

Macrocyclic Di-Zinc(II) Alkyl and Alkoxide Complexes: Reactivity towards CO₂ and Investigations in Polymerization Catalysis

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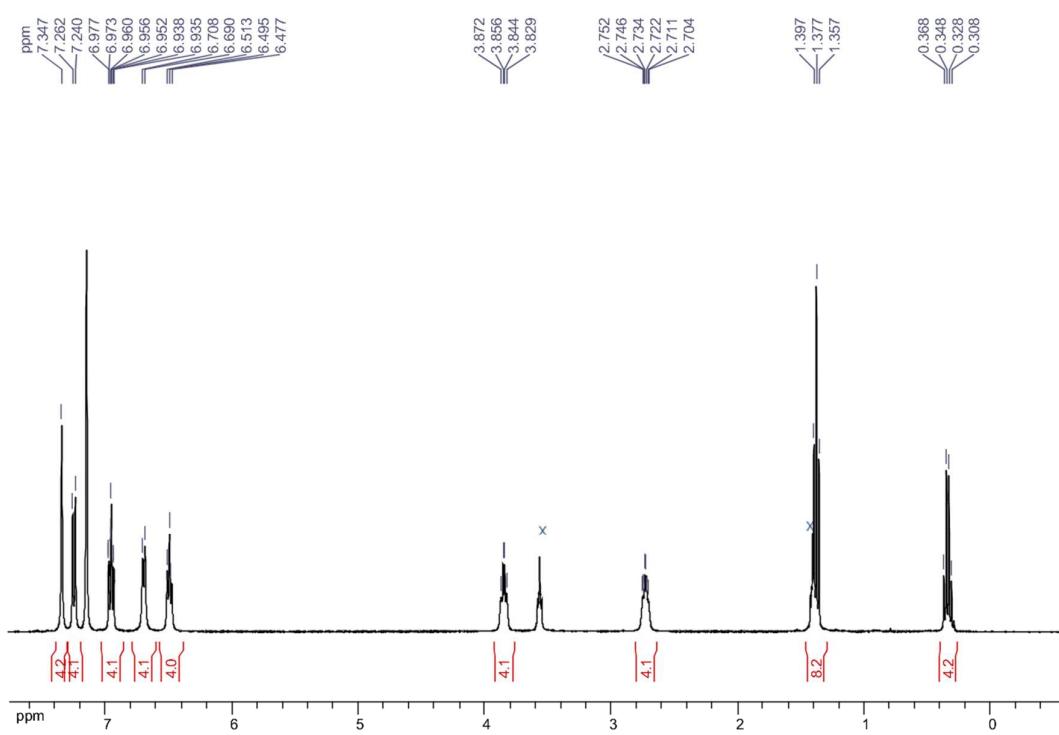


Figure S1: ^1H NMR spectrum (C_6D_6 , 298 K) of **1** showing only 1 isomer in C_6D_6 (x = free residual THF).

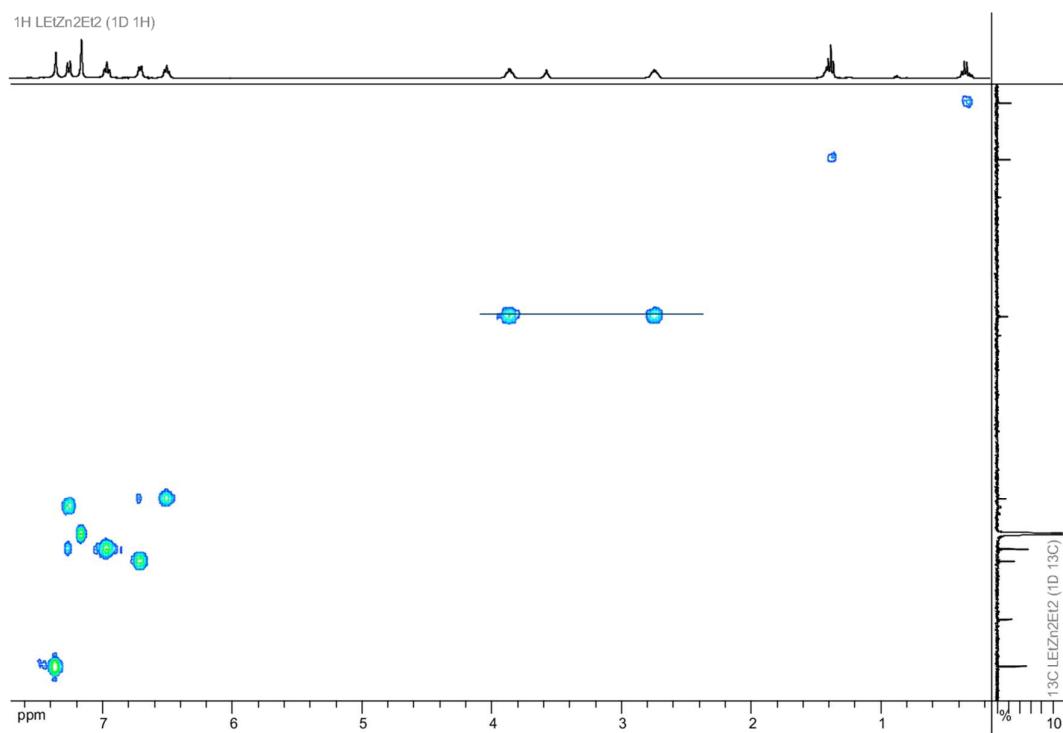


Figure S2: $\{^1\text{H}-^{13}\text{C}\}$ HSQC NMR spectrum (C_6D_6 , 298 K) of **1**.

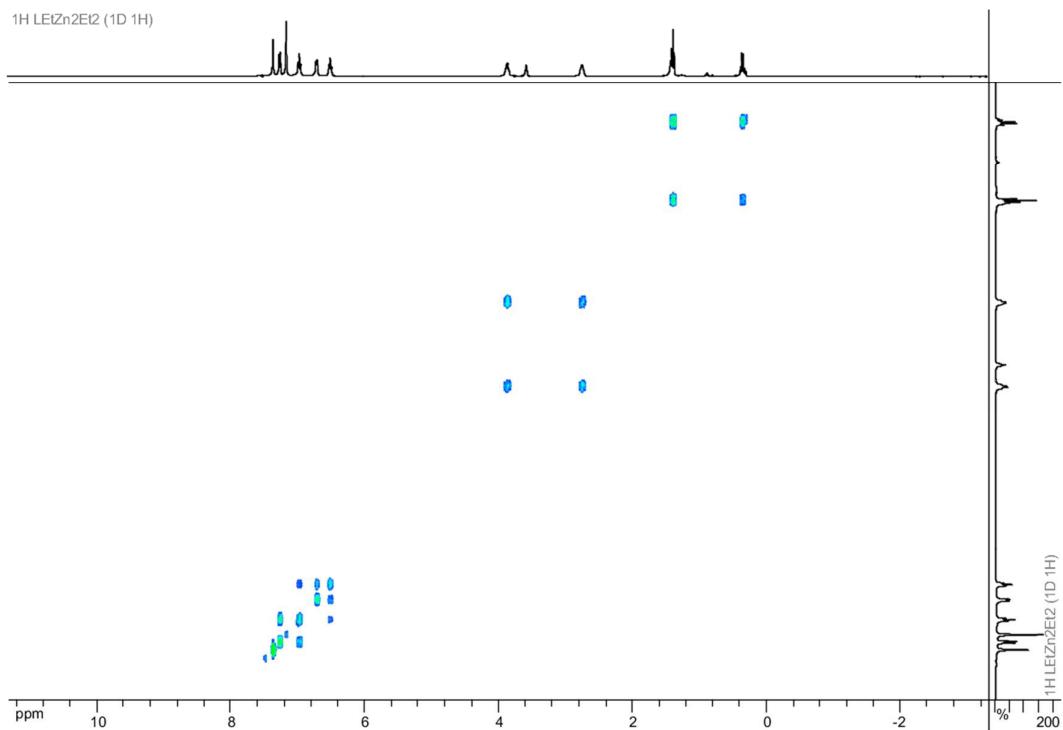


Figure S3: ^1H COSY NMR spectrum (C_6D_6 , 268 K) of **1**.

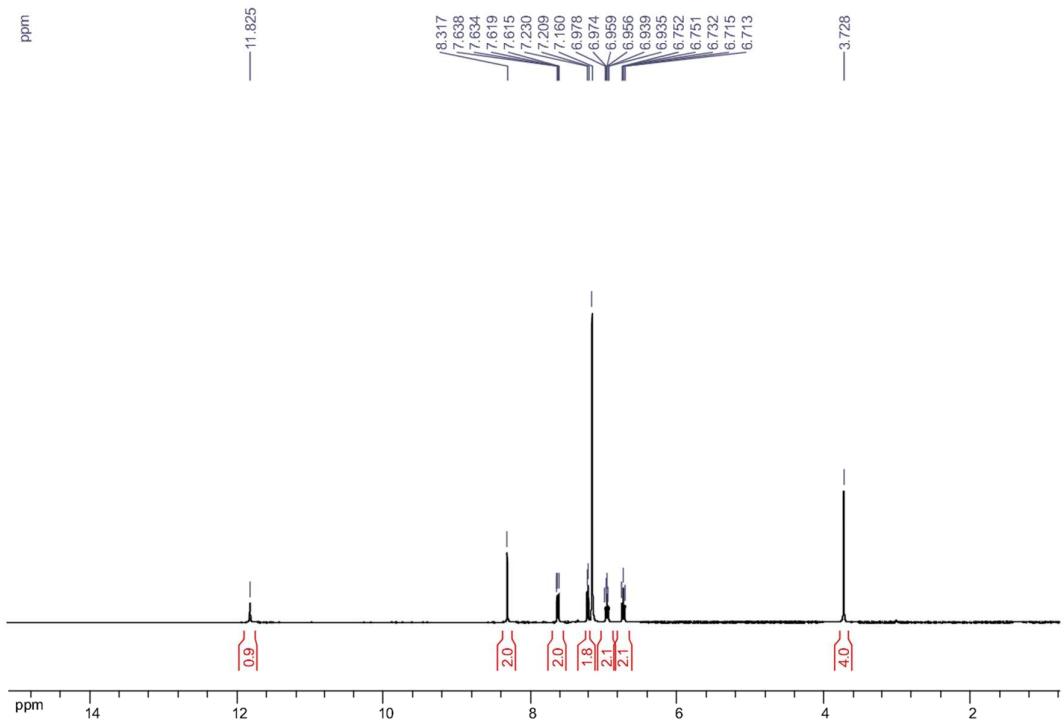


Figure S4: ^1H NMR spectrum (C_6D_6 , 298 K) of $\text{H}_2\text{L}^{\text{Et}}$ in C_6D_6 .

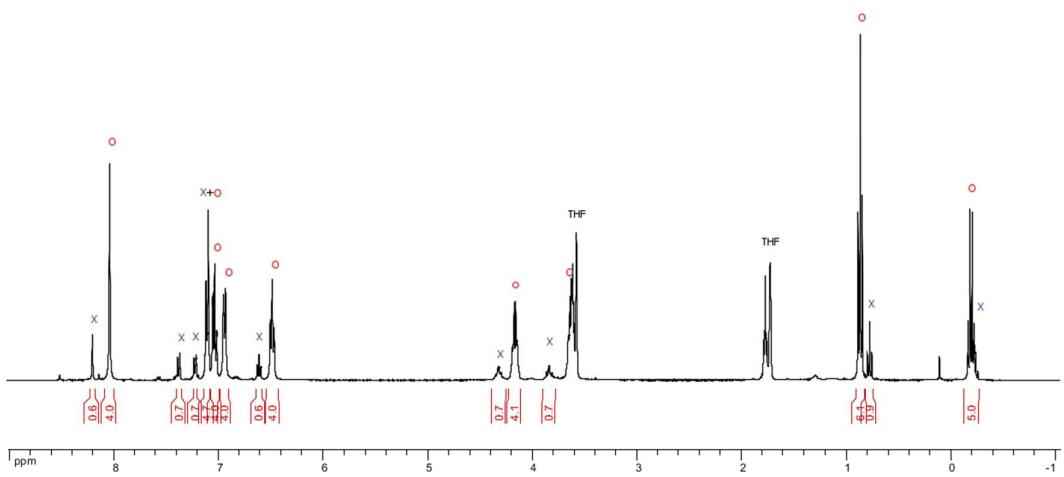


Figure S5: ^1H NMR spectrum (298 K) of **1** showing the presence of two main isomers (X and O) in $\text{THF}-d_8$.

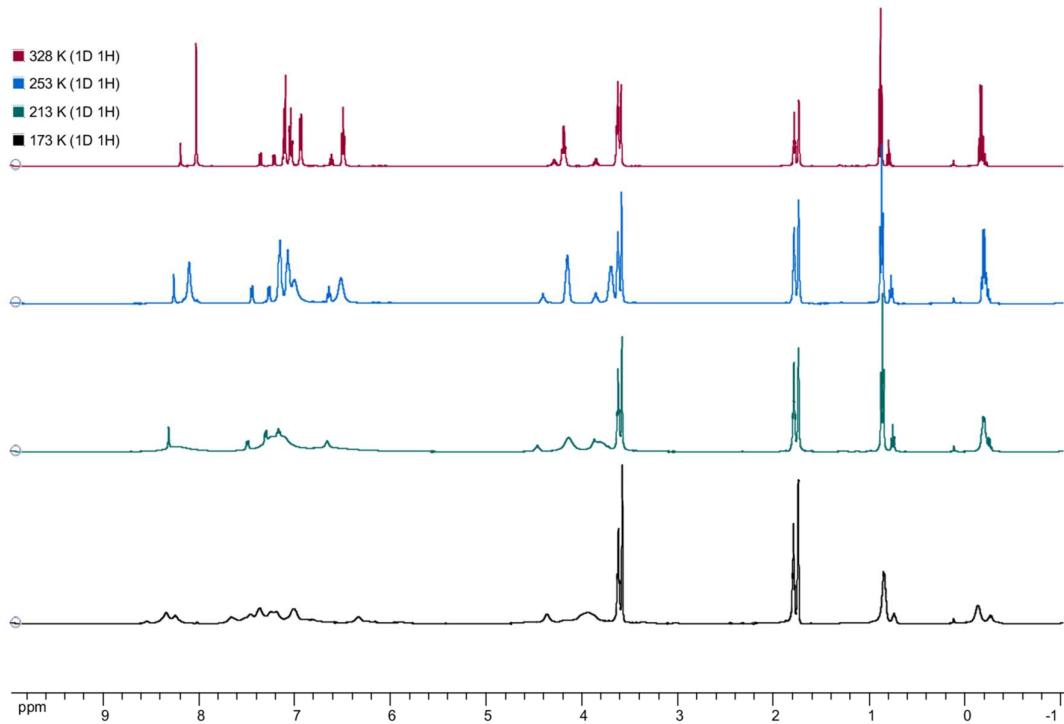


Figure S6: Variable temperature ¹H NMR spectra of **1** in THF-d₈ between 173 K and 328 K.

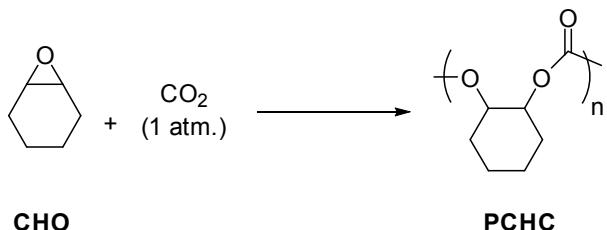


Table S1: Investigated conditions for ROCOP of CHO/CO₂.

Entry	Cat.	Co-cat. (iPA) (eq.)	CHO (eq.)	CO ₂ (bar)	T (°C)	T (h)	Conv. (%)
1	1	-	1000	1	80	20	0
2	1	2	1000	1	80	20	0
3	2	-	1000	1	80	35	0
4	2	-	1000	1	100	13	0

Reaction conditions: cat. = 1 eq., 80 °C, epoxide as solvent.

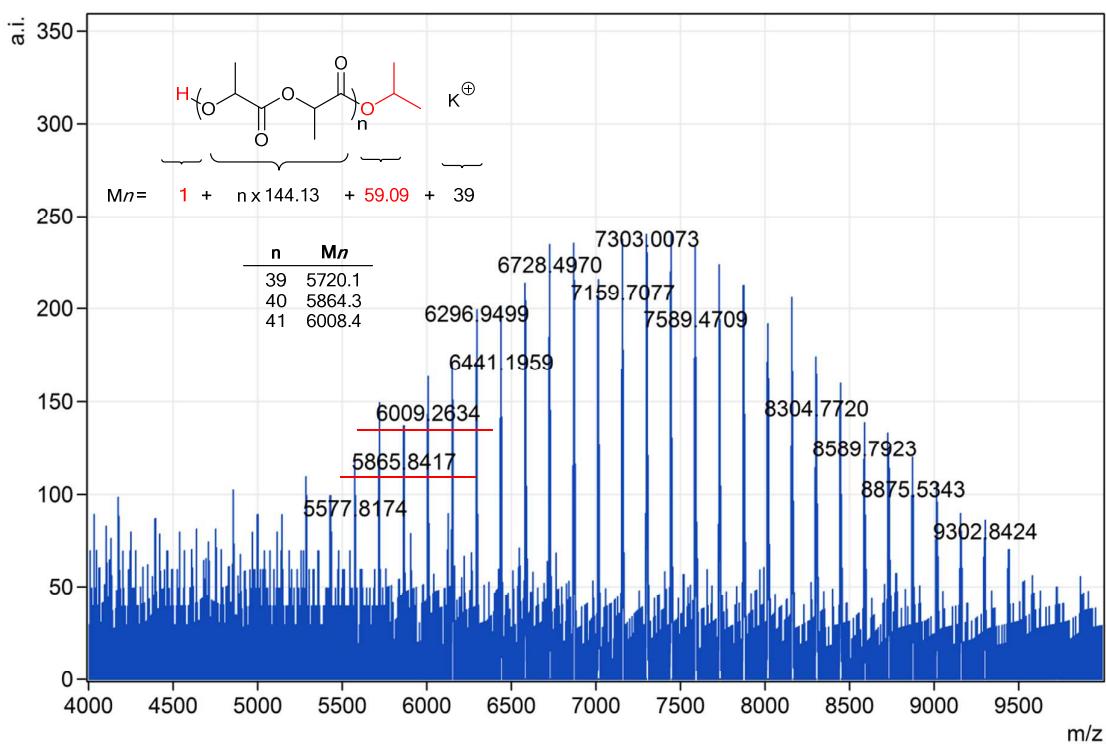


Figure S7: MALDI-ToF spectrum of PLA ($M_n = 6,550 \text{ g/mol}^{-1}$, $D = 1.08$).

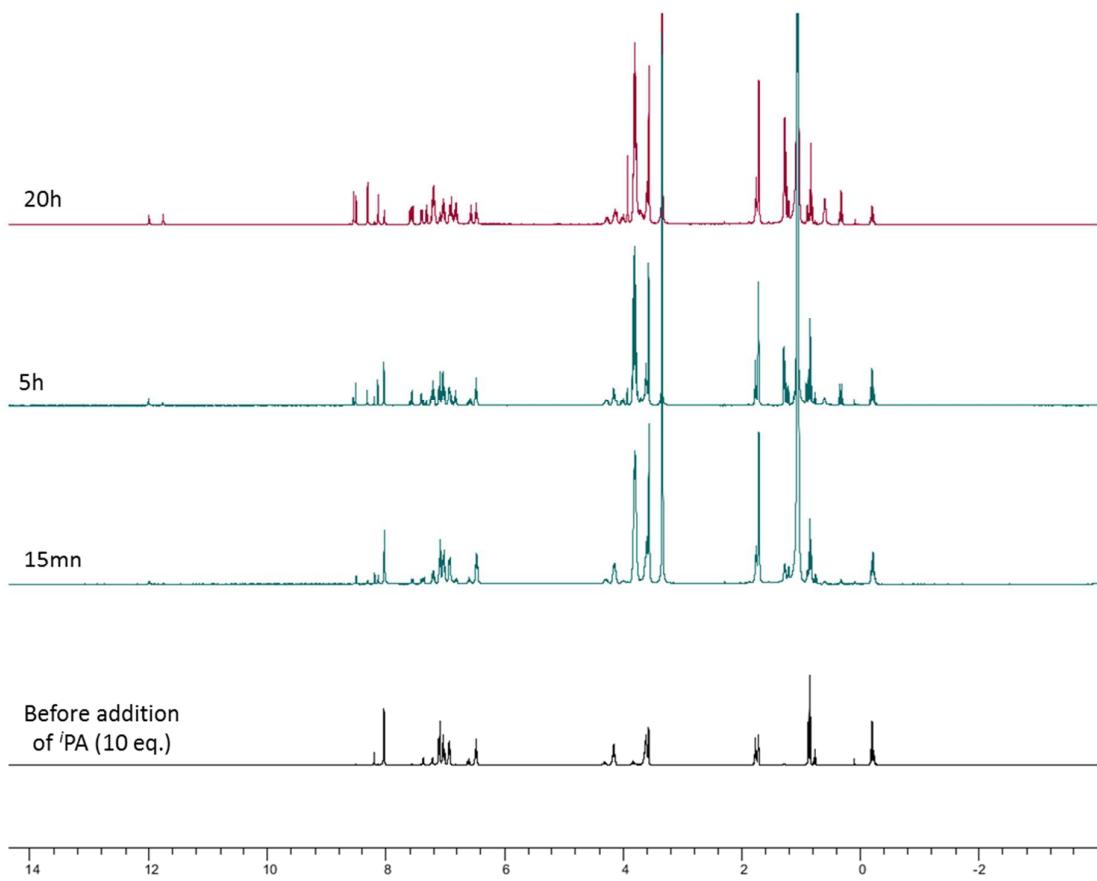


Figure S8: ^1H NMR spectra ($25\text{ }^\circ\text{C}$, THF-d8) of **1** with time showing the stability of the ethyl group and the slow protonation of the ligand (11.76 ppm and 12.00 ppm) in the presence of 10 equivalents of ^1PA .

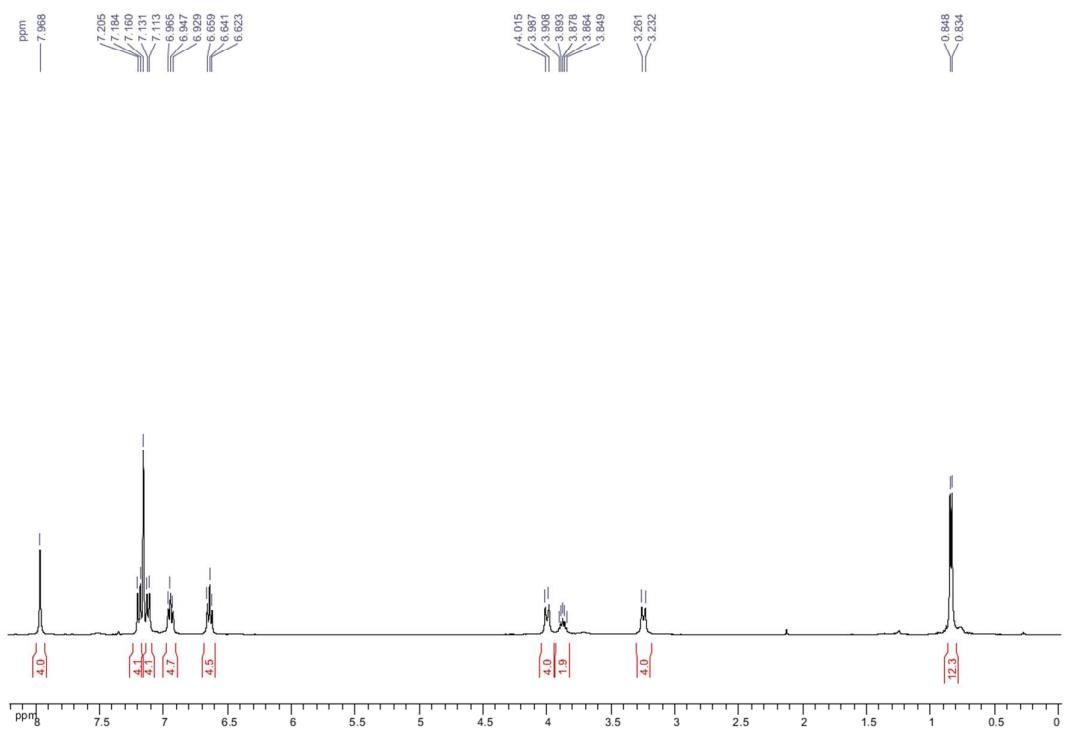


Figure S9: ^1H NMR spectrum of **2** in C_6D_6 at room temperature.

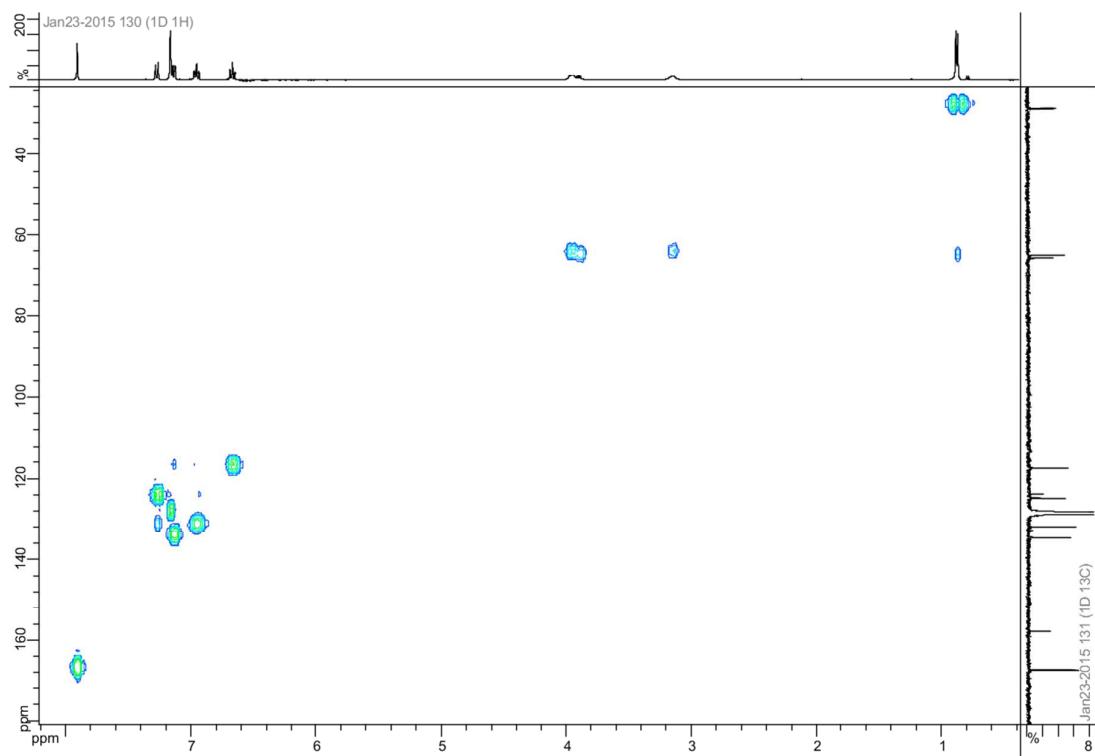


Figure S10: $\{^1\text{H}-^{13}\text{C}\}$ HSQC NMR spectrum (C_6D_6 , 298 K) of **2**.

Temperature increase showing formation and equilibrium between **3a** (T), **3b** (X) and **2**(O) under CO₂.

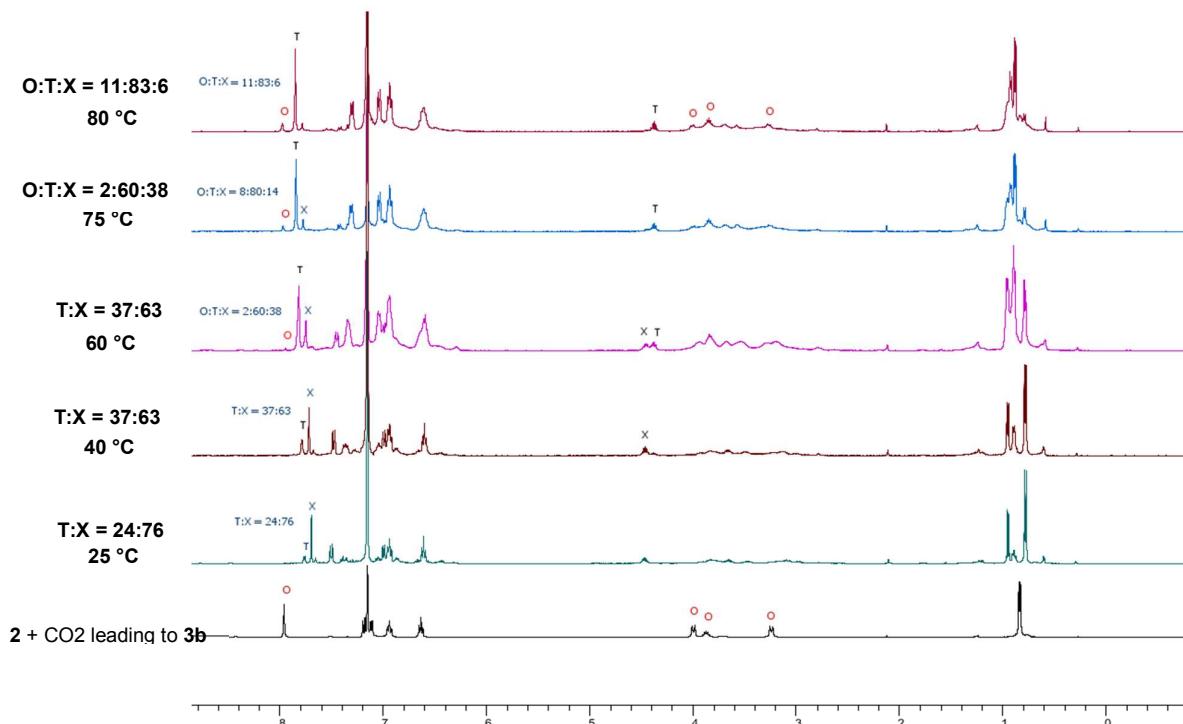


Figure S11: ¹H NMR spectra showing CO₂ insertion into **2** leading to **3b**. From bottom to top: **2** in C₆D₆ (black), after CO₂ addition at room temperature (green), ¹H NMR spectra at variable temperatures with the ratio of the different species (O, X and T) based on the integration of the imine signals (lhs).

Proposed ¹H chemical shifts attributed to intermediate **3a** at 75 °C in C₆D₆ (spectrum in blue in Figure S11): ¹H NMR (400 MHz, C₆D₆): 7.85 (s, N=CH), 7.30 (d, *J* = 7.6 Hz, aryl-H), 7.04 (d, *J* = 8.0 Hz), 6.93 (dd, *J* = 8 Hz, *J* = 8 Hz), 6.66-6.55 (m, aryl-H), 4.38 (sept, *J* = 6.0 Hz, CH-iPr), 4.01 (br, ethyl chain), 3.84 (sept, *J* = 6.0 Hz), 3.68 (br, ethyl chain), 3.57 (br, ethyl chain), 3.26 (br, ethyl chain), 0.92 (d, *J* = 6.0 Hz, iPr), 0.88 (d, *J* = 6.0 Hz).

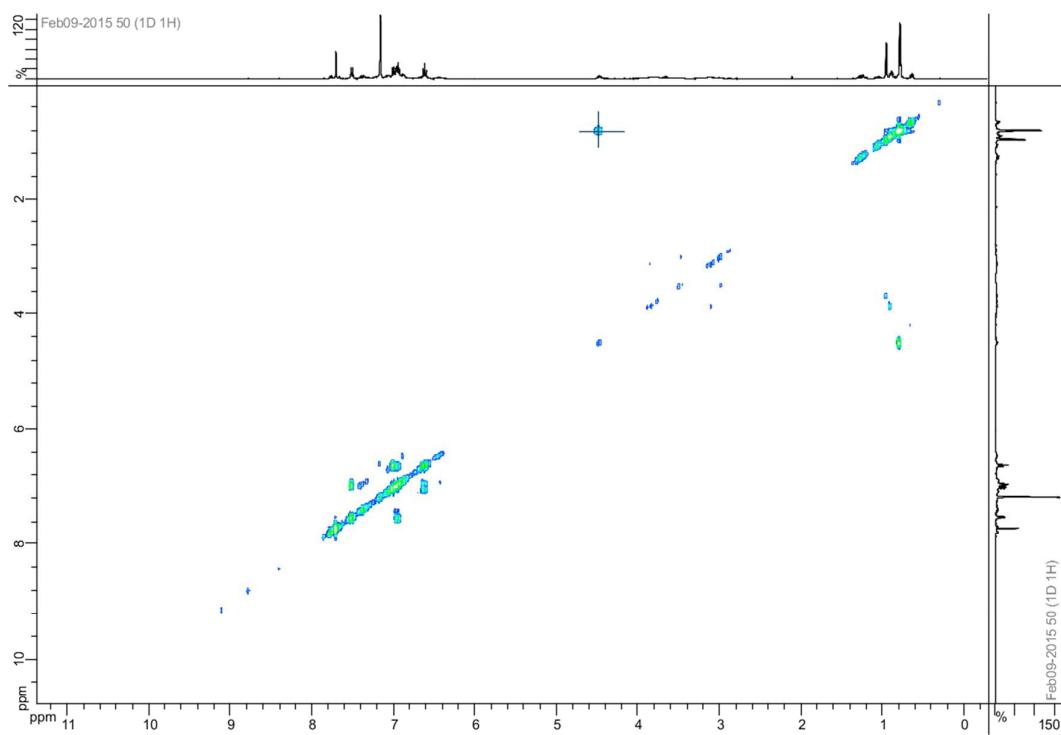


Figure S12: ^1H COSY NMR spectrum after CO_2 addition to **2** in C_6D_6 .

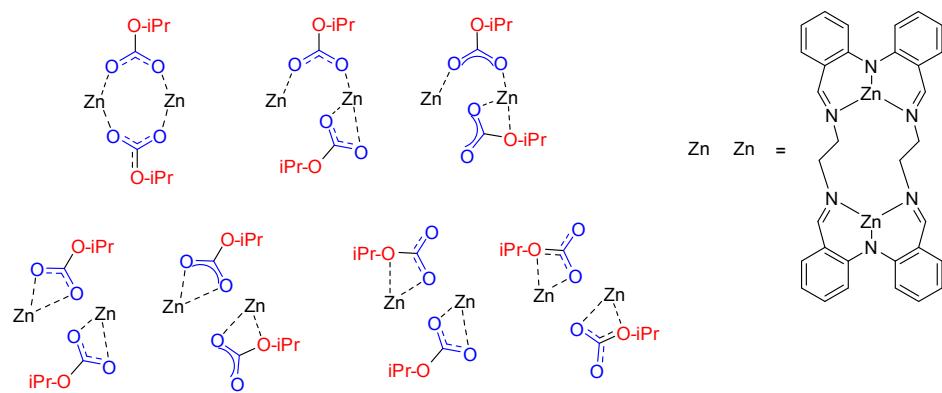


Figure S13: Different coordination modes of the carbonate groups for complex **3b**.

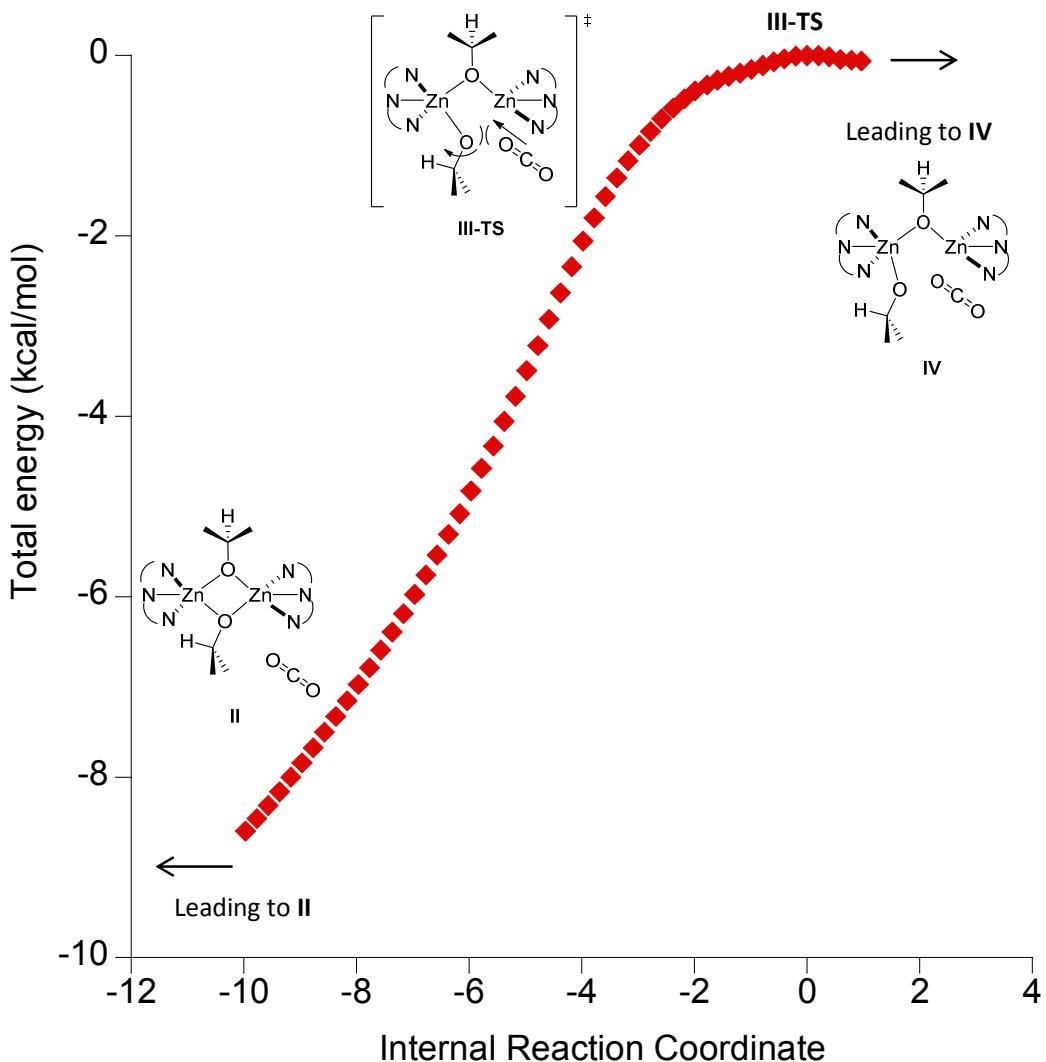


Figure S14: Forward and reverse IRC calculations from III-TS leading to II and IV, respectively.

Reverse IRC calculation (follow the path only in the reverse direction):

```
IRC=(reverse,maxpoints=50,recalc=5,calcfc,maxcycle=40,tight,cartesian,lqa,stepsize=10) rwb97xd/6-31g(d) scrf=(cpcm,solvent=benzene)
```

Forward IRC calculation (follow the path only in the forward direction):

```
IRC=(forward,maxpoints=50,recalc=8,calcfc,maxcycle=40,tight,cartesian,lqa,stepsize=20) rwb97xd/6-31g(d) scrf=(cpcm,solvent=benzene)
```

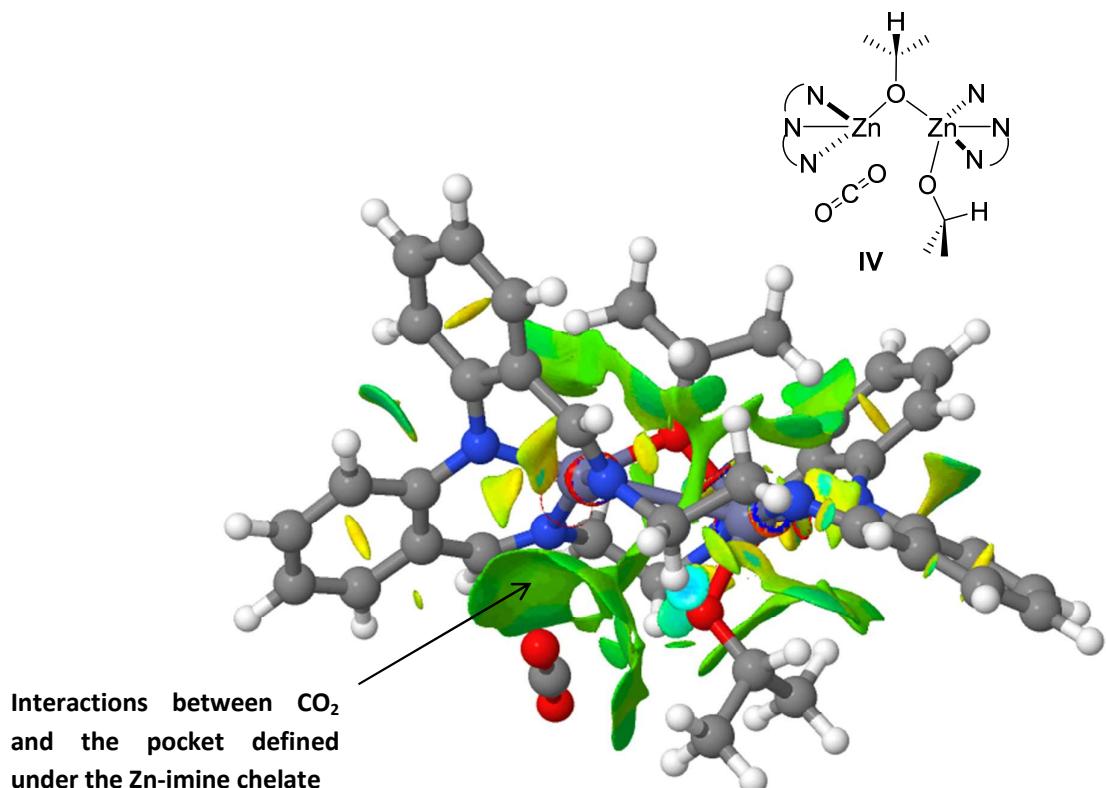


Figure S15: Non covalent interactions (NCI) in **IV** showing interaction between CO_2 and the free pocket.

The following parameters are used to create the NCI surface:¹

```
isosurface parameters [0.5 1 0 0.05 0.95 1.00] NCI density.cube colorscheme "bgyor";color isosurface range 0.04 -0.04
```

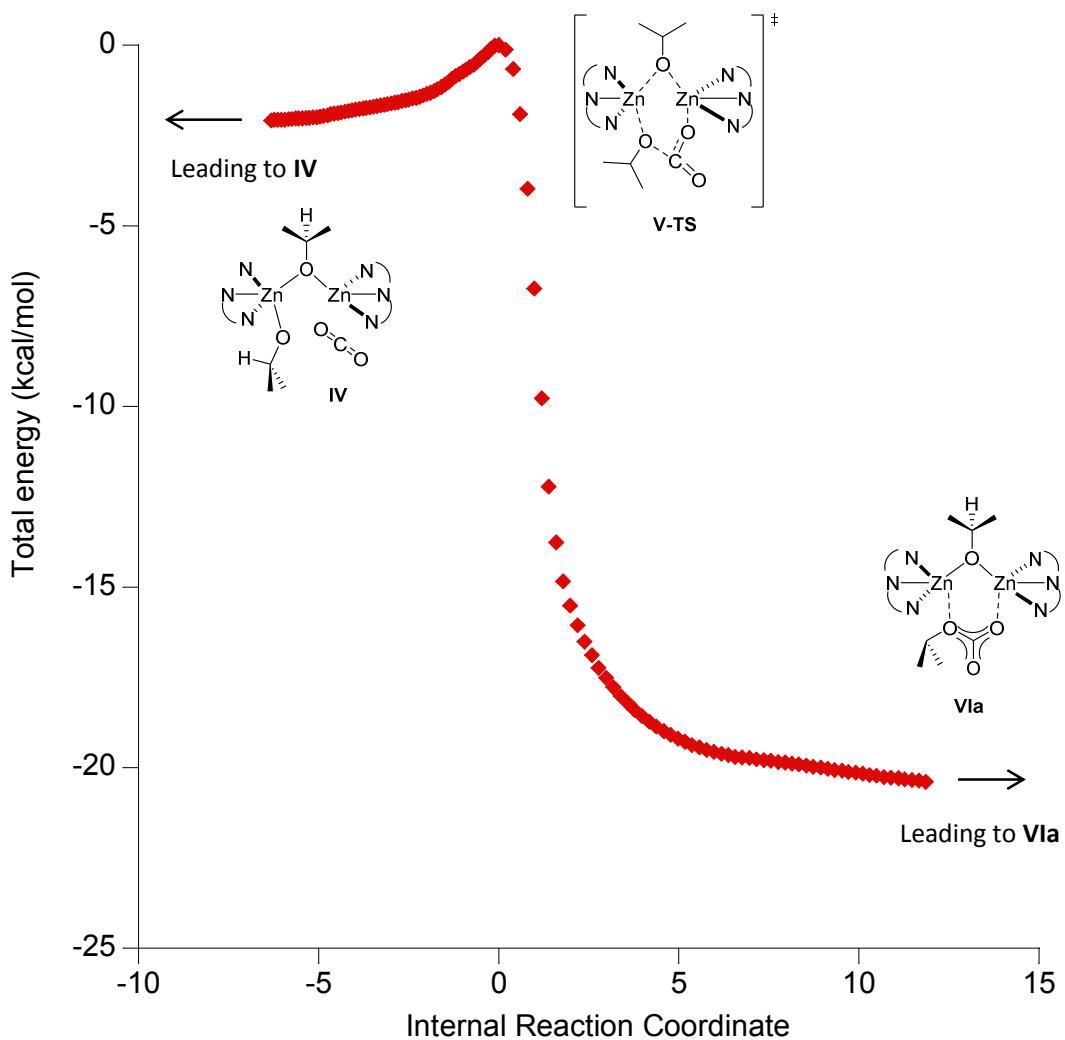


Figure S16: Forward and reverse IRC calculations from **V-TS** leading to **IV** and **VIa**, respectively.

Reverse IRC calculation (follow the path only in the reverse direction):

```
IRC=(reverse,maxpoints=100,recalc=5,calcfc,maxcycle=40,tight,cartesian,lqa,stepsize=10)
rwb97xd/6-31g(d) scrf=(cpcm,solvent=benzene)
```

Forward IRC calculation (follow the path only in the forward direction):

```
IRC=(forward,maxpoints=60,recalc=8,calcfc,maxcycle=40,tight,cartesian,lqa,stepsize=20)
rwb97xd/6-31g(d) scrf=(cpcm,solvent=benzene)
```

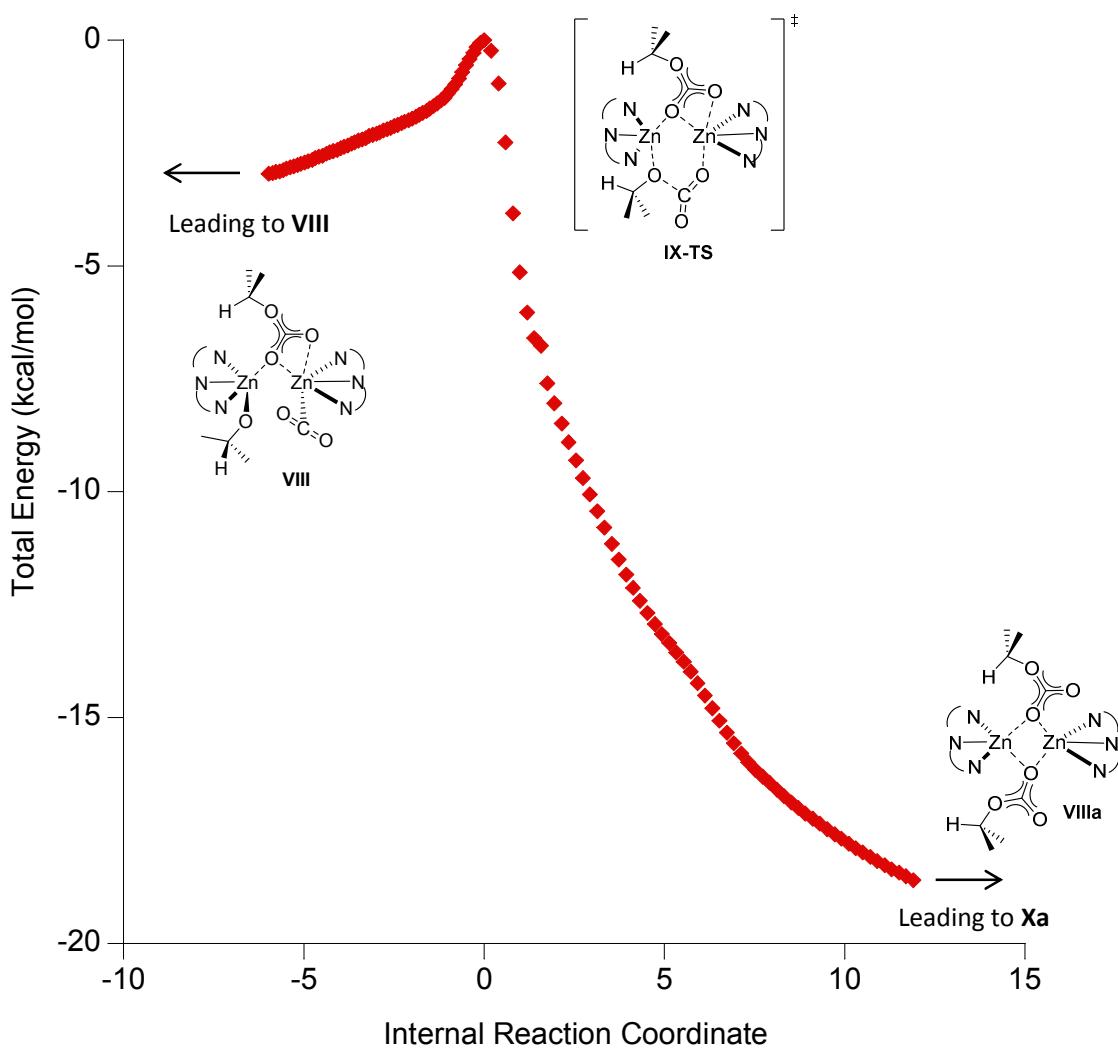


Figure S17: Plot showing both the forward and reverse IRC calculations from **IX-TS** leading to **VIII** and **Xa**, respectively.

Reverse IRC calculation (follow the path only in the reverse direction):

```
IRC=(reverse,maxpoints=100,recalc=5,calcfc,maxcycle=40,tight,cartesian,lqa,stepsize=10)
rwB97xd/6-31g(d) scrf=(cpcm,solvent=benzene)
```

Forward IRC calculation (follow the path only in the forward direction):

```
IRC=(forward,maxpoints=60,recalc=8,calcfc,maxcycle=40,tight,cartesian,lqa,stepsize=20)
rwB97xd/6-31g(d) scrf=(cpcm,solvent=benzene)
```

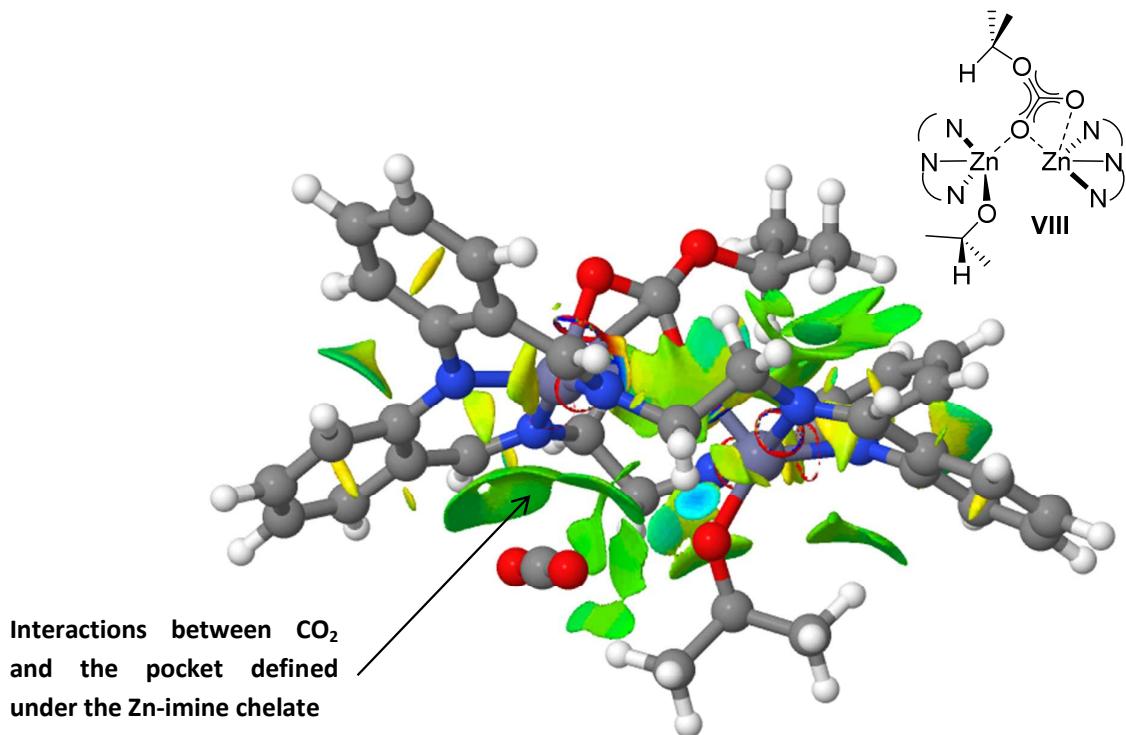


Figure S18: Non covalent interactions (NCI) in **VIII** showing interaction between CO_2 and the free pocket.

The following parameters are used to create the NCI surface:¹

```
isosurface parameters [0.5 1 0 0.05 0.95 1.00] NCI density.cube colorscheme "bgyor";color isosurface range 0.04 -0.04
```

- Johnson, E. R.; Keinan, S.; Mori-Sánchez, P.; Contreras-García, J.; Cohen, A. J.; Yang, W., Revealing Noncovalent Interactions. *Journal of the American Chemical Society* **2010**, 132 (18), 6498-6506.

X-ray crystallography

Table S2. Crystallographic Data for compounds **1**, **2** and **3a**.

data	1	2	3a
chemical formula	C ₃₆ H ₃₈ N ₆ Zn ₂	C ₃₈ H ₄₂ N ₆ O ₂ Zn ₂	C ₃₉ H ₄₂ N ₆ O ₄ Zn ₂
solvent	C ₆ H ₆	—	—
fw	763.57	745.51	789.52
T (°C)	-100	-100	-100
space group	P-1 (no. 2)	P-1 (no. 2)	C2/c (no. 15)
a (Å)	10.8554(4)	12.0878(5)	37.6404(5)
b (Å)	11.4026(5)	12.1033(6)	16.9073(2)
c (Å)	15.3400(6)	13.5035(5)	17.4493(2)
α (deg)	95.001(3)	92.669(3)	90
β (deg)	104.463(3)	106.799(4)	90.1883(12)
γ (deg)	93.974(3)	108.762(4)	90
V (Å ³)	1823.43(13)	1769.46(14)	11104.6(2)
Z	2	2	12 [c]
ρ _{calcd} (g cm ⁻³)	1.391	1.399	1.417
λ (Å)	1.54184	0.71073	1.54184
μ (mm ⁻¹)	1.911	1.398	1.985
R ₁ (obs) [a]	0.0347	0.0348	0.0443
wR ₂ (all) [b]	0.0993	0.0838	0.1465

[a] $R_1 = \sum |F_o| - |F_c| | / \sum |F_o|$. [b] $wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$. [c] There are two independent complexes, one of which has crystallographic C₂ symmetry.

Table 1 provides a summary of the crystallographic data for compounds **1**, **2** and **3a**. Data were collected using Agilent Xcalibur PX Ultra A (**1** and **3a**) and Xcalibur 3 E (**2**) diffractometers, and the structures were refined using the SHELXTL and SHELX-97 program systems. CCDC 1416267 to 1416269.

The X-ray crystal structure of **1**

Both the C41-based ethyl ligand and the C51-based benzene solvent molecule in the structure of **1** were found to be disordered, and two orientations were identified in each case of *ca.* 63:37 and 91:9% occupancy respectively. The geometries of each pair of orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientations were refined anisotropically (those of the minor occupancy orientations were refined isotropically).

The X-ray crystal structure of **2**

The O50-based bridging iso-propoxide ligand in the structure of **2** was found to be disordered. Two orientations (sharing a common oxygen site) were identified of *ca.* 55 and 44% occupancy, their geometries were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically).

The X-ray crystal structure of **3a**

The structure of **3a** was found to contain two crystallographically independent complexes, **3a-I** and **3a-II**. Whilst complex **3a-I** sits in a general position, complex **3a-II** is situated across a C_2 axis (that bisects the Zn3 \cdots Zn3A, N61 \cdots N61A and N77 \cdots N77A vectors). Both the O80-based iso-propoxide and O90-based carbonate bridging ligands are disordered about this axis, and this was modelled by using one complete 50% occupancy orientation for each ligand, with the operation of the C_2 axis generating a second 50% occupancy orientation for each group.

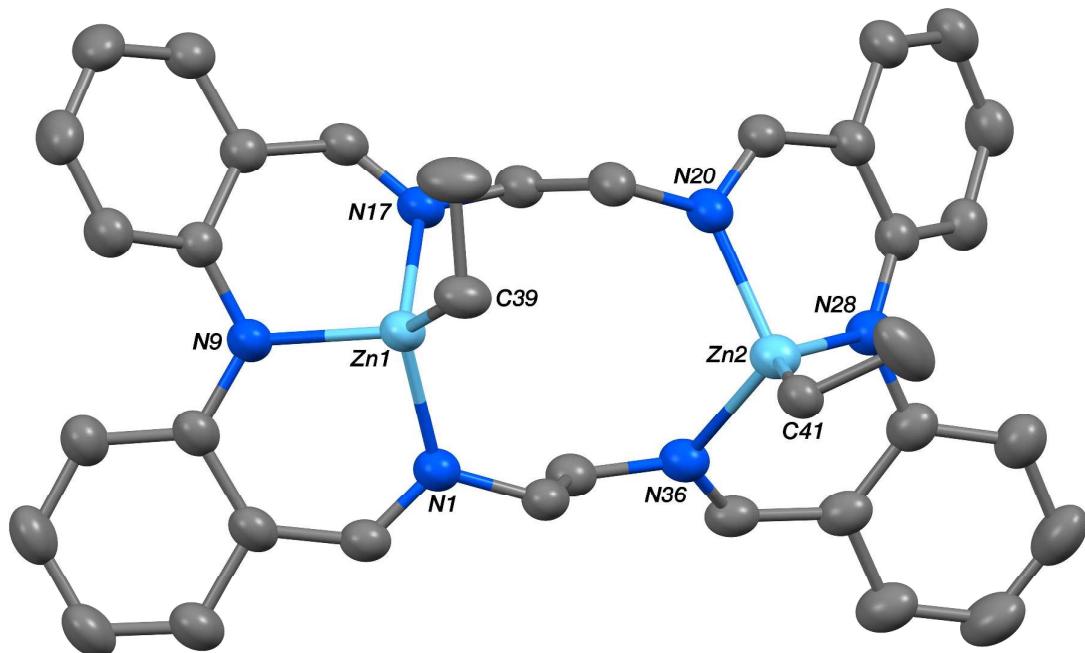


Figure S19: The crystal structure of **1** (50% probability ellipsoids).

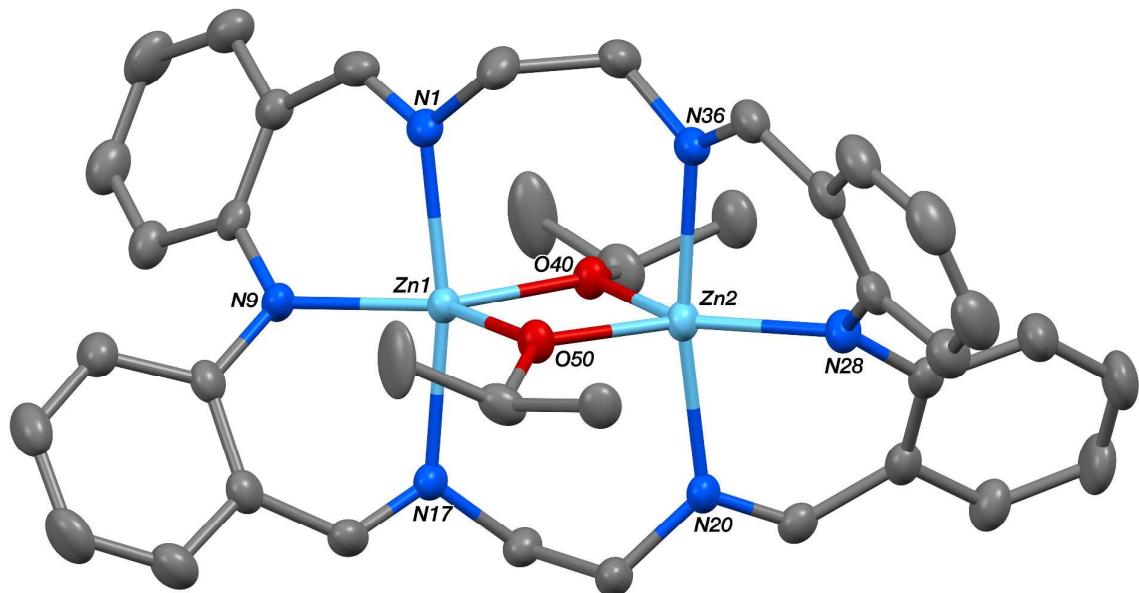


Figure S20: The crystal structure of **2** (50% probability ellipsoids).

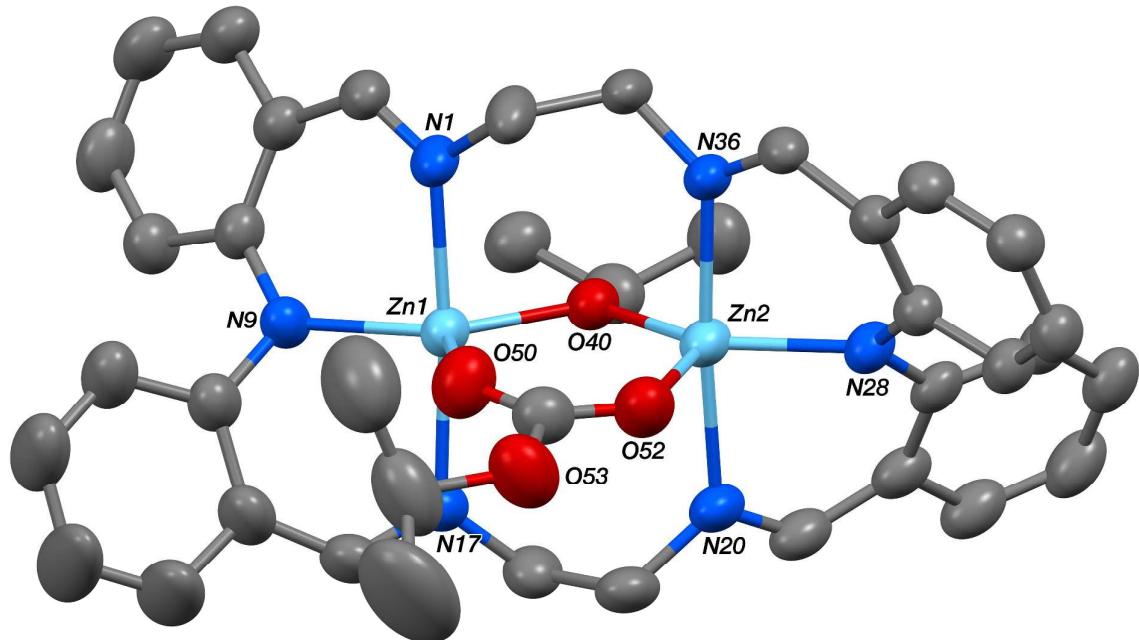


Figure S21: The structure of one (**3a-I**) of the two independent complexes present in the crystal of **3a** (50% probability ellipsoids).

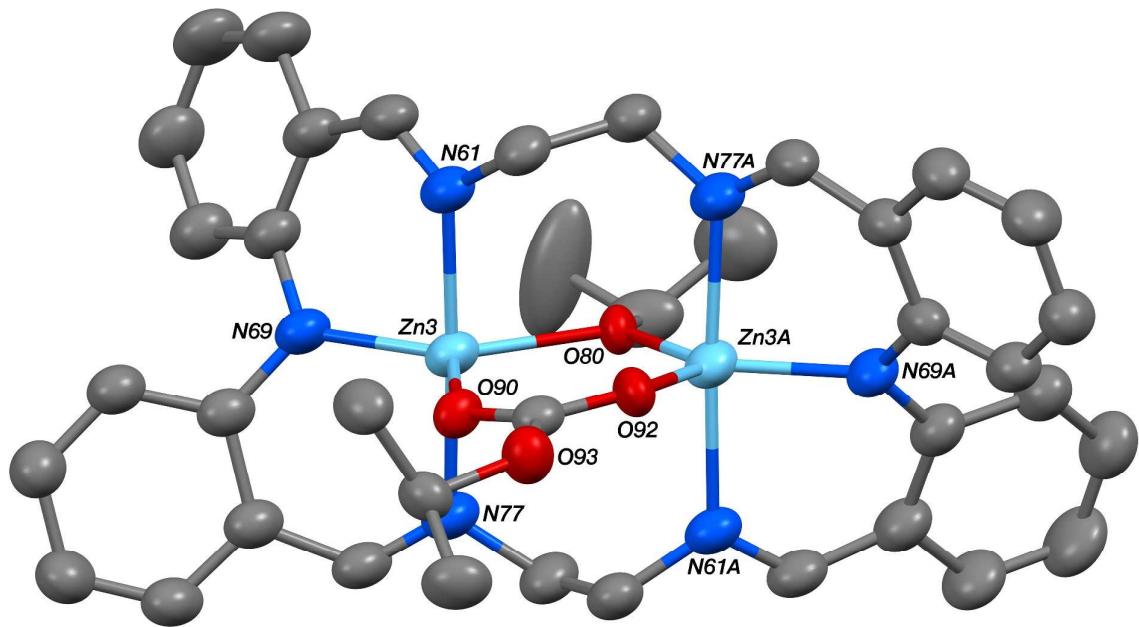


Figure 22: The structure of one (**3a-II**) of the two independent complexes present in the crystal of **3a** (50% probability ellipsoids). This independent complex sits across a C_2 axis that bisects the $Zn3 \cdots Zn3A$ and $N61 \cdots N61A$ vectors; the bridging iso-propoxide and carbonate ligands are disordered about this axis.

Optimized geometries and computed Free Gibbs Energy

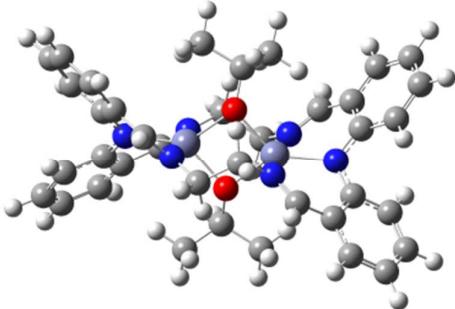
Full coordinates for all the geometries are available via the corresponding Gaussian 09 output files, stored in the digital repository. In addition, a web-enhanced table is available [here](#).

In addition, full coordinates for all the geometries, together with their 3 lowest calculated vibrations and their computed Free Gibbs Energy are reported below.

Table S3: Free energy profile for the reaction between 2 and two molecules of CO₂ (figure 9 and figure 10).

Structure	ΔG (kcal/mol)	Digital repository
I	0	10000490
II	+4.6	10003463
III-TS	+20.2	10002875
IV	+18.4	10000487
V-TS	+22.9	109089
VIa	+3.9	109174
VIb	-6.4	10000491
VII	+8.5	10000489
VIII	+13.5	10000486
IX-TS	+19.0	109088
Xa	-2.1	109177
Xb	-6.8	10000561
Xc	-5.8	10000562

I



O 1

Zn 4.35573600 2.30723700 2.27308100
Zn 5.61782800 2.01482300 4.89627300
N 5.11605700 4.32382700 1.92533700
C 5.47992200 4.67453600 0.74980200
H 6.03211100 5.61579100 0.61602100
C 5.22449700 3.93779600 -0.47815500
C 5.98144200 4.30511900 -1.60520300
H 6.74480900 5.07153600 -1.48892200
C 5.77907900 3.72288100 -2.84110800
H 6.38213300 4.01230100 -3.69532900
C 4.77316900 2.75729700 -2.96781500
H 4.59693900 2.28106000 -3.92839200
C 4.00577300 2.38969200 -1.87933800
H 3.23844700 1.62953000 -1.98905600
C 4.20613000 2.95574100 -0.59873900
N 3.47930000 2.52501800 0.49273200
C 2.13196800 2.30859800 0.35455300
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H 1.81530200 3.91172000 -1.05216400
C -0.03676600 2.95886100 -0.57280200
H -0.61083300 3.62086000 -1.21556400
C -0.69224600 1.96245500 0.16436900
H -1.76680800 1.83323000 0.09171300
C 0.06546200 1.14337900 0.97513900
H -0.41730800 0.34840000 1.53976600
C 1.46011400 1.29595100 1.09678400
C 2.15327100 0.30375600 1.89520500
H 1.56094100 -0.59441100 2.12170800
N 3.36175500 0.37231400 2.32232600
C 3.85944200 -0.79951900 3.02727500
H 4.88202500 -0.99625100 2.69149000
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H 5.76711800 -1.97438900 5.45036100
C 7.17551700 -0.54180100 6.22856400
C 8.13337300 -1.56464500 6.36460400
H 7.92879900 -2.52776600 5.90160600

C 9.30925900 -1.37751000 7.06126400
H 10.04110200 -2.17416300 7.14170500
C 9.53081700 -0.13442300 7.67048600
H 10.45055600 0.04087200 8.22210200
C 8.60346400 0.88183800 7.56769500
H 8.80133200 1.84264600 8.03211600
C 7.39949700 0.72714900 6.83410900
N 6.52361200 1.76895700 6.66009500
C 6.34612700 2.67958900 7.67979900
C 6.22826700 2.25836700 9.02536900
H 6.32141300 1.19814700 9.23969800
C 5.97186000 3.15043500 10.04828700
H 5.86775800 2.77804600 11.06382200
C 5.83081500 4.51904800 9.78769400
H 5.62726400 5.21982800 10.59048100
C 5.96617400 4.95896100 8.48561800
H 5.88169600 6.02070100 8.26402300
C 6.21370000 4.07038300 7.42369200
C 6.42593200 4.66011500 6.11127600
H 6.63796100 5.73887300 6.11954800
N 6.39747700 4.03686100 4.99336200
C 6.69971000 4.81079300 3.80020700
H 7.33514900 4.19864500 3.15504400
H 7.25610600 5.71854800 4.07199800
C 5.44308500 5.23282500 3.01172900
H 4.59027500 5.26522800 3.69386300
H 5.60851300 6.24481600 2.61689900
O 6.12351900 1.75036000 2.99238000
C 7.05695200 0.82798400 2.51115100
H 6.87360200 -0.16620500 2.96185600
C 6.92538500 0.68577600 0.99600200
H 5.91370300 0.35578800 0.73045400
H 7.64116700 -0.04056000 0.59428500
H 7.10075300 1.65410600 0.51079100
C 8.46760600 1.24937200 2.91993100
H 8.71399300 2.21971300 2.47228300
H 9.21552700 0.51661400 2.59529100
H 8.53514400 1.34487400 4.01004000
O 3.89366400 2.68898000 4.16839400
C 2.60786500 2.74166300 4.71315300
H 2.05884500 1.80865500 4.48093500
C 1.81691400 3.89094000 4.08850400
H 1.75911200 3.77118200 3.00017900
H 2.30699300 4.84788100 4.30413200
H 0.79349300 3.93073300 4.47960200
C 2.68424800 2.87234600 6.23300000
H 3.20848600 2.01269900 6.66766300
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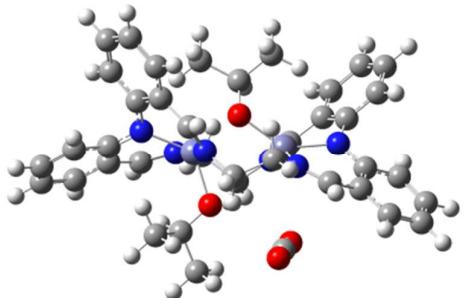
Sum of electronic and thermal Free Energies =

- 5509.501325

Frequencies--

16.4757 29.0920 35.6514

II



0 1

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 Zn 0.16585000 1.06955500 -1.41638000
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 C -1.09723000 -2.67568900 6.15503800
 H -1.41830500 -2.70303700 7.19090900
 C -1.12901300 -3.82917600 5.35959400
 H -1.49380100 -4.76439600 5.77614600
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 H -2.71898200 -1.05402500 -0.90724700
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 C -1.49096000 -1.23365100 -2.68840400
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 C -2.76835000 0.04290800 2.02803000
 H -2.19199000 0.17067200 2.96700900
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 H -4.41753500 1.12566100 2.96320400
 H -4.52717700 1.01746500 1.19812300
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 H -4.07010100 -1.49334500 1.22327500
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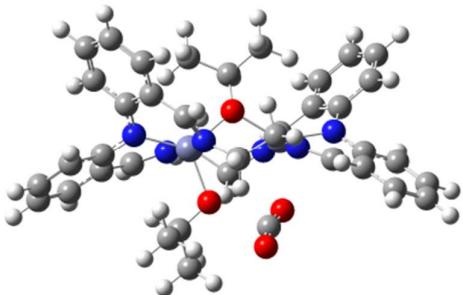
Sum of electronic and thermal Free Energies=

- 5698.002374

Frequencies --

10.2995 19.9926 27.5757

III-TS



0 1

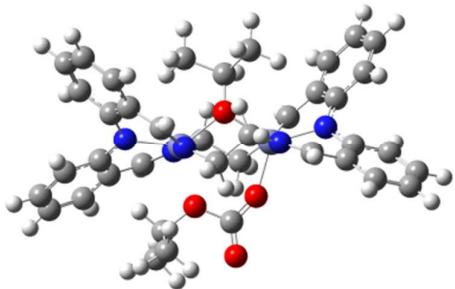
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C	31.28598300	11.21325800	6.49042200
C	30.85899200	11.18198400	7.83194600
H	30.97786900	12.08218200	8.43109200
C	30.29394400	10.05647300	8.39505000
H	29.96421800	10.05774100	9.42860200
C	30.15186000	8.91513300	7.59555000
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C	30.57330200	8.91526700	6.28129400
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N	31.53308300	10.04385500	4.34951000
C	32.10825600	8.89106400	3.86179300
C	33.01130500	8.13459100	4.65150300
H	33.22027800	8.47818600	5.65948200
C	33.64006100	7.00359300	4.17232800
H	34.33458900	6.46998800	4.81560500
C	33.40205600	6.54661400	2.86981300
H	33.89197400	5.65536800	2.49236200
C	32.52736800	7.26179000	2.07803700
H	32.32202900	6.92533200	1.06392600
C	31.88708300	8.42955900	2.53495000
C	30.98831200	9.07091700	1.59350600
H	30.69577700	8.44707400	0.73655400
N	30.54708200	10.26968700	1.66898300
C	29.68605900	10.72049200	0.58726300
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H	31.49125500	10.96533100	-0.56315300
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C	30.19136200	14.87547500	-1.82034000
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C	29.27450600	16.68094600	-3.18503300
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C	30.29127400	17.52074800	-2.70711000

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H	32.00958300	17.73604800	-1.46637400
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C	34.17523400	16.22357100	-1.46689500
H	33.78384600	15.96164800	-2.44501600
C	35.41607900	16.82494500	-1.35408200
H	35.99142900	17.03105000	-2.25209600
C	35.93481200	17.15715100	-0.09898700
H	36.90711900	17.62938600	-0.00772000
C	35.18397000	16.87253100	1.02609500
H	35.57048900	17.12825300	2.00995700
C	33.92688400	16.24908000	0.93788100
C	33.23681200	16.01086800	2.20195900
H	33.62643200	16.58592700	3.05239500
N	32.27465900	15.18989700	2.40065900
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H	31.73471800	16.05580100	4.23486200
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H	32.83593200	14.62235800	5.61236500
O	29.59353800	12.74123800	3.15183500
C	28.73985400	12.41060800	4.21836600
H	29.34521900	12.13533800	5.09770200
C	27.89639800	13.61160200	4.65499000
H	28.54526300	14.46950200	4.86525000
H	27.33148100	13.37975200	5.56584800
H	27.17819600	13.90093400	3.88036000
C	27.86463700	11.19890100	3.88362400
H	28.49630900	10.34278900	3.62163500
H	27.21623900	11.42437500	3.02992900
H	27.23449600	10.91297600	4.73487000
C	28.65170900	14.00940200	1.58229900
O	29.54319300	14.77714000	1.48977200
O	27.62898700	13.46987100	1.40203200
O	32.53092200	12.36818000	1.77468000
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H	35.51553500	11.16985900	2.76715500
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Sum of electronic and thermal Free Energies= -5697.995139

Frequencies –
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IVa



O 1

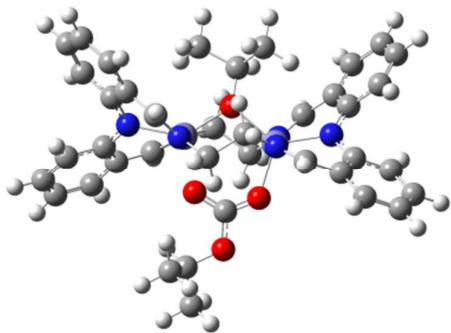
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H 2.80073400 0.80214900 -0.13552500
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Sum of electronic and thermal Free Energies= -5698.025507

Frequencies –
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IVb



0 1

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H	-2.58868400	-2.04473500	6.80083300
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H	-5.73977200	-0.07319300	0.15975600
H	-5.68893600	-0.96400700	1.69630400
C	-2.44028700	1.07789400	0.34108200
O	-2.01213600	0.03193500	0.89225600
O	-1.84376800	1.77831700	-0.51549800
O	0.96666700	-0.06493000	-0.49142000
C	2.37183100	-0.12708800	-0.52880300
H	2.79404200	0.81575400	-0.13735900
C	2.88488700	-1.26869100	0.34563300
H	2.56851500	-1.13717200	1.38652900
H	3.97897100	-1.32273900	0.32419100
H	2.48571200	-2.22626600	-0.01194800
C	2.85399000	-0.27726000	-1.97078400
H	2.46368600	0.53086300	-2.59882300
H	2.51075500	-1.23245300	-2.38594400
H	3.94823000	-0.25019200	-2.02587000

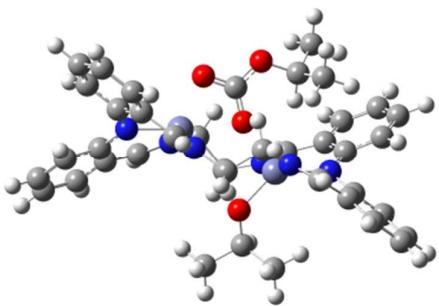
Sum of electronic and thermal Free Energies=

-5698.041961

Frequencies –

12.2631 18.6929 23.1349

v



0 1

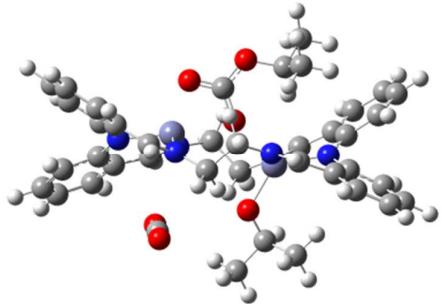
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 H 0.83015000 0.70849100 4.42954900
 C -0.26379100 -1.14900400 4.30266900
 C -0.62820600 -0.98289900 5.65232100
 H -0.34485600 -0.05952900 6.15245000
 C -1.33703200 -1.94297700 6.34579300
 H -1.61213600 -1.78720800 7.38343200
 C -1.69790200 -3.11536100 5.67338700
 H -2.27551600 -3.87994800 6.18547500
 C -1.33964500 -3.31059300 4.35388700
 H -1.64093500 -4.22101000 3.84613500
 C -0.59923900 -2.35203000 3.62241100
 N -0.28930800 -2.56000900 2.28756100
 C 0.09132300 -3.82056300 1.89485700
 C 0.81632400 -4.67790000 2.76514400
 H 1.05861600 -4.31390800 3.75796600
 C 1.23579300 -5.93645100 2.38590400
 H 1.79987800 -6.54044200 3.09147100
 C 0.95399600 -6.43487700 1.10760200
 H 1.27357500 -7.42815800 0.81140500
 C 0.26860900 -5.61956100 0.23141500
 H 0.05035100 -5.97672600 -0.77268900
 C -0.14850300 -4.31956800 0.57879700
 C -0.79518800 -3.57368300 -0.48561300
 H -1.11644200 -4.17770600 -1.34517600
 N -0.96984000 -2.30517100 -0.51978700
 C -1.58721900 -1.73269400 -1.70780600
 H -2.20852900 -0.89591200 -1.38367700
 H -2.22696700 -2.47862900 -2.19635900
 C -0.54887400 -1.21346400 -2.73003200
 H 0.44234500 -1.58203800 -2.46083700
 H -0.78511400 -1.62701000 -3.71711600
 N -0.49372800 0.24746500 -2.82784500
 C -1.21688700 0.77665300 -3.75842400
 H -1.83573800 0.09859600 -4.35757400
 C -1.33942100 2.16214900 -4.13717500
 C -2.40403500 2.44245800 -5.02329100
 H -3.03961700 1.61746900 -5.33746800
 C -2.66707000 3.71213500 -5.48308200
 H -3.49615800 3.90222800 -6.15575600
 C -1.83632000 4.75589100 -5.04682100

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 C -0.77307200 4.51903100 -4.20474200
 H -0.16486300 5.35304000 -3.87414800
 C -0.45991500 3.21502400 -3.72739000
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 H 1.92275800 4.19656400 -4.83656800
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 H 3.76583500 5.80317100 -4.56578900
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 C 3.09421600 5.20899800 -1.30721000
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 H 1.63905200 4.39461300 0.67656900
 N 0.84680500 2.65460100 -0.05083900
 C 0.35326300 2.34108900 1.29002800
 H -0.61940400 1.84770200 1.17860400
 H 0.21574400 3.26908100 1.85807000
 C 1.30964700 1.39998900 2.05828200
 H 2.14314200 1.12292000 1.40817100
 H 1.72913900 1.91643500 2.93249000
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 C -3.15067200 0.02003500 0.89639900
 H -3.42448800 -0.96979300 0.46938500
 C -3.49822200 -0.03154700 2.38932900
 H -2.91920700 -0.81394000 2.89419100
 H -4.56350100 -0.23557900 2.55514600
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 C -3.99877200 1.07141800 0.17627500
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 H -3.78800400 2.06412200 0.59282600
 H -5.07300400 0.87419900 0.27708600
 O 1.13071600 -0.39214300 -0.29737300
 C 2.24438000 -0.41001200 -0.89898400
 O 2.54169000 0.46813700 -1.75143900
 O 3.14417500 -1.36442800 -0.67964600
 C 2.80827600 -2.43118400 0.24143000
 H 1.72690100 -2.55530000 0.22164100
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 H 2.75127100 -1.15578600 1.98531500
 H 4.34240400 -1.89954200 1.66837900
 H 3.00464300 -2.86982300 2.33299000
 C 3.46495200 -3.69133300 -0.28864200
 H 3.12097500 -3.90570100 -1.30476200
 H 3.19293800 -4.53527900 0.35318300
 H 4.55533000 -3.59068000 -0.30060900

Sum of electronic and thermal Free Energies= -5698.018188

Frequencies –
 13.0782 23.2071 32.7994

VI



0 1

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Zn	0.68698400	1.47673500	-1.75235300
N	0.62766700	0.23251400	2.45150600
C	0.56034200	-0.00218800	3.70754300
H	0.98960800	0.72785200	4.40635600
C	-0.08996300	-1.14071200	4.34034300
C	-0.34017800	-0.99138500	5.71808400
H	-0.01175100	-0.07571500	6.20439200
C	-0.99603100	-1.95527900	6.45617400
H	-1.18478000	-1.81049400	7.51443500
C	-1.42275300	-3.11464400	5.80017800
H	-1.96686500	-3.88008900	6.34651700
C	-1.17382700	-3.29572300	4.45403300
H	-1.52882400	-4.19502600	3.96183900
C	-0.48487100	-2.33546900	3.67527500
N	-0.28934600	-2.52487100	2.31644200
C	0.02226700	-3.78581200	1.86634100
C	0.76531700	-4.69335700	2.66810400
H	1.08435600	-4.36584400	3.65167300
C	1.10825600	-5.95813000	2.23631500
H	1.68838800	-6.60121900	2.89251300
C	0.72965800	-6.41138300	0.96662800
H	0.98729600	-7.40916900	0.62824300
C	0.03538400	-5.54361600	0.14988100
H	-0.24915800	-5.86301900	-0.85037500
C	-0.30594200	-4.23639200	0.55014700
C	-0.94853000	-3.43108800	-0.47366800
H	-1.31113000	-3.99215500	-1.34545500
N	-1.06807200	-2.15639500	-0.46413700
C	-1.66229400	-1.50363200	-1.62429000
H	-2.14154000	-0.58976100	-1.26498000
H	-2.43013500	-2.14881600	-2.06904300
C	-0.60929300	-1.14534500	-2.70084900
H	0.35933200	-1.55467700	-2.40906400
H	-0.88430000	-1.62040500	-3.64974600
N	-0.46297400	0.29683000	-2.91043400
C	-1.02905600	0.77616700	-3.96692900
H	-1.58663900	0.07216600	-4.59472800
C	-1.06777300	2.13515500	-4.44926800
C	-1.99216000	2.35377500	-5.49447900
H	-2.55460000	1.50084400	-5.86725800
C	-2.21565700	3.59923800	-6.03591000
H	-2.93849400	3.74035800	-6.83189800
C	-1.49853000	4.68256500	-5.50896000

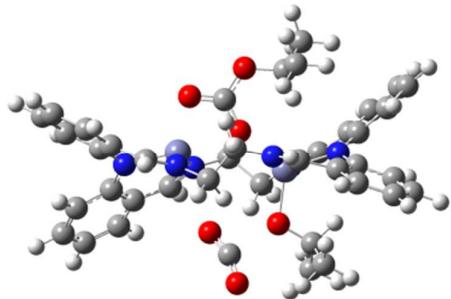
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H	-0.05200800	5.36990800	-4.11089300
C	-0.28617900	3.22535600	-3.95373800
N	0.63117900	3.04510300	-2.95864000
C	1.61864700	3.99572700	-2.73523900
C	2.34801300	4.58058200	-3.79057500
H	2.11925800	4.27678400	-4.80684400
C	3.34502400	5.51071300	-3.55857900
H	3.88864700	5.92773600	-4.40137400
C	3.66025600	5.91065700	-2.25621000
H	4.43543700	6.64713200	-2.07388000
C	2.96931300	5.34134900	-1.20437900
H	3.20499300	5.63227600	-0.18347100
C	1.97114600	4.37247000	-1.41360900
C	1.35472600	3.82854300	-0.21207700
H	1.46901400	4.44816700	0.68502100
N	0.74741000	2.70290200	-0.09681600
C	0.26001200	2.34807300	1.23822600
H	-0.68832100	1.81128800	1.13276400
H	0.05910100	3.26194000	1.80905400
C	1.26487600	1.46238000	2.00886900
H	2.09334000	1.19676700	1.34807000
H	1.68487300	2.01342400	2.86129500
O	-1.99634900	0.28629900	0.93653700
C	-3.27593300	-0.19661400	1.19708000
H	-3.43226300	-1.18337000	0.70941200
C	-3.51257000	-0.39680800	2.69928800
H	-2.79555100	-1.11358700	3.11373700
H	-4.52368600	-0.76918700	2.90651600
H	-3.37827100	0.55769500	3.22343800
C	-4.32315300	0.75698100	0.61796000
H	-4.18611200	0.86314700	-0.46286000
H	-4.21245400	1.74667000	1.07944900
H	-5.34442900	0.40325400	0.80376400
O	1.04866900	-0.32097000	-0.30408800
C	2.16834800	-0.35734600	-0.88939600
O	2.49865300	0.51495800	-1.73931300
O	3.05163300	-1.32630700	-0.66389600
C	2.69546500	-2.38891600	0.25261100
H	1.60994600	-2.46039600	0.26826300
C	3.21084600	-2.05371000	1.64023500
H	2.76017200	-1.12802000	2.00591800
H	4.30059000	-1.94522400	1.63018500
H	2.94131500	-2.85599000	2.33397200
C	3.27264600	-3.67269800	-0.31226400
H	2.88017100	-3.86016300	-1.31614100
H	2.98508400	-4.50984900	0.33168200
H	4.36530900	-3.62273000	-0.36530000
C	-2.44138000	3.18960800	-0.81009600
O	-2.27942100	3.87653900	0.11702200
O	-2.61566300	2.52898400	-1.75247500

Sum of electronic and thermal Free Energies= -5886.540912

Frequencies –

23.2807 26.4665 31.5503

VII-TS



O 1

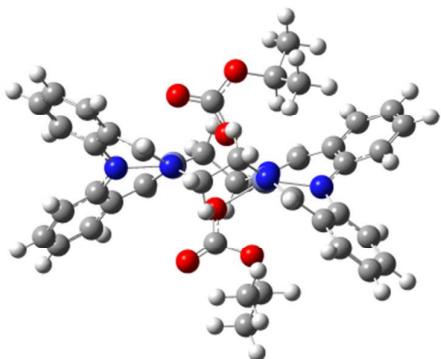
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C	32.35747600	12.70160000	5.92107100
H	32.83091600	13.40228100	6.62034400
C	31.62718000	11.61256800	6.54718800
C	31.32232600	11.80372400	7.90897000
H	31.67514200	12.71118500	8.39349500
C	30.57967100	10.89165000	8.62969100
H	30.34717300	11.06714100	9.67443200
C	30.12534500	9.74193700	7.97395000
H	29.51357400	9.01938700	8.50687200
C	30.43361200	9.51598800	6.64724900
H	30.05906100	8.62423900	6.15572800
C	31.20887400	10.42327800	5.88638000
N	31.47186100	10.19716600	4.54766700
C	31.70883800	8.91071100	4.12475500
C	32.37224200	7.97255300	4.95781300
H	32.68209600	8.29547700	5.94612600
C	32.64869800	6.68362400	4.54946100
H	33.17091800	6.01419400	5.22744200
C	32.27473500	6.23893100	3.27549200
H	32.48033800	5.22330500	2.95525200
C	31.64917400	7.13385600	2.43253800
H	31.36570400	6.81669000	1.43135600
C	31.37802000	8.46418700	2.80939200
C	30.79045700	9.28793500	1.76562200
H	30.38693500	8.72872100	0.91126900
N	30.75307400	10.56798100	1.73332200
C	30.17868700	11.20696600	0.55500600
H	29.66064300	12.10693000	0.89010700
H	29.43991800	10.53992500	0.09245900
C	31.24549400	11.58420500	-0.50261300
H	32.20571900	11.14721700	-0.22286200
H	30.96373900	11.14169100	-1.46503300
N	31.42025000	13.02784400	-0.67440600
C	30.78634100	13.56422600	-1.66225300
H	30.15659300	12.90346600	-2.26883800
C	30.76358700	14.94170700	-2.09470300
C	29.77189600	15.23196200	-3.05833600
H	29.13242700	14.41938600	-3.39558000
C	29.57871600	16.49698200	-3.56438900

H	28.80401200	16.69307100	-4.29735600
C	30.40327100	17.52730800	-3.09018500
H	30.25578200	18.54404100	-3.44436400
C	31.39774500	17.27990600	-2.16975800
H	32.00085600	18.10578900	-1.81119300
C	31.64440200	15.97925100	-1.65017900
N	32.62340400	15.73047400	-0.73324700
C	33.65452700	16.63824500	-0.53151800
C	34.36899000	17.20741300	-1.60448800
H	34.08941600	16.92872000	-2.61543300
C	35.41390400	18.08956200	-1.39546800
H	35.94505400	18.49630000	-2.25111600
C	35.79248200	18.45457100	-0.09977800
H	36.60562700	19.15349600	0.06424200
C	35.11171700	17.90451000	0.96905800
H	35.39288600	18.17405500	1.98433500
C	34.06432300	16.98453200	0.78259600
C	33.44181300	16.47180600	1.99596900
H	33.59160200	17.09002500	2.88897500
N	32.78014400	15.37814500	2.11552900
C	32.26393100	15.05077500	3.44146000
H	31.30206200	14.55766200	3.31093200
H	32.08624800	15.96841500	4.01385900
C	33.19180400	14.10472800	4.23084800
H	34.00917700	13.77795500	3.58453700
H	33.63409600	14.62782900	5.08861800
O	29.57763400	12.69799900	3.40457300
C	28.57664100	11.91827900	4.02700300
H	28.98944300	10.91670500	4.23506700
C	28.15812900	12.51553600	5.37073700
H	29.03229500	12.61637100	6.02286200
H	27.43020500	11.87035700	5.87779700
H	27.71210200	13.50428000	5.22913800
C	27.37990200	11.70064100	3.09756200
H	27.71333800	11.25575500	2.15347100
H	26.87246100	12.64514600	2.87772800
H	26.65097000	11.02090600	3.55481600
O	32.88860200	12.34559800	1.94498700
C	33.99609900	12.24064200	1.34265300
O	34.36566600	13.08613600	0.48388900
O	34.82456100	11.22288200	1.56185200
C	34.42558700	10.18773800	2.49146700
H	33.33846700	10.16425600	2.50975500
C	34.95898500	10.51311800	3.87469100
H	34.55109900	11.46112900	4.23361000
H	36.05234000	10.57351400	3.86104300
H	34.65608600	9.73004800	4.57652000
C	34.94409500	8.87363800	1.93958300
H	34.53560300	8.68896900	0.94162900
H	34.62790600	8.05791000	2.59762800
H	36.03734300	8.87692800	1.87750300
C	28.96752600	14.42006400	2.44094600
O	28.09991700	14.84084700	3.11872100
O	29.71635300	14.41077900	1.52274200

Sum of electronic and thermal Free Energies= -
5886.531820

Frequencies –
-202.6476 22.5788 23.3578

VIIIa



O 1

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Zn	0.46600900	1.39080800	-1.41705500
N	0.55831500	0.09315300	2.27455900
C	0.05083700	-0.06884400	3.44189300
H	0.33055700	0.63344500	4.23808300
C	-0.89736600	-1.09104600	3.84435200
C	-1.59990900	-0.85441300	5.04020600
H	-1.41244300	0.07200500	5.57833600
C	-2.52228900	-1.75706000	5.53099300
H	-3.06452600	-1.55083500	6.44756900
C	-2.73609700	-2.94688100	4.82432100
H	-3.46154300	-3.66978400	5.18663700
C	-2.03976500	-3.21245400	3.66030200
H	-2.22048700	-4.13569300	3.11866900
C	-1.10308000	-2.29788100	3.12987600
N	-0.45467200	-2.54930800	1.93549000
C	0.07640700	-3.79449200	1.71550700
C	0.58397900	-4.58634700	2.77807000
H	0.51339900	-4.19849100	3.78881100
C	1.19739000	-5.80146500	2.55490600
H	1.59355700	-6.35641100	3.40087600
C	1.32737700	-6.31877400	1.25823700
H	1.80712100	-7.27618000	1.08656300
C	0.82043600	-5.58266000	0.20778500
H	0.89587400	-5.96918000	-0.80629900
C	0.21069400	-4.32753600	0.40134400
C	-0.30281600	-3.67496100	-0.78583300
H	-0.43347200	-4.33280200	-1.65479100
N	-0.59033100	-2.42910600	-0.90776200
C	-1.12382300	-1.99989700	-2.19410900
H	-1.97387400	-1.33888600	-2.00575500
H	-1.49127700	-2.87239800	-2.74934400
C	-0.09635200	-1.25486500	-3.07455700
H	0.91529900	-1.52922000	-2.76950900
H	-0.22780400	-1.59186500	-4.11017200
N	-0.23562900	0.19667000	-3.01317600
C	-1.00248300	0.71544800	-3.90539600
H	-1.48248900	0.04484600	-4.63046900
C	-1.34194100	2.11218000	-4.07809900
C	-2.43379700	2.38011200	-4.92834900
H	-2.96165800	1.53842300	-5.37137600
C	-2.84632900	3.66620900	-5.20450100
H	-3.69614700	3.85022700	-5.85306900

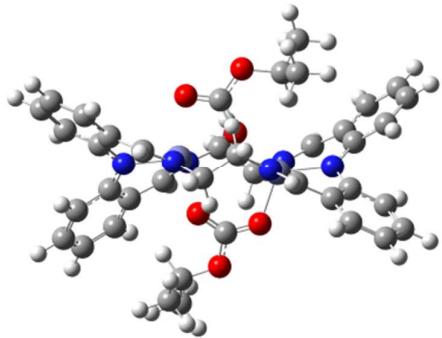
C	-2.14158600	4.73001000	-4.62417700
H	-2.45480900	5.75346500	-4.81148000
C	-1.05686100	4.49850400	-3.80417900
H	-0.53512100	5.33587600	-3.35279300
C	-0.61153500	3.18748100	-3.50182200
N	0.44272500	2.96023100	-2.65070100
C	1.51380200	3.82324200	-2.66357000
C	1.98234300	4.40918100	-3.86513100
H	1.46571800	4.17223300	-4.78938300
C	3.08396200	5.23981800	-3.89117200
H	3.41564200	5.65097300	-4.84074200
C	3.78201000	5.54831400	-2.71589700
H	4.64422500	6.20627600	-2.73699000
C	3.34450900	4.99479500	-1.53116100
H	3.86511500	5.22443100	-0.60406700
C	2.23755700	4.12567100	-1.47850800
C	1.85870800	3.65992300	-0.16199300
H	2.29231600	4.23686000	0.66492500
N	1.08532400	2.67445900	0.12624500
C	0.80958200	2.47186500	1.54164700
H	-0.27412400	2.41052300	1.67634400
C	1.15272300	3.34389800	2.11335500
C	1.48124800	1.21323600	2.12701000
H	2.30196800	0.90536900	1.47657400
H	1.91075500	1.46785100	3.10382900
O	-2.51882900	0.17813100	1.33472600
C	-3.58002900	0.55238100	2.23977600
H	-3.61818200	-0.31870000	2.90086600
C	-3.21345300	1.77423500	3.07163300
H	-2.22844900	1.64020900	3.52975300
H	-3.94691400	1.89597800	3.87543600
H	-3.20103700	2.67867300	2.46101100
C	-4.90943000	0.68536200	1.51082800
H	-5.11823000	-0.22082600	0.93386500
H	-4.89771800	1.54338000	0.83549000
H	-5.71410700	0.81979800	2.24119800
O	1.40911900	-0.34727700	-0.53586100
C	2.56472400	-0.19268400	-1.07727200
O	2.84736600	0.79517100	-1.75831900
O	3.49597100	-1.14625100	-0.91270000
C	3.13503600	-2.37561100	-0.24828400
H	2.09104300	-2.58793100	-0.48178400
C	3.31020000	-2.24294900	1.25633200
H	2.65223200	-1.47138100	1.66506300
H	4.34826100	-1.98996400	1.49713300
H	3.05668900	-3.19099000	1.74227800
C	4.01303000	-3.46040400	-0.84682800
H	3.86884300	-3.51982300	-1.92951600
H	3.75050700	-4.42706200	-0.40507200
H	5.07073400	-3.26030100	-0.64653400
C	-2.07307600	1.04132000	0.38128400
O	-2.55596900	2.14102900	0.17531300
O	-1.06847600	0.50893000	-0.23958300

Sum of electronic and thermal Free Energies=

-5886.565437

Frequencies –

12.6034 23.7094 25.6170

VIIIb

0 1

Zn	-0.43091800	-1.08042100	0.91619800
Zn	0.28961500	1.42155600	-1.49426900
N	0.09517200	0.21675800	2.47244800
C	-0.23427100	-0.07025800	3.67659100
H	0.03659700	0.62966600	4.47790000
C	-0.93672800	-1.26597400	4.12307100
C	-1.55330800	-1.17833000	5.38461300
H	-1.51493900	-0.22872300	5.91371400
C	-2.20266300	-2.25331700	5.95835600
H	-2.68333800	-2.15763300	6.92609200
C	-2.22175300	-3.46785300	5.26394100
H	-2.73136100	-4.32812600	5.68896500
C	-1.60605700	-3.58780600	4.03288100
H	-1.64260800	-4.53353100	3.50143800
C	-0.94413400	-2.50129700	3.41713000
N	-0.38035700	-2.62465800	2.16254200
C	0.32878200	-3.74324800	1.82566100
C	1.04764100	-4.50044500	2.78836500
H	1.00825200	-4.18325900	3.82504600
C	1.81539900	-5.59123600	2.44004000
H	2.36423700	-6.11976000	3.21497600
C	1.90366500	-6.01796900	1.10714200
H	2.50070300	-6.88194200	0.83572400
C	1.20734800	-5.31077000	0.15060700
H	1.25966700	-5.62320300	-0.89016700
C	0.44044200	-4.17010600	0.46663800
C	-0.20997400	-3.53577400	-0.66295400
H	-0.26378000	-4.16936500	-1.55803000
N	-0.69253200	-2.34536800	-0.73463700
C	-1.29887300	-1.98063400	-2.01368700
H	-2.16074500	-1.33707500	-1.82525400
H	-1.67682900	-2.88541100	-2.50503500
C	-0.33208800	-1.27631600	-2.99457100
H	0.70150300	-1.50635200	-2.72233400
H	-0.50303200	-1.69074000	-3.99659900
N	-0.48393500	0.17411000	-3.03257300
C	-1.09192300	0.66116200	-4.05168900
H	-1.47411000	-0.03036500	-4.81394800
C	-1.38491300	2.06054700	-4.30927300
C	-2.38974700	2.29809300	-5.26751200
H	-2.85660000	1.44041000	-5.74643000
C	-2.80447200	3.57172600	-5.59779800
H	-3.58811800	3.72856500	-6.33107100

C	-2.18771700	4.65478600	-4.95885800
H	-2.50503200	5.66959600	-5.18251700
C	-1.18223300	4.45401800	-4.03490500
H	-0.72779100	5.30858100	-3.54473600
C	-0.73201800	3.15790800	-3.67729100
N	0.23780700	2.97681100	-2.71904700
C	1.25639200	3.90623400	-2.61194500
C	1.83655200	4.49493100	-3.75973300
H	1.44976200	4.21114300	-4.73304400
C	2.88337400	5.39114900	-3.67318700
H	3.30586300	5.80356900	-4.58515300
C	3.40862800	5.76216900	-2.42980400
H	4.22673200	6.47103700	-2.36082200
C	2.85856100	5.20646100	-1.29287100
H	3.24596500	5.48652800	-0.31591200
C	1.80674600	4.27232200	-1.35324100
C	1.29770200	3.80771600	-0.07291800
H	1.54096400	4.45889700	0.77646600
N	0.61365600	2.74383300	0.14401400
C	0.14909100	2.53350400	1.51386100
H	-0.91478800	2.29117600	1.47878000
H	0.25194900	3.46605400	2.08277200
C	0.90240200	1.40885700	2.25299600
H	1.76878700	1.10462400	1.66108100
H	1.26949300	1.79707100	3.21207600
O	-3.40202500	1.12325900	-0.29665700
C	-3.20084500	2.08842300	-1.35327600
H	-2.37293700	1.74244600	-1.96932200
C	-4.47017900	2.09248000	-2.18513900
H	-4.66873900	1.09463800	-2.58745100
H	-4.35254200	2.78655200	-3.02320400
H	-5.33021200	2.40601700	-1.58421900
C	-2.86995400	3.44879900	-0.76390900
H	-1.91586000	3.42334300	-0.23191100
H	-3.65816700	3.77036900	-0.07530900
H	-2.78263100	4.18450800	-1.56965700
O	1.58741700	-0.84230300	0.34098000
C	2.22088700	-0.57105200	-0.70181200
O	1.99039000	0.38752600	-1.49373700
O	3.25507500	-1.34322100	-1.07357500
C	3.59111000	-2.47056400	-0.23348400
H	2.67057200	-2.84519600	0.21607900
C	4.54463900	-2.02091700	0.86146400
H	4.07133100	-1.25847800	1.48647200
H	5.46248000	-1.60784800	0.42938500
H	4.80928800	-2.87080300	1.49904900
C	4.17828800	-3.52442800	-1.15445300
H	3.45784400	-3.79397200	-1.93279800
H	4.41512400	-4.42520700	-0.57960000
H	5.09336700	-3.16183300	-1.63446900
C	-2.36740100	0.40370500	0.14517200
O	-1.19226300	0.60346000	-0.31956800
O	-2.58699800	-0.46447500	1.00525500

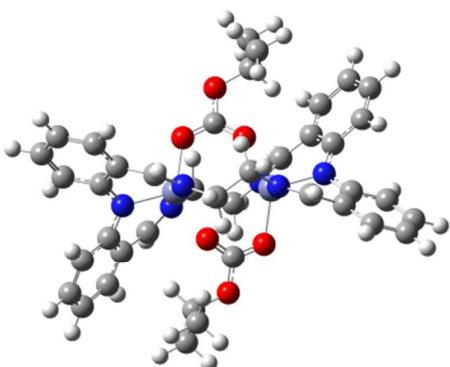
Sum of electronic and thermal Free Energies=

-5886.572884

Frequencies –

11.8136 23.4465 28.8366

VIIIc



O 1

Zn	31.28554400	11.90978000	3.55210000
Zn	32.15493900	14.21487100	1.12148000
N	32.20880500	13.11925700	5.01993400
C	31.89461200	12.91547600	6.24640600
H	32.37082000	13.53201200	7.02032400
C	30.98558600	11.89735300	6.76264500
C	30.45792800	12.12655800	8.04668600
H	30.67790500	13.07302900	8.53562100
C	29.67533200	11.19017800	8.69321100
H	29.26435000	11.39520200	9.67598100
C	29.43332500	9.96683400	8.05746200
H	28.82026400	9.21408200	8.54530900
C	29.95683700	9.70595600	6.80617600
H	29.74923500	8.75861100	6.31865800
C	30.73723000	10.65673100	6.11028000
N	31.19161800	10.41515300	4.83077100
C	31.69455600	9.19084600	4.47979100
C	32.36953800	8.36238300	5.41205900
H	32.46001900	8.71052700	6.43587700
C	32.94267300	7.16166500	5.04629400
H	33.47174400	6.57820400	5.79503000
C	32.85823300	6.69405900	3.72824600
H	33.30159000	5.74614500	3.44303600
C	32.18994300	7.46943200	2.80299100
H	32.10144200	7.12145800	1.77601000
C	31.62666500	8.71689800	3.13440600
C	30.94385900	9.40152100	2.04865600
H	30.64170200	8.74435300	1.22217400
N	30.66840800	10.65264900	1.96505700
C	29.89178800	11.07511500	0.80476100
H	29.11170500	11.75797700	1.15225800
H	29.39267900	10.20452700	0.35951700
C	30.71806300	11.75100200	-0.30522500
H	31.72866600	11.33373800	-0.31671100
H	30.24680400	11.50134600	-1.26480800
N	30.83093900	13.20001300	-0.18001500
C	30.09432400	13.90390700	-0.96098800
H	29.38577100	13.38374800	-1.61929400
C	30.07761500	15.35152600	-1.09249000
C	28.91605700	15.89170000	-1.67767400
H	28.11806000	15.20873800	-1.96074200
C	28.75741600	17.24657000	-1.88356100

H	27.84536700	17.64018800	-2.31909500
C	29.80933000	18.09853700	-1.52212600
H	29.70916600	19.17126500	-1.66336500
C	30.97474700	17.59798600	-0.97859900
H	31.76849100	18.28048300	-0.69328600
C	31.15965100	16.21289300	-0.73652500
N	32.28794400	15.72856600	-0.12876700
C	33.50358300	16.36466800	-0.28368300
C	33.92298400	16.85365400	-1.54131500
H	33.24696500	16.74567800	-2.38379400
C	35.16651200	17.42734800	-1.72398600
H	35.45307700	17.77080500	-2.71417500
C	36.05783900	17.55907500	-0.65317900
H	37.03358400	18.01131600	-0.79501400
C	35.66244400	17.11186300	0.59232200
H	36.33158500	17.22790000	1.44204500
C	34.41120300	16.50446900	0.80288200
C	34.07445100	16.18690400	2.18673800
H	34.62497600	16.77467300	2.93331100
N	33.19784500	15.34373500	2.59149200
C	32.89152800	15.33834600	4.01967000
H	31.81362200	15.48497500	4.11761300
H	33.39095500	16.18792300	4.50390500
C	33.30152100	14.05306000	4.75943000
H	34.04484800	13.51523600	4.16616700
H	33.77363800	14.33773400	5.70891700
O	33.20266800	11.78389700	2.79459700
C	33.74071200	11.88290500	1.66683100
O	33.51878200	12.78274700	0.81355400
O	34.64304100	10.96714500	1.28347800
C	34.95837500	9.90230100	2.20922200
H	34.05368200	9.66149500	2.76964100
C	36.04302200	10.36824300	3.16733600
H	35.69803900	11.23370700	3.74008500
H	36.95113900	10.64273500	2.61975400
H	36.28905100	9.56753200	3.87231400
C	35.37127700	8.71207800	1.36314600
H	34.56517200	8.43132200	0.67872900
H	35.58495000	7.85676300	2.01155400
H	36.26695800	8.93976000	0.77532900
O	30.56155800	14.56543500	2.36848200
C	29.54046400	13.98745100	2.81318900
O	29.52760900	12.88094700	3.41200200
O	28.33710200	14.55824200	2.66198100
C	28.27462300	15.84739400	2.01068500
H	29.06346600	15.88687600	1.25810800
C	28.49540500	16.94342700	3.04113300
H	29.48042800	16.83767500	3.50474700
H	27.72861500	16.89915600	3.82181500
H	28.44703500	17.92493100	2.55863600
C	26.91654400	15.91849600	1.33741800
H	26.80710500	15.10726200	0.61129100
H	26.81962500	16.86934600	0.80464600
H	26.10992600	15.84318300	2.07429200

Sum of electronic and thermal Free Energies= -5886.571258

Frequencies –
10.8869 17.8091 23.1847

CO₂



0 1
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O 0.00000000 0.00000000 1.16471100
O 0.00000000 0.00000000 -1.16471100

Sum of electronic and thermal Free Energies=

-188.530371

Frequencies –

651.5571 651.5571 1401.0504