Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting information

Designing Dual-Atom Cobalt Catalysts Anchored on Amino-Functionalized MOFs for Efficient CO_2 Photoreduction

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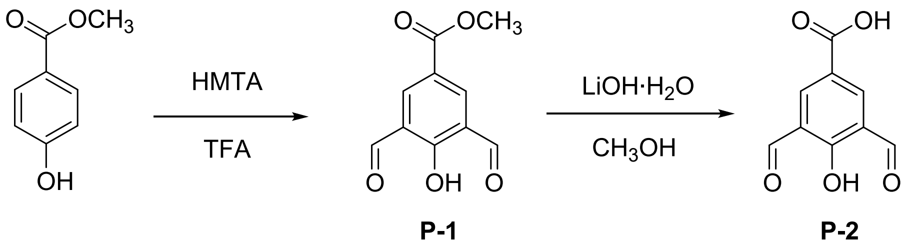
1. Materials and Instruments

All chemicals were purchased from commercial ways and used without further purification. The water used was prepared by using a Milli-Q ultrapure water purification system. Powder X-ray diffraction (PXRD) tests were conducted on a SmartLab 9 KW X-ray diffractometer (Rigaku, Japan). Scanning electron microscopy (SEM) images were collected on a scanning electron microscope Quanta250FEG (FEI, America). High-resolution transmission electron microscopy (HRTEM) images and element mapping were collected on a Talos F200X (FEI, America). Fourier transform infrared (FT-IR) spectra were analyzed on a PerkinElmer Frontier Mid-IR FT-IR spectrometer using KBr pellets. UV-Vis DRS was acquired on a UV-3600 spectrophotometer (Shimadzu, Japan) with Ba_2SO_4 as the background. X-ray photoelectron spectroscopy (XPS) were performed on an ESCALAB250Xi X-ray spectrometer (Thermo Scientific, America) and the test data were calibrated versus C 1s binding energy (284.6 eV). The contents of Co and Zr were quantified by inductively coupled plasma-mass spectrometer (ICP-MS, iCAP RQ, Germany). CO_2 adsorption measurement was carried out using a multi-station specific surface micropore and vapor analyzer (BELSORP-Mas, MicrotracBEL, Japan) at 298 K. In-situ FTIR spectra were recorded on Nicolet Is50 FTIR (Thermo Scientific, America). An F-4600 fluorescence spectrometer (Hitachi, Japan) was employed to demonstrate the quenching mode of the excited photosensitive part of the catalyst. ^{1}H NMR spectra were obtained on a Bruck AVANCE III HD spectrometer at 400 MHz, and referenced to the proton resonance resulting from DMSO-d_6 (δ 2.50). Amounts of CO evolution were detected by Shimadzu GC-2014 gas chromatography equipped with a thermal conductivity detector (TCD) and a flame conductivity detector (FID). Isotope labeling experiment was performed in $^{13}CO_2$ atmosphere, and the products were analyzed by gas chromatography- mass spectrometer (GC-MS, Agilent 7980B). Mott-Schottky, Transient photocurrent response (TPR) and electrochemical impedance (EIS) measurements were operated on a CHI760E workstation (Chenhua Instrument, Shanghai, China) equipped with a standard three-electrode system, with catalyst-coated Fluorine-doped tin oxide transparent conductive film glass (FTO) as working electrode, Pt plate as counter electrode, and Ag/AgCl as reference electrode. 2 mg catalyst was dispersed in a mixture of 960 μL ethanol and 40 μL Nafion, and then 100 μL suspension was added dropwise onto the surface of a FTO plate with an area of 1×1 cm and dried naturally to obtain the working electrode. 0.5 M Na_2SO_4 solution was used as electrolyte. Mott-Schottky plots were measured at frequencies of 500, 1000, and 1500 Hz, respectively. Photo responsive signals were recorded under chopped light with a bias potential of + 0.6 V. EIS tests were performed with a bias potential of + 0.6 V.

2. Synthesis and Characterization of Ligand and Complexes

2.1 Synthesis of methyl 3,5-diformyl-4-hydroxybenzoate (P-1) and 3,5-diformyl-4-hydroxybenzoic acid (P-2)



Scheme S1. Synthesis of P-1 and P-2.[1]

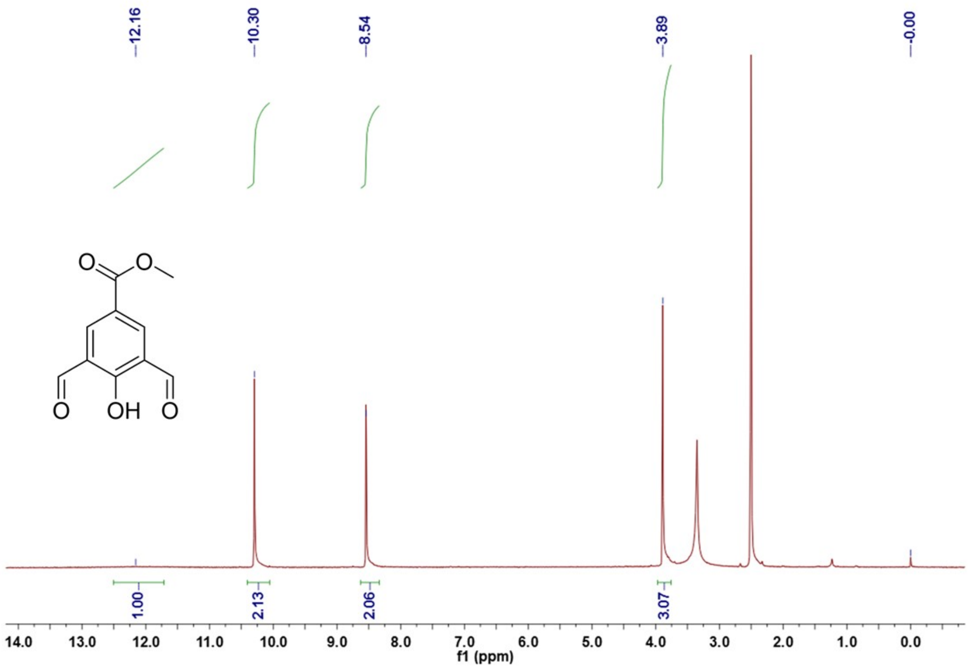


Figure S1. ^{1}H NMR spectrum of P-1. [400 MHz, DMSO-d$_6$, δ 12.16 (s, 1H), 10.30 (s, 2H), 8.54 (s, 2H), 3.07 (s, 3H)].

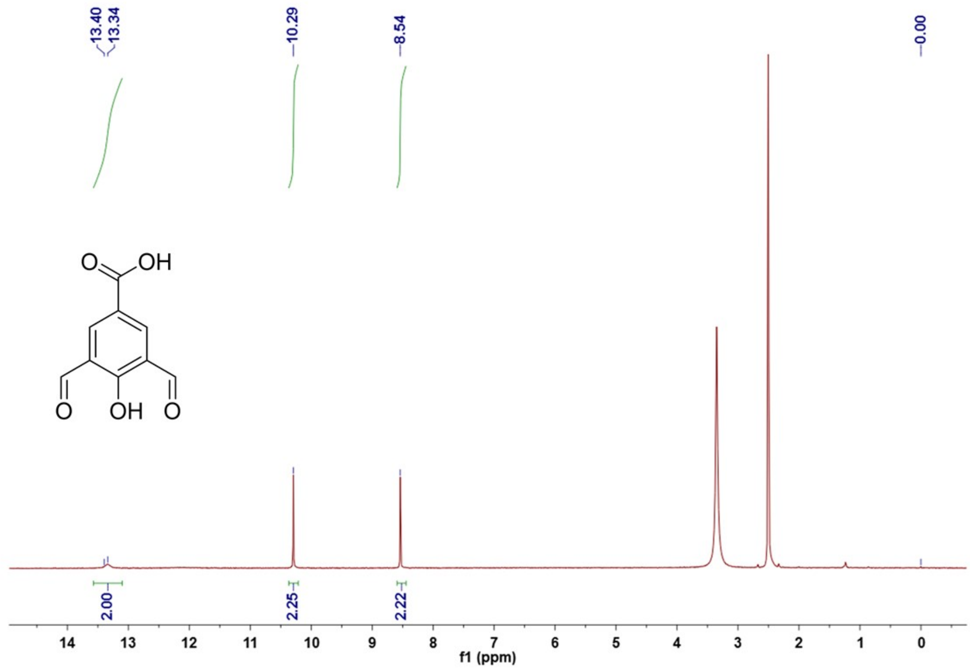
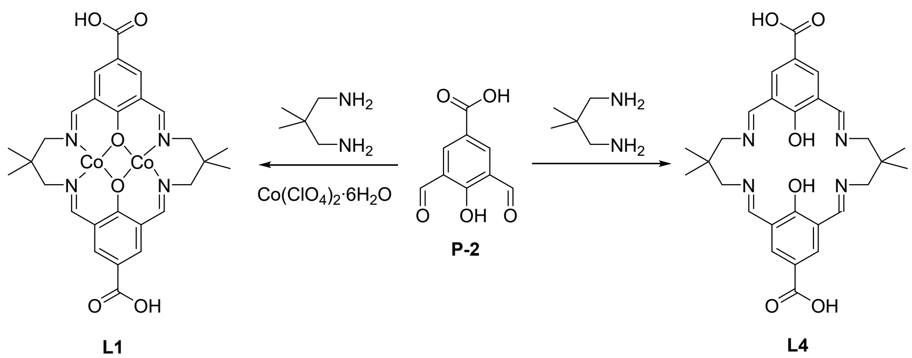


Figure S2. ^{1}H NMR spectrum of P-2. [400 MHz, DMSO-d_6, δ 10.34-10.40 (d, 2H), 10.29 (s, 2H), 8.54 (s, 2H)].

2.2 Synthesis of L1 and L4

L1 was synthesized in accordance with previously reported literatures.[2, 3] L4 was synthesized through a Schiff-based reaction. P-2 was dissolved in ethanol, to which 1 eq 2, 2-dimethyl-1, 3-malonediamine was added. The mixed solution was stirred at room temperature for 24 h. Finally, the orange powder was collected by centrifugation and dried.



Scheme S2. Synthesis of L1 and L4.

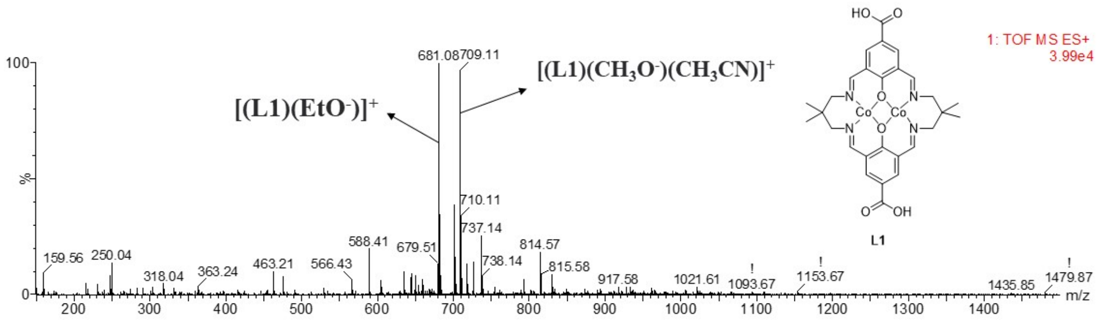


Figure S3. Mass of L1 in CH_3OH solution, m/z =681.08 $[(L1)(EtO^-)]^+$, *m/z* = 709.11 $[(L1)(CH_3O^-)(CH_3CN)]^+$.

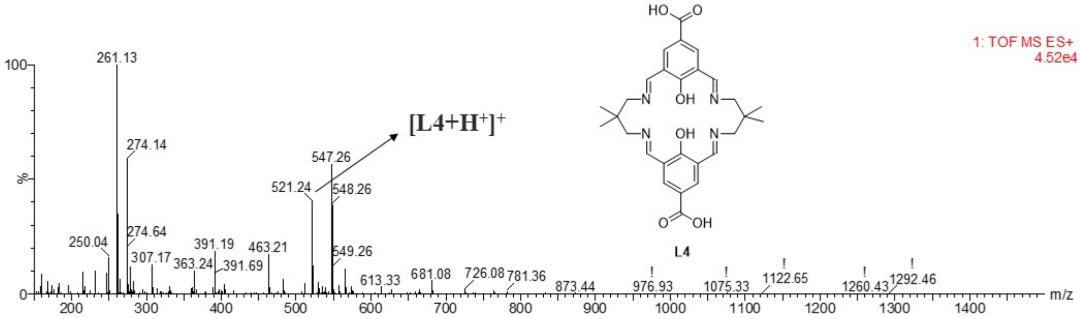
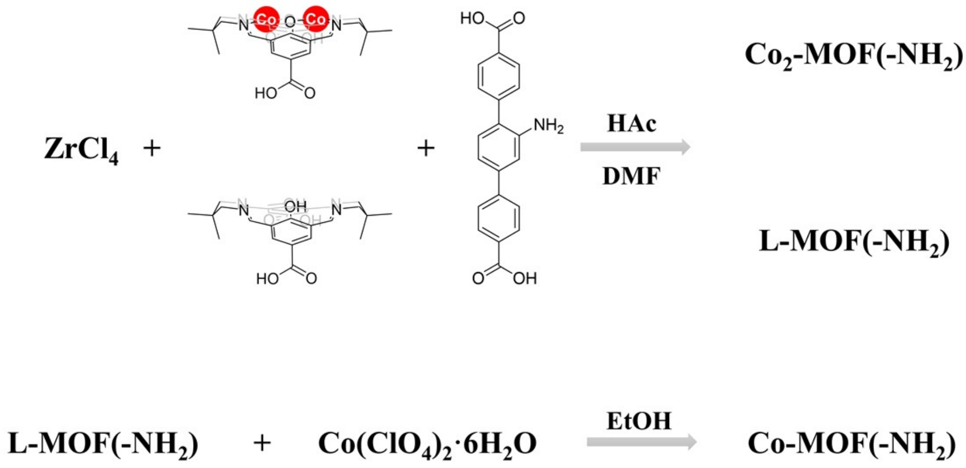


Figure S4. Mass spectrum of L4 in CH_3CN solution, *m/z* =521.24 $[L4+H^+]^+$.

3. Synthesis and Characterization of Co_2-MOF(-NH_2), Co-MOF(-NH_2), L-MOF(-NH_2) and Co_2-MOF



Scheme S3. Synthesis of Co_2-MOF(-NH_2), Co-MOF(-NH_2) and L-MOF(-NH_2).

The photocatalyst Co_2-MOF(-NH_2) required for this work was synthesized by a solvothermal reaction with slight modification to a previously reported procedure.[4, 5]

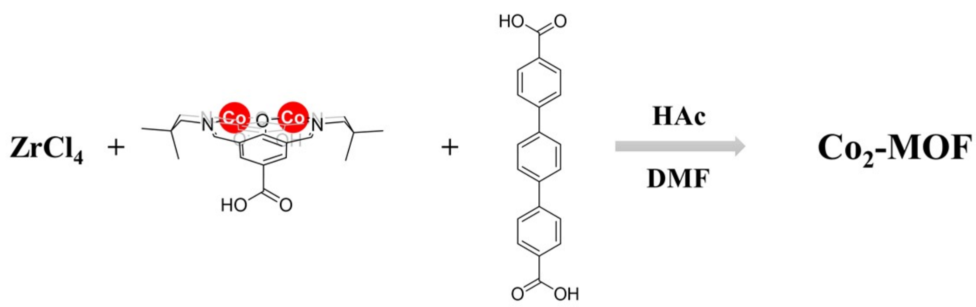
5.2 mg $ZrCl_4$ (0.0222 mmol), 6.6 mg L1 (0.0074 mmol), 12.3 mg 2'-amino-[1,1':4',1"-terphenyl]-4,4"-dicarboxylic acid (L2, 0.0370 mmol), 600 μL acetic acid were dissolved in 6 mL DMF by ultrasound. Then the mixture was transferred into a 15 mL vial, which was sealed and heated at 120 °C for 24 h. After cooling to room temperature, the light yellow powder was collected by centrifugation, washed with DMF and acetonitrile for 3 times. In addition, by changing the ratio of L1 and L2, we have synthesized a series of Co_2-MOFs(-NH_2). The dosage of the chemicals was listed below:

Table S1. The dosage of the chemicals during the synthesis of Co_2-MOFs(-NH_2) with different ratios of L1 and L2.

Samples	L1:L2	m ($ZrCl_4$) (mg)	m (**L1**) (mg)	m (**L2**) (mg)
Co_2-MOF(-NH_2)-1	1:1		19.9	7.4
Co_2-MOF(-NH_2)-2	1:2		13.3	9.9
Co_2-MOF(-NH_2)	1:5	5.2	6.6	12.3
Co_2-MOF(-NH_2)-10	1:10		3.6	13.4
Co_2-MOF(-NH_2)-20	1:20		1.9	14.1

The preparation of L-MOF(-NH_2) follows the same method as Co_2-MOF(-NH_2) except substitute 3.8 mg L4 (0.0074 mmol) for 6.6 mg L1.

The mononuclear Co-MOF(-NH_2) was prepared with the reaction of $Co(ClO_4)_2 \cdot 6H_2O$ and L-MOF(-NH_2): 20 mg L-MOF(-NH_2) was added to a mixed solution containing 2 mg $Co(ClO_4)_2 \cdot 6H_2O$ and 5 mL methanol and then stirred at room temperature for 24 h. Finally, the yellow powder was collected by centrifugation and dried.



Scheme S4. Synthesis of Co_2-MOF.

The preparation of Co_2-MOF follows the same method as Co_2-MOF(-NH_2) except substitute 11.8 mg [1,1':4',1''-terphenyl]-4,4''-dicarboxylic acid (L3, 0.0370 mmol) for 12.3 mg L2.

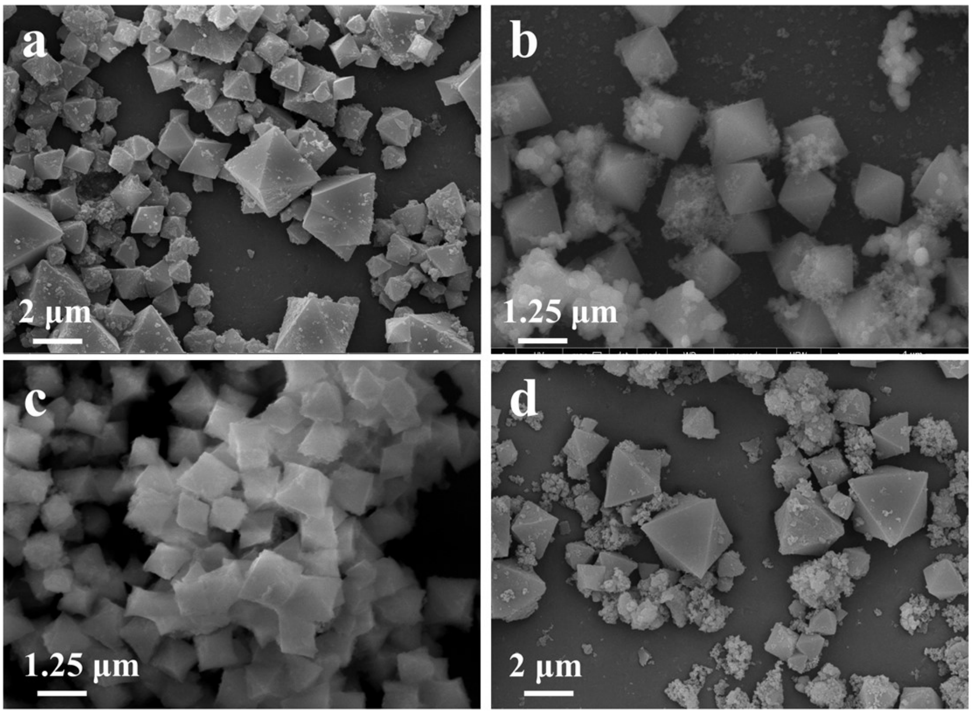


Figure S5. SEM images of Co_2-MOF(-NH_2), Co-MOF(-NH_2), L-MOF(-NH_2) and Co_2-MOF.

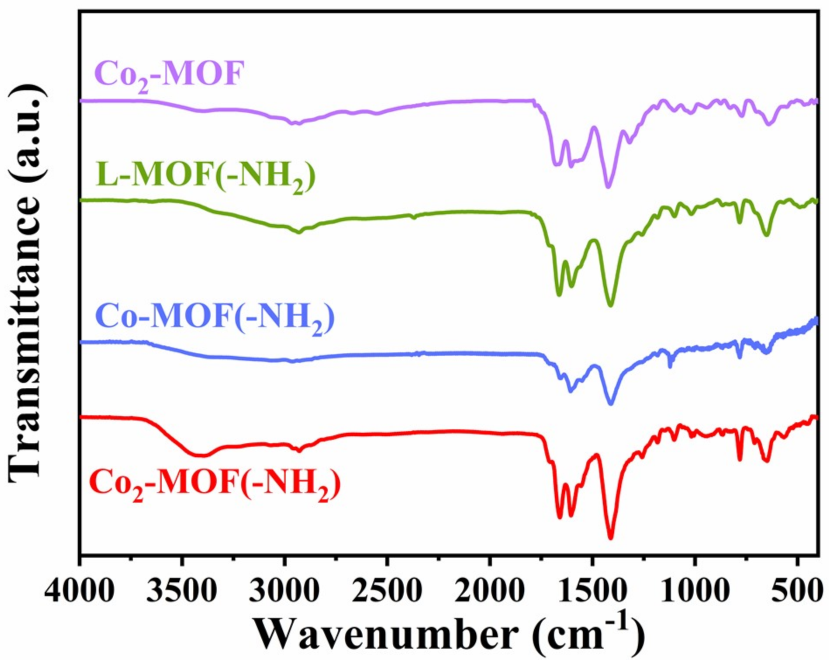


Figure S6. IR spectrum of Co$_2$-MOF(-NH$_2$) (red), Co-MOF(-NH$_2$) (blue), L-MOF(-NH$_2$) (green) and Co$_2$-MOF (purple).

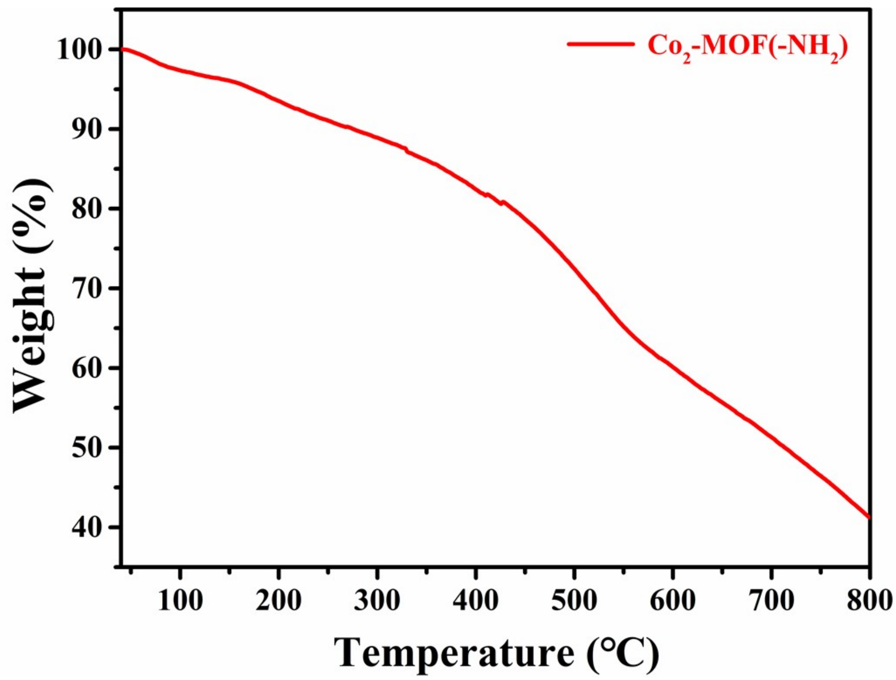


Figure S7. TG curves of Co$_2$-MOF(-NH$_2$).

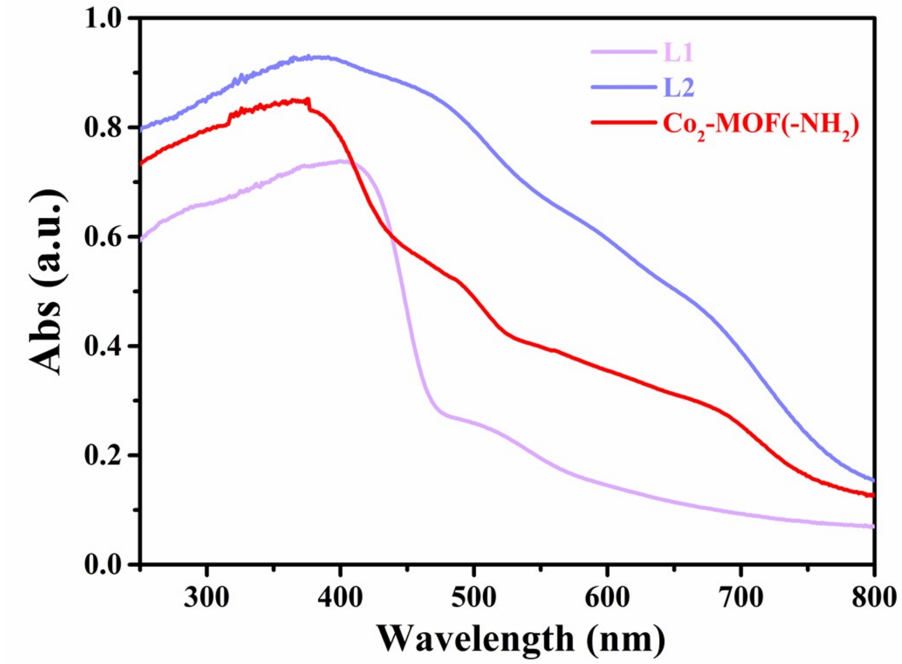


Figure S8. UV-Vis DRS of L1, L2 and Co_2-MOF(-NH_2).

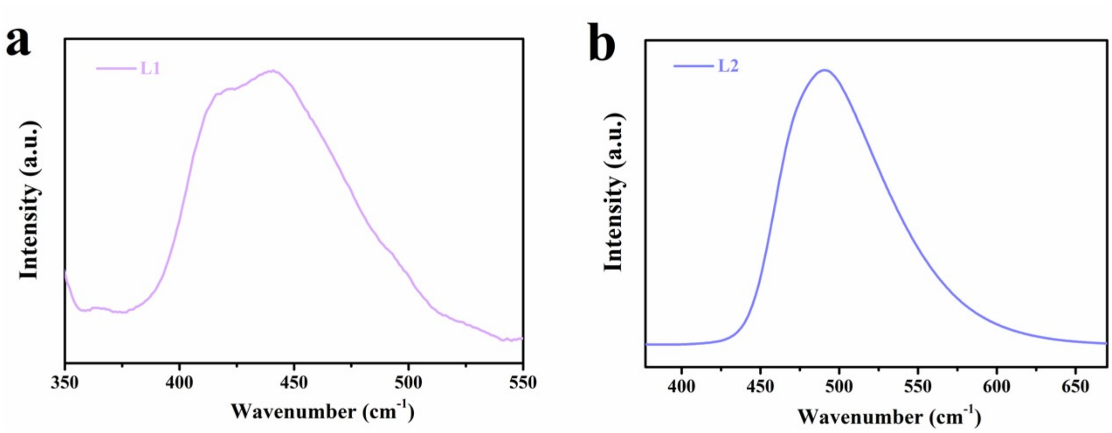


Figure S9. The PL spectra of L1 and L2.

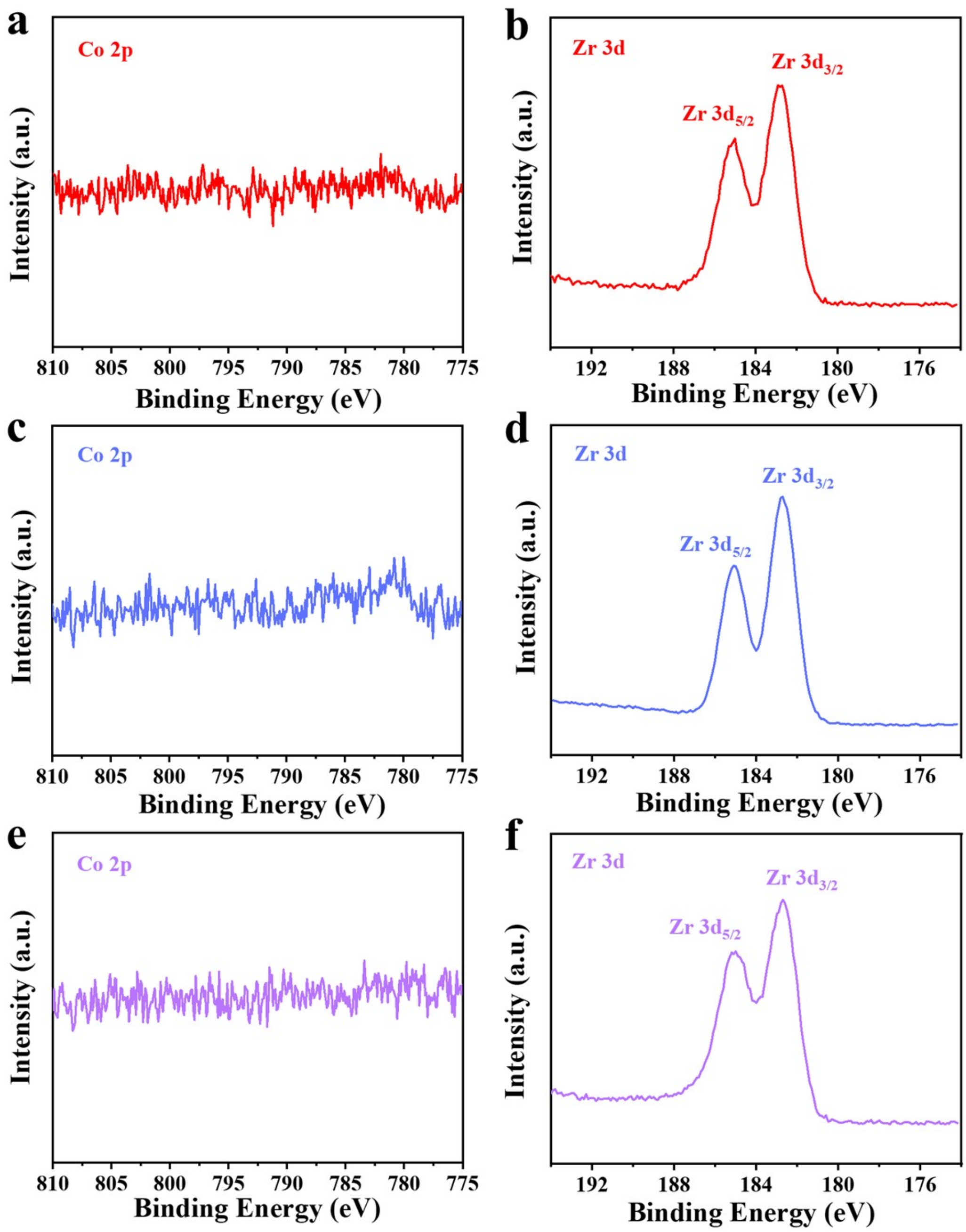


Figure S10. X-ray photoelectron spectroscopy (XPS) of Co 2p and Zr 3d for Co_2-MOF(-NH_2) (a, b), Co-MOF(-NH_2) (c, d) and Co_2-MOF (e, f).

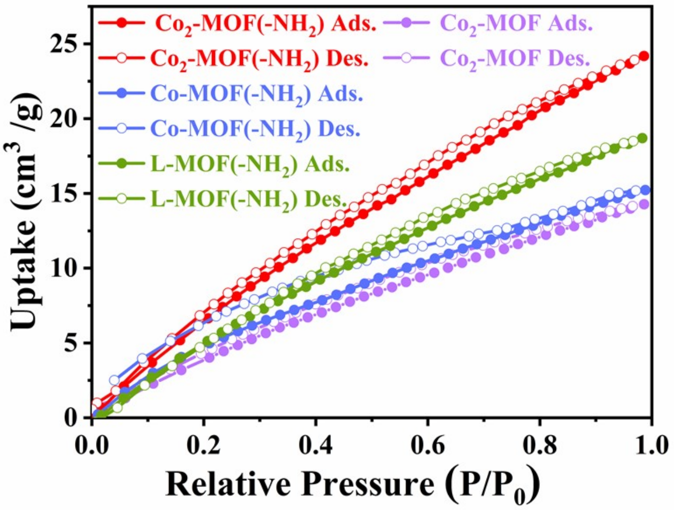


Figure S11. CO_2 adsorption/desorption isotherms of Co_2-MOF(-NH_2) (red), Co-MOF(-NH_2) (blue), L-MOF(-NH_2) (green) and Co_2-MOF (purple) at 298 K.

4. Photo-catalytic CO_2 reduction experiment

The photocatalytic CO_2 reduction reaction was conducted in a 17.5 mL special quartz tube with a rubber hose. 1 mg Co_2-MOF(-NH_2), Co-MOF(-NH_2), L-MOF(-NH_2) or Co_2-MOF as catalyst was dispersed in a 5 mL mixed solution of CH_3CN and H_2O (v/v =4/1) containing 0.025 M BIH as sacrificial reductant. The reaction system was degassed with Ar to remove O_2 and other gases, and pumped with CO_2 for 30 minutes until saturated. Then a 300 W Xe lamp with full spectrum was used as the light source. After irradiation for 10 h at room temperature, the gas products were detected by gas chromatograph (GC-2014, Shimadzu, Japanese). Each photocatalytic reaction is repeated at least 3 times to ensure data reliability.

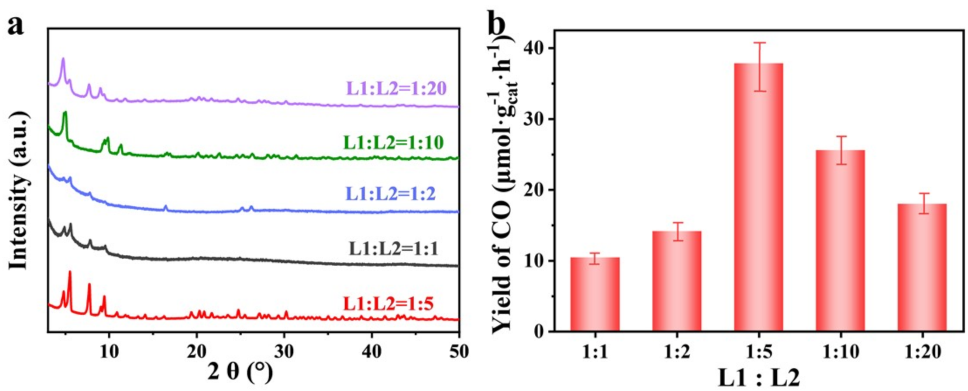


Figure S12. (a) PXRD patterns and (b) CO production of Co_2-MOF(-NH_2) with ratio of L1 and L2 from 1:1 to 1:20.

Table S2. The ICP analysis of MOFs

Samples	ω_{Co} (%)	ω_{Zr} (%)	n_{Co}: n_{Zr}
Co_2-MOF(-NH_2) (L1: L2 = 1:20)	0.79	30.56	1: 25.0
Co_2-MOF(-NH_2) (L1: L2 = 1:10)	1.05	19.69	1: 12.3
Co_2-MOF(-NH_2) (L1: L2 = 1: 5)	1.55	12.32	1: 9.1
Co_2-MOF(-NH_2) (L1: L2 = 1: 2)	2.80	19.42	1: 4.5
Co_2-MOF(-NH_2) (L1: L2 = 1: 1)	3.19	11.16	1: 2.3
Co-MOF(-NH_2)	0.88	18.02	1:13.2
Co_2-MOF	1.24	20.52	1: 10.7
Co_2-MOF(-NH_2) (after reaction)	1.30	22.84	1: 11.3

Table S3. The ICP analysis of Co in Co-MOF(-NH_2).

Samples (inventory ratio)	ω_{Co} (%)
Co-MOF(-NH_2) (L-MOF(-NH_2): $Co(ClO_4)_2 \cdot 6H_2O$ = 10:1)	0.88
Co-MOF(-NH_2) (L-MOF(-NH_2): $Co(ClO_4)_2 \cdot 6H_2O$ = 5:1)	0.92
Co-MOF(-NH_2) (L-MOF(-NH_2): $Co(ClO_4)_2 \cdot 6H_2O$ = 2.5:1)	0.92

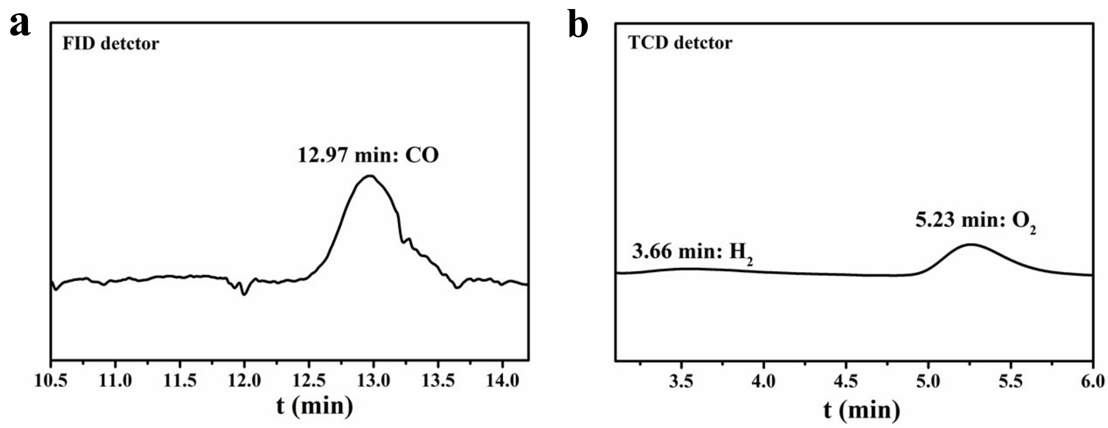


Figure S13. Gas chromatography (GC) of the Co_2-MOF (-NH_2) photocatalysis CO_2 reduction.

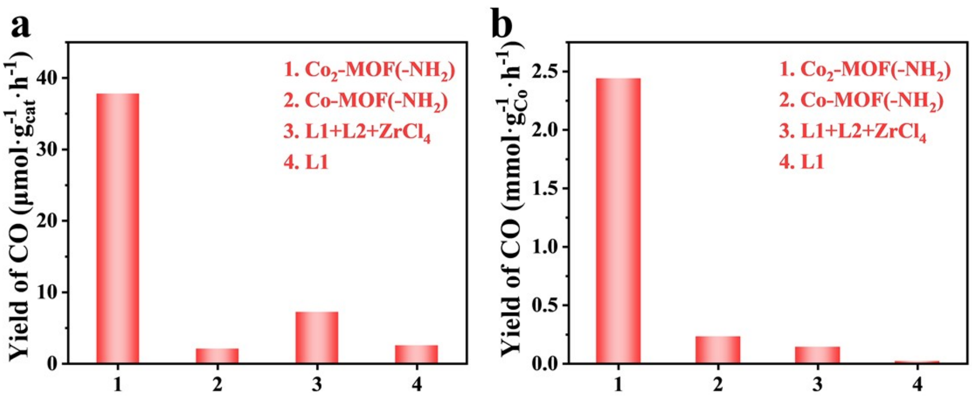


Figure S14. CO production vs. cat. (a) and Co content (b) of Co_2-MOF(-NH_2), Co-MOF(-NH_2), the mixed sample (L1, L2 and $ZrCl_4$) and L1 (in homogeneous phase).

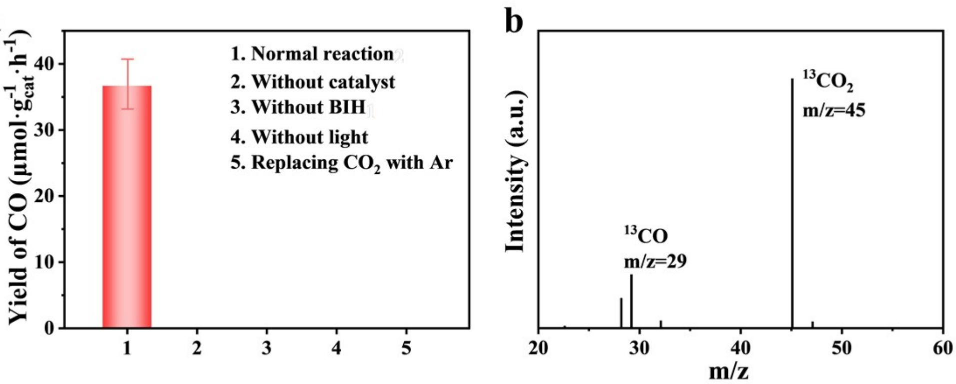


Figure S15. (a) CO production of Co_2-MOF(-NH_2) compared the corresponding blank experiments; (b) mass spectrum of produced ^{13}CO via isotope $^{13}CO_2$ reduction under visible light.

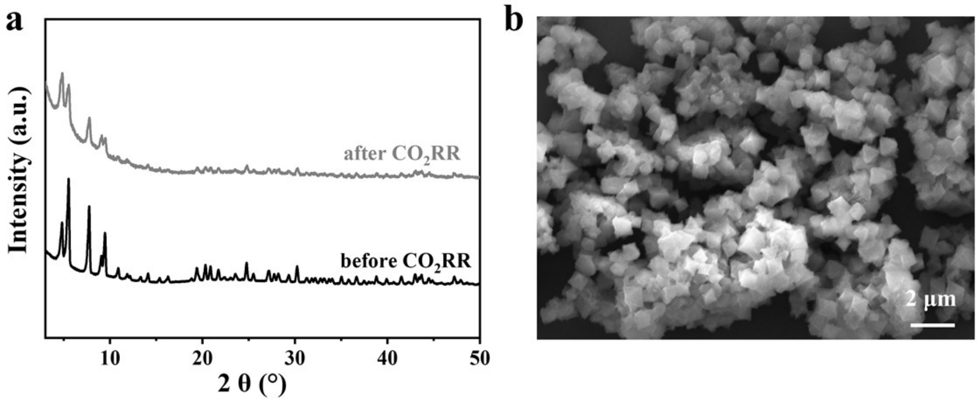


Figure S16. PXRD patterns and SEM images of Co_2-MOF(-NH_2) after CO_2RR.

Table S4. A comparison of photocatalytic CO_2 reduction activities of recently reported MOF-based catalysts without additional photosensitizer.

Catalyst	Reaction agent	Light source	Major product	Yield ($\mu mol \cdot g^{-1} \cdot h^{-1}$)	Ref.
Co_2-MOF(-NH_2)	CH_3CN/H_2O, BIH	300 W Xe lamp, 780 nm > λ > 320 nm	CO	37.8	**This work**
PCN-222	CH_3CN, TEOA	300 W Xe lamp, 800 nm > λ > 420 nm	$HCOO^-$	60	Jiang et al.[6]
NNU-28	CH_3CN, TEOA	300 W Xe lamp, 800 nm > λ > 420 nm	$HCOO^-$	52.8	Chen et al.[7]
MOF-525-Zn	CH_3CN, TEOA	300 W Xe lamp, 800 nm > λ > 420 nm	CO	200.6	Ye et al.[8]
Re-MOF-NH_2	TEA	300 W Xe lamp, 700 nm > λ > 400 nm	CO	1.5	Ryu et al.[9]
Ag⊂Re_3-MOF	CH_3CN, TEA	300 W Xe lamp, 700 nm > λ > 400 nm	CO	7 (TON)	Yaghi et al.[10]
Zr-SDCA-NH_2	CH_3CN, TEOA	300 W Xe lamp, 800 nm > λ > 420 nm	$HCOO^-$	96.2 ($\mu mol\ h^{-1}\ mmol_{MOF}^{-1}$)	Sun et al.[11]
Zn-MOF	CH_3CN, MeOH, TEOA	120 W Xe lamp, 800 nm > λ > 420 nm	CO	117.8 (TON)	Ye et al.[12]

Zn_2GeO_4/Mg-MOF-74	CH_3CN, H_2O	300 W Xe lamp, 1100 nm > λ > 200 nm	CO	1.44	Zhao et al.[13]
UiO-68(Zr)-F	Acetone, TEOA	300 W Xe lamp, 780 > λ > 400 nm	CO	2.1	Wei et al.[14]
UiO-68(Zr)-NH_2				2.2	
UiO-68(Zr)-CH_3				10.9	
UiO-68(Zr)-OCH_3				19.7	
AUBM-4	CH_3CN, TEOA	150 W Xe lamp, 800 nm > λ > 420 nm	$HCOO^-$	366	Mahmoud et al.[15]
mPT-Cu/Re	DMA, H_2O, BIH	13.9 W Solid state plasma light, 700 nm > λ > 350 nm	CO	1328 (TON)	Lin et al.[16]

5. Photophysical and Electrochemical Data

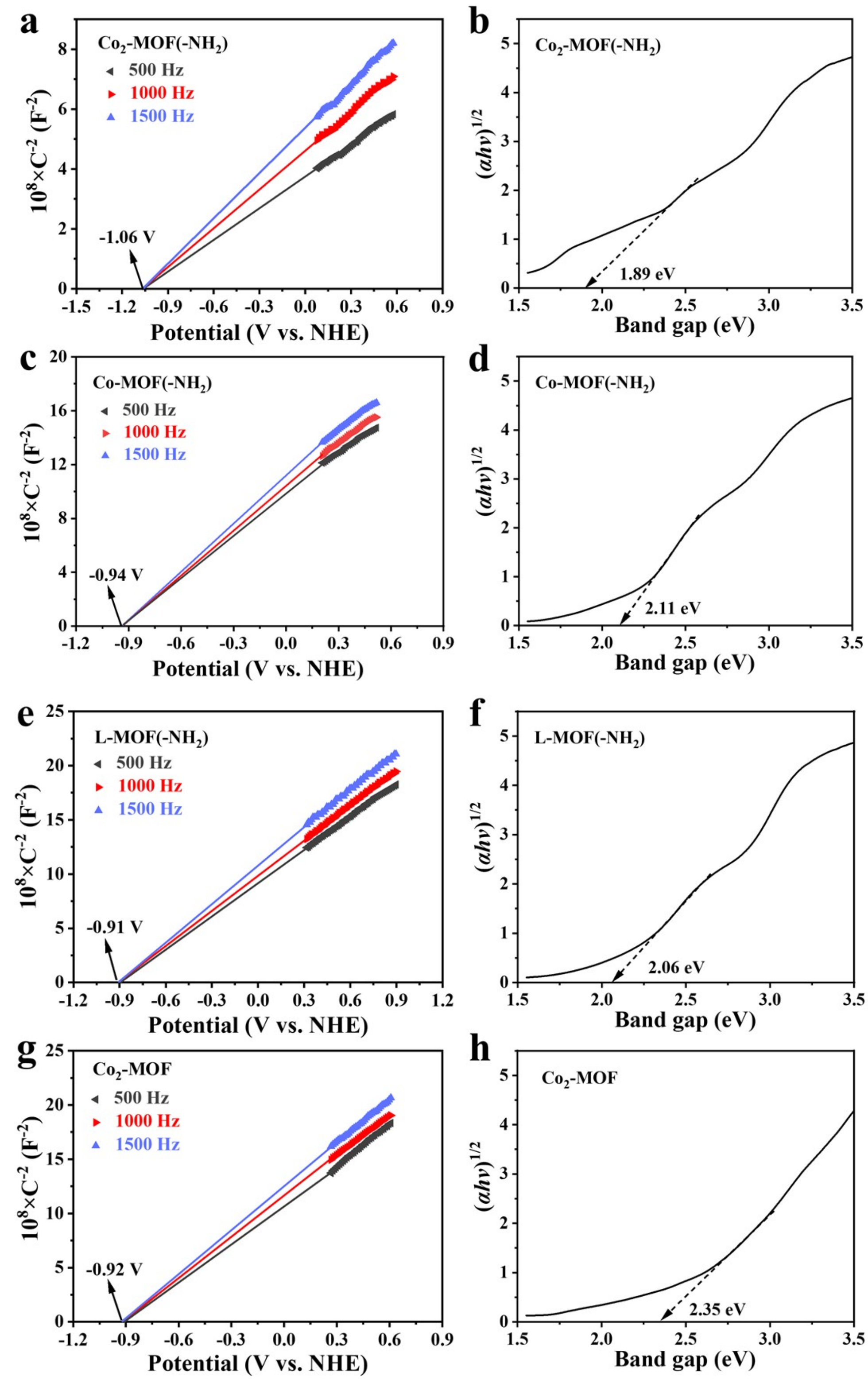


Figure S17. Mott-Schottky plots in 0.5 M Na_2SO_4 aqueous solution and Tauc plots of $(\alpha h\nu)^{1/2}$ vs. photon energy of (a) Co_2-MOF(-NH_2), (b) Co-MOF(-NH_2), (c) L-MOF(-NH_2) and (d) Co_2-MOF.

6. Mechanism Investigations

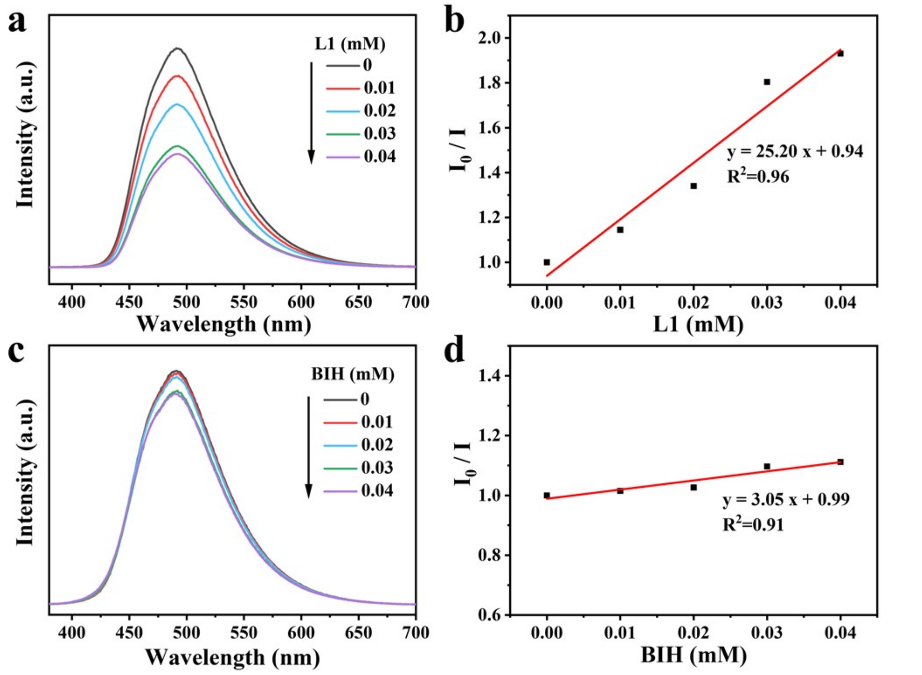


Figure S18. Fluorescence spectra of a CH_3CN/H_2O (v:v = 4:1) solution containing 0.4 mM L2 in the presence of 0-0.04 mM L1 (a) or BIH (c), respectively. Linear plots of fluorescent intensity ratio in the absence (I_0) and presence (I) of L1 (or BIH) versus the concentrations of L1 (b) or BIH (d).

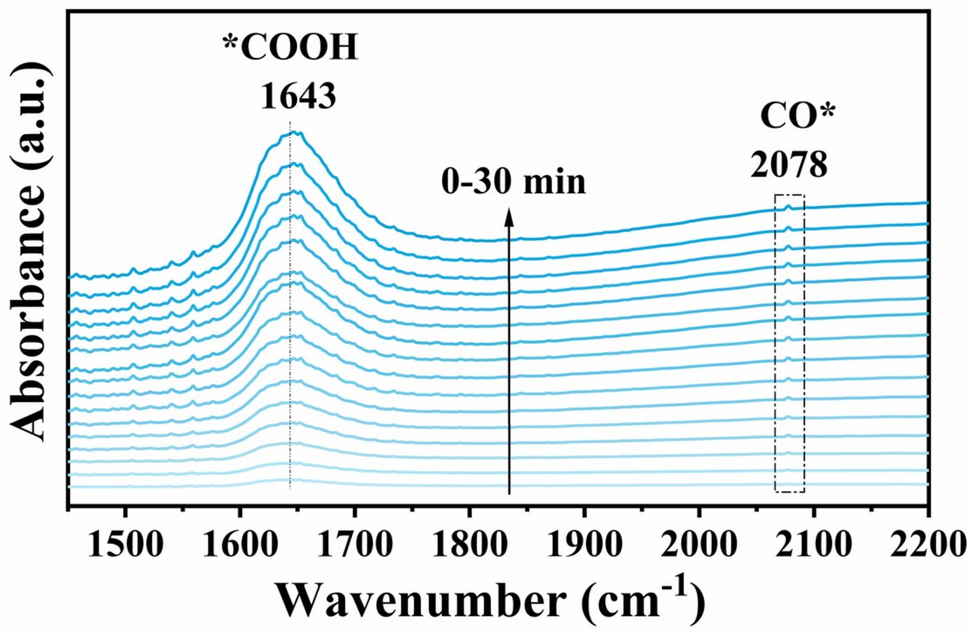


Figure S19. In situ FTIR spectra of Co-MOF($-NH_2$).

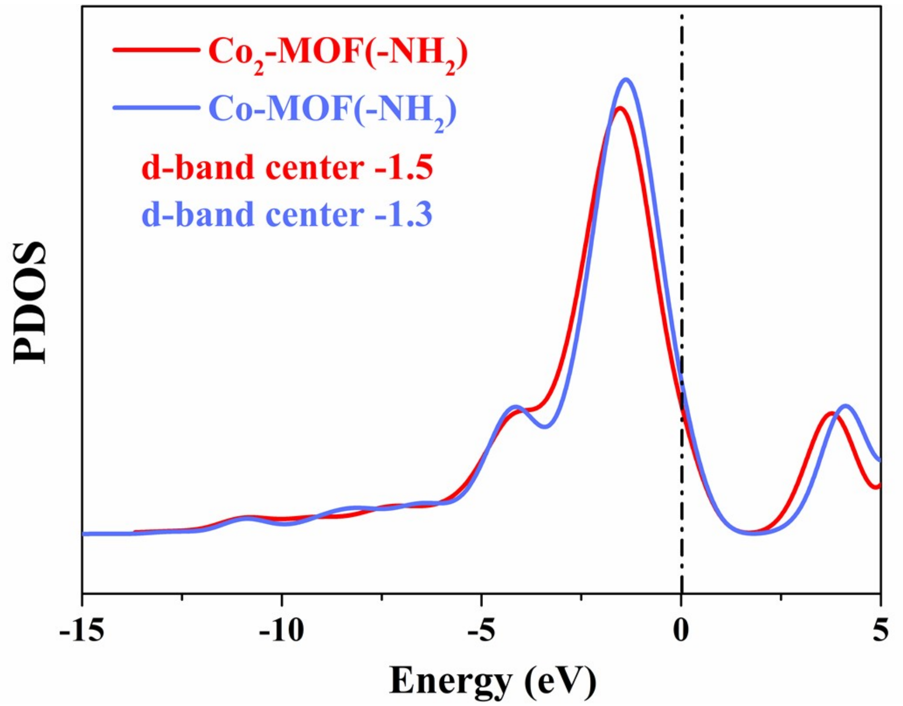


Figure S20. PDOS of d band center value of Co on Co_2-MOF(-NH_2) and Co-MOF(-NH_2).

7. Density Functional Theory (DFT) Calculations.

The density functional theory calculations were performed using the hybrid B3LYP-D3 functional (with the Grimme's D3 dispersion correction)[17-19] as implemented in the Gaussian16 program.[20] The solvation effects of acetonitrile was taken into account by using the SMD-flavor[21] of self-consistent reaction field (SCRF) theory. All geometries were optimized with no constraint of freedom by using the SDD pseudopotential[22] for Co, 6-31G (d) basis set for the C, N, O and H elements. The harmonic frequencies were then computed analytically at the same level of theory as the geometry optimizations to characterize the nature of all stationary points as minima states and to gain the Gibbs free energy correction. In order to obtain more accurate relative energies, single point calculations using the def2tzvp basis set were performed based on the B3LYP-D3/mix basis set optimized molecular geometries. The solvation free energy was calculated based on the M06/def2tzvp basis set.[23] Gibbs free energy was calculated using zero-point energy and thermal corrections, and the contributions from $\Delta G_{298oCH3CN}$ (H^+) = -266.48 kcal/mol in acetonitrile, while $\Delta G_{298oCH3CN}$ (H^+) is the sum of $\Delta G_{298ogas}$ (H^+) = -6.28 kcal/mol and the solvation energy change of H^+ in acetonitrile (-260.2 kcal/mol)[24-26] and the 3D structures of molecules were generated using CYL View.[27]

Cartesian coordination

Cat.-Co_2

	X	Y	Z
Co	-0.0218000	-1.4940000	-0.6090000
Co	0.0208000	1.4924000	-0.6185000
O	1.2114000	-0.0032000	-0.4702000
O	-1.2150000	0.0294000	-0.4841000
O	7.0286000	-1.2203000	1.7782000
O	7.0289000	1.0459000	1.7630000
H	7.9261000	0.9088000	2.1257000
O	-7.0316000	1.2162000	1.7843000
O	-7.0217000	-1.0500000	1.7661000
H	-7.9186000	-0.9172000	2.1310000
N	-1.4709000	-2.7637000	-0.6591000
N	1.3905000	-2.8054000	-0.6489000
N	1.4619000	2.7531000	-0.6618000
N	-1.3845000	2.7985000	-0.6523000
C	-1.3026000	-4.1402000	-1.1652000
H	-2.2040000	-4.7152000	-0.9292000
H	-1.2325000	-4.0763000	-2.2583000
C	-0.0713000	-4.8650000	-0.6131000
C	-0.0901000	-6.2991000	-1.1740000
H	-0.9827000	-6.8338000	-0.8345000
H	0.7831000	-6.8601000	-0.8267000
H	-0.0854000	-6.3074000	-2.2698000
C	-0.0792000	-4.8970000	0.9215000
H	-0.0656000	-3.8933000	1.3610000
H	0.7935000	-5.4393000	1.2998000
H	-0.9719000	-5.4120000	1.2914000
C	1.1867000	-4.1781000	-1.1529000
H	2.0681000	-4.7787000	-0.9057000
H	1.1304000	-4.1148000	-2.2468000
C	2.5771000	-2.5387000	-0.2036000
H	3.2878000	-3.3654000	-0.1521000
C	3.1277000	-1.2622000	0.1846000
C	6.4846000	-0.1645000	1.5502000
C	2.6444000	2.4613000	-0.2107000
H	3.3680000	3.2763000	-0.1563000
C	1.2975000	4.1309000	-1.1671000
H	1.2244000	4.0653000	-2.2595000
H	2.2025000	4.7012000	-0.9337000
C	0.0730000	4.8615000	-0.6120000
C	0.0841000	4.8956000	0.9226000
H	0.0666000	3.8922000	1.3615000
H	-0.7851000	5.4435000	1.3011000
H	0.9796000	5.4080000	1.2894000
C	0.0943000	6.2942000	-1.1761000
H	0.9880000	6.8278000	-0.8378000
H	-0.7776000	6.8576000	-0.8292000
H	0.0889000	6.3007000	-2.2719000
C	-1.1840000	4.1750000	-1.1495000
H	-2.0658000	4.7722000	-0.8955000
H	-1.1324000	4.1159000	-2.2435000
C	-2.5736000	2.5371000	-0.2013000
H	-3.2750000	3.3707000	-0.1384000
C	-3.1322000	1.2673000	0.1816000
C	-4.4363000	1.2616000	0.7029000
H	-4.9587000	2.1961000	0.8871000
C	-5.1014000	0.0733000	0.9881000
C	-4.4719000	-1.1342000	0.6957000
H	-5.0065000	-2.0633000	0.8655000
C	-3.1661000	-1.1745000	0.1744000
C	-2.4687000	0.0381000	-0.0454000
C	-6.4833000	0.1634000	1.5535000
C	-2.6517000	-2.4639000	-0.2189000

C	4.4313000	-1.2557000	0.7027000
H	4.9544000	-2.1904000	0.8844000
C	5.1018000	-0.0678000	0.9881000
C	4.4770000	1.1403000	0.6986000
H	5.0124000	2.0691000	0.8677000
C	3.1684000	1.1797000	0.1799000
C	2.4673000	-0.0290000	-0.0382000

Int.-1

	X	Y	Z				
Co	-0.0020000	-1.5747000	-0.6692000	C	4.5690000	1.2065000	0.5499000
Co	0.0018000	1.5201000	-0.5110000	H	5.0951000	2.1396000	0.7217000
O	1.2372000	0.0698000	-0.4212000	C	3.2250000	1.2321000	0.1358000
O	-1.2428000	0.0644000	-0.4379000	C	2.5103000	0.0240000	-0.0984000
O	7.2391000	-1.1389000	1.3321000	C	6.6420000	-0.0947000	1.1783000
O	7.1980000	1.1186000	1.3988000	C	2.6492000	2.5125000	-0.1354000
H	8.1165000	0.9542000	1.6848000	H	3.3533000	3.3432000	-0.0541000
O	-7.2564000	1.1256000	1.3837000	C	1.2505000	4.2126000	-0.9130000
O	-7.1933000	-1.1322000	1.3399000	H	1.2043000	4.2353000	-2.0093000
H	-8.1140000	-0.9933000	1.6323000	H	2.1337000	4.7886000	-0.6142000
N	-1.5137000	-2.8706000	-0.5727000	C	-0.0028000	4.8782000	-0.3449000
N	1.4948000	-2.8490000	-0.6871000	C	-0.0370000	4.8004000	1.1873000
N	1.4371000	2.8076000	-0.5104000	H	-0.0365000	3.7663000	1.5450000
N	-1.4308000	2.8098000	-0.5550000	H	-0.9342000	5.2929000	1.5779000
C	-1.2881000	-4.2915000	-0.8589000	H	0.8340000	5.3070000	1.6172000
H	-2.1361000	-4.8852000	-0.4892000	C	0.0049000	6.3481000	-0.8004000
H	-1.2621000	-4.4061000	-1.9507000	H	0.8812000	6.8711000	-0.4034000
C	0.0173000	-4.8641000	-0.2719000	H	-0.8863000	6.8699000	-0.4367000
C	0.0184000	-6.3740000	-0.5760000	H	0.0255000	6.4335000	-1.8931000
H	-0.8445000	-6.8641000	-0.1131000	C	-1.2276000	4.2081000	-0.9686000
H	0.9223000	-6.8483000	-0.1799000	H	-2.1246000	4.7870000	-0.7212000
H	-0.0204000	-6.5684000	-1.6545000	H	-1.1267000	4.2162000	-2.0612000
C	0.0828000	-4.6407000	1.2450000	C	-2.6469000	2.5243000	-0.1905000
H	0.0695000	-3.5766000	1.4995000	H	-3.3528000	3.3553000	-0.1343000
H	0.9981000	-5.0772000	1.6602000	C	-3.2234000	1.2481000	0.1045000
H	-0.7695000	-5.1181000	1.7414000	C	-4.5636000	1.2349000	0.5191000
C	1.2560000	-4.2667000	-0.9749000	H	-5.1000000	2.1660000	0.6751000
H	2.1383000	-4.8587000	-0.6939000	C	-5.2351000	0.0390000	0.7310000
H	1.1286000	-4.3646000	-2.0606000	C	-4.5580000	-1.1586000	0.4851000
C	2.6780000	-2.5424000	-0.2569000	H	-5.0927000	-2.0929000	0.6209000
H	3.4001000	-3.3505000	-0.1017000	C	-3.2224000	-1.2045000	0.0631000
C	3.2109000	-1.2209000	0.0304000	C	-2.5121000	0.0308000	-0.1011000
				C	-6.6498000	0.0951000	1.1805000

C	4.5431000	-1.1879000	0.4564000	C	-2.7031000	-2.5383000	-0.1972000
H	5.0882000	-2.1192000	0.5785000	H	-3.4460000	-3.3324000	-0.0620000
C	5.2288000	-0.0006000	0.7310000				

Int.-2

	X	Y	Z				
				H	5.0986000	-2.0014000	-1.0418000
Co	-0.0195000	1.4732000	0.3922000	C	3.2082000	-1.1308000	-0.4922000
Co	0.0182000	-1.4112000	0.2916000	C	2.4862000	0.0816000	-0.3340000
O	1.2070000	0.0549000	-0.0916000	C	6.6046000	0.2389000	-1.5729000
O	-1.2091000	0.0244000	-0.0894000	C	2.6611000	-2.4067000	-0.0857000
O	7.1943000	1.2865000	-1.7327000	H	3.3819000	-3.2275000	-0.1042000
O	7.1646000	-0.9722000	-1.7869000	C	1.3021000	-3.9906000	0.9759000
H	8.0830000	-0.8086000	-2.0740000	H	1.2200000	-3.8327000	2.0564000
O	-7.1967000	-1.1048000	-1.7939000	H	2.1966000	-4.5952000	0.7840000
O	-7.1669000	1.1536000	-1.7267000	C	0.0620000	-4.7424000	0.4779000
H	-8.0851000	1.0050000	-2.0221000	C	0.0628000	-4.8715000	-1.0510000
N	-1.4892000	2.7354000	0.5226000	H	0.0499000	-3.8939000	-1.5438000
N	1.4166000	2.7733000	0.5244000	H	-0.8147000	-5.4321000	-1.3919000
N	1.4791000	-2.6597000	0.3795000	H	0.9542000	-5.4093000	-1.3927000
N	-1.4093000	-2.6979000	0.3812000	C	0.0809000	-6.1373000	1.1274000
C	-1.3067000	4.0527000	1.1457000	H	0.9724000	-6.6949000	0.8213000
H	-2.1980000	4.6654000	0.9641000	H	-0.7958000	-6.7183000	0.8225000
H	-1.2353000	3.8873000	2.2280000	H	0.0808000	-6.0707000	2.2213000
C	-0.0629000	4.8130000	0.6663000	C	-1.1971000	-4.0239000	0.9772000
C	-0.0813000	6.1953000	1.3428000	H	-2.0756000	-4.6517000	0.7858000
H	-0.9724000	6.7588000	1.0473000	H	-1.1184000	-3.8641000	2.0576000
H	0.7953000	6.7816000	1.0489000	C	-2.5973000	-2.4767000	-0.0843000
H	-0.0811000	6.1096000	2.4356000	H	-3.2972000	-3.3152000	-0.1032000
C	-0.0633000	4.9730000	-0.8600000	C	-3.1769000	-1.2148000	-0.4911000
H	-0.0511000	4.0070000	-1.3751000	C	-4.5117000	-1.1949000	-0.9063000
H	0.8147000	5.5398000	-1.1887000	H	-5.0556000	-2.1242000	-1.0486000
H	-0.9540000	5.5186000	-1.1903000	C	-5.1940000	0.0052000	-1.1234000
C	1.1991000	4.0849000	1.1483000	C	-4.5489000	1.2096000	-0.8436000
H	2.0747000	4.7203000	0.9694000	H	-5.1012000	2.1395000	-0.9308000
H	1.1293000	3.9165000	2.2303000	C	-3.2099000	1.2383000	-0.4250000
C	2.6011000	2.5629000	0.0424000	C	-2.4882000	0.0174000	-0.3331000
H	3.3017000	3.4014000	0.0510000	C	-6.6067000	-0.0677000	-1.5780000
C	3.1749000	1.3222000	-0.4244000	C	-2.6681000	2.4930000	0.0408000
C	4.5111000	1.3266000	-0.8422000	H	-3.3895000	3.3139000	0.0490000
H	5.0543000	2.2625000	-0.9361000	C	0.0126000	-0.8411000	2.2333000
C	5.1918000	0.1415000	-1.1227000	O	-0.0036000	0.4024000	2.2994000
C	4.5454000	-1.0777000	-0.9067000	O	0.0260000	-1.7943000	2.9776000

Int.-3

	X	Y	Z
Co	-0.1300000	1.4839000	0.3301000
Co	0.0538000	-1.4505000	0.5637000
O	1.1103000	0.1604000	-0.3371000
O	-1.2942000	-0.0907000	0.2359000
O	7.1279000	1.5707000	-1.7099000
O	7.2178000	-0.6790000	-1.5284000
H	8.1407000	-0.4884000	-1.7818000
O	-7.1597000	-1.4905000	-1.7587000
O	-7.2834000	0.7525000	-1.5188000
H	-8.1861000	0.5643000	-1.8385000
N	-1.6713000	2.6194000	0.6389000
N	1.1844000	2.9145000	0.1679000
N	1.6045000	-2.5717000	0.5440000
N	-1.3052000	-2.9390000	0.2331000
C	-1.5064000	3.9664000	1.1892000
H	-2.4755000	4.4799000	1.1944000
H	-1.1814000	3.8582000	2.2309000
C	-0.4828000	4.8150000	0.4180000
C	-0.5383000	6.2401000	0.9964000
H	-1.5254000	6.6850000	0.8335000
H	0.2015000	6.8850000	0.5108000
H	-0.3375000	6.2461000	2.0741000
C	-0.7997000	4.8442000	-1.0833000
H	-0.7281000	3.8508000	-1.5375000
H	-0.1010000	5.5039000	-1.6091000
H	-1.8125000	5.2236000	-1.2593000
C	0.9253000	4.2716000	0.6779000
H	1.6622000	4.9632000	0.2519000
H	1.0965000	4.2383000	1.7620000
C	2.3698000	2.7364000	-0.3291000
H	3.0010000	3.6212000	-0.4452000
C	3.0360000	1.4965000	-0.6391000
C	4.3922000	1.5443000	-0.9814000
H	4.8861000	2.4979000	-1.1444000
C	5.1531000	0.3814000	-1.0935000
C	4.5591000	-0.8449000	-0.7817000
H	5.1728000	-1.7400000	-0.7874000
C	3.2053000	-0.9446000	-0.4346000
C	2.3971000	0.2343000	-0.4650000
C	6.5815000	0.5137000	-1.4729000
C	2.7454000	-2.2395000	0.0336000
H	3.5134000	-3.0165000	-0.0062000
C	1.4665000	-3.9477000	1.0252000
H	1.1666000	-3.8967000	2.0776000
H	2.4406000	-4.4501000	0.9770000
C	0.4376000	-4.7757000	0.2234000
C	0.6938000	-4.6652000	-1.2857000
H	0.5386000	-3.6460000	-1.6536000
H	0.0186000	-5.3284000	-1.8371000
H	1.7210000	-4.9591000	-1.5298000
C	0.5833000	-6.2395000	0.6765000
H	1.5750000	-6.6266000	0.4202000
H	-0.1596000	-6.8752000	0.1833000
H	0.4497000	-6.3405000	1.7599000
C	-0.9918000	-4.3344000	0.5680000
H	-1.7076000	-5.0065000	0.0752000
H	-1.1379000	-4.4375000	1.6514000
C	-2.4989000	-2.7160000	-0.2043000
H	-3.1480000	-3.5776000	-0.3964000
C	-3.1498000	-1.4369000	-0.4103000
C	-4.4769000	-1.4641000	-0.8525000
H	-4.9474000	-2.4114000	-1.0994000
C	-5.2430000	-0.3041000	-0.9761000
C	-4.6767000	0.9156000	-0.6091000
H	-5.2806000	1.8161000	-0.6541000
C	-3.3472000	0.9993000	-0.1739000
C	-2.5481000	-0.1785000	-0.1092000
C	-6.6421000	-0.4365000	-1.4554000
C	-2.8716000	2.2822000	0.2920000
H	-3.6521000	3.0416000	0.3858000
C	0.4683000	-0.5327000	2.2262000
O	0.3727000	0.7086000	2.3173000
O	0.8713000	-1.2142000	3.3140000
H	1.0190000	-0.5664000	4.0384000

Int.-4

	X	Y	Z				
				C	3.1406000	-1.1339000	-0.3875000
Co	-0.0232000	1.5150000	0.5822000	C	2.4444000	0.0744000	-0.1373000
Co	0.0348000	-1.4764000	0.6399000	C	6.3361000	0.2297000	-2.0101000
O	1.2335000	0.0568000	0.3914000	C	2.6565000	-2.4320000	0.0327000
O	-1.1842000	0.0041000	0.2509000	H	3.3891000	-3.2355000	-0.0668000
O	6.8527000	1.2854000	-2.2952000	C	1.3437000	-4.1223000	1.0131000
O	6.8769000	-0.9799000	-2.2377000	H	1.2321000	-4.0814000	2.1038000
H	7.7455000	-0.8415000	-2.6639000	H	2.2585000	-4.6852000	0.7989000
O	-6.8774000	-1.2374000	-2.2578000	C	0.1385000	-4.8492000	0.3996000
O	-6.8982000	1.0282000	-2.2231000	C	0.2069000	-4.8427000	-1.1338000
H	-7.7767000	0.8857000	-2.6269000	H	0.1864000	-3.8285000	-1.5471000
N	-1.4638000	2.7544000	0.4791000	H	-0.6379000	-5.3950000	-1.5584000
N	1.3591000	2.8247000	0.5063000	H	1.1244000	-5.3294000	-1.4811000
N	1.5071000	-2.7389000	0.5389000	C	0.1566000	-6.2955000	0.9275000
N	-1.3581000	-2.8126000	0.4324000	H	1.0681000	-6.8109000	0.6090000
C	-1.3271000	4.0888000	1.0842000	H	-0.6957000	-6.8597000	0.5362000
H	-2.2409000	4.6584000	0.8866000	H	0.1122000	-6.3292000	2.0220000
H	-1.2549000	3.9295000	2.1655000	C	-1.1557000	-4.1953000	0.8998000
C	-0.1113000	4.8754000	0.5833000	H	-2.0135000	-4.8038000	0.5944000
C	-0.1529000	6.2651000	1.2445000	H	-1.1507000	-4.1667000	1.9969000
H	-1.0506000	6.8102000	0.9367000	C	-2.5073000	-2.5496000	-0.0997000
H	0.7145000	6.8619000	0.9455000	H	-3.1939000	-3.3862000	-0.2434000
H	-0.1571000	6.1938000	2.3379000	C	-3.0559000	-1.2670000	-0.4829000
C	-0.1222000	5.0127000	-0.9454000	C	-4.3315000	-1.2623000	-1.0648000
H	-0.0827000	4.0418000	-1.4522000	H	-4.8385000	-2.1982000	-1.2827000
H	0.7344000	5.6036000	-1.2860000	C	-4.9986000	-0.0760000	-1.3703000
H	-1.0291000	5.5273000	-1.2795000	C	-4.3981000	1.1353000	-1.0454000
C	1.1600000	4.1742000	1.0693000	H	-4.9332000	2.0608000	-1.2321000
H	2.0363000	4.7842000	0.8277000	C	-3.1150000	1.1789000	-0.4676000
H	1.1222000	4.0620000	2.1587000	C	-2.4173000	-0.0285000	-0.2202000
C	2.5184000	2.5752000	-0.0232000	C	-6.3529000	-0.1795000	-1.9956000
H	3.1997000	3.4211000	-0.1283000	C	-2.6173000	2.4576000	-0.0339000
C	3.0698000	1.3115000	-0.4366000	H	-3.3420000	3.2705000	-0.1037000
C	4.3357000	1.3163000	-1.0455000	O	-0.0826000	1.4460000	2.3762000
H	4.8310000	2.2540000	-1.2817000	H	0.8352000	1.5392000	2.6909000
C	4.9968000	0.1315000	-1.3520000	C	-0.1151000	-1.3319000	2.7188000
C	4.4053000	-1.0807000	-0.9983000	O	-0.2386000	-1.3861000	3.8437000
H	4.9410000	-2.0042000	-1.1942000				

Cat.-Co

	X	Y	Z				
Co	-0.0232420	-1.3126130	-0.7352420	H	-1.2535550	-3.9482570	-2.2925030
O	-1.2504040	0.1263320	-0.6664560	H	-2.2185860	-4.5619820	-0.9472990
O	1.2545090	0.0817030	-0.6663740	C	-0.0849650	-4.7041560	-0.6475060
O	-6.9261740	1.4059830	1.8923120	C	-0.0857530	-4.7121750	0.8865120
O	-6.9035940	-0.8457010	1.9704470	H	-0.0677360	-3.6981920	1.2956910
H	-7.7627670	-0.6327440	2.3784900	H	0.7903520	-5.2472210	1.2705130
O	6.9435430	-1.0025290	1.9953510	H	-0.9808350	-5.2155760	1.2696730
O	6.8990540	1.2460700	1.8634240	C	-0.1109500	-6.1453540	-1.1828370
H	7.7611740	1.0834940	2.2882590	H	-1.0058710	-6.6730110	-0.8350450
N	1.6195440	2.8702570	-1.0614990	H	0.7636680	-6.7052740	-0.8339450
N	-1.5142020	2.9275130	-1.0630610	H	-0.1106300	-6.1667300	-2.2793300
N	-1.4811820	-2.6075680	-0.7127670	C	1.1771720	-4.0262420	-1.1953040
N	1.3866510	-2.6598670	-0.7113640	H	2.0527340	-4.6397760	-0.9451860
C	1.3682170	4.2595140	-1.3773330	H	1.1120170	-3.9912350	-2.2913010
H	2.2188840	4.9009960	-1.0752310	C	2.5658420	-2.4149520	-0.2135550
H	1.2672520	4.3444390	-2.4680470	H	3.2456350	-3.2647730	-0.1030560
C	0.0879660	4.8450790	-0.7274140	C	3.1157010	-1.1526400	0.1577600
C	0.1158620	6.3635910	-0.9833780	C	4.3875080	-1.1357950	0.7505650
H	1.0098140	6.8182200	-0.5417870	H	4.8859450	-2.0671930	1.0045560
H	-0.7610800	6.8505380	-0.5422520	C	5.0354100	0.0599830	1.0191700
H	0.1201960	6.5871410	-2.0577490	C	4.4094970	1.2638580	0.6304590
C	0.0823420	4.5707730	0.7809470	H	4.9318740	2.1989230	0.8080920
H	0.0629920	3.4966530	0.9798410	C	3.1663640	1.3064290	0.0174380
H	-0.7965640	5.0256390	1.2541640	C	2.4400310	0.0728240	-0.1873450
H	0.9765800	4.9939750	1.2549730	C	6.3591010	0.0132510	1.6625580
C	-1.2123950	4.3069190	-1.3783930	C	2.6750330	2.6273780	-0.3925240
H	-2.0391880	4.9788530	-1.0767760	H	3.3493630	3.4499750	-0.0859020
H	-1.1075500	4.3883090	-2.4690180				
C	-2.5783830	2.7235730	-0.3947110				
H	-3.2229790	3.5691510	-0.0880700				
C	-3.1169800	1.4206870	0.0143550				
C	-4.3593420	1.4203460	0.6259700				
H	-4.8613960	2.3658300	0.8113810				
C	-5.0307740	0.2412010	1.0150490				
C	-4.4293650	-0.9788030	0.7480370				
H	-4.9474020	-1.9006150	0.9943040				
C	-3.1563270	-1.0391580	0.1551130				
C	-2.4359900	0.1606910	-0.1892350				
C	-6.3515220	0.3598080	1.6536730				

C	-2.6514690	-2.3195590	-0.2161950
H	-3.3609290	-3.1451490	-0.1067390
C	-1.3210010	-3.9805830	-1.1965400

Int.-1

	X	Y	Z				
Co	-0.0199230	-1.3123470	-0.5687130	C	-4.7122020	-0.9864470	0.2910390
O	-1.3461620	0.1836850	-0.4562550	H	-5.2578470	-1.9172140	0.4201070
O	1.3497370	0.1443160	-0.4535320	C	-3.3528830	-1.0414790	-0.0435760
O	-7.4519190	1.3204890	0.9856770	C	-2.5914800	0.1893690	-0.2160410
O	-7.3954220	-0.9268080	0.9769110	C	-6.7971240	0.3001130	0.8218420
H	-8.3153050	-0.7084390	1.2103100	C	-2.7787170	-2.3418580	-0.2165830
O	7.4595000	-1.0225990	0.9922850	H	-3.4945850	-3.1652480	-0.0877000
O	7.3944510	1.2242610	0.9697650	C	-1.3239870	-4.0889450	-0.7336320
H	8.3155160	1.0124480	1.2047680	H	-1.2440710	-4.2756630	-1.8157210
N	1.6615650	2.9693850	-0.7793990	H	-2.1980150	-4.6608960	-0.3787020
N	-1.5743510	3.0167950	-0.7827670	C	-0.0652920	-4.6673580	-0.0628460
N	-1.5406180	-2.6626180	-0.5181240	C	-0.0543380	-4.3691250	1.4410900
N	1.4639560	-2.7065390	-0.5265830	H	-0.0397540	-3.2920760	1.6235620
C	1.3560550	4.3763690	-0.8832060	H	0.8304810	-4.8106290	1.9164440
H	2.1944120	4.9999700	-0.5077730	H	-0.9457120	-4.7880420	1.9246760
H	1.2247240	4.6240000	-1.9473750	C	-0.0878990	-6.1896630	-0.2889000
C	0.0692750	4.8131360	-0.1317140	H	-0.9789980	-6.6389600	0.1653580
C	0.0917900	6.3517170	-0.0692120	H	0.7932110	-6.6642160	0.1590040
H	0.9830370	6.7097130	0.4597700	H	-0.0952150	-6.4349790	-1.3588290
H	-0.7900700	6.7355620	0.4572460	C	1.2035260	-4.1249790	-0.7448420
H	0.0995790	6.7917030	-1.0757060	H	2.0637160	-4.7237050	-0.4007980
C	0.0584620	4.2272430	1.2844170	H	1.1069960	-4.3047400	-1.8266460
H	0.0422220	3.1359510	1.2394000	C	2.7105360	-2.4235060	-0.2251090
H	-0.8258660	4.5677160	1.8384430	H	3.4031820	-3.2667950	-0.0999880
H	0.9508970	4.5413830	1.8411180	C	3.3209670	-1.1399530	-0.0473940
C	-1.2273650	4.4141420	-0.8874540	C	4.6796350	-1.1222500	0.2865380
H	-2.0480640	5.0627340	-0.5158290	H	5.2135610	-2.0605470	0.4158970
H	-1.0849180	4.6563720	-1.9514300	C	5.3881700	0.0667710	0.4640340
C	-2.7177980	2.7565110	-0.2814020	C	4.7039590	1.2867240	0.2768600
H	-3.3861230	3.5856710	0.0304510	H	5.2500810	2.2174800	0.4000000
C	-3.3229320	1.4376800	-0.0778340	C	3.3621450	1.3388120	-0.0728500
C	-4.6643650	1.4223130	0.2714130	C	2.5948260	0.1128440	-0.2146240
H	-5.1982910	2.3606860	0.3956920	C	6.8013290	-0.0047380	0.8226340
C	-5.3845640	0.2243810	0.4632410	C	2.7949530	2.6745190	-0.2746150
				H	3.4857160	3.4841380	0.0411580

Int.-2

	X	Y	Z				
Co	-0.0195410	-1.2602710	1.0130380	C	3.1182840	-1.0301370	-0.3617940
O	1.5059210	0.1183500	0.9672200	C	2.5478220	0.1594060	0.2618850
O	-1.2400680	0.2657470	0.4177390	C	6.2502240	0.3390700	-2.0031010
O	6.9003240	1.3568160	-2.1953120	C	2.5322360	-2.3348590	-0.2142320
O	6.6841980	-0.8599050	-2.5117350	H	3.1639190	-3.1528870	-0.5910370
H	7.5117430	-0.6339210	-2.9727210	C	1.1193440	-4.0820850	0.4440930
O	-7.0076390	-0.4077580	-2.2228130	H	1.0726720	-4.3017710	1.5158080
O	-6.8047230	1.8279480	-2.0827660	H	1.9478070	-4.6636880	0.0069440
H	-7.6718850	1.6953260	-2.5058130	C	-0.1990690	-4.5489670	-0.2062490
N	-1.4240550	3.0836530	0.8358420	C	-0.2551900	-4.1367180	-1.6819130
N	1.7072340	2.9594650	1.1237230	H	-0.2158420	-3.0497180	-1.7900720
N	1.3934920	-2.6559260	0.3095540	H	-1.1817830	-4.4909850	-2.1508060
N	-1.6076110	-2.5643400	0.4163080	H	0.5895820	-4.5648520	-2.2361010
C	-1.1171690	4.4463790	1.1989370	C	-0.2405690	-6.0822240	-0.0864280
H	-1.8989230	5.1483390	0.8396830	H	0.6098400	-6.5387190	-0.6068380
H	-1.1079070	4.5098850	2.2970040	H	-1.1598410	-6.4837780	-0.5289990
C	0.2502410	4.9620130	0.6816680	H	-0.2039810	-6.3976880	0.9634100
C	0.2870930	6.4779440	0.9494250	C	-1.4205150	-4.0017190	0.5652020
H	-0.5366750	6.9872190	0.4352740	H	-2.3190770	-4.5375350	0.2170740
H	1.2277180	6.9157770	0.5950100	H	-1.2829960	-4.2186090	1.6287890
H	0.1986670	6.6946330	2.0222210	C	-2.7210430	-2.1870810	-0.1201550
C	0.3793660	4.6932270	-0.8218130	H	-3.4321760	-2.9703400	-0.4213310
H	0.3370080	3.6202170	-1.0213440	C	-3.1909620	-0.8495790	-0.3758550
H	1.3310820	5.0808410	-1.2072460	C	-4.4468840	-0.7302210	-0.9703830
H	-0.4348740	5.1808090	-1.3732950	H	-5.0056150	-1.6240750	-1.2370910
C	1.4525700	4.3425160	1.4454540	C	-5.0247380	0.5117830	-1.2397110
H	2.3390440	4.9778030	1.2386080	C	-4.3146150	1.6688590	-0.8545400
H	1.2437850	4.4150150	2.5223230	H	-4.7730370	2.6393940	-1.0233450
C	2.8038050	2.7104520	0.5246210	C	-3.0679980	1.6196670	-0.2534030
H	3.5130880	3.5326780	0.2961640	C	-2.4141880	0.3334430	-0.0350370
C	3.2716550	1.4093980	0.0404230	C	-6.3365010	0.5553440	-1.8776770
C	4.4464830	1.4074010	-0.6880330	C	-2.4956460	2.8999690	0.1710170
H	4.9781600	2.3426520	-0.8449330	H	-3.1290950	3.7664450	-0.1121220
C	5.0003300	0.2396630	-1.2570340	C	-0.1329080	-2.0560470	2.8859840
C	4.3161940	-0.9624870	-1.0780980	O	-0.4623750	-0.9193880	3.2155060
H	4.7251560	-1.8735190	-1.5065870	O	0.0772020	-3.1798170	3.3048910

Int.-3

	X	Y	Z				
Co	-0.1766940	-1.2490170	0.9571050	C	2.7772370	-1.2482210	-0.6524580
O	1.3957750	-0.1178300	0.9676340	C	2.3920710	-0.1201430	0.1892400
O	-1.0085490	0.3218030	-0.0139150	C	6.0228280	-0.0370340	-2.2016520
O	6.8024940	0.9042770	-2.2600100	C	2.0655880	-2.5051500	-0.6511010
O	6.2771060	-1.1818580	-2.9173010	H	2.6283190	-3.3460450	-1.0878970
H	7.1158270	-0.9899380	-3.3733760	C	0.5459890	-4.1381470	0.0112110
O	-7.0951480	0.3108310	-1.8599100	H	0.8566650	-4.4281060	1.0245640
O	-6.5368470	2.4803010	-2.0652130	H	1.1136290	-4.7687480	-0.6952850
H	-7.4501090	2.4385820	-2.4009770	C	-0.9519850	-4.4418400	-0.1390800
N	-1.0668090	3.2024070	0.7631410	C	-1.4263650	-4.0603960	-1.5472140
N	1.8931480	2.6480120	1.3795670	H	-1.2299230	-3.0056040	-1.7561740
N	0.9055940	-2.7374310	-0.1512730	H	-2.5022110	-4.2394670	-1.6667680
N	-1.8365250	-2.2666250	0.7371300	H	-0.8999390	-4.6595500	-2.3005270
C	-0.6550240	4.5324800	1.1489330	C	-1.1456640	-5.9504830	0.0889430
H	-1.2652070	5.3095660	0.6431860	H	-0.5491390	-6.5342690	-0.6224460
H	-0.8389460	4.6338000	2.2291090	H	-2.1967520	-6.2334390	-0.0425030
C	0.8331620	4.8647330	0.8910200	H	-0.8419740	-6.2400100	1.1025450
C	1.0362240	6.3425250	1.2720270	C	-1.7791960	-3.7101660	0.9502720
H	0.3688300	6.9934990	0.6943850	H	-2.7982840	-4.1259580	0.9387340
H	2.0675390	6.6578650	1.0751510	H	-1.3493340	-3.8939320	1.9358010
H	0.8307770	6.5105780	2.3373860	C	-2.9285760	-1.8309780	0.1950650
C	1.1608900	4.6602760	-0.5927490	H	-3.7391930	-2.5532080	0.0451040
H	0.9784860	3.6247590	-0.8883590	C	-3.2314090	-0.4988430	-0.2477000
H	2.2123470	4.8963220	-0.7990550	C	-4.5121050	-0.2586120	-0.7447380
H	0.5376700	5.3143180	-1.2163290	H	-5.2278140	-1.0739220	-0.8148240
C	1.7927220	4.0286370	1.7845630	C	-4.9118940	1.0118190	-1.1637680
H	2.7807810	4.5333480	1.7636410	C	-4.0083680	2.0806840	-0.9771000
H	1.4228460	4.0722350	2.8183350	H	-4.3435780	3.0894740	-1.2017760
C	2.9674470	2.3207730	0.7767470	C	-2.7328820	1.9033490	-0.4664370
H	3.7809870	3.0647000	0.6513210	C	-2.2355780	0.5561970	-0.2195640
C	3.2659540	1.0471320	0.1221810	C	-6.2543100	1.1865720	-1.7078990
C	4.4131090	1.0200630	-0.6518020	C	-2.0165120	3.1234860	-0.0822910
H	5.0525770	1.8985040	-0.6858210	H	-2.4623480	4.0443410	-0.5106140
C	4.7918390	-0.0947940	-1.4239050	C	0.3047500	-2.1176870	2.6039300
C	3.9518580	-1.2110450	-1.4030200	O	-0.4370160	-2.3966170	3.5427720
H	4.2257990	-2.0873850	-1.9840730	O	1.6445900	-2.4485340	2.7571760
				H	1.6945050	-2.8134960	3.6659630

Int.-4

	X	Y	Z				
Co	-0.0295000	-1.2542000	-0.8629000	C	-3.1869000	-0.9842000	0.2081000
O	-1.4315000	0.1785000	-0.9485000	C	-2.5146000	0.2065000	-0.2942000
O	1.4920000	0.2504000	-1.0393000	C	-6.2899000	0.4827000	1.8263000
O	-6.8880000	1.5240000	2.0600000	C	-2.6992000	-2.3296000	-0.0043000
O	-6.8155000	-0.7169000	2.2395000	H	-3.3733000	-3.1140000	0.3760000
H	-7.6443000	-0.4675000	2.6859000	C	-1.3694000	-4.1143000	-0.7297000
O	6.8585000	-0.8837000	2.2240000	H	-1.3595000	-4.3553000	-1.8039000
O	6.8327000	1.3626000	2.1141000	H	-2.1901000	-4.6960000	-0.2747000
H	7.6518000	1.1541000	2.5979000	C	-0.0333000	-4.5935000	-0.1193000
N	1.6772000	3.0705000	-0.9920000	C	0.0532000	-4.2142000	1.3646000
N	-1.5081000	3.0030000	-1.0210000	H	0.0190000	-3.1283000	1.4995000
N	-1.6145000	-2.6940000	-0.5873000	H	0.9882000	-4.5915000	1.7994000
N	1.4573000	-2.6191000	-0.6771000	H	-0.7792000	-4.6677000	1.9190000
C	1.3846000	4.4706000	-1.1737000	C	0.0077000	-6.1238000	-0.2843000
H	2.1907000	5.1140000	-0.7617000	H	-0.8425000	-6.5925000	0.2249000
H	1.3294000	4.6751000	-2.2536000	H	0.9260000	-6.5366000	0.1490000
C	0.0476000	4.9333000	-0.5364000	H	-0.0289000	-6.4180000	-1.3418000
C	0.0059000	6.4680000	-0.6594000	C	1.1777000	-4.0287000	-0.9011000
H	0.8681000	6.9255000	-0.1597000	H	2.0650000	-4.6265000	-0.6378000
H	-0.9038000	6.8731000	-0.2008000	H	0.9965000	-4.1776000	-1.9758000
H	0.0210000	6.7834000	-1.7112000	C	2.5998000	-2.3182000	-0.1576000
C	-0.0021000	4.5266000	0.9404000	H	3.2639000	-3.1517000	0.1117000
H	0.0371000	3.4396000	1.0376000	C	3.1546000	-1.0166000	0.1157000
H	-0.9272000	4.8818000	1.4119000	C	4.3641000	-0.9952000	0.8049000
H	0.8463000	4.9556000	1.4891000	H	4.8231000	-1.9298000	1.1187000
C	-1.1997000	4.3889000	-1.2876000	C	5.0230000	0.1967000	1.1245000
H	-2.0551000	5.0472000	-1.0292000	C	4.4277000	1.4094000	0.7189000
H	-1.0201000	4.5013000	-2.3667000	H	4.9234000	2.3424000	0.9737000
C	-2.6198000	2.7760000	-0.4382000	C	3.2398000	1.4602000	0.0089000
H	-3.2877000	3.6219000	-0.1742000	C	2.5422000	0.2266000	-0.3501000
C	-3.1720000	1.4807000	-0.0322000	C	6.2835000	0.1314000	1.8520000
C	-4.3778000	1.5129000	0.6486000	C	2.7327000	2.7895000	-0.3320000
H	-4.8588000	2.4693000	0.8378000	H	3.3765000	3.6070000	0.0550000
C	-5.0193000	0.3532000	1.1226000	C	-0.0613000	-1.4008000	-2.6784000
C	-4.4003000	-0.8783000	0.8859000	O	-0.0775000	-1.4662000	-3.8248000
H	-4.8834000	-1.7856000	1.2378000	O	-0.0770000	2.3495000	-2.1156000
				H	-0.1095000	2.6252000	-3.1098000

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