Electronic Supplementary Information

The synergistic catalysis effect within a dinuclear nickel complex for efficient and selective electrocatalytic reduction of CO_2 to CO

Li-Ming Cao,[+a] *Hai-Hua Huang,*[+a] *Jia-Wei Wang,*[a] *Di-Chang Zhong,**[b] *and Tong-Bu Lu**[ab]

[a]MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry, Sun Yat-Sen University, Guangzhou 510275, China.
[b]Institute for New Energy Materials & Low Carbon Technologies, School of Materials Science & Engineering, Tianjin University of Technology, Tianjin 300384, China.
[+] These authors contributed equally.

1. Experimental Details

Materials. All of the chemicals are commercially available and used without further purification. All solutions were prepared with Milli-Q ultrapure water (> 18 MΩ) unless otherwise stated. Electrodes and other accessories were all purchased from GaussUnion Co., Ltd.

Characterizations. Electrochemical measurements were carried out using an electrochemical workstation (CHI 760E). All potentials were referenced against $Ag/AgNO_3$ (0.10 M) reference electrode, and the potential of $Ag/AgNO_3$ (0.10 M) reference electrode was calibrated using ferrocene/ferrocenium ($Fc^{0/+}$) as an external standard, and converted to the normal hydrogen electrode (NHE) by adding 0.60 V to the measured potentials. Unless otherwise stated, all potentials were footnoted as vs. NHE. Gas composition was analyzed on an Agilent 7820A gas chromatography

equipped with a thermal conductivity detector (TCD) and a TDX-01 packed column, the oven temperature was kept at 60 °C, the inlet and detector temperature were set at 80 °C and 200 °C, respectively. All experiments were conducted at room temperature (24~25 °C). Energy dispersive X-ray (EDX) spectra were collected by a field emission scanning electron microscope (FEI, Quanta 400).

Synthesis of 1, 2 and 3. The complexes **1**, **2** and **3** were synthesized according to literature methods.[1, 2] **1** ESI-MS: m/z calcd 337.19 (M^{2+}), 387.17 (M^{2+} + $HClO_4$), 437.15 (M^{2+} + $2HClO_4$); found: 337.19 (M^{2+}), 387.17 (M^{2+} + $HClO_4$), 437.15 (M^{2+} + $2HClO_4$); Elemental analysis: calcd (%) for $C_{32}H_{66}Cl_4N_8Ni_2O_{18}$ (**1**·$2H_2O$): C 34.62, H 5.99, N 10.09; found: C 34.80, H 5.84, N 10.01. **2** ESI-MS: m/z calcd 188.1 (M^{2+}), 475.1 (M^{2+} + ClO_4^-); found: 188.1 (M^{2+}), 475.1 (M^{2+} + ClO_4^-); Elemental analysis: calcd (%) for $C_{19}H_{36}Cl_2N_4NiO_9$ (**2**·H_2O): C 38.41, H 6.11, N 9.43; found: C 38.56, H 5.82, N 9.48. **3** ESI-MS: m/z calcd 337.19 (M^{2+}), 387.17 (M^{2+} + $HClO_4$), 437.15 (M^{2+} + $2HClO_4$); found: 337.19 (M^{2+}), 387.17 (M^{2+} + $HClO_4$), 437.15 (M^{2+} + $2HClO_4$); Elemental analysis: calcd (%) for $C_{32}H_{66}Cl_4N_8Ni_2O_{18}$ (**3**·$2H_2O$): C 34.62, H 5.99, N 10.09; found: C 34.72, H 5.91, N 10.08.

Cyclic Voltammetry (CV). CV experiments were performed in a gas-tight three-neck flask (Synthware) with a three-electrode system, where a 0.071 cm^2 glassy carbon (GC) electrode, a platinum wire auxiliary electrode, and an $Ag/AgNO_3$ (0.1 M) reference electrode were placed in a 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) CH_3CN solution with or without a certain amount of water. Prior to experiments, the glassy carbon (GC) electrode was polished with 0.3 and 0.05 μm Al_2O_3 slurry for 5 min each to obtain a mirror surface, followed by sonication in distilled water for ~60 seconds to remove debris, and was thoroughly rinsed with Milli-Q ultrapure water. The electrolyte solution was saturated with argon or CO_2 by purging with argon or CO_2 for 15 min prior to each experiment, respectively.

Controlled-Potential Electrolysis (CPE). CPE experiments were performed in a gas-tight three-neck flask with a three-electrode system under stirring, where a 1 cm × 1

cm GC plate (1.5 cm^2 immersed in electrolyte), a platinum wire auxiliary electrode, and an $Ag/AgNO_3$ (0.10 M) reference electrode were placed in a 0.1 M $TBAPF_6$ CH_3CN/H_2O (*v*/*v* = 4:1) solution. The electrolyte solution (20.0 mL) was saturated with CO_2 by purging with gas for 20 min prior to each experiment, respectively. The volume of head space in the flask was measured as 31.0 mL. The generated gas samples in the head space were analyzed by gas chromatography.

DFT Calculations

All the calculations were performed with Gaussian 09 program.[3] All the structures were fully optimized at the BP86[4]/BSI level of theory (BSI designated the basis set combination of SDD[5] for Ni atom and 6-31g(d) for non-metal atoms). Frequency analysis calculations were performed to characterize the structures to be the minima or transition states. IRC calculations were adopted to confirm the connection of the transition state and its two relevant minimum. With BP86/BSI optimized geometries, the energy results were refined by single-point calculations at the BP86/BSII level of theory (BSII designated SDD for Ni atom, 6-311+g(d) for O and N atoms, and 6-311g(d) for C and H atoms). As for the solvation effect of the mixed solvent (water/acetonitrile = 1:4), the dielectric constant is 45.36 is set according to the reference[6] with the SMD continuum model at the BP86/BSII level of theory. The 3D optimized structures were drawn by CYLview visualization program.[7]

The standard Gibbs free energy was calculated by the equation (1),

$$G^{\Theta}_{(sol)} = E^{\Theta}_{(gas)} + \Delta G_{solv} + \varepsilon_{ZPE} + G^{\Theta}_{298K} + RT\ln(24.5) \quad (1)$$

Where the $E^{\Theta}_{(gas)}$ designates the electronic energy in the gas phase, ΔG_{solv} is the solvation free energy from 1M gas sphere to 1M aqueous sphere. ε_{ZPE} is the gas sphere zero-point energy and the G^{Θ}_{298K} is the thermal contribution to Gibbs free energy at 298.15K. Finally, in order to take the free energy change (RTln(24.5)) from 1M of an ideal gas of 1 atm (24.5 L, 298.15K) to the 1M solution.

For the redox potentials calculation, the result was calculated by,

$$-nE^{\Theta}F = \Delta G^{\Theta}_{(sol)} \qquad (2)$$

where $\Delta G^{\Theta}_{(sol)}$ is the free energy change of the reduction process at standard conditions, n is the number of electrons, F is the Faraday constant.

Finally, since the experimental observed redox potential results were reported versus the normal hydrogen electrode (NHE), the calculated redox potential is referenced to NHE by subtracting 4.48 V.[8]

k_{cat}, TOF, and TON Calculations

$$j = \frac{[\mathbf{1}]D^{\frac{1}{2}}(2k_{cat})^{\frac{1}{2}}F}{1 + \exp[\frac{F}{RT}(E - E_{cat})]} \qquad (1)$$

$$\mathrm{TOF} = \frac{k_{cat}}{1 + \exp[\frac{F}{RT}(E - E_{cat})]} \qquad (2)$$

$$\mathrm{TON} = \frac{k_{cat}}{1 + \exp[\frac{F}{RT}(E - E_{cat})]} \times t \qquad (3)$$

We applied Eq. (1) to calculate an intrinsic catalytic rate (k_{cat}) of **1** and **2** based on the number of catalyst molecules in the diffusion layer of the cathode. In Eq. (1), [**1**] is the concentration of catalysts (**1**, 0.5 mM; **2**,1.0 mM; **3**, 0.5 mM), E is the applied potential in CPE (-1.16 V vs NHE), E_{cat} is the standard potential for catalysis (namely the $E_{1/2}$ of $Ni^{II/I}$ couple at -1.18 V vs NHE of **1**, -1.15 V vs NHE of **2**, -1.14 V vs NHE of **3**), T is the environmental temperature (298.15 K), and j is the averaged electrolytic current density (**1**, 0.60 mA/cm^2; **2**, 0.42 mA/cm^2; **3**, 0.40 mA/cm^2). TOFs and TONs could be calculated based on Eq. (2) and Eq. (3).

2. Supplementary Figures

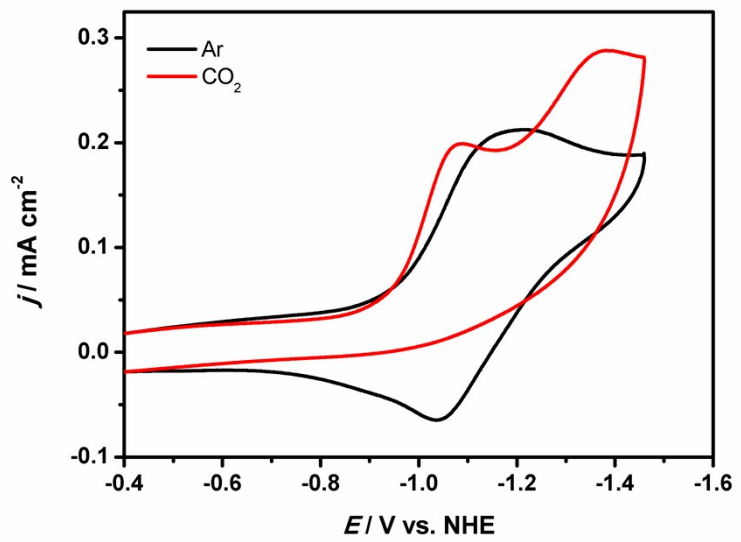


Fig. S1 CVs of 0.5 mM **1** in CH_3CN under Ar/CO_2 atmosphere, with 0.1 M tetra(*n*-butyl)ammonium hexafluorophosphate ($TBAPF_6$) as the supporting electrolyte (scan rate: 100 mV/s).

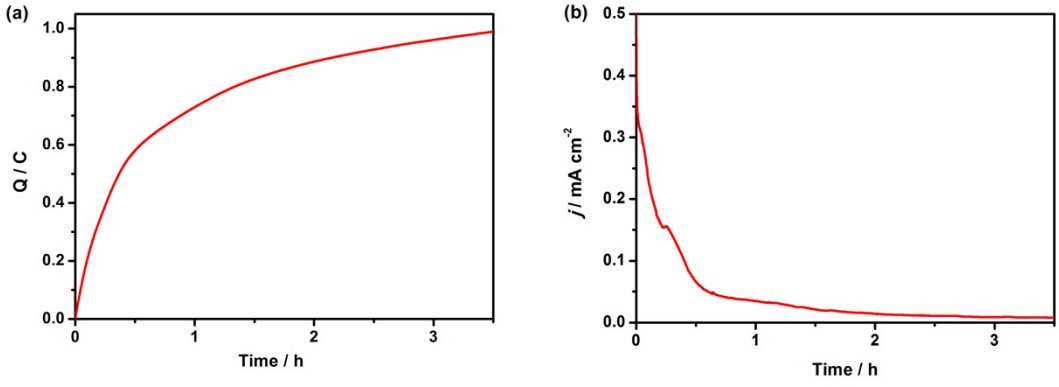


Fig. S2 (a) Chronocoulometric plot and (b) Current density trace obtained from CPE at -1.21 V vs NHE in CH_3CN with 0.5 mM **1** and 0.1 M $TBAPF_6$ at a GC plate (1.5 cm^2) under argon.

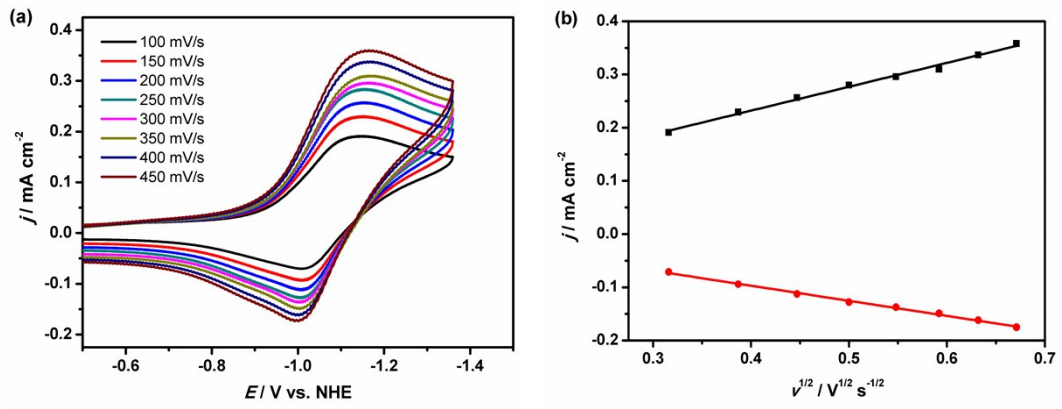


Fig. S3 (a) Scan-rate dependent CVs of 0.5 mM **1** in a 0.1 M $TBAPF_6$ anhydrous CH_3CN under argon. (b) Plots of the peak current versus the square root of the scan rate, showing that both the cathodic (-1.18 V) and anodic (-1.00 V) currents increase linearly with the square root of the scan rate (v). This behavior is indicative of a freely-diffusing species, where the electrode reaction is controlled by mass transport. We applied Eq. (4) to calculate the D_{cat}. Here n = 2 is the number of electrons transferred in this process, F is the Faraday constant, A = 1.5 cm^2 is the electrode surface, c_{cat} is the concentration of catalyst, and v is the scan rate.

$$j = 0.4633nFAc_{cat}\left(\frac{nFvD_{cat}}{RT}\right)^{1/2} \quad (4)$$

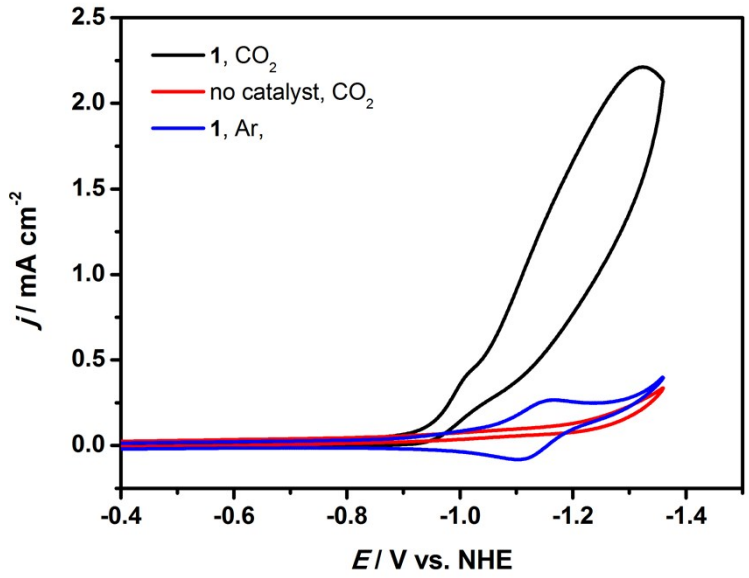


Fig. S4 CVs of 0.5 mM **1** in CH_3CN/H_2O (*v*/*v* = 4:1) containing 0.1 M $TBAPF_6$ under CO_2 (black) and Ar (blue), respectively, and control experiment in the absence of **1** (red) (scan rate: 100 mV/s).

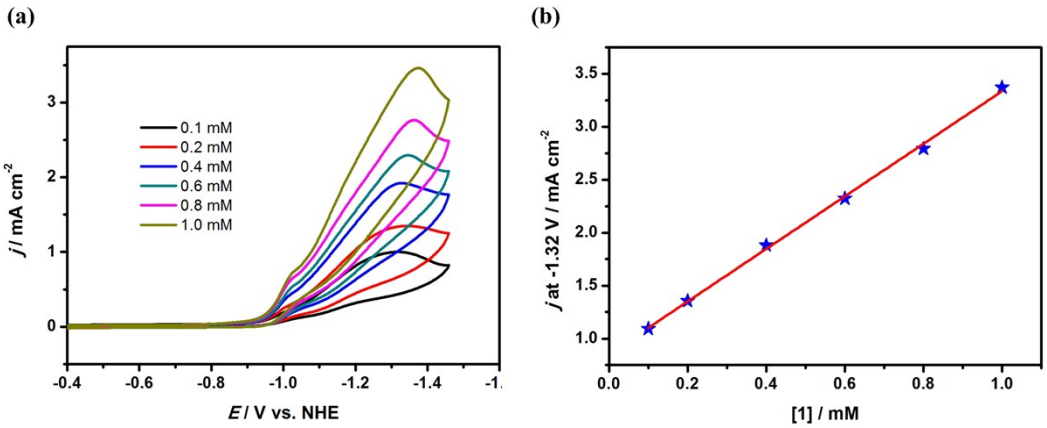


Fig. S5 (a) CVs of **1** at different concentrations in 0.1 M $TBAPF_6$ CH_3CN/H_2O (*v*:*v* = 4:1) under CO_2 atmosphere (scan rate: 100 mV/s), and (b) Plot of the catalytic current densities versus the catalyst concentrations.

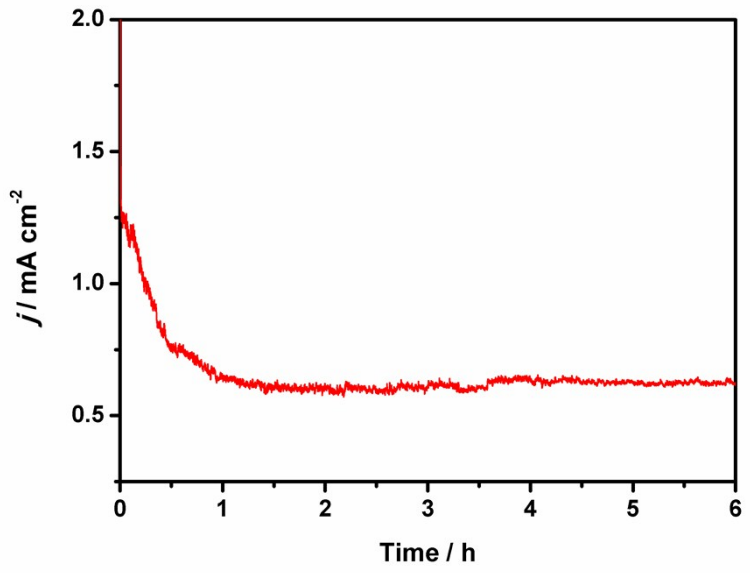


Fig. S6 Current density trace during a 6 h CPE with 0.5 mM **1** in a 0.1 M $TBAPF_6$ CH_3CN/H_2O (v/v = 4:1) solution at a GC plate (1.5 cm^2) under a CO_2 atmosphere.

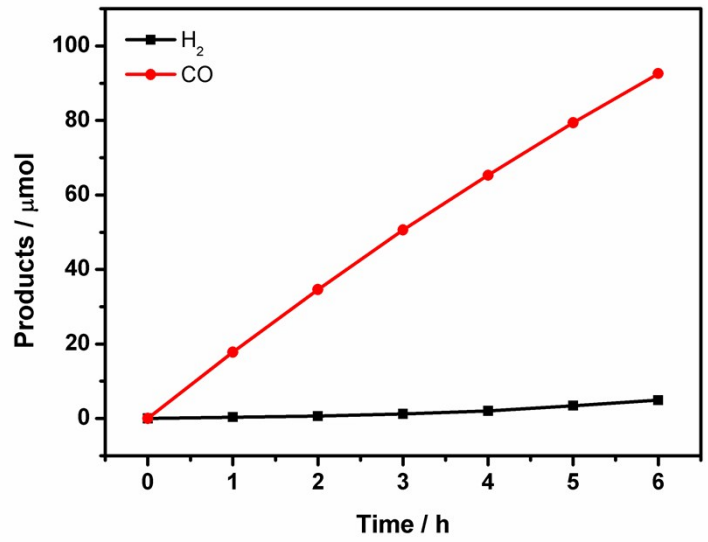


Fig. S7 Time-dependent electrocatalytic evolution of CO and H_2 during a 6 h CPE at -1.16 V vs NHE under CO_2 atmosphere with 0.5 mM **1** in 0.1 M $TBAPF_6$ CH_3CN/H_2O (v:v = 4:1) at a GC plate (1.5 cm^2).

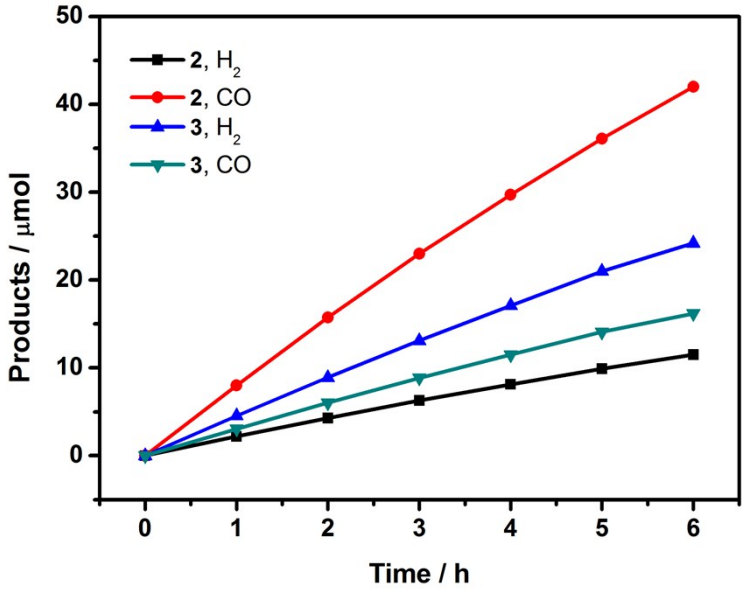


Fig. S8 Time-dependent electrocatalytic evolution of CO and H_2 during a 6 h CPE at -1.16 V vs NHE under CO_2 atmosphere in 0.1 M $TBAPF_6$ CH_3CN/H_2O (*v*:*v* = 4:1) at a GC plate (1.5 cm^2) in the presence of 1.0 mM **2** and 0.5 mM **3**, respectively.

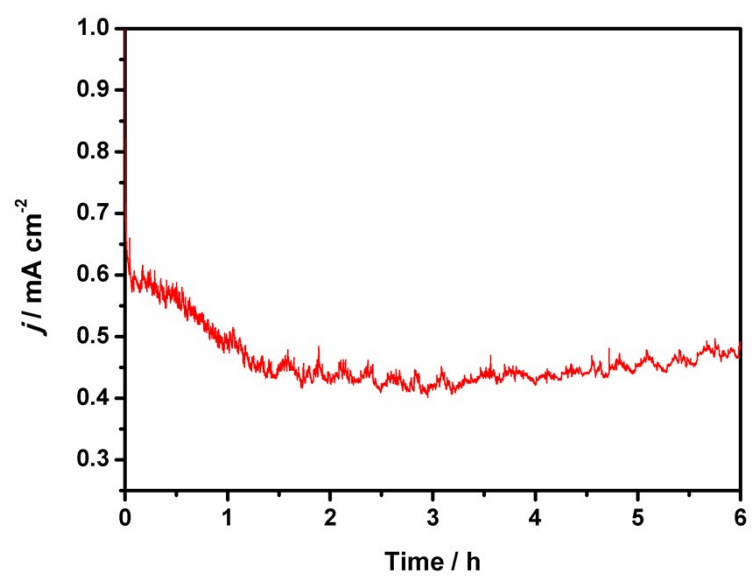


Fig. S9 Current density trace during a 6 h CPE with 1.0 mM **2** in a 0.1 M $TBAPF_6$ CH_3CN/H_2O (*v*/*v* = 4:1) solution at a GC plate (1.5 cm^2) under a CO_2 atmosphere.

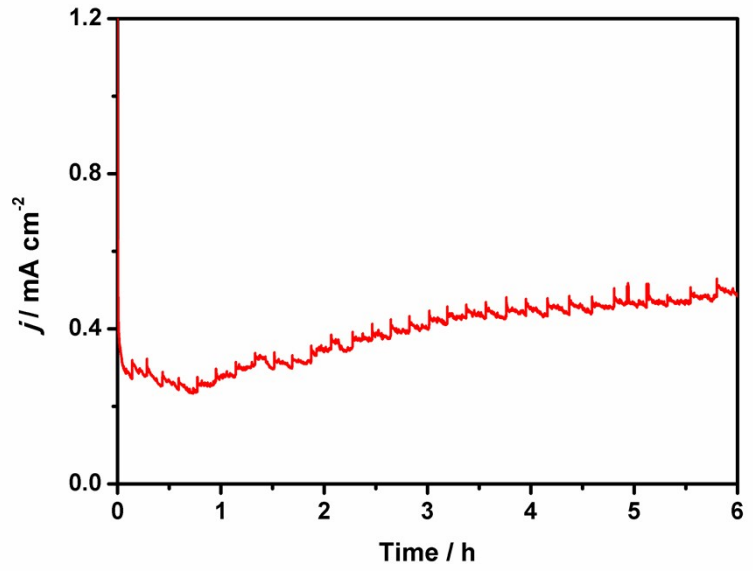


Fig. S10 Current density trace during a 6 h CPE with 0.5 mM **3** in a 0.1 M $TBAPF_6$ CH_3CN/H_2O (*v*/*v* = 4:1) solution at a GC plate (1.5 cm^2) under a CO_2 atmosphere.

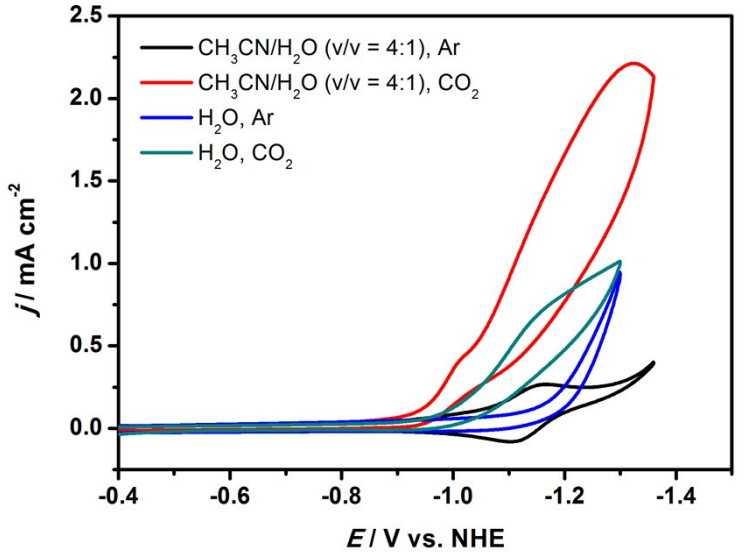


Fig. S11 CVs of 0.5 mM **1** in CH_3CN/H_2O (*v*/*v* = 4:1) containing 0.1 M $TBAPF_6$ under CO_2 (red) and Ar (black), respectively, and CVs of 0.5 mM **1** in H_2O containing 0.1 M KCl under CO_2 (cyan) and Ar (blue), respectively (scan rate: 100 mV/s).

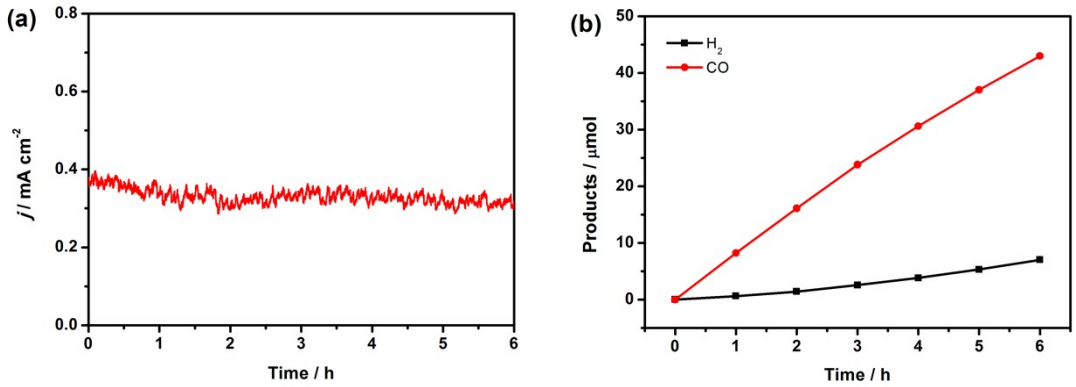


Fig. S12 (a) Current density trace during a 6 h CPE with 0.5 mM **1** in a 0.1 M KCl H_2O solution at a GC plate (1.5 cm^2) under CO_2 atmosphere. (b) Time-dependent electrocatalytic evolution of CO and H_2 during a 6 h CPE at -1.16 V vs NHE under CO_2 atmosphere with 0.5 mM **1** in 0.1 M KCl H_2O solution at a GC plate (1.5 cm^2).

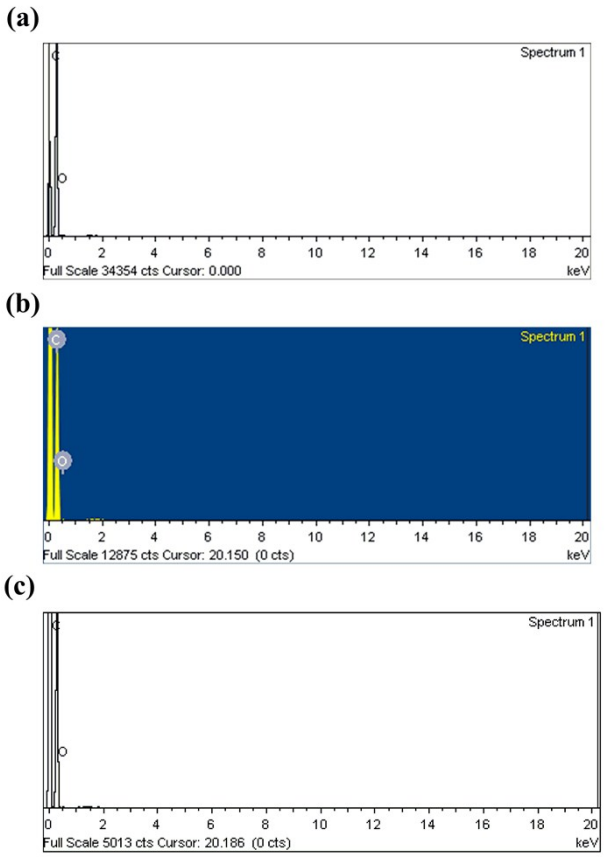


Fig. S13 EDX results of the GC plate after 6 h CPE at -1.16 V, (a) **1** (atomic%: C: 96.10%; O: 3.90%), (b) **2** (atomic%: C: 97.76%; O: 2.24%) and **3** (atomic%: C: 97.15%; O: 2.85%).

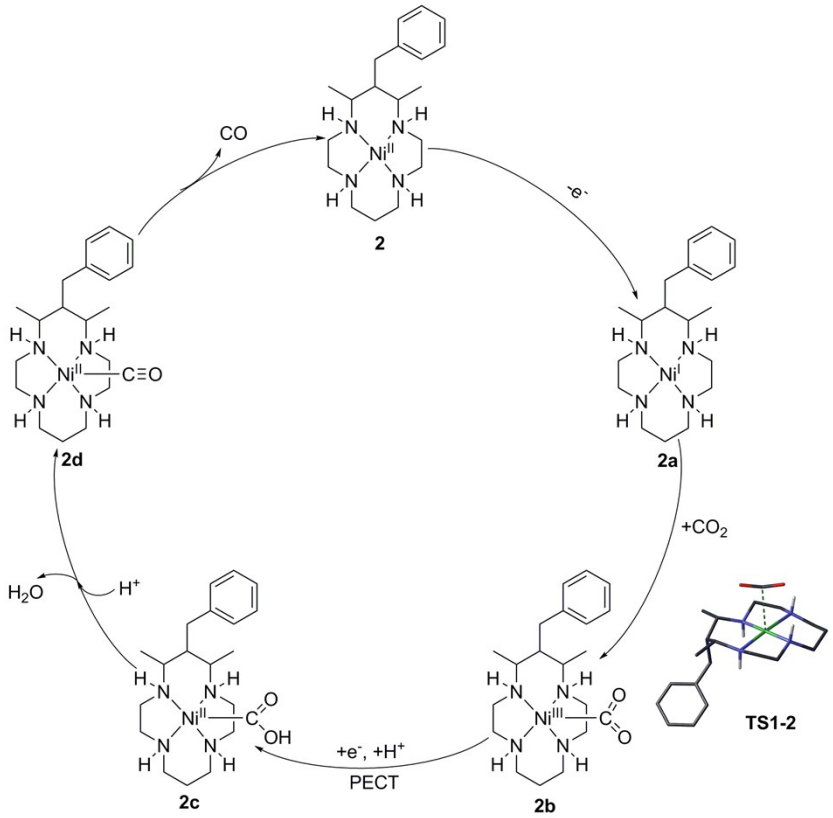
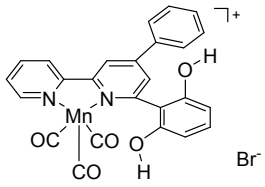
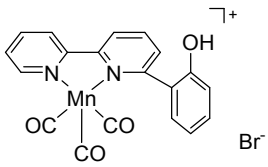
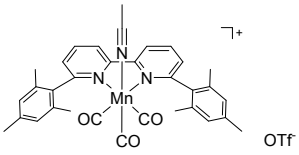
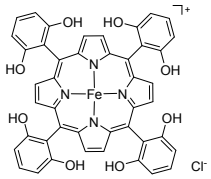
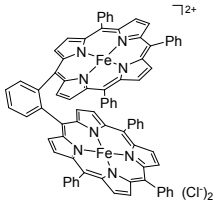
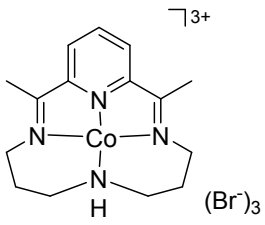
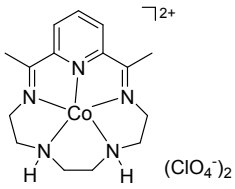
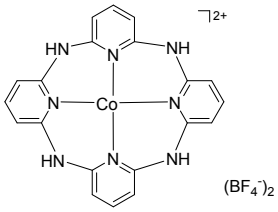
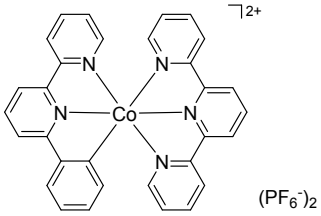
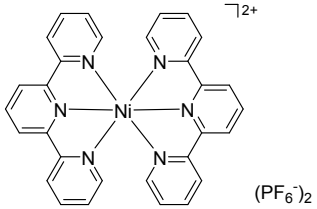
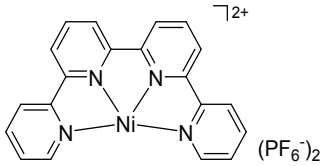
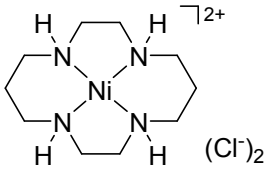
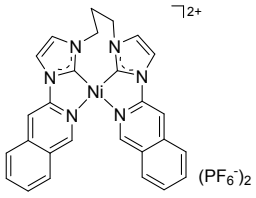
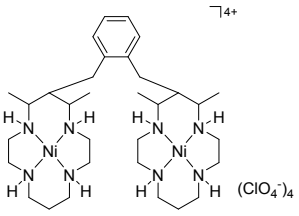


Fig. S14 Proposed mechanism of electrochemical CO_2-to-CO conversion catalyzed by **2**.

3. Supplementary Table

Table S1 Comparison of the catalytic performances

Entry	Catalyst	Solvent	E_{cat} (V vs NHE)	F(CO) (%)	TOF(CO) (s^{-1})[a]	TON (CO)[a]	Ref.
1		CH_3CN	-1.56	70			9
2		CH_3CN + 5% H_2O	-1.26	86			10
3		CH_3CN + 0.2 M Mg	-0.96	96			11
4		DMF + 2 M H_2O	-1.16	94	3470	5.0×10^7	12
5		DMF:H_2O (9:1)	-1.35	95	4300	1.54×10^8	13
6		CH_3CN + 10 M H_2O	-1.36	45			14
7		DMF	-1.26	82			15

8		DMF	-2.15	98	170	1.22×10^6	[16]
9		DMF + 5% H_2O	-1.29	20			[17]
10		DMF + 5% H_2O	-1.08	18			[17]
11		CH_3CN	-1.46	35			[18]
12		H_2O	-1.30	90	90	3.2×10^5	[19]
13		CH_3CN	-1.56	22			[20]
14		CH_3CN/H_2O (v/v = 4:1)	-1.16	95	190	4.1×10^6	This work

[a] The TON and TOF values were calculated based on the number of the catalyst molecules in the diffusion layer.

References

1 K. T. Szacilowski, P. Xie, A. Y. S. Malkhasian, M. J. Heeg, M. Y. Udugala-Ganehenege, L. E. Wenger and J. F. Endicott, *Inorg. Chem.*, 2005, **44**, 6019-6033.

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Optimized Coordinates (xyz) Optimized at the BP86/BSI Level of theory

1

Ni	-5.09518400	-0.94980800	0.09744800
N	-4.31195600	0.02241500	-1.44579100
H	-3.38950100	-0.41776700	-1.61389800
N	-3.85952500	-0.07034500	1.38446600
H	-2.95275300	-0.55041400	1.24008500
N	-5.89395200	-1.87402200	1.64344500
H	-6.68117800	-1.24865100	1.89908800
N	-6.31436000	-1.81063500	-1.18835500
H	-7.14143700	-1.18427200	-1.17578700
C	-4.07873700	1.52099800	-1.27775300
H	-5.06694100	1.91201600	-0.96650400
C	-3.69934900	2.19394000	-2.61158100
H	-2.78931200	1.76321600	-3.06604200
H	-3.50985600	3.26593300	-2.44062600
H	-4.51157800	2.14327700	-3.35282900
C	-3.08350600	1.86367600	-0.13618500
H	-3.20127700	2.95802400	-0.06264400
C	-3.60611700	1.42862800	1.25655400
H	-4.61149100	1.87717400	1.37226900
C	-2.70527300	1.95600900	2.39024800
H	-3.19040100	1.89739000	3.37690900
H	-2.47755200	3.01903900	2.20824900
H	-1.74210000	1.41629000	2.44069100
C	-4.32044800	-0.41561700	2.78111200
H	-5.08992700	0.32430000	3.06576800
H	-3.49334900	-0.33629700	3.50532000
C	-4.89683300	-1.81418200	2.76236600
H	-4.12244100	-2.57449600	2.55758700
H	-5.37337000	-2.06785700	3.72724300

C	-6.46972100	-3.26135400	1.52664600
H	-6.93666200	-3.51442200	2.49673700
H	-5.62420400	-3.95424500	1.37014000
C	-7.48455300	-3.38196300	0.39560300
H	-8.32901600	-2.67781300	0.53451900
H	-7.93156700	-4.39120100	0.43969900
C	-6.83562400	-3.20709000	-0.97271800
H	-5.98372200	-3.89882200	-1.09566900
H	-7.56249800	-3.42272500	-1.77792900
C	-5.68496100	-1.68429600	-2.54420200
H	-6.41771500	-1.91180400	-3.34020000
H	-4.87312100	-2.43020000	-2.60790900
C	-5.16373500	-0.26903900	-2.65966900
H	-4.59286700	-0.12688500	-3.59168700
H	-5.99874300	0.45424700	-2.65970400
C	-1.54592300	1.62429800	-0.42271100
H	-1.15762700	0.82082600	0.23386400
H	-1.42812300	1.23890300	-1.45617300
C	-0.67358800	2.89590500	-0.24264400
C	-1.25028500	4.14822500	-0.56253100
H	-2.23507500	4.18928600	-1.03761700
C	-0.62456300	5.37527300	-0.31315300
H	-1.12067800	6.31187400	-0.58524900
C	0.62488200	5.37522500	0.31271000
H	1.12115000	6.31179000	0.58465200
C	1.25042700	4.14812000	0.56223800
H	2.23526000	4.18908400	1.03725000
C	0.67352600	2.89584800	0.24254400
C	1.54577000	1.62419800	0.42262000
H	1.15738000	0.82069600	-0.23386400
H	1.42805800	1.23890000	1.45612800
Ni	5.09519500	-0.94980900	-0.09735100
N	4.31202500	0.02263700	1.44578100
H	3.38962500	-0.41759300	1.61406500
N	3.85935100	-0.07069400	-1.38442900
H	2.95263500	-0.55082000	-1.23988300
N	5.89392100	-1.87423000	-1.64325000
H	6.68104900	-1.24880800	-1.89906800
N	6.31456700	-1.81028700	1.18849500
H	7.14160100	-1.18387200	1.17572600
C	4.07866100	1.52117000	1.27747600
H	5.06680600	1.91221800	0.96608000
C	3.69930100	2.19435600	2.61118800
H	2.78934000	1.76363900	3.06580500

H	3.50968400	3.26629300	2.44000800
H	4.51158700	2.14394300	3.35239000
C	3.08331600	1.86355100	0.13592400
H	3.20102400	2.95789400	0.06217000
C	3.60581500	1.42827900	-1.25678600
H	4.61113100	1.87690200	-1.37270900
C	2.70477400	1.95534000	-2.39047000
H	1.74164100	1.41552600	-2.44067100
H	3.18977500	1.89656400	-3.37718400
H	2.47697900	3.01838700	-2.20865900
C	4.32018400	-0.41618500	-2.78105100
H	5.08957200	0.32374800	-3.06591200
H	3.49301500	-0.33707500	-3.50520200
C	4.89669600	-1.81469400	-2.76209300
H	4.12239200	-2.57504000	-2.55710200
H	5.37317000	-2.06850700	-3.72696500
C	6.46986100	-3.26147500	-1.52627200
H	6.93677300	-3.51464000	-2.49635100
H	5.62443600	-3.95444200	-1.36960500
C	7.48477100	-3.38179600	-0.39526800
H	7.93187300	-4.39100100	-0.43921900
H	8.32916200	-2.67759300	-0.53435400
C	6.83590500	-3.20674500	0.97306100
H	5.98405000	-3.89850800	1.09617000
H	7.56283600	-3.42220400	1.77826600
C	5.68529800	-1.68374000	2.54438300
H	6.41815700	-1.91102500	3.34034800
H	4.87353400	-2.42970800	2.60832100
C	5.16395400	-0.26850900	2.65962800
H	4.59316900	-0.12622800	3.59167800
H	5.99889700	0.45485200	2.65943800

1a

Ni	3.88425900	-1.08005400	-0.27566600
N	3.87929400	0.29198600	1.29661500
H	2.96223500	0.23845300	1.76890200
N	2.79593900	0.11649600	-1.59705300
H	1.80424600	-0.02940500	-1.34530700
N	4.00372600	-2.43377400	-1.85263300
H	4.93657800	-2.26725900	-2.26541100
N	5.01878000	-2.28232700	0.98795000
H	5.99767100	-2.11810200	0.69980400
C	4.07804900	1.71298600	0.85055800
H	5.01765100	1.69858300	0.26352500

C	4.26780400	2.69829500	2.02248300
H	3.37827900	2.75197700	2.67708900
H	4.46583100	3.71405300	1.63825000
H	5.13049800	2.42508200	2.65208500
C	2.94897600	2.18520700	-0.11620200
H	3.18530100	3.25351200	-0.27286400
C	3.05534200	1.59744800	-1.55436100
H	4.11506600	1.70616600	-1.85796300
C	2.18309500	2.38036500	-2.55610300
H	2.41185100	2.10480900	-3.59908200
H	2.35731700	3.46491500	-2.45756200
H	1.10560200	2.20639900	-2.38092900
C	2.99320900	-0.47854200	-2.95360800
H	3.97077800	-0.12354600	-3.32987600
H	2.22379300	-0.15482400	-3.68018000
C	2.99087600	-2.00649000	-2.85140900
H	2.00685500	-2.36376600	-2.49380800
H	3.16301900	-2.45688500	-3.85028900
C	3.91986200	-3.88444800	-1.51940400
H	4.02661200	-4.49887900	-2.43767600
H	2.90611600	-4.06840400	-1.11759400
C	4.97605100	-4.31302700	-0.49012500
H	5.99227200	-4.06607900	-0.86121100
H	4.95008800	-5.41597500	-0.42225700
C	4.78151700	-3.75191100	0.92642700
H	3.74421300	-3.93015200	1.26570400
H	5.45440700	-4.28282100	1.63147600
C	4.85847700	-1.71779500	2.35301600
H	5.63032900	-2.08767300	3.05812900
H	3.87512800	-2.04877600	2.73595500
C	4.90922100	-0.18972000	2.26636000
H	4.78480500	0.24744500	3.27489600
H	5.89685300	0.13171700	1.88603700
C	1.50698000	2.13897700	0.50792800
H	0.97508200	1.23371700	0.16018700
H	1.60224000	2.01195000	1.60613600
C	0.66595600	3.39704400	0.24999100
C	1.26845400	4.64318600	0.54648500
H	2.26812900	4.65729700	0.99610800
C	0.63687300	5.86488800	0.29316400
H	1.14006200	6.80545400	0.53938000
C	-0.63684400	5.86487700	-0.29338900
H	-1.14000200	6.80543400	-0.53970500
C	-1.26845800	4.64316800	-0.54659300

H	-2.26812500	4.65726700	-0.99623700
C	-0.66600000	3.39703700	-0.24997200
C	-1.50704000	2.13896100	-0.50782400
H	-0.97511900	1.23370900	-0.16009500
H	-1.60236800	2.01190600	-1.60602400
Ni	-3.88424700	-1.08008900	0.27564200
N	-3.87939000	0.29208200	-1.29652700
H	-2.96235900	0.23859600	-1.76887200
N	-2.79586700	0.11636400	1.59706700
H	-1.80418700	-0.02950300	1.34525100
N	-4.00361500	-2.43393700	1.85250700
H	-4.93644400	-2.26745900	2.26535200
N	-5.01884100	-2.28226500	-0.98800200
H	-5.99771500	-2.11807000	-0.69978300
C	-4.07812800	1.71304400	-0.85033600
H	-5.01769300	1.69858900	-0.26324600
C	-4.26795600	2.69846200	-2.02215900
H	-3.37847900	2.75218800	-2.67682900
H	-4.46593400	3.71418800	-1.63781800
H	-5.13070300	2.42532300	-2.65172000
C	-2.94899900	2.18518500	0.11639400
H	-3.18530300	3.25348100	0.27314200
C	-3.05529200	1.59731500	1.55451300
H	-4.11500400	1.70599600	1.85817300
C	-2.18300800	2.38015700	2.55628200
H	-1.10552200	2.20622000	2.38104200
H	-2.41171200	2.10450600	3.59924700
H	-2.35724900	3.46471400	2.45784400
C	-2.99305300	-0.47878700	2.95358500
H	-3.97060300	-0.12383200	3.32993800
H	-2.22359800	-0.15512100	3.68013900
C	-2.99071100	-2.00672600	2.85126000
H	-2.00670700	-2.36396500	2.49357500
H	-3.16279400	-2.45720400	3.85011300
C	-3.91976300	-3.88458400	1.51915800
H	-4.02645700	-4.49908700	2.43738900
H	-2.90603900	-4.06850300	1.11727600
C	-4.97600900	-4.31308700	0.48990600
H	-4.95004200	-5.41602900	0.42194700
H	-5.99221000	-4.06617800	0.86107200
C	-4.78156400	-3.75185300	-0.92661300
H	-3.74427900	-3.93006100	-1.26596800
H	-5.45449400	-4.28270900	-1.63166400
C	-4.85862300	-1.71762300	-2.35303100

H	-5.63051400	-2.08744900	-3.05812800
H	-3.87529400	-2.04856600	-2.73605400
C	-4.90937100	-0.18955400	-2.26624900
H	-4.78501800	0.24769100	-3.27475800
H	-5.89698300	0.13184600	-1.88584200

1b

Ni	-3.52060400	-0.97864200	0.18042600
N	-3.29532900	-0.00197000	-1.64686200
H	-2.29398000	-0.04771700	-1.89671800
N	-2.93829900	0.63187000	1.37813200
H	-1.90668200	0.61768200	1.42848900
N	-3.88940500	-1.97190300	1.97249400
H	-4.91087000	-1.89128500	2.10853700
N	-4.20913500	-2.58891500	-0.95546900
H	-5.23918400	-2.51892300	-0.90258200
C	-3.69876200	1.44616200	-1.63317400
H	-4.75630100	1.44702500	-1.30317800
C	-3.64325200	2.10187400	-3.02891900
H	-2.63462700	2.05231400	-3.47949000
H	-3.93091600	3.16564500	-2.96440900
H	-4.34554800	1.62382500	-3.73150400
C	-2.89284900	2.26270000	-0.57541200
H	-3.22151200	3.30219600	-0.75644700
C	-3.34293100	1.99826200	0.89491400
H	-4.45054700	1.97267400	0.87771100
C	-2.90651400	3.11807800	1.86061900
H	-3.40214600	3.01967400	2.84096400
H	-3.17800500	4.10750900	1.45610500
H	-1.81362400	3.12140500	2.02059500
C	-3.43833600	0.31589900	2.75175800
H	-4.51523300	0.56731700	2.77696800
H	-2.94089200	0.91796200	3.53514500
C	-3.23542600	-1.17366700	3.04199500
H	-2.15824000	-1.42154600	3.02681300
H	-3.62078800	-1.42348900	4.05124000
C	-3.55059500	-3.42212600	2.02761200
H	-3.79384500	-3.83877500	3.02717800
H	-2.45626200	-3.50574100	1.89453300
C	-4.27858600	-4.23301600	0.94508000
H	-5.37530100	-4.09314000	1.04010400
H	-4.10326900	-5.30460900	1.15189400
C	-3.83778200	-3.95798600	-0.50056000
H	-2.73851100	-4.04422700	-0.58567600

H	-4.27868100	-4.72275700	-1.17328900
C	-3.81784600	-2.30909800	-2.36197700
H	-4.37999900	-2.92944700	-3.08911600
H	-2.74719700	-2.56475200	-2.46470400
C	-4.03710400	-0.82203400	-2.65208300
H	-3.73699300	-0.59610200	-3.69264500
H	-5.11023500	-0.57152400	-2.55613800
C	-1.34681700	2.23397700	-0.82634300
H	-0.91270700	1.33476300	-0.35055600
H	-1.18618100	2.09204200	-1.91417800
C	-0.59234700	3.49863500	-0.39691800
C	-1.10769000	4.74296600	-0.83083600
H	-1.97475700	4.75806900	-1.50194600
C	-0.55093400	5.96400800	-0.43621800
H	-0.98035500	6.90515900	-0.79447000
C	0.54733500	5.96407800	0.43646500
H	0.97638600	6.90527900	0.79502700
C	1.10458600	4.74313100	0.83069000
H	1.97162200	4.75841900	1.50182800
C	0.58975400	3.49873300	0.39636300
C	1.34439600	2.23406700	0.82549200
H	0.91120300	1.33522000	0.34820600
H	1.18246600	2.09088100	1.91297900
Ni	3.52074800	-0.97697800	-0.18055300
N	3.29355000	-0.00142200	1.64702500
H	2.29201000	-0.04817200	1.89595900
N	2.93882500	0.63388100	-1.37800200
H	1.90726600	0.61933400	-1.42929300
N	3.89150600	-1.96917600	-1.97283300
H	4.91304300	-1.88806900	-2.10805100
N	4.20946700	-2.58743100	0.95504900
H	5.23950000	-2.51670900	0.90283800
C	3.69587500	1.44702900	1.63463200
H	4.75383000	1.44892700	1.30595100
C	3.63822800	2.10191100	3.03067200
H	2.62906500	2.05160700	3.47994800
H	3.92543300	3.16585900	2.96710600
H	4.33988400	1.62385000	3.73388800
C	2.89069100	2.26364000	0.57637100
H	3.21873100	3.30318200	0.75827800
C	3.34248000	2.00016800	-0.89362200
H	4.45008700	1.97499300	-0.87528400
C	2.90657900	3.12030900	-1.85918200
H	1.81383300	3.12333800	-2.02016600

H	3.40314500	3.02253800	-2.83912100
H	3.17735700	4.10963800	-1.45395200
C	3.44015900	0.31880400	-2.75136300
H	4.51698200	0.57065200	-2.77555500
H	2.94312100	0.92106200	-3.53484800
C	3.23801700	-1.17070300	-3.04246600
H	2.16091300	-1.41896700	-3.02817000
H	3.62423500	-1.41993600	-4.05152300
C	3.55336200	-3.41952600	-2.02885000
H	3.79736200	-3.83556600	-3.02848200
H	2.45899900	-3.50368800	-1.89641100
C	4.28113700	-4.23058600	-0.94629600
H	4.10649300	-5.30216300	-1.15375500
H	5.37783700	-4.09010800	-1.04061800
C	3.83933200	-3.95654900	0.49922600
H	2.74006800	-4.04360200	0.58368600
H	4.28036600	-4.72133900	1.17184000
C	3.81713000	-2.30857200	2.36146100
H	4.37932900	-2.92884100	3.08862800
H	2.74662500	-2.56508600	2.46344100
C	4.03510800	-0.82148700	2.65242600
H	3.73397800	-0.59628000	3.69284900
H	5.10814100	-0.57015300	2.55750500
O	0.10028600	-1.57559500	1.18043600
C	0.00453200	-1.57528400	-0.00036200
O	-0.09326200	-1.57532000	-1.18097900

1c

Ni	-3.36066100	0.56704300	0.22581700
N	-2.54341600	1.29989500	-1.45699300
H	-1.67503400	0.73165800	-1.52201800
N	-2.01976200	1.52491300	1.42739600
H	-1.20646100	0.87231200	1.33400700
N	-4.17442700	-0.14867900	1.92395800
H	-4.94489600	0.51669700	2.11216400
N	-4.67401400	-0.41828500	-0.99199800
H	-5.48901300	0.21459500	-1.06342200
C	-2.21065200	2.76918000	-1.42103600
H	-3.13942000	3.26943900	-1.08024400
C	-1.85760400	3.34542900	-2.80894500
H	-1.00531600	2.82735800	-3.28373400
H	-1.59027100	4.41140500	-2.70894000
H	-2.70998200	3.29691300	-3.50598700
C	-1.10948300	3.08642400	-0.37070800

H	-0.95080200	4.17602000	-0.47987400
C	-1.60885300	2.93700100	1.09310000
H	-2.54587300	3.52562400	1.16205100
C	-0.60634900	3.51622800	2.11091900
H	-1.06290000	3.64243700	3.10642500
H	-0.25985100	4.50982000	1.78183700
H	0.28515300	2.87438300	2.21594100
C	-2.51523900	1.40172400	2.83171000
H	-3.25626100	2.20554800	3.00295300
H	-1.70650800	1.53222200	3.57287100
C	-3.15865200	0.03153100	3.00375400
H	-2.40214100	-0.76164700	2.87641000
H	-3.61091100	-0.07220200	4.00953800
C	-4.76910000	-1.51942500	1.94416900
H	-5.23775100	-1.70184900	2.93191000
H	-3.93526800	-2.23595100	1.83587700
C	-5.79620600	-1.73352400	0.82835800
H	-6.60136900	-0.97332800	0.89035700
H	-6.29236000	-2.70526300	1.00330300
C	-5.18530600	-1.75625700	-0.57571700
H	-4.32754300	-2.45292800	-0.60435600
H	-5.93045900	-2.11737500	-1.31236700
C	-4.01585900	-0.45698900	-2.32823400
H	-4.72234600	-0.75442700	-3.12795200
H	-3.21122500	-1.21175900	-2.27628900
C	-3.42998300	0.92248900	-2.59887300
H	-2.89146200	0.93139600	-3.56382800
H	-4.23953800	1.67371100	-2.66188000
C	0.26067800	2.39418400	-0.68156000
H	0.29180400	1.41840900	-0.17171800
H	0.28130200	2.16099900	-1.76479800
C	1.50590300	3.22777800	-0.36256900
C	1.60682700	4.50820300	-0.95631800
H	0.81300100	4.84608300	-1.63429700
C	2.68902500	5.36077100	-0.71109200
H	2.73165600	6.34523800	-1.18830300
C	3.70949900	4.94427800	0.15934300
H	4.55207400	5.60555700	0.38602100
C	3.64017300	3.67072100	0.73276100
H	4.43905200	3.34883300	1.41249600
C	2.57027900	2.78383900	0.46942300
C	2.61037600	1.41204700	1.13652800
H	1.67192400	0.86269300	0.96211500
H	2.65111600	1.57559400	2.23126500

Ni	1.89134700	-2.09598400	-0.25030500
N	2.63339600	-1.56293200	1.65769700
H	1.82017000	-0.99981200	1.96428700
N	2.75062900	-0.48146200	-1.30582000
H	2.03546200	0.26188900	-1.31535600
N	1.68650300	-2.98475900	-2.15372100
H	2.52131700	-3.57638300	-2.30046400
N	1.51222400	-3.95320600	0.65394100
H	2.34669200	-4.53483600	0.46894800
C	3.88748800	-0.74433400	1.73908300
H	4.69342300	-1.40373200	1.35771400
C	4.25191000	-0.35436600	3.18721900
H	3.43204200	0.18510100	3.69491300
H	5.14282300	0.29716500	3.19647000
H	4.49767100	-1.24033800	3.79573100
C	3.82249100	0.49241800	0.78728000
H	4.73941500	1.06493200	1.02552500
C	4.00655100	0.10053500	-0.71247900
H	4.73493500	-0.73591000	-0.72616700
C	4.58971100	1.23694600	-1.57762500
H	3.86304100	2.05110800	-1.73712800
H	4.92013800	0.86208300	-2.56113400
H	5.47456000	1.67556800	-1.08640500
C	2.92442500	-0.94720200	-2.71759800
H	3.87974900	-1.50437700	-2.76613400
H	3.00467400	-0.10322700	-3.42682600
C	1.76116600	-1.85815600	-3.11838400
H	0.80302200	-1.31677100	-3.04373900
H	1.89114200	-2.20884700	-4.16185100
C	0.48591400	-3.84998400	-2.32795200
H	0.43123600	-4.22287900	-3.37143300
H	-0.38943900	-3.20336800	-2.14624200
C	0.48802300	-5.04319000	-1.35989900
H	-0.35147800	-5.70531900	-1.63991000
H	1.40223800	-5.65494500	-1.51031400
C	0.33279100	-4.69533300	0.12913500
H	-0.55071300	-4.05007600	0.28350300
H	0.17588700	-5.62610300	0.71215700
C	1.47164700	-3.69105700	2.11624900
H	1.48973800	-4.62851900	2.70697700
H	0.52450400	-3.16504100	2.32784400
C	2.66216400	-2.80066800	2.48577900
H	2.63873700	-2.58408100	3.57012600
H	3.61453700	-3.32652100	2.27861500

O	-0.10681300	-0.77681200	1.19258900
C	0.10692000	-1.17223700	0.00545100
O	-0.56054100	-1.00157100	-1.04889400

1d

Ni	2.94485700	0.28136700	-0.26514100
N	2.67618400	1.51357100	1.41592700
H	1.78599600	1.23209900	1.85640900
N	1.91128100	1.47198200	-1.64818100
H	0.98500700	1.01152400	-1.68248800
N	3.76188900	-0.65080600	-1.95475300
H	4.68711700	-0.20998000	-2.09959200
N	4.39479000	-0.67961300	0.92562800
H	5.29899600	-0.23855600	0.68349700
C	2.54759400	2.98753600	1.09179200
H	3.48386700	3.24806000	0.55869100
C	2.46142800	3.86163300	2.35678900
H	1.57284800	3.62698100	2.97139900
H	2.39919000	4.92501700	2.06996900
H	3.35376800	3.76003300	2.99565100
C	1.35649500	3.24282000	0.11789200
H	1.23597100	4.34173700	0.13436300
C	1.71257300	2.94644000	-1.36836400
H	2.70720600	3.40289400	-1.54207700
C	0.71838300	3.58126000	-2.35873500
H	1.08790600	3.53273100	-3.39608900
H	0.57060300	4.64750600	-2.12005900
H	-0.27265600	3.09708000	-2.31459500
C	2.54816000	1.21840100	-2.98639400
H	3.45283800	1.85175800	-3.05357600
H	1.88155100	1.51262800	-3.81567400
C	2.90873300	-0.26139100	-3.11840900
H	1.99891300	-0.88273500	-3.08377100
H	3.42414300	-0.45065800	-4.07870400
C	3.99975200	-2.12439500	-1.84008700
H	4.36445600	-2.51792300	-2.80855900
H	3.02101800	-2.59390200	-1.63623000
C	5.01000500	-2.46599900	-0.73490200
H	5.98501000	-1.97946100	-0.94383000
H	5.21629900	-3.55012000	-0.79012300
C	4.56129300	-2.15035200	0.69926100
H	3.58605400	-2.62592700	0.91151800
H	5.29612600	-2.55868700	1.41979800
C	4.09562300	-0.30010000	2.33615500

H	4.93350500	-0.54236400	3.01709600
H	3.22407200	-0.89726200	2.66510900
C	3.78135400	1.19660200	2.38123000
H	3.53200500	1.50364100	3.41191300
H	4.66924400	1.78004000	2.07419200
C	0.00507600	2.64075600	0.63226200
H	-0.09192600	1.60092300	0.26735600
H	0.07336800	2.56823900	1.73911500
C	-1.25063900	3.45999500	0.31243200
C	-1.27113200	4.80324800	0.75700700
H	-0.41454000	5.19678700	1.31866200
C	-2.35649000	5.65128800	0.51159900
H	-2.33786200	6.68523600	0.87010500
C	-3.46201100	5.16341900	-0.20418800
H	-4.31126100	5.81637700	-0.42858600
C	-3.46945700	3.83032000	-0.62680100
H	-4.33508900	3.45889900	-1.18922300
C	-2.39331200	2.95035400	-0.36349100
C	-2.52897400	1.51452200	-0.86785100
H	-1.59446500	0.94818900	-0.71734300
H	-2.66227500	1.56103900	-1.96647800
Ni	-1.78052900	-2.02361400	0.30434000
N	-2.90526800	-1.43872200	-1.40842300
H	-2.18813000	-0.92713600	-1.94869100
N	-2.35924800	-0.38159700	1.55354300
H	-1.61956100	0.33077200	1.45428400
N	-1.38977600	-2.98217000	2.15726500
H	-2.27243900	-3.46515900	2.39826500
N	-1.88564500	-3.93919800	-0.57554300
H	-2.74462300	-4.38293800	-0.20645800
C	-4.09035100	-0.52648200	-1.21020100
H	-4.83674600	-1.13433000	-0.66122000
C	-4.72671000	-0.10014000	-2.54824300
H	-4.00965600	0.41644700	-3.21187100
H	-5.57148700	0.58519500	-2.36486700
H	-5.13499300	-0.96223000	-3.10078400
C	-3.73143200	0.69139400	-0.30472000
H	-4.62255000	1.34353100	-0.37109500
C	-3.66140000	0.31172200	1.20565200
H	-4.44174200	-0.45643000	1.37816900
C	-3.94755700	1.49618600	2.14900600
H	-3.14236100	2.25033100	2.12154600
H	-4.09031600	1.16385600	3.19089100
H	-4.87945100	2.00207100	1.84656600

C	-2.32519700	-0.86812000	2.97121400
H	-3.30354300	-1.33803700	3.18467500
H	-2.20391900	-0.04046100	3.69217900
C	-1.21058800	-1.89965600	3.16096100
H	-0.21608400	-1.44176400	2.98836900
H	-1.21457700	-2.28585400	4.19895900
C	-0.32027300	-4.02533000	2.15428700
H	-0.15202200	-4.40259500	3.18231600
H	0.61692200	-3.53558900	1.82453200
C	-0.66118400	-5.19825400	1.22322300
H	0.12036700	-5.96858500	1.35195300
H	-1.59898300	-5.68358200	1.56349800
C	-0.75503300	-4.86609600	-0.27370700
H	0.17150800	-4.37885500	-0.62887800
H	-0.87413900	-5.80531200	-0.84887600
C	-2.11558800	-3.70545100	-2.03029900
H	-2.37587800	-4.64264300	-2.55856800
H	-1.17342600	-3.32231100	-2.45939200
C	-3.23957000	-2.67931200	-2.17873300
H	-3.41398100	-2.46506800	-3.24792100
H	-4.18397500	-3.08523300	-1.76906400
O	1.20988300	-1.04013900	0.24496100
C	-0.06948200	-1.28860000	-0.48837300
O	-0.00019700	-0.87887100	-1.63805800
H	1.12012000	-1.41836300	1.14901300

1e

Ni	4.23228500	-1.02798800	-0.15761500
N	4.05194900	0.36797500	1.40248900
H	3.09585800	0.14552100	1.72314900
N	3.28437400	0.19572100	-1.58916600
H	2.32192200	-0.12585000	-1.39483000
N	4.88257100	-2.14922700	-1.80607100
H	5.80387500	-1.78454200	-2.10182200
N	5.57039100	-2.01283300	1.12478100
H	6.51836900	-1.64407700	0.93807900
C	4.12433500	1.82202900	1.02258000
H	5.11462700	1.94318700	0.53833700
C	4.09034400	2.75568000	2.24997600
H	3.13926600	2.68379400	2.80790800
H	4.22119400	3.80387000	1.93197600
H	4.91109700	2.53885200	2.95239800
C	3.05329700	2.22366600	-0.03917500
H	3.23851700	3.30555400	-0.16066700

C	3.34326600	1.69387800	-1.47585200
H	4.39838800	1.95240400	-1.69458400
C	2.45136500	2.39028000	-2.52271200
H	2.77429300	2.16560500	-3.55241400
H	2.49634900	3.48491500	-2.39863300
H	1.39304200	2.08924700	-2.41727600
C	3.68312700	-0.31669200	-2.93715200
H	4.61837800	0.20005200	-3.22422900
H	2.93148900	-0.08232100	-3.71246500
C	3.90394500	-1.83116600	-2.88459000
H	2.96246100	-2.34981000	-2.63204300
H	4.24516700	-2.20243800	-3.87011800
C	5.04747100	-3.61493900	-1.55721800
H	5.35815200	-4.11879700	-2.49328500
H	4.05145700	-4.01170900	-1.28763300
C	6.06482300	-3.91410700	-0.44593300
H	7.04940200	-3.46881500	-0.69696300
H	6.23635300	-5.00561300	-0.43620400
C	5.64173300	-3.49741800	0.97068900
H	4.64119300	-3.90132000	1.21202000
H	6.34937600	-3.91775500	1.71173400
C	5.17618500	-1.56017700	2.48916700
H	5.91927600	-1.85943700	3.25308400
H	4.21839700	-2.05178500	2.73461700
C	5.01519900	-0.03750800	2.47468300
H	4.69877000	0.31418400	3.47278900
H	5.98544800	0.44448100	2.25051900
C	1.55803800	2.08122800	0.43580700
H	1.08643800	1.21924000	-0.07159900
H	1.55218000	1.81911000	1.51420600
C	0.70975300	3.35113900	0.23219200
C	1.30373900	4.59568600	0.55215700
H	2.29870900	4.61215800	1.00877000
C	0.67506600	5.82291400	0.31619100
H	1.17795000	6.75807300	0.58168000
C	-0.59085400	5.83323400	-0.28341500
H	-1.08887500	6.77634300	-0.52911000
C	-1.22347800	4.61360000	-0.54551300
H	-2.21891900	4.64068600	-1.00190400
C	-0.62982500	3.36223600	-0.25441900
C	-1.49567400	2.10803800	-0.48378900
H	-0.99548900	1.21454400	-0.06332100
H	-1.55882700	1.91656700	-1.57521300
Ni	-4.08511900	-1.03892400	0.12591500

N	-4.07554700	0.46538300	-1.38876200
H	-3.19689400	0.34987400	-1.91718300
N	-3.04741200	0.14615100	1.58377000
H	-2.05110100	-0.07796300	1.43706200
N	-4.75938600	-2.11577900	1.80923300
H	-5.63089900	-1.66237200	2.13261700
N	-5.69339100	-1.83337000	-0.97951000
H	-6.55656500	-1.38204600	-0.63175400
C	-4.10826200	1.89608300	-0.89986700
H	-5.05598100	1.97650200	-0.33059000
C	-4.17291200	2.90062400	-2.06774700
H	-3.26654800	2.87080500	-2.69962300
H	-4.27794300	3.92605200	-1.67506900
H	-5.04542900	2.72599900	-2.71696800
C	-2.95647900	2.23752800	0.09290900
H	-3.11760100	3.31637500	0.26947500
C	-3.16458600	1.65358700	1.51816200
H	-4.21726100	1.86229600	1.79303100
C	-2.24596300	2.33526900	2.55014800
H	-1.18449000	2.07815200	2.37972300
H	-2.51029500	2.06202300	3.58473400
H	-2.33184700	3.43156100	2.47084000
C	-3.42752400	-0.39299200	2.93482600
H	-4.33075900	0.15490300	3.26170900
H	-2.64222900	-0.20447900	3.68750900
C	-3.72686200	-1.88944500	2.85728200
H	-2.82712600	-2.46338200	2.56942300
H	-4.05693900	-2.26341800	3.84591400
C	-5.07748500	-3.56020100	1.57802100
H	-5.35615600	-4.03491800	2.53894100
H	-4.15060200	-4.04885000	1.22574400
C	-6.21211400	-3.75099000	0.56268300
H	-6.46134900	-4.82703200	0.53737200
H	-7.13394400	-3.24934400	0.92261800
C	-5.89959200	-3.31140300	-0.87390400
H	-4.97964600	-3.80077900	-1.24281700
H	-6.72624700	-3.61783000	-1.54397300
C	-5.47481000	-1.35419200	-2.37241800
H	-6.34629500	-1.56757300	-3.02108000
H	-4.61063000	-1.90466800	-2.78649800
C	-5.20944900	0.14936400	-2.32784000
H	-5.01482600	0.52988000	-3.34530900
H	-6.10578400	0.67359300	-1.94753700
O	2.53871700	-1.79069100	0.25187800

C	-2.65614000	-2.09333500	-0.47892200
O	-1.71374800	-2.63181600	-0.88103000
H	2.60675300	-2.76100100	0.38617200

TS1-1

Ni	-3.51014500	-0.96730300	0.15393900
N	-3.19100500	-0.08460400	-1.71068200
H	-2.17825200	-0.13857800	-1.90704300
N	-2.98183300	0.70325400	1.29372600
H	-1.95280400	0.70612600	1.38390600
N	-3.97565600	-1.86080300	1.97665100
H	-5.00011600	-1.75249100	2.06271400
N	-4.15952200	-2.62653400	-0.92847700
H	-5.18974700	-2.54148000	-0.93568000
C	-3.59785300	1.35990900	-1.79117000
H	-4.67090500	1.37052600	-1.51595800
C	-3.47284300	1.94573000	-3.21349200
H	-2.44285500	1.87878300	-3.61005700
H	-3.76633200	3.00982600	-3.21757900
H	-4.13732000	1.42896300	-3.92547200
C	-2.85350000	2.23357800	-0.73347000
H	-3.17694300	3.26080900	-0.98295900
C	-3.38433900	2.03503000	0.72028400
H	-4.48819100	1.98207900	0.63838100
C	-3.03534200	3.21213500	1.65309400
H	-3.59518700	3.15162300	2.60148200
H	-3.30026800	4.17269900	1.18047800
H	-1.95682500	3.25066800	1.88613700
C	-3.53346400	0.45627400	2.66126100
H	-4.60937200	0.71143700	2.63428100
H	-3.06280000	1.09498000	3.43201700
C	-3.35210000	-1.01852200	3.02993800
H	-2.27736100	-1.27571800	3.06464500
H	-3.77466200	-1.21711900	4.03587200
C	-3.67218500	-3.31218600	2.12606200
H	-3.97791900	-3.66981300	3.13135000
H	-2.57436800	-3.42493900	2.05780200
C	-4.35879000	-4.16520100	1.04900800
H	-5.45574400	-3.99976800	1.07590200
H	-4.21779200	-5.22748800	1.32003300
C	-3.83408000	-3.97389300	-0.38178500
H	-2.73312400	-4.07677200	-0.39857900
H	-4.24773400	-4.76830500	-1.03731400
C	-3.69002200	-2.42763600	-2.32427400

H	-4.21726800	-3.08427100	-3.04583400
H	-2.61751200	-2.69404500	-2.35470100
C	-3.88126900	-0.95764700	-2.70799700
H	-3.52228100	-0.79129400	-3.74112700
H	-4.95629300	-0.69790700	-2.68681900
C	-1.29683900	2.20300900	-0.89982600
H	-0.89074200	1.30449200	-0.39851000
H	-1.08010100	2.05737300	-1.97744300
C	-0.56681800	3.46789400	-0.43246000
C	-1.04937500	4.71100100	-0.90601100
H	-1.86907000	4.72349800	-1.63435200
C	-0.52101800	5.93287200	-0.47646000
H	-0.92368700	6.87324600	-0.86641100
C	0.51235300	5.93519700	0.47264600
H	0.91429600	6.87739000	0.85892500
C	1.04140000	4.71533000	0.90691500
H	1.86116400	4.73084400	1.63521400
C	0.55926800	3.47027700	0.43815000
C	1.29191800	2.20850400	0.90947600
H	0.88241800	1.30694900	0.41648200
H	1.08271900	2.07027600	1.98955300
Ni	3.47674100	-0.96633800	-0.14752500
N	3.19163700	-0.07504500	1.71879800
H	2.18297100	-0.12830000	1.93416500
N	2.95627000	0.70315500	-1.29358200
H	1.92762400	0.71291200	-1.38584400
N	3.93350900	-1.86903500	-1.96851400
H	4.95880100	-1.76804300	-2.05454000
N	4.14113000	-2.62221500	0.93234000
H	5.17146000	-2.53803800	0.91893200
C	3.60043600	1.36966200	1.78695100
H	4.67092900	1.37762400	1.50157100
C	3.48948600	1.96272100	3.20734000
H	2.46292600	1.89953300	3.61326500
H	3.78456800	3.02633500	3.20324600
H	4.15960500	1.44869300	3.91598500
C	2.84718700	2.23862800	0.73168400
H	3.17178900	3.26705800	0.97475100
C	3.36808100	2.03442400	-0.72486700
H	4.47223500	1.97664100	-0.64965200
C	3.01900600	3.21052000	-1.65882700
H	1.93938700	3.25306800	-1.88571900
H	3.57343000	3.14535900	-2.61008100
H	3.29065500	4.17103200	-1.18998800

C	3.50786100	0.44833000	-2.66018700
H	4.58541000	0.69674800	-2.63288000
H	3.04196700	1.08840800	-3.43247500
C	3.31667600	-1.02596800	-3.02555600
H	2.24074200	-1.27601300	-3.06097700
H	3.74052600	-1.23035800	-4.02962500
C	3.62085200	-3.31931100	-2.11204600
H	3.91765000	-3.68089800	-3.11847700
H	2.52295100	-3.42532900	-2.03643300
C	4.31133000	-4.17327900	-1.03817400
H	4.15902500	-5.23552300	-1.30308300
H	5.40929800	-4.01706100	-1.07783600
C	3.80492200	-3.97217300	0.39789200
H	2.70418200	-4.07250900	0.43073700
H	4.22551100	-4.76344900	1.05261700
C	3.70015600	-2.41600900	2.33670300
H	4.24338000	-3.06834200	3.05003700
H	2.62903500	-2.68255600	2.39104500
C	3.89993000	-0.94392200	2.70774800
H	3.56038300	-0.77104900	3.74619700
H	4.97456200	-0.68489700	2.66500700
O	0.19885800	-1.68442100	1.14972400
C	0.17393500	-1.62011400	-0.03357200
O	0.06936900	-1.56681600	-1.21354300

2

Ni	1.47487900	-0.07979000	0.20689000
N	-0.29687100	-0.63454100	0.86464800
H	-0.86593900	-0.90212400	0.03499200
C	-1.10946600	0.41593700	1.59306500
H	-0.44354500	0.78789300	2.39658100
N	0.99334900	1.81789300	-0.15042600
H	0.71829400	1.78067600	-1.14937800
C	-1.39234500	1.60033800	0.62852100
H	-2.17333800	2.20070600	1.13041500
N	3.31032500	0.42183700	-0.34943400
H	3.83308400	0.43398800	0.54508200
C	-0.14925900	2.52352700	0.56517700
H	0.21198000	2.68219700	1.59855300
N	2.04694500	-1.93980800	0.54153000
H	2.60632700	-1.86905800	1.41122600
C	2.27099400	2.60740300	-0.08806500
H	2.54942700	2.71523800	0.97527600
H	2.13765100	3.61701000	-0.51120700

C	3.31088700	1.83167500	-0.86891800
H	4.31644000	2.28106000	-0.78452100
H	3.04954400	1.79076600	-1.94162000
C	4.05501900	-0.49354300	-1.28349700
H	3.48693400	-0.52484500	-2.23010900
H	5.04120900	-0.04080800	-1.49865600
C	4.23262000	-1.89438900	-0.70404400
H	4.83833500	-2.48570100	-1.41365500
H	4.82429000	-1.85989100	0.23350600
C	2.91050100	-2.62403500	-0.48291700
H	3.09699100	-3.65930000	-0.14049000
H	2.32600700	-2.68065000	-1.41822600
C	0.84026300	-2.77138000	0.87448300
H	0.38077600	-3.08846200	-0.07835200
H	1.13288400	-3.68009800	1.43042500
C	-0.10286200	-1.89032400	1.66598700
H	0.32450700	-1.61181000	2.64607500
H	-1.06659600	-2.39628200	1.84197000
C	-2.36302200	-0.16940900	2.27450900
H	-2.09454000	-0.82587000	3.11845000
H	-3.01268000	-0.71884000	1.57607900
H	-2.95472200	0.66007800	2.69689800
C	-0.44480600	3.89624800	-0.07027300
H	-0.59068700	3.83454600	-1.16367500
H	0.34840300	4.63330500	0.13334000
H	-1.37250300	4.30560400	0.36451500
C	-1.92504900	1.24496200	-0.79926000
H	-1.10371600	0.84377500	-1.43057800
H	-2.22921900	2.19456700	-1.27692900
C	-3.07712600	0.25499500	-0.87383600
C	-4.36761100	0.60262800	-0.42228700
H	-4.55837900	1.60842000	-0.02827900
C	-5.41779400	-0.32566600	-0.48499900
H	-6.41658900	-0.03876400	-0.14015500
C	-5.19646100	-1.61522800	-1.00206300
H	-6.02075800	-2.33337400	-1.05607000
C	-3.92368400	-1.96692800	-1.47646700
H	-3.75449100	-2.95487500	-1.91771700
C	-2.87372500	-1.03271700	-1.41592400
H	-1.90068100	-1.28718900	-1.86605400

2a

Ni	1.58066500	-0.06849200	0.12717800
N	-0.20147300	-0.97183500	0.74370300

H	-0.75498400	-1.24053000	-0.08624000
C	-1.07016900	-0.07497400	1.57639300
H	-0.42336000	0.24243800	2.41885400
N	0.82058200	1.86779200	-0.12597100
H	0.43579000	1.88550500	-1.08491500
C	-1.43689500	1.21870800	0.78074200
H	-2.25788400	1.68446200	1.35979300
N	3.41415700	0.78059600	-0.38328800
H	3.89945600	0.90242600	0.52085100
C	-0.28830300	2.27677300	0.80187200
H	0.15956900	2.25887800	1.81478000
N	2.43365800	-1.94803500	0.42672100
H	2.91535100	-1.87994700	1.33835900
C	2.00017400	2.77831300	-0.11451800
H	2.30710700	2.91384700	0.93964800
H	1.77370600	3.78046900	-0.52661800
C	3.13288700	2.13748100	-0.92229500
H	4.03018000	2.78926000	-0.91599400
H	2.82247000	2.01611700	-1.97693600
C	4.30734500	-0.02476300	-1.26319800
H	3.79380400	-0.14029700	-2.23544300
H	5.25557000	0.52012800	-1.45627300
C	4.62600200	-1.40544400	-0.66958200
H	5.39967400	-1.87241900	-1.30628500
H	5.09730700	-1.28899000	0.32879900
C	3.44356200	-2.38194700	-0.57804200
H	3.82205900	-3.39749900	-0.33577400
H	2.92874000	-2.44792700	-1.55439600
C	1.30931400	-2.90616300	0.59179900
H	0.93198100	-3.15293400	-0.41806500
H	1.62990200	-3.85601700	1.06612000
C	0.20566500	-2.23798700	1.41737300
H	0.58768800	-1.97479500	2.42175900
H	-0.63928400	-2.93904700	1.55488700
C	-2.29576900	-0.79742100	2.17365900
H	-1.98737900	-1.57462900	2.89418500
H	-2.92251700	-1.26715500	1.39795400
H	-2.92810300	-0.08016200	2.72475600
C	-0.80150500	3.70642000	0.53477300
H	-1.17421800	3.83232600	-0.49817200
H	-0.01240700	4.45903500	0.70043000
H	-1.62937900	3.95113500	1.22268900
C	-1.97619700	0.99231400	-0.66621300
H	-1.20191200	0.49484600	-1.28514000

H	-2.12857100	1.99035300	-1.12142500
C	-3.27456900	0.21042500	-0.79225700
C	-4.48183100	0.72243700	-0.27146900
H	-4.48853500	1.69991500	0.22706900
C	-5.67845500	0.00064400	-0.39113900
H	-6.60651200	0.41595000	0.01650000
C	-5.69069700	-1.24635800	-1.03977200
H	-6.62601400	-1.80776700	-1.13518700
C	-4.50082300	-1.76021500	-1.57748300
H	-4.50365700	-2.72224600	-2.10152200
C	-3.30456800	-1.03295700	-1.45575000
H	-2.38373700	-1.42827500	-1.90753300

2b

Ni	1.43677700	-0.08517600	0.00442600
N	-0.34163400	-0.91415200	0.74288000
H	-0.88054400	-1.24373200	-0.07585800
C	-1.23702300	0.03529700	1.49135400
H	-0.60266400	0.44449100	2.29650900
N	0.59412200	1.77787700	-0.48060300
H	0.15893000	1.64183100	-1.40847200
C	-1.62868000	1.23811600	0.56956200
H	-2.42434800	1.76568500	1.12973700
N	3.10644300	0.63139900	-1.03216100
H	3.79402100	0.74523000	-0.27015100
C	-0.48246100	2.29408600	0.43570000
H	0.00250400	2.38624600	1.42224900
N	2.17091000	-2.03704300	0.15621500
H	2.85222900	-1.93513900	0.92565400
C	1.76042200	2.68354300	-0.68535400
H	2.19328700	2.90108800	0.30714800
H	1.47467500	3.64759200	-1.14676600
C	2.77137500	1.97037600	-1.59169900
H	3.67268500	2.59609500	-1.73931600
H	2.32206100	1.80732600	-2.58995800
C	3.70112900	-0.29350300	-2.03887700
H	2.95811800	-0.42689800	-2.84835800
H	4.59902300	0.17100200	-2.49591600
C	4.08122800	-1.65664800	-1.44025900
H	4.66481200	-2.20145900	-2.20466400
H	4.76562500	-1.51618200	-0.58062400
C	2.90341600	-2.55586200	-1.03319400
H	3.27610900	-3.58144400	-0.83252900
H	2.17692100	-2.63130500	-1.86471800

C	1.05924700	-2.92119600	0.59924200
H	0.53215300	-3.27125800	-0.30881700
H	1.42906800	-3.82108700	1.12771000
C	0.08534800	-2.13469800	1.48652000
H	0.57281900	-1.80840500	2.42281400
H	-0.76821100	-2.78233800	1.76051500
C	-2.44565300	-0.66446800	2.14347400
H	-2.12063900	-1.35336600	2.94226500
H	-3.05495300	-1.22608900	1.41668100
H	-3.10224600	0.08580600	2.61628700
C	-1.00678500	3.68251600	0.01908300
H	-1.40484700	3.69869900	-1.01223800
H	-0.21884000	4.45123100	0.08824000
H	-1.81934400	3.99710600	0.69672900
C	-2.23578200	0.86047900	-0.81789100
H	-1.51295700	0.26027600	-1.40855500
H	-2.37041600	1.80094000	-1.38704400
C	-3.56605800	0.12174100	-0.80081400
C	-4.72876300	0.74238500	-0.29790600
H	-4.67720900	1.77043200	0.08212100
C	-5.95585500	0.06329700	-0.28549400
H	-6.84865600	0.56233900	0.10651200
C	-6.04403200	-1.24846500	-0.78243400
H	-7.00317800	-1.77661700	-0.77450000
C	-4.89903100	-1.87191800	-1.30168900
H	-4.96088900	-2.88757900	-1.70742700
C	-3.67205900	-1.18745500	-1.31184800
H	-2.78604900	-1.67463100	-1.74341500
C	2.39655700	0.42051400	1.82934800
O	1.60441200	1.07481700	2.48557800
O	3.52471900	-0.06061100	1.77804400

2c

Ni	1.42525600	-0.07326600	-0.00847100
N	-0.37821000	-0.95698000	0.64569300
H	-0.94365500	-1.28140200	-0.15595700
C	-1.23306100	-0.00175000	1.43270800
H	-0.56302200	0.39372000	2.21779900
N	0.54239800	1.75287600	-0.59250300
H	0.07374900	1.62808100	-1.50449000
C	-1.64186200	1.21395900	0.53672800
H	-2.41503000	1.74310100	1.12615500
N	3.10366700	0.62782700	-1.09173700
H	3.75388400	0.79774100	-0.30827000

C	-0.48837000	2.25876200	0.38025300
H	0.04138600	2.31710200	1.34832200
N	2.19597300	-2.03361500	0.11828200
H	2.82619200	-1.90184400	0.92661600
C	1.70563300	2.65580800	-0.81660900
H	2.13460600	2.89253900	0.17309000
H	1.41564700	3.60880400	-1.29812300
C	2.72835200	1.93288700	-1.70071500
H	3.61118900	2.57764500	-1.87932500
H	2.27922500	1.71678600	-2.68902200
C	3.77163100	-0.29829900	-2.04673500
H	3.06945000	-0.47634700	-2.88355700
H	4.67368000	0.18330400	-2.47788500
C	4.16759700	-1.63292600	-1.39650500
H	4.80276100	-2.17794700	-2.11848800
H	4.80724500	-1.44857400	-0.51080900
C	3.00082900	-2.55841600	-1.01807100
H	3.39660000	-3.56574200	-0.77251200
H	2.31825600	-2.68042700	-1.88069400
C	1.07867800	-2.93251200	0.51266500
H	0.58542700	-3.27421200	-0.41749800
H	1.43997100	-3.83755700	1.03955600
C	0.06944500	-2.17293100	1.38233800
H	0.53623600	-1.83934700	2.32633100
H	-0.77280100	-2.84198000	1.64001700
C	-2.42662200	-0.69202300	2.12143000
H	-2.08232100	-1.39627900	2.89861500
H	-3.07035500	-1.23570600	1.41077600
H	-3.05359000	0.06133000	2.62831600
C	-1.01303200	3.66202700	0.01843100
H	-1.46528100	3.70356900	-0.98976600
H	-0.21107000	4.41822200	0.05965500
H	-1.78337200	3.97409200	0.74476300
C	-2.29264100	0.85591400	-0.83595000
H	-1.59045300	0.25918300	-1.45409100
H	-2.43927900	1.80388300	-1.38978100
C	-3.62497600	0.12241700	-0.78647600
C	-4.76902500	0.74254100	-0.24182100
H	-4.70110800	1.76682900	0.14557700
C	-5.99749600	0.06750200	-0.19579200
H	-6.87554300	0.56604200	0.22887100
C	-6.10598400	-1.23983600	-0.70030100
H	-7.06611400	-1.76519000	-0.66579400
C	-4.98039200	-1.86246200	-1.26131500

H	-5.05876700	-2.87452200	-1.67324000
C	-3.75196700	-1.18191700	-1.30528200
H	-2.88213800	-1.66822100	-1.76950900
C	2.16078700	0.48695500	1.75583300
O	1.67666800	1.18160000	2.64778300
O	3.46648600	-0.01700600	1.94654900
H	3.76404500	0.30307100	2.83986700

2d

Ni	1.15130700	-0.02590500	-0.03067300
N	-0.63930600	-0.88650200	0.67640800
H	-1.22004800	-1.16707900	-0.13330700
C	-1.48943200	0.03901400	1.51161500
H	-0.81550200	0.41110400	2.30878100
N	0.25603000	1.83413400	-0.48338800
H	-0.24003300	1.70927900	-1.38236300
C	-1.91882900	1.27831100	0.65963500
H	-2.68164400	1.78779600	1.27761500
N	2.73851900	0.70183700	-1.24396600
H	3.55968900	0.79528000	-0.61579000
C	-0.77209100	2.33028800	0.50789300
H	-0.24036900	2.39506700	1.47695200
N	1.81679600	-2.00798500	-0.11837100
H	2.60292900	-2.00064100	0.57280600
C	1.40502300	2.75194300	-0.74727800
H	1.89980300	2.96348200	0.21781200
H	1.07444400	3.71741500	-1.17017200
C	2.35471900	2.06533500	-1.73179100
H	3.24604200	2.69322800	-1.91477200
H	1.84483100	1.93826800	-2.70473300
C	3.15117700	-0.19781900	-2.37085200
H	2.30286200	-0.25436900	-3.07850300
H	3.99379200	0.27105100	-2.91662500
C	3.54592800	-1.60590700	-1.90958200
H	4.00558600	-2.11848200	-2.77398600
H	4.33096700	-1.55919000	-1.13104000
C	2.38232100	-2.47648700	-1.42047000
H	2.72769400	-3.52332900	-1.30783400
H	1.56656400	-2.48517600	-2.16855400
C	0.72282100	-2.89948100	0.37223600
H	0.13582600	-3.22858600	-0.50579500
H	1.13153000	-3.81001100	0.84824200
C	-0.18970800	-2.14718600	1.34328300
H	0.34537000	-1.87211600	2.27016500

H	-1.04388600	-2.78740200	1.62625700
C	-2.66025400	-0.68697500	2.20021900
H	-2.29735800	-1.40318300	2.95670000
H	-3.30546000	-1.21853500	1.48279700
H	-3.28909400	0.04659000	2.73190800
C	-1.29538300	3.73706900	0.16156800
H	-1.73113400	3.79202300	-0.85200500
H	-0.50195500	4.49917400	0.23357800
H	-2.08072600	4.02830500	0.87965000
C	-2.59328300	0.95435400	-0.71159700
H	-1.89224600	0.40672000	-1.37663800
H	-2.78531100	1.91928600	-1.21961100
C	-3.89571800	0.16956500	-0.66115700
C	-5.04712000	0.71839100	-0.05466000
H	-5.01096700	1.72323800	0.38404000
C	-6.24814400	-0.00300800	-0.02456900
H	-7.13573600	0.43757900	0.44096500
C	-6.31987500	-1.28426500	-0.60321400
H	-7.26075700	-1.84328400	-0.58297700
C	-5.18565100	-1.83531000	-1.22334200
H	-5.24145100	-2.82177800	-1.69520500
C	-3.98470800	-1.10890900	-1.25308600
H	-3.11327800	-1.52988800	-1.77566900
C	1.85738700	0.48638700	1.66410700
O	2.20575300	0.92817600	2.66901900
O	3.97843700	-1.52439600	1.65984400
H	4.44065900	-2.07603900	2.32304900
H	4.62486700	-0.82772100	1.36957500
O	5.31517400	0.67677200	0.58572000
H	6.16060800	0.52583700	0.10991400
H	5.54202700	1.34475400	1.26843200

TS1-2

Ni	1.35623400	-0.13083200	-0.16810200
N	-0.37477500	-0.94199100	0.67219800
H	-0.95684700	-1.29048700	-0.10762200
C	-1.22460400	0.02614200	1.44787500
H	-0.55585600	0.42981300	2.23040700
N	0.54948800	1.75141900	-0.59246000
H	0.08115800	1.63585800	-1.50663000
C	-1.63578900	1.23155900	0.53984900
H	-2.40993100	1.76758200	1.12208700
N	3.07905200	0.60579700	-1.08594600
H	3.72984600	0.77428500	-0.30271800

C	-0.48348000	2.27388200	0.36612400
H	0.03577100	2.35979700	1.33827700
N	2.18157900	-2.01806200	0.14804900
H	2.82581400	-1.89226300	0.94458200
C	1.71579500	2.65024500	-0.82086700
H	2.14911900	2.89501300	0.16624500
H	1.43354300	3.60451200	-1.30556500
C	2.73487200	1.91648300	-1.69988900
H	3.62847100	2.54907800	-1.87128800
H	2.28786900	1.70786700	-2.69028600
C	3.76097500	-0.32064700	-2.03433200
H	3.06646300	-0.50246700	-2.87600900
H	4.66789900	0.16000200	-2.45723700
C	4.15085100	-1.65261300	-1.37584300
H	4.78113700	-2.20710000	-2.09506500
H	4.79705000	-1.46587800	-0.49465700
C	2.98107400	-2.56785600	-0.98425300
H	3.37158400	-3.57452900	-0.72650800
H	2.29343600	-2.69338400	-1.84146400
C	1.07821500	-2.91993000	0.57534600
H	0.57667400	-3.28319400	-0.34137400
H	1.44987700	-3.81079700	1.11957000
C	0.07582300	-2.14128600	1.43537300
H	0.54989600	-1.78896000	2.36999400
H	-0.76262800	-2.80518900	1.71930300
C	-2.41898100	-0.64688000	2.15356300
H	-2.07589300	-1.34283500	2.93868600
H	-3.06562600	-1.19779900	1.45127400
H	-3.04275400	0.11566600	2.65083900
C	-1.01011000	3.67131800	-0.01879400
H	-1.45263100	3.69310300	-1.03163000
H	-0.21045400	4.43036800	0.01452600
H	-1.78864200	3.99375600	0.69429500
C	-2.28452500	0.85312600	-0.82836900
H	-1.57871400	0.24730500	-1.43247400
H	-2.43118700	1.79237500	-1.39671400
C	-3.61794500	0.12231100	-0.76690000
C	-4.76200700	0.75388900	-0.23551200
H	-4.69331700	1.78559500	0.13175800
C	-5.99144300	0.08150100	-0.17782300
H	-6.86949700	0.58925500	0.23581600
C	-6.10069600	-1.23519500	-0.65718500
H	-7.06144800	-1.75877400	-0.61374600
C	-4.97519100	-1.86951700	-1.20517400

H	-5.05442600	-2.88912500	-1.59788900
C	-3.74582100	-1.19147400	-1.26128600
H	-2.87621000	-1.68697600	-1.71573700
C	2.65773700	0.58212100	2.24317200
O	1.75476600	1.12406100	2.79680700
O	3.70898200	0.10576300	1.93075200