Supplementary materials

Chemical fixation of CO_2 into cyclic carbonates catalyzed by bimetal mixed MOFs: the role of the interaction between Co and Zn

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Catalyst characterization

The as-prepared compounds were characterized using a Nicolet 5700 spectrometer, with potassium bromide being used as fixative, for Fourier transform infrared (FT-IR) spectra. The measurement was conducted at the wavenumber range of 400 to 4000 cm^{-1} (2 cm^{-1} resolution). The powder X-ray diffraction (PXRD) patterns of the $[M_1M_2][(BDC)(DABCO)_{0.5}]$ (M_1, M_2=Co, Ni, Zn) were determined by Rigaku D/max-A instrument equipped with Cu kα radiation, with the data collected in 2θ range of 5-60° with a scan speed of 10 °/min. X-ray photoelectron spectroscopy (XPS) of the synthesized MOFs were recorded on an ESCALAB-250 spectrometer using Al Kα (1486.6 eV) irradiation. The binding energies (B.E.) value were internally calibrated according to the adventitious carbon deposit C (1s) peak at 284.8 eV, while the specific surface area (BET) and pore characteristics of the $[M_1M_2][(BDC)(DABCO)_{0.5}]$ were measured using a Beishide 3H-2000 analyzer at liquid nitrogen temperature (-196 °C) after the samples have been treated at 120 °C for 12 h. Furthermore, the thermogravimetric (TG) profile of the CZ-BDO sample was recorded on a thermal analyzer SDT Q600 under nitrogen atmosphere at a temperature range of 30-800 °C and heating rate of 10 °/min. The distribution and amount of acid/basic sites were measured through temperature-programmed desorption of NH_3 (NH_3-TPD) using the TP-5056 instrument equipped with a TCD detector. CO_2-adsorption curves of all the compounds were detected by CO_2 physisorption at room temperature (25 ˚C) with the use of a Beishide 3H-2000 analyzer after the studied samples were degassed at 120 ˚C for 6 h. Concentrations of Co, Zn and Ni inside bimetal samples were measured using Inductively conducted plasma-optical emission spectrometry (ICP-OES, Varian 720-ES)

Table S1. The concentrations of Co, Zn and Ni inside the bimetal samples, as determined by ICP-OES.

sample	Weight (g)	Detected element	Content (mg/kg)	Atomic ratio
NZ-BDO	0.0708	Zn	32800.5	1Zn:3.55Ni

	0.0708	Ni	105220.7	
CZ-BDO	0.0507	Zn	90734.5	1Zn:1.02Co
	0.0507	Co	80042.9	
CN-BDO	0.0656	Ni	110901.5	1Co:2.99Ni
	0.0656	Co	37229.2	

Table S2. Textural properties of the bimetal samples

Samples	S_{BET}[a] (m^2g^{-1})	S_{micro}[c] (m^2g^{-1})	S_{meso}[c] (m^2g^{-1})	V_{total}[b] (cm^3g^{-1})	V_{micro}[c] (cm^3g^{-1})	D_{avera} (nm)	V_{total}[d] (m^3g^{-1})
Ni-BDO	1629.05	1547.27	81.78	0.986	0.799	10.00	22.34
Zn-BDO	1342.51	1255.30	87.21	0.786	0.655	6.77	9.94
Co-BDO	1296.87	1154.78	142.09	0.800	0.598	6.32	15.36
NZ-BDO	897.13	805.05	92.08	0.613	0.419	6.91	12.79
CZ-BDO	1298.13	1179.57	115.56	0.780	0.611	6.32	17.49
CN-BDO	1417.34	1338.79	78.55	0.861	0.695	9.76	18.76

[a] BET method. [b] Volume adsorbed at $p/p_0 = 0.98$. [c] *t*-plot method. [d] Volume adsorbed at $p/p_0 = 0.50$.

Table S3. The bond length between the different elements within bimetal samples*

Distance ($1*10^{-10}$)	Co-BDO	Ni-BDO	Zn-BDO	CN-BDO	CZ-BDO	NZ-BDO
Co-Co	2.24945					
Ni-Ni		2.42095				
Zn-Zn			2.76632			
Co-Ni				2.40280		
Co-Zn					2.62130	
Ni-Zn						2.50917
Co-N	2.20713			2.20884	2.19154	
Ni-N		2.41059		2.38816		2.39780
Zn-N			2.12479		2.12624	2.14407
Co-O	1.92563			1.95050	1.94621	
Ni-O		1.90603		1.89601		1.90051
Zn-O			2.07578		2.07394	2.08705

*The geometry optimization of all the basic unit was performed on Gaussian 09 program equipped with the M06 method, and the mixed basis sets consisting of ECP-based LANL2DZ (for metal atom) and 6-31G(d) (for other atoms) were employed for searching optimal structure.

Raman

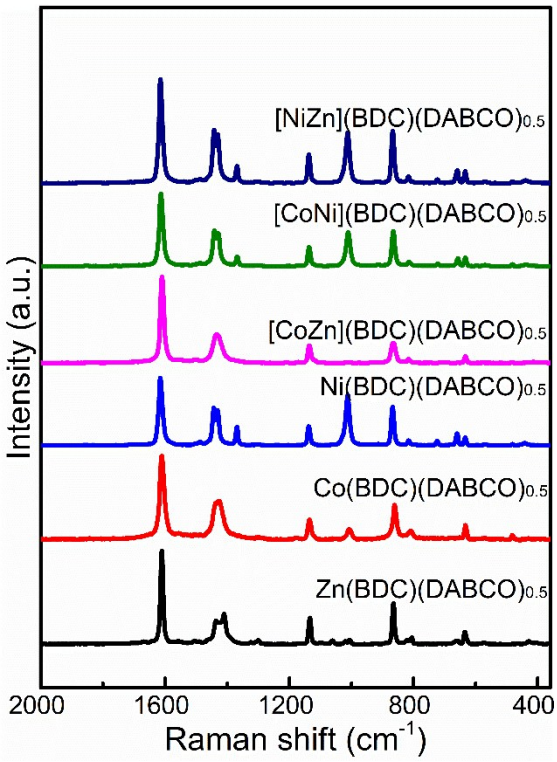

Fig.S1 Raman spectra of the as prepared $[M_1M_2](BDC)(DABCO)_{0.5}$ (M_1, M_2 = Co, Ni, Zn) compounds.

SEM

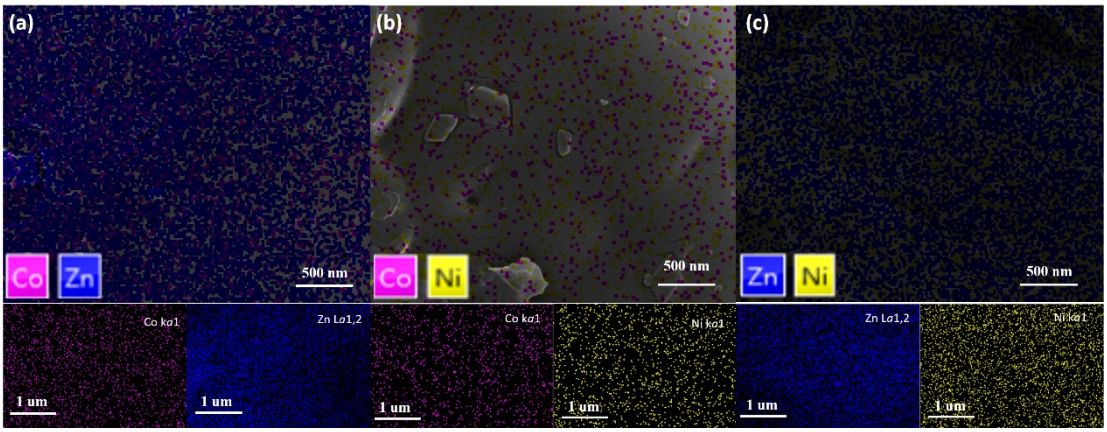

Fig.S2 EDS spectra of the CZ-BDO, CN-BDO, NZ-BDO samples.

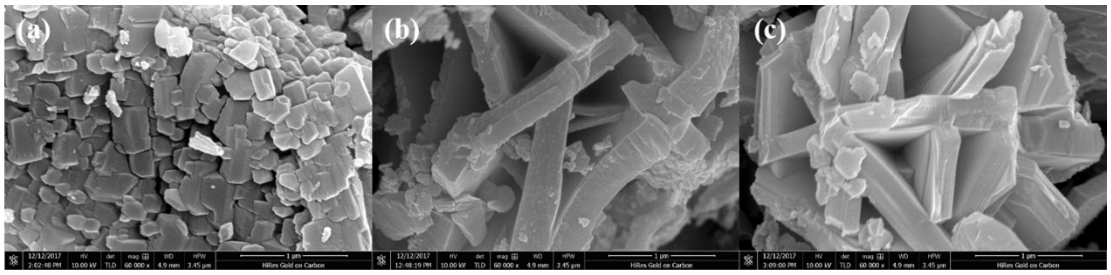

Fig.S3 SEM images of the Zn-BDO, Co-BDO, CZ-BDO samples.

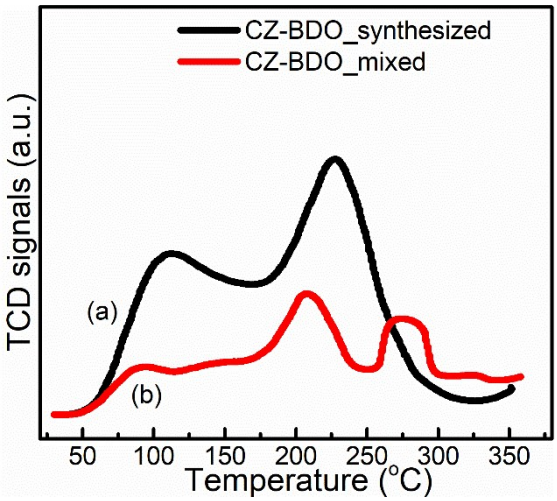

Fig.S4 NH_3-TPD profiles of the CZ-BDO samples. (a) synthesized CZ-BDO, (b) mixed CZ-BDO.

It can be seen that NH_3-TPD profile of the synthesized CZ-BDO was obviously larger than that of the equal mass mechanically mixed sample (1Co-BDO:1Zn-BDO), which may be ascribed to the simultaneous presence of Co and Zn ions within the crystal structure.

Leaching experiment

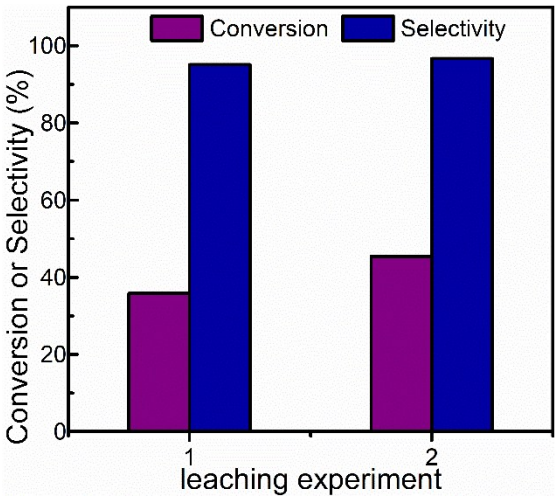

Fig.S5 The results of the leaching experiment. 100 ˚C, 3.0MPa, 0.5 wt.% catalyst of ECH.

1 represents the system with catalyst, which was heated at 100 ˚C for 3h.

2 represents the system without catalyst, which was heated at 100 ˚C for another 4h.

Table S4. The concentrations of Co, Zn within the catalyst-free liquid, as determined by ICP-OES.

sample	Weight	Detected element	Content	Lost rate

catalyst-free liquid	1.4163g	Co	77.1 mg/kg	2.27%
	1.4163g	Zn	88.2 mg/kg	2.61%

The catalyst-free liquid was determined by ICP-OES, only slight lost rate was detected both for Co, Zn elements (**Table S4**), suggesting that the CZ-BDO sample can be kept stable during the liquid reaction. In addition, it can also be drawn that the primary factor for the decreasing catalytic activity was associated with the adsorbed organic components covering the active sites instead of structure collapse during the liquid reaction.

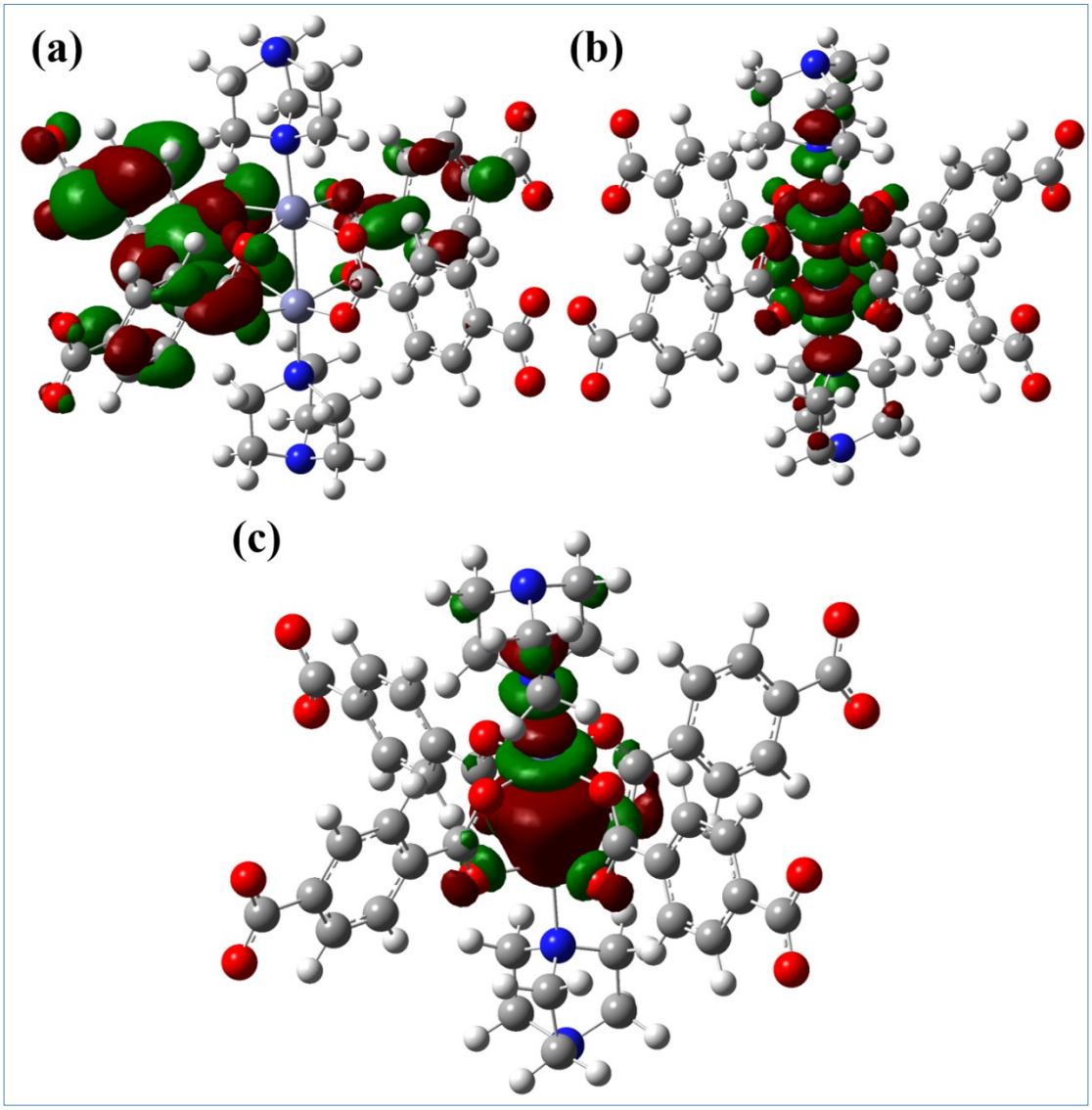

Fig.S6 DFT-calculated frontier molecular orbitals (LUMO) of (a) Zn-BDO, (b) Co-BDO, and (c) CZ-BDO. M06//ECP-based LANL2DZ (for metal atom) and 6-31G(d) (for other atoms).

The LUMOs of Zn-BDO, Co-BDO, and CZ-BDO are shown in **Fig.S6**. Compared with the Zn-BDO and Co-BDO, the LUMO of CZ-BDO focused mainly on the Co-Zn

bridge (**Fig.S6c**), indicating that epoxide can be easily activated via coordination with metal node. In other words, the unoccupied orbital became changed after the Zn (Co) ions were substituted by Co (Zn) ions, resulting in a new LUMO forming around Co and Zn ions, which could result into the newly-formed LUMO to easily receive electrons from the epoxides during the coupling process.

Stability test

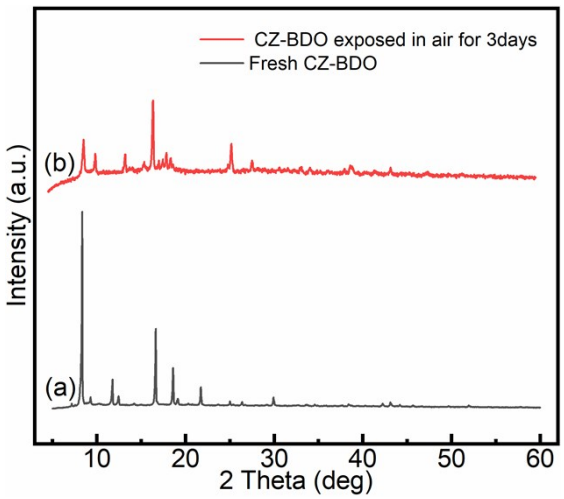

Fig.S7 X-ray diffractograms of CZ-BDO samples, (a) fresh sample, (b) the sample exposed in ambient for 3day.

The CZ-BDO was firstly washed with DMF and then dried at 60^{o}C for 48h. Subsequently, the pretreated sample was exposed in ambient for 3days, and characterized by XRD. It can be seen from **Fig.S7** that XRD pattern of the CZ-BDO was not in consist with that of the same sample exposed to the air, suggesting that bimetal mixed sample of CZ-BDO could be easily degraded in moisture environment. However, the liquid reaction system only included the epoxide and CO2, and the water molecule was not being introduced, as a result the reaction system was not affected by the moisture environment.

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N	-0.65251300	-0.40576300	3.25371500
C	-0.69010100	2.49954700	0.07701800
C	8.11827800	2.12689200	1.09477200
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C	6.62469700	1.74322600	0.88957700
C	-1.84908500	6.66912700	0.27814700
C	3.89769000	1.04602900	0.51208000
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C	5.78284100	1.49508900	1.98233900
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C	5.59860200	6.17808200	-0.06044300
C	-6.18716700	5.67288800	0.03449600
C	1.61566400	1.88311100	-0.01505600
C	-2.98008300	2.70671500	0.01237600
C	4.54375300	5.04453900	-0.04834600
C	-5.05077600	4.62103500	0.02672200
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C	3.02229600	3.59520700	1.16635500
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C	4.14178300	4.42426100	-1.23353600
C	3.19734300	3.40637800	-1.22874300
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H	2.57421900	3.26138900	2.10157500
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H	-4.86962900	4.62781200	-2.09126100
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C	-4.04230500	-4.53346600	1.23656300
H	-2.62729300	-3.18110600	2.15591400
C	-4.27637200	-4.34366400	-1.14043600
H	-3.04889400	-2.83857900	-2.09133800
C	4.49800000	-4.01223000	1.16221100
H	3.11487000	-2.64826500	2.11462600
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H	4.96847500	-4.36428100	2.07979200
H	4.76201400	-4.55109100	-2.15331900
C	-5.70123200	-6.10013700	0.06713000
C	6.10591100	-5.60168100	-0.04693800
O	-5.96337000	-6.56945800	1.19721100
O	-6.16052900	-6.41288600	-1.05424500
O	6.54182400	-5.92354400	1.08111200
O	6.45129800	-6.00141100	-1.18143600
C	1.37119400	0.29010500	-4.07777600
C	-0.26693400	-1.44680400	-4.04953100
H	-1.24205800	-1.72573500	-3.62744800
H	0.47962300	-2.11260100	-3.59366600
C	1.41905800	0.19595700	-5.62370400

H	2.09325300	-0.37983700	-3.58998500
C	-0.24960700	-1.50172600	-5.59805800
N	0.10923800	-0.19331800	-6.15941900
H	-1.23466000	-1.78013400	-6.00423900
H	0.47787400	-2.23952600	-5.97108600
H	2.15395600	-0.55092100	-5.96245600
H	1.69734600	1.15890900	-6.07980400
C	-0.88464000	0.79040600	-5.71461900
H	-1.85545800	0.51281300	-6.15405600
H	-0.60134300	1.76681900	-6.13803700
C	-0.87300700	0.83456700	4.22426200
C	1.46746700	0.40432700	4.03154900
C	-0.72510100	0.79652700	5.76716600
H	-1.86074700	0.48165500	3.89443500
H	2.20313000	-0.21621300	3.50128600
C	1.59211400	0.29350600	5.57201200
N	0.32425800	-0.14920000	6.16388800
H	0.76281000	-2.17892900	5.95504000
H	-1.66278800	0.48727200	6.25500400
H	-0.45540500	1.78404000	6.17331600
H	2.36788400	-0.43088700	5.86490200
H	1.85806600	1.26006100	6.02796500
O	6.03347400	6.48815500	-1.19226700
O	5.88898400	6.64686900	1.06302000
C	-0.08431600	-1.41234800	4.06602500
C	-0.00636200	-1.46919600	5.61274200
H	-0.96390700	-1.78631700	6.05486700
H	0.67606600	-2.03977900	3.57941800
H	-1.06002400	-1.73786100	3.67936000
Ni	-0.03956800	0.03727500	1.20887200
Ni	-0.05665800	0.03272100	-1.21023700

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%chk=Zn-BDO.chk
%nprocshared=28
%mem=120GB
opt genecp M06 geom=connectivity scf=maxcycle=500 test

O	-4.98913300	7.53107200	-1.13837000
O	-5.21634000	7.38192100	1.10952600
N	-0.00602600	-0.12258500	-3.41985300
N	0.12523000	-0.01130500	3.42187700
C	-1.50079800	2.16979000	-0.00212400
C	6.93760200	4.82596300	-0.11442800
C	-4.80201500	7.01510300	-0.01331600
C	2.09219800	1.52099300	-0.03546300
C	-2.34096600	3.40194900	-0.00481200
C	5.65751700	3.95614000	-0.09405300
C	-3.93057200	5.73593300	-0.01021700
C	3.32162700	2.36660600	-0.05614100
C	-2.87670800	3.90646800	1.18497900
C	4.90806500	3.80701500	1.07441000
C	-3.65653500	5.05562300	1.17799900
C	3.75985800	3.02607100	1.09735900
C	-2.61162700	4.08155900	-1.19727400
C	-3.39530900	5.22803400	-1.19568500
C	5.21783700	3.29641300	-1.24330500
C	4.07012100	2.51471000	-1.22881600
H	-2.66610000	3.37380600	2.11250700
H	5.26682100	4.33027800	1.96035400
H	-4.08291600	5.46845500	2.09187800
H	3.17443100	2.91690700	2.01002800
H	-2.19173400	3.68723500	-2.12276800
H	-3.62139800	5.77310100	-2.11175900
H	5.81660300	3.42432400	-2.14473000
H	3.73339500	1.99593900	-2.12602400
C	-0.69779100	1.03555200	-4.02183900
H	-0.26086000	1.94748300	-3.59504500
H	-0.30846300	2.03303100	3.52972100
H	1.90465400	1.07677500	3.46089100
H	1.85781200	0.79791600	-3.59283400
H	-1.74257800	1.00108000	-3.68471000
O	-0.99737000	1.79691100	-1.10182300
O	-1.84159200	-0.90825500	-1.06586600
O	0.90316500	-1.75501900	-1.08953100
O	1.72463300	0.98699300	-1.12250900
C	-2.19396600	-1.41680800	0.03816000
C	1.43143500	-2.10804300	0.00468400
O	-1.33964400	1.56807200	1.09957400
O	-1.56501100	-1.26416900	1.12600000
C	-3.42776900	-2.25577000	0.05776900
O	1.28807000	-1.48651700	1.09755000
C	2.27754200	-3.33606800	0.00607800
O	1.48819500	1.38146700	1.06768600
C	-3.84442300	-2.89206200	1.23209600
C	-4.19464200	-2.43209300	-1.09914900
C	2.84080800	-3.81811600	1.19261800
C	2.52861600	-4.03460700	-1.17989900
C	-4.98916200	-3.67813000	1.24455700
H	-3.24494500	-2.76063500	2.13254700
C	-5.33879100	-3.21892000	-1.07818600
H	-3.87552700	-1.93179900	-2.01314100
C	3.62698300	-4.96280200	1.18922400
H	2.64690600	-3.27276800	2.11680700
C	3.31883200	-5.17646600	-1.17537600
H	2.08782700	-3.66022200	-2.10439200
C	-5.75641400	-3.85614500	0.09175000
H	-5.33091400	-4.18397100	2.14717400
H	-5.95121500	-3.36896100	-1.96693000
C	3.88077800	-5.66133900	0.00723400
H	4.07420100	-5.35805700	2.10087600
H	3.52951700	-5.73575700	-2.08650400
C	-7.03096300	-4.73408200	0.11014700
C	4.75911300	-6.93593800	0.00792100
O	-7.31362300	-5.24144900	1.21896300
O	-7.62725200	-4.83246600	-0.98601100
O	5.19806300	-7.28063000	1.12820900
O	4.92538200	-7.46962100	-1.11193000
C	1.39574500	-0.15072500	-3.89211200
C	-0.67823100	-1.36974400	-3.84870000
H	-1.66840400	-1.39419800	-3.37834900
H	-0.10389200	-2.20186700	-3.42174100
C	1.40614100	-0.37146700	-5.41968900

H	1.91285800	-0.94487900	-3.33907800
C	-0.73456400	-1.40484300	-5.39025100
N	0.04796800	-0.30791900	-5.96800000
H	-1.76791900	-1.30493800	-5.75468300
H	-0.34118000	-2.35403200	-5.78294100
H	1.82412000	-1.35552100	-5.67879000
H	2.01966000	0.38728400	-5.92771000
C	-0.55944700	0.96090400	-5.55785100
H	-1.53834900	1.05162100	-6.05149900
H	0.07550300	1.77396900	-5.94036400
C	-0.63660400	1.10573200	4.01660400
C	1.54689700	0.10387700	3.81878900
C	-0.41036300	1.11076100	5.54401500
H	-1.69059000	0.96295800	3.74294000
H	2.10389600	-0.66262900	3.26599400
C	1.65447200	-0.05361300	5.35004800
N	0.32530800	-0.08340600	5.96859000
H	0.10830100	-2.16133600	5.88251500
H	-1.36586300	1.14077100	6.08847100
H	0.17171500	1.99004700	5.85771100
H	2.16857400	-0.98764000	5.62137400
H	2.22517300	0.77383200	5.79689300
O	7.51594300	4.89878600	-1.22213600
O	7.24229600	5.35300600	0.97927800
C	-0.40966400	-1.29235200	3.93275400
C	-0.38566500	-1.26668300	5.47568600
H	-1.40471100	-1.24009200	5.88994900
H	0.21477600	-2.08906700	3.50757000
H	-1.41653600	-1.42395900	3.51883900
Zn	-0.05165200	0.02275100	-1.35716700
Zn	-0.02606300	0.04694700	1.35998600

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%mem=120GB
opt genecp M06 geom=connectivity scf=maxcycle=500 test

Zn	0.00815944	-0.00816328	1.58015821
O	-7.12047082	5.32744831	0.31626108
O	-6.84108200	5.35360907	-1.92011139
N	-0.23778610	0.17128059	3.50622967
N	0.39014288	-0.37121732	-3.31731288
C	-1.85417876	1.33425171	-0.20624655
C	-4.70896542	-6.80884364	-0.19812297
C	-6.47023348	4.94150738	-0.74282801
C	-1.23905365	-2.06256763	0.00384496
C	-3.06257455	2.27842703	-0.34744646
C	-3.80035124	-5.56655529	-0.14562122
C	-5.26187036	3.99708113	-0.60284170
C	-2.14706375	-3.30529631	-0.04954962
C	-3.46165460	2.72191609	-1.61558028
C	-3.38357077	-4.95224654	-1.33432695
C	-4.56134000	3.58130975	-1.74325167
C	-2.55686511	-3.82159214	-1.28630684
C	-3.76322412	2.69412570	0.79278238
C	-4.86279443	3.55342759	0.66511888
C	-3.39029085	-5.05039956	1.09099863
C	-2.56363591	-3.91986451	1.13903620
H	-2.92681064	2.40444335	-2.48627513
H	-3.69656414	-5.34645492	-2.27855160
H	-4.86608416	3.91999807	-2.71141423
H	-2.23859932	-3.35257312	-2.19386514
H	-3.45856692	2.35537248	1.76094257
H	-5.39767363	3.87079650	1.53580387
H	-3.70840966	-5.51950488	1.99854637
H	-2.25050731	-3.52585732	2.08328680
C	-1.59768150	0.58417333	3.83574709
H	-2.21491230	-0.28639357	3.75803901
H	-1.57195249	0.38097717	-3.64581366
H	-0.84081934	-1.96417225	-3.67692991
H	-0.39956307	-1.94056225	3.69968986
H	-1.98191807	1.34680952	3.19105015
O	-1.53456712	0.95363136	0.99292743
O	0.99906023	1.56997716	1.18679006
O	1.62865212	-0.96893777	1.36190562
O	-0.89045705	-1.63441117	1.17637817
C	1.32496463	2.03123906	0.01670372
C	2.12045900	-1.38188842	0.23419715
O	-1.24642484	0.97847905	-1.29671347
O	1.09835083	1.44309089	-1.12646450
C	2.05156428	3.38844728	-0.02397667
O	1.67490327	-1.06468558	-0.95793846
C	3.34494691	-2.31339869	0.30194297
O	-0.88130970	-1.53651596	-1.13424392
C	2.43490700	3.94212428	-1.25302773
C	2.32948907	4.06981932	1.16863930
C	3.92962446	-2.78981289	-0.87923489
C	3.87460489	-2.68460828	1.54520651
C	3.09658597	5.17703037	-1.28926554
H	2.22244177	3.42207432	-2.16370217
C	2.99114460	5.30461040	1.13239717
H	2.03648437	3.64717943	2.10697347
C	5.04389543	-3.63751136	-0.81708311
H	3.52532100	-2.50636883	-1.82849071
C	4.98882116	-3.53226355	1.60732214
H	3.42824333	-2.32080488	2.44707407
C	3.37484266	5.85818732	-0.09650921
H	3.38934083	5.59979291	-2.22759728
H	3.20340970	5.82474226	2.04305312
C	5.57347543	-4.00871665	0.42619779
H	5.49032979	-4.00131355	-1.71888788
H	5.39316938	-3.81568200	2.55657559
C	4.10226223	7.21502704	-0.13606479
C	6.79791104	-4.94022242	0.49455349
O	4.45883546	7.72925413	-1.27704214
O	4.36037940	7.84733496	0.97160910
O	7.34085663	-5.38277218	-0.60214465
O	7.28961312	-5.28478539	1.64905590
C	0.01403049	-1.08852895	4.19756664
C	0.66788981	1.16593249	4.07091811
H	0.25311496	2.12679207	3.84822722
H	1.66187061	1.11204594	3.67846628

C	-0.67651588	-0.97821512	5.59789464
H	1.07610081	-1.20063019	4.26362849
C	0.75020727	0.87764929	5.60717011
N	-0.55974567	0.40626882	6.02644847
H	1.06195389	1.77314444	6.10295428
H	1.44312139	0.09272494	5.82770138
H	-0.20675214	-1.67315694	6.26219089
H	-1.72295233	-1.19464580	5.54313165
C	-1.54993830	1.17121851	5.28591637
H	-1.21841346	2.18854233	5.29216359
H	-2.53311693	1.11793926	5.70475496
C	-0.59130325	0.39917819	-4.07346071
C	0.21217218	-1.77407951	-3.67614924
C	-0.68190330	-0.25748059	-5.49140077
H	-0.23883071	1.40903732	-4.10294520
H	0.69189167	-2.45282673	-3.00230359
C	0.86792085	-1.96407860	-5.08462357
N	0.64924212	-0.73471210	-5.82948962
H	2.57507728	0.15412323	-5.75619523
H	-1.06295299	0.47008878	-6.17721287
H	-1.32366264	-1.11363991	-5.49261464
H	1.92750293	-2.09574659	-5.01521595
H	0.43458741	-2.82695018	-5.54567942
O	-5.09585318	-7.37905415	0.90577867
O	-5.08987118	-7.28835939	-1.34630607
C	1.71245955	0.03265981	-3.78280100
C	1.59835417	0.24654289	-5.32912705
H	1.19818507	1.20952759	-5.56869230
H	2.38894176	-0.75325588	-3.51896581
H	2.05546895	0.95106899	-3.35413268
Co	0.20157965	-0.10644848	-1.48597618

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%chk=CN-BDO.chk
%nprocshared=28
%mem=120GB
opt genecp M06 geom=connectivity scf=maxcycle=500 test

O	-7.12047082	5.32744831	0.31626108
O	-6.84108200	5.35360907	-1.92011139
N	-0.23778610	0.17128059	3.50622967
N	0.39014288	-0.37121732	-3.31731288
C	-1.85417876	1.33425171	-0.20624655
C	-4.70896542	-6.80884364	-0.19812297
C	-6.47023348	4.94150738	-0.74282801
C	-1.23905365	-2.06256763	0.00384496
C	-3.06257455	2.27842703	-0.34744646
C	-3.80035124	-5.56655529	-0.14562122
C	-5.26187036	3.99708113	-0.60284170
C	-2.14706375	-3.30529631	-0.04954962
C	-3.46165460	2.72191609	-1.61558028
C	-3.38357077	-4.95224654	-1.33432695
C	-4.56134000	3.58130975	-1.74325167
C	-2.55686511	-3.82159214	-1.28630684
C	-3.76322412	2.69412570	0.79278238
C	-4.86279443	3.55342759	0.66511888
C	-3.39029085	-5.05039956	1.09099863
C	-2.56363591	-3.91986451	1.13903620
H	-2.92681064	2.40444335	-2.48627513
H	-3.69656414	-5.34645492	-2.27855160
H	-4.86608416	3.91999807	-2.71141423
H	-2.23859932	-3.35257312	-2.19386514
H	-3.45856692	2.35537248	1.76094257
H	-5.39767363	3.87079650	1.53580387
H	-3.70840966	-5.51950488	1.99854637
H	-2.25050731	-3.52585732	2.08328680
C	-1.59768150	0.58417333	3.83574709
H	-2.21491230	-0.28639357	3.75803901
H	-1.57195249	0.38097717	-3.64581366
H	-0.84081934	-1.96417225	-3.67692991
H	-0.39956307	-1.94056225	3.69968986
H	-1.98191807	1.34680952	3.19105015
O	-1.53456712	0.95363136	0.99292743
O	0.99906023	1.56997716	1.18679006
O	1.62865212	-0.96893777	1.36190562
O	-0.89045705	-1.63441117	1.17637817
C	1.32496463	2.03123906	0.01670372
C	2.12045900	-1.38188842	0.23419715
O	-1.24642484	0.97847905	-1.29671347
O	1.09835083	1.44309089	-1.12646450
C	2.05156428	3.38844728	-0.02397667
O	1.67490327	-1.06468558	-0.95793846
C	3.34494691	-2.31339869	0.30194297
O	-0.88130970	-1.53651596	-1.13424392
C	2.43490700	3.94212428	-1.25302773
C	2.32948907	4.06981932	1.16863930
C	3.92962446	-2.78981289	-0.87923489
C	3.87460489	-2.68460828	1.54520651
C	3.09658597	5.17703037	-1.28926554
H	2.22244177	3.42207432	-2.16370217
C	2.99114460	5.30461040	1.13239717
H	2.03648437	3.64717943	2.10697347
C	5.04389543	-3.63751136	-0.81708311
H	3.52532100	-2.50636883	-1.82849071
C	4.98882116	-3.53226355	1.60732214
H	3.42824333	-2.32080488	2.44707407
C	3.37484266	5.85818732	-0.09650921
H	3.38934083	5.59979291	-2.22759728
H	3.20340970	5.82474226	2.04305312
C	5.57347543	-4.00871665	0.42619779
H	5.49032979	-4.00131355	-1.71888788
H	5.39316938	-3.81568200	2.55657559
C	4.10226223	7.21502704	-0.13606479
C	6.79791104	-4.94022242	0.49455349
O	4.45883546	7.72925413	-1.27704214
O	4.36037940	7.84733496	0.97160910
O	7.34085663	-5.38277218	-0.60214465
O	7.28961312	-5.28478539	1.64905590
C	0.01403049	-1.08852895	4.19756664
C	0.66788981	1.16593249	4.07091811
H	0.25311496	2.12679207	3.84822722
H	1.66187061	1.11204594	3.67846628
C	-0.67651588	-0.97821512	5.59789464

H	1.07610081	-1.20063019	4.26362849
C	0.75020727	0.87764929	5.60717011
N	-0.55974567	0.40626882	6.02644847
H	1.06195389	1.77314444	6.10295428
H	1.44312139	0.09272494	5.82770138
H	-0.20675214	-1.67315694	6.26219089
H	-1.72295233	-1.19464580	5.54313165
C	-1.54993830	1.17121851	5.28591637
H	-1.21841346	2.18854233	5.29216359
H	-2.53311693	1.11793926	5.70475496
C	-0.59130325	0.39917819	-4.07346071
C	0.21217218	-1.77407951	-3.67614924
C	-0.68190330	-0.25748059	-5.49140077
H	-0.23883071	1.40903732	-4.10294520
H	0.69189167	-2.45282673	-3.00230359
C	0.86792085	-1.96407860	-5.08462357
N	0.64924212	-0.73471210	-5.82948962
H	2.57507728	0.15412323	-5.75619523
H	-1.06295299	0.47008878	-6.17721287
H	-1.32366264	-1.11363991	-5.49261464
H	1.92750293	-2.09574659	-5.01521595
H	0.43458741	-2.82695018	-5.54567942
O	-5.09585318	-7.37905415	0.90577867
O	-5.08987118	-7.28835939	-1.34630607
C	1.71245955	0.03265981	-3.78280100
C	1.59835417	0.24654289	-5.32912705
H	1.19818507	1.20952759	-5.56869230
H	2.38894176	-0.75325588	-3.51896581
H	2.05546895	0.95106899	-3.35413268
Co	0.20157965	-0.10644848	-1.48597618
Ni	0.00815944	-0.00816328	1.58015821

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%chk=NZ-BDO.chk
%nprocshared=28
%mem=120GB
opt genecp M06 geom=connectivity scf=maxcycle=500 test

O	-2.39075900	8.74319100	-0.76447400
O	-2.41103000	8.63281600	1.50705900
N	0.75895400	0.31779700	-3.47639200
N	-0.65251300	-0.40576300	3.25371500
C	-0.69010100	2.49954700	0.07701800
C	8.11827800	2.12689200	1.09477200
C	-2.25990100	8.16807900	0.34742800
C	2.46046100	0.67672900	0.30825400
C	-1.09327500	3.93638700	0.15028000
C	6.62469700	1.74322600	0.88957700
C	-1.84908500	6.66912700	0.27814700
C	3.89769000	1.04602900	0.51208000
C	-1.28241900	4.57534300	1.38748900
C	5.78284100	1.49508900	1.98233900
C	-1.65340500	5.91733600	1.44505000
C	4.44383700	1.15204500	1.80220700
C	-1.29027500	4.68635000	-1.02134900
C	-1.66172100	6.02750000	-0.95369900
C	6.07676400	1.63604600	-0.39590700
C	4.73903400	1.29490000	-0.58492500
H	-1.12997800	4.00076900	2.29634700
H	6.21950600	1.58263500	2.97334800
H	-1.80275900	6.42671500	2.39295700
H	3.79841600	0.96043100	2.65428200
H	-1.15039700	4.19618200	-1.98043100
H	-1.81783000	6.62187300	-1.84970800
H	6.74004900	1.83020800	-1.23431200
H	4.32419400	1.21662900	-1.58588100
C	1.21129900	1.72203200	-3.67781600
H	1.98112600	1.91662100	-2.92952200
H	-0.89729800	1.63091400	3.66281000
H	1.16928700	0.40090800	3.89546500
H	2.66137600	-0.37192200	-2.97182900
H	0.36604300	2.37623400	-3.45161900
O	-0.48014200	1.98618100	-1.06998400
O	-1.90552900	-0.47216300	-1.61231700
O	0.60197200	-1.87427900	-1.24255700
O	2.01022500	0.60545700	-0.87751800
C	-2.51791000	-0.59998900	-0.49906600
C	0.65533700	-2.46416900	-0.11574600
O	-0.56577100	1.85597200	1.17162300
O	-1.96443200	-0.44675100	0.63975000
C	-3.96918800	-0.95621200	-0.53755700
O	0.41905800	-1.88545300	0.99644700
C	1.02117200	-3.91308000	-0.08902700
O	1.75823000	0.45512500	1.35405700
C	-4.75030700	-0.97480400	0.63015200
C	-4.58688800	-1.28640700	-1.75590700
C	1.26256800	-4.58167900	1.12302100
C	1.13519100	-4.64313300	-1.28422900
C	-6.10045900	-1.31602500	0.57678100
H	-4.28328200	-0.70643900	1.57330900
C	-5.93635900	-1.63006600	-1.79847100
H	-3.98522600	-1.27232900	-2.65987400
C	1.60687500	-5.93211300	1.13370900
H	1.18586000	-4.02144000	2.05045300
C	1.47537800	-5.99404200	-1.26316500
H	0.94502700	-4.13207800	-2.22361500
C	-6.71849100	-1.65227100	-0.63566700
H	-6.71965900	-1.33324700	1.46930300
H	-6.42904900	-1.89139700	-2.73087600
C	1.71857300	-6.66407600	-0.05648600
H	1.80089000	-6.46335800	2.06131200
H	1.56405100	-6.57410500	-2.17755900
C	-8.22518600	-2.03612000	-0.69048400
C	2.10077300	-8.17220600	-0.03980300
O	-8.82231400	-2.03643600	0.41709200
O	-8.67167000	-2.30334600	-1.83658300
O	2.28242700	-8.66977300	1.10154000
O	2.18208200	-8.71980700	-1.17009200
C	1.90626700	-0.59782200	-3.72585400
C	-0.32019200	0.01305500	-4.44980400
H	-1.16357700	0.67549100	-4.23419600
H	-0.65708600	-1.01105800	-4.26476600
C	2.42338500	-0.39460200	-5.18156900

H	1.55999400	-1.61690000	-3.54158100
C	0.22023500	0.20095200	-5.90182400
N	1.63018400	0.62984300	-5.89087400
H	-0.36070500	0.95729700	-6.44470300
H	0.15459100	-0.73473600	-6.47133300
H	2.36388500	-1.32609200	-5.75869300
H	3.47163100	-0.07228500	-5.18763800
C	1.72665600	1.89609300	-5.13756000
H	1.14478800	2.65430000	-5.67679200
H	2.77521300	2.21744400	-5.15115900
C	-1.45883600	0.70568300	3.80988900
C	0.60460200	-0.52475200	4.03104200
C	-1.76593500	0.43306400	5.31558000
H	-2.36837300	0.78235100	3.20877800
H	1.19132800	-1.32923500	3.58097300
C	0.27383200	-0.79893200	5.53111000
N	-1.18389700	-0.85080400	5.75298500
H	-1.32169000	-2.87647800	5.24472400
H	-2.84699900	0.39318300	5.50022500
H	-1.35391200	1.22505400	5.95448000
H	0.69922500	-1.75447400	5.86347100
H	0.68657400	-0.01445800	6.17888700
O	8.77500200	2.32198700	0.03869300
O	8.49748500	2.19900400	2.29253100
C	-1.42038100	-1.66893800	3.39828500
C	-1.74195500	-1.92196100	4.90297300
H	-2.82453400	-1.96053500	5.07851600
H	-0.81759300	-2.46703300	2.96187900
H	-2.32175300	-1.57309100	2.79038700
Zn	-0.09729300	-0.01851000	1.12246900
Ni	0.01951500	0.05841900	-1.47401000

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