.3246331	-1.2952736	-5.3863494
H	-2.8801279	-0.0316346	5.2081516
H	0.5604321	2.6701254	-5.2723464
H	0.2662391	-2.3851806	-5.4161164
C	-1.1365029	-0.1430606	6.4910296
C	0.5389701	0.8793454	-6.4913194
C	0.4559791	-0.5384266	-6.5303064
H	-1.7197859	-0.1438666	7.4166956
H	0.5033571	-1.0399936	-7.5015274
H	0.6540651	1.4248344	-7.4326804
H	1.7841971	-4.4064306	-3.3718454
H	2.3863521	-3.0213586	-3.0832754
H	4.2586631	1.5162564	3.6801486
H	2.8579851	2.1023914	3.4452856
H	-1.8412709	3.0328154	-3.4720344
H	-0.9127009	4.0543444	-4.1491914
H	-3.3115319	-2.2554846	2.9247246
H	-4.7230769	-1.6585846	3.0381436

Ni₅⁻

Ni	0.0094906	-0.0480790	0.0406497
Ni	0.1406086	-2.0018860	3.0282017
O	-0.7971064	-2.3956670	4.8737787
O	-0.0618144	-3.9804620	3.6575517
O	-0.9362884	-4.4350490	5.5815857
N	-1.5301774	-1.9689080	1.9046517
N	-1.5266334	-1.3350900	0.7504317
N	-2.6888044	-1.4025560	0.1542797
N	0.1497996	0.7027910	2.0402447
N	0.2503346	-0.0530510	3.1097027
N	-0.6049954	-3.6370760	4.7441677
C	-2.7786884	-2.4858380	2.0887057
C	-3.3789294	-3.2318480	3.1259277
H	-2.8572044	-3.5138090	4.0395037
C	-4.7005734	-3.5840520	2.9604947
H	-5.1980714	-4.1588210	3.7469577
C	-5.4433754	-3.2155970	1.8096547
H	-6.4920854	-3.5181070	1.7387757
C	-4.8783094	-2.4799660	0.7926107
H	-5.4493574	-2.1777140	-0.0880603
C	-3.5252854	-2.1188980	0.9494517
C	0.3640776	0.7528650	4.1959747
C	0.5127856	0.4758540	5.5681387
H	0.5353956	-0.5524460	5.9387407
C	0.6166606	1.5676820	6.4027607
H	0.7336196	1.4112080	7.4790497
Ni	0.1901896	3.4523670	0.9819807
Ni	-3.0923854	-0.7022870	-1.7136993
Ni	2.7974306	-0.9071540	-2.1014573
O	1.4501146	4.9134850	1.9429137
O	-4.1888494	-0.1143300	-3.4596243
O	3.7047306	-2.5546420	-3.1247323
O	0.5107246	5.3724860	0.0818727
O	-5.1983104	-0.2847220	-1.5863703
O	4.9253096	-1.2086050	-2.0034223
O	-6.3249874	0.1929290	-3.3665113
O	5.8522486	-2.7861920	-3.1504233
O	1.6695876	6.8878590	1.0946987
O	-1.3478924	4.3849980	2.1042147
O	-3.6867694	-2.6552420	-2.2665023
O	3.2048366	0.1698140	-3.8797723
N	1.7396436	2.5231160	-0.0313863
N	-2.5047604	1.2285630	-1.2539393
N	2.4530136	-1.9440060	-0.3320673
N	1.4720986	-1.5592380	0.4541107

N	1.5719546	1.3037280	-0.4990063
N	-1.4455674	1.4162200	-0.4949943
N	1.4192706	-2.2835040	1.5479887
N	-1.2338864	2.6873990	-0.2542033
N	2.6096876	0.8980740	-1.1906023
N	-0.1497174	-0.8397980	-1.9222413
N	0.1838886	1.9723020	2.3549277
N	-1.2863394	-1.0927160	-2.5248563
N	0.8780056	-1.1464230	-2.6764223
N	1.2200146	5.7685440	1.0459807
N	-5.2773314	-0.0675340	-2.8255053
N	4.8649066	-2.1985760	-2.7782193
C	-3.0230314	2.4551410	-1.5441743
C	3.0881076	-2.9861520	0.2769717
C	2.9720536	2.9476120	-0.4262783
C	-4.1198694	2.8847940	-2.3225853
C	4.1893916	-3.7942990	-0.0804413
C	3.7036486	4.1334460	-0.1983533
H	-4.7547974	2.2027000	-2.8866203
H	4.7272136	-3.6935840	-1.0224673
H	3.3371716	4.9443080	0.4304567
C	-4.3524954	4.2414240	-2.3854473
C	4.5794896	-4.7594940	0.8223237
C	4.9529046	4.2202890	-0.7729193
H	-5.1921854	4.6075190	-2.9833033
H	5.4298236	-5.4020200	0.5763397
H	5.5492956	5.1232310	-0.6128843
C	-3.5299514	5.1816900	-1.7129833
C	3.9170276	-4.9472670	2.0627017
C	5.4979946	3.1693540	-1.5554153
H	-3.7604434	6.2470940	-1.8041943
H	4.2791606	-5.7230750	2.7434437
H	6.4953316	3.2948830	-1.9873983
C	-2.4455774	4.7834440	-0.9641433
C	2.8339936	-4.1783750	2.4238397
C	4.8086736	1.9976340	-1.7712253
H	-1.7920164	5.5003280	-0.4618683
H	2.3118886	-4.3178800	3.3731467
H	5.2269196	1.1804680	-2.3615923
C	-2.2018854	3.3971290	-0.8894673
C	2.4231276	-3.1965900	1.5020757
C	3.5292276	1.8981970	-1.1870953
C	0.3218866	2.0718440	3.7039007
C	-1.0039554	-1.5923940	-3.7568373
C	0.4017036	-1.6344370	-3.8521403
C	0.4323226	3.1802700	4.5671857

C	1.0465556	-2.1218210	-5.0074913
C	-1.8268744	-2.0100830	-4.8228223
H	0.4092476	4.2023030	4.1815037
H	2.1357866	-2.1797310	-5.0720713
H	-2.9159754	-1.9626660	-4.7540973
C	0.5781746	2.9000000	5.9087437
C	0.2320356	-2.5346280	-6.0394793
C	-1.1846324	-2.4730400	-5.9505263
H	0.6699726	3.7244810	6.6218277
H	-1.7791824	-2.8064600	-6.8062893
H	0.6840116	-2.9237310	-6.9566753
H	-4.6202734	-2.8997740	-2.1699553
H	-3.1962114	-3.3674470	-1.8270643
H	2.4450396	0.6903240	-4.1854943
H	3.4867736	-0.3352930	-4.6581853
H	-2.1761724	3.8796780	2.1172227
H	-1.6134574	5.2876100	1.8679627
H	1.3471036	-1.9493520	3.8036757

***COO-**

Ni	-0.0292913	-0.0180089	-0.0147047
Ni	-3.0936053	-1.6267429	-1.0346177
O	-3.8116813	-3.1225219	-2.3864227
O	-4.3193073	-3.2496229	-0.3175417
O	-5.1565263	-4.6704079	-1.7101367
N	-1.2769623	-2.7606759	-0.6407547
N	-0.2483873	-2.1319689	-0.1234137
N	0.7754737	-2.9338539	0.0830893
N	-0.9088493	0.0815901	-1.9572197
N	-2.0396623	-0.4873339	-2.2962637
N	-4.4589853	-3.7056969	-1.4783247
C	-0.9139013	-4.0631979	-0.7988507
C	-1.5826623	-5.1899219	-1.3281047
H	-2.5903263	-5.1383769	-1.7440877
C	-0.8925093	-6.3831589	-1.3364537
H	-1.3774863	-7.2758709	-1.7425407
C	0.4358347	-6.4898649	-0.8480177
H	0.9363657	-7.4619949	-0.8870957
C	1.1095417	-5.3998989	-0.3426877
H	2.1407127	-5.4718099	0.0126783
C	0.4106807	-4.1753709	-0.3246707
C	-2.2721163	-0.2022729	-3.6038717
C	-3.3302023	-0.5409979	-4.4714077
H	-4.1674193	-1.1628679	-4.1431437
C	-3.2533673	-0.0543339	-5.7586777
H	-4.0512793	-0.2886689	-6.4694307
Ni	1.2567417	1.9095761	-2.8073217
Ni	2.4839877	-2.4313419	1.0364983
Ni	-0.7330053	2.2080801	2.7678203
O	0.7466307	3.5039391	-4.1714897
O	4.4830357	-2.5554709	1.8172723
O	-1.4701053	2.2900841	4.7848513
O	2.6589927	3.4818751	-3.2229927
O	3.8823277	-3.8669479	0.2437893
O	-2.2080693	3.6723391	3.3344073
O	5.8468727	-4.0766329	1.1167763
O	-2.8688833	3.8227551	5.3844523
O	2.2097877	5.0060291	-4.6858497
O	2.0247867	0.9844561	-4.5571327
O	2.0698997	-3.9223779	2.4890493
O	0.7039677	3.5912851	3.4977333
N	0.4533327	2.8450021	-1.1469557
N	2.9419887	-0.9442119	-0.3284407
N	-2.1439183	0.8602101	2.0951453
N	-1.9249743	0.1847631	0.9809353

N	0.1559037	2.1211931	-0.0875627
N	1.9703727	-0.1950869	-0.8071667
N	-2.9394493	-0.5844559	0.6701283
N	2.4119037	0.6706051	-1.6889407
N	-0.2585823	2.8660191	0.9103813
N	0.8668347	-0.1249749	1.9262943
N	-0.3694003	0.7318661	-2.9657687
N	1.7093077	-1.0588299	2.2970183
N	0.6128827	0.7113301	2.9050203
N	1.8849137	4.0277481	-4.0558727
N	4.7730907	-3.5250699	1.0669903
N	-2.2010003	3.2885031	4.5315243
C	4.1005957	-0.5450059	-0.9235557
C	-3.3752553	0.5042621	2.5538343
C	0.2088267	4.1487471	-0.8367437
C	5.4454217	-0.9549849	-0.7921987
C	-4.1274033	0.8666931	3.6930453
C	0.3135387	5.3525511	-1.5685937
H	5.7681967	-1.7259899	-0.0930947
H	-3.7542603	1.5403021	4.4644053
H	0.6133767	5.3886551	-2.6160077
C	6.3785767	-0.3073989	-1.5722217
C	-5.3759033	0.2986161	3.8280053
C	-0.0232823	6.5162801	-0.9123507
H	7.4304647	-0.5971569	-1.4932377
H	-5.9839843	0.5558681	4.7005023
H	0.0411597	7.4668061	-1.4501947
C	6.0221557	0.7354461	-2.4653077
C	-5.8968083	-0.6169869	2.8781733
C	-0.4619073	6.5221691	0.4369583
H	6.8078067	1.2204181	-3.0519867
H	-6.8952663	-1.0348689	3.0375933
H	-0.7144793	7.4776371	0.9062883
C	4.7184957	1.1590131	-2.5963977
C	-5.1708643	-0.9963309	1.7709813
C	-0.5841093	5.3581971	1.1615393
H	4.4441217	1.9811411	-3.2613227
H	-5.5578073	-1.7137979	1.0430933
H	-0.9267833	5.3541141	2.1978113
C	3.7539637	0.4974301	-1.8086427
C	-3.8913213	-0.4226839	1.6250703
C	-0.2433613	4.1607441	0.4993263
C	-1.1910263	0.5904461	-4.0380787
C	2.0378987	-0.8354529	3.5967093
C	1.3214457	0.3110341	3.9927693
C	-1.1228373	1.0835881	-5.3571857

C	1.4143767	0.8194451	5.3041503
C	2.8931127	-1.5145609	4.4879953
H	-0.2874383	1.7035201	-5.6902397
H	0.8362897	1.6920591	5.6180453
H	3.4508257	-2.4001039	4.1745143
C	-2.1648083	0.7479071	-6.1943727
C	2.2504707	0.1458661	6.1684173
C	2.9830457	-1.0025169	5.7643883
H	-2.1595193	1.1081871	-7.2275137
H	3.6337867	-1.4931039	6.4942763
H	2.3539697	0.4992061	7.1986483
H	2.2972577	-4.8368159	2.2587823
H	1.1307747	-3.9571459	2.7310763
H	1.6028407	3.4051921	3.1834303
H	0.7891757	3.6627671	4.4610483
H	2.1170257	0.0215921	-4.4828117
H	2.8773137	1.2903501	-4.9034437
C	-4.8593563	-0.4012509	-1.4720567
O	-4.5533153	0.7613191	-1.4387207
O	-5.7794673	-1.1598249	-1.6525217

*OCO-

Ni	-0.0129292	0.0301146	-0.0115112
Ni	3.2859728	-1.4677524	0.4310638
O	4.2825448	-3.2046434	1.2423088
O	4.6506868	-2.6162814	-0.7770362
O	5.8196818	-4.2030244	0.1025628
N	1.6374058	-2.5926614	-0.2455792
N	0.5154978	-1.9758804	-0.5500532
N	-0.3946462	-2.8085814	-0.9999432
N	0.9523038	-0.3207364	1.8539268
N	2.1537218	-0.8295764	1.9809388
N	4.9518428	-3.3652314	0.1871508
C	1.4537408	-3.9198964	-0.4953222
C	2.2752328	-5.0576354	-0.3306412
H	3.2756698	-5.0082534	0.0995498
C	1.7438088	-6.2749954	-0.6973112
H	2.3518598	-7.1765934	-0.5790312
C	0.4259608	-6.4019184	-1.2068592
H	0.0556208	-7.3963124	-1.4729022
C	-0.3976882	-5.3081944	-1.3546552
H	-1.4257722	-5.4034664	-1.7126742
C	0.1403628	-4.0565534	-0.9911812
C	2.4504938	-0.8755884	3.3049068
C	3.5860928	-1.3329894	4.0049548
H	4.4477138	-1.7561794	3.4826538
C	3.5473858	-1.2231194	5.3778388
H	4.4040728	-1.5629964	5.9674918
Ni	-1.3714242	0.8508306	3.2474398
Ni	-2.2141262	-2.3066274	-1.6857232
Ni	0.2867668	3.0416346	-2.0179632
O	-0.9898112	2.0613396	4.9886478
O	-4.2244302	-2.4447804	-2.3919992
O	0.9475378	3.7992726	-3.9170592
O	-2.9578032	1.9690296	4.1657198
O	-3.3686072	-4.1388774	-1.4142812
O	1.5066538	4.8114906	-2.1229542
O	-5.3546982	-4.2782374	-2.2492072
O	2.0736568	5.6383446	-4.0362452
O	-2.6110902	3.0877926	5.9805128
O	-1.8221492	-0.6498714	4.6862698
O	-1.7143172	-3.1442854	-3.5689802
O	-1.3559522	4.3575066	-2.3111182
N	-0.8697762	2.3387466	1.9005008
N	-2.7544612	-1.4694734	0.1084358
N	1.8912908	1.7658196	-1.7644512
N	1.7829788	0.7574366	-0.9209222

N	-0.4840392	2.0031156	0.6869898
N	-1.8987182	-0.6877124	0.7349028
N	2.8917528	0.0635336	-0.8444382
N	-2.3925952	-0.2272464	1.8586048
N	-0.2106502	3.0554286	-0.0473982
N	-0.9805222	0.3787356	-1.8779282
N	0.4276788	-0.0219274	3.0196698
N	-1.7549242	-0.4955494	-2.4730682
N	-0.8743092	1.4862396	-2.5742922
N	-2.2014532	2.3915346	5.0822648
N	-4.3465122	-3.6469144	-2.0331982
N	1.5238248	4.7859756	-3.3806032
C	-3.8875702	-1.5293684	0.8637048
C	3.1482248	1.7268206	-2.2878492
C	-0.8394272	3.6987456	1.9794228
C	-5.1216882	-2.1985844	0.7092978
C	3.8213718	2.5112046	-3.2506012
C	-1.1239142	4.6142026	3.0167978
H	-5.3621072	-2.8295794	-0.1456462
H	3.3498668	3.3352066	-3.7849052
H	-1.4285692	4.3111706	4.0175548
C	-6.0591772	-2.0239764	1.7039628
C	5.1255438	2.1710916	-3.5368842
C	-0.9757222	5.9535836	2.7308508
H	-7.0261692	-2.5276214	1.6149748
H	5.6750028	2.7555756	-4.2808322
H	-1.1823052	6.6893816	3.5134928
C	-5.8149602	-1.2073304	2.8378188
C	5.7786278	1.0804186	-2.9066612
C	-0.5527432	6.4110376	1.4564838
H	-6.6002082	-1.1006884	3.5919388
H	6.8165188	0.8598306	-3.1731662
H	-0.4488162	7.4871736	1.2895188
C	-4.6189532	-0.5461554	3.0047758
C	5.1345378	0.2937226	-1.9785502
C	-0.2650332	5.5348936	0.4344218
H	-4.4282772	0.0942586	3.8689388
H	5.6247158	-0.5577964	-1.4994042
H	0.0717678	5.8800406	-0.5451352
C	-3.6499082	-0.7228394	1.9964428
C	3.7976988	0.6308896	-1.6810992
C	-0.4149702	4.1610406	0.7159498
C	1.3324908	-0.3461534	3.9805188
C	-2.1962502	0.0586566	-3.6333892
C	-1.6177442	1.3419716	-3.7017422
C	1.3084258	-0.2310164	5.3858298

C	-1.8509432	2.1983416	-4.7968042
C	-3.0524592	-0.4153494	-4.6483132
H	0.4467388	0.1944216	5.9055738
H	-1.3849722	3.1842916	-4.8590632
H	-3.5111992	-1.4043864	-4.5886452
C	2.4265768	-0.6746484	6.0581648
C	-2.6837622	1.7213366	-5.7856592
C	-3.2805082	0.4343076	-5.7091172
H	2.4580178	-0.6058624	7.1496068
H	-3.9387812	0.1123906	-6.5215462
H	-2.8955922	2.3475976	-6.6573552
H	-1.8160072	-4.1041354	-3.6667752
H	-0.7921982	-2.9693074	-3.8157042
H	-2.2129542	3.9326146	-2.1490992
H	-1.4541732	4.7871096	-3.1748242
H	-1.9036002	-1.5440094	4.3186338
H	-2.6144402	-0.5362484	5.2341508
C	6.0148798	-0.7819394	1.1856758
O	7.0729998	-0.3407464	1.5944558
O	4.8456888	-0.3389414	1.1810408

*CO₂⁻

Ni	0.1115904	0.0799518	0.0258515
Ni	-2.5552176	1.6945828	1.8741525
O	-2.9075436	2.2371038	3.7170265
O	-3.3465016	3.4645608	2.0542675
O	-3.7843986	4.1952698	4.0517175
N	-0.3596156	2.4053938	1.9082755
N	0.5195764	1.7818258	1.1664565
N	1.7447994	2.2394878	1.3408115
N	-1.0340246	-0.6945072	1.6211935
N	-2.0437806	-0.0798442	2.1954665
N	-3.3773376	3.3481148	3.3196625
C	0.3162064	3.3384198	2.6261935
C	-0.1104916	4.2875868	3.5788155
H	-1.1567806	4.3838918	3.8786975
C	0.8570644	5.0987268	4.1303885
H	0.5694314	5.8478138	4.8738485
C	2.2251704	4.9873728	3.7648135
H	2.9519354	5.6533788	4.2395425
C	2.6590914	4.0650398	2.8371035
H	3.7141214	3.9715838	2.5677395
C	1.6756164	3.2332478	2.2630105
C	-2.5660486	-0.9033752	3.1447575
C	-3.6339906	-0.7566302	4.0510905
H	-4.2088806	0.1702218	4.1106705
C	-3.8961906	-1.8333432	4.8696335
H	-4.7143896	-1.7684772	5.5926475
Ni	0.4321124	-3.2626402	1.3812025
Ni	3.3431124	1.7398248	0.2079545
Ni	-0.9896616	-0.0478702	-3.4253585
O	-0.7349706	-5.0408072	1.6987275
O	5.3948264	1.6109528	-0.4427335
O	-1.5553876	1.1820378	-5.0846135
O	1.2511024	-5.1970292	0.9326975
O	4.9446694	2.1028098	1.5856575
O	-2.7110706	-0.5507142	-4.6174605
O	7.0007604	2.0745178	0.9254765
O	-3.1926116	0.6111738	-6.3733505
O	0.1320104	-6.9913582	1.3732645
O	1.0965854	-3.6071002	3.3639375
O	3.5499784	3.7906488	-0.3143265
O	0.0992124	-1.1606062	-4.8650145
N	-0.3245526	-2.9341592	-0.5192955
N	3.1818064	-0.2698922	0.6555965
N	-2.1180786	0.9872328	-2.0248075
N	-1.7745086	0.9182998	-0.7605575

N	-0.3303086	-1.7161272	-1.0203085
N	1.9830164	-0.8095402	0.7181625
N	-2.6673736	1.5033568	0.0059325
N	2.0356074	-2.0700992	1.0746015
N	-0.8390836	-1.6861512	-2.2288195
N	1.1571494	0.8835668	-1.6087365
N	-0.8570956	-1.8865152	2.1293005
N	2.3242974	1.4787168	-1.5236305
N	0.7137794	0.8599808	-2.8427065
N	0.2160034	-5.7868502	1.3442865
N	5.8225904	1.9418008	0.6950035
N	-2.5079266	0.4150528	-5.3984255
C	4.0867114	-1.2346542	0.9845235
C	-3.2984816	1.6666718	-2.1047235
C	-0.8700086	-3.7633492	-1.4531255
C	5.4959264	-1.2506792	1.0709825
C	-4.1147236	2.0578578	-3.1876035
C	-1.1380986	-5.1501492	-1.4773855
H	6.1195344	-0.3900892	0.8294955
H	-3.8627916	1.8624848	-4.2290895
H	-0.9300906	-5.8153522	-0.6402055
C	6.0880854	-2.4352462	1.4520925
C	-5.2688656	2.7477838	-2.8879635
C	-1.7133116	-5.6578922	-2.6213845
H	7.1783184	-2.4838212	1.5259795
H	-5.9226276	3.0687598	-3.7038625
H	-1.9369996	-6.7274312	-2.6722665
C	5.3305754	-3.5988912	1.7416565
C	-5.6320986	3.0651438	-1.5549575
C	-2.0327916	-4.8382632	-3.7344665
H	5.8568174	-4.5119402	2.0352765
H	-6.5590186	3.6173708	-1.3757765
H	-2.4914496	-5.2983302	-4.6147085
C	3.9566024	-3.6062852	1.6493815
C	-4.8408456	2.7063298	-0.4864405
C	-1.7867526	-3.4841222	-3.7270135
H	3.3695754	-4.5040702	1.8549325
H	-5.1067506	2.9698708	0.5396755
H	-2.0385116	-2.8446532	-4.5748925
C	3.3403914	-2.3987842	1.2633185
C	-3.6597706	1.9989728	-0.7837835
C	-1.1971646	-2.9538532	-2.5610765
C	-1.7972016	-2.0813352	3.0935005
C	2.6833404	1.8693168	-2.7745765
C	1.6344514	1.4769008	-3.6288945
C	-2.0796626	-3.1781912	3.9326625

C	1.6687354	1.7521748	-5.0113865
C	3.8289404	2.5254808	-3.2694135
H	-1.4933046	-4.0972282	3.8826115
H	0.8401404	1.4796328	-5.6695275
H	4.6481094	2.8153448	-2.6084725
C	-3.1332796	-3.0294142	4.8074305
C	2.7893484	2.4014028	-5.4817925
C	3.8584274	2.7754988	-4.6239585
H	-3.3934046	-3.8535962	5.4777765
H	4.7263504	3.2810248	-5.0575925
H	2.8623764	2.6399778	-6.5469335
H	4.0872904	4.3430038	0.2751815
H	2.6983684	4.2522028	-0.3734875
H	1.0018174	-1.3830022	-4.5870215
H	0.2005424	-0.7850052	-5.7534215
H	1.5251804	-2.8343952	3.7650455
H	1.7188614	-4.3364332	3.5124295
C	-5.6753206	0.5394478	1.7461155
O	-5.5384876	-0.2934192	0.9534205
O	-5.8084006	1.3773118	2.5382205

***COOH**

Ni	0.0476405	0.0407813	0.0152088
Ni	-2.9667785	-1.4697227	-1.2239332
O	-3.6559685	-2.8461657	-2.6199252
O	-4.3604955	-2.9598937	-0.6139082
O	-5.1724345	-4.2968807	-2.1048432
N	-1.3920005	-2.6260107	-0.6208902
N	-0.3738505	-2.0521597	-0.0131632
N	0.5265535	-2.9257607	0.3581738
N	-0.6305625	0.0798353	-2.0007752
N	-1.7424085	-0.4691227	-2.4272382
N	-4.4355085	-3.4003197	-1.7893312
C	-1.1426565	-3.9665987	-0.6687712
C	-1.8319095	-5.0707687	-1.2180822
H	-2.7681495	-4.9841047	-1.7677332
C	-1.2503395	-6.3114527	-1.0706792
H	-1.7569695	-7.1854107	-1.4902542
C	-0.0100105	-6.4936077	-0.4082112
H	0.4041655	-7.5027857	-0.3281482
C	0.6856885	-5.4292047	0.1185818
H	1.6561875	-5.5541317	0.6052568
C	0.0979205	-4.1561077	-0.0235272
C	-1.8355265	-0.2566707	-3.7663582
C	-2.8101645	-0.6088497	-4.7216662
H	-3.7005145	-1.1824197	-4.4497462
C	-2.5750615	-0.2050607	-6.0177462
H	-3.3018245	-0.4549887	-6.7960432
Ni	1.7217465	1.7223183	-2.7192262
Ni	2.2104705	-2.5043867	1.4167928
Ni	-0.8098975	2.4297303	2.6038788
O	1.4015095	3.2712823	-4.1660902
O	4.1356355	-2.7435557	2.3457838
O	-1.7832065	2.6769553	4.5098438
O	3.2637305	3.1674063	-3.1280582
O	3.4932045	-4.1372307	0.8624168
O	-2.2777175	3.9682653	2.8833738
O	5.3633075	-4.4616287	1.8933118
O	-3.1741095	4.3007133	4.8195048
O	2.9938795	4.6321513	-4.6924302
O	2.5494535	0.6694583	-4.3699872
O	1.5455135	-3.8018367	2.9548168
O	0.5861835	3.8087223	3.4013088
N	0.8419575	2.7845003	-1.1803742
N	2.9007675	-1.1925377	-0.0279532
N	-2.2044155	1.0743313	1.8675698
N	-1.9282115	0.3759773	0.7893468

N	0.3702825	2.1390363	-0.1352142
N	2.0628455	-0.3427137	-0.5843112
N	-2.9368495	-0.3895637	0.4410638
N	2.6602965	0.4358253	-1.4537272
N	-0.1189325	2.9570023	0.7665178
N	0.7339575	-0.0133547	2.0281048
N	0.0296365	0.6456003	-2.9799002
N	1.4975275	-0.9641867	2.5103058
N	0.4641785	0.8971273	2.9340608
N	2.5714315	3.7183543	-4.0257852
N	4.3632595	-3.8087717	1.7138068
N	-2.4338195	3.6784263	4.0977228
C	4.1329175	-0.9619027	-0.5621392
C	-3.4674755	0.7485643	2.2622468
C	0.6453385	4.1151713	-0.9639382
C	5.4020755	-1.5470467	-0.3614182
C	-4.2711155	1.1519543	3.3505818
C	0.9202185	5.2694563	-1.7297192
H	5.5838615	-2.3534757	0.3472628
H	-3.9138965	1.8283423	4.1267778
H	1.3544735	5.2320653	-2.7283252
C	6.4504655	-1.0419297	-1.0991732
C	-5.5378335	0.6163903	3.4271778
C	0.5780675	6.4842473	-1.1776062
H	7.4475425	-1.4722557	-0.9670112
H	-6.1864575	0.9029243	4.2600218
H	0.7733255	7.3986753	-1.7454162
C	6.2832125	0.0252053	-2.0188372
C	-6.0260375	-0.3047867	2.4659898
C	-0.0287165	6.5886973	0.1006598
H	7.1552745	0.3909493	-2.5685492
H	-7.0419575	-0.6952097	2.5752458
H	-0.2790845	7.5810653	0.4869648
C	5.0549475	0.6118493	-2.2248162
C	-5.2491695	-0.7278157	1.4108088
C	-0.3150505	5.4744643	0.8564258
H	4.9218925	1.4466563	-2.9164132
H	-5.6169385	-1.4510747	0.6801768
H	-0.7872535	5.5467133	1.8376148
C	3.9737105	0.0944353	-1.4834032
C	-3.9490155	-0.1903797	1.3273178
C	0.0301185	4.2252343	0.3008128
C	-0.6838245	0.4705433	-4.1244522
C	1.7571095	-0.6723457	3.8125958
C	1.0819415	0.5336473	4.0878788
C	-0.4544215	0.8777473	-5.4543582

C	1.1228475	1.1236633	5.3673908
C	2.5191425	-1.3321727	4.7983718
H	0.4411695	1.4404163	-5.7265182
H	0.5833865	2.0480133	5.5870938
H	3.0525895	-2.2597967	4.5769788
C	-1.4138825	0.5283433	-6.3793582
C	1.8641615	0.4664003	6.3250408
C	2.5565655	-0.7422887	6.0429778
H	-1.2830425	0.8215553	-7.4251102
H	3.1337865	-1.2150707	6.8430828
H	1.9247955	0.8824323	7.3350448
H	1.6707405	-4.7523677	2.8068598
H	0.5976655	-3.7052677	3.1392728
H	1.5117865	3.5512733	3.2666418
H	0.5228455	4.0234223	4.3448318
H	2.5527225	-0.2940427	-4.2541142
H	3.4586465	0.8898063	-4.6273472
C	-4.4056045	-0.2211317	-1.7888022
O	-5.5236405	-0.8666567	-2.0011652
H	-6.2269195	-0.2349157	-2.2658772
O	-4.1966435	0.9457733	-1.8890022

***OCOH**

Ni	-0.0660254	0.0010857	-0.0430792
Ni	3.0893986	-1.7411343	-0.1613122
O	4.1208566	-3.4867763	0.4921378
O	4.3255396	-2.8337693	-1.5292192
O	5.4571666	-4.5398153	-0.8396042
N	1.3453596	-2.7046403	-0.6482962
N	0.2246476	-2.0154723	-0.6929162
N	-0.8058054	-2.7789893	-0.9575692
N	1.1333706	-0.4783963	1.6363598
N	2.2775946	-1.1203553	1.5741168
N	4.6712176	-3.6486943	-0.6335092
C	1.0379526	-4.0093683	-0.8929262
C	1.8078366	-5.1915363	-0.9560022
H	2.8836266	-5.2139783	-0.7827942
C	1.1347496	-6.3632603	-1.2262312
H	1.6990746	-7.2988413	-1.2791622
C	-0.2696604	-6.4001733	-1.4244212
H	-0.7503034	-7.3627883	-1.6222282
C	-1.0378564	-5.2594463	-1.3592032
H	-2.1233444	-5.2845903	-1.4823012
C	-0.3577684	-4.0535903	-1.0941252
C	2.7313766	-1.2882933	2.8444298
C	3.8737716	-1.9257313	3.3725108
H	4.5893856	-2.4495703	2.7322538
C	4.0234866	-1.8898603	4.7423268
H	4.8922046	-2.3739053	5.1982938
Ni	-0.8544784	0.8255497	3.3937588
Ni	-2.6765114	-2.1282533	-1.3749592
Ni	0.1308646	3.0347187	-2.0219972
O	-0.0969444	1.9156827	5.0853018
O	-4.7825904	-2.1561313	-1.8052912
O	0.5634286	3.7706267	-3.9921062
O	-2.1671354	2.0424837	4.5797228
O	-3.8640764	-3.8738453	-0.9301202
O	1.3968276	4.7578307	-2.2919682
O	-5.9464624	-3.9479603	-1.4982602
O	1.7336946	5.5655767	-4.2656912
O	-1.4401914	3.0262137	6.3601148
O	-1.2630854	-0.6870563	4.8277398
O	-2.4890164	-2.9807013	-3.3099152
O	-1.4673724	4.4278527	-2.0810312
N	-0.4051714	2.2999777	2.0193278
N	-2.9013024	-1.2425933	0.4589658
N	1.7120066	1.7025767	-1.9707522
N	1.6382956	0.6498187	-1.1845042

N	-0.2748624	1.9791767	0.7485728
N	-1.8848344	-0.5832913	0.9713678
N	2.7158416	-0.0929743	-1.2622862
N	-2.1761264	-0.0741673	2.1436698
N	-0.0923254	3.0366497	-0.0053642
N	-1.2603604	0.4385587	-1.7299592
N	0.8011856	-0.2019613	2.8731028
N	-2.1863504	-0.3607533	-2.1998872
N	-1.1638274	1.5385677	-2.4379342
N	-1.2427234	2.3463567	5.3822318
N	-4.8997044	-3.3500143	-1.4217012
N	1.2424556	4.7336517	-3.5404392
C	-3.9345224	-1.1619213	1.3434658
C	2.9124676	1.6518067	-2.6138522
C	-0.2874884	3.6534077	2.1153688
C	-5.2566494	-1.6564253	1.3333868
C	3.5297856	2.4810787	-3.5758812
C	-0.3095094	4.5486247	3.2069848
H	-5.6750234	-2.2269733	0.5043228
H	3.0595366	3.3731777	-3.9888262
H	-0.4093274	4.2256357	4.2423628
C	-6.0410264	-1.3680513	2.4291788
C	4.7820136	2.1081227	-4.0133662
C	-0.1589424	5.8879127	2.9225678
H	-7.0721304	-1.7323813	2.4542908
H	5.2883156	2.7256537	-4.7609492
H	-0.1669494	6.6097517	3.7444208
C	-5.5604584	-0.6020603	3.5226878
C	5.4368446	0.9457937	-3.5304532
C	0.0154866	6.3629937	1.5970878
H	-6.2340694	-0.3962313	4.3595708
H	6.4321256	0.7024877	-3.9137022
H	0.1276006	7.4385737	1.4322598
C	-4.2761924	-0.1051903	3.5468048
C	4.8477406	0.1207917	-2.5984222
C	0.0547876	5.5043327	0.5217728
H	-3.9061714	0.5054737	4.3747358
H	5.3390706	-0.7794513	-2.2229932
H	0.1952356	5.8624577	-0.4995152
C	-3.4619374	-0.4032603	2.4350628
C	3.5642836	0.4907627	-2.1484042
C	-0.0956604	4.1303077	0.8015628
C	1.7802276	-0.6782083	3.6867248
C	-2.7492884	0.2399797	-3.2818072
C	-2.0784134	1.4686667	-3.4405602
C	1.9479946	-0.6410383	5.0860848

C	-2.3956664	2.3484447	-4.4952532
C	-3.7910024	-0.1486023	-4.1488682
H	1.2165866	-0.1515373	5.7327348
H	-1.8542034	3.2864287	-4.6378312
H	-4.3225444	-1.0927353	-4.0076302
C	3.0787556	-1.2481913	5.5868888
C	-3.4080524	1.9543857	-5.3425162
C	-4.1015914	0.7265257	-5.1672702
H	3.2558616	-1.2458533	6.6663138
H	-4.9042214	0.4731047	-5.8660832
H	-3.6895804	2.6017397	-6.1783512
H	-2.6041544	-3.9414703	-3.3764072
H	-1.6235884	-2.8078573	-3.7135432
H	-2.3038954	4.0775677	-1.7365322
H	-1.6974064	4.8359447	-2.9300822
H	-1.3560414	-1.5660763	4.4271068
H	-2.0678294	-0.5733233	5.3574378
C	5.8873516	-1.0269063	1.0831708
O	4.9584576	-0.6875233	0.4041028
O	6.8977216	-0.3742993	1.5291828
H	6.8782826	0.5733527	1.2542248

***OCHO**

Ni	-0.0978130	-0.0205327	-0.0227146
Ni	2.6394440	-2.2270037	0.9038694
O	3.1265580	-3.9248067	2.0874474
O	3.8028390	-3.8363107	0.0644304
O	4.4502080	-5.4572957	1.3368644
N	0.8368030	-2.9795957	0.2518364
N	-0.1142000	-2.1541607	-0.1330226
N	-1.2200550	-2.7893167	-0.4367286
N	0.7234540	-0.2426617	1.9449554
N	1.7163270	-1.0459637	2.2459734
N	3.8240940	-4.4387547	1.1700114
C	0.3260090	-4.2439947	0.2070094
C	0.8573500	-5.5182237	0.5057814
H	1.8728860	-5.6744867	0.8667594
C	0.0224270	-6.6021317	0.3411454
H	0.4022910	-7.6028547	0.5664704
C	-1.3179900	-6.4635547	-0.1013016
H	-1.9367910	-7.3598057	-0.2020596
C	-1.8549660	-5.2306937	-0.3949816
H	-2.8925010	-5.1127267	-0.7164486
C	-1.0060340	-4.1158747	-0.2379156
C	1.9611840	-0.9307847	3.5762344
C	2.9058270	-1.5523947	4.4175424
H	3.6204910	-2.2795737	4.0240444
C	2.8772550	-1.1882577	5.7460164
H	3.5904330	-1.6393387	6.4423934
Ni	-1.1609840	1.8078623	2.9258864
Ni	-2.8648330	-1.9739867	-1.3148756
Ni	1.0072350	2.3001603	-2.5878426
O	-0.4559700	3.2161213	4.4016404
O	-4.8890810	-1.8362837	-2.0426466
O	1.8738200	2.3378633	-4.5359776
O	-2.3560800	3.5076713	3.4735624
O	-4.3760730	-3.2924577	-0.5686006
O	2.6339450	3.6510903	-3.0346966
O	-6.3845800	-3.2379237	-1.3601736
O	3.3999640	3.7765843	-5.0502776
O	-1.7094150	4.8603303	5.0274354
O	-2.0670730	0.8646563	4.5952454
O	-2.6340930	-3.3463167	-2.9192086
O	-0.2410800	3.8542683	-3.2968516
N	-0.2238130	2.7636783	1.3452164
N	-3.1511570	-0.5668487	0.1730634
N	2.2817140	0.8418733	-1.8534046
N	1.8389080	0.0434483	-0.8979456

N	-0.0069830	2.1032903	0.2271434
N	-2.1006370	-0.0015907	0.7317544
N	2.7918480	-0.7684827	-0.4941386
N	-2.4421900	0.8137233	1.7003284
N	0.4910340	2.8761023	-0.7083966
N	-0.9124460	0.1313043	-1.9875836
N	0.2870400	0.4007833	3.0018954
N	-1.8935470	-0.6115877	-2.4451706
N	-0.4654570	0.9575623	-2.9017006
N	-1.5168940	3.8915043	4.3322704
N	-5.2563450	-2.8094447	-1.3310296
N	2.6576680	3.2805663	-4.2365716
C	-4.2601210	-0.0858557	0.8031844
C	3.5817630	0.5341083	-2.0812316
C	0.1660540	4.0538143	1.1422954
C	-5.6452820	-0.2936227	0.6206864
C	4.5316930	0.9866403	-3.0471166
C	0.2016410	5.1957393	1.9724024
H	-6.0549270	-0.9194557	-0.1717616
H	4.3287590	1.7731313	-3.7735386
H	-0.0898840	5.1791243	3.0224194
C	-6.4977930	0.3764153	1.4709494
C	5.7727950	0.3212433	-3.0687826
C	0.6733760	6.3631663	1.4126804
H	-7.5771200	0.2418233	1.3549014
H	6.4952760	0.6053323	-3.8397226
H	0.7183320	7.2661933	2.0285074
C	-6.0233430	1.2500853	2.4827904
C	6.1179170	-0.6748347	-2.1837446
C	1.1149380	6.4310163	0.0661144
H	-6.7482880	1.7587283	3.1248764
H	7.0986580	-1.1556577	-2.2480356
H	1.4818610	7.3857823	-0.3221126
C	-4.6782280	1.4828993	2.6607234
C	5.2484640	-1.0811397	-1.0419016
C	1.1025530	5.3253303	-0.7533266
H	-4.3073330	2.1754913	3.4188774
H	5.2109430	-2.1762467	-0.9046456
H	1.4523380	5.3677123	-1.7861146
C	-3.7964370	0.7994103	1.7989624
C	3.8994010	-0.4909957	-1.1877566
C	0.6204340	4.1257863	-0.1913526
C	1.0345110	0.0093613	4.0687444
C	-2.1198530	-0.2548197	-3.7370876
C	-1.1875370	0.7586783	-4.0358136
C	1.0185700	0.3756693	5.4303624

C	-1.1295170	1.3528333	-5.3133176
C	-3.0552800	-0.6988117	-4.6937536
H	0.3064700	1.1070993	5.8173794
H	-0.3850160	2.1165083	-5.5518206
H	-3.7864050	-1.4753247	-4.4597586
C	1.9473450	-0.2363087	6.2441084
C	-2.0442800	0.9056383	-6.2421086
C	-2.9980490	-0.1013967	-5.9343686
H	1.9742730	0.0154363	7.3084494
H	-3.7035790	-0.4108137	-6.7110206
H	-2.0390610	1.3335083	-7.2489606
H	-3.0887280	-4.2012447	-2.8631026
H	-1.7105090	-3.5709847	-3.1142206
H	-1.1689930	3.7619523	-3.0289436
H	-0.2733250	4.0263353	-4.2507796
H	-2.3770010	-0.0379997	4.4206974
H	-2.8196800	1.3080303	5.0171114
C	5.5215550	-0.8725307	1.3549994
O	5.9329890	-0.5464957	0.1585734
O	4.5485120	-1.5411657	1.6366014
H	6.1941710	-0.4487467	2.1268424

***CO**

Ni	0.0241512	-0.0003132	0.0232755
Ni	2.7529852	-1.3261992	2.0363415
O	4.7066482	-2.9783792	3.3364905
O	4.1840472	-2.3709162	1.3200295
O	5.8943982	-3.6060622	1.6533865
N	1.5288792	-2.4541162	1.1347685
N	0.6612202	-2.0085272	0.2374435
N	0.0437732	-2.9823212	-0.3636205
N	0.3192692	0.1378108	2.1622505
N	1.3136112	-0.3993492	2.8321645
N	4.9580932	-3.0086882	2.1385835
C	1.4776222	-3.8099542	1.1299755
C	2.1480622	-4.7955292	1.8795175
H	2.8630202	-4.5310712	2.6638535
C	1.8280942	-6.1059372	1.5938565
H	2.3193992	-6.9096302	2.1503545
C	0.8707722	-6.4507682	0.6016555
H	0.6584582	-7.5090382	0.4232165
C	0.1995822	-5.4914362	-0.1255495
H	-0.5542488	-5.7532082	-0.8735105
C	0.5169772	-4.1461472	0.1536035
C	1.1519952	-0.1252072	4.1555265
C	1.8986082	-0.4738642	5.2963895
H	2.7791992	-1.1204422	5.2307735
C	1.4443372	0.0234988	6.4986805
H	1.9871702	-0.2186782	7.4167025
Ni	-2.1003558	1.6147248	2.4823435
Ni	-1.7226878	-2.5436322	-1.8837615
Ni	1.2219152	2.2949978	-2.5243535
O	-3.8329928	3.2474818	4.1036215
O	-3.6708348	-4.2311042	-3.0125165
O	2.7088862	4.0041478	-4.2431015
O	-3.6929968	2.5847098	2.0450345
O	-2.6154168	-4.0544932	-1.1312505
O	2.2628012	3.8505838	-2.1295015
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O	3.7884533	-1.9379701	-2.7188183

References

1. G. Sheldrick, SHELXT - Integrated space-group and crystal-structure determination. *Acta Crystallogr., Sect. A: Found. Crystallogr.* 71, 3-8 (2015).
2. G. Sheldrick, Crystal structure refinement with SHELXL. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* 71, 3-8 (2015).
3. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* 42, 339-341 (2009).
4. A. Spek, PLATON SQUEEZE: a tool for the calculation of the disordered solvent contribution to the calculated structure factors. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* 71, 9-18 (2015).