

## Supporting Information

### **Using nature's blueprint porous organic polymeric nanotraps enables the interfacial activation of the hosted amine and CO<sub>2</sub>**

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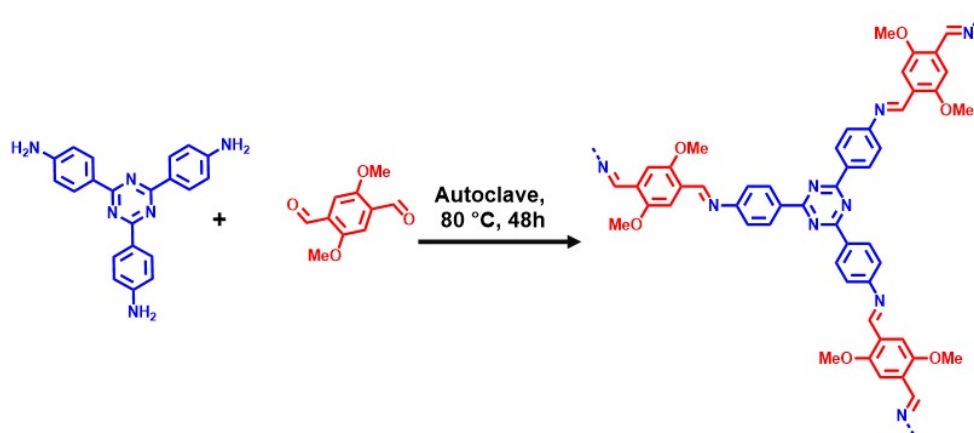
## Materials and methods:

### 1. Materials:

4,4',4''-(1,3,5-triazine-2,4,6-triyl)trianiline (TRI), 2,5-dimethoxyterephthalaldehyde, L-Histidine, ZnCl<sub>2</sub>, N-methylaniline (NMA), phenylsilane (PhSiH<sub>3</sub>), 4,4'-bipiperidine, Piperidine, Morpholine, Piperazine were purchased from Sigma-Aldrich and TCI chemicals. 1,4-dioxane, N-Butanol, N, N-dimethylformamide (DMF), dichloroethane (DCE), Methanol (MeOH), Tetrahydrofuran (THF), Chloroform (CHCl<sub>3</sub>), Acetone, dimethyl sulfoxide (DMSO), acetonitrile (ACN), dimethylacetamide (DMAc), dichloromethane (DCM), Aqueous Acetic Acid (CH<sub>3</sub>COOH) and ethanol (EtOH) were purchased from Finar Chemicals and used without any further purification.

### Synthesis of T-POP:

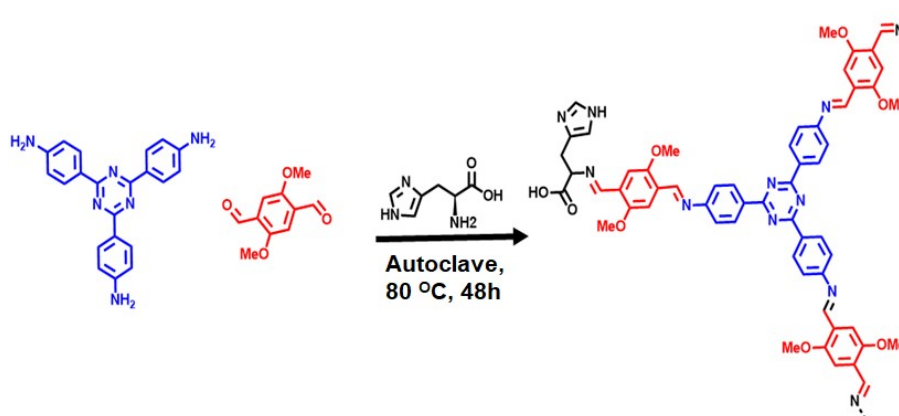
In a 100 mL round-bottom flask, 4,4',4''-(1,3,5-triazine-2,4,6-triyl)trianiline (87 mg, 0.45 mmol) and 2,5-dimethoxyterephthalaldehyde (106 mg, 0.3 mmol) were dissolved in a solvent mixture of 1,4-dioxane, n-butanol, and methanol (12:12:3 ratio) and sonicated for uniform dispersion. The reaction mixture was then stirred at room temperature under a nitrogen (N<sub>2</sub>) atmosphere for 15 minutes, followed by the addition of 0.5 mL of aqueous acetic acid (6 M) and further stirring for a few minutes. The resulting mixture was transferred into a Teflon-lined autoclave, sealed, and heated in an oven at 80 °C for 2 days to facilitate polymerization. After completion, the reaction mixture was cooled, and the solid product was filtered, washed with ethanol and water, the resulting solid was further purified using a Soxhlet extractor with a mixed solvent of methanol, chloroform and acetone for 72 h. Finally, the purified precipitate was filtered and dried under vacuum at 80 °C to remove all solvent. This resulted in formation of T-POP.



**Scheme S1:** Schematic representation of pristine T-POP synthesis.

### Synthesis of His-POP:

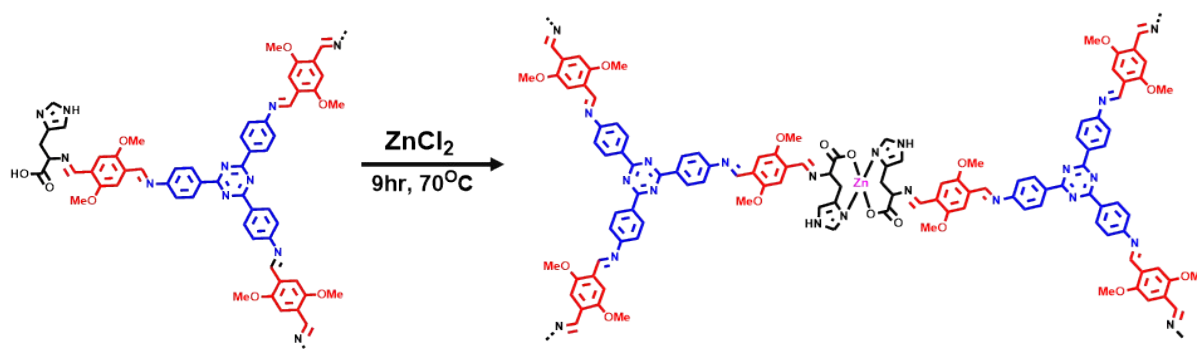
In a 100 mL round-bottom flask, 4,4',4''-(1,3,5-triazine-2,4,6-triyl)trianiline (87 mg, 0.45 mmol) and 2,5-dimethoxyterephthalaldehyde (106 mg, 0.3 mmol) were dissolved in a solvent mixture of 1,4-dioxane, n-butanol, and methanol (12:12:3 ratio) and sonicated for uniform dispersion. The reaction mixture was then stirred at room temperature under a nitrogen ( $N_2$ ) atmosphere for 15 minutes, followed by the addition of 0.5 mL of aqueous acetic acid (6 M) and further stirring for a few minutes. In a separate beaker, L-Histidine (47 mg, 0.3 mmol) was dissolved in 5 mL of aqueous acetic acid and added to the reaction mixture, which was then stirred for 1-2 h at room temperature under  $N_2$  atmosphere. The resulting mixture was transferred into a Teflon-lined autoclave, sealed, and heated in an oven at 80 °C for 2 days to facilitate polymerization. After completion, the reaction mixture was cooled, and the solid product was filtered, washed with ethanol and water, the resulting solid was further purified using a Soxhlet extractor with a mixed solvent of methanol, chloroform and acetone for 72 h. Finally, the purified precipitate was filtered and dried under vacuum at 80 °C to remove all solvent.



**Scheme S2:** Schematic representation of pristine **His-POP** synthesis.

### Incorporation of Zn-Metal active site in as-synthesized His-POP:

The Zn (II) metallic site was successfully anchored into the **His-POP** backbone by reacting with Zn (II) chloride. Initially, 30 mg of Zn (II) chloride ( $ZnCl_2$ ) was added to 100 mg of the as-synthesized **His-POP** in a round-bottom flask, to which 50-60 mL of ethanol was added. The resulting solution was then stirred for 9 h at 70 °C, after which it was filtered off. The final precipitate was dried under vacuum at 80 °C for 24 h and denoted as **Zn@His-POP**.



**Scheme S3:** Schematic representation of designing **Zn@His-POP** via embedding Zn-sites into the polymeric backbone.

## 2. Characterization Technique Details:

The powder X-ray diffraction (XRD) patterns were obtained using a Rigaku Miniflex X-ray diffractometer from Rigaku Corporation in Japan. These patterns were collected using Ni-filtered Cu K $\alpha$  radiation ( $\lambda = 1.5406 \text{ \AA}$ ) at a scan speed of  $2^\circ/\text{min}$  with a range of  $10$  to  $80^\circ$  at  $30 \text{ kV}$  and  $15 \text{ mA}$ .

FT-IR spectra of the catalysts were recorded on a DIGILAB IR spectrometer in the USA using the KBr disc method. Solid-state  $^{13}\text{C}$  CP MAS NMR studies were conducted on a Bruker Avance III HD  $400 \text{ MHz}$  NMR spectrometer.

Thermogravimetric analysis (TGA) of all samples was carried out using a TGA Instruments thermal analyzer TA-SDT Q-600 under a nitrogen atmosphere at a heating rate of  $10 \text{ }^\circ\text{C min}^{-1}$  from  $25$  to  $700 \text{ }^\circ\text{C}$ . Before conducting the TGA analysis, we kept the sample in a vacuum oven at  $80 \text{ }^\circ\text{C}$  for  $10 \text{ h}$ .

The catalyst's morphology was examined via scanning electron microscopy (SEM) using the FEI Verios 460L field-emission SEM (FE-SEM) equipped with an electron diffraction spectroscopy (EDS) detector for elemental mapping. Transmission electron microscopy (TEM) images were taken at  $100 \text{ kV}$  using a JEOL 1010 TEM.

The surface area was determined through the Brunauer-Emmett-Teller (BET) method. The average pore volume and pore size were measured by Non-local density functional theory (NLDFT) method. The BET surface area, pore volume and pore sizes were determined by using the  $\text{N}_2$  adsorption-desorption method using BEL Sorb II Instruments, Japan at liquid nitrogen temperature. Before the measurement the samples were degassed at  $130 \text{ }^\circ\text{C}$  for  $2 \text{ h}$ .

The low-pressure  $\text{CO}_2$  adsorption experiments were carried out using a Quantachrome iSorb-HP high-pressure gas sorption analyzer at  $273 \text{ K}$  and  $298 \text{ K}$ , up to  $1 \text{ bar}$ . Before the adsorption measurements, the samples underwent drying at  $110 \text{ }^\circ\text{C}$  for  $24 \text{ h}$ .

X-ray photoelectron spectroscopy (XPS) analysis was conducted using a Thermo Scientific K-Alpha instrument, utilizing monochromatic Al K $\alpha$  radiation with a photon energy of 1486.6 eV. To correct the binding energies (B.E) for both core levels and valence band maxima, an internal reference peak of the C 1s peak centred at 284.8 eV was employed.

Experiments were performed on the JNM-ECZ600R (JEOL Ltd.) at 14.1 T (600 MHz) solid-state NMR spectrometer equipped with a triple-channel  $^1\text{H}/^{13}\text{C}/^{14}\text{N}$  1 mm MAS probes at a MAS frequency of 70 kHz. The  $^{14}\text{N}$  and  $^{13}\text{C}$  edited experiments were recorded with a recycle delay of 5 and 5 Sec, respectively. The T-HMQC (TRAPDOR-heteronuclear multiple-quantum correlation) experiment was used to record 2D  $^1\text{H}$ - $^{14}\text{N}$  correlation spectra with 96 scans, for a total experimental time of approximately 7.5 h, corresponding to acquisition times of 5 ms and 0.8 ms in  $^1\text{H}$  and  $^{14}\text{N}$  dimensions, respectively. Two-proton-detected two-dimensional  $^1\text{H}$ - $^{13}\text{C}$  heteronuclear correlation spectra with a CP contact time of 100  $\mu\text{s}$  and 2 ms were recorded with 96 and 512 points, corresponding to acquisition times of 3.34 ms and 5 ms in the  $^{13}\text{C}$  and  $^1\text{H}$  dimensions, respectively.

**Product Analysis by Gas Chromatography (GC-FID):** All the reactants, products, and intermediates are confirmed and analysed by GC (Model QP 5050 supplied by M/S. Shimadzu Instruments Corporation, Japan) and GC (Shimadzu 2010), respectively. The GC is equipped with a flame ionization detector (FID) and an INNO Wax capillary column (diameter: 0.25 mm, length: 30 m) for separating the reaction mixtures. The product and reactant mixture, which was collected from the reactor, was added to the organic solvents (methanol or acetone), and an equal amount of an internal standard (anisole) was added before starting the GC analysis. The GC programming conditions are different for different reactions. The temperature of the injector is 250  $^\circ\text{C}$ , the temperature of the oven/column is usually 80-280  $^\circ\text{C}$  with the ramping rate of 10  $^\circ\text{C min}^{-1}$ , and the holding time is 3 and 5 minutes for the start and the end time of the analysis, respectively. The FID temperature is 300  $^\circ\text{C}$ .

#### **Computational details:**

All calculations were performed using Gaussian 16 Rev.C.01.<sup>1</sup> Geometries and frequencies optimizations were investigated using the unrestricted open-shell M06-2X functional<sup>2</sup> combined with the Ahlrichs family basis set def2-SVP.<sup>3,4</sup> The HOMO, LUMO distributions and ESP map of the **His-POP** and the **Zn@His-POP** complexes were analyzed by Chemcraft.<sup>5</sup> Charge density difference (CDD) map was visualized using the Multiwfn code.<sup>6</sup>

The interaction free energies ( $\Delta G_{\text{int}}$ ) between **His-POP** and **Zn@His-POP** complexes with the  $\text{CO}_2$  molecule were calculated *via* the following equation:

$$\Delta G_{\text{int}} = G(\text{CO}_2/\text{His-POP}) - G(\text{CO}_2) - G(\text{His-POP})$$

$$\Delta G_{\text{int}} = G(\text{CO}_2/\text{Zn@His-POP}) - G(\text{CO}_2) - G(\text{Zn@His-POP})$$

### Experimental Section:

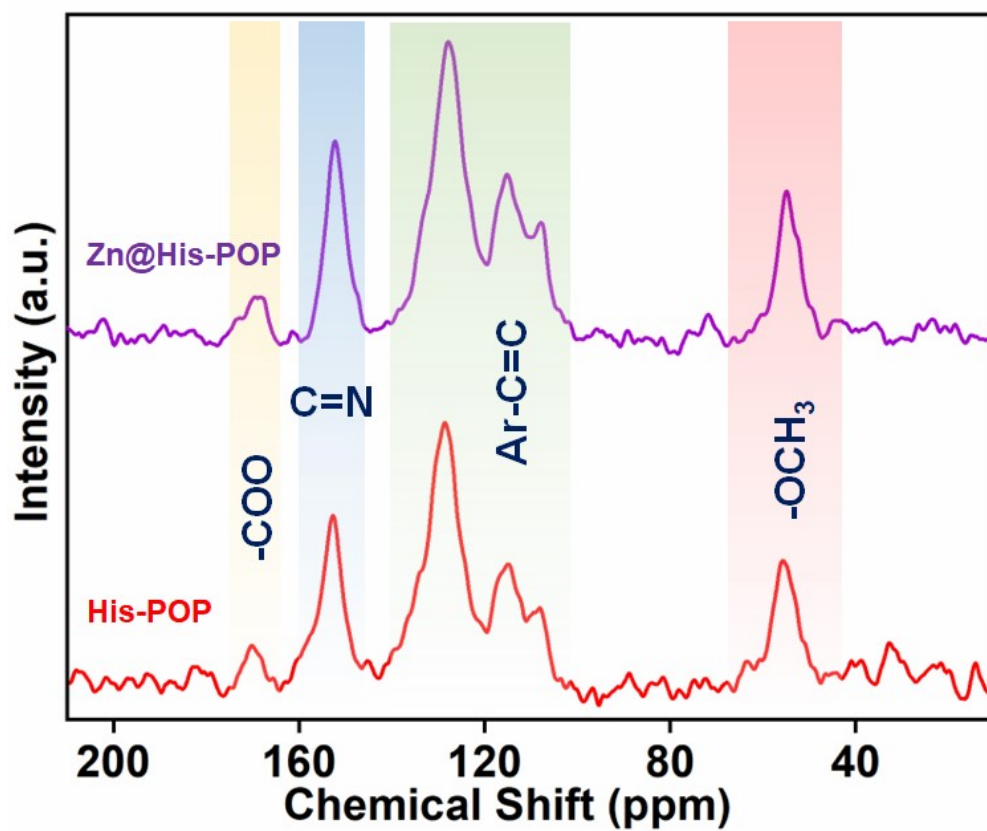
#### Reaction condition screening of the synthesis of N-formylation products:

For the reductive N-formylation of amines using CO<sub>2</sub>, a 100 mL single-neck round-bottom flask was charged with N-methylaniline (1 mmol, 1 equiv.) and phenylsilane (2 mmol, 2 equiv.). Subsequently, the **Zn@His-POP** catalyst (20 mg) was added, followed by the addition of 5-10 mL of N, N-dimethylformamide (DMF) as the reaction medium. The mixture was stirred to achieve a homogeneous solution, then the flask was sealed with a septum. Carbon dioxide (CO<sub>2</sub>) gas was continuously purged into the reaction system at approximately 80 °C. The reaction was allowed to proceed for 12 h under sustained CO<sub>2</sub> flow to ensure optimal conversion.

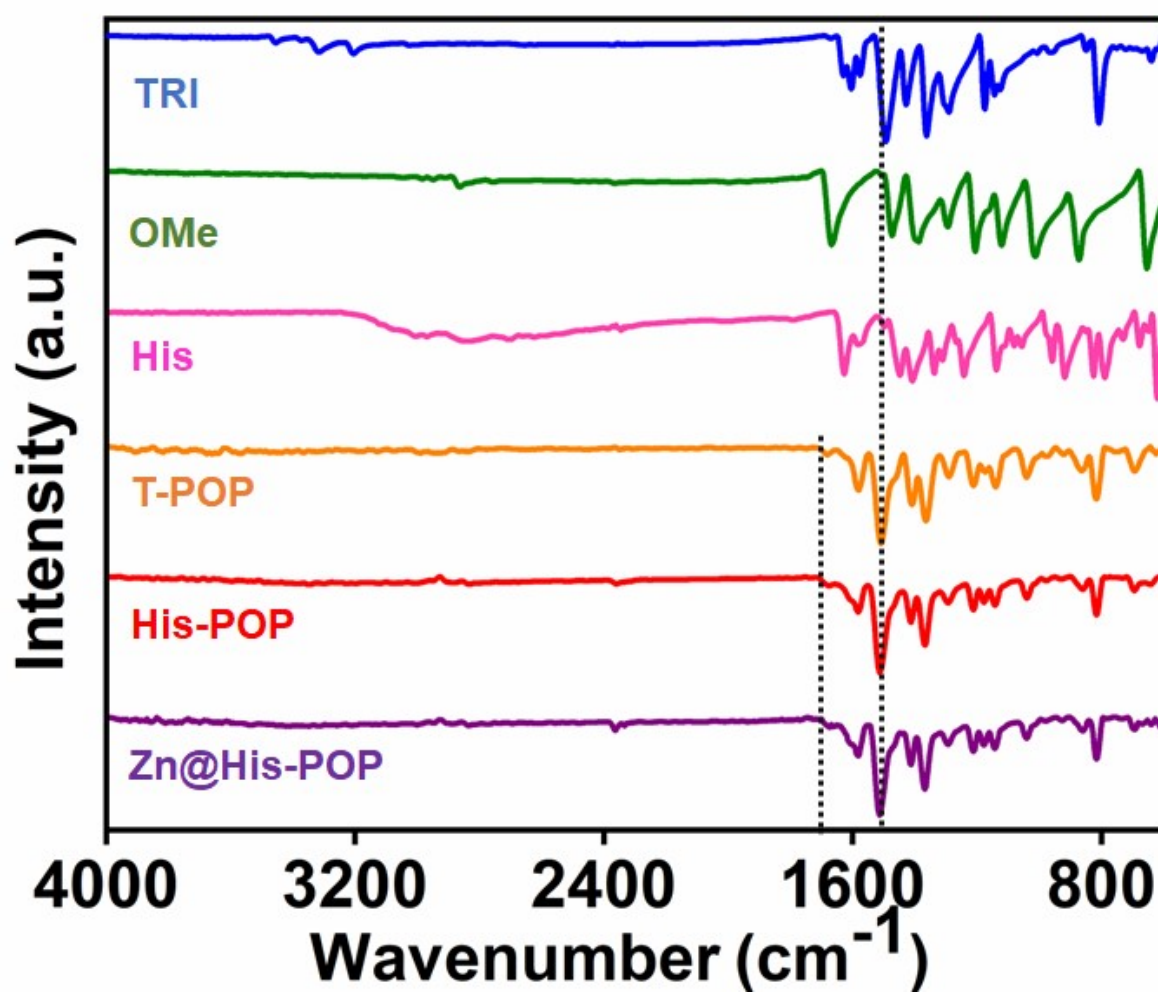


**Scheme S4:** Schematic representation of N-Formylation reaction by using **Zn@His-POP** as a Catalyst.

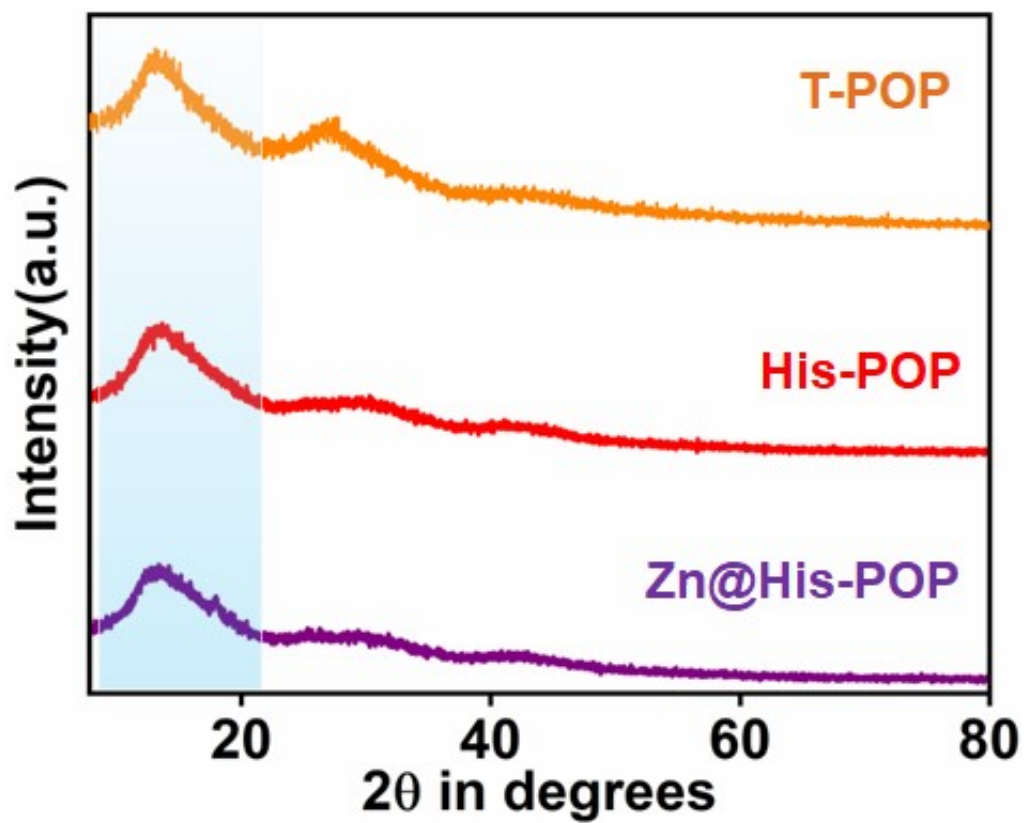
After the reaction was completed, the mixture was allowed to cool naturally to ambient temperature. The solid precipitate formed was then carefully isolated through vacuum filtration to ensure maximum recovery. To remove any unreacted substrates, byproducts, or residual solvent, the precipitate was thoroughly washed multiple times with DMF. The purified solid was subsequently dried under reduced pressure before being analyzed by <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy, and gas chromatography-mass spectrometry (GC-MS) to confirm product formation and assess purity.



**Figure S1:**  $^{13}\text{C}$  cross polarization (CP) solid-state MAS NMR spectrum of **His-POP** and **Zn@His-POP** respectively.



**Figure S2:** FT-IR analysis of the T-POP, His-POP and Zn@His-POP along with their respective monomer, respectively.



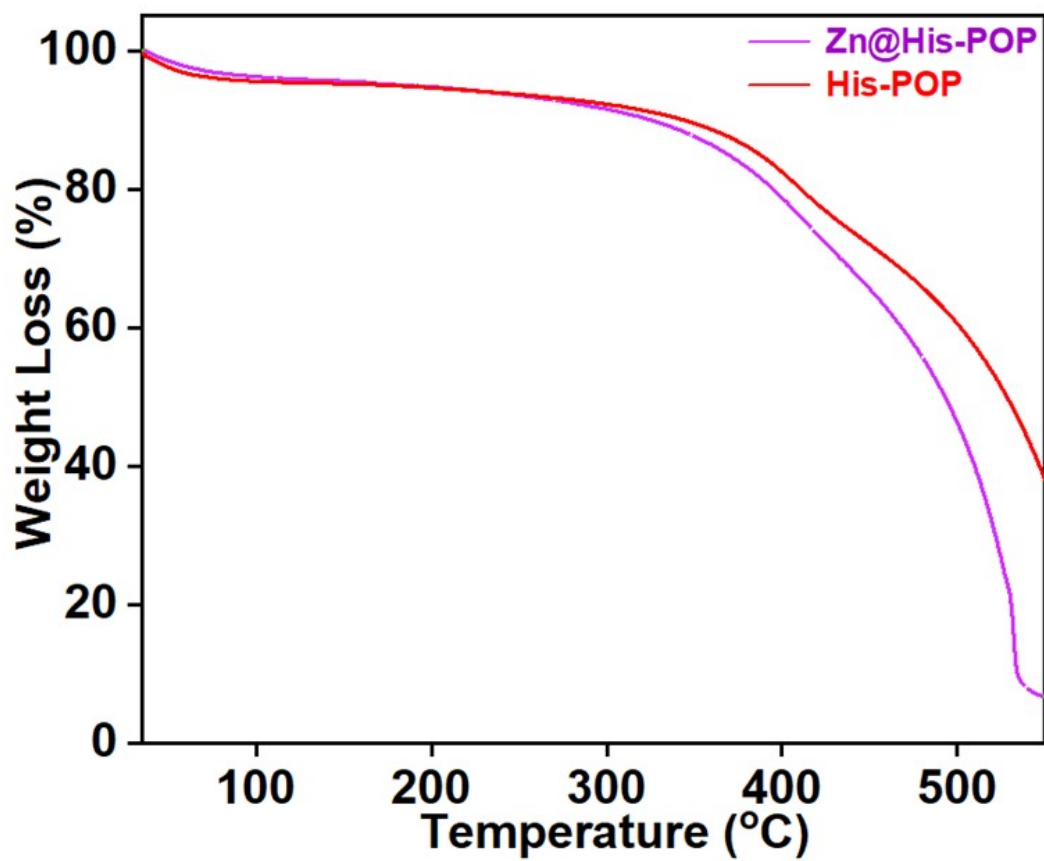
**Figure S3:** Wide angle Powder X-ray Diffraction (PXRD) pattern for the T-POP, His-POP and Zn@His-POP respectively.

**Table S1:** CHN analysis of **His-POP** and **Zn@His-POP**, respectively.

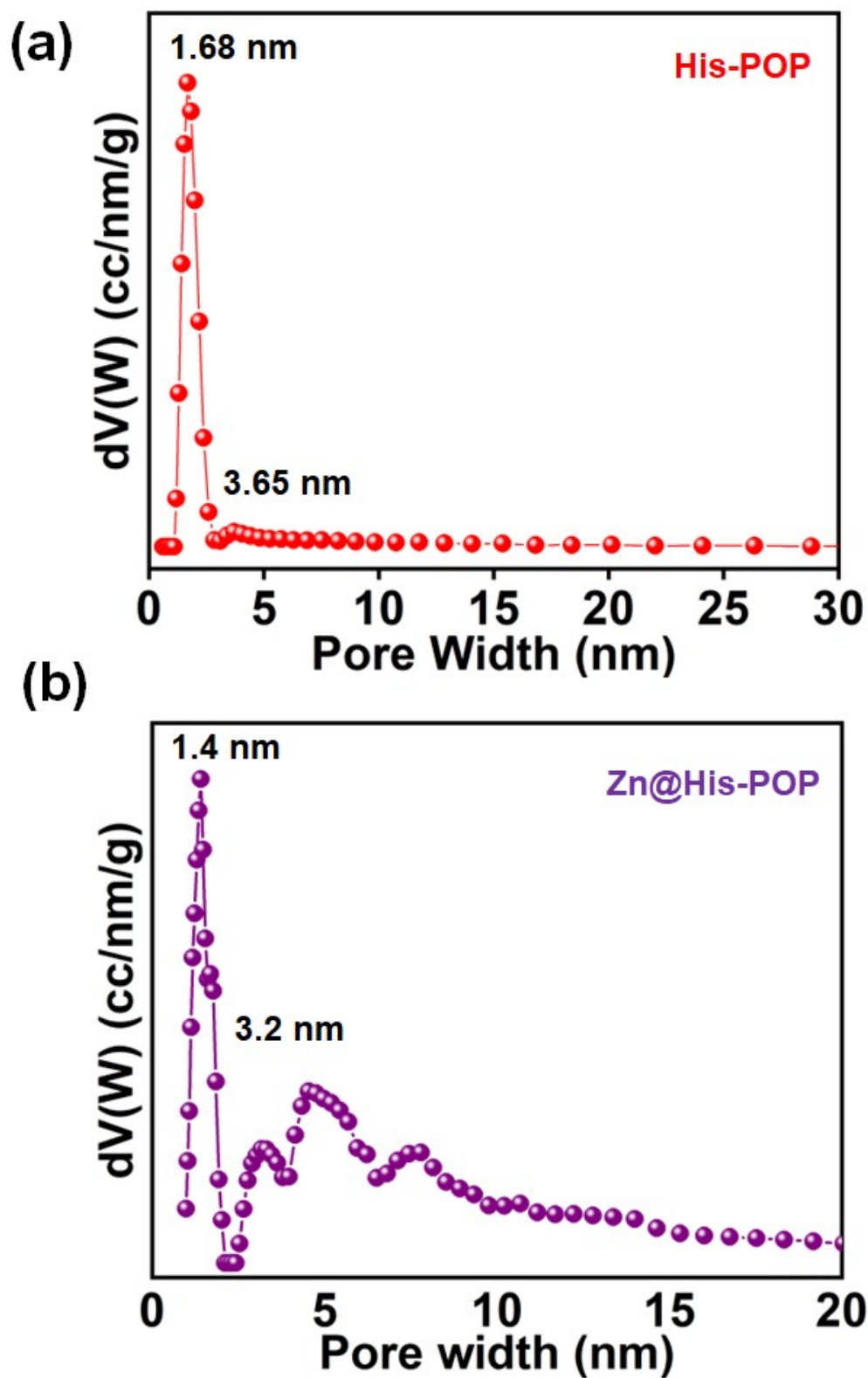
<b>Elements in weight %</b>	<b>His-POP</b>	<b>Zn@His-POP</b>
<b>C</b>	67.86	61.60
<b>H</b>	13.40	12.38
<b>N</b>	5.53	4.92

**Table S2: ICP-MS Analysis of Zn@His-POP.**

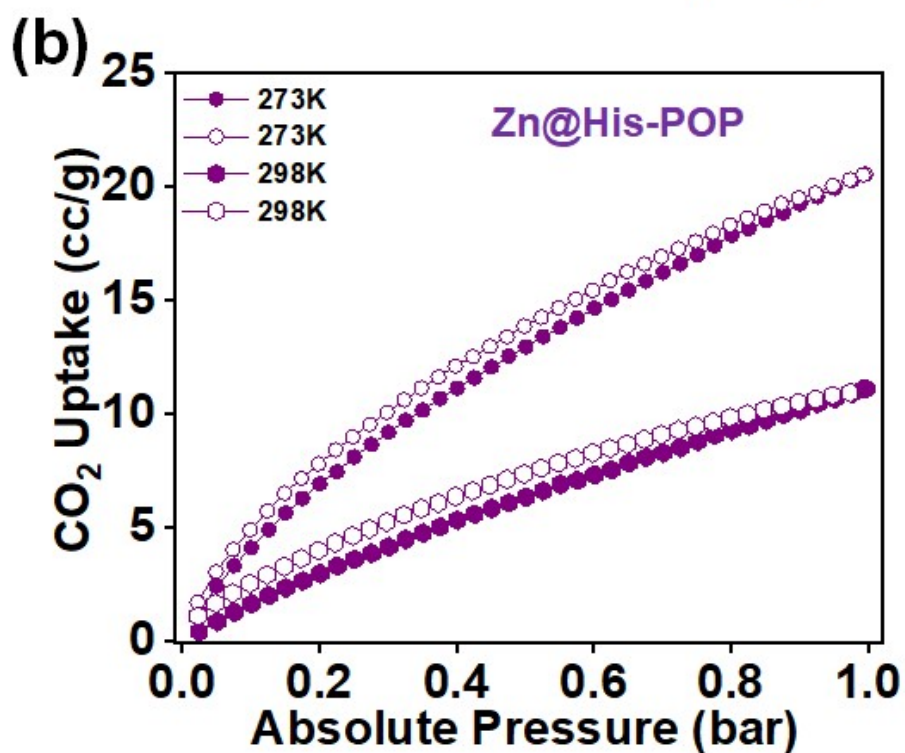
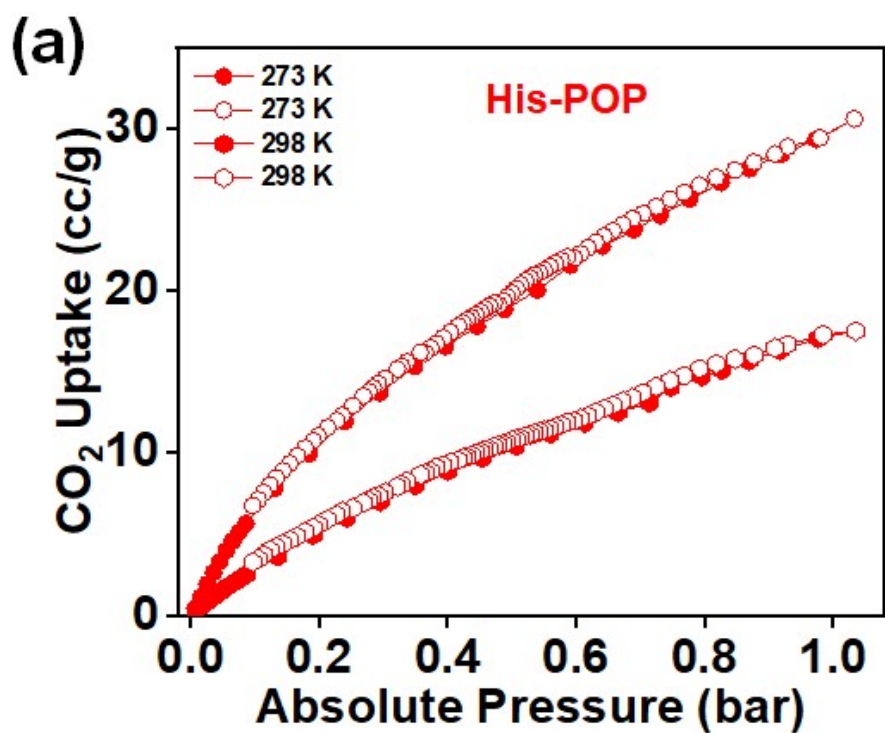
<b>Sl. No</b>	<b>Sample Name</b>	<b>Test Parameter</b>	<b>UOM</b>	<b>Result</b>
1.	<b>Zn@His-POP</b>	Zinc as Zn	Wt.%	4.01
2.	Reused <b>Zn@His-POP</b>	Zinc as Zn	Wt.%	3.21



**Figure S4:** Thermogravimetric (TGA) analysis spectra of His-POP and Zn@His-POP, respectively



**Figure S5:** Pore-size distributions as calculated by NLDFT for His-POP (a) and Zn@His-POP (b), respectively.



**Figure S6:** CO<sub>2</sub> Adsorption-Desorption isotherms analysis at 273 K and 298 K for His-POP (a) and Zn@His-POP (b), respectively.

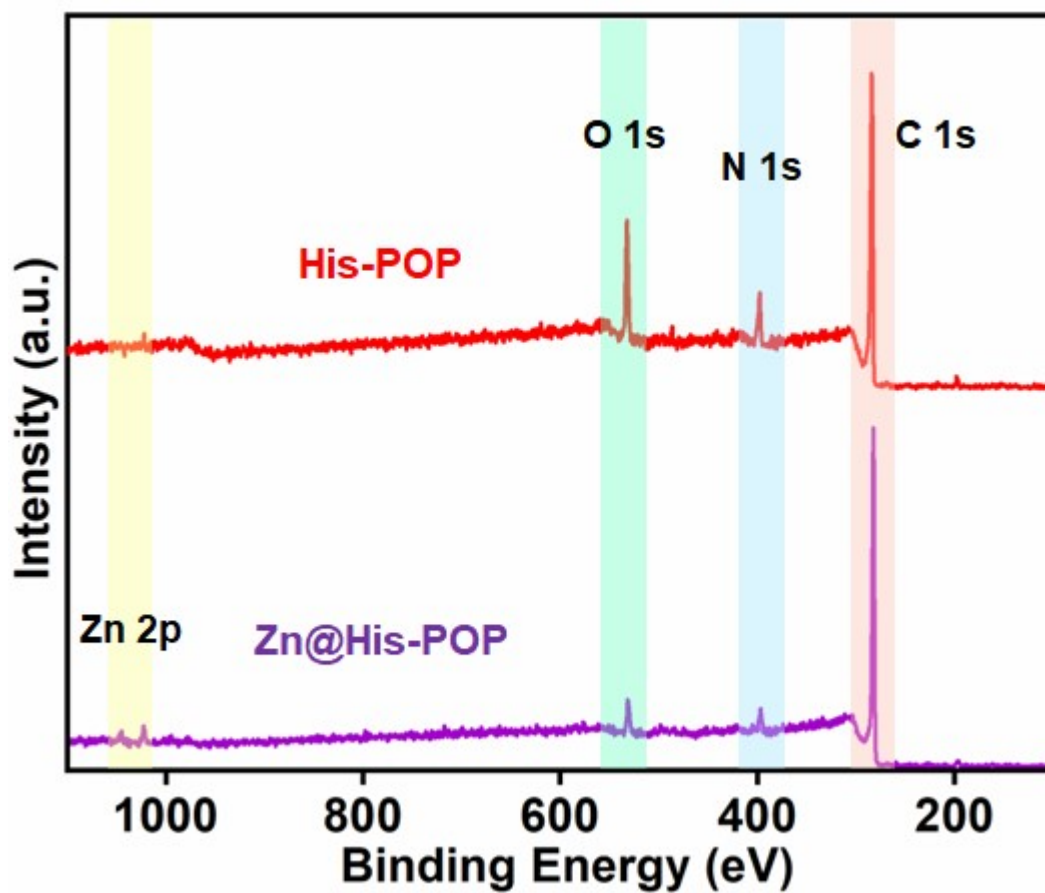
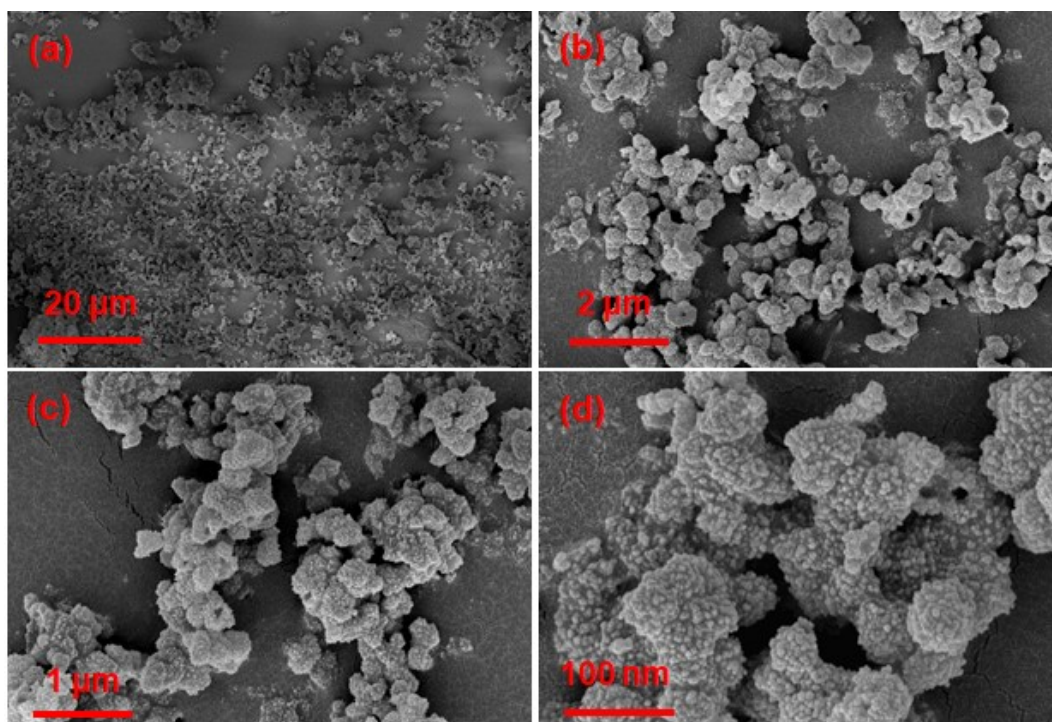
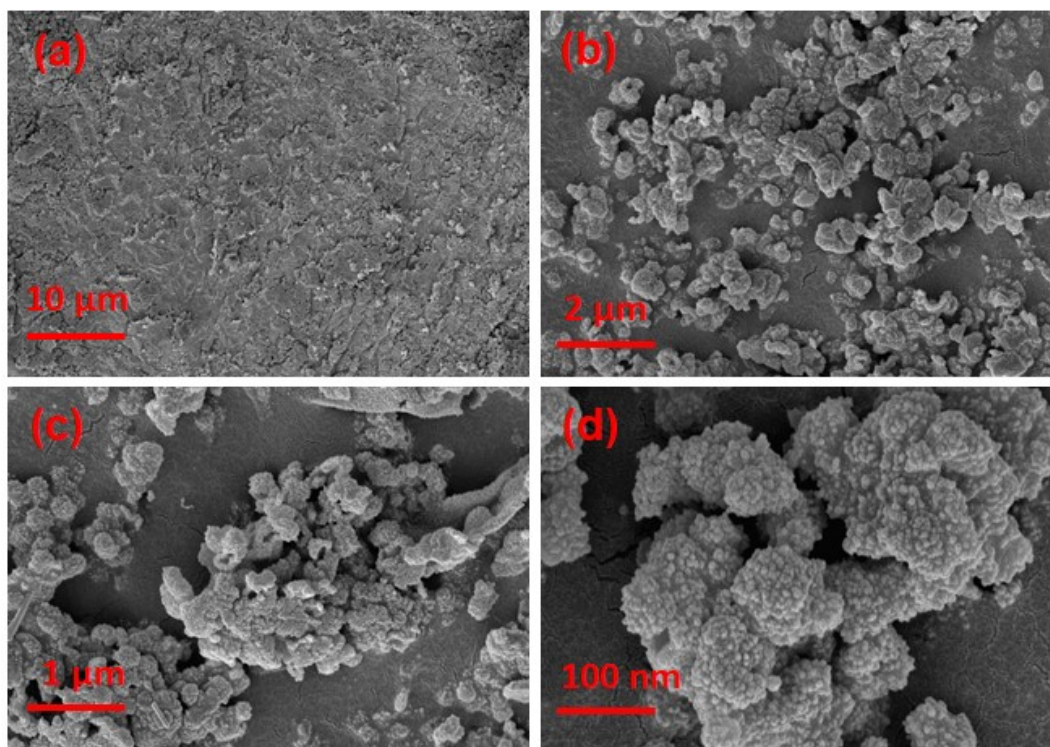


Figure S7: X-ray photoelectron survey spectrum of His-POP and Zn@His-POP respectively



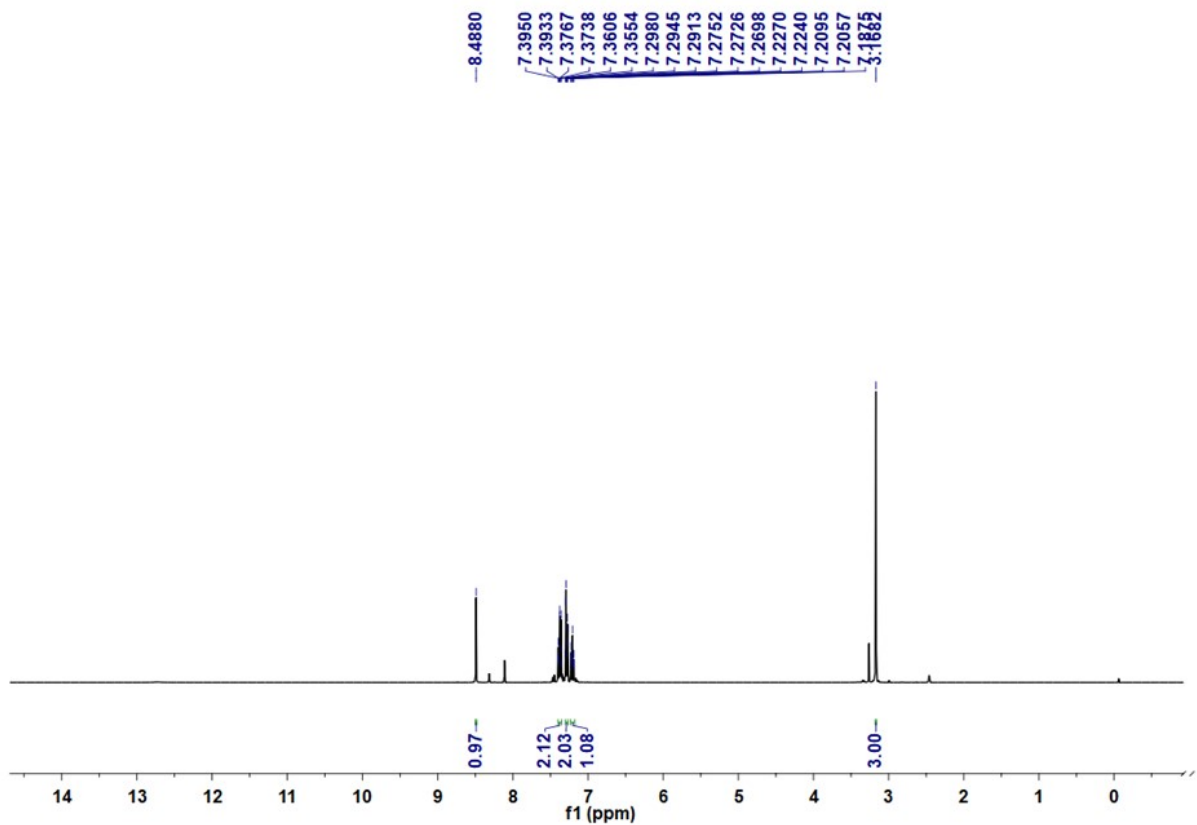
**Figure S8:** Field emission scanning electron microscopy (FE-SEM) images of **His-POP** (a-d), respectively.



**Figure S9:** Field emission scanning electron microscopy (FE-SEM) images of Zn@His-POP (a-d), respectively.

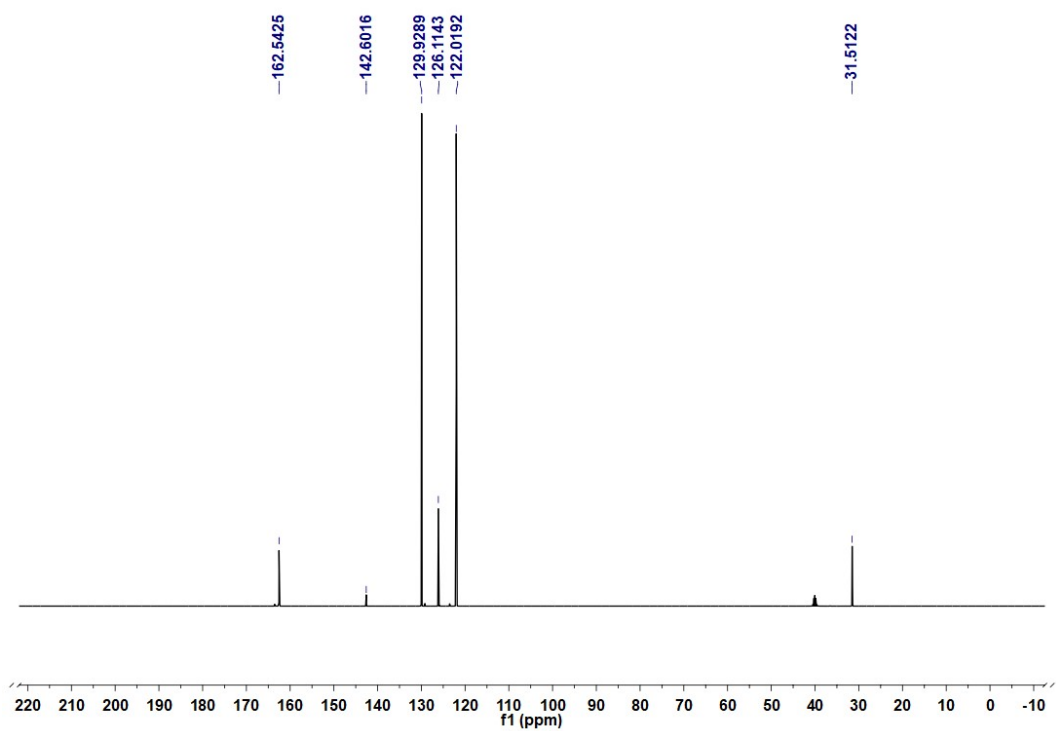
**Table S3:** Parameters obtained after fitting the XAS data of **Zn@His-POP**.

<b>Sample</b>	<b>First Shell</b>	<b>Coordination Number (N)</b>	<b>R(Å)</b>	<b><math>\sigma^2(10^{-2}\text{Å}^2)</math></b>	<b><math>\Delta E_0</math> (eV)</b>
<b>Zn@His-POP</b>	<b>O1.1</b>	<b>2</b>	<b>2.0167</b>	<b>0.187</b>	<b>6.12</b>
	<b>N2.1</b>	<b>2</b>	<b>1.5761</b>	<b>0.002</b>	<b>-155.70</b>



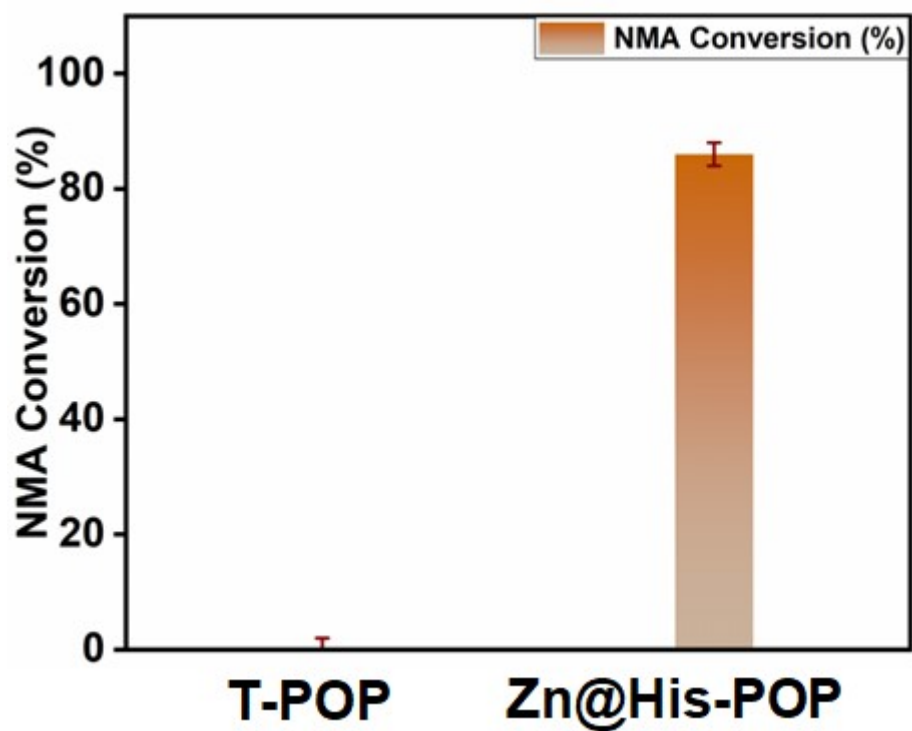
**Figure S10:**  $^1\text{H}$  NMR spectrum of **N-methyl-N-phenylformamide**.

$^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  8.49 (s), 7.40-7.35 (m), ( $J = 8.6, 1.3\text{Hz}$ ), 7.23-7.18(m), 3.17(s)

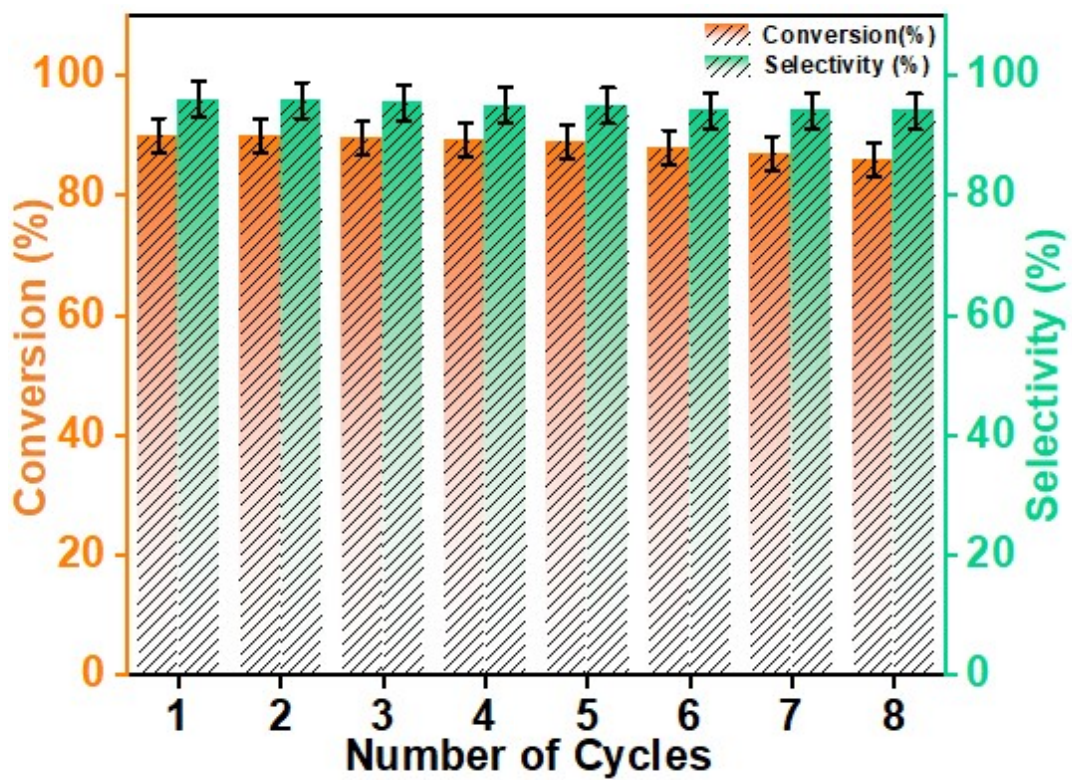


**Figure S11:**  $^{13}\text{C}$  NMR spectrum of **N-methyl-N-phenylformamide**.

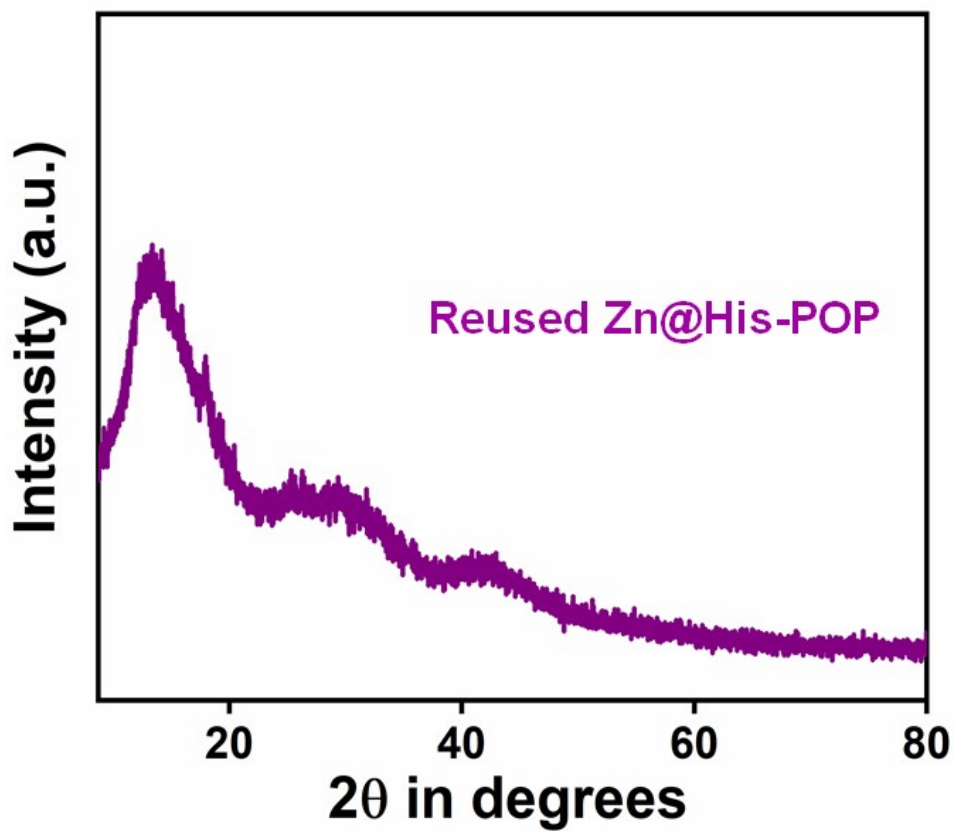
$^{13}\text{C}$  NMR (101 MHz, DMSO)  $\delta$  162.54, 142.60, 129.93, 126.11, 122.02, 31.51



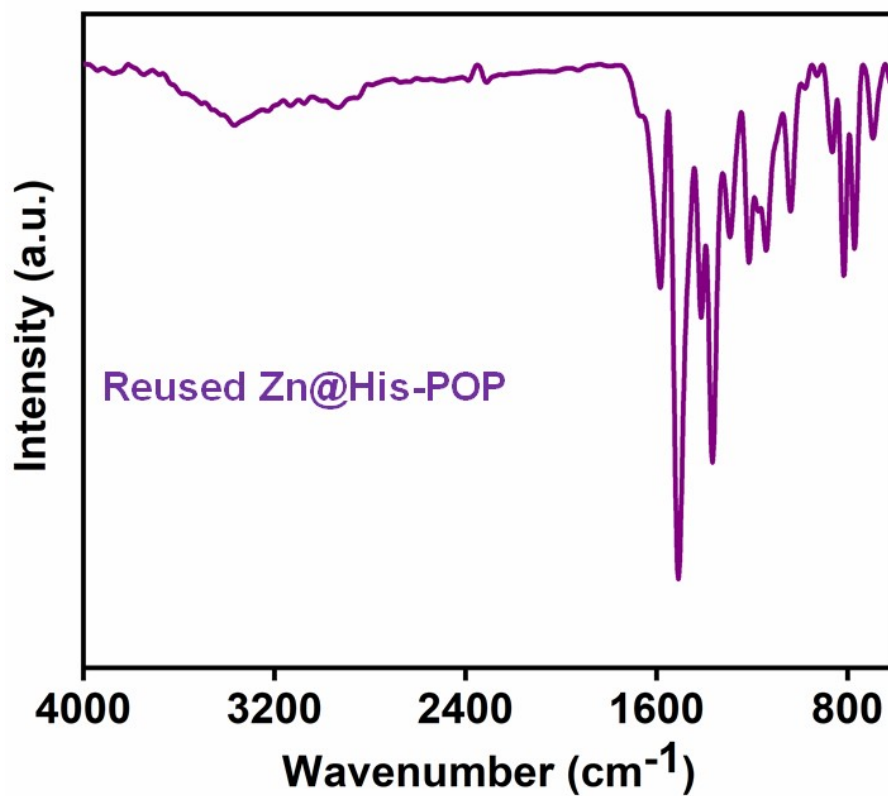
**Figure S12:** Comparison in the catalytic performance for N-formylation reaction with **T-POP** and **Zn@His-POP** respectively.



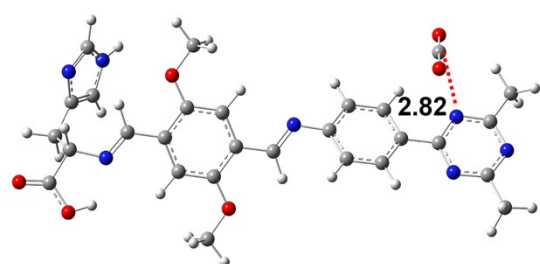
**Figure S13:** Reusability potential diagram of Zn@His-POP catalyst.



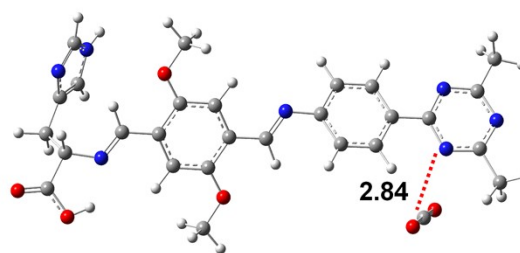
**Figure S14:** Wide angle Powder X-ray Diffraction (PXRD) pattern for the Reused Zn@His-POP catalyst..



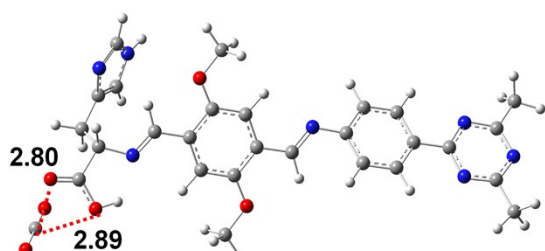
**Figure S15:** FT-IR spectrum of the reused Zn@His-POP catalyst.



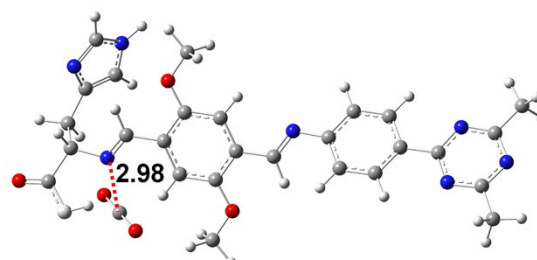
N8 (CO<sub>2</sub>/HisPOP-cp1),  $\Delta G_{\text{int}} = 10.0$



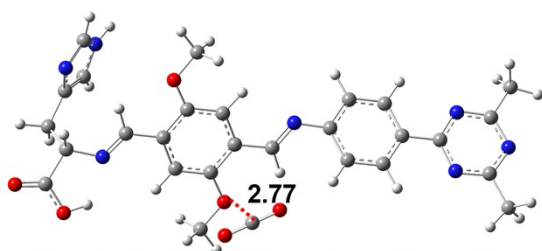
N6 (CO<sub>2</sub>/HisPOP-cp3),  $\Delta G_{\text{int}} = 11.8$



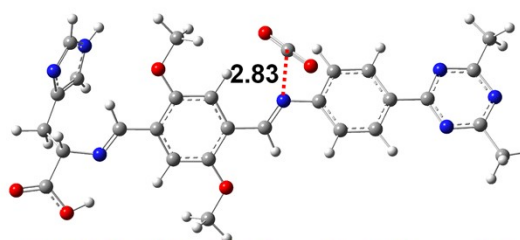
COO (CO<sub>2</sub>/HisPOP-cp2),  $\Delta G_{\text{int}} = 6.5$



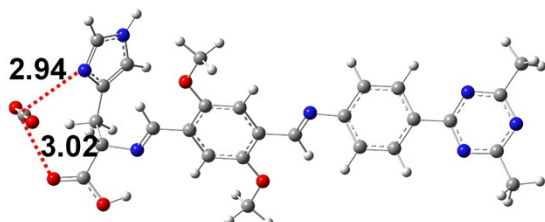
N32 (CO<sub>2</sub>/HisPOP-cp4),  $\Delta G_{\text{int}} = 3.9$



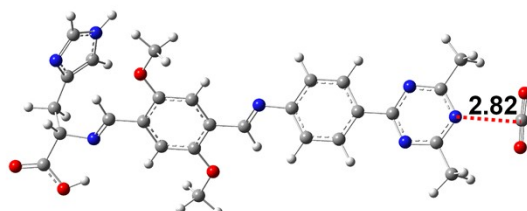
O33 (CO<sub>2</sub>/HisPOP-cp5),  $\Delta G_{\text{int}} = 8.1$



N19 (CO<sub>2</sub>/HisPOP-cp6),  $\Delta G_{\text{int}} = 2.9$



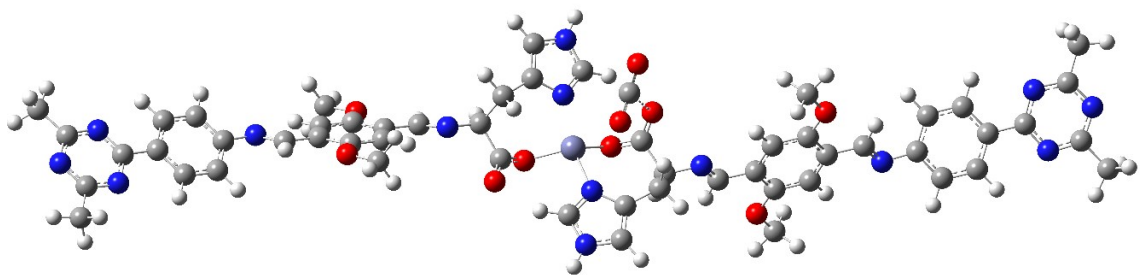
N57 (CO<sub>2</sub>/HisPOP-cp7),  $\Delta G_{\text{int}} = 9.4$



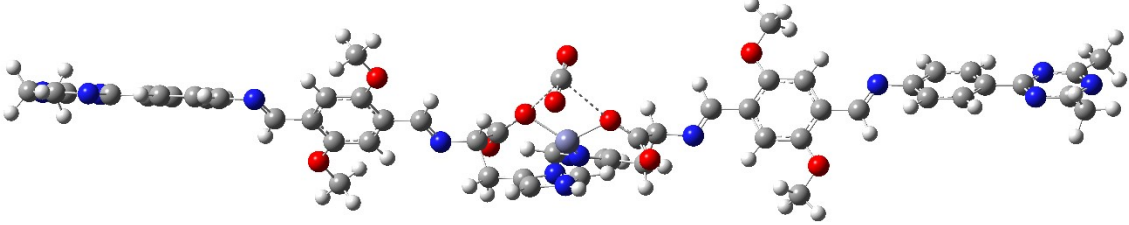
N42 (CO<sub>2</sub>/HisPOP-cp7),  $\Delta G_{\text{int}} = 15.1$

**Figure S16:** Eight possible interaction configurations of the His-POP with the CO<sub>2</sub> molecule at different active sites. All calculations were performed at the uM06-2X/def2-SVP level of theory. The Gibbs free energies of interaction ( $\Delta G_{\text{int}}$ , kcal/mol) were also mentioned.

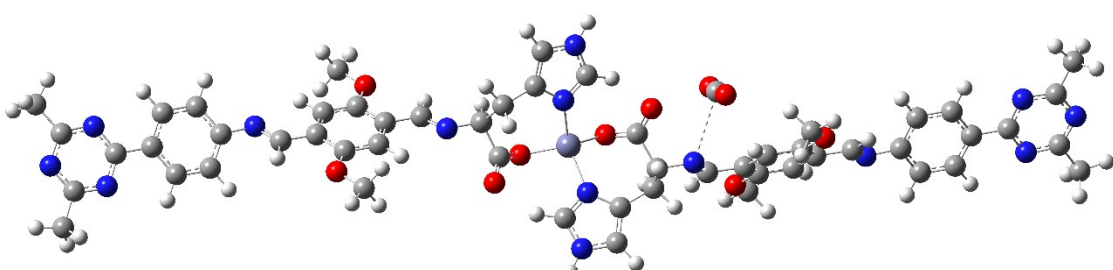
**Table S4:** Cartesian coordinates and corresponding thermochemistry data for seven possible interactions of the **Zn@His-POP** polymer with the CO<sub>2</sub> molecule. All calculations were performed at the uM06-2X/def2-SVP level of theory. Values in parentheses are the relative enthalpies / relative free energies of each configuration compared to the most stable one (units are in kcal/mol).

Cartesian coordinates				Optimized structure
<b>COO (7.6 / 3.3)</b>				
				
0 1				Zero-point correction= 1.033779 (Hartree/Particle)
C	19.35930800	-1.94769700	-0.47554500	Thermal correction to Energy= 1.110368
N	20.30673600	-1.02303500	-0.33969800	Thermal correction to Enthalpy= 1.111313
C	19.87744500	0.20464500	-0.02600100	Thermal correction to Gibbs Free Energy= 0.896412
C	17.71691800	-0.46404800	-0.00767000	Sum of electronic and zero-point Energies= -5420.069485
N	18.05513900	-1.71478700	-0.31930900	Sum of electronic and thermal Energies= -5419.992896
N	18.60173800	0.52899500	0.14861200	Sum of electronic and thermal Enthalpies= -5419.991952
C	16.28082100	-0.15135500	0.17530200	Sum of electronic and thermal Free Energies= -5420.206853
C	15.87397900	1.14726600	0.51302000	
C	15.31568200	-1.15477500	0.02555100	
C	14.52951500	1.43481100	0.69570000	
H	16.63453200	1.91807000	0.63593500	
C	13.96768000	-0.86573400	0.19349500	
H	15.64551300	-2.16454500	-0.21859900	
C	13.55632400	0.43876000	0.51627700	
H	14.19767100	2.43625500	0.97085100	
H	13.22183000	-1.65709100	0.10426800	
N	12.21431000	0.78242600	0.70867200	
C	11.32150500	0.30017900	-0.06322400	
H	11.57462600	-0.33931700	-0.92406400	
C	9.89343500	0.58142400	0.13608700	
C	9.47820500	1.38020100	1.20753600	
C	8.93849200	0.04100800	-0.74904100	
C	8.12782800	1.65124300	1.41317200	
H	10.25917200	1.77113200	1.85843100	
C	7.58695400	0.31307400	-0.54195200	
C	7.17382200	1.11029300	0.52747800	
H	6.80161800	-0.08215500	-1.18539800	
C	5.73412000	1.37239500	0.72805300	
H	5.45954900	1.92106800	1.64481900	
N	4.87156600	0.97375900	-0.11139800	
O	9.40422200	-0.72747700	-1.76083200	
O	7.65658700	2.41704200	2.42619700	
C	8.47289900	-1.28395900	-2.65377900	
H	7.76651500	-1.95087500	-2.13392700	
H	7.90221700	-0.50049900	-3.17795300	
H	9.04765900	-1.86292800	-3.38467100	
C	8.58052900	2.94457700	3.34193400	
H	8.00266300	3.51089700	4.08033900	
H	9.14036800	2.14517400	3.85415100	
H	9.29735400	3.61972600	2.84661300	
C	3.48136500	1.23595800	0.16120800	
H	3.32847100	1.84258500	1.07218700	
C	2.70862400	-0.08721800	0.33191400	
O	1.73056000	-0.02406500	1.16201800	
O	2.99327700	-1.05387900	-0.36366100	
C	2.89679800	1.96906400	-1.06966500	
H	3.60520300	2.76446600	-1.34051500	
H	2.88798000	1.25078200	-1.90265200	

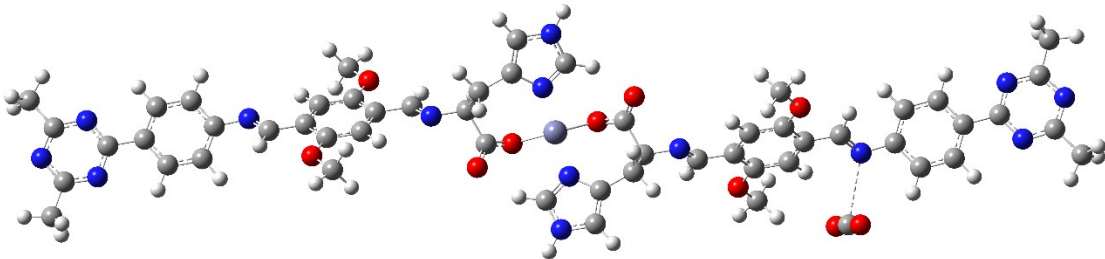
C	1.55019400	2.61074700	-0.91775400
C	1.26413500	3.93700300	-1.11889400
N	-0.08895300	4.07573900	-0.91869000
H	1.90699600	4.76853400	-1.38793500
C	-0.59604100	2.87281900	-0.60045500
H	-0.62394900	4.93177800	-0.98668900
H	-1.64877100	2.66927200	-0.37012600
N	0.36706200	1.96759600	-0.60068500
Zn	-0.01358500	0.15867000	0.31175800
C	-19.56046800	1.55418500	-0.86092800
N	-20.46434400	0.61641500	-0.58773900
C	-19.98163200	-0.52260500	-0.07829500
C	-17.85648100	0.24861200	-0.14722500
N	-18.24934000	1.41515000	-0.65769500
N	-18.69495500	-0.75029900	0.15739500
C	-16.41052200	0.04110500	0.09728900
C	-15.94900800	-1.16550700	0.64232200
C	-15.49116500	1.05427900	-0.20114300
C	-14.59608500	-1.35328900	0.88234600
H	-16.67443100	-1.94347800	0.87924100
C	-14.13410600	0.86276500	0.02460100
H	-15.86356700	1.99487600	-0.60691900
C	-13.66770000	-0.35174400	0.55604500
H	-14.22217800	-2.28046800	1.31736200
H	-13.42500700	1.66575100	-0.18252600
N	-12.31539400	-0.59645100	0.81514000
C	-11.42934700	-0.19978100	-0.01133100
H	-11.69250900	0.28708200	-0.96414100
C	-9.99519300	-0.38724500	0.24632700
C	-9.56997300	-0.99476100	1.43325500
C	-9.04521200	0.04573200	-0.70090500
C	-8.21479200	-1.18148000	1.69246300
H	-10.34745200	-1.30980600	2.12794500
C	-7.68847900	-0.14324700	-0.44071800
C	-7.26584100	-0.75193500	0.74259400
H	-6.90652600	0.17550000	-1.12913300
C	-5.82222300	-0.93776200	0.99263200
H	-5.54364100	-1.30662500	1.99440400
N	-4.96080000	-0.67918100	0.09951800
O	-9.52072900	0.63289800	-1.82369800
O	-7.73395200	-1.76489700	2.81660200
C	-8.59444400	1.08510700	-2.77849600
H	-7.92112900	1.84767400	-2.35522700
H	-7.98736100	0.25451400	-3.17333700
H	-9.17659200	1.52709000	-3.59431500
C	-8.65378100	-2.17629700	3.79377400
H	-8.06894200	-2.60036700	4.61721900
H	-9.24791200	-1.32743400	4.16968700
H	-9.34009100	-2.94497300	3.40236500
C	-3.56914000	-0.85569100	0.42536200
H	-3.41684800	-1.36088700	1.39745600
C	-2.84365300	0.50643400	0.47923300
O	-1.73596000	0.47528900	1.13525200
O	-3.29451200	1.46540300	-0.12192800
C	-2.92812900	-1.70211900	-0.70594900
H	-3.66540800	-2.46492900	-0.99121400
H	-2.79604500	-1.05135000	-1.58532200
C	-1.65115800	-2.41351400	-0.38316100
C	-1.47143700	-3.76559300	-0.24020500
N	-0.13485500	-3.94982000	0.02820700
H	-2.17478300	-4.58852000	-0.31275500
C	0.46339200	-2.74791400	0.04513300
H	0.33449900	-4.83482000	0.17168700
H	1.52834600	-2.56484000	0.20903700
N	-0.42404300	-1.80225300	-0.20980300
C	-20.97050100	-1.60215800	0.24170800
H	-21.52051400	-1.87641000	-0.66910100
H	-20.45982400	-2.47857900	0.65244000
H	-21.70821700	-1.22129400	0.96137600
C	-20.03353700	2.85557400	-1.43462800
H	-19.72990700	3.67993700	-0.77472500
H	-19.55117400	3.02506400	-2.40721100
H	-21.12172700	2.84592300	-1.55021800
C	19.77159400	-3.34566500	-0.82519700
H	19.43936200	-4.03428700	-0.03593300

H	19.27382100	-3.65434000	-1.75470600	
H	20.85829700	-3.40289600	-0.94097900	
C	20.91634900	1.27282700	0.13338700	
H	20.44824800	2.22315000	0.40794200	
H	21.63988100	0.96889900	0.90219400	
H	21.47326300	1.38417000	-0.80737300	
C	1.51178700	-1.44244600	-2.53750400	
O	1.11084400	-0.35808000	-2.44322500	
O	1.86734600	-2.53158800	-2.67971900	
<b>Zn (5.7 / 14.5)</b>				
				
O 1				Zero-point correction= 1.033733 (Hartree/Particle)
C	-19.29599000	-2.15420200	-0.75942200	Thermal correction to Energy= 1.109516
N	-20.22478800	-1.22766200	-0.98282300	Thermal correction to Enthalpy= 1.110461
C	-19.76751400	0.01116100	-1.19748600	Thermal correction to Gibbs Free Energy= 0.900560
C	-17.61758700	-0.65140800	-0.96451400	Sum of electronic and zero-point Energies= -5420.069421
N	-17.98413200	-1.91292800	-0.74086300	Sum of electronic and thermal Energies= -5419.993637
N	-18.48218200	0.34440200	-1.19767000	Sum of electronic and thermal Enthalpies= -5419.992693
C	-16.17197800	-0.32922600	-0.95397900	Sum of electronic and thermal Free Energies= -5420.202594
C	-15.73435400	0.98086200	-1.19512100	
C	-15.22685000	-1.33472400	-0.71659100	
C	-14.37948200	1.27736400	-1.19805500	
H	-16.47834600	1.75358500	-1.38754600	
C	-13.87029200	-1.03715400	-0.70406300	
H	-15.57820700	-2.35282200	-0.54910000	
C	-13.43012300	0.27812200	-0.93043400	
H	-14.02214500	2.28811500	-1.39659500	
H	-13.13636600	-1.82923700	-0.54767800	
N	-12.07678200	0.63064000	-0.94268100	
C	-11.28447100	0.12765500	-0.07974100	
H	-11.63946700	-0.53769200	0.72362500	
C	-9.84434100	0.41786700	-0.09133600	
C	-9.30343800	1.24551500	-1.08164200	
C	-9.00420100	-0.14252500	0.89230600	
C	-7.93960800	1.52540200	-1.10998200	
H	-9.99934000	1.65108200	-1.81486700	
C	-7.63901000	0.13859500	0.86299300	
C	-7.10037500	0.96434900	-0.12593500	
H	-6.93799700	-0.26964300	1.59032200	
C	-5.64927300	1.23856600	-0.13813900	
H	-5.26898200	1.82023200	-0.99477200	
N	-4.89222900	0.81604300	0.78728900	
O	-9.58851700	-0.93741400	1.81872600	
O	-7.35027500	2.31826600	-2.03653000	
C	-8.77300600	-1.51494100	2.80634000	
H	-8.00414300	-2.16704800	2.36171800	
H	-8.27563300	-0.74433900	3.41712500	
H	-9.43146100	-2.11351000	3.44506100	
C	-8.15602400	2.86945200	-3.04530000	
H	-7.49375300	3.45674100	-3.69054300	
H	-8.64391000	2.08354600	-3.64457400	
H	-8.93214000	3.52952700	-2.62465300	
C	-3.48446000	1.10439600	0.69673000	
H	-3.22532700	1.72741200	-0.17855600	
C	-2.66320500	-0.19696800	0.63731600	
O	-1.59699200	-0.11773100	-0.08584100	
O	-2.98498500	-1.14431800	1.33568600	
C	-3.06167400	1.83132800	1.99829700	
H	-3.81732300	2.60158600	2.20562300	
H	-3.11612800	1.09612100	2.81595200	
C	-1.72632500	2.50815600	1.96514400	
C	-1.50068500	3.85913600	2.00667000	
N	-0.13766400	4.02320000	1.94893000	
H	-2.19153400	4.69274100	2.07503900	
C	0.43215700	2.81119400	1.86923800	

H	0.36399900	4.90169100	1.93975400
H	1.50687900	2.63048000	1.75761900
N	-0.49967100	1.87241100	1.89128300
Zn	0.01769700	0.09334300	0.97029000
C	19.44176000	1.41893900	-0.80099900
N	20.29832800	0.43637400	-1.06917900
C	19.75034900	-0.75936900	-1.31369100
C	17.65719500	0.04638300	-1.02207800
N	18.11642100	1.27094800	-0.76641000
N	18.44465900	-1.00029300	-1.30114400
C	16.19270800	-0.17326400	-0.99524600
C	15.66010500	-1.44118700	-1.26875700
C	15.32460900	0.88768300	-0.70967900
C	14.28793500	-1.64200700	-1.25597900
H	16.34471800	-2.25735500	-1.49853300
C	13.95076200	0.68535600	-0.68139300
H	15.74916600	1.87294300	-0.51708200
C	13.41563300	-0.58813500	-0.94008800
H	13.85711200	-2.61837000	-1.47919300
H	13.27711500	1.52134100	-0.48684300
N	12.04123400	-0.84672900	-0.93781600
C	11.29839900	-0.31761700	-0.04699800
H	11.70933000	0.29937000	0.76822600
C	9.84240700	-0.51432100	-0.03985100
C	9.23317400	-1.27808200	-1.04177600
C	9.05666100	0.06921100	0.97480300
C	7.85432800	-1.47261400	-1.05060900
H	9.88891800	-1.70525700	-1.79931200
C	7.67639000	-0.12714000	0.96548200
C	7.06989200	-0.89038700	-0.03431100
H	7.01559500	0.30331200	1.71721300
C	5.60498500	-1.07659400	-0.02347700
H	5.17118000	-1.59444600	-0.89548500
N	4.89623700	-0.65257900	0.93884800
O	9.70554700	0.80113200	1.90993400
O	7.20005000	-2.20117800	-1.98619300
C	8.94456200	1.40185400	2.92702000
H	8.20942300	2.11071300	2.51338600
H	8.41173800	0.64744900	3.52806000
H	9.64971600	1.94247500	3.56751500
C	7.95020600	-2.76412800	-3.03075900
H	7.24056900	-3.28806300	-3.68016400
H	8.47217500	-1.98824700	-3.61414600
H	8.69363900	-3.48342700	-2.65003600
C	3.46981700	-0.84471700	0.86975100
H	3.16124500	-1.44661500	-0.00447500
C	2.75445400	0.52413900	0.79562800
O	1.68115400	0.52936900	0.07684300
O	3.17596700	1.45679300	1.45548000
C	3.02626200	-1.54258100	2.18022800
H	3.79770300	-2.28147000	2.43665500
H	3.03640000	-0.78519600	2.98023200
C	1.71563500	-2.26555600	2.13747400
C	1.50642900	-3.59971200	2.37404100
N	0.15392900	-3.80872000	2.23600000
H	2.20129000	-4.39367900	2.62649800
C	-0.42731900	-2.63987500	1.92223500
H	-0.33227400	-4.69014100	2.33995000
H	-1.49314400	-2.48191500	1.72387600
N	0.48897600	-1.68810500	1.86425600
C	20.68443900	-1.88995400	-1.62186500
H	21.39581000	-2.01413000	-0.79395400
H	20.12372200	-2.81600000	-1.78202200
H	21.27183000	-1.64461500	-2.51761000
C	19.98904500	2.78599000	-0.52135900
H	19.61238800	3.49201000	-1.27473000
H	19.62984800	3.13406900	0.45663900
H	21.08309100	2.76768800	-0.53997500
C	-19.73991900	-3.56420900	-0.51176600
H	-19.29548700	-4.22702400	-1.26708500
H	-19.37275600	-3.89839900	0.46839500
H	-20.83167100	-3.63010200	-0.54835600
C	-20.78489000	1.08097800	-1.45463100
H	-20.29421500	2.04889700	-1.59598800
H	-21.37096400	0.82081800	-2.34703500

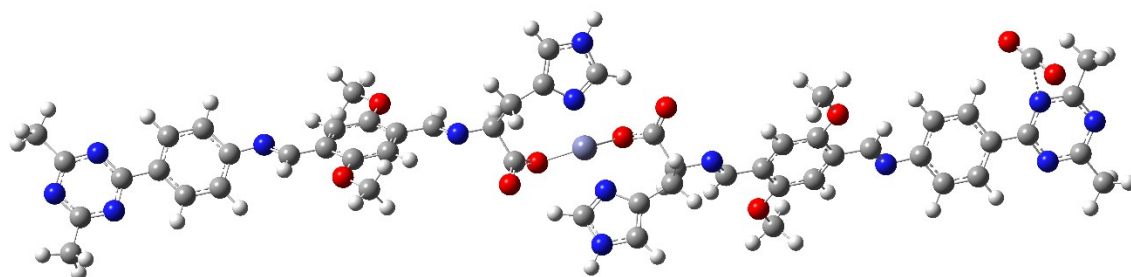
H	-21.48685600	1.12979500	-0.61094600	
C	-0.22310100	1.65436900	-1.76987200	
O	0.03210700	0.82146800	-2.52580900	
O	-0.48369300	2.52200400	-1.04481000	
<b>N32 (0.0 / 0.0)</b>				
				
0 1				Zero-point correction= 1.034040 (Hartree/Particle)
C	-19.72827900	-1.68950300	-0.27575600	Thermal correction to Energy= 1.110526
N	-20.61358300	-0.72381400	-0.50967300	Thermal correction to Enthalpy= 1.111470
C	-20.09871200	0.47395600	-0.80988400	Thermal correction to Gibbs Free Energy= 0.898213
C	-17.98035200	-0.29829300	-0.63166600	Sum of electronic and zero-point Energies= -5420.072300
N	-18.40553000	-1.52347700	-0.32525300	Sum of electronic and thermal Energies= -5419.995815
N	-18.79826800	0.73219400	-0.88193200	Sum of electronic and thermal Enthalpies= -5419.994871
C	-16.52024600	-0.05885300	-0.69868700	Sum of electronic and thermal Free Energies= -5420.208127
C	-16.02354600	1.21066700	-1.02659700	
C	-15.62126000	-1.10277100	-0.44803400	
C	-14.65612400	1.42990600	-1.10088600	
H	-16.73253800	2.01326100	-1.22859500	
C	-14.25128500	-0.88179800	-0.50731000	
H	-16.01924100	-2.08980400	-0.21258900	
C	-13.75118600	0.39373800	-0.82018000	
H	-14.25369900	2.40766100	-1.36689200	
H	-13.55519800	-1.70510900	-0.33961100	
N	-12.38304100	0.67108100	-0.90545400	
C	-11.57996700	0.16619800	-0.05367100	
H	-11.93186400	-0.44387100	0.79374200	
C	-10.12936000	0.38374600	-0.13725300	
C	-9.59354000	1.14422600	-1.18270000	
C	-9.27490000	-0.17577700	0.83445500	
C	-8.22099900	1.35943700	-1.27674900	
H	-10.30054900	1.55233300	-1.90376200	
C	-7.90093400	0.04107800	0.73968200	
C	-7.36772600	0.80146000	-0.30314700	
H	-7.18922500	-0.36981500	1.45501800	
C	-5.90810100	1.01184100	-0.38164000	
H	-5.53678600	1.53145600	-1.28104800	
N	-5.13511100	0.60684400	0.53835700	
O	-9.85506400	-0.90577100	1.81522900	
O	-7.63578000	2.08664100	-2.25821400	
C	-9.02558100	-1.48313600	2.79134200	
H	-8.30548500	-2.18577500	2.34211000	
H	-8.46964700	-0.71402400	3.35144100	
H	-9.68282400	-2.02672000	3.47860700	
C	-8.45691000	2.63110200	-3.25820100	
H	-7.79636500	3.16072800	-3.95321100	
H	-9.00205500	1.84372200	-3.80378300	
H	-9.18623700	3.34225000	-2.83703700	
C	-3.71962400	0.82565600	0.38261200	
H	-3.47561800	1.42426800	-0.51402800	
C	-2.97634600	-0.52554300	0.28250300	
O	-1.94170700	-0.51018500	-0.48596500	
O	-3.34367200	-1.46323700	0.96973700	
C	-3.21258100	1.54656000	1.65638200	
H	-3.97019900	2.29075900	1.93787700	
H	-3.18383300	0.80194700	2.46778600	
C	-1.90438000	2.26631900	1.53920600	
C	-1.68524500	3.60378600	1.74771000	
N	-0.34029200	3.80959500	1.54796700	
H	-2.36828400	4.40174900	2.01924500	
C	0.22593300	2.63544200	1.22478400	
H	0.15150200	4.69107900	1.62059600	
H	1.28649900	2.48364400	0.99349800	
N	-0.69175300	1.68328800	1.22019500	

Zn	-0.23159200	-0.11345900	0.31496900
C	19.26546600	1.61777400	-0.11030000
N	20.16591800	0.73132700	-0.55012800
C	19.66716400	-0.39187200	-1.06061200
C	17.53837800	0.27657000	-0.68812500
N	17.95123800	1.43523300	-0.15820600
N	18.36373200	-0.66207300	-1.14979300
C	16.08042800	0.02643200	-0.76294400
C	15.59428400	-1.16511900	-1.31997000
C	15.17313900	0.98276700	-0.29131000
C	14.22908700	-1.39386800	-1.40249700
H	16.31017900	-1.89790100	-1.69190600
C	13.80545200	0.74907900	-0.35881800
H	15.56179000	1.91322100	0.12230700
C	13.31668000	-0.45072100	-0.90274200
H	13.83453000	-2.30904800	-1.84464100
H	13.10149300	1.50929600	-0.01674800
N	11.95069600	-0.73219600	-1.00772500
C	11.16579400	-0.42402300	-0.05169800
H	11.53337300	0.00837300	0.89277500
C	9.71563900	-0.64310200	-0.14267800
C	9.15846900	-1.17614200	-1.31000300
C	8.88376400	-0.31600300	0.94794700
C	7.78535200	-1.38583700	-1.41486300
H	9.84873800	-1.41056800	-2.11928500
C	7.51012100	-0.53165500	0.84337600
C	6.95304200	-1.05299600	-0.32731400
H	6.82603800	-0.30481200	1.66074700
C	5.49310900	-1.24798400	-0.42255800
H	5.12687100	-1.78731300	-1.31187100
N	4.71277700	-0.80354400	0.47343100
O	9.48124400	0.19445500	2.04752400
O	7.18040900	-1.89368300	-2.51411100
C	8.67040500	0.52774200	3.14872900
H	7.90287000	1.26930600	2.87718700
H	8.16951100	-0.36471100	3.55801100
H	9.33622000	0.94868200	3.90966300
C	7.97929800	-2.20856900	-3.62494900
H	7.30425500	-2.58877400	-4.39920500
H	8.50455800	-1.31809700	-4.00651700
H	8.72350900	-2.98360800	-3.37892400
C	3.29745400	-1.03468500	0.33099500
H	3.05466400	-1.68631200	-0.52777900
C	2.54119500	0.29946900	0.15630300
O	1.46855900	0.21918900	-0.54352600
O	2.93843000	1.29737600	0.74202500
C	2.80190200	-1.68339600	1.64918300
H	3.56846600	-2.40446100	1.96437000
H	2.77980600	-0.89317000	2.41665300
C	1.49778100	-2.41794900	1.59588600
C	1.29892900	-3.74848000	1.86188500
N	-0.05052100	-3.97177300	1.71959200
H	1.99831400	-4.53009600	2.13943900
C	-0.63913900	-2.81451600	1.37480700
H	-0.53135000	-4.85345000	1.84410500
H	-1.70936800	-2.67533300	1.18045600
N	0.26941300	-1.85670600	1.30086100
C	20.62124200	-1.42925900	-1.57048300
H	20.47502900	-2.36637400	-1.01550300
H	20.40415100	-1.64132900	-2.62637000
H	21.65336500	-1.08320300	-1.45833700
C	19.79042300	2.89666000	0.46812900
H	20.36397800	3.43559200	-0.29897800
H	18.96596300	3.52071000	0.82656600
H	20.48369800	2.67094700	1.28974500
C	-20.23782400	-3.05734700	0.06466000
H	-19.87753600	-3.77904600	-0.68160600
H	-19.83385800	-3.36893100	1.03765700
H	-21.33185900	-3.05881600	0.09100600
C	-21.06588400	1.58666600	-1.07844700
H	-20.52937400	2.50781800	-1.32594100
H	-21.73249800	1.30160300	-1.90390200
H	-21.69776100	1.74350900	-0.19323000
C	5.48650300	1.93077900	0.89848900
O	5.53004800	1.88580400	2.05655300

O	5.52922200	2.02932800	-0.25205500	
<b>N19 (19.2 / 13.8)</b>				
				
0 1				Zero-point correction= 1.033841 (Hartree/Particle)
C	-19.83751100	-1.73417300	-0.80895000	Thermal correction to Energy= 1.110604
N	-20.72656100	-0.77366000	-1.04993800	Thermal correction to Enthalpy= 1.111548
C	-20.21807300	0.44296500	-1.27613300	Thermal correction to Gibbs Free Energy= 0.896203
C	-18.09832800	-0.30294700	-1.01943900	Sum of electronic and zero-point Energies= -5420.065225
N	-18.51708300	-1.54590000	-0.78379400	Sum of electronic and thermal Energies= -5419.988462
N	-18.92039500	0.72401300	-1.27072100	Sum of electronic and thermal Enthalpies= -5419.987518
C	-16.64118500	-0.03839900	-1.00126800	Sum of electronic and thermal Free Energies= -5420.202862
C	-16.15078900	1.25139300	-1.25024700	
C	-15.73787300	-1.07801900	-0.74825400	
C	-14.78544200	1.49459800	-1.24465400	
H	-16.86257200	2.05078600	-1.45511500	
C	-14.37077300	-0.83373300	-0.72787300	
H	-16.12986600	-2.08017400	-0.57476300	
C	-13.87779100	0.46156200	-0.96107500	
H	-14.38719100	2.48884600	-1.44860900	
H	-13.66990600	-1.65276800	-0.55918600	
N	-12.51224800	0.76363900	-0.96411300	
C	-11.74409900	0.23283200	-0.09595800	
H	-12.12720100	-0.42074600	0.70413100	
C	-10.29527100	0.47587700	-0.09538000	
C	-9.72108500	1.29546100	-1.07368900	
C	-9.48061500	-0.11926100	0.88926200	
C	-8.34938100	1.53471100	-1.08782800	
H	-10.39809500	1.72893200	-1.80861100	
C	-8.10741200	0.12114200	0.87406000	
C	-7.53592200	0.94036800	-0.10173200	
H	-7.42505500	-0.31568400	1.60251000	
C	-6.07745700	1.17292200	-0.09740100	
H	-5.67116900	1.74663200	-0.94740100	
N	-5.34384000	0.72534600	0.83501300	
O	-10.09614900	-0.90565300	1.80262800	
O	-7.72861200	2.31839600	-2.00165400	
C	-9.30615500	-1.51824200	2.78995500	
H	-8.55348600	-2.18801700	2.34397000	
H	-8.79105200	-0.76963300	3.41328400	
H	-9.98728300	-2.10388700	3.41675400	
C	-8.50812200	2.89838900	-3.01480000	
H	-7.82295100	3.47029100	-3.64987700	
H	-9.01226600	2.13029400	-3.62365300	
H	-9.26932100	3.57789600	-2.59779400	
C	-3.92509100	0.96618700	0.76045000	
H	-3.64699500	1.62248500	-0.08433700	
C	-3.16555200	-0.37153400	0.60884600	
O	-2.11768700	-0.31242000	-0.13845100	
O	-3.53816400	-1.34359800	1.24397400	
C	-3.48472700	1.60475300	2.09981200	
H	-4.25799500	2.32823600	2.39274900	
H	-3.49136900	0.80785800	2.86042600	
C	-2.17516300	2.33161300	2.09116100	
C	-1.96838900	3.64491200	2.42701000	
N	-0.61812800	3.86869400	2.29253700	
H	-2.66341800	4.41468100	2.74545000	
C	-0.03707300	2.72903300	1.88308900	
H	-0.13220100	4.74014000	2.46095000	
H	1.03190500	2.59836400	1.67607800	
N	-0.95058100	1.78049300	1.76079400	
Zn	-0.42787600	0.07502500	0.71197200	
C	18.81193800	2.39698800	-1.06751300	
N	19.78431300	1.50336700	-0.90357200	

C	19.38542300	0.23980400	-0.71893100
C	17.20416800	0.81865100	-0.86608500
N	17.51104900	2.10124000	-1.05620300
N	18.11537100	-0.14705100	-0.69277900
C	15.77310300	0.43639800	-0.84291300
C	15.39807300	-0.90035600	-0.64816100
C	14.78025100	1.40630000	-1.02198100
C	14.05879400	-1.26194000	-0.63756300
H	16.17927500	-1.64722400	-0.50838700
C	13.43767500	1.04974900	-0.99895100
H	15.08204700	2.44105500	-1.18390200
C	13.06051200	-0.28816600	-0.79859000
H	13.76329100	-2.29822700	-0.47474100
H	12.66460500	1.80174900	-1.16503100
N	11.71305900	-0.67721600	-0.79392700
C	10.88434100	-0.00745400	-0.09183600
H	11.21910600	0.80147900	0.57748700
C	9.43933900	-0.26903400	-0.11655800
C	8.86792000	-1.00192500	-1.16345600
C	8.62096200	0.25044800	0.90733900
C	7.49405700	-1.23779300	-1.20096300
H	9.53414800	-1.36369700	-1.94549100
C	7.24851900	0.01105800	0.87039900
C	6.67991500	-0.72713900	-0.16985200
H	6.56444900	0.38646900	1.63086500
C	5.22053600	-0.95497700	-0.18983900
H	4.81505700	-1.45088400	-1.08776300
N	4.48660600	-0.58847000	0.77693500
O	9.23660100	0.95853400	1.88168500
O	6.87478000	-1.93248900	-2.18220100
C	8.44310600	1.51302200	2.90058700
H	7.69763200	2.21443100	2.49270600
H	7.91946600	0.72937800	3.47127200
H	9.12359900	2.05264900	3.56794100
C	7.65255800	-2.39980000	-3.25710100
H	6.96861800	-2.92636000	-3.93136400
H	8.12464500	-1.56425800	-3.79961600
H	8.43944500	-3.09005500	-2.91645700
C	3.06736700	-0.81806400	0.68000300
H	2.78810900	-1.38898100	-0.22428900
C	2.31074200	0.52990200	0.65893300
O	1.26375100	0.54631400	-0.09151400
O	2.68501200	1.43457700	1.38600000
C	2.62585800	-1.58281000	1.95122800
H	3.39884200	-2.33113200	2.17414800
H	2.63096100	-0.86323700	2.78535800
C	1.31659300	-2.30553700	1.86943500
C	1.10901100	-3.64505000	2.07645100
N	-0.24074100	-3.85457300	1.91649300
H	1.80306600	-4.44204500	2.32159000
C	-0.82063700	-2.68072600	1.61677300
H	-0.72697800	-4.73823100	1.99807100
H	-1.88903200	-2.53021000	1.42028800
N	0.09313100	-1.72495300	1.58951200
C	20.45337700	-0.79465800	-0.53218400
H	21.08342900	-0.52033300	0.32499600
H	20.00651800	-1.78093700	-0.37353600
H	21.10378900	-0.81255900	-1.41771500
C	19.18970900	3.83144000	-1.28193800
H	18.81056200	4.16833700	-2.25686300
H	18.71203200	4.45666200	-0.51528400
H	20.27718300	3.94729100	-1.24226900
C	-20.33969700	-3.12247600	-0.55012100
H	-19.94147900	-3.80434900	-1.31447800
H	-19.96788900	-3.47355300	0.42214700
H	-21.43380300	-3.13922000	-0.56655400
C	-21.18952400	1.54960400	-1.55421700
H	-20.65956500	2.49633200	-1.69727800
H	-21.77411300	1.30518600	-2.45208300
H	-21.89953200	1.63276800	-0.72006300
C	11.20169000	-3.51176300	-1.01057700
O	11.65086000	-3.58419800	0.05174700
O	10.75088700	-3.49633600	-2.07698500

# N6 (20.4/19.7)

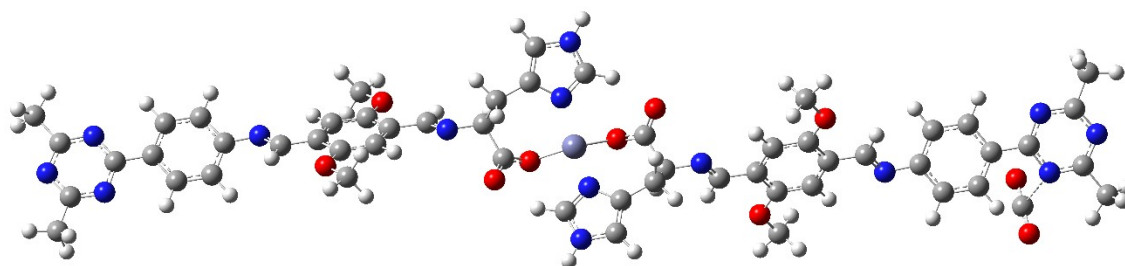


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C	-20.04665700	-1.85839000	-0.35930700
N	-20.93206000	-0.99359700	-0.84845900
C	-20.41913500	0.11881300	-1.38639000
C	-18.30237200	-0.53809500	-0.93540400
N	-18.72573000	-1.67338300	-0.38064900
N	-19.12055300	0.38803100	-1.45154900
C	-16.84431500	-0.28267500	-0.98413700
C	-16.34822400	0.89124200	-1.56885800
C	-15.94579000	-1.21912000	-0.45845400
C	-14.98188000	1.12222200	-1.62552500
H	-17.05638100	1.60869800	-1.98289800
C	-14.57778100	-0.98279500	-0.50034400
H	-16.34228300	-2.13648400	-0.02338700
C	-14.07908500	0.20007300	-1.07230000
H	-14.57934600	2.02358300	-2.08838000
H	-13.88019600	-1.72833700	-0.11557400
N	-12.71186100	0.48267500	-1.15334800
C	-11.94985900	0.20989900	-0.16827000
H	-12.34025300	-0.19145500	0.78076100
C	-10.49878000	0.43088800	-0.22978700
C	-9.91373300	0.92655800	-1.40049600
C	-9.69276600	0.13803500	0.88911200
C	-8.53923300	1.13613000	-1.47684200
H	-10.58456600	1.13571300	-2.23272800
C	-8.31676800	0.34877200	0.81153800
C	-7.73421200	0.84300700	-0.35729900
H	-7.64065500	0.13421000	1.63851800
C	-6.27243400	1.04589900	-0.41508400
H	-5.85660500	1.33130500	-1.39611900
N	-5.54664300	0.88780600	0.61260600
O	-10.31882000	-0.34365000	1.98797200
O	-7.90770000	1.61511600	-2.57519700
C	-9.53725300	-0.65553800	3.11316800
H	-8.79194600	-1.43332500	2.88168100
H	-9.01413400	0.23482100	3.49769900
H	-10.22599000	-1.02899100	3.87865300
C	-8.67869700	1.88682400	-3.71632500
H	-7.98596800	2.24478800	-4.48564000
H	-9.19023200	0.98120000	-4.08105700
H	-9.43304600	2.66527900	-3.51630700
C	-4.12394800	1.07086400	0.47653600
H	-3.83301600	1.42283300	-0.53005400
C	-3.38867500	-0.25919900	0.76003500
O	-2.34706800	-0.46451600	0.03009900
O	-3.77244900	-0.96789900	1.67530200
C	-3.67374800	2.09150600	1.54927900
H	-4.43431000	2.88308200	1.59573700
H	-3.69327500	1.57473800	2.52196900
C	-2.35184800	2.75653900	1.31696800
C	-2.12031200	4.10528300	1.23008000
N	-0.76732700	4.25161100	1.03118300
H	-2.79986400	4.94845800	1.29540200
C	-0.20881400	3.03067800	0.99294600
H	-0.26550500	5.12329100	0.92042300
H	0.85627000	2.82303700	0.83428000
N	-1.13927900	2.10782000	1.17116300
Zn	-0.64686400	0.15180600	0.70705700
C	18.79396800	0.95033500	-1.31828700
N	19.63838900	-0.07204200	-1.43708200

Zero-point correction=	1.034000 (Hartree/Particle)
Thermal correction to Energy=	1.110543
Thermal correction to Enthalpy=	1.111487
Thermal correction to Gibbs Free Energy=	0.897931
Sum of electronic and zero-point Energies=	-5420.064546
Sum of electronic and thermal Energies=	-5419.988003
Sum of electronic and thermal Enthalpies=	-5419.987059
Sum of electronic and thermal Free Energies=	-5420.200615

C	19.08247500	-1.28669600	-1.42860100
C	16.99873700	-0.42821500	-1.22522900
N	17.47152700	0.82122200	-1.20793700
N	17.77575500	-1.51095200	-1.32808900
C	15.53526300	-0.62756600	-1.12585600
C	15.00590800	-1.92226800	-1.02117700
C	14.66365100	0.46868300	-1.15688100
C	13.63536200	-2.11449500	-0.93835600
H	15.69243100	-2.76856900	-1.01381800
C	13.29057700	0.27816800	-1.06224800
H	15.07383300	1.47239500	-1.26987800
C	12.75975500	-1.01650200	-0.93431800
H	13.20806400	-3.11489400	-0.86565600
H	12.61508200	1.13307300	-1.11902000
N	11.38710900	-1.26710800	-0.84758500
C	10.64703000	-0.50470900	-0.14276600
H	11.06036300	0.32250200	0.45648300
C	9.19222900	-0.69392300	-0.06949400
C	8.57998500	-1.71438600	-0.80605200
C	8.41035800	0.15458900	0.74049100
C	7.20201200	-1.90584100	-0.74931700
H	9.23287300	-2.33966700	-1.41361600
C	7.03073100	-0.03898000	0.79736000
C	6.42126900	-1.05803900	0.06266700
H	6.37276500	0.58703900	1.39928300
C	4.95719900	-1.23745900	0.13728900
H	4.52121300	-1.98823400	-0.54311000
N	4.25159700	-0.55459200	0.93965700
O	9.06219900	1.12478300	1.42223000
O	6.54485100	-2.87342100	-1.43229600
C	8.30557200	1.99118000	2.22932500
H	7.56538700	2.55023300	1.63473000
H	7.77929600	1.44045000	3.02554500
H	9.01294700	2.69414100	2.68234800
C	7.29104800	-3.71236500	-2.27480100
H	6.57967300	-4.40278300	-2.74078700
H	7.80692600	-3.13700800	-3.06071700
H	8.03920100	-4.29001900	-1.70765300
C	2.82630900	-0.76662700	0.94101800
H	2.51702300	-1.58811100	0.26923100
C	2.09544200	0.52340700	0.50298300
O	1.04177100	0.32836000	-0.21242200
O	2.49373600	1.60121900	0.91126200
C	2.39626500	-1.07684100	2.39514400
H	3.16092000	-1.73091800	2.83630700
H	2.42698800	-0.12911300	2.95588700
C	1.07450600	-1.76135200	2.56123100
C	0.84722200	-2.95629900	3.19418900
N	-0.50735500	-3.18137900	3.11660600
H	1.53067800	-3.64307400	3.68228400
C	-1.07093700	-2.15870900	2.45286200
H	-1.00704100	-3.98116400	3.48346200
H	-2.13857600	-2.06084600	2.22198400
N	-0.14196700	-1.28112300	2.11205900
C	20.00071400	-2.46381600	-1.55492800
H	20.81465600	-2.37792600	-0.82330500
H	19.44771200	-3.39709600	-1.41051000
H	20.46070300	-2.45828400	-2.55366900
C	19.37153300	2.33287900	-1.27713200
H	18.61761100	3.07089400	-1.57677700
H	19.69371300	2.55077400	-0.24728900
H	20.25408300	2.39146600	-1.92455400
C	-20.55388700	-3.12711900	0.25679300
H	-20.14479300	-3.98875800	-0.28891400
H	-20.19696800	-3.20129000	1.29317500
H	-21.64767200	-3.15069100	0.23049500
C	-21.38620400	1.11470700	-1.95090100
H	-20.85365400	1.99406300	-2.32606000
H	-21.95894700	0.64665500	-2.76375800
H	-22.10715600	1.40703600	-1.17539400
C	16.77408500	2.82860300	0.66999600
O	17.50858800	2.29767700	1.38888600
O	16.03933300	3.39678300	-0.01965100

# N8 (21.0/18.9)

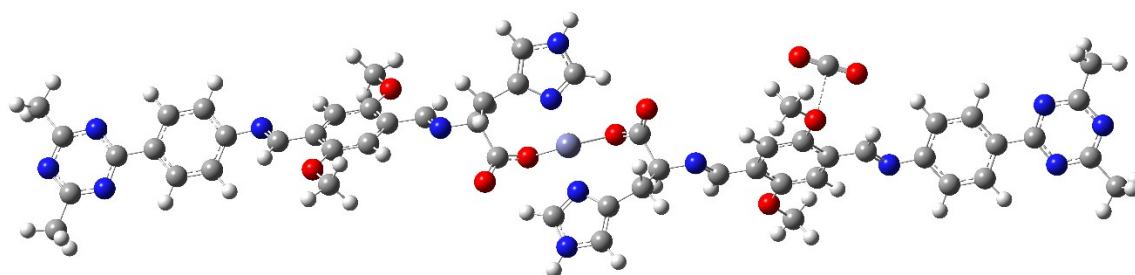


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C	-20.05479300	-2.06957700	0.05111400
N	-20.93931200	-1.37036600	-0.65586800
C	-20.42606200	-0.43781900	-1.46628900
C	-18.31066200	-0.93969600	-0.84267100
N	-18.73437600	-1.88947700	-0.00949200
N	-19.12796700	-0.18849500	-1.59187000
C	-16.85329300	-0.69719800	-0.94698100
C	-16.35751600	0.28369700	-1.81762500
C	-15.95507900	-1.45530600	-0.18590800
C	-14.99184700	0.50100500	-1.92289500
H	-17.06531300	0.86136900	-2.41172100
C	-14.58780500	-1.22903300	-0.27851500
H	-16.35110100	-2.22778300	0.47326000
C	-14.08968100	-0.23564800	-1.13874600
H	-14.58930800	1.25093100	-2.60427700
H	-13.89035300	-1.84158100	0.29493900
N	-12.72359100	0.02751400	-1.28123400
C	-11.96798700	0.02811000	-0.25435300
H	-12.36299500	-0.11703300	0.76400500
C	-10.51880900	0.24393700	-0.36248400
C	-9.92955000	0.43120200	-1.61796700
C	-9.71936100	0.26082500	0.79854000
C	-8.55765600	0.63724400	-1.73782900
H	-10.59531000	0.40927500	-2.47972700
C	-8.34608800	0.46863200	0.67732100
C	-7.75962100	0.65679600	-0.57589300
H	-7.67521000	0.48668400	1.53564600
C	-6.30161500	0.87075900	-0.67488100
H	-5.88035200	0.90643700	-1.69374800
N	-5.58510000	0.99857200	0.36345200
O	-10.34901000	0.06668100	1.98059400
O	-7.92261600	0.82863800	-2.91884000
C	-9.57474300	0.07096500	3.15306700
H	-8.81453600	-0.72641400	3.13555000
H	-9.07023400	1.03996900	3.29720400
H	-10.26563300	-0.10440800	3.98475800
C	-8.68640700	0.78504200	-4.09577500
H	-7.99149500	0.94444700	-4.92737400
H	-9.18130300	-0.19218200	-4.21800800
H	-9.45380300	1.57626900	-4.10709200
C	-4.16596700	1.18106000	0.19395700
H	-3.87052800	1.26999900	-0.86747300
C	-3.39787200	-0.00689400	0.81703300
O	-2.33382000	-0.35333400	0.17846900
O	-3.78071800	-0.47354700	1.87664500
C	-3.75998000	2.45797400	0.96920800
H	-4.54442900	3.20960300	0.80535100
H	-3.77750300	2.20963100	2.04233000
C	-2.45562600	3.08327300	0.58074500
C	-2.26440300	4.36831000	0.14214300
N	-0.91323800	4.50348700	-0.07601200
H	-2.97063300	5.17496700	-0.02383400
C	-0.31665300	3.33592100	0.21559700
H	-0.43669900	5.33184500	-0.40864900
H	0.75703700	3.13070700	0.12824300
N	-1.22124000	2.46144700	0.62318800
Zn	-0.66527100	0.46925500	0.69531300
C	18.76817600	1.53322700	-1.15858500
N	19.65728300	0.55510500	-0.99775900
C	19.14967000	-0.64893600	-0.71620100
C	17.02841700	0.14487900	-0.75890000

Zero-point correction=	1.033609 (Hartree/Particle)
Thermal correction to Energy=	1.110381
Thermal correction to Enthalpy=	1.11326
Thermal correction to Gibbs Free Energy=	0.895731
Sum of electronic and zero-point Energies=	-5420.064567
Sum of electronic and thermal Energies=	-5419.987794
Sum of electronic and thermal Enthalpies=	-5419.986850
Sum of electronic and thermal Free Energies=	-5420.202445

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N	17.85089000	-0.89878500	-0.58975300
C	15.57370800	-0.09163400	-0.62039300
C	15.09248700	-1.33207200	-0.17521700
C	14.66193400	0.91958600	-0.94455800
C	13.72824700	-1.55700000	-0.06728200
H	15.80588300	-2.11456300	0.08746300
C	13.29529200	0.70071900	-0.82540500
H	15.04660700	1.87533300	-1.30047300
C	12.81116100	-0.53798500	-0.37196100
H	13.33896500	-2.51853100	0.26835700
H	12.58804300	1.48047200	-1.11216200
N	11.44721000	-0.81743100	-0.24572700
C	10.66019900	0.06788800	0.22602800
H	11.02611500	1.03849200	0.59793200
C	9.21210600	-0.15842000	0.32237500
C	8.65761000	-1.35836200	-0.13746800
C	8.37841700	0.83473800	0.87544300
C	7.28667700	-1.58759600	-0.05507500
H	9.34877500	-2.08975600	-0.55421700
C	7.00598800	0.60343100	0.95843500
C	6.45413200	-0.59447000	0.50002600
H	6.30952700	1.33381300	1.36900400
C	4.99595800	-0.80985500	0.59433900
H	4.60517800	-1.72678500	0.12186100
N	4.24586300	0.02589500	1.18316000
O	8.97555400	1.97405500	1.29557600
O	6.68400600	-2.72462100	-0.47730000
C	8.16628700	2.98390700	1.84317700
H	7.42071900	3.34048600	1.11451000
H	7.64122800	2.63184100	2.74571500
H	8.83471700	3.80892600	2.11207600
C	7.48269100	-3.71846400	-1.06468600
H	6.80997000	-4.53488600	-1.34881900
H	7.99687100	-3.34161800	-1.96380900
H	8.23693300	-4.09915200	-0.35670700
C	2.82899500	-0.23441300	1.21425200
H	2.56523400	-1.21395500	0.77528700
C	2.06922500	0.86761700	0.44055600
O	1.03896300	0.45337200	-0.21284700
O	2.42512900	2.02833900	0.55479400
C	2.36989600	-0.17114700	2.69103600
H	3.14300300	-0.65847600	3.30094900
H	2.35563700	0.89038000	2.98517900
C	1.06652500	-0.83750100	3.00774400
C	0.86113500	-1.83613400	3.92465400
N	-0.48357100	-2.12221300	3.88740000
H	1.55350800	-2.34836900	4.58438400
C	-1.06245400	-1.32629000	2.97337700
H	-0.96704600	-2.81737400	4.44141000
H	-2.12683100	-1.32987400	2.70909400
N	-0.15312600	-0.53340000	2.43135900
C	20.11172700	-1.78169500	-0.52436100
H	20.63751800	-1.64824600	0.43271700
H	19.57900700	-2.73870300	-0.51064500
H	20.87084300	-1.76379000	-1.31657700
C	19.27060600	2.90432700	-1.49438400
H	18.90152500	3.19354300	-2.48866000
H	18.86917400	3.63130300	-0.77575600
H	20.36477200	2.92048400	-1.48520500
C	-20.56237300	-3.13407000	0.97617400
H	-20.17010400	-4.11085200	0.65989700
H	-20.18859200	-2.94870600	1.99228400
H	-21.65658600	-3.15143500	0.97038700
C	-21.39243300	0.36964400	-2.27859400
H	-20.85754100	1.09814200	-2.89567000
H	-21.98653600	-0.30149500	-2.91414200
H	-22.09460900	0.88359700	-1.60777000
C	16.96443400	-2.96610600	-2.29020100
O	17.20045000	-3.82077900	-1.54601900
O	16.72464000	-2.13870500	-3.06129500

**O88 (15.7/13.0)**

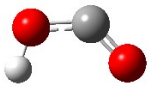
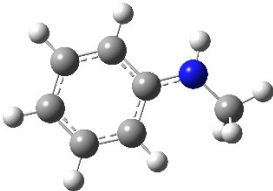
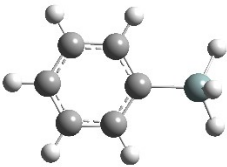


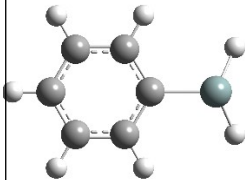
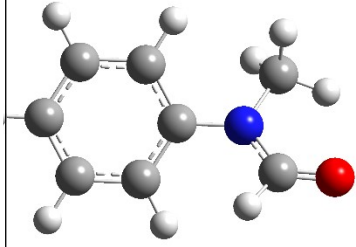
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N	-20.67210000	-0.75351800	-1.05635300
C	-20.14916700	0.45011200	-1.31656000
C	-18.03849400	-0.31310600	-1.03690600
N	-18.47204400	-1.54379000	-0.76617000
N	-18.84825800	0.71587200	-1.31807400
C	-16.57832000	-0.06545700	-1.02541500
C	-16.07245300	1.21004100	-1.31401000
C	-15.68759500	-1.10734100	-0.73936000
C	-14.70430900	1.43699600	-1.31535700
H	-16.77457800	2.01111100	-1.54407600
C	-14.31767600	-0.87877400	-0.72545000
H	-16.09155600	-2.09887200	-0.53501200
C	-13.80919600	0.40251600	-0.99908200
H	-14.29419500	2.41953300	-1.55018800
H	-13.62652600	-1.70025800	-0.53055900
N	-12.44002800	0.68714600	-1.01140800
C	-11.67926900	0.17834000	-0.12380900
H	-12.07135400	-0.44049100	0.69927200
C	-10.22727300	0.40172000	-0.13124300
C	-9.64126200	1.17174100	-1.14226900
C	-9.42149900	-0.16290700	0.87833900
C	-8.26630100	1.39062500	-1.16520800
H	-10.31172400	1.58364100	-1.89537400
C	-8.04503500	0.05753900	0.85461200
C	-7.46169400	0.82673200	-0.15429200
H	-7.36930200	-0.35750700	1.60174900
C	-6.00002100	1.03818700	-0.15863800
H	-5.58424700	1.56292500	-1.03530100
N	-5.27419000	0.62681100	0.79627500
O	-10.04825600	-0.90172400	1.82321600
O	-7.63417400	2.12655000	-2.11044200
C	-9.26698000	-1.48428300	2.83538300
H	-8.52371000	-2.18223300	2.41771200
H	-8.74136800	-0.71797600	3.42765500
H	-9.95629700	-2.03401700	3.48532000
C	-8.40528500	2.67590200	-3.14680000
H	-7.71197000	3.21140300	-3.80438300
H	-8.92060000	1.89099700	-3.72405000
H	-9.15656100	3.38276900	-2.75822600
C	-3.85206000	0.84294200	0.71254400
H	-3.56235500	1.44106300	-0.17067700
C	-3.11114000	-0.51222500	0.64851900
O	-2.06429600	-0.51752000	-0.10250000
O	-3.49560100	-1.43481200	1.34725100
C	-3.40625800	1.55830200	2.01061700
H	-4.17040800	2.30867500	2.25598900
H	-3.42422000	0.81075700	2.81958600
C	-2.08740300	2.26632100	1.95853300
C	-1.86335700	3.59438200	2.21607600
N	-0.51057800	3.79247900	2.06748500
H	-2.54804700	4.39040500	2.48911900
C	0.05521300	2.62337800	1.72549900
H	-0.01316700	4.66596100	2.18390600
H	1.12219800	2.46658400	1.52652600
N	-0.87050700	1.68098800	1.65998300
Zn	-0.36877500	-0.09149200	0.71740000
C	19.05742300	1.44182800	-0.79844000
N	19.93417500	0.47149100	-1.04527700
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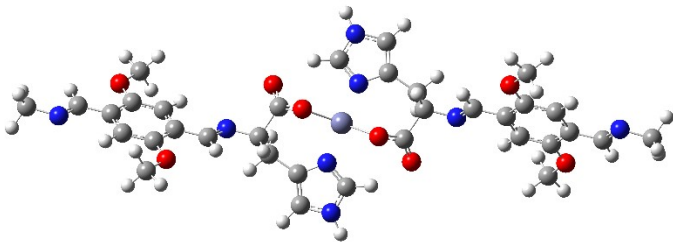
Zero-point correction=	1.033895 (Hartree/Particle)
Thermal correction to Energy=	1.110523
Thermal correction to Enthalpy=	1.111468
Thermal correction to Gibbs Free Energy=	0.897168
Sum of electronic and zero-point Energies=	-5420.066450
Sum of electronic and thermal Energies=	-5419.989822
Sum of electronic and thermal Enthalpies=	-5419.988877
Sum of electronic and thermal Free Energies=	-5420.203176

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N	18.10805000	-0.99848400	-1.28757100
C	15.83830700	-0.20687900	-1.02006700
C	15.33192100	-1.48717400	-1.28624900
C	14.94822700	0.84227200	-0.75833800
C	13.96335100	-1.71207100	-1.28922300
H	16.03390600	-2.29351400	-1.49755800
C	13.57751100	0.61757800	-0.74496000
H	15.35324600	1.83688200	-0.57191000
C	13.07084600	-0.66911400	-0.99610700
H	13.55282400	-2.69835100	-1.50727400
H	12.88130600	1.43983000	-0.57212700
N	11.69891900	-0.94292700	-1.00849500
C	10.94831600	-0.41509500	-0.12479800
H	11.35196300	0.20242400	0.69271200
C	9.49023000	-0.61059600	-0.13689700
C	8.90075900	-1.40515700	-1.12689500
C	8.68261900	-0.01089500	0.84954500
C	7.52484900	-1.61927400	-1.14455000
H	9.57125900	-1.84521900	-1.86381500
C	7.30590100	-0.22601400	0.83346600
C	6.72076900	-1.02580000	-0.15000400
H	6.63208100	0.21867500	1.56516000
C	5.25930000	-1.23941700	-0.14515500
H	4.84170100	-1.78450500	-1.00838300
N	4.53647400	-0.80903300	0.80343100
O	9.30869800	0.77936000	1.76130600
O	6.89172200	-2.38002700	-2.06790300
C	8.54221500	1.28808200	2.82866800
H	7.76182700	1.97441600	2.46553600
H	8.07373000	0.47212900	3.40121400
H	9.23616100	1.83516400	3.47638000
C	7.66168000	-2.96300800	-3.08724700
H	6.96629400	-3.51354100	-3.72995800
H	8.18157100	-2.19741400	-3.68575600
H	8.40861400	-3.66207500	-2.67712800
C	3.11440300	-1.03017900	0.72977700
H	2.82352000	-1.65223500	-0.13629000
C	2.37057200	0.32139700	0.63165700
O	1.32518300	0.30581200	-0.12111600
O	2.75175200	1.26064900	1.30949200
C	2.67344000	-1.71042900	2.04793600
H	3.43710700	-2.45568200	2.30996200
H	2.69617600	-0.94137300	2.83634600
C	1.35288800	-2.41678800	2.01979600
C	1.12721300	-3.73666200	2.31527700
N	-0.22629300	-3.93636000	2.17602800
H	1.81125100	-4.52596300	2.60871200
C	-0.79093800	-2.77626200	1.80267900
H	-0.72485300	-4.80532400	2.31831400
H	-1.85818300	-2.62400600	1.60118200
N	0.13620800	-1.83775200	1.70825300
C	20.36637200	-1.85306900	-1.57044000
H	21.07680200	-1.94964000	-0.73815000
H	19.82410000	-2.79212000	-1.71797800
H	20.95232400	-1.61144800	-2.46823400
C	19.57784800	2.82060000	-0.52465900
H	19.19338200	3.51464600	-1.28510800
H	19.20576400	3.16846800	0.44864000
H	20.67216600	2.82203000	-0.53534100
C	-20.31323800	-3.09135400	-0.48865800
H	-19.91325200	-3.80208800	-1.22519700
H	-19.95567600	-3.41325600	0.49900200
H	-21.40722800	-3.09809500	-0.51606100
C	-21.10723900	1.55958600	-1.62779600
H	-20.56682200	2.49793000	-1.78617700
H	-21.68459900	1.30152200	-2.52661900
H	-21.82514900	1.66705500	-0.80334600
C	9.52757200	2.84222100	-0.05014000
O	8.48631400	3.18025800	0.32088300
O	10.57231300	2.52940600	-0.43651700

**Table S4:** Cartesian coordinates, optimized structures, and the corresponding thermochemistry data of all the reactants, transition states, and product complexes involved in the N-formylation reaction catalysed by the **Zn@His-POP** polymer at the uM06-2X/def2-SVP(GD3) level of theory.

Cartesian coordinates				Thermochemistry data	
<b>HOCO</b>					
					
0 2				Zero-point correction=	0.020994 (Hartree/Particle)
C	0.00000000	0.43650500	0.00000000	Thermal correction to Energy=	0.024171
O	1.13965100	0.18423500	0.00000000	Thermal correction to Enthalpy=	0.025115
O	-1.04390700	-0.35355500	0.00000000	Thermal correction to Gibbs Free Energy=	-0.003410
H	-0.76595600	-1.26447700	0.00000000	Sum of electronic and zero-point Energies=	-188.873382
				Sum of electronic and thermal Energies=	-188.870204
				Sum of electronic and thermal Enthalpies=	-188.869260
				Sum of electronic and thermal Free Energies=	-188.897785
<b>N-methylaniline (NMA)</b>					
					
0 1				Zero-point correction=	0.146411 (Hartree/Particle)
C	2.30735000	-0.34390700	0.02665800	Thermal correction to Energy=	0.153659
C	1.34845600	-1.35233800	-0.00705000	Thermal correction to Enthalpy=	0.154603
C	-0.01319300	-1.05353800	-0.03705100	Thermal correction to Gibbs Free Energy=	0.115120
C	-0.44636600	0.28443300	-0.04209200	Sum of electronic and zero-point Energies=	-326.373519
C	0.52985500	1.30066300	-0.00576000	Sum of electronic and thermal Energies=	-326.366271
C	1.88121400	0.98691500	0.02878800	Sum of electronic and thermal Enthalpies=	-326.365327
H	3.36962200	-0.58685400	0.05283900	Sum of electronic and thermal Free Energies=	-326.404809
H	1.65896500	-2.39892700	-0.00584000		
H	-0.73978400	-1.86522500	-0.05774800		
H	0.20948000	2.34518800	-0.01003800		
H	2.61439500	1.79514700	0.05706500		
N	-1.78360600	0.61502400	-0.10033300		
H	-2.00970100	1.56700700	0.15085200		
C	-2.82034400	-0.36686100	0.06958500		
H	-2.73812200	-0.92336700	1.02214200		
H	-3.79654200	0.13207300	0.04470400		
H	-2.80490200	-1.10241900	-0.75011400		
<b>PhSiH<sub>3</sub></b>					
					
0 1				Zero-point correction=	0.116470 (Hartree/Particle)
C	-2.34782300	-0.00037000	0.01120400	Thermal correction to Energy=	0.123444
C	-1.64865200	-1.20689600	0.00353600	Thermal correction to Enthalpy=	0.124388
C	-0.25454700	-1.20359100	-0.01083400	Thermal correction to Gibbs Free Energy=	0.084504
C	0.46569700	0.00045700	-0.01602800	Sum of electronic and zero-point Energies=	-522.431873
C	-0.25513300	1.20397100	-0.01080100	Sum of electronic and thermal Energies=	-522.424899
C	-1.64942000	1.20641400	0.00349600	Sum of electronic and thermal Enthalpies=	-522.423955
H	-3.43902900	-0.00072900	0.01990600	Sum of electronic and thermal Free Energies=	-522.463839
H	-2.19141700	-2.15353600	0.00550500		
H	0.27835100	-2.15810100	-0.02293300		
H	0.27733900	2.15865100	-0.02284700		
H	-2.19268800	2.15276500	0.00546700		

Si	2.34513900	0.00008000	0.00665900	
H	2.86615700	-0.03117400	1.40086400	
H	2.85526000	-1.20066800	-0.70800400	
H	2.85335200	1.23176300	-0.65461700	
<b>PhSiH<sub>2</sub>* radical</b>				
				
0 2				Zero-point correction= 0.107117 (Hartree/Particle)
C	2.29599400	0.00007300	0.01176500	Thermal correction to Energy= 0.113709
C	1.59638300	-1.20705200	0.00616700	Thermal correction to Enthalpy= 0.114653
C	0.20353100	-1.20607500	-0.00514300	Thermal correction to Gibbs Free Energy= 0.075798
C	-0.51917700	-0.00008400	-0.00565900	Sum of electronic and zero-point Energies= -521.798350
C	0.20340400	1.20599300	-0.00514500	Sum of electronic and thermal Energies= -521.791758
C	1.59625800	1.20712400	0.00616400	Sum of electronic and thermal Enthalpies= -521.790814
H	3.38707900	0.00012700	0.02098000	Sum of electronic and thermal Free Energies= -521.829669
H	2.13938800	-2.15358300	0.01235700	
H	-0.33015200	-2.16009700	-0.00740300	
H	-0.33037900	2.15995900	-0.00740100	
H	2.13915900	2.15371500	0.01235400	
Si	-2.38240000	-0.00000800	-0.08106600	
H	-2.95503900	-1.23054200	0.52759600	
H	-2.95480400	1.23065400	0.52755700	
<b>N-methyl-N-phenylformamide (NMPF)</b>				
				
C	-2.94931600	-0.18826500	0.07268000	Zero-point correction= 0.157188 (Hartree/Particle)
C	-2.34062800	1.04296600	0.30817000	Thermal correction to Energy= 0.165924
C	-0.95478700	1.17076000	0.25511200	Thermal correction to Enthalpy= 0.166868
C	-0.15383600	0.06071500	-0.04463500	Thermal correction to Gibbs Free Energy= 0.123177
C	-0.77067800	-1.17019400	-0.31363400	Sum of electronic and zero-point Energies= -439.578803
C	-2.15545800	-1.29135800	-0.23809400	Sum of electronic and thermal Energies= -439.570067
H	-4.03432400	-0.28518400	0.11874100	Sum of electronic and thermal Enthalpies= -439.569123
H	-2.94856700	1.91761000	0.54439000	Sum of electronic and thermal Free Energies= -439.612814
H	-0.49125700	2.13588100	0.45892900	
H	-0.16811500	-2.02797300	-0.61247800	
H	-2.61819400	-2.25666800	-0.44875000	
N	1.25021200	0.19308100	-0.09848800	
C	1.84972800	1.45549700	-0.49417100	
H	1.84165800	2.18806900	0.32816400	
H	2.89123800	1.25840300	-0.76958800	
H	1.30467800	1.87157100	-1.35130100	
C	2.08342500	-0.81280000	0.33014100	
O	3.28671600	-0.75844400	0.30561800	
H	1.52696800	-1.68965300	0.72294600	
<b>Zn@His-POP</b>				

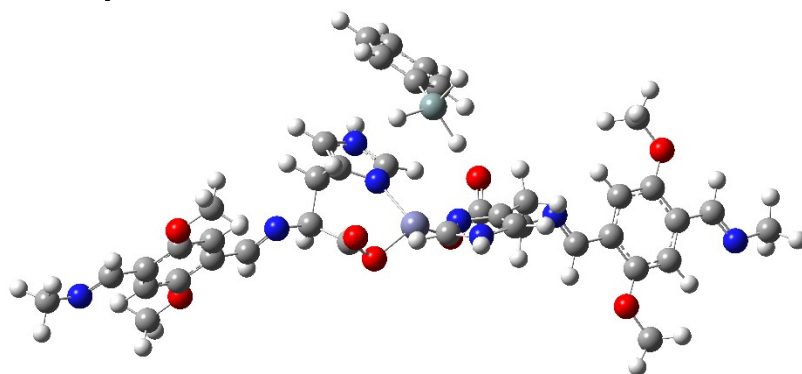


0 1			
N	12.07466400	-0.10798700	1.57720200
C	11.30103700	-0.56356000	0.68223300
H	11.66102000	-1.22467400	-0.12515300
C	9.86081400	-0.24001900	0.65847600
C	9.31526400	0.58510900	1.64573200
C	9.03222400	-0.76236400	-0.35390400
C	7.95787400	0.90092400	1.64351500
H	10.00338200	0.95889600	2.40288700
C	7.67485900	-0.44552900	-0.35708800
C	7.13028300	0.37952400	0.63010000
H	6.98351700	-0.82416500	-1.10930600
C	5.68831300	0.69424100	0.60754600
H	5.30071000	1.26788300	1.46652700
N	4.94435700	0.31620200	-0.34767600
O	9.62050800	-1.55967100	-1.27918700
O	7.36696200	1.69599000	2.56894600
C	8.81244700	-2.10794600	-2.28771500
H	8.01687200	-2.74328700	-1.86587900
H	8.34737200	-1.32099400	-2.90360800
H	9.46812900	-2.71907600	-2.91770700
C	8.16145900	2.20616500	3.60672500
H	7.49988200	2.80134000	4.24569500
H	8.61181400	1.39680700	4.20434600
H	8.96714000	2.85055600	3.21831800
C	3.54238700	0.64353200	-0.28592300
H	3.29017700	1.27539700	0.58537800
C	2.69481400	-0.64688400	-0.21335700
O	1.65059600	-0.56438700	0.53755900
O	3.00299800	-1.60194300	-0.90639400
C	3.16941400	1.37367200	-1.59861500
H	3.99434800	2.05604300	-1.84564700
H	3.13416900	0.61533400	-2.39688500
C	1.91179800	2.18658600	-1.56879400
C	1.79605900	3.52268300	-1.85454800
N	0.46329700	3.83242900	-1.71418300
H	2.54324600	4.25514100	-2.14123600
C	-0.19537300	2.72015000	-1.34921300
H	0.03835500	4.74075100	-1.84895600
H	-1.27168500	2.65466900	-1.14878800
N	0.65129400	1.70789100	-1.26158800
Zn	-0.00000400	0.00003500	-0.28953000
N	-12.07465400	0.10776700	1.57723200
C	-11.30105100	0.56343300	0.68229000
H	-11.66103700	1.22460900	-0.12504600
C	-9.86082100	0.23992200	0.65849800
C	-9.31524800	-0.58525200	1.64570200
C	-9.03224900	0.76234100	-0.35385900
C	-7.95785200	-0.90104200	1.64345600
H	-10.00335500	-0.95909400	2.40284000
C	-7.67487800	0.44553300	-0.35707100
C	-7.13027800	-0.37956800	0.63006500
H	-6.98354900	0.82422500	-1.10927400
C	-5.68830300	-0.69426000	0.60748300
H	-5.30068900	-1.26795400	1.46642400
N	-4.94435700	-0.31614700	-0.34771700
O	-9.62055600	1.55968900	-1.27909100
O	-7.36691800	-1.69615100	2.56883600
C	-8.81251400	2.10803100	-2.28759800
H	-8.01694800	2.74336600	-1.86573700
H	-8.34743000	1.32112000	-2.90353700
H	-9.46821400	2.71918200	-2.91755300
C	-8.16139400	-2.20639100	3.60659900
H	-7.49980100	-2.80159000	4.24552900

Zero-point correction=	0.711308 (Hartree/Particle)
Thermal correction to Energy=	0.761624
Thermal correction to Enthalpy=	0.762568
Thermal correction to Gibbs Free Energy=	0.617487
Sum of electronic and zero-point Energies=	-4134.099331
Sum of electronic and thermal Energies=	-4134.049015
Sum of electronic and thermal Enthalpies=	-4134.048071
Sum of electronic and thermal Free Energies=	-4134.193152

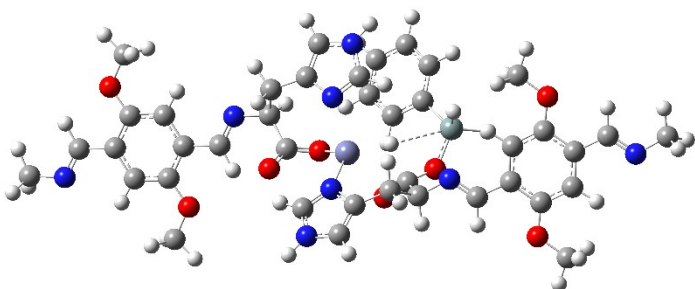
H	-8.61175200	-1.39707100	4.20426700
H	-8.96707100	-2.85077400	3.21816900
C	-3.54238300	-0.64347000	-0.28599200
H	-3.29016500	-1.27538900	0.58526700
C	-2.69481900	0.64694700	-0.21334500
O	-1.65060800	0.56441600	0.53757900
O	-3.00300000	1.60204300	-0.90633200
C	-3.16940900	-1.37352100	-1.59873300
H	-3.99434100	-2.05587800	-1.84581100
H	-3.13416500	-0.61512900	-2.39695300
C	-1.91179100	-2.18643300	-1.56896200
C	-1.79604600	-3.52250800	-1.85481400
N	-0.46328600	-3.83226300	-1.71445500
H	-2.54322800	-4.25494700	-2.14156500
C	0.19537800	-2.72000900	-1.34939400
H	-0.03834000	-4.74057400	-1.84929000
H	1.27168700	-2.65454200	-1.14894900
N	-0.65129200	-1.70775900	-1.26170400
C	13.46534900	-0.47500200	1.52522400
H	13.74746700	-0.97653200	2.46356500
H	13.71756000	-1.13844400	0.67713200
H	14.08248100	0.43408800	1.46003500
C	-13.46534900	0.47475100	1.52532300
H	-13.74752400	0.97597700	2.46380400
H	-13.71754300	1.13847500	0.67746200
H	-14.08248300	-0.43432900	1.45977600

### R1 complex



0 1				Zero-point correction=	0.829438 (Hartree/Particle)
N	11.99924400	-1.66753300	-1.21757000	Thermal correction to Energy=	0.888145
C	11.21883000	-0.73673200	-0.85503500	Thermal correction to Enthalpy=	0.889089
H	11.57394300	0.29368400	-0.68007600	Thermal correction to Gibbs Free Energy=	0.725674
C	9.77644300	-0.96851100	-0.64141900	Sum of electronic and zero-point Energies=	-4656.549126
C	9.23745300	-2.24163700	-0.84527800	Sum of electronic and thermal Energies=	-4656.490419
C	8.93950800	0.08914600	-0.23493600	Sum of electronic and thermal Enthalpies=	-4656.489475
C	7.87847100	-2.48228400	-0.65107200	Sum of electronic and thermal Free Energies=	-4656.652890
H	9.93196000	-3.01979400	-1.15927900		
C	7.58062200	-0.15140700	-0.03975600		
C	7.04241400	-1.42466500	-0.24331800		
H	6.88364100	0.62698600	0.26894100		
C	5.59953300	-1.65293500	-0.03229000		
H	5.22315800	-2.65870000	-0.28468300		
N	4.84241800	-0.73671900	0.41113800		
O	9.52209000	1.30044800	-0.05765600		
O	7.29425100	-3.69235400	-0.82881400		
C	8.70721600	2.37385300	0.33480200		
H	7.91889700	2.57425200	-0.40889900		
H	8.23242000	2.18328100	1.31111000		
H	9.35961700	3.25024600	0.41572000		
C	8.09955200	-4.75945300	-1.25509500		
H	7.44284600	-5.63140900	-1.34758100		
H	8.56303200	-4.54865600	-2.23269900		
H	8.89568100	-4.98012300	-0.52527700		
C	3.44178400	-1.03572000	0.57600500		
H	3.20105800	-2.08988500	0.34768000		
C	2.59179100	-0.13687100	-0.34894700		
O	1.58426400	-0.72441100	-0.89331300		
O	2.86480400	1.05039700	-0.44797200		
C	3.06104300	-0.70530000	2.03573600		
H	3.85673600	-1.09724100	2.68459800		

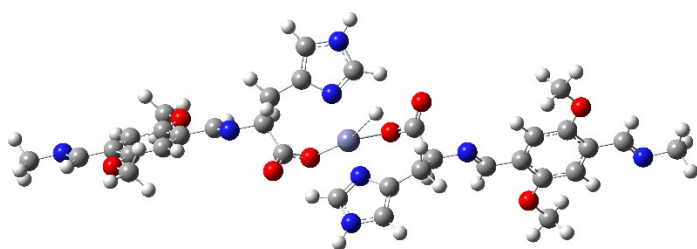
H	3.08298100	0.39177000	2.13414100
C	1.76461100	-1.26770000	2.53515800
C	1.59572000	-2.01260500	3.67418900
N	0.25302600	-2.29636100	3.75437400
H	2.31431400	-2.35181500	4.41280300
C	-0.36158700	-1.74778400	2.69357900
H	-0.20738900	-2.83615700	4.47579700
H	-1.43513700	-1.81893100	2.47872700
N	0.52300000	-1.11200400	1.94262900
Zn	-0.10178100	-0.52712000	0.04910800
N	-12.26347000	-1.53584300	-0.99414300
C	-11.46301500	-1.23318400	-0.05887200
H	-11.80253000	-1.08767600	0.98137700
C	-10.01726000	-1.05399700	-0.29760600
C	-9.49633700	-1.22561600	-1.58312600
C	-9.15860700	-0.71345700	0.76579800
C	-8.13444100	-1.06327000	-1.83009900
H	-10.20709700	-1.48908400	-2.36536100
C	-7.79661000	-0.54995700	0.51873600
C	-7.27679800	-0.72085000	-0.76669400
H	-7.08257200	-0.29418500	1.30094600
C	-5.82953900	-0.54645000	-0.99978100
H	-5.46569500	-0.78882300	-2.01276300
N	-5.05582100	-0.14536300	-0.07846500
O	-9.72390000	-0.56575900	1.98924100
O	-7.56654300	-1.21271200	-3.05205200
C	-8.88688000	-0.23939200	3.06790300
H	-8.11960900	-1.01342200	3.23139000
H	-8.38436300	0.72870300	2.90916800
H	-9.52811700	-0.17234400	3.95368800
C	-8.39250600	-1.58257600	-4.12410900
H	-7.74642900	-1.66487400	-5.00503100
H	-8.88087500	-2.55348700	-3.94001300
H	-9.17038100	-0.82487700	-4.31401100
C	-3.65168900	-0.02090800	-0.37751400
H	-3.42565100	-0.20386500	-1.44419400
C	-2.83351200	-1.02096400	0.47117300
O	-1.77653200	-1.48296000	-0.10450500
O	-3.17554400	-1.24933400	1.61912200
C	-3.20774500	1.41057200	0.01868200
H	-4.03137900	2.09317300	-0.23130600
H	-3.09725500	1.43577600	1.11504600
C	-1.97728800	1.92317000	-0.66060500
C	-1.86772200	3.04356300	-1.44362200
N	-0.56061500	3.09487300	-1.86557500
H	-2.60521600	3.78714000	-1.72689100
C	0.09384300	2.04935700	-1.34031900
H	-0.11822100	3.85803000	-2.36615800
H	1.15944000	1.83869800	-1.46274900
N	-0.73226500	1.32359100	-0.60461300
C	13.39160300	-1.35433400	-1.40361600
H	13.68697200	-1.59650800	-2.43592900
H	13.63893700	-0.29562200	-1.20136300
H	14.00203500	-1.99285200	-0.74693500
C	-13.65753500	-1.69199400	-0.67242100
H	-13.98664900	-2.70503600	-0.94996300
H	-13.88783100	-1.52304200	0.39597100
H	-14.25444600	-0.99346900	-1.27852900
C	1.13966400	6.07945300	-1.08118800
C	-0.01759500	6.11144400	-0.30161800
C	-0.21608300	5.14697400	0.68777300
C	0.73136700	4.13800900	0.91245300
C	1.89400800	4.12017600	0.12319400
C	2.09579900	5.08367400	-0.86599300
H	1.30051200	6.83578400	-1.85208200
H	-0.76542000	6.89008300	-0.46327600
H	-1.13391700	5.17596200	1.28144100
H	2.62405500	3.31369100	0.24200300
H	3.00165400	5.05298900	-1.47418100
Si	0.45061100	2.79768300	2.20330000
H	0.92553700	3.24237800	3.54336800
H	-1.00178600	2.48585800	2.30921200
H	1.21049400	1.58739400	1.80472900
<b>TS1</b>			



0 1				Zero-point correction=	0.827960 (Hartree/Particle)
N	11.58076700	0.18439500	-0.32929300	Thermal correction to Energy=	0.885170
C	10.54981100	0.71898300	0.17813700	Thermal correction to Enthalpy=	0.886114
H	10.58512400	1.69495200	0.69249500	Thermal correction to Gibbs Free Energy=	0.728021
C	9.22542300	0.06836600	0.11427300	Sum of electronic and zero-point Energies=	-4656.514705
C	9.08553100	-1.16617500	-0.52446000	Sum of electronic and thermal Energies=	-4656.457495
C	8.10105100	0.68823200	0.69404600	Sum of electronic and thermal Enthalpies=	-4656.456551
C	7.84440700	-1.79697500	-0.59940000	Sum of electronic and thermal Free Energies=	-4656.614644
H	9.98885700	-1.59714900	-0.95424800		
C	6.86113700	0.05662400	0.62310000		
C	6.72007200	-1.17601400	-0.02097100		
H	5.95909900	0.48735400	1.05603000		
C	5.39273000	-1.81283100	-0.10540100		
H	5.34516800	-2.77001600	-0.65113500		
N	4.36354700	-1.27584500	0.40801200		
O	8.30140600	1.88620000	1.29655600		
O	7.64173500	-2.99141400	-1.20392200		
C	7.19119500	2.53645100	1.85588900		
H	6.41954800	2.74064100	1.09521400		
H	6.74014500	1.93988600	2.66585000		
H	7.55587300	3.48445200	2.26652600		
C	8.73728800	-3.61844600	-1.81846100		
H	8.36124600	-4.55018300	-2.25468300		
H	9.16404900	-2.98982600	-2.61675500		
H	9.52880700	-3.85249400	-1.08802000		
C	3.09298400	-1.93248400	0.24235500		
H	3.19046200	-2.90921200	-0.27494300		
C	2.17330500	-1.13754600	-0.72320300		
O	1.13439500	-1.66736800	-1.13394500		
O	2.88021000	-0.33668700	-1.57894500		
C	2.49756100	-2.15855900	1.64210400		
H	3.20942400	-2.78467500	2.19793000		
H	2.46692500	-1.17920500	2.14143900		
C	1.14914600	-2.79933200	1.70811800		
C	0.82960600	-4.08897900	2.04109600		
N	-0.54134000	-4.17185200	1.95469400		
H	1.45276200	-4.92942000	2.32774000		
C	-1.01776900	-2.96986100	1.58236200		
H	-1.10586500	-4.99279400	2.12861000		
H	-2.06145700	-2.72366700	1.38527800		
N	-0.02129100	-2.11970900	1.43973800		
Zn	-0.01551700	-0.35746300	0.36714200		
N	-11.93681700	-1.43636700	-0.63637200		
C	-11.32824600	-0.41134200	-0.20487800		
H	-11.86580100	0.46134300	0.20531600		
C	-9.85556200	-0.31324500	-0.22139700		
C	-9.09096900	-1.36865100	-0.72583000		
C	-9.21464800	0.84091300	0.26835500		
C	-7.69898300	-1.29655100	-0.75049700		
H	-9.63931800	-2.23527500	-1.09277600		
C	-7.82298700	0.91239600	0.24348900		
C	-7.05716700	-0.14271900	-0.25806100		
H	-7.27312900	1.77897300	0.60797500		
C	-5.58109400	-0.04854000	-0.27625300		
H	-5.04768700	-0.93353200	-0.64789600		
N	-4.99579100	1.00145700	0.13090700		
O	-10.01173900	1.83150200	0.74346400		
O	-6.90423300	-2.28279700	-1.22955000		
C	-9.39869500	2.99393200	1.23255900		
H	-8.73958700	2.77331900	2.08832200		
H	-8.80664900	3.49741200	0.45066400		
H	-10.20410400	3.66059900	1.56037800		
C	-7.51366500	-3.44257900	-1.72883000		

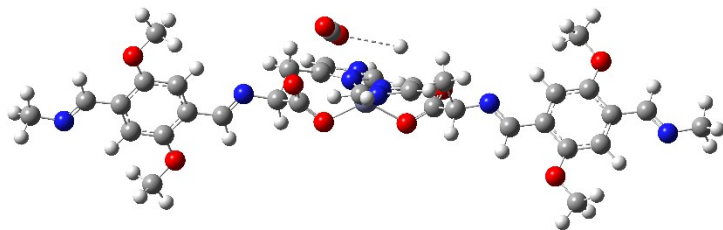
H	-6.70555800	-4.10279100	-2.06229400
H	-8.10444100	-3.95474000	-0.95146400
H	-8.17306000	-3.21640000	-2.58293600
C	-3.55510100	1.11405800	0.08080600
H	-3.29822700	1.79925100	-0.74300200
C	-2.71577400	-0.16556900	-0.05249500
O	-1.62688500	-0.01906200	-0.71220600
O	-3.04986900	-1.15613600	0.58958300
C	-3.08573500	1.75752100	1.40782600
H	-3.78018100	2.57857900	1.63148500
H	-3.20551100	0.99835100	2.19651000
C	-1.69153200	2.30355800	1.40824100
C	-1.34812800	3.63141800	1.45789500
N	0.02369200	3.67356500	1.44057900
H	-1.96376200	4.52372800	1.50459500
C	0.47182900	2.40784000	1.37177200
H	0.60269600	4.50075300	1.37977000
H	1.52384500	2.13810400	1.29526500
N	-0.53000700	1.55334600	1.36216700
C	12.83334100	0.88556000	-0.22469500
H	13.23632200	1.06688500	-1.23270800
H	12.75772400	1.85142800	0.30832100
H	13.56652700	0.24976700	0.29450500
C	-13.37489800	-1.44600700	-0.58301800
H	-13.71443800	-2.30724700	0.01251900
H	-13.80920300	-0.52355300	-0.15439600
H	-13.77873900	-1.58970900	-1.59689400
C	-0.31522200	4.02004800	-1.89881400
C	0.94156000	4.58625100	-1.67044700
C	2.05963300	3.76329000	-1.53407100
C	1.94477000	2.36939600	-1.64836600
C	0.68100500	1.81952000	-1.90581700
C	-0.44619200	2.63635300	-2.01133800
H	-1.19460900	4.66067500	-1.99088800
H	1.04872500	5.67115200	-1.60073300
H	3.03622000	4.21989100	-1.34223900
H	0.56724700	0.73618900	-2.02495700
H	-1.41813000	2.16878600	-2.17327100
Si	3.40931600	1.23509800	-1.35869000
H	4.48001800	1.43584600	-2.36553700
H	3.96426300	1.52225200	-0.00871100
H	1.72785900	0.04718200	0.36953800

### P1 complex



0 2				Zero-point correction=	0.713653 (Hartree/Particle)
N	12.02553300	-0.99872000	1.41530600	Thermal correction to Energy=	0.765050
C	11.26979200	-0.90731900	0.40165300	Thermal correction to Enthalpy=	0.765995
H	11.64354800	-1.05836500	-0.62597900	Thermal correction to Gibbs Free Energy=	0.619432
C	9.83307200	-0.59155000	0.52652000	Sum of electronic and zero-point Energies=	-4134.597330
C	9.27040000	-0.39128600	1.79002100	Sum of electronic and thermal Energies=	-4134.545932
C	9.02492300	-0.49411300	-0.62310000	Sum of electronic and thermal Enthalpies=	-4134.544988
C	7.91592100	-0.09452800	1.93061400	Sum of electronic and thermal Free Energies=	-4134.691551
H	9.94315400	-0.47960400	2.64213600		
C	7.67057300	-0.19620500	-0.48278700		
C	7.10880500	0.00415600	0.78061600		
H	6.99450100	-0.11432700	-1.33327400		
C	5.67020300	0.31251700	0.90090200		
H	5.26698400	0.36911200	1.92623000		
N	4.94634300	0.49417100	-0.12470000		
O	9.62889400	-0.70369100	-1.81863200		
O	7.30942700	0.11336700	3.12502800		
C	8.84141400	-0.62783100	-2.97827000		
H	8.03040700	-1.37390700	-2.96432800		
H	8.39821800	0.37405900	-3.09944100		
H	9.50734000	-0.83258300	-3.82379500		

C	8.08339100	-0.00590500	4.28918900
H	7.41177300	0.18266700	5.13391600
H	8.51300500	-1.01643900	4.38547600
H	8.90318700	0.73090200	4.30559800
C	3.54558100	0.76939000	0.07189900
H	3.27529600	0.86890800	1.13901400
C	2.68761900	-0.35815200	-0.54458900
O	1.63903900	-0.67035400	0.13594100
O	2.99244300	-0.80892700	-1.63658200
C	3.21094600	2.07366600	-0.68828900
H	4.02774300	2.78592300	-0.50691100
H	3.22817700	1.83451100	-1.76346500
C	1.93138900	2.75441600	-0.30936200
C	1.79036800	4.05494700	0.10313200
N	0.44462500	4.24983800	0.31040700
H	2.52823000	4.83527900	0.25691000
C	-0.19736600	3.10223400	0.03832400
H	0.00047700	5.10304600	0.62450900
H	-1.27930500	2.94292600	0.12403700
N	0.67328200	2.18265900	-0.34524000
Zn	-0.00501700	0.21951800	-0.35745500
N	-12.01024500	-0.74643500	1.59629400
C	-11.26999300	0.06470900	0.96298000
H	-11.66194000	0.99872400	0.52420700
C	-9.82805800	-0.18494600	0.76807400
C	-9.24260200	-1.33915300	1.29556800
C	-9.03788700	0.73755500	0.05468500
C	-7.88281100	-1.59286400	1.12525800
H	-9.90209400	-2.01549500	1.83788800
C	-7.67819400	0.48351300	-0.11655400
C	-7.09365800	-0.67061300	0.41089700
H	-7.01530800	1.16229600	-0.65219800
C	-5.64967100	-0.91127200	0.22083700
H	-5.22829500	-1.78885300	0.73990100
N	-4.94155800	-0.14122300	-0.49636800
O	-9.66370200	1.83910300	-0.42780800
O	-7.25427500	-2.69254700	1.60822300
C	-8.89437300	2.78158900	-1.12831200
H	-8.09208900	3.19642500	-0.49682800
H	-8.44146500	2.34065400	-2.03126500
H	-9.57633500	3.58682800	-1.42289900
C	-8.00960500	-3.61406900	2.34907800
H	-7.32188600	-4.40962800	2.65617300
H	-8.44805200	-3.14676300	3.24597600
H	-8.82124800	-4.04952100	1.74342300
C	-3.53378000	-0.42594400	-0.61578000
H	-3.24406200	-1.36567400	-0.11088800
C	-2.70589600	0.72733600	-0.00386000
O	-1.65479700	0.35370200	0.64033000
O	-3.03382300	1.88191000	-0.22420900
C	-3.19788600	-0.50356300	-2.12239400
H	-4.00703000	-1.06062400	-2.61495300
H	-3.23767000	0.52547500	-2.51563300
C	-1.91014300	-1.17718100	-2.48984700
C	-1.76297600	-2.20461000	-3.38639400
N	-0.41921300	-2.49446700	-3.42525500
H	-2.49676600	-2.73572100	-3.98344700
C	0.21699600	-1.67402500	-2.57333200
H	0.02712500	-3.20884700	-3.98583900
H	1.29554600	-1.67227500	-2.37447300
N	-0.65513000	-0.86220500	-1.99933800
C	13.41420300	-1.31125300	1.20261100
H	13.67036300	-2.23236100	1.74806600
H	13.68130100	-1.44220700	0.13745500
H	14.03957500	-0.51226100	1.62936700
C	-13.40537800	-0.42367400	1.74036900
H	-13.66252200	-0.37803300	2.80965800
H	-13.69070800	0.53295300	1.26446400
H	-14.01545300	-1.23105600	1.30733500
H	-1.35625700	1.88664800	-2.29065400
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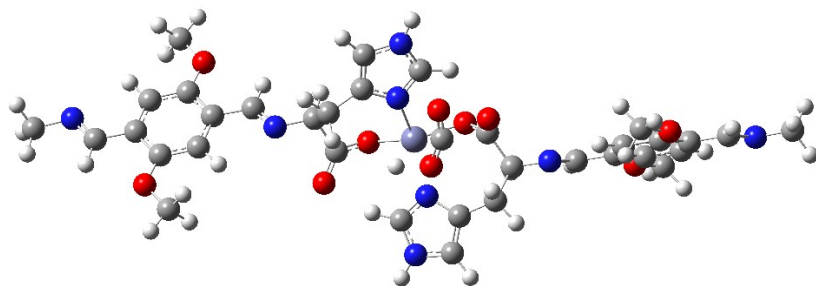


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C	-11.31583400	-0.29403600	-0.48002800
H	-11.59848900	-1.19386300	0.09347900
C	-9.88292700	0.06098900	-0.46017100
C	-9.43249100	1.18145900	-1.16359800
C	-8.96612300	-0.72691300	0.26300700
C	-8.08393500	1.53333300	-1.15993800
H	-10.18628800	1.75204600	-1.70463600
C	-7.61765800	-0.37428500	0.26794800
C	-7.16815400	0.74618500	-0.43518000
H	-6.86116100	-0.94766200	0.80272500
C	-5.73330100	1.09284600	-0.41801600
H	-5.42484100	1.92730900	-1.07059600
N	-4.90899600	0.45573200	0.30519600
O	-9.46455200	-1.80286600	0.91989700
O	-7.58271900	2.60725500	-1.81821100
C	-8.56854300	-2.61316900	1.63511900
H	-7.80196400	-3.04796500	0.97343600
H	-8.06508100	-2.04725500	2.43583800
H	-9.16156600	-3.41934100	2.08080400
C	-8.46844600	3.39502700	-2.56887100
H	-7.87072300	4.19079800	-3.02676800
H	-8.95797000	2.80637200	-3.36189600
H	-9.24610200	3.84632800	-1.93109400
C	-3.52045000	0.83699400	0.25170300
H	-3.34154700	1.71885000	-0.39010100
C	-2.66219800	-0.32582900	-0.28634200
O	-1.63997300	0.04373400	-0.97033600
O	-2.93354500	-1.47971900	0.02062200
C	-3.06578300	1.13503100	1.70013400
H	-3.84563000	1.75516600	2.16389200
H	-3.05549000	0.17718600	2.24161700
C	-1.76246800	1.85288800	1.88546600
C	-1.57703300	3.02337300	2.57713400
N	-0.22701300	3.28333000	2.54347300
H	-2.28732900	3.66907800	3.08278200
C	0.37552900	2.30443400	1.84769600
H	0.24490300	4.07538100	2.96006600
H	1.45086900	2.23484200	1.64248500
N	-0.52483300	1.42557000	1.44327000
Zn	0.05258700	0.07051600	-0.00505700
N	12.34000000	0.72936200	-0.74046000
C	11.46430700	0.63947800	0.17174100
H	11.72038600	0.71908900	1.24255800
C	10.03709800	0.42132800	-0.13624300
C	9.61874500	0.31464800	-1.46554200
C	9.09319900	0.32350000	0.90475700
C	8.27594300	0.11109300	-1.77805900
H	10.39235700	0.39868400	-2.22776400
C	7.75036500	0.11902100	0.59228400
C	7.33310200	0.01170600	-0.73659400
H	6.97330200	0.04390100	1.35227200
C	5.90310100	-0.19746400	-1.03806100
H	5.61879000	-0.16334800	-2.10371400
N	5.05677800	-0.39657800	-0.11525500
O	9.56110900	0.44049500	2.17178600
O	7.80484400	-0.00369800	-3.04421300
C	8.63768100	0.36211500	3.22625000
H	7.87879900	1.15830600	3.15756600
H	8.12592000	-0.61398600	3.24162400
H	9.20865100	0.48485500	4.15319100
C	8.71660900	0.12347800	-4.10292100
H	8.14015500	0.01887300	-5.02866900
H	9.21114500	1.10856700	-4.09255300

Zero-point correction=	0.727173 (Hartree/Particle)
Thermal correction to Energy=	0.782299
Thermal correction to Enthalpy=	0.783243
Thermal correction to Gibbs Free Energy=	0.627933
Sum of electronic and zero-point Energies=	-4322.968698
Sum of electronic and thermal Energies=	-4322.913572
Sum of electronic and thermal Enthalpies=	-4322.912628
Sum of electronic and thermal Free Energies=	-4323.067938

H	9.48958700	-0.66163400	-4.06611100
C	3.67403100	-0.56174900	-0.48201300
H	3.52329000	-0.62954100	-1.57542300
C	2.82498700	0.61571500	0.04283000
O	1.73831800	0.80645300	-0.61958500
O	3.16649400	1.21678700	1.04797300
C	3.16887700	-1.86079600	0.19583000
H	3.96011500	-2.61346900	0.07359100
H	3.09229800	-1.66210300	1.27723500
C	1.90203100	-2.46542700	-0.32847200
C	1.78269900	-3.67949700	-0.95614000
N	0.44719600	-3.83719000	-1.24301300
H	2.52998300	-4.42409900	-1.20979800
C	-0.20997300	-2.75130600	-0.80494800
H	0.01756000	-4.63221700	-1.69835000
H	-1.28790400	-2.58278900	-0.88524700
N	0.63813900	-1.91094200	-0.23716600
C	-13.54401800	-0.02270300	-1.08381700
H	-13.89775200	-0.20418800	-2.11021800
H	-13.71614600	-0.93397700	-0.48138400
H	-14.16448700	0.79182500	-0.67988200
C	13.70882400	0.94290800	-0.35051800
H	14.08126600	1.87005800	-0.81231200
H	13.85334200	1.00726200	0.74401300
H	14.33376800	0.12628900	-0.74320500
H	1.39968200	-0.41848800	2.21339200
C	-1.46912400	-2.49786700	1.98029700
O	-1.13747900	-1.41998600	2.25401600
O	-1.75545000	-3.59233500	1.75209700

## TS2



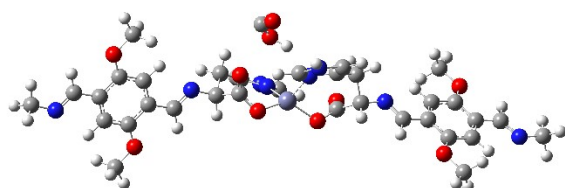
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N	-12.16922500	0.14632900	0.98564600
C	-11.27480200	0.64231800	0.23672900
H	-11.50385400	1.40656000	-0.52613200
C	-9.86048600	0.22992300	0.33400300
C	-9.47713800	-0.72875500	1.27578700
C	-8.89416300	0.80057700	-0.51746400
C	-8.14729700	-1.13133900	1.38568700
H	-10.26696400	-1.13437700	1.90676600
C	-7.56442000	0.39755400	-0.40831800
C	-7.18175900	-0.56118600	0.53337200
H	-6.77236800	0.80660000	-1.03468000
C	-5.76580600	-0.96616600	0.63237500
H	-5.51574100	-1.67105900	1.44323600
N	-4.89261000	-0.51833800	-0.17158400
O	-9.32901900	1.72706000	-1.40642100
O	-7.71031800	-2.05624500	2.27500900
C	-8.38366900	2.31997300	-2.25810700
H	-7.60740600	2.85569000	-1.68800200
H	-7.89571400	1.57035900	-2.90220200
H	-8.92969600	3.03366900	-2.88478000
C	-8.64567900	-2.62190600	3.15475500
H	-8.09484900	-3.32390200	3.79031800
H	-9.11905300	-1.85362500	3.78771900
H	-9.43348500	-3.16716800	2.60960700
C	-3.52762800	-0.94751000	0.00100100
H	-3.40892700	-1.68153900	0.81813500
C	-2.61866000	0.26051700	0.29953200
O	-1.72802200	0.05725500	1.20392400
O	-2.72108000	1.27051900	-0.38727000
C	-3.04823400	-1.54827800	-1.33758100
H	-3.82004600	-2.24736200	-1.68902300

Zero-point correction=	0.726609 (Hartree/Particle)
Thermal correction to Energy=	0.781248
Thermal correction to Enthalpy=	0.782192
Thermal correction to Gibbs Free Energy=	0.627161
Sum of electronic and zero-point Energies=	-4322.928808
Sum of electronic and thermal Energies=	-4322.874168
Sum of electronic and thermal Enthalpies=	-4322.873224
Sum of electronic and thermal Free Energies=	-4323.028255

H	-3.00731300	-0.71925100	-2.06101200
C	-1.74718200	-2.29205600	-1.31129200
C	-1.53419200	-3.55925800	-1.79054500
N	-0.19861200	-3.82422000	-1.60168500
H	-2.21713600	-4.27054300	-2.24292600
C	0.36831300	-2.75485800	-1.01927800
H	0.28786800	-4.67745000	-1.84448400
H	1.42650800	-2.67913500	-0.74108000
N	-0.53971600	-1.81017200	-0.83618400
Zn	0.01801600	-0.20102400	0.36452000
N	12.31707200	-0.19886500	0.74107600
C	11.42272400	-0.50149300	-0.10484600
H	11.66510100	-0.96935000	-1.07484900
C	9.99085700	-0.24830300	0.15029700
C	9.58972500	0.33355400	1.35608100
C	9.02543400	-0.59474200	-0.81512100
C	8.24308300	0.57811100	1.61852400
H	10.37973000	0.57954800	2.06449700
C	7.67860900	-0.34889200	-0.55329100
C	7.27864600	0.23319200	0.65194400
H	6.88575700	-0.60277300	-1.25612000
C	5.84454700	0.47413000	0.90585100
H	5.57932500	0.81682900	1.92070400
N	4.97396100	0.28710100	0.00336600
O	9.47738400	-1.16131500	-1.96086600
O	7.78804900	1.14165200	2.76475300
C	8.53272000	-1.53288200	-2.93051300
H	7.82168900	-2.27681300	-2.53613500
H	7.96604000	-0.66081700	-3.29562600
H	9.09340100	-1.97304200	-3.76249000
C	8.72359400	1.46175000	3.76008300
H	8.15862800	1.88200600	4.59940000
H	9.27019000	0.56754500	4.10168300
H	9.45250500	2.20792200	3.40350200
C	3.59049300	0.51199000	0.33476400
H	3.45874100	0.96816000	1.33389800
C	2.80689100	-0.81949000	0.30936700
O	1.72749100	-0.81434200	1.01555000
O	3.19306100	-1.73849700	-0.39011400
C	2.99242800	1.44850800	-0.74882400
H	3.78722100	2.14428900	-1.04979700
H	2.75474300	0.83958400	-1.63798200
C	1.80777700	2.26669700	-0.34345400
C	1.74063800	3.63123900	-0.22983400
N	0.45622100	3.92009700	0.16963200
H	2.49062800	4.39707700	-0.39699700
C	-0.22096600	2.76758200	0.28475200
H	0.06343100	4.84151900	0.31242100
H	-1.27900400	2.67277200	0.52883000
N	0.56558000	1.75293100	-0.02399600
C	-13.52356500	0.60571200	0.82406800
H	-13.88557600	1.02175100	1.77664900
H	-13.64131100	1.37025200	0.03376700
H	-14.17538200	-0.24977800	0.58990000
C	13.68907500	-0.48203200	0.41127400
H	14.11978500	-1.14762300	1.17485600
H	13.81906500	-0.94935200	-0.58257700
H	14.27418400	0.44971900	0.44420600
H	0.40406200	0.35102600	-2.39287800
C	-1.26309800	1.71667100	-2.57078600
O	-0.87460000	0.57428900	-2.60765300
O	-1.14730100	2.87133100	-2.50263300

### P2 complex

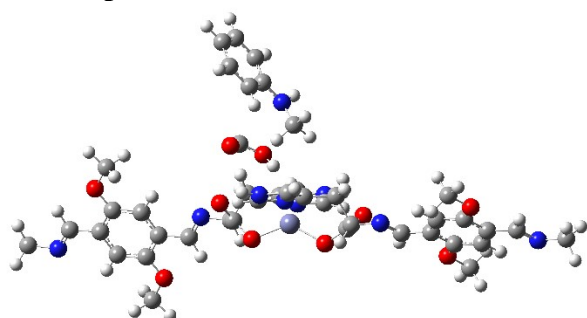


0 2			Zero-point correction=	0.734513 (Hartree/Particle)
N	-12.09095300	-0.78963000	Thermal correction to Energy=	0.789291
C	-11.28046000	0.02910400	Thermal correction to Enthalpy=	0.790235

H	-11.60749200	1.00353300	0.29241800	Thermal correction to Gibbs Free Energy=	0.634013
C	-9.83832900	-0.26557400	0.58085600	Sum of electronic and zero-point Energies=	-4322.967428
C	-9.33254000	-1.47294800	1.07035700	Sum of electronic and thermal Energies=	-4322.912650
C	-8.96838600	0.66732700	-0.01711500	Sum of electronic and thermal Enthalpies=	-4322.911706
C	-7.97420200	-1.76989800	0.97503000	Sum of electronic and thermal Free Energies=	-4323.067928
H	-10.05182300	-2.15465500	1.52249700		
C	-7.61007200	0.36992800	-0.11360000		
C	-7.10529600	-0.83741500	0.37588400		
H	-6.88834000	1.05371600	-0.55934800		
C	-5.66133100	-1.12332000	0.26694500		
H	-5.30868100	-2.05013800	0.75061100		
N	-4.87828500	-0.33596700	-0.34596800		
O	-9.51933900	1.82065500	-0.46756200		
O	-7.42015600	-2.92183700	1.42696500		
C	-8.67022500	2.77344400	-1.05365900		
H	-7.89888100	3.11585900	-0.34506900		
H	-8.17268500	2.37130400	-1.95110100		
H	-9.30118400	3.62194000	-1.34010700		
C	-8.25754900	-3.85592000	2.05529700		
H	-7.62175800	-4.69569000	2.35657200		
H	-8.74028700	-3.42704200	2.94864400		
H	-9.04028500	-4.22072100	1.37014700		
C	-3.47698400	-0.66842500	-0.39359400		
H	-3.25327200	-1.64252100	0.07888800		
C	-2.65363200	0.41931600	0.32704200		
O	-1.67027700	-0.02263900	1.03640300		
O	-2.91620100	1.59585800	0.13531500		
C	-3.04661500	-0.67962000	-1.87693900		
H	-3.83097600	-1.19852600	-2.44528600		
H	-3.03382300	0.36490700	-2.22346000		
C	-1.75030100	-1.36230900	-2.19038200		
C	-1.56726000	-2.33933700	-3.13446900		
N	-0.23260800	-2.66777800	-3.10046800		
H	-2.27182400	-2.81019300	-3.81178300		
C	0.36445300	-1.91917200	-2.16044300		
H	0.23268000	-3.36056700	-3.67262200		
H	1.42568700	-1.96595900	-1.88856800		
N	-0.52279500	-1.11392000	-1.59740900		
Zn	0.02839000	-0.12752100	0.13070500		
N	12.30596700	-0.88188800	0.80162800		
C	11.43167500	-0.82319600	-0.11429000		
H	11.68570700	-0.95942800	-1.17981600		
C	10.00813200	-0.56775400	0.18309900		
C	9.59341100	-0.38940900	1.50558600		
C	9.06464700	-0.50640700	-0.86124200		
C	8.25421900	-0.14995600	1.80868000		
H	10.36667700	-0.44817300	2.27051000		
C	7.72561500	-0.26618200	-0.55855000		
C	7.31179800	-0.08762200	0.76396200		
H	6.94944700	-0.21576000	-1.32143900		
C	5.88632900	0.15754200	1.05696800		
H	5.60685400	0.19189500	2.12383500		
N	5.03727600	0.31115200	0.12736600		
O	9.52953500	-0.69230900	-2.12095000		
O	7.78686200	0.03394500	3.06772200		
C	8.60664600	-0.65132500	-3.17788500		
H	7.83529500	-1.43102100	-3.06966900		
H	8.11057100	0.33092600	-3.24137100		
H	9.17464400	-0.82888700	-4.09771000		
C	8.69818200	-0.05541800	4.13113400		
H	8.12465200	0.10359000	5.05088100		
H	9.17695500	-1.04752100	4.16863700		
H	9.48318300	0.71469500	4.05500800		
C	3.66084100	0.52131100	0.49215200		
H	3.51423500	0.63371100	1.58211800		
C	2.77766400	-0.64119500	-0.00099800		
O	1.71979100	-0.83362000	0.71109700		
O	3.06420500	-1.21847400	-1.03559700		
C	3.17251500	1.79902100	-0.23844600		
H	3.97290200	2.54697400	-0.15582200		
H	3.07843600	1.55260300	-1.30790100		
C	1.91795500	2.42774000	0.28228500		
C	1.82001800	3.62414300	0.94103600		
N	0.48505700	3.80143200	1.22537900		
H	2.58099900	4.34580500	1.21881300		

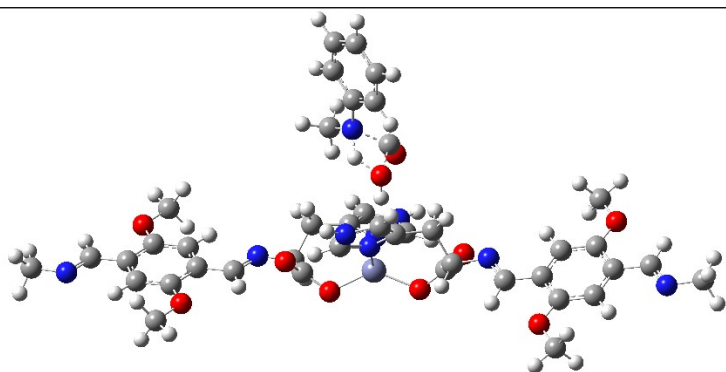
C	-0.19508900	2.75145300	0.75291500
H	0.06435400	4.60203700	1.68040400
H	-1.27982300	2.61165500	0.81918700
N	0.63853600	1.90020800	0.16418300
C	-13.48045400	-0.42133200	1.29511000
H	-13.80917900	-0.43202200	2.34553400
H	-13.69829500	0.57343400	0.86387800
H	-14.08710800	-1.17558500	0.77101600
C	13.67128200	-1.13625500	0.42391900
H	14.02828700	-2.04565000	0.93093200
H	13.81494800	-1.25623900	-0.66597300
H	14.30906000	-0.31167200	0.77723000
H	-0.30500600	1.96316500	-1.67403100
C	-1.82337000	2.98163000	-2.12969800
O	-1.08912000	1.89976800	-2.26353000
O	-1.61300400	3.96924600	-1.51609600

### R3 complex



0 2				Zero-point correction=	0.882167 (Hartree/Particle)
N	11.98097000	-2.33625100	-0.69340200	Thermal correction to Energy=	0.945948
C	11.18665100	-1.35442700	-0.58323700	Thermal correction to Enthalpy=	0.946892
H	11.53731300	-0.30815200	-0.61115300	Thermal correction to Gibbs Free Energy=	0.768241
C	9.73285100	-1.54396600	-0.40965600	Sum of electronic and zero-point Energies=	-4649.348906
C	9.19793000	-2.83455300	-0.37068000	Sum of electronic and thermal Energies=	-4649.285124
C	8.88130400	-0.42844600	-0.28635200	Sum of electronic and thermal Enthalpies=	-4649.284180
C	7.82822100	-3.03599100	-0.21064500	Sum of electronic and thermal Free Energies=	-4649.462832
H	9.90430700	-3.65759700	-0.47147400		
C	7.51155300	-0.62991000	-0.12472900		
C	6.97768600	-1.92050200	-0.08619600		
H	6.80320500	0.19260600	-0.03045600		
C	5.52237200	-2.10379400	0.07766100		
H	5.14795000	-3.13887800	0.00180300		
N	4.75419800	-1.11639100	0.28661200		
O	9.45999400	0.79568800	-0.33676000		
O	7.24608400	-4.25966800	-0.16227800		
C	8.62954500	1.92376100	-0.23194300		
H	7.88700600	1.95436300	-1.04550200		
H	8.09799600	1.94409100	0.73323700		
H	9.28164700	2.80106100	-0.30359600		
C	8.06727700	-5.38785400	-0.30837500		
H	7.41143800	-6.26365700	-0.25267800		
H	8.58693300	-5.38476000	-1.28047900		
H	8.81944500	-5.44578700	0.49540800		
C	3.34099200	-1.36540800	0.41330600		
H	3.08952000	-2.44064000	0.36022600		
C	2.57437700	-0.63090300	-0.70549300		
O	1.59142700	-1.29292200	-1.21732900		
O	2.87221800	0.52057800	-0.97846700		
C	2.87818200	-0.76947000	1.76107300		
H	3.62160900	-1.04851400	2.52062700		
H	2.90979000	0.32611600	1.66288200		
C	1.54108200	-1.21763300	2.26699900		
C	1.28862400	-1.73395200	3.51165700		
N	-0.06181000	-1.98708600	3.56135500		
H	1.95522300	-1.93136600	4.34445300		
C	-0.60104200	-1.64244200	2.38206800		
H	-0.57374600	-2.37771100	4.34188300		
H	-1.65822000	-1.74661600	2.11220900		
N	0.33836100	-1.16600500	1.57989700		
Zn	-0.12993400	-0.95217800	-0.42345500		
N	-12.12036100	-2.30819100	0.53077700		
C	-11.49823500	-1.36232300	-0.03928400		

H	-12.02144700	-0.49691400	-0.48180200
C	-10.02589900	-1.35407200	-0.15070600
C	-9.28034200	-2.41031800	0.37854900
C	-9.36761300	-0.28541600	-0.78966600
C	-7.88931000	-2.42254500	0.28472600
H	-9.84215700	-3.20972100	0.85990900
C	-7.97727400	-0.29772400	-0.88316500
C	-7.23007000	-1.35199300	-0.35158100
H	-7.41595900	0.50060400	-1.36643400
C	-5.75593500	-1.34912700	-0.45731800
H	-5.24183500	-2.19595500	0.01661200
N	-5.15006300	-0.40688500	-1.05479100
O	-10.14779300	0.70866300	-1.28339000
O	-7.11263600	-3.41840700	0.77269500
C	-9.51904700	1.78471400	-1.92632800
H	-8.83541600	2.31777000	-1.24518500
H	-8.95016900	1.45024000	-2.80944000
H	-10.31345600	2.46778300	-2.24681900
C	-7.74028800	-4.49553500	1.41559900
H	-6.94457500	-5.17900400	1.73135300
H	-8.30593800	-4.16228400	2.30115800
H	-8.42643200	-5.02661700	0.73563700
C	-3.71059400	-0.42133500	-1.19875800
H	-3.47393000	-0.73231400	-2.22880700
C	-2.89640500	-1.29622100	-0.22898900
O	-1.82816500	-1.80746300	-0.73326200
O	-3.23430000	-1.35975200	0.94555100
C	-3.21069000	1.03224200	-0.99815000
H	-3.98435500	1.68609300	-1.42186700
H	-3.18522700	1.22550400	0.08721400
C	-1.90553800	1.39641300	-1.63415900
C	-1.72517900	2.28626300	-2.65972000
N	-0.37217700	2.31996700	-2.91039300
H	-2.44118300	2.88453900	-3.21340900
C	0.23869700	1.47722200	-2.06913100
H	0.10555400	2.89893500	-3.59019200
H	1.31778300	1.28822800	-2.02690600
N	-0.65771400	0.90801200	-1.26994600
C	13.38367500	-2.06078600	-0.86066200
H	13.73713200	-2.51513000	-1.79886400
H	13.62525200	-0.98171600	-0.87445200
H	13.95111900	-2.54084900	-0.04878400
C	-13.55639400	-2.23705600	0.59486600
H	-13.87846000	-2.27076700	1.64684300
H	-13.97718000	-1.33014200	0.12221400
H	-13.98932500	-3.12415300	0.10788100
H	0.38712200	1.70678000	0.41585700
C	1.89042600	2.83667400	0.52237500
O	1.11478600	1.90917100	1.04238800
O	1.79920400	3.41835000	-0.50217300
C	1.54950800	8.27792600	0.87049600
C	0.91679900	7.64191900	-0.19420700
C	0.26959500	6.41955500	-0.02270500
C	0.25051300	5.79945700	1.23805100
C	0.89361500	6.44595700	2.31106500
C	1.53071700	7.66516100	2.12573200
H	2.05169100	9.23478300	0.72743600
H	0.92255700	8.10268300	-1.18384900
H	-0.21045700	5.93942700	-0.87472900
H	0.89079200	5.97248200	3.29567500
H	2.02099700	8.14430600	2.97515100
N	-0.35892900	4.57647100	1.43638300
H	-0.51532800	4.31311900	2.39923800
C	-1.22155600	3.98701100	0.45005200
H	-0.65392100	3.74415900	-0.46461100
H	-1.64164600	3.05286300	0.84679200
H	-2.06355000	4.64320700	0.15757500
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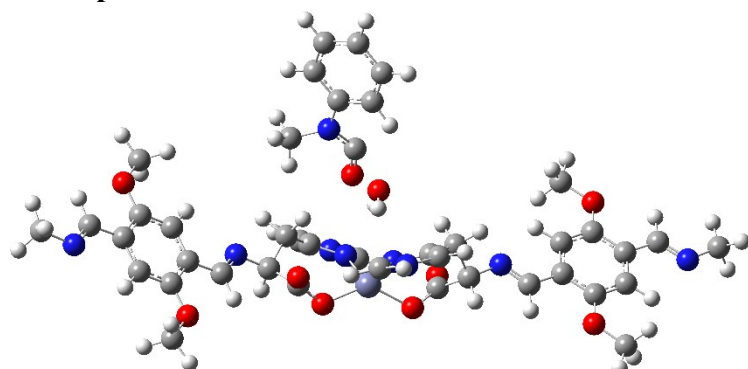


0 2			
N	12.32037700	-1.54158600	0.03093400
C	11.44682600	-0.72841000	-0.39662800
H	11.71760200	0.19121700	-0.94391000
C	10.00278600	-0.95602100	-0.19153600
C	9.56582400	-2.10027200	0.48176900
C	9.06183300	-0.02592400	-0.67503300
C	8.20717300	-2.33574600	0.68355000
H	10.33823600	-2.78367700	0.83225900
C	7.70296200	-0.26060600	-0.47169500
C	7.26721800	-1.40436600	0.20169000
H	6.92811600	0.41731100	-0.82840600
C	5.82117900	-1.62946900	0.39620600
H	5.53106600	-2.60197200	0.82942200
N	4.96922500	-0.74792200	0.07266700
O	9.54802300	1.06025100	-1.32398500
O	7.71743100	-3.42256900	1.32995500
C	8.62821700	1.99190200	-1.83185100
H	7.95200900	1.52970400	-2.56904200
H	8.02186900	2.43885100	-1.02728400
H	9.21486300	2.77739800	-2.32077700
C	8.63015200	-4.38175400	1.79366500
H	8.04020600	-5.17535300	2.26530100
H	9.21939900	-4.81027600	0.96646900
H	9.32247700	-3.95344900	2.53699700
C	3.57289100	-1.04307200	0.26604000
H	3.40758900	-2.00880100	0.77904100
C	2.84160000	-1.08037100	-1.09514500
O	1.83130500	-1.88366100	-1.14246800
O	3.19140500	-0.32390200	-1.98254200
C	2.95788400	0.11283800	1.09963100
H	3.72672600	0.44990100	1.80791900
H	2.75672300	0.96235900	0.42700700
C	1.73469500	-0.22093000	1.89278200
C	1.58255100	-0.14061300	3.25256300
N	0.28840300	-0.52509700	3.51857600
H	2.27882900	0.15716400	4.02928100
C	-0.31180200	-0.83047200	2.35669700
H	-0.14863400	-0.57748800	4.42964400
H	-1.34616600	-1.17147600	2.24167500
N	0.53542700	-0.65090200	1.35761200
Zn	0.10153400	-1.30220800	-0.55212800
N	-11.88883400	-2.04039000	0.97167400
C	-11.25111300	-1.31231700	0.15316000
H	-11.75934600	-0.59803500	-0.51775300
C	-9.78012300	-1.37072200	0.04045600
C	-9.05289500	-2.25027600	0.84632100
C	-9.10435300	-0.54507700	-0.87868500
C	-7.66345700	-2.32309100	0.75496600
H	-9.62734500	-2.86590100	1.53726500
C	-7.71565900	-0.61711400	-0.96896000
C	-6.98663200	-1.49445600	-0.16207700
H	-7.14124900	-0.00428700	-1.66211900
C	-5.51374800	-1.56020700	-0.27251100
H	-5.01447300	-2.26793400	0.40234100
N	-4.89393300	-0.82270100	-1.09944600
O	-9.86706400	0.28500200	-1.63443500
O	-6.90456700	-3.15713100	1.50363500
C	-9.22121200	1.10743200	-2.56833800
H	-8.51755900	1.80008200	-2.07764400

Zero-point correction=	0.878761 (Hartree/Particle)
Thermal correction to Energy=	0.941005
Thermal correction to Enthalpy=	0.941949
Thermal correction to Gibbs Free Energy=	0.768061
Sum of electronic and zero-point Energies=	-4649.294603
Sum of electronic and thermal Energies=	-4649.232360
Sum of electronic and thermal Enthalpies=	-4649.231416
Sum of electronic and thermal Free Energies=	-4649.405304

H	-8.67001000	0.51348500	-3.31588200
H	-10.00318800	1.68587200	-3.07273700
C	-7.54919100	-3.99262700	2.42758600
H	-6.76530900	-4.57624900	2.92239300
H	-8.09955500	-3.40859800	3.18342800
H	-8.25269200	-4.67894900	1.92826800
C	-3.45783300	-0.91450300	-1.25490100
H	-3.25488800	-1.48178100	-2.17725400
C	-2.64673700	-1.54909000	-0.10731900
O	-1.60106500	-2.20010200	-0.47990100
O	-2.97037600	-1.31711600	1.04955200
C	-2.91467200	0.52738400	-1.44111500
H	-3.71389800	1.09487100	-1.93701300
H	-2.78397400	0.96780100	-0.43690000
C	-1.66839300	0.68322800	-2.25498500
C	-1.54796600	1.31546600	-3.46407900
N	-0.22955700	1.20452400	-3.82830300
H	-2.28459600	1.82680800	-4.07461400
C	0.42696900	0.54519000	-2.86693400
H	0.20706700	1.62723800	-4.63756500
H	1.49586400	0.30121300	-2.87846800
N	-0.41518600	0.21371400	-1.89586800
C	13.70641900	-1.24165400	-0.21461100
H	14.16562400	-2.06681900	-0.78015900
H	13.86445300	-0.29832800	-0.76978200
H	14.24461600	-1.18329400	0.74382100
C	-13.32235000	-1.92067500	1.01528200
H	-13.63642600	-1.64410000	2.03332800
H	-13.72737600	-1.17773300	0.30320300
H	-13.77847200	-2.89982400	0.80372100
H	0.21581600	1.50751700	-0.35509700
C	0.22921900	3.63613400	-0.72754900
O	0.34610900	2.27927100	0.22651800
O	0.08491700	3.45278400	-1.90710400
C	-0.09543000	6.95561700	3.09973400
C	-1.25326500	7.08846400	2.34037800
C	-1.57233600	6.14715200	1.35961300
C	-0.72595500	5.05906300	1.14069600
C	0.44051900	4.91958100	1.90628500
C	0.74897500	5.86617500	2.87593700
H	0.15051300	7.69539700	3.86220600
H	-1.92179200	7.93498200	2.50376500
H	-2.48083400	6.27485700	0.77311800
H	1.09407900	4.06349200	1.73313700
H	1.66038500	5.75088900	3.46439300
N	-1.01328500	4.05681400	0.15593100
H	-0.67941800	2.89049500	0.53612700
C	-2.23590200	4.19990500	-0.62868700
H	-2.21680900	5.12828400	-1.21777200
H	-2.29391100	3.35294400	-1.32231800
H	-3.10881700	4.19848200	0.03634400

### P3 complex

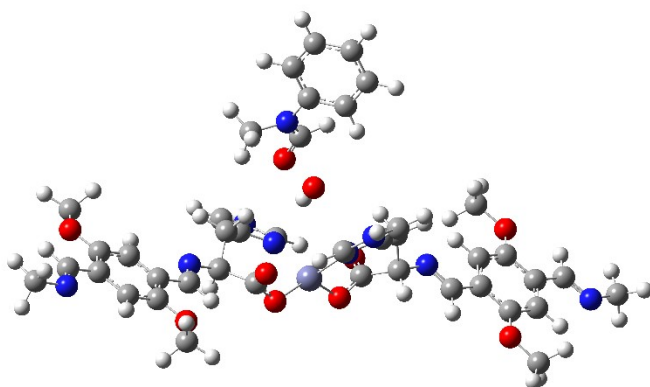


0 2				Zero-point correction=	0.881453 (Hartree/Particle)
N	12.33571100	-0.25647400	0.14562200	Thermal correction to Energy=	0.945556
C	11.30766900	0.45515600	-0.06375400	Thermal correction to Enthalpy=	0.946500
H	11.37736600	1.51806000	-0.35347500	Thermal correction to Gibbs Free Energy=	0.767677
C	9.94211700	-0.09050900	0.06579700	Sum of electronic and zero-point Energies=	-4649.363326
C	9.75707600	-1.42945700	0.42142500	Sum of electronic and thermal Energies=	-4649.299224
C	8.82344700	0.73204700	-0.17140700	Sum of electronic and thermal Enthalpies=	-4649.298280

C	8.47675400	-1.96522700	0.54674200	Sum of electronic and thermal Free Energies=	-4649.477102
H	10.65830200	-2.01710600	0.59155000		
C	7.54286100	0.19627200	-0.04536600		
C	7.35883100	-1.14179200	0.31111000		
H	6.64017300	0.77945000	-0.22433900		
C	5.99092000	-1.68347700	0.43060200		
H	5.90992300	-2.77011500	0.60540800		
N	4.97314400	-0.93460800	0.32979100		
O	9.06903600	2.01916900	-0.51806600		
O	8.22820500	-3.25309300	0.89109500		
C	7.97017200	2.85407600	-0.77743100		
H	7.36218300	2.47176000	-1.61324100		
H	7.32539300	2.95846500	0.11031300		
H	8.37775000	3.83515900	-1.04489700		
C	9.32385100	-4.10519500	1.09525200		
H	8.91420400	-5.09076800	1.34252100		
H	9.94483400	-4.18727800	0.18821800		
H	9.95680600	-3.75606000	1.92756600		
C	3.67028200	-1.53878700	0.42465000		
H	3.70705400	-2.59377200	0.75609600		
C	2.94342500	-1.49467400	-0.93480500		
O	1.93739000	-2.30282600	-0.99958300		
O	3.28459900	-0.69946000	-1.79033600		
C	2.84278700	-0.70473400	1.43973300		
H	3.51524200	-0.45986300	2.27305400		
H	2.56170800	0.25121400	0.96936100		
C	1.62124300	-1.35073000	2.01463000		
C	1.46755400	-1.89546800	3.26261900		
N	0.16421800	-2.33278100	3.33467800		
H	2.16659200	-1.99538000	4.08626600		
C	-0.44464600	-2.05700000	2.17067400		
H	-0.27565800	-2.78474500	4.12636500		
H	-1.48404900	-2.29752300	1.91918700		
N	0.40741200	-1.45380600	1.35565400		
Zn	0.16413800	-1.62081500	-0.71074800		
N	-11.82629100	-1.37904800	0.98650300		
C	-11.03154200	-0.45451700	0.63944300		
H	-11.35140500	0.59971800	0.56923900		
C	-9.61947400	-0.72533500	0.30422700		
C	-9.12523000	-2.03070600	0.36736800		
C	-8.76556600	0.32683300	-0.07915900		
C	-7.79484000	-2.30835200	0.05679500		
H	-9.83035400	-2.80452500	0.66800200		
C	-7.43587100	0.04908100	-0.39002100		
C	-6.93947200	-1.25519100	-0.32379700		
H	-6.73006300	0.82209900	-0.69049400		
C	-5.52528700	-1.52986700	-0.65064300		
H	-5.19338400	-2.56632100	-0.49717800		
N	-4.76019700	-0.60988000	-1.07441600		
O	-9.30532700	1.57147200	-0.12030200		
O	-7.25898000	-3.55120100	0.09250100		
C	-8.47543900	2.63892000	-0.49087900		
H	-7.62829200	2.75193700	0.20563900		
H	-8.07979200	2.50681500	-1.51151000		
H	-9.09252300	3.54374200	-0.45799000		
C	-8.07972800	-4.61699900	0.48980700		
H	-7.45826900	-5.51867400	0.46196400		
H	-8.46250400	-4.47087900	1.51319700		
H	-8.93502300	-4.74413400	-0.19401600		
C	-3.38870400	-0.93400400	-1.40494600		
H	-3.35367500	-1.39917900	-2.40445000		
C	-2.66727900	-1.88600200	-0.42418600		
O	-1.58646300	-2.39817900	-0.90223900		
O	-3.08839400	-2.04074200	0.71035200		
C	-2.59143500	0.39677500	-1.46620800		
H	-3.30891800	1.14847000	-1.82067100		
H	-2.30015100	0.69743300	-0.44466400		
C	-1.38331500	0.45469400	-2.34648600		
C	-1.26623500	1.04328900	-3.57823300		
N	0.04610300	0.88972900	-3.95559400		
H	-1.99664500	1.55790000	-4.19399000		
C	0.69889300	0.24381200	-2.98011500		
H	0.47771900	1.26295600	-4.79115700		
H	1.75939000	-0.02620200	-2.98038000		
N	-0.13992600	-0.03733000	-1.99432200		

C	13.62914200	0.35657500	-0.00468700
H	14.20946900	-0.19273000	-0.76173100
H	13.58360700	1.42259900	-0.29544800
H	14.18810800	0.27022700	0.93962700
C	-13.18680600	-1.02629300	1.29594400
H	-13.42143100	-1.33794500	2.32521400
H	-13.39914500	0.05425000	1.19381700
H	-13.86933200	-1.58546200	0.63786800
H	0.49761400	1.34436000	-0.29655400
C	0.14351900	3.75377200	-0.99484400
O	0.31719300	1.55449200	0.63073400
O	0.34442800	3.11922500	-1.98617200
C	-1.05161600	6.25265900	3.19178600
C	-1.98815300	6.57929300	2.21497100
C	-1.97712000	5.93150300	0.97974200
C	-1.02193200	4.94482000	0.72118100
C	-0.09347200	4.59228600	1.70907500
C	-0.10867200	5.25657500	2.93077600
H	-1.06142400	6.76300200	4.15549400
H	-2.73509700	7.35096500	2.40725200
H	-2.70625300	6.20745800	0.21793800
H	0.59876800	3.77259400	1.51356000
H	0.61640000	4.97772000	3.69697000
N	-1.00008700	4.28484500	-0.53470600
H	0.09650800	0.70412000	1.03128600
C	-2.22276200	4.15882300	-1.32096000
H	-2.48326300	5.10566300	-1.81714300
H	-2.05101400	3.39026500	-2.08381100
H	-3.05141200	3.85165700	-0.66827000

### P4 complex



0 2				Zero-point correction=	0.880611 (Hartree/Particle)
N	-12.29826200	-1.68849000	-0.05517600	Thermal correction to Energy=	0.944338
C	-11.44965000	-0.85306900	0.37955400	Thermal correction to Enthalpy=	0.945282
H	-11.74777900	0.05154100	0.93755400	Thermal correction to Gibbs Free Energy=	0.767506
C	-9.99962200	-1.03325900	0.16927100	Sum of electronic and zero-point Energies=	-4649.331523
C	-9.52859800	-2.15600500	-0.51705500	Sum of electronic and thermal Energies=	-4649.267796
C	-9.08695800	-0.08011200	0.66183700	Sum of electronic and thermal Enthalpies=	-4649.266851
C	-8.16356700	-2.34742900	-0.72280800	Sum of electronic and thermal Free Energies=	-4649.444627
H	-10.27990500	-2.85932700	-0.87394000		
C	-7.72182700	-0.27066800	0.45472500		
C	-7.25187800	-1.39312900	-0.23147600		
H	-6.96767500	0.42610800	0.81924700		
C	-5.79983000	-1.57441600	-0.42654200		
H	-5.48173900	-2.53419000	-0.86813000		
N	-4.97314800	-0.67264400	-0.09246400		
O	-9.60566700	0.98326900	1.32383900		
O	-7.64162700	-3.41156400	-1.38101700		
C	-8.71436900	1.93458200	1.84489100		
H	-8.02465500	1.48274000	2.57604400		
H	-8.12147700	2.41052000	1.04681800		
H	-9.32417100	2.69553700	2.34426500		
C	-8.52426700	-4.39657900	-1.84909800		
H	-7.91021600	-5.16755000	-2.32737800		
H	-9.09723800	-4.84914100	-1.02329500		
H	-9.23179100	-3.98584800	-2.58799500		
C	-3.56828600	-0.93176700	-0.28029200		
H	-3.37750000	-1.88213500	-0.81225900		
C	-2.85186800	-0.98525000	1.09117800		

O	-1.86817200	-1.81731500	1.15632900
O	-3.19357300	-0.21192800	1.96779100
C	-2.97030300	0.25438900	-1.08030800
H	-3.73686800	0.59756400	-1.78824300
H	-2.79636300	1.08509100	-0.37591200
C	-1.72971200	-0.03735400	-1.86334300
C	-1.52739900	0.15650100	-3.20461500
N	-0.22967300	-0.22675600	-3.45632600
H	-2.19054400	0.52888100	-3.97808400
C	0.32356800	-0.64030000	-2.30615000
H	0.24246200	-0.20365200	-4.35091900
H	1.34784600	-1.01234700	-2.19006000
N	-0.55873500	-0.53486000	-1.32577700
Zn	-0.13101300	-1.23945300	0.56558300
N	11.88033800	-2.11033800	-0.93077100
C	11.23382800	-1.33955600	-0.15946700
H	11.73413800	-0.57932300	0.46541800
C	9.76370400	-1.40582600	-0.04311500
C	9.04512200	-2.33979700	-0.79395800
C	9.07935100	-0.53217600	0.82359700
C	7.65641600	-2.41972600	-0.69861000
H	9.62570400	-2.99109700	-1.44597700
C	7.69127400	-0.61164900	0.91785200
C	6.97090600	-1.54281100	0.16568700
H	7.10989400	0.03727500	1.57123300
C	5.49788000	-1.61288400	0.27775300
H	5.00385700	-2.35460700	-0.36336700
N	4.87325000	-0.84039600	1.06800800
O	9.83346100	0.35071200	1.52696900
O	6.90584700	-3.30555700	-1.39439500
C	9.17777000	1.22709400	2.40290400
H	8.46869800	1.87882200	1.86614100
H	8.63027000	0.67909200	3.18740800
H	9.95313300	1.84515700	2.86919700
C	7.55797100	-4.18595300	-2.26971500
H	6.77963800	-4.80501600	-2.72896100
H	8.10152700	-3.64078500	-3.05884800
H	8.26918300	-4.83528600	-1.73311600
C	3.43683000	-0.93382600	1.22268500
H	3.23393400	-1.50685700	2.14175300
C	2.63028300	-1.56725400	0.06998300
O	1.55007000	-2.16547700	0.43527600
O	2.98960100	-1.38761900	-1.08448300
C	2.88818300	0.50695700	1.41442500
H	3.70393300	1.08658200	1.86703500
H	2.69258200	0.93925600	0.41804500
C	1.67591200	0.66158800	2.27733600
C	1.59314400	1.26931600	3.50237300
N	0.27798500	1.17841800	3.88934300
H	2.35269200	1.74835900	4.11108700
C	-0.40994200	0.55526500	2.92486700
H	-0.13336400	1.58638000	4.71870900
H	-1.48361800	0.33913000	2.94506000
N	0.40733200	0.22663900	1.93475700
C	-13.69245900	-1.43519800	0.19655900
H	-14.12387300	-2.28059200	0.75404100
H	-13.87889800	-0.50343300	0.76233900
H	-14.23458800	-1.38362000	-0.76003200
C	13.31239600	-1.97724600	-0.98127700
H	13.62476600	-1.76263100	-2.01470800
H	13.70804600	-1.18559000	-0.31798500
H	13.77973100	-2.93541100	-0.70717000
H	0.17937100	1.64333000	0.25664600
C	-0.30876700	4.05685600	0.96029900
O	0.35681800	1.92960600	-0.66645400
O	-0.25609300	3.34441200	1.93944400
C	0.26110600	6.63630600	-3.33829300
C	1.27226100	6.98357800	-2.44273500
C	1.44400400	6.26646100	-1.26169500
C	0.60562800	5.18422000	-0.97280800
C	-0.38615600	4.81074900	-1.88739400
C	-0.56430200	5.54914500	-3.05534500
H	0.12555400	7.20410600	-4.25944800
H	1.92929800	7.82711000	-2.65928900
H	2.22354100	6.55267300	-0.55486100

H	-0.97729000	3.91464200	-1.69497700
H	-1.34187000	5.25458000	-3.76173400
N	0.77355600	4.45661300	0.23148300
C	2.10991200	4.08834900	0.67106600
H	2.63651800	4.94198800	1.12439800
H	2.01074700	3.29748900	1.42461400
H	2.68809800	3.71427500	-0.18402000
H	-1.26331100	4.45949100	0.56172600

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