

## Supporting Information

# Disclosing the Microscopic Mechanism and Adsorption Properties of CO<sub>2</sub> Capture in N-isopropylethylenediamine Appended M<sub>2</sub>(dobpdc) Series

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**Table S1.** The calculated total energies E (eV) of nonmagnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) states, magnetic moment ( $\mu_B$ ) on each metal atom, and total magnetic moment ( $M_{tot}$ ) per unit cell of bare M<sub>2</sub>(dobpdc), i-2-M<sub>2</sub>(dobpdc) and CO<sub>2</sub>-i-2-M<sub>2</sub>(dobpdc) (M=Mg, Sc-Zn).

		bare M <sub>2</sub> (dobpdc)			i-2-M <sub>2</sub> (dobpdc)			CO <sub>2</sub> -i-2-M <sub>2</sub> (dobpdc)		
		NM	FM	AFM	NM	FM	AFM	NM	FM	AFM
<b>Mg</b>	E	-602.63861	—	—	-717.99188	—	—	-741.62403	—	—
<b>Sc</b>	1	0	0.763	0.763	0	0.706	0.705	0	0.755	0.755
	2	0	0.764	0.764	0	0.758	0.758	0	0.619	0.619
	3	0	0.764	0.764	0	0.514	0.513	0	0.085	0.085
	4	0	0.763	-0.763	0	0.754	-0.754	0	0.73	-0.73
	5	0	0.764	-0.764	0	0.756	-0.756	0	0.76	-0.76
	6	0	0.764	-0.764	0	0.749	-0.749	0	0.76	-0.76
	$M_{tot}$	0	5.039	0	0	4.856	-0.2	0	4.708	-0.321
	E	-617.18732	-618.18644	-618.18536	-732.45058	-733.48321	-733.48201	-756.57349	-757.15017	-757.14906
<b>Ti</b>	1	0	1.698	1.698	0	1.671	1.669	0	1.671	1.673
	2	0	1.698	1.698	0	1.672	1.672	0	1.655	1.683
	3	0	1.698	1.698	0	1.621	1.622	0	1.591	1.589
	4	0	1.698	-1.698	0	1.694	-1.694	0	1.692	-1.691
	5	0	1.698	-1.698	0	1.696	-1.696	0	1.698	-1.698
	6	0	1.698	-1.698	0	1.695	-1.696	0	1.693	-1.694
	$M_{tot}$	0	10.644	0	0	10.574	-0.059	0	10.559	-0.058
	E	-621.15931	-623.67881	-623.67909	-736.54050	-739.06248	-739.05951	-760.06054	-762.55774	-762.53817
<b>V</b>	1	0	2.828	2.828	0	2.822	2.808	0	2.822	2.815

	2	0	2.828	2.828	0	2.826	2.814	0	2.826	2.815
	3	0	2.828	2.828	0	2.822	-0.961	0	2.823	-0.989
	4	0	2.828	-2.828	0	2.828	-2.828	0	2.828	-2.828
	5	0	2.828	-2.828	0	2.827	-2.827	0	2.827	-2.828
	6	0	2.828	-2.828	0	2.828	-2.828	0	2.827	-2.827
	M <sub>tot</sub>	0	17.005	0	0	16.993	-3.808	0	17	-3.812
	E	-610.93827	-623.01889	-623.01893	-726.67462	-738.55029	-737.75614	-750.09828	-762.05027	-761.25830
Cr	1	0	3.823	3.823	0	3.823	3.823	0	3.822	3.822
	2	0	3.823	3.823	0	3.823	3.823	0	3.822	3.822
	3	0	3.823	3.823	0	3.82	3.82	0	3.824	3.824
	4	0	3.823	-3.823	0	3.824	-3.824	0	3.823	-3.823
	5	0	3.823	-3.823	0	3.824	-3.824	0	3.824	-3.824
	6	0	3.823	-3.823	0	3.823	-3.823	0	3.822	-3.821
	M <sub>tot</sub>	0	22.805	0	0	22.825	0.017	0	22.834	0.029
E	-607.52638	-625.94929	-625.94915	-722.84902	-741.00324	-741.00225	-746.29439	-764.53468	-764.53550	
Mn	1	0	4.632	4.632	0	4.629	4.629	0	4.631	4.633
	2	0	4.632	4.632	0	4.634	4.633	0	4.632	4.639
	3	0	4.631	4.632	0	4.643	4.643	0	4.645	4.637
	4	0	4.632	-4.632	0	4.631	-4.63	0	4.631	-4.631
	5	0	4.632	-4.632	0	4.633	-4.632	0	4.633	-4.632
	6	0	4.631	-4.632	0	4.631	-4.63	0	4.63	-4.63
	M <sub>tot</sub>	0	28.564	0	0	28.581	0.013	0	28.589	0.012
E	-601.23761	-624.33141	-624.33617	-716.52826	-739.62940	-739.62594	-739.89192	-763.19802	-763.19305	
Fe	1	0	3.735	3.735	0	3.735	3.735	0	3.734	3.733
	2	0	3.735	3.735	0	3.735	3.734	0	3.731	3.731
	3	0	3.735	3.735	0	3.751	3.75	0	3.759	3.758
	4	0	3.735	-3.735	0	3.735	-3.734	0	3.735	-3.735
	5	0	3.735	-3.735	0	3.737	-3.736	0	3.737	-3.737
	6	0	3.735	-3.735	0	3.734	-3.734	0	3.734	-3.734
	M <sub>tot</sub>	0	23.386	0	0	23.402	0.016	0	23.407	0.022
E	-600.67892	-613.35593	-613.34910	-716.25356	-728.68899	-728.68698	-739.59510	-752.17401	-752.17535	
Co	1	0	2.688	2.687	0	2.688	-0.999	0	2.687	1.004
	2	0	2.688	2.687	0	2.688	2.691	0	2.682	-0.995
	3	0	2.688	2.687	0	2.717	2.712	0	2.731	2.729
	4	0	2.688	-2.687	0	2.685	-2.684	0	2.686	-2.684
	5	0	2.688	-2.687	0	2.689	-2.688	0	2.691	-2.688
	6	0	2.688	-2.687	0	2.686	-2.683	0	2.685	-2.684
	M <sub>tot</sub>	0	17.533	0	0	17.549	-3.886	0	17.552	-5.82
E	-594.02985	-603.13903	-603.14027	-709.49953	-718.46554	-717.90536	-732.73641	-741.91145	-740.81157	

<b>Ni</b>	1	0	1.792	1.792	0	1.793	1.793	0	1.791	1.791
	2	0	1.792	1.792	0	1.795	1.794	0	1.790	1.790
	3	0	1.792	1.792	0	1.797	1.797	0	1.813	1.813
	4	0	1.792	-1.792	0	1.791	-1.791	0	1.791	-1.791
	5	0	1.792	-1.792	0	1.792	-1.792	0	1.792	-1.792
	6	0	1.792	-1.792	0	1.791	-1.790	0	1.790	-1.790
	M <sub>tot</sub>	0	11.840	0	0	11.845	0.007	0	11.857	0.019
	E	-584.97719	-590.44668	-590.44764	-700.26965	-705.90009	-705.90096	-723.39517	-729.31908	-729.31941
<b>Cu</b>	1	0	0.614	0.612	0	0.615	0.612	0	0.618	-0.616
	2	0	0.614	0.612	0	0.615	-0.609	0	0.615	-0.612
	3	0	0.614	0.612	0	0.652	-0.648	0	0.653	-0.651
	4	0	0.614	-0.612	0	0.612	0.612	0	0.613	0.611
	5	0	0.614	-0.612	0	0.613	0.612	0	0.614	0.612
	6	0	0.614	-0.612	0	0.613	0.611	0	0.614	0.612
	M <sub>tot</sub>	0	5.617	0	0	5.623	1.863	0	5.629	-0.015
	E	-581.24204	-583.03377	-583.04411	-696.07513	-698.15057	-698.15172	-719.59135	-721.55560	-721.56716
<b>Zn</b>	E	-582.66110	—	—	-698.20007	—	—	-721.60287	—	—

**Table S2.** Computed lattice parameters ( $a$ ,  $b$ ,  $c$  in Å) and unit cell volumes ( $V$  in Å<sup>3</sup>) for M<sub>2</sub>(dobpdc), i-2-M<sub>2</sub>(dobpdc) and CO<sub>2</sub>-i-2-M<sub>2</sub>(dobpdc) (M=Mg, Sc-Zn).

M	bare			i-2-MOF				CO <sub>2</sub> -i-2-MOF			
	$a=b$	$c$	$V$	$a$	$b$	$c$	$V$	$a$	$b$	$c$	$V$
Mg	21.562	6.865	2763.185	21.007	22.096	6.828	2716.778	20.617	22.199	6.844	2678.900
Sc	22.008	7.348	3079.520	21.700	22.405	7.258	2998.205	20.858	22.610	7.243	2909.417
Ti	21.738	7.106	2905.493	21.302	22.230	7.054	2842.047	20.854	22.297	7.059	2785.721
V	21.667	7.058	2867.533	21.089	22.257	7.013	2810.950	21.040	22.232	7.021	2769.176
Cr	21.874	6.534	2705.074	21.474	22.119	6.470	2650.100	21.090	22.053	6.515	2607.962
Mn	21.761	7.028	2884.095	21.463	22.327	6.922	2823.934	20.925	22.224	6.927	2759.851
Fe	21.709	6.859	2798.241	21.080	22.347	6.808	2742.601	20.631	22.289	6.838	2688.097
Co	21.550	6.787	2727.426	21.035	22.041	6.777	2687.068	20.416	22.058	6.796	2634.493
Ni	21.451	6.723	2677.874	20.812	22.061	6.707	2636.196	20.371	22.000	6.729	2580.455
Cu	21.687	6.121	2491.816	21.222	21.799	6.191	2455.128	20.946	21.744	6.196	2428.113
Zn	21.632	6.703	2714.944	21.338	22.025	6.391	2589.460	20.799	21.942	6.490	2552.740

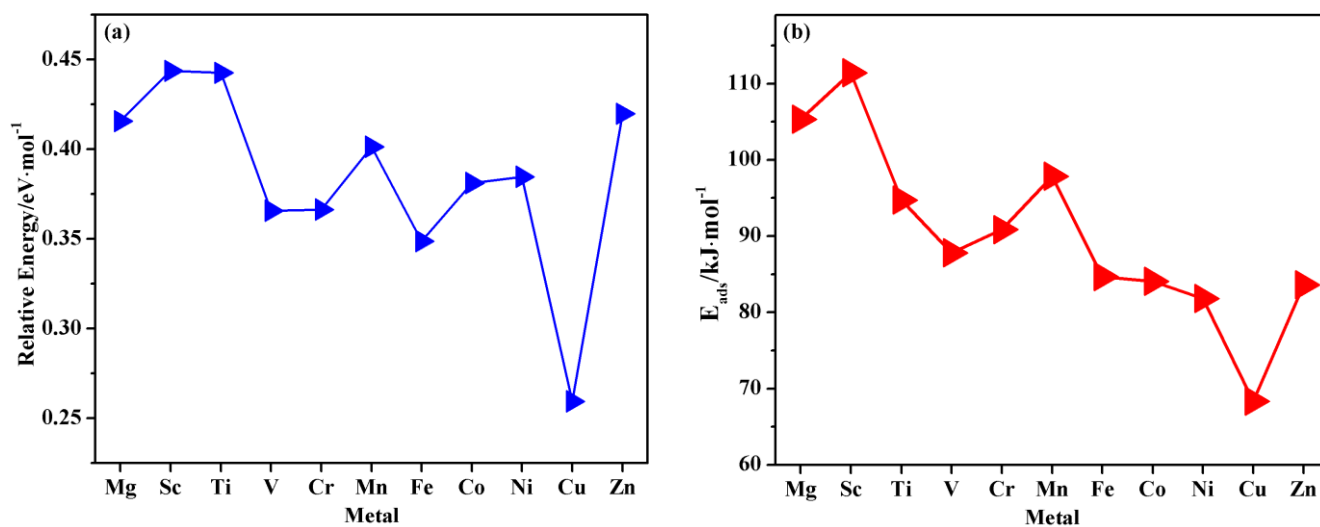


**Table S3.** The experimental values of lattice parameters ( $a$ ,  $b$ ,  $c$  in Å) and unit cell volumes ( $V$  in Å<sup>3</sup>) for available experimental structures of M<sub>2</sub>(dobpdc), i-2-M<sub>2</sub>(dobpdc) and CO<sub>2</sub>-i-2-M<sub>2</sub>(dobpdc) (M=Mg, Sc–Zn).

M	bare			i-2-M			CO <sub>2</sub> -i-2-M		
	$a=b$	$c$	V	$a=b$	$c$	V	$a=b$	$c$	V
Mg	21.446	6.824	2718	—	—	—	—	—	—
Sc	—	—	—	—	—	—	—	—	—
Ti	—	—	—	—	—	—	—	—	—
V	—	—	—	—	—	—	—	—	—
Cr	—	—	—	—	—	—	—	—	—
Mn	21.629	6.958	2819	—	—	—	—	—	—
Fe	21.848	6.814	2817	—	—	—	—	—	—
Co	21.537	6.798	2731	—	—	—	—	—	—
Ni	21.579	6.809	2745	—	—	—	—	—	—
Cu	—	—	—	—	—	—	—	—	—
Zn	21.547	6.775	2724	21.682	6.874	2799	21.652	6.839	2777

**Table S4.** The binding energies ( $E_b$ ) of i-2 with  $M_2(\text{dobpdc})$  and  $\text{CO}_2$  with i-2- $M_2(\text{dobpdc})$ , and the bond lengths (d) of M-N bond in i-2- $M_2(\text{dobpdc})$  and O-M bond in  $\text{CO}_2$ -i-2- $M_2(\text{dobpdc})$  (M=Mg, Sc-Zn).

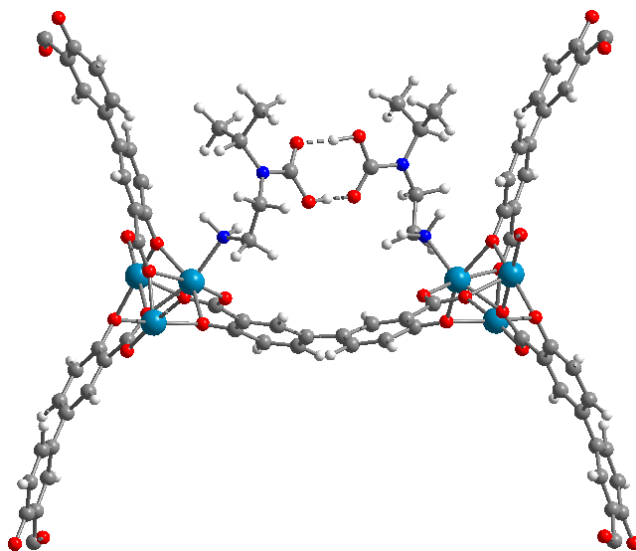
M	$E_b$ (kJ/mol)		d (Å)	
	i-2	$\text{CO}_2$	M-N	O-M
Mg	160.41	65.25	2.226	2.033
Sc	154.96	68.61	2.399	2.144
Ti	163.34	52.04	2.316	2.163
V	177.60	52.49	2.260	2.153
Cr	131.53	55.53	2.349	2.312
Mn	155.08	59.12	2.268	2.116
Fe	158.46	51.05	2.224	2.113
Co	157.83	47.27	2.153	2.048
Ni	170.07	44.68	2.139	2.038
Cu	137.60	43.33	2.135	2.236
Zn	178.33	43.12	2.084	2.011



**Fig. S1.** (a) The relative energies of experimental motif  $\text{CO}_2\text{-i-2-M}_2(\text{dobpdc})\text{-I}$  (see Fig.3) and present study discovered more stable conformation  $\text{CO}_2\text{-i-2-M}_2(\text{dobpdc})\text{-II}$  ( $M=\text{Mg}, \text{Sc-Zn}$ ), and (b) the binding energies of  $\text{CO}_2$  in  $\text{i-2-M}_2(\text{dobpdc})$  ( $M=\text{Mg}, \text{Sc-Zn}$ ) for the more stable conformation.

**Table S5.** The binding energies ( $E_b$ ) and bond lengths of  $\text{O-M}$  bond ( $d_{\text{O-M}}$ ) in present study discovered more stable conformation  $\text{CO}_2\text{-i-2-M}_2(\text{dobpdc})\text{-II}$  (see Fig.3) ( $M=\text{Mg}, \text{Sc-Zn}$ ).

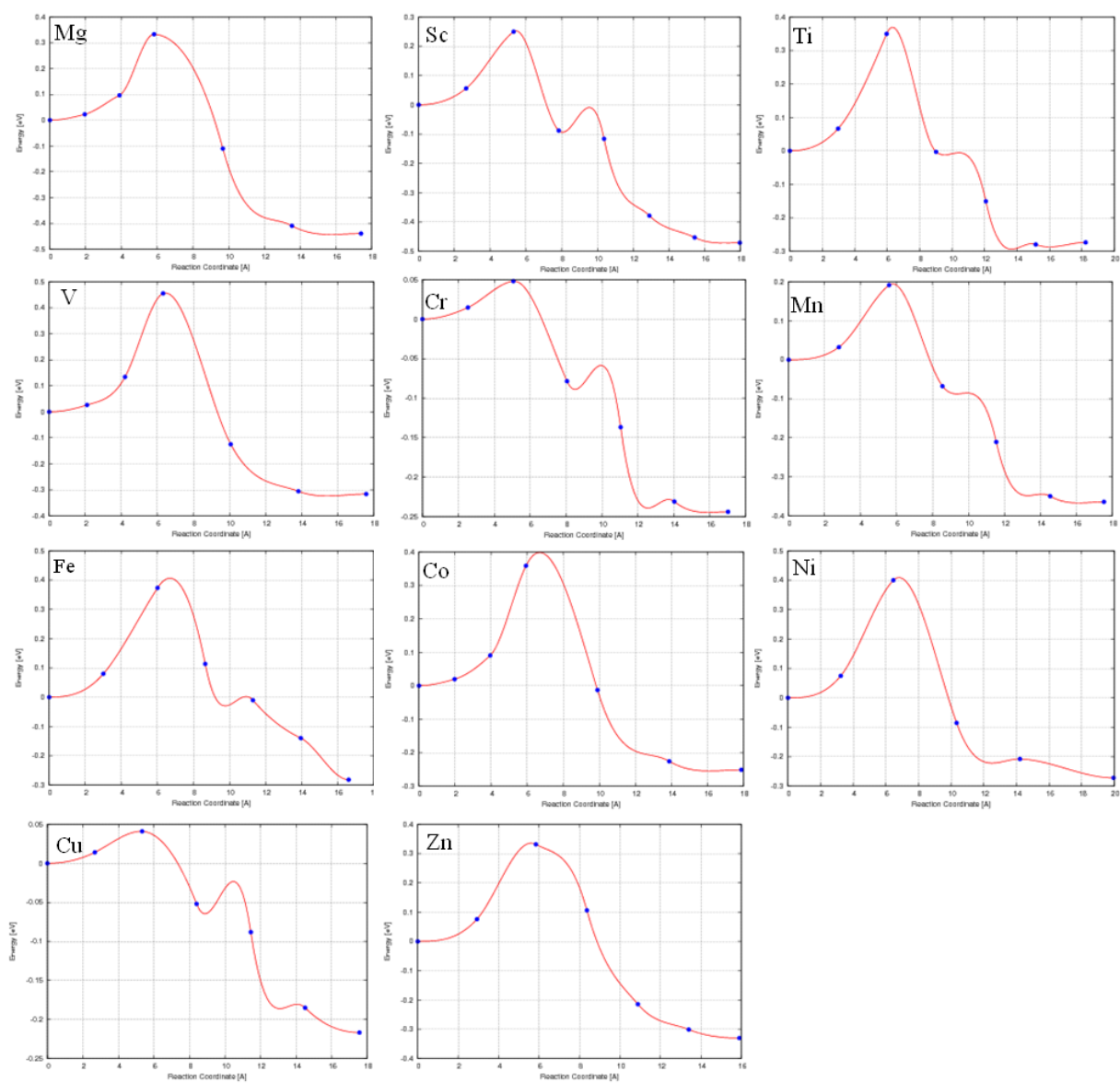
	Mg	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
$E_b(\text{kJ/mol})$	105.34	111.41	94.73	87.79	90.87	97.84	84.69	84.05	81.78	68.36	83.61
$d_{\text{O-M}}(\text{\AA})$	2.018	2.120	2.154	2.143	2.255	2.080	2.120	2.058	2.053	2.166	1.990



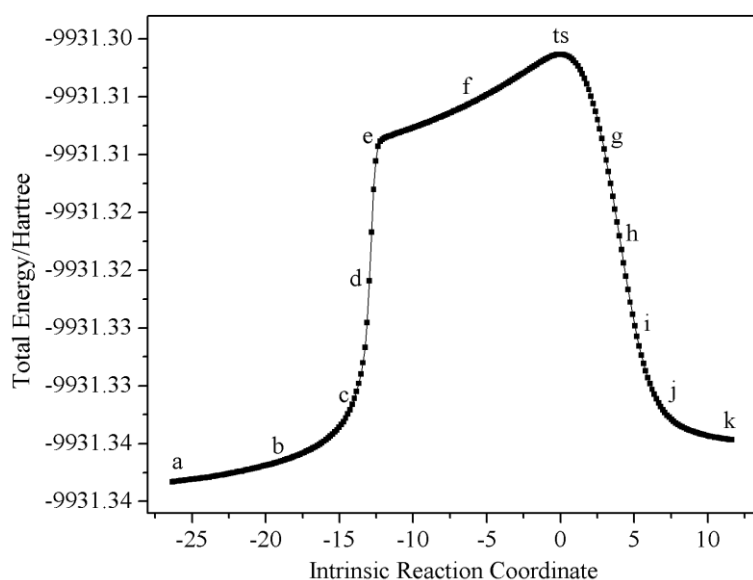
**Fig. S2.** The “pairs structure” proposed by Planas et al. of CO<sub>2</sub> adsorption on i-2-Zn<sub>2</sub>(dobpdc).

**Table S6.** The CO<sub>2</sub> binding energies ( $E_b$ : kJ/mol) of pair model and the difference of  $E_b$  for pair model and the experimental chain model.

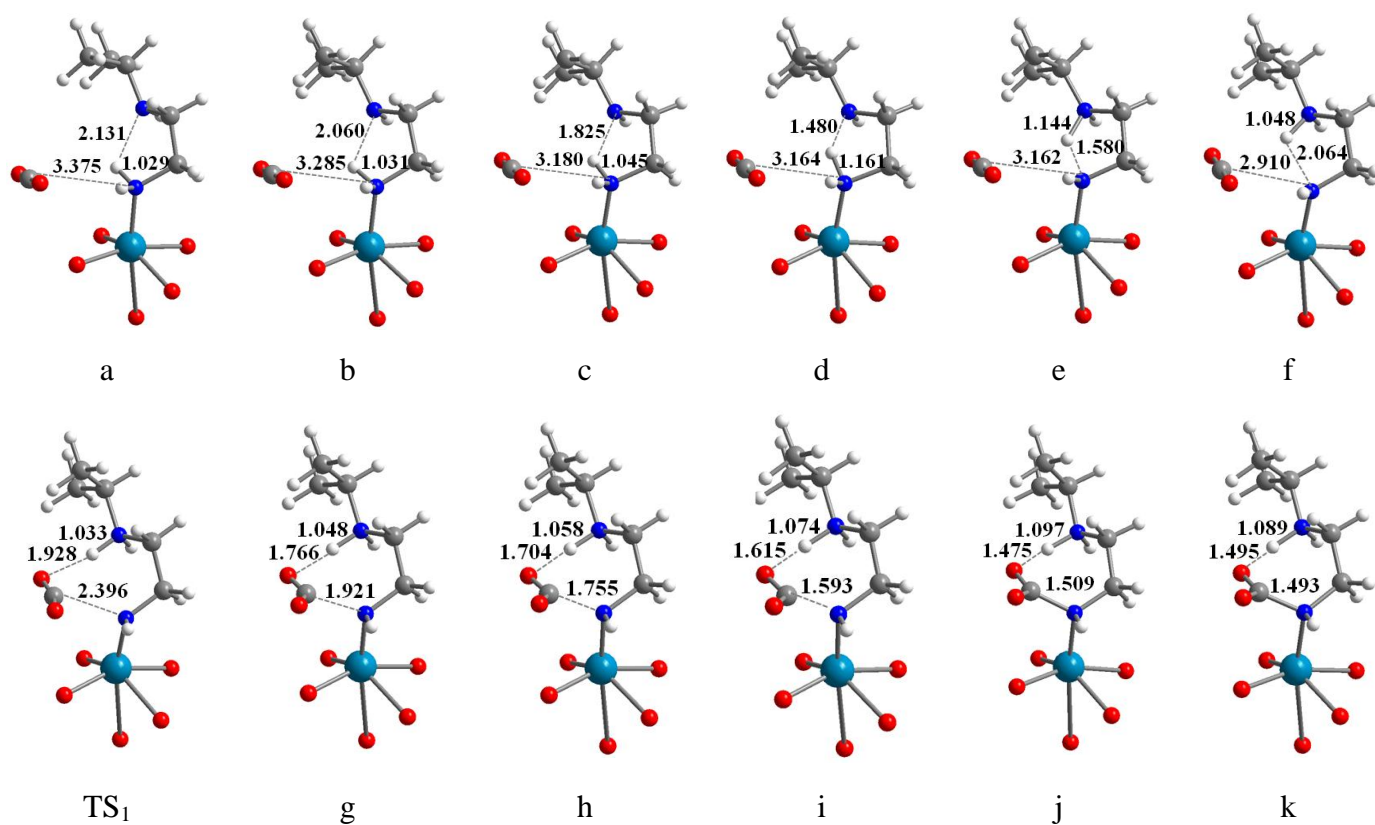
	Mg	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
pair model	42.23	46.85	43.85	41.88	39.53	48.77	38.72	39.63	37.48	35.24	19.47
difference	23.02	21.76	8.18	10.62	16.00	10.35	12.33	7.65	7.20	8.10	23.65



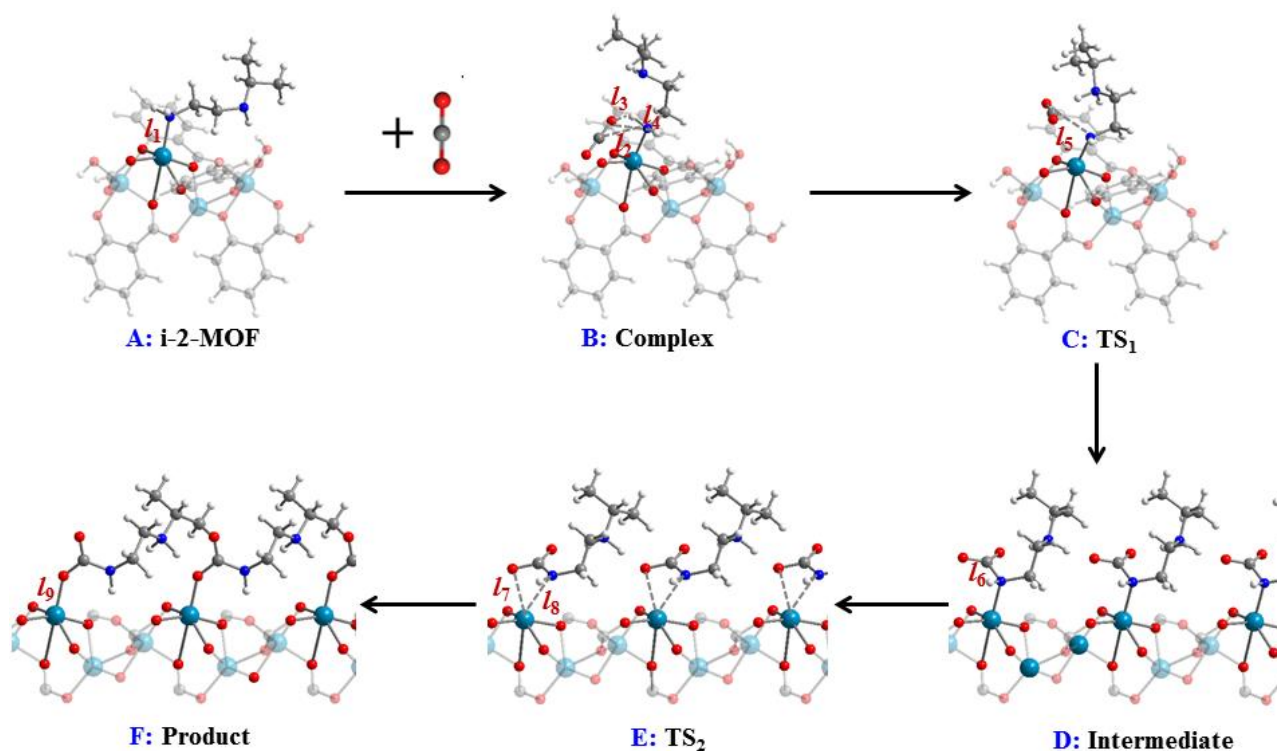
**Fig. S3.** The energy profiles of different images during the climbing image nudged elastic band (CI-NEB) calculations.



**Fig. S4.** The detailed Intrinsic Reaction Coordinate (IRC) curves of the transition state (TS<sub>1</sub>) of CO<sub>2</sub> adsorption in *i*-2-Zn<sub>2</sub>(dobpdc).



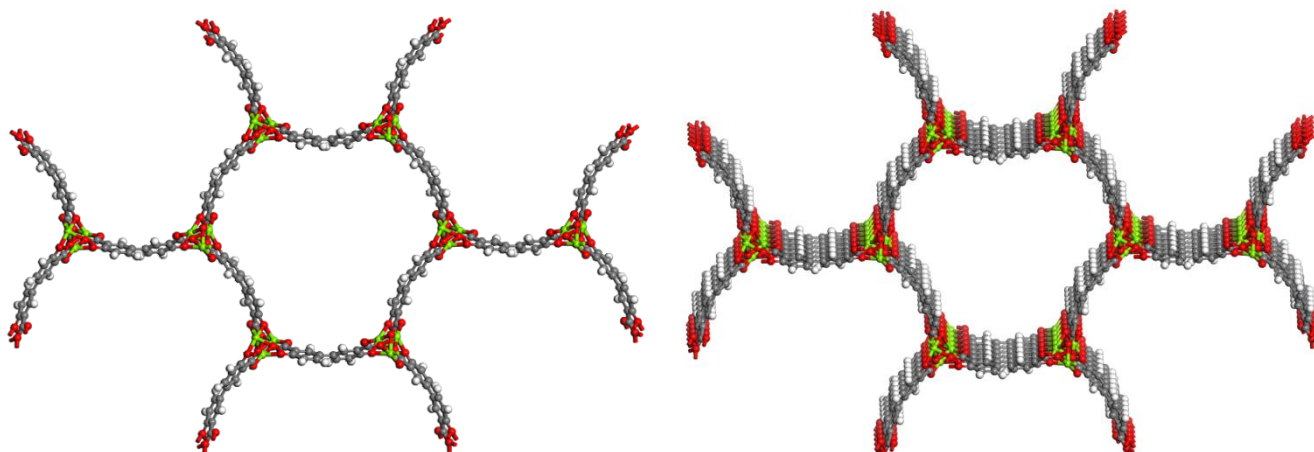
**Fig. S5.** The illustrative structures of selected points along the IRC of the transition state (TS<sub>1</sub>) of CO<sub>2</sub> adsorption in *i*-2-Zn<sub>2</sub>(dobpdc). Cyan blue, red, blue, gray, and white spheres represent Zn, O, N, C, and H atoms, respectively. The bond lengths are in Å.



**Fig. S6.** The key distances ( $l_i$  in Å) between two atoms of important intermediates of CO<sub>2</sub> adsorption in  $i-2-M_2(\text{dobpdc})$  ( $M=\text{Mg, Sc-Zn}$ ) are given in the bottom table with the above corresponding structures of important intermediates in reaction process.

	$l_1(\text{N-M})$	$l_2(\text{C-N})$	$l_3(\text{H-O})$	$l_4(\text{H-O})$	$l_5(\text{C-N})$	$l_6(\text{C-N})$	$l_7(\text{O-M})$	$l_8(\text{N-M})$	$l_9(\text{O-M})$
Mg	2.218	4.021	2.441	3.246	2.505	1.473	2.760	2.910	2.033
Sc	2.332	3.743	3.255	2.404	2.256	1.480	2.919	2.687	2.144
Ti	2.272	4.137	2.631	3.167	2.431	1.475	3.047	2.703	2.163
V	2.208	3.857	2.810	3.122	2.390	1.481	2.813	2.938	2.153
Cr	2.179	3.976	2.576	2.945	2.368	1.434	3.195	3.055	2.312
Mn	2.090	3.984	2.523	3.105	2.565	1.473	2.787	2.564	2.116
Fe	2.010	4.289	2.836	3.303	2.549	1.469	2.957	2.986	2.113
Co	1.951	4.186	2.739	3.152	2.398	1.469	2.984	2.864	2.048
Ni	1.903	3.894	2.934	2.579	2.408	1.476	3.102	3.057	2.038
Cu	2.253	3.870	2.500	2.991	2.420	1.417	3.345	3.209	2.236
Zn	2.090	3.885	2.525	2.913	2.396	1.483	2.557	2.878	2.011

The optimized geometry structures and corresponding lattices and coordinates (in VASP format) are listed below:



front view

oblique view

Mg<sub>2</sub>(dobpdc)

1.00000000000000

21.5622144298226672 -0.0061177974149995 0.0002390088389067

-10.7864053828879243 18.6703665593549673 -0.0002390088389067

0.0000746199744972 -0.0000430818623629 6.8649102810386049

Mg O C H

6 18 42 18

Direct

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0.2804895678449739 0.6230311640816524 0.1422979362980428

0.3768964627581539 0.6573213751748810 0.4756357055045441

0.7194382136860540 0.3426646126153869 0.1910513972736112

0.6230311640816524 0.2804895678449739 0.8577020487019595

0.6573213751748810 0.3768964627581539 0.5243642944954559

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0.3665444817686279 0.7132218720965469 0.2471804240854567

0.3927403577100677 0.7951659475161748 0.0157945838355218

0.2448708063028491 0.6665728260722190 0.9404582618148112

0.2867284085854038 0.6531595698204029 0.5804828686849461

0.2047587789502927 0.5973380601507117 0.3491610096149671

0.3333485713838655 0.5781241602045668 0.2738137545570538

0.3467408247580295 0.6333921014054624 0.9138072000506341

0.4025833487291024 0.6073137461464171 0.6825158389778565

0.7551230959419826 0.4218623937637105 0.3928603158548682

0.7132218720965469 0.3665444817686279 0.7528195759145433

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0.6665728260722190 0.2448708063028491 0.0595417231851911

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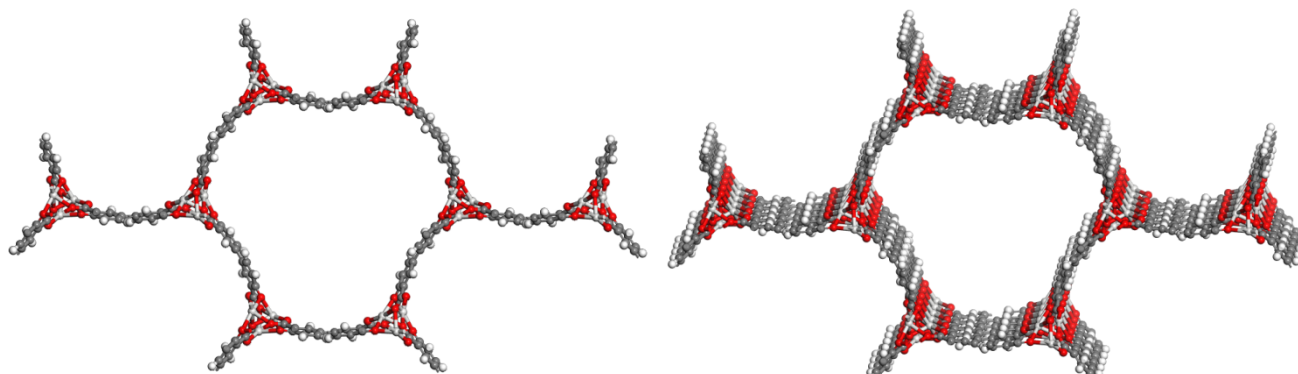
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0.6333921014054624 0.3467408247580295 0.0861928139493671



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front view

oblique view

Sc<sub>2</sub>(dobpdc)

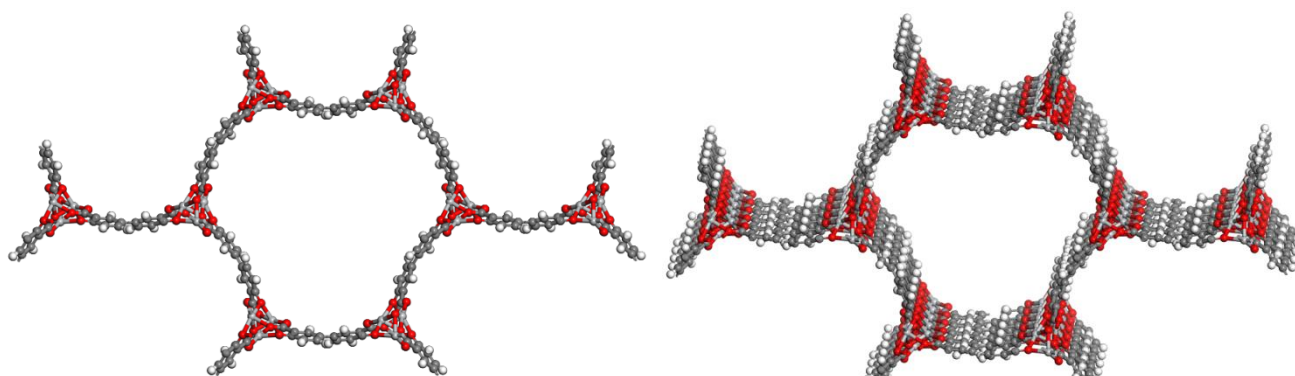
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front view

oblique view

Ti<sub>2</sub>(dobpdc)

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Ti O C H

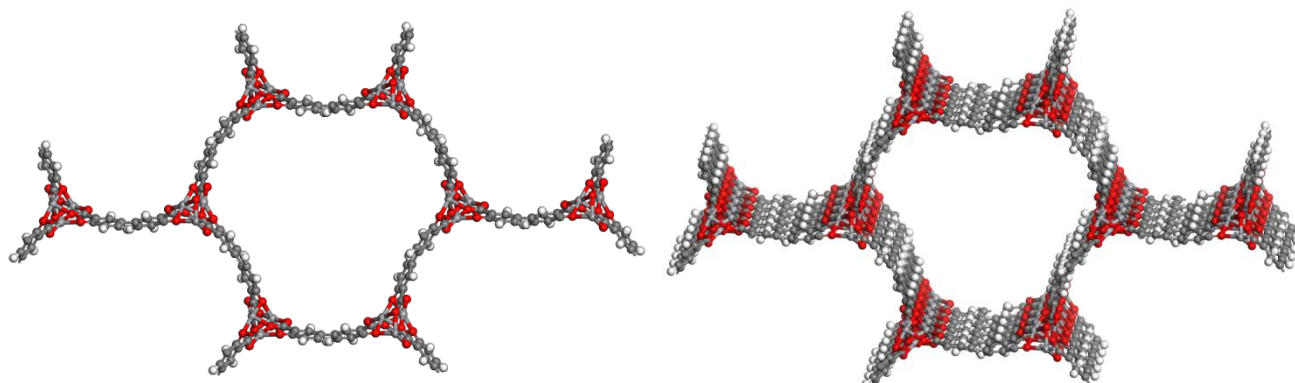
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front view

oblique view

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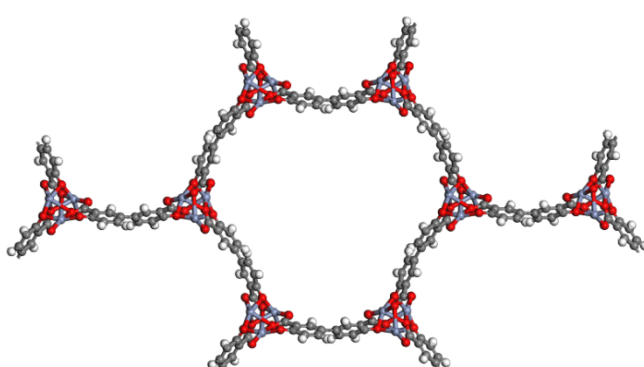
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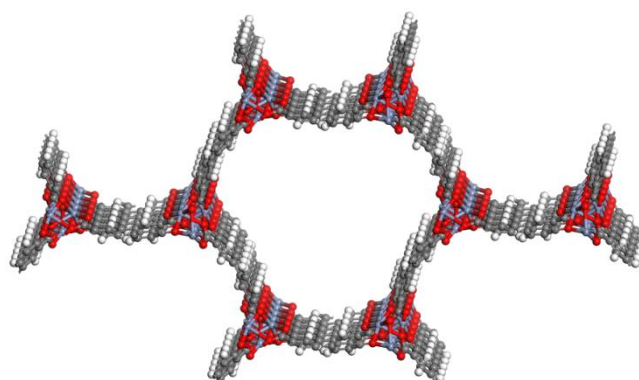
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front view



oblique view

Cr<sub>2</sub>(dobpdc)

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Cr O C H

6 18 42 18

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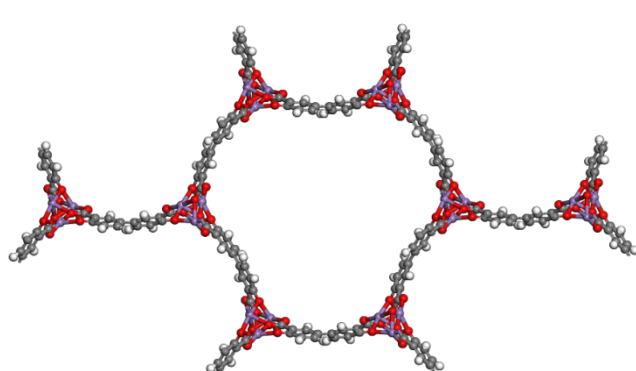
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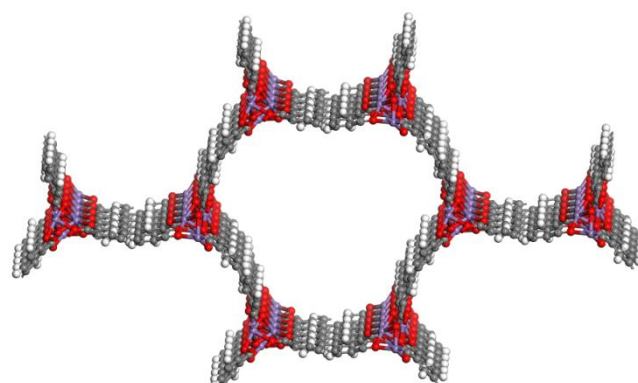
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front view



oblique view

Mn<sub>2</sub>(dobpdc)

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Mn O C H

6 18 42 18

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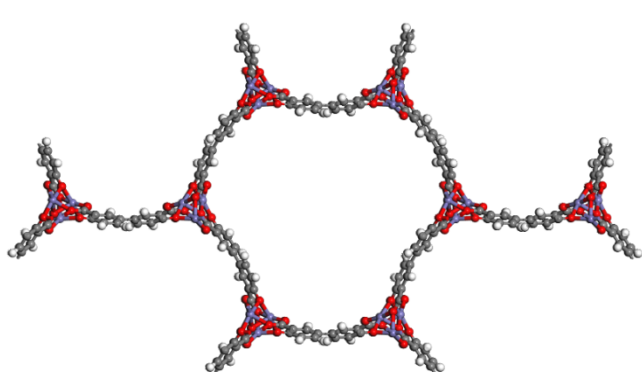
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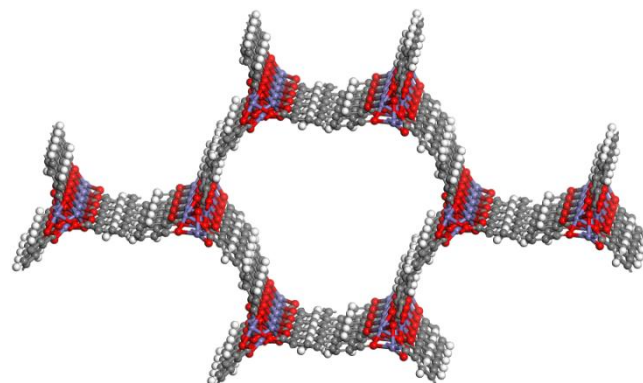
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front view



oblique view

Fe<sub>2</sub>(dobpdc)

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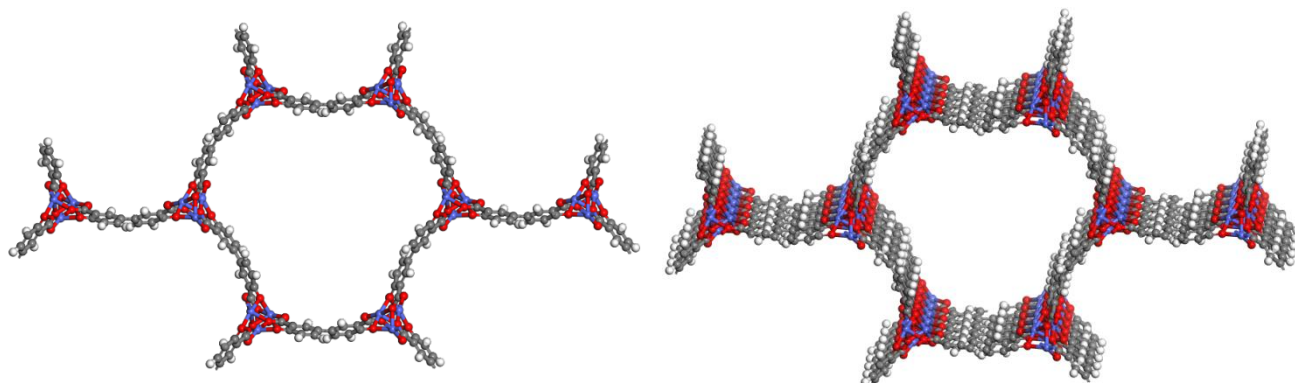
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Fe	O	C	H
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Direct

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front view

oblique view

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Co O C H

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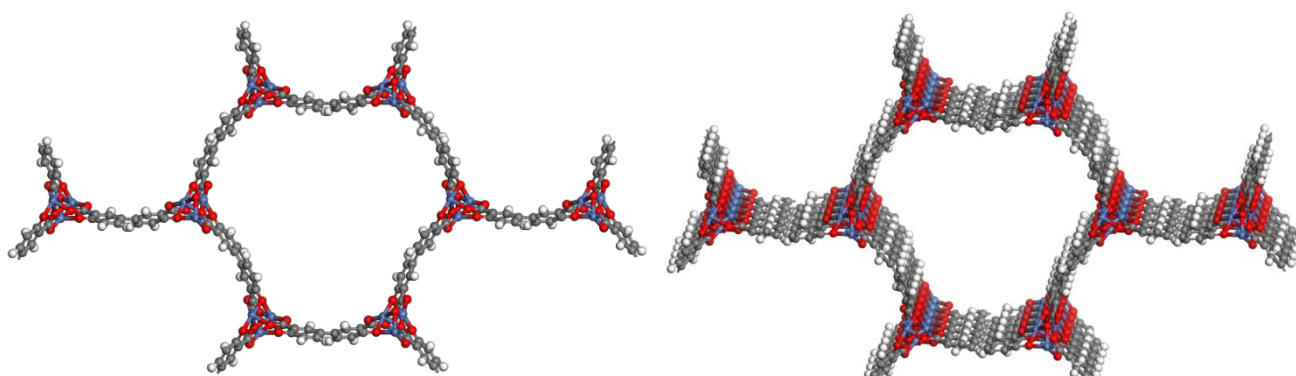
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front view

oblique view

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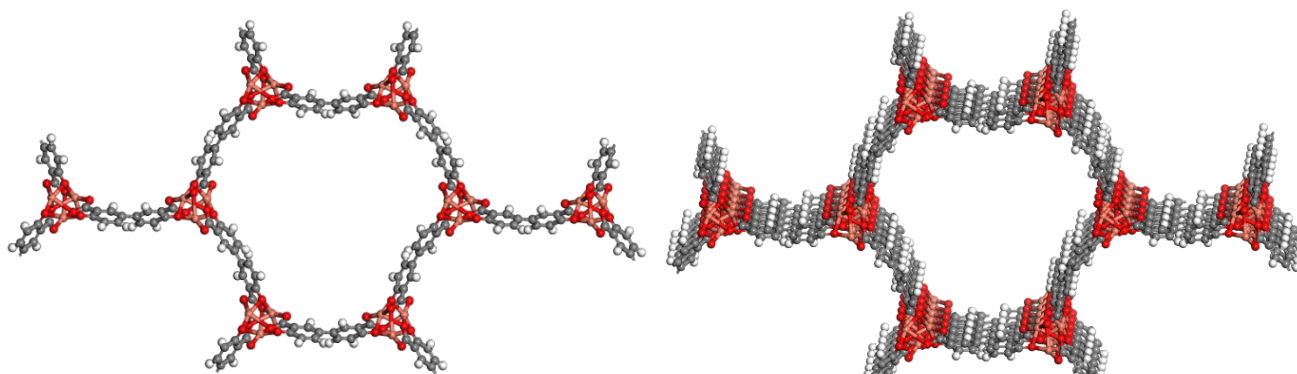
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front view

oblique view

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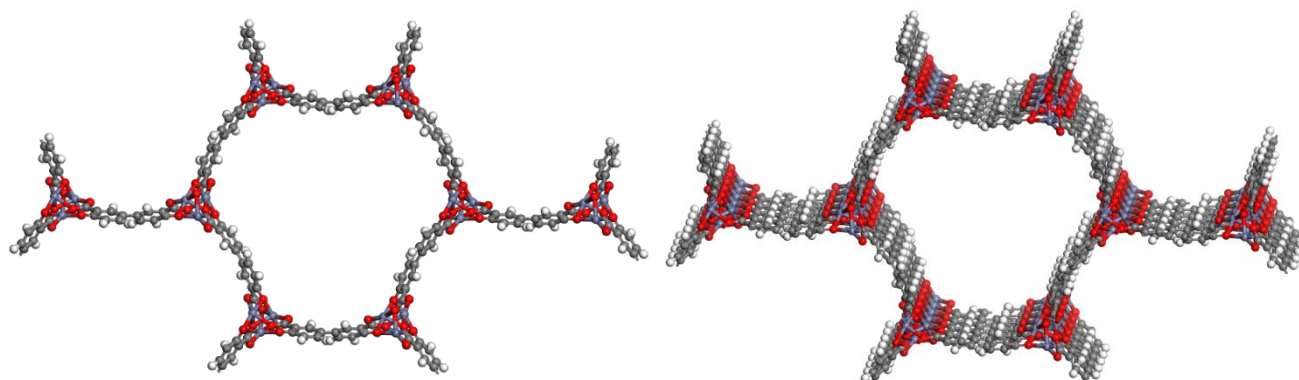
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front view

oblique view

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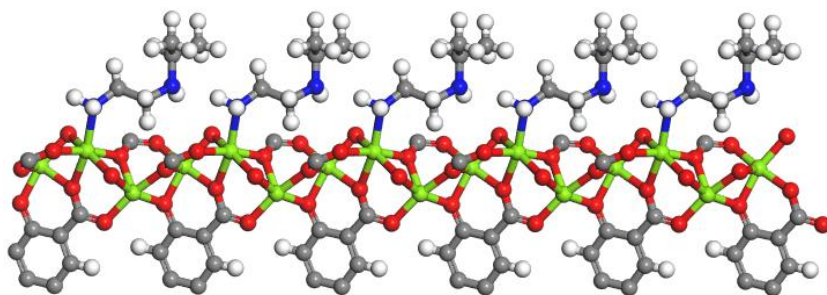
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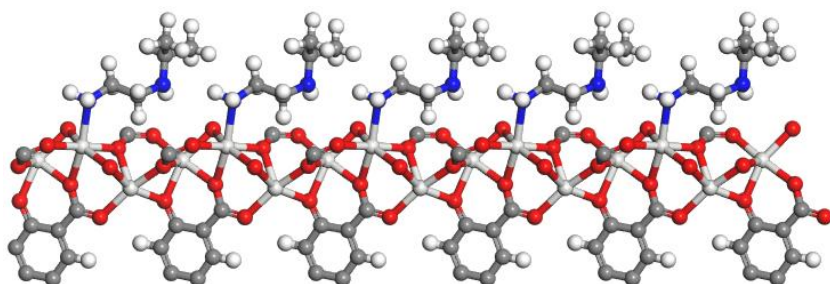
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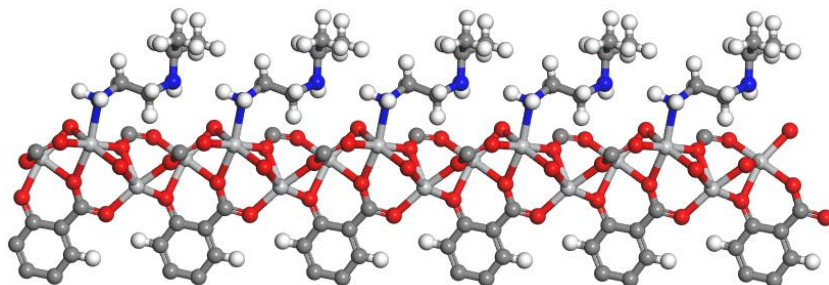
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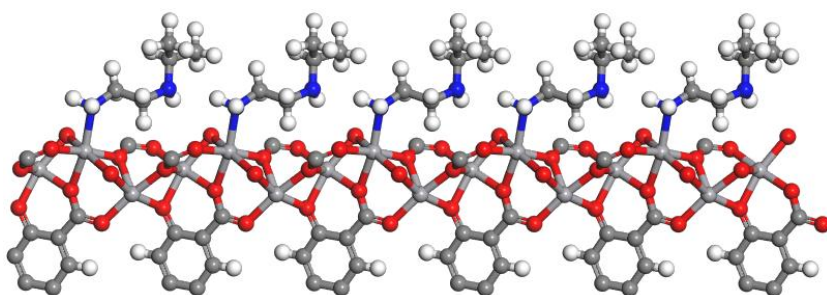
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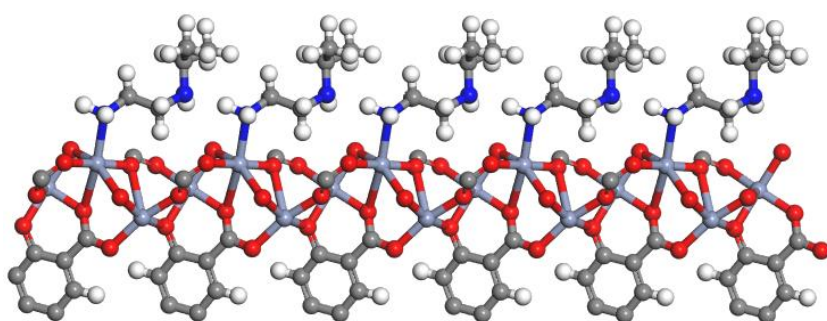
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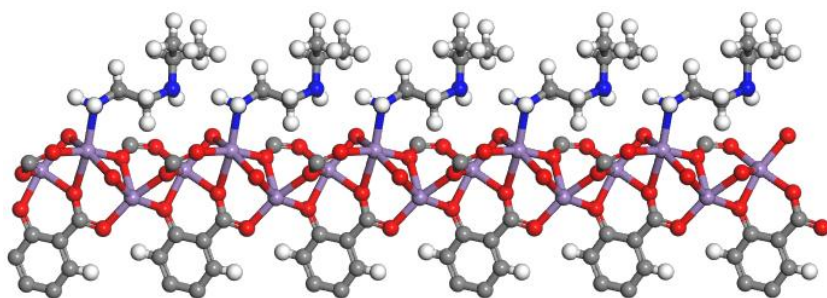
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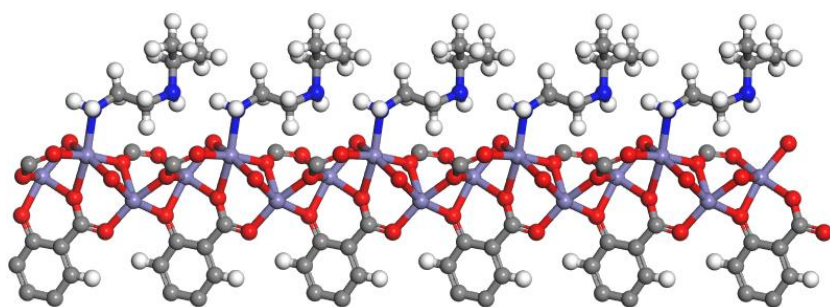
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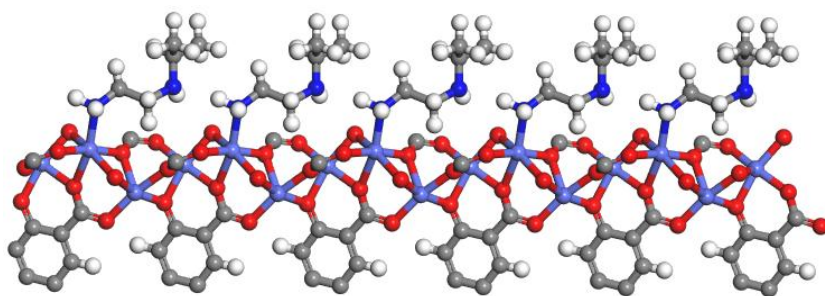
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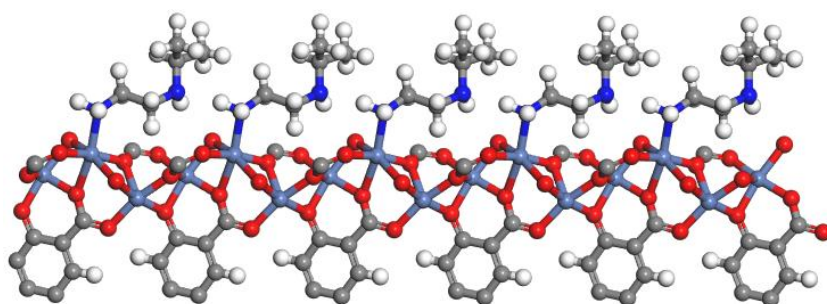
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i-2-Ni<sub>2</sub>(dobpdc)

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6 18 47 32 2

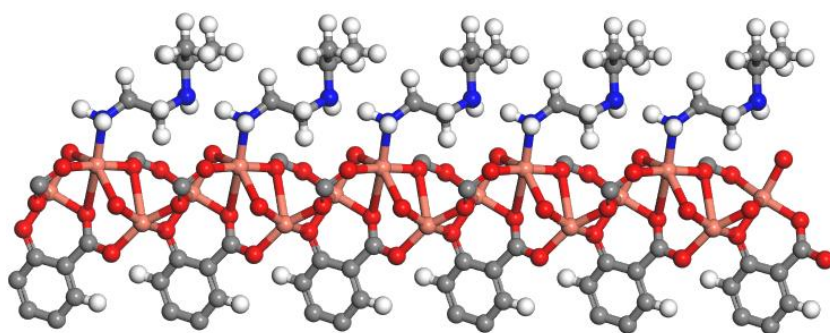
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i-2-Cu<sub>2</sub>(dobpdc)

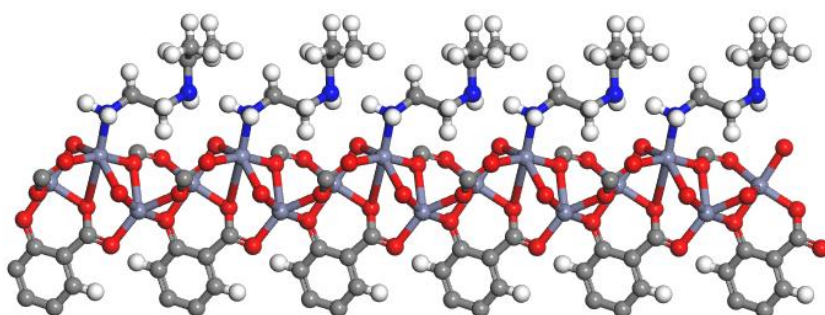
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i-2-Zn<sub>2</sub>(dobpdc)

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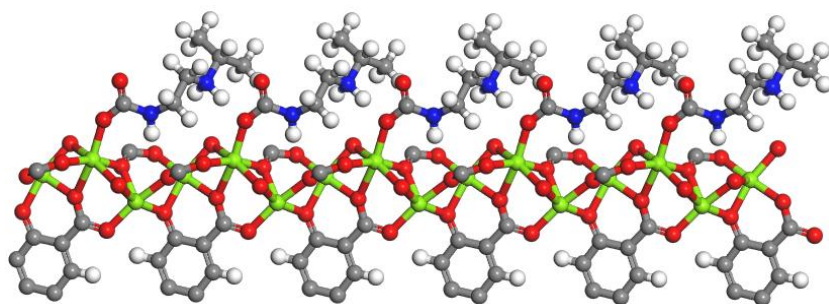
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0.5852818493354306	0.4185319243114307	0.3570654925149981
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0.0652684684155389	0.5677437015193902	0.4432011296703990
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experimental-CO<sub>2</sub>-i-2-Mg<sub>2</sub>(dobpdc)

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Mg	O	C	H	N
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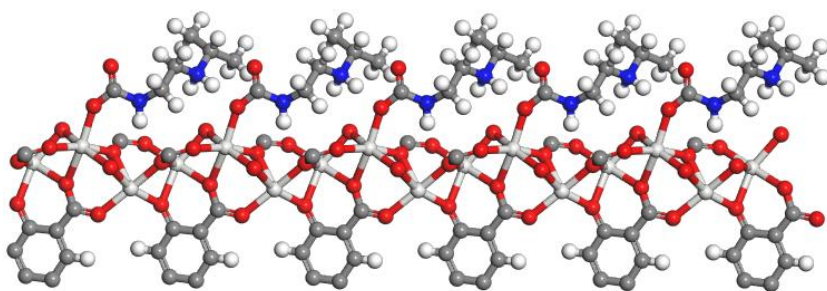
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0.5895380612893817	0.2922225156322469	0.8846079221983629
0.6192409717387761	0.3853082449314726	0.5508042517669480
0.4286760832595533	0.7847687365030609	0.6279070834053115
0.3676201663108785	0.7428632026180964	0.2628620952572760
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0.2413360562286542	0.7012820122575079	0.9580178289646497
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0.3208628690147748	0.6055170158882106	0.2887524505252017
0.3417754981054912	0.6617405208536340	0.9351509569873144
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0.5348006726895207	0.3357311458642087	0.7504487433544185
0.5944071737349006	0.3532119453591918	0.1139978272665871
0.5635106116393587	0.4051384878589133	0.3423117968262375
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experimental-CO<sub>2</sub>-i-2-Sc<sub>2</sub>(dobpdc)

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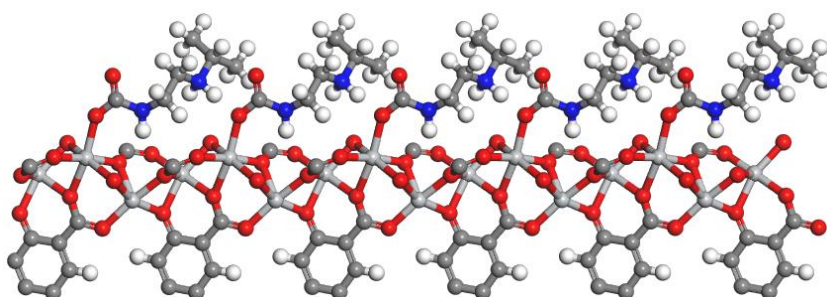
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Direct

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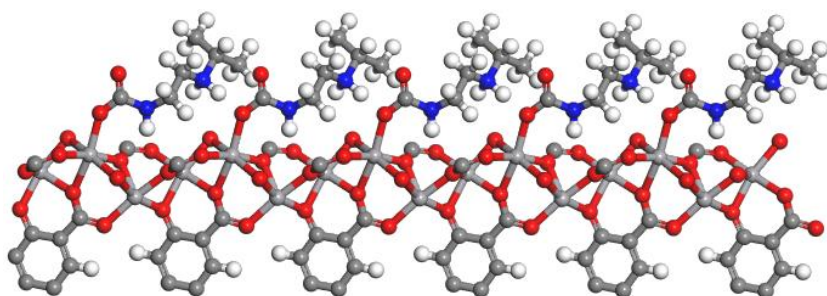
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Direct

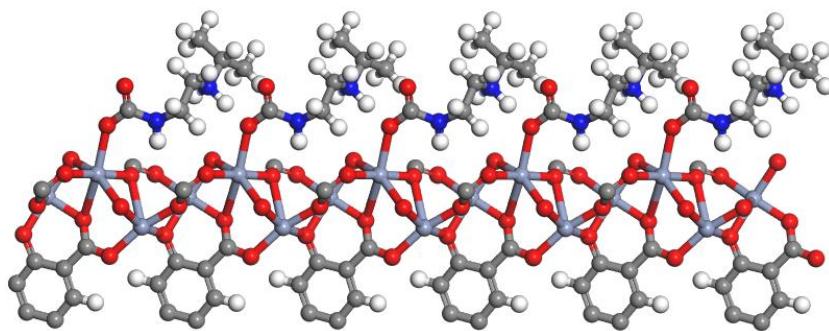
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experimental-CO<sub>2</sub>-i-2-Cr<sub>2</sub>(dobpdc)

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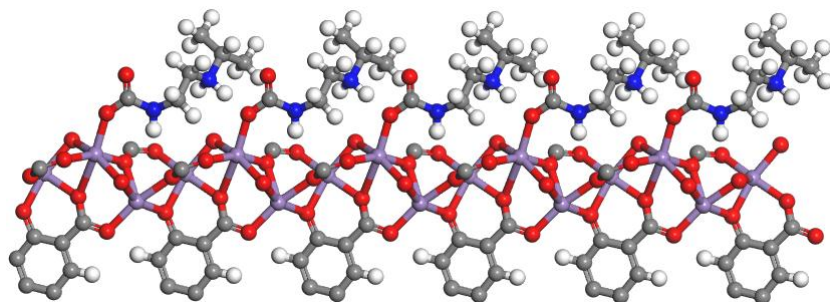
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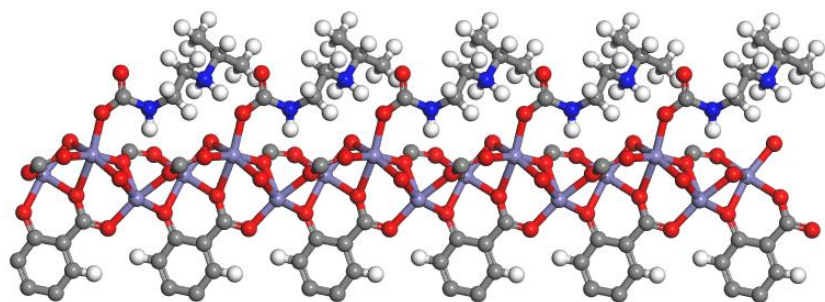
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experimental-CO<sub>2</sub>-i-2-Fe<sub>2</sub>(dobpdc)

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Direct

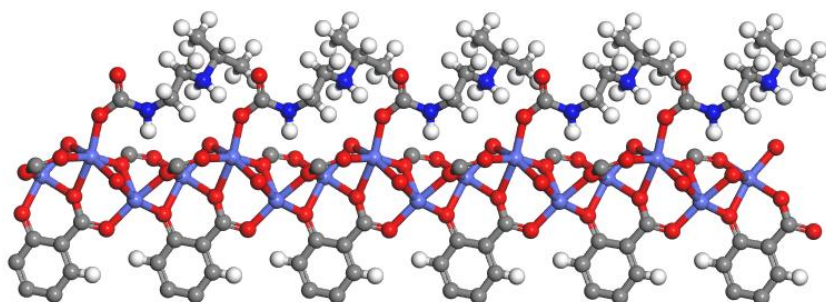
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experimental-CO<sub>2</sub>-i-2-Co<sub>2</sub>(dobpdc)

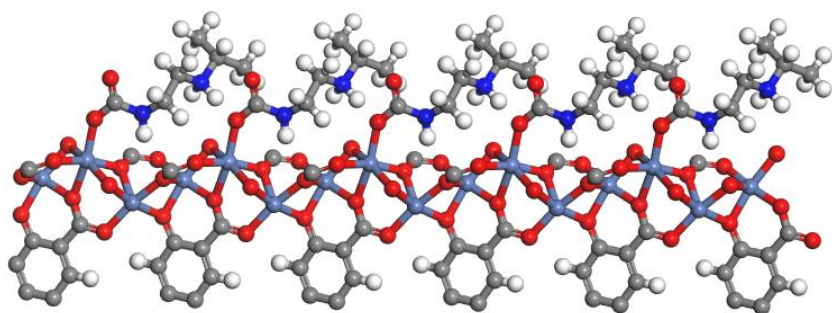
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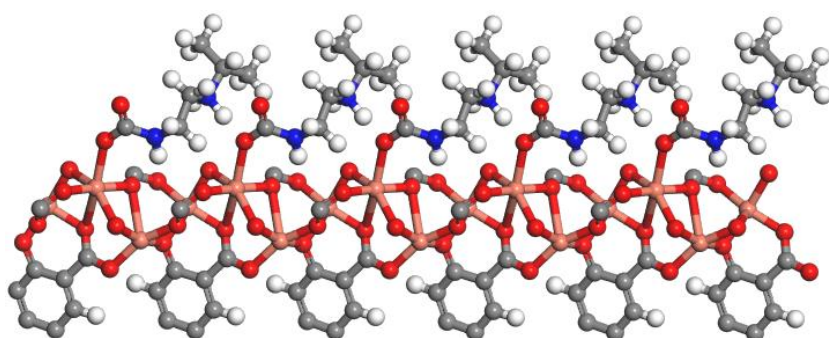
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experimental-CO<sub>2</sub>-i-2-Cu<sub>2</sub>(dobpdc)

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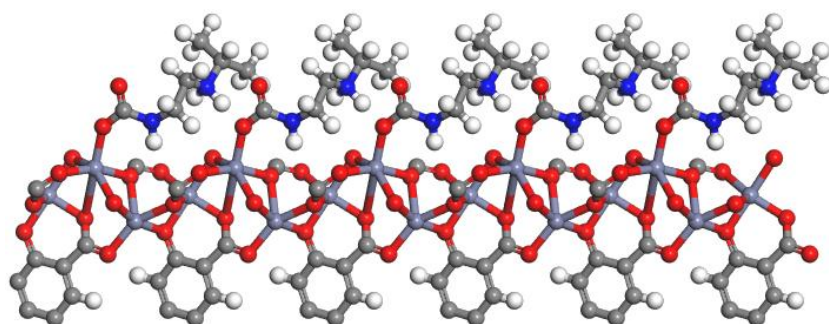
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experimental-CO<sub>2</sub>-i-2-Zn<sub>2</sub>(dobpdc)

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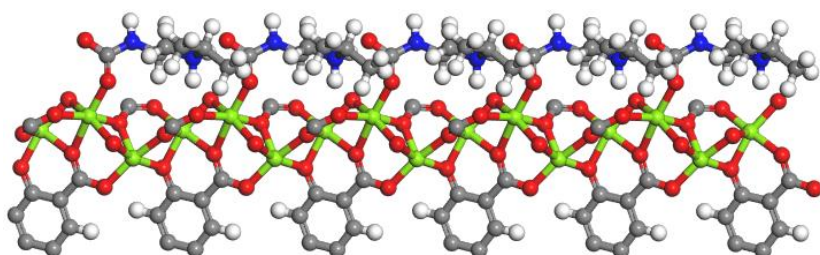
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0.3068800184951002	0.4959624516001497	0.4831758113721847
0.5736028376806033	0.6594120203755836	0.9189059165249702
0.6570859083988410	0.7439264267996748	0.6803027879286319
0.8934029269952575	0.5025930122958329	0.9454741984546686
0.9599001689654543	0.6154720705116716	0.3715235920240687
0.8293386341620419	0.5452064246299599	0.2414003083632394
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0.5951892245971351	0.0401699888485894	0.0373990214209314
0.6494202188726348	0.1632522209101808	0.9092312932622448
0.4796806918556840	0.4442694121004109	0.2599488755853869
0.3603781519237188	0.3981869341208082	0.6819446294176785
0.4269856795217706	0.3379546332864720	0.5615861768533179
0.5168699166625643	0.6752538175039362	0.7442583091674848
0.5709955423846225	0.7753135699500646	0.5465385961961218
0.5847238695740415	0.8279165669510178	0.7513516232393087
0.6678450859836076	0.7925409035898099	0.9129941643252266
0.4723264905609170	0.7044334532941150	0.0224597256156471
0.6229413794083811	0.9267321371863915	0.4476496498435480
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more stable-CO<sub>2</sub>-i-2-Mg<sub>2</sub>(dobpdc)

1.0000000000000000

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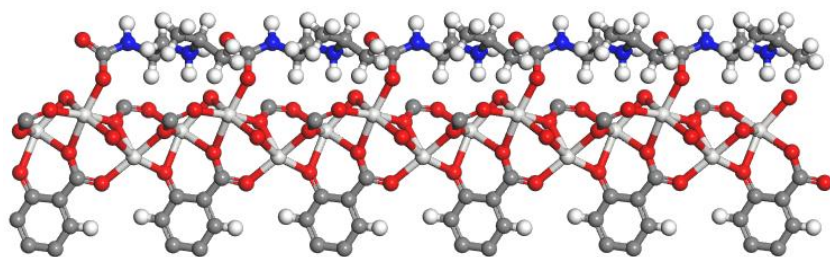
Mg	O	C	H	N
6	20	48	32	2

Direct

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0.6178710137802028	0.2853589570466823	0.8714980987763639
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0.4336645097660039	0.7734215975012049	0.6133143048444722
0.3721308173901434	0.7337395674916394	0.2545518616180189
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0.2518958179684319	0.6926699423813290	0.9464396545400575
0.2943433254701304	0.6712346923233454	0.5839282065524785
0.2063644783212908	0.6209378328556667	0.3546591439333753
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0.3514204104011114	0.6506619095118964	0.9247839946400234
0.4091661169659844	0.6214049010046026	0.6987782342020026
0.4943903456855239	0.7020810132941264	0.3280644396651482
0.6004013777432604	0.7768371650857091	0.4908142163324953
0.7452424118138978	0.4308456608354660	0.4061509863567494
0.7058823814346695	0.3758153138893832	0.7698121713624317
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0.5888325778070680	0.4009278239810428	0.3313569014351216

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0.5025321718758420	0.9217824937398760	0.2614373735317912
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0.1837890987615296	0.6623110531580778	0.8670601620532423
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0.3750326184721260	0.5563997330080852	0.9999004685979429
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0.4289096732027815	0.3941487521702243	0.7732856840274138
0.4697074782410624	0.3641167166679224	0.7005755854927003
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0.5971271453332463	0.6263209651139761	0.6391688469927033

0.5491672383425055	0.5818876886425670	0.4682555544948670
0.6074348842872155	0.5805255461484293	0.7921590407335088
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0.5996163376432264	0.0057766447280798	0.6688680317463707
0.5303685614542459	0.8837867061298752	0.7997950921837997
0.0855569163031547	0.5836635508025196	0.4512345653871037
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0.5757237201606600	0.7129740705580758	0.6222706621112053
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0.6516031418929487	0.7275247585043019	0.9158468030027720
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0.9844935152924847	0.6010749178148984	0.3536920716704302
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0.5712179470746435	0.0962803085648574	0.5718779412317971
0.6100118066643958	0.0266018215693578	0.0160458284490801
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0.4973032525649401	0.4296650595482063	0.2369412543414740
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0.4967060495282638	0.5381861397230168	0.5217392224758655
0.5778463752560867	0.5584011050741182	0.3880510214748512
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more stable-CO<sub>2</sub>-i-2-Sc<sub>2</sub>(dobpdc)

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Sc	O	C	H	N
6	20	48	32	2

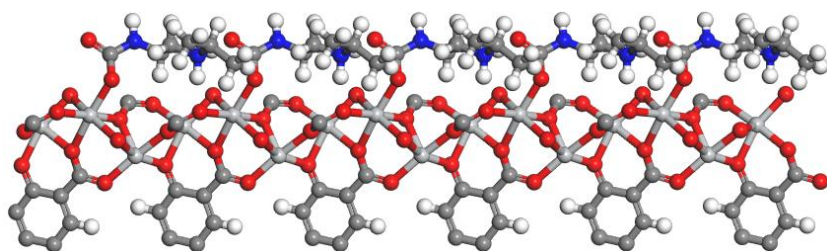
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0.4423520064455302	0.7741993751976537	0.6050838082007165
0.3759439124003972	0.7379226623490152	0.2681090428682907
0.4121665121052098	0.8194339913199237	0.0443394835448908
0.2408702141409294	0.6960856162663172	0.9353740945783051
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0.2095172294076091	0.6365757189325587	0.3680060905758817
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0.3495043488581409	0.6520008117825860	0.9212979989479523
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0.4906884467634151	0.6939663020700846	0.3354215776559952
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0.6649357905991961	0.2911755632531294	0.4320950664502297
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0.5580648033334193	0.3303818237196353	0.7477771542970769
0.6113457500216590	0.3380765845167033	0.1012092930580133
0.5780287672279629	0.3916086343421836	0.3148035539418059
0.4781698041597651	0.8383714010186626	0.5251410254124474
0.4694531263982308	0.8528364510306896	0.3362718952644063
0.5093416215412304	0.9221667441912317	0.2703319419339505
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0.5645771329819295	0.9613082583431045	0.5643853114111645
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0.9980578875692350	0.6125863072113797	0.9761685972286487
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more stable-CO<sub>2</sub>-i-2-Ti<sub>2</sub>(dobpdc)

1.00000000000000

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Ti	O	C	H	N
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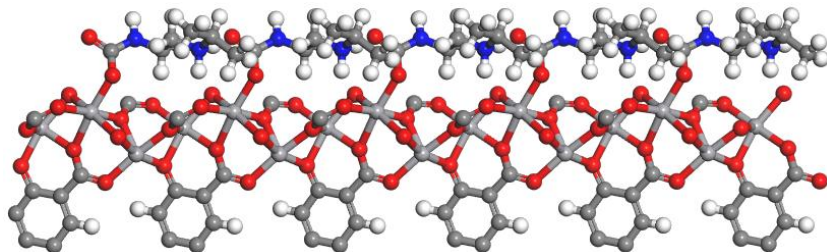
Direct

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0.5595126899413326	0.3311651437451108	0.7346413222716857
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0.6083669545460764	0.0097668107368802	0.6609691667913912
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0.6469124839435746	0.7191360649487224	0.9152931418016935
0.5670961080815790	0.6499409605201880	0.0256361638818409
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more stable-CO<sub>2</sub>-i-2-V<sub>2</sub>(dobpdc)

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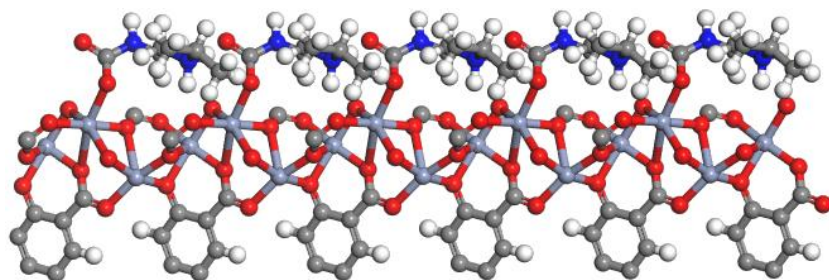
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6	20	48	32	2

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0.4908922523030261	0.6899384560892650	0.3211900560671159
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0.5084731323958777	0.9327893413640653	0.1171259110785163
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more stable-CO<sub>2</sub>-i-2-Cr<sub>2</sub>(dobpdc)  
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Cr	O	C	H	N
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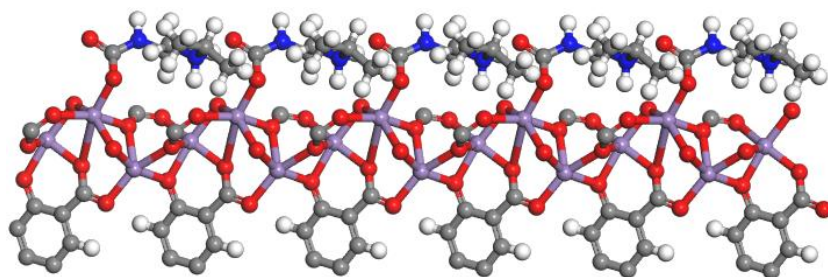
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0.0068743930898034	0.6239496389134170	0.0193900897673974
0.1342927309207100	0.6846343624586394	0.1459067557502211
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0.3687302527677345	0.4046803253936804	0.3395429310650852
0.3213311188234309	0.4821920149482389	0.4733733935301491
0.5783235118653529	0.7078404193660615	0.6007327226362247
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0.5781075426903716	0.6644134305721647	0.0315323953872723
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0.5102901347645212	0.6369935935121678	0.7161960782677341
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more stable-CO<sub>2</sub>-i-2-Mn<sub>2</sub>(dobpdc)

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Mn	O	C	H	N
6	20	48	32	2

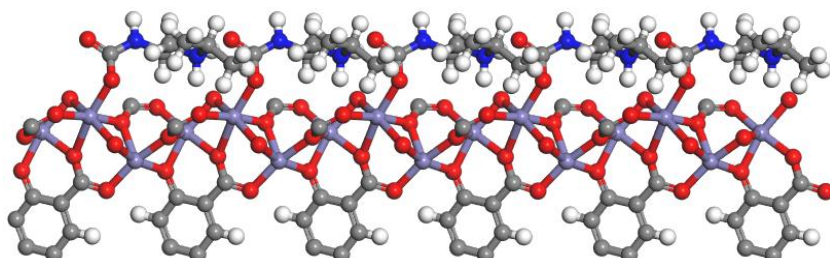
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0.4155847600122229	0.6798845323205498	0.4426340397559017
0.7225866320289356	0.3564784193168791	0.2253884309380823
0.6134335538944882	0.2819139880634651	0.8881917264808195
0.6431119082248813	0.3856474321423278	0.5535653106813569
0.4403032128875211	0.7726245662961801	0.6005695219166967
0.3860552322382773	0.7343059478090268	0.2177547984673680
0.4074973323042386	0.8205241341895189	0.0047294490387131

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0.2847133205711927	0.6889133708805346	0.5377026465352941
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0.3314982448490724	0.5914934920722743	0.2836321333634331
0.3379801157793381	0.6381068945412522	0.8896430106407252
0.4162243771834753	0.6220536590566184	0.7044463194853634
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0.6090612399813793	0.7756900355689638	0.4780951081332248
0.7449359841305281	0.4406008475126697	0.4210046973486499
0.7072044808372979	0.3888560160870966	0.8083361714320176
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0.5855469720632485	0.4089896039862779	0.3385884001107726
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0.3721522068795267	0.5528973776207877	0.9962387154076922
0.3959119203377739	0.5070767731111445	0.9249331603129249
0.3965596860717682	0.4543979750503837	0.0412229296605133
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0.5242471227547369	0.3783006517464713	0.0262998702266515
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0.4628790509726528	0.3578407335381542	0.7049306123394246
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0.5947571666507088	0.6169723549062525	0.6323595740586612
0.5445171820577670	0.5716327637979219	0.4640254350582040
0.6030672452136727	0.5719378200179719	0.7932881899195081
0.4938688199825378	0.9340155267085279	0.1056707805358030
0.6032457180167228	0.0035719508452488	0.6720680108457699
0.5358872247436466	0.8807522049652832	0.7947142802756701
0.0769014379483011	0.5853521235143830	0.4540541195958312
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0.4157672761902660	0.5147128509429493	0.7733215394160382
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0.5189291456157648	0.7354123958442358	0.9439948365737436
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more stable-CO<sub>2</sub>-i-2-Fe<sub>2</sub>(dobpdc)

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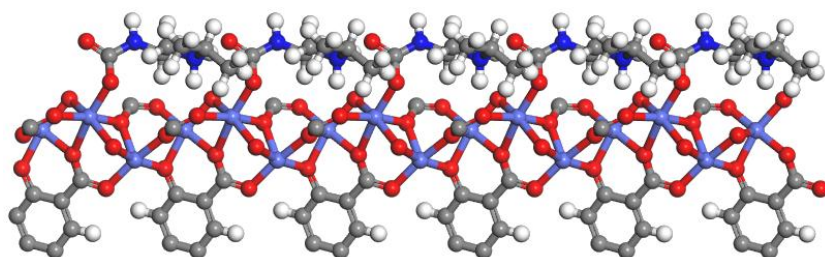
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6	20	48	32	2

Direct

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0.4948484776176446	0.6967633755363252	0.3118313015222025
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0.7063417342103977	0.3849309353671796	0.7835346328431460
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more stable-CO<sub>2</sub>-i-2-CO<sub>2</sub>(dobpdc)

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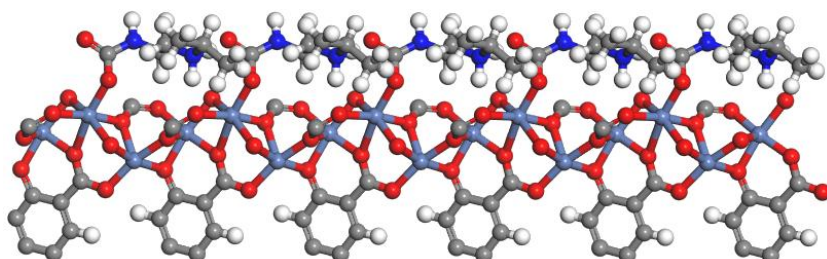
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more stable-CO<sub>2</sub>-i-2-Ni<sub>2</sub>(dobpdc)

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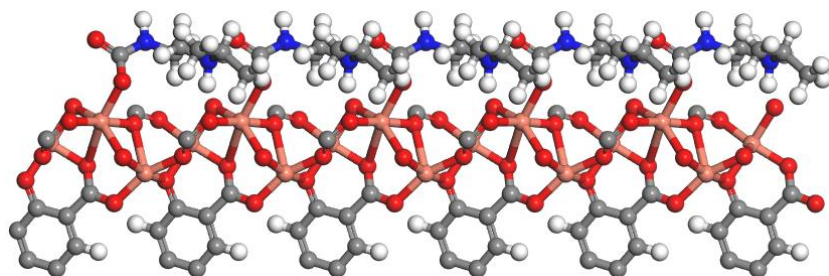
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0.6253839339269779	0.5343047279656732	0.7069840884224478
0.5509938280534120	0.5293919693208525	0.8536840708081117
0.6490399814407539	0.6529350838462207	0.5662207188566074
0.5963370942933702	0.7806172389725945	0.1484315564224481
0.5613541148054508	0.6578068032354915	0.7096482077957484



more stable-CO<sub>2</sub>-i-2-Cu<sub>2</sub>(dobpdc)

1.00000000000000

20.6761631499431289	0.0224495347899948	0.0395668945304480
-10.4763858830187875	18.8590104676172032	0.0433404656035511
-0.0638811942300004	-0.0225305026605096	6.2744415211284643

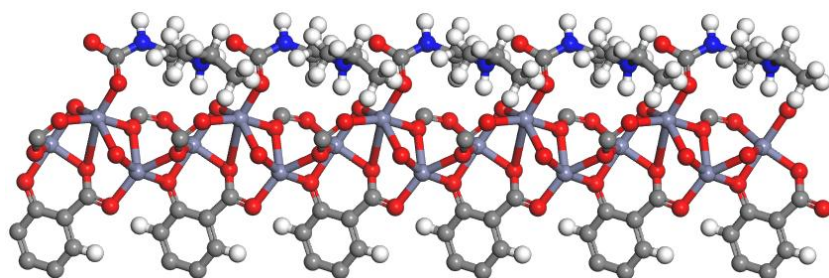
Cu	O	C	H	N
6	20	48	32	2

Direct

0.3413199209151614	0.7467831381664425	0.7787318303940154
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0.4093728229247660	0.6847495685745812	0.4410360865373875
0.7212099581514337	0.3459601972143744	0.2529769059558902
0.6031080905080515	0.2780295513653357	0.9179113677516852
0.6485170644842881	0.3906499349761390	0.5843585218835301
0.4350602862999082	0.7697728862905393	0.6236444129935350
0.3949734405909169	0.7318272986488878	0.1950640472341547
0.3944699761513206	0.8174115610332606	0.9994826628517686
0.2504888378225729	0.6995977125101689	0.9531890453733496
0.2883724440649189	0.7038564599591268	0.5199154956449092
0.2026905218261703	0.6140282442668195	0.3324020547335280
0.3270839736870954	0.5931763594970931	0.2902640392663258
0.3252806717926120	0.6292750127439106	0.8552690688901095
0.4169405257843479	0.6266272304458198	0.6781138050630489
0.5120956439214126	0.7025737587620497	0.2989119113551695
0.6109858181581274	0.7864310237384231	0.4828060315175051
0.7391017342226505	0.4344274141482316	0.4125506942677575
0.7018063352373431	0.4001342248324917	0.8466621411477462
0.7933577120619901	0.4003848511646808	0.0352964098428998
0.6764765153778640	0.2588094516013726	0.0790348028432746
0.6774293036564316	0.2954788003751148	0.5127403673550717
0.5880550772745750	0.2089173550535719	0.6985388133552846

0.5562869719971175	0.3222070984487928	0.7421814381709666
0.5930003897037963	0.3199071922680474	0.1784870928979458
0.5916195950003384	0.4069606957936074	0.3635488846798722
0.4726440552990496	0.8351759587342897	0.5389043555456539
0.4609207164128506	0.8518700869543849	0.3270972501948179
0.4975989169137804	0.9225310543427057	0.2575636671672328
0.5484960440548576	0.9770416069351384	0.3875178519014852
0.5630579361589625	0.9591905023801672	0.5914259305888621
0.5264475621244173	0.8901803663710623	0.6662556319434643
0.4136763779587795	0.7973615731314609	0.1690352622745266
0.1816623382000486	0.6682435648184963	0.8698480682747274
0.1645625575964402	0.6397659829382221	0.6599433788056572
0.0904629655054237	0.6017005160144038	0.5931911226837414
0.0326627516438620	0.5941864422365981	0.7235624299142458
0.0506993907306352	0.6267419960503986	0.9251388875687852
0.1232176095942137	0.6631229708729336	0.9975002640733948
0.2222037726914152	0.6528187160027699	0.4995907654485521
0.3468265091147344	0.5485461843840724	0.2026389017343391
0.3741957744923710	0.5560832362829231	0.9908531171773376
0.4007440976477028	0.5112451329600702	0.9187682571427374
0.3987486431148000	0.4570240864237434	0.0456932849178031
0.3669592985688226	0.4469950434260781	0.2487367026813061
0.3410319915866467	0.4909892173325474	0.3257131637118320
0.3724171538241450	0.6075179914322462	0.8367243351120308
0.5733385547913628	0.7608937363143298	0.3117830613344807
0.5791537895441152	0.7640297412537080	0.9228183408917872
0.6044946458852678	0.7084042662672019	0.8961573219716570
0.8069734680557659	0.4740015525840136	0.4988495121200529
0.8262038612064657	0.4642882381358433	0.7099653973818079
0.9000972072986215	0.5029704878904866	0.7790401161910907
0.9549316407515605	0.5539125414408588	0.6497583865594478
0.9339852586246238	0.5661569152006436	0.4467744951381292
0.8619382205612709	0.5275606426401538	0.3721281346600733
0.7707650886951569	0.4183119578306744	0.8685530521464031
0.6500728376975786	0.1935367669122598	0.1645471825431102
0.6211538210916743	0.1759981924360616	0.3745139316773276
0.5876220593321619	0.1051519898559405	0.4425812835549223
0.5852779116079248	0.0514731414727834	0.3136045877802616
0.6186489919802014	0.0704800895769537	0.1121253095049610
0.6505564062327664	0.1396721663505573	0.0384313226993598
0.6285972614094817	0.2297661977674110	0.5330973748573484
0.5153251624452295	0.3490784235623110	0.8257500723175468
0.5251288381391888	0.3759019170290046	0.0372736682600348
0.4854262438982673	0.4095461807444138	0.1045681750200558
0.4339832288294403	0.4154447599710167	0.9727958076365724
0.4209543137360257	0.3843259577524023	0.7694199472641827

0.4600220572249754	0.3514279494461690	0.6971860438945257
0.5732724062940520	0.3676007704487247	0.1979056157091819
0.6027213051911673	0.6212340673144183	0.6162840698598870
0.5512328235459094	0.5727620599376237	0.4420544503632939
0.6143197250379444	0.5788917418869417	0.7936288314478688
0.4843925426965043	0.9337606730984476	0.0983801186626678
0.6047705558715393	0.0008543328197277	0.6915852298035645
0.5382287464257729	0.8767522828176695	0.8241401334542360
0.0793202505117350	0.5776792851563783	0.4352091657729815
0.0064191383252989	0.6237994669021845	0.0253697758039593
0.1368323266374887	0.6883539190277546	0.1536681330179803
0.4234322817787728	0.5197936132057421	0.7584934986435314
0.3625701624340394	0.4032696354272360	0.3469448200617720
0.3157510824327119	0.4825512134818339	0.4824480191212857
0.5833582951296421	0.7097552681431267	0.5851677924812293
0.6004867538544758	0.8025104446461881	0.7916206935042638
0.5184912029370210	0.7381651719999525	0.9145758819169956
0.6650327232524873	0.7340561972079271	0.8828551417516337
0.5865401043573684	0.6721945674247394	0.0328266401673503
0.9136323016975041	0.4917054766833076	0.9377603617236971
0.9756896293950987	0.6074553760291082	0.3468879825079796
0.8462478880801712	0.5372529966040602	0.2143742179930399
0.5626952839296067	0.0929900026520443	0.6002205556806786
0.6196188883274871	0.0295836481091882	0.0126216781461608
0.6762322915893577	0.1539528463337589	0.8820418657535711
0.4969126596806177	0.4322968974947869	0.2639826223946145
0.3788815112934287	0.3859351743256809	0.6670414871999171
0.4494055328673525	0.3271609884683926	0.5397390254130769
0.5147609517926384	0.6399785182788946	0.7067476342110197
0.5344344216409453	0.6015229910363402	0.3298809592047931
0.5008335464908029	0.5298629417052041	0.5124789361271098
0.5787218502135261	0.5480284174987347	0.3550147391228720
0.6561634474042108	0.8382507640898993	0.1423369286066816
0.6558816891910197	0.6127224547480665	0.9113953051608235
0.6334053007303737	0.5442100207524661	0.7223374993625953
0.5623580864818720	0.5445471234544215	0.8769240668203864
0.6565920615942957	0.6586268834012898	0.5470874642988832
0.6033813035013154	0.7984438347381086	0.1265311404414433
0.5721918386821869	0.6675718781716569	0.6964875790630956



more stable-CO<sub>2</sub>-i-2-Zn<sub>2</sub>(dobpdc)

1.00000000000000

20.7386006095635551	0.0655814203208497	-0.0135376356003786
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-0.0805845249966124	-0.0468867434036519	6.4701722835968560

Zn	O	C	H	N
6	20	48	32	2

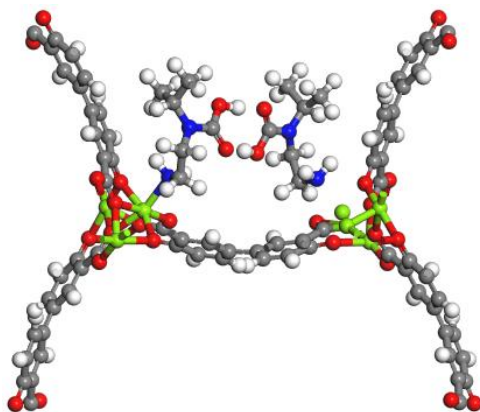
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0.4223835170021530	0.6866062470450629	0.4373195151017271
0.7186631192175952	0.3488408715889832	0.2370516832530072
0.6098317376022351	0.2818697414324021	0.9002449652659550
0.6448312062509345	0.3832985270955120	0.5661051545467259
0.4378390628182274	0.7708212297077282	0.6047770109746153
0.3890230946515629	0.7340029876980054	0.1997496727602837
0.3986408375227768	0.8193265357676225	0.9889857279652787
0.2496508611492914	0.6978676876427130	0.9499638281725069
0.2842022396785779	0.7014625106419459	0.5209713730877183
0.1976137684501396	0.6123407456536896	0.3421460916750760
0.3363919064479504	0.5994046511425637	0.2942494795735584
0.3351724773471574	0.6379007419035716	0.8689383529447383
0.4218009109667449	0.6274288530809571	0.6924118566830160
0.5129074072151667	0.7031003889524357	0.2902694584013901
0.6099430215612145	0.7834777200481895	0.4824726164992228
0.7396214149794034	0.4349903242238540	0.4157829249761420
0.7018934795306109	0.3922796977707037	0.8354444469803468
0.7963672304416960	0.4042510770670447	0.0312037343536034
0.6765958852713823	0.2577042250049644	0.0814411486087820
0.6688473891963440	0.2949271547011776	0.4997935322230873
0.5889881861428208	0.2063758541852465	0.6904907965583078
0.5545664045051666	0.3226168486739809	0.7429340593683662
0.5998474793695010	0.3278235170467667	0.1655700523454726
0.5864544316229825	0.4060202561288335	0.3575936345817325
0.4723786042248719	0.8360833726041790	0.5230621424545134
0.4603341400258358	0.8529231397170918	0.3175708007646847
0.4967080589230832	0.9232565791867202	0.2524257547472217
0.5463487990418088	0.9776446577010773	0.3799635174091094
0.5600120833713760	0.9600552837949721	0.5790942120995553
0.5242937131006045	0.8913717252214823	0.6489092978774238
0.4128165997172246	0.7997351611947963	0.1615141364748496
0.1806661726761405	0.6656080284364521	0.8717957789627988
0.1627601253441568	0.6377103109087727	0.6670152138258203
0.0887108979516640	0.5999876743752068	0.6034507886542571
0.0315014058272283	0.5918588418906054	0.7309394320988432
0.0500266113181738	0.6230707394374946	0.9286651252525360

0.1224605443666533	0.6589807804190286	0.9978836069038692
0.2180527273787547	0.6504372092339779	0.5063705803831908
0.3519645397763327	0.5526738521561967	0.2031915615551654
0.3767071784859226	0.5587921140909557	0.9956361101358979
0.4004569739192689	0.5122066662866871	0.9228097207354793
0.3987655714037643	0.4582196802840102	0.0439213656541568
0.3690358750725267	0.4494465219087047	0.2425688081510700
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0.5829421621740707	0.7637910592059285	0.9312673007432650
0.6050831811466466	0.7064022442697038	0.8978779443634366
0.8071011284183598	0.4733854124980823	0.5041863823672514
0.8257121062792763	0.4638114755468337	0.7101234654728259
0.8992698767318430	0.5026829562616228	0.7798014579436696
0.9542846621444809	0.5525395188432256	0.6569068998706058
0.9338982926787551	0.5641206432822585	0.4582106913588930
0.8623911784848914	0.5257844285100219	0.3834486823570629
0.7722258470338730	0.4170853885834447	0.8635358200457404
0.6484364799195248	0.1927060465414669	0.1649973255308339
0.6200582015056710	0.1758462710088864	0.3686714747380933
0.5866613529282958	0.1053316886896027	0.4336510233670552
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0.6146864136299115	0.0695706342763032	0.1118036260332858
0.6467528888931398	0.1382474414574943	0.0416316848350462
0.6253441225390901	0.2280643173372852	0.5244702526789027
0.5149326277167035	0.3506140403777422	0.8256732103983282
0.5245245436895871	0.3767535714243877	0.0322309017906903
0.4842700418838319	0.4097882826772121	0.0980243009210895
0.4334652737434013	0.4166398663509341	0.9705915676175607
0.4214441679074952	0.3870871691596705	0.7708582322897186
0.4606941879918480	0.3546296638042108	0.7003263784802130
0.5733941761685770	0.3705267392877403	0.1900969814532374
0.6010882315490633	0.6197572610560940	0.6226963140179862
0.5500290860995349	0.5732577677736970	0.4498559207755335
0.6107473364486040	0.5761231542253640	0.7931828697743839
0.4838086002569355	0.9341267101722011	0.0971897604176277
0.6003528662979249	0.0014646042119679	0.6795256829362657
0.5355961512328378	0.8782451894336916	0.8030010586014527
0.0773034419427958	0.5769711527320567	0.4485938496064179
0.0064232215837805	0.6197032364997668	0.0284992929613779
0.1362313175504184	0.6833215046313583	0.1508553669947403
0.4214269621563531	0.5196698364319943	0.7660046173600321
0.3646726265709717	0.4059876584006403	0.3374419655199219
0.3223545513329569	0.4878293416464601	0.4738783564769591
0.5825532721297506	0.7080262232880870	0.5941678591963822



0.6059433535406171	0.8037916505660121	0.8099828463194569
0.5228549470979615	0.7409171099526191	0.9215673166077281
0.6651243049132560	0.7298986654433008	0.8862859896577291
0.5862352529140864	0.6696541436556913	0.0276306864287363
0.9123104785491734	0.4919467489080347	0.9349411059449082
0.9755074805735688	0.6045267651658577	0.3616015736052560
0.8472884520081578	0.5350144914289388	0.2290110723829244
0.5627998813535342	0.0938654627095588	0.5871566555024543
0.6144818313094760	0.0285848719389818	0.0133030443965083
0.6714411985661783	0.1518077620204679	0.8893535693200505
0.4951414382182904	0.4315209201799277	0.2542075216628703
0.3800612372623817	0.3894694002194541	0.6701040670289160
0.4507025762357202	0.3314634834370054	0.5458780581004916
0.5144128590529320	0.6397370063127852	0.7147877419348134
0.5363653327571711	0.6033608779079458	0.3380450598505433
0.4982106953741550	0.5323772735372359	0.5134833386215831
0.5760229509857027	0.5465061883886690	0.3691045889382352
0.6600366708318290	0.8353805691255332	0.1522919772794395
0.6523029777361913	0.6084704156261651	0.9094957851590024
0.6286448278219723	0.5408521467977820	0.7228224635974101
0.5586360110858237	0.5428523589602179	0.8713321131143488
0.6552151808931654	0.6562784763910656	0.5591960321233458
0.6081543289764966	0.7951989389563821	0.1338482866263888
0.5717557648149452	0.6668281596923649	0.7024098141682913



pair-CO<sub>2</sub>-i-2-Mg<sub>2</sub>(dobpdc)

1.0000000000000000

20.8226524968228972	-0.0437186884573209	-0.0080842102330091
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Mg	H	C	O	N
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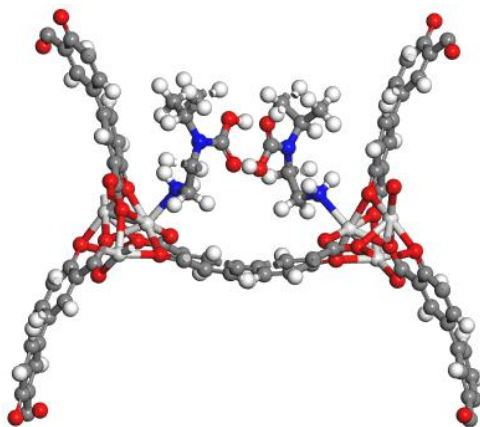
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0.3051243315720551	0.6086503383070100	0.8418749246781241

0.3646305503933097	0.6996945418561671	0.1808065620132854
0.4105687916283647	0.6382613739906678	0.5220108482137011
0.5338926655652935	0.3915444552967516	0.7631671123911420
0.6840771512217513	0.0974266733630679	0.1200437804795151
0.6231242156614514	0.9754102442304027	0.9916041865580166
0.5960842564862232	0.0588258552226866	0.4423748519873023
0.0144873864835132	0.5519292179703971	0.6424529450929135
0.8953948634021804	0.4776653826284674	0.7829096708477126
0.9424336796842151	0.4514386788048375	0.0884511836855632
0.4315424342169029	0.3686729438017250	0.3188610608750811
0.5075452773604681	0.3149681926790047	0.4516539662340310
0.4472062760937973	0.4818675214398813	0.2207952641985611
0.0282766923692344	0.5670888677601174	0.9892570027354741
0.1514814885296646	0.6296967645412552	0.8616529298855260
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Sc H C O N

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Direct

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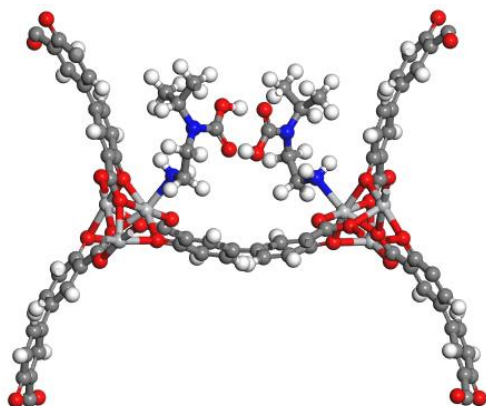
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Ti H C O N

6 46 54 22 4

Direct

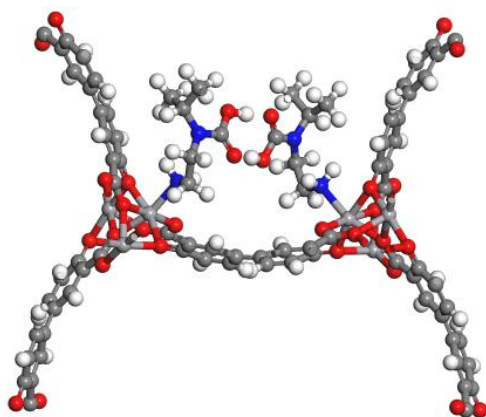
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V H C O N

6 46 54 22 4

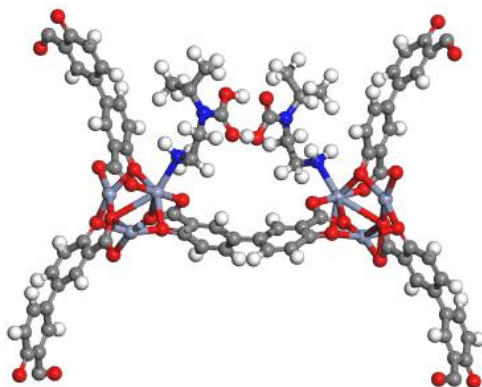
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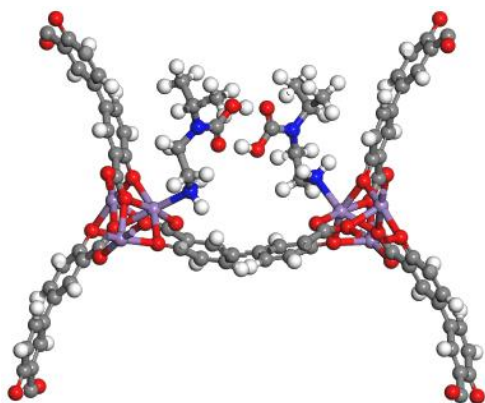
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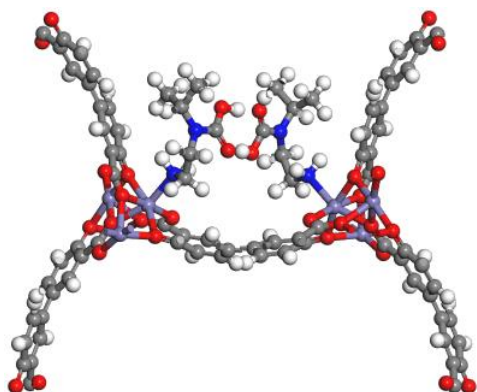
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Fe H C O N

6 46 54 22 4

Direct

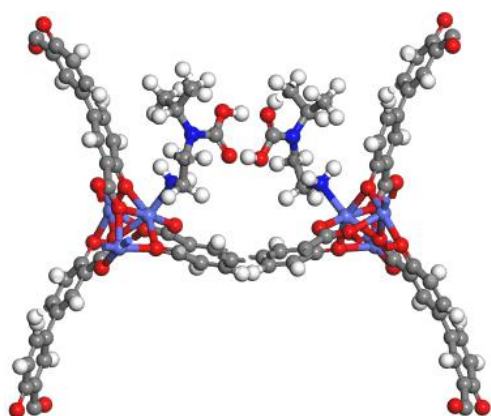
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Co H C O N

6 46 54 22 4

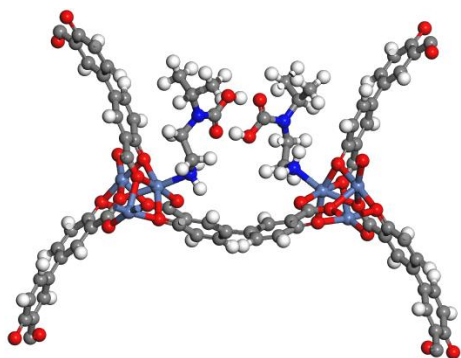
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pair-CO<sub>2</sub>-i-2-Ni<sub>2</sub>(dobpdc)

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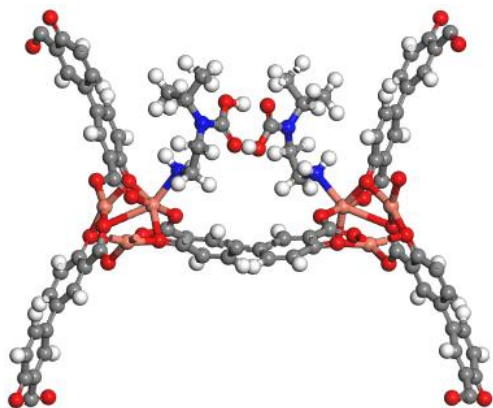
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Direct

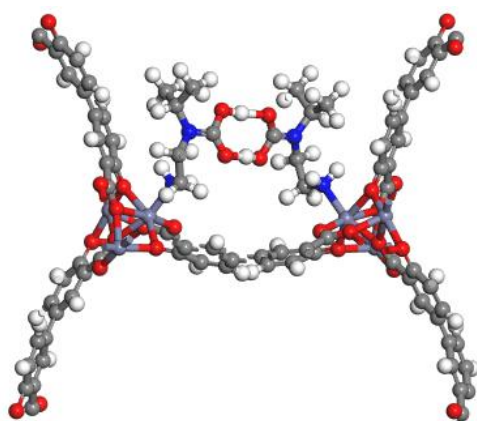
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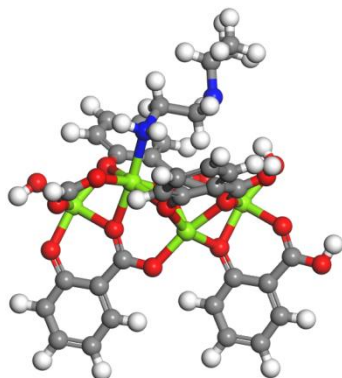
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The optimized structures (A–F) and coordinate files in the reaction pathway are listed as follows:



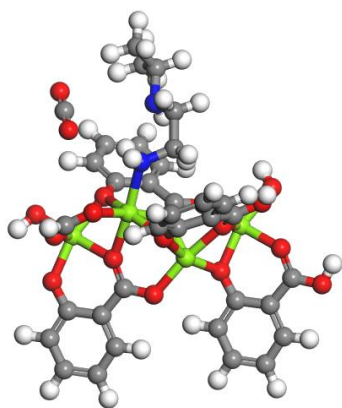
Mg–(A) i–2–MOF

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O	-1	-0.07681800	2.58829200	-1.16085200
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O	-1	-3.71292500	2.03002300	1.48902000
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C	-1	-0.52241800	4.99284000	-1.13301500
C	-1	0.02277900	6.28738400	-1.18904800
C	-1	1.38290900	6.52221900	-1.37913000
C	-1	2.22033700	5.39852900	-1.53587200
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C	-1	-2.06495900	1.03799300	2.91129500
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H	-1	1.23040700	-5.01227600	-1.93055000
H	-1	4.29019600	2.58787200	0.19345100
H	-1	2.37571000	3.24492400	-1.59729800
H	-1	-1.11824300	-0.51244400	6.34724000
H	-1	0.47134500	-0.65845600	4.44581500
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H	0	-3.01488800	-3.89889500	1.04633400
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H	0	-3.94807900	-1.64879200	1.15785400
H	0	-0.94430400	-3.52093600	2.03083800
H	0	-4.49759200	-4.07845300	-0.79222700
N	0	-1.37140300	-2.68236300	1.64202000
H	0	-1.28146900	-3.66817700	-5.19033000
H	-1	0.13490300	-5.43401700	-4.10567500
O	-1	3.53411800	-4.40038600	-1.05286300
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H	-1	7.33078300	-1.28738400	-0.36433600
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Mg-(B) Complex

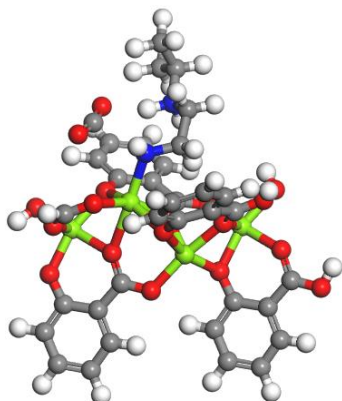


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O	-1	-1.37812500	-4.23139400	-2.01380400
O	-1	-3.00920000	-0.69462500	-1.20426100
O	-1	-3.63644300	-3.35285000	-1.02244900
O	-1	-5.79277100	-3.92516400	-1.02495400
O	-1	-1.57617600	-2.19470800	0.42106400
O	-1	-1.73624800	-4.26464000	1.22336600
H	0	-0.56002300	-4.20042300	-2.52208100
C	-1	-4.33903000	-0.52691100	-1.28613800
C	-1	-5.27521700	-1.60666200	-1.23002500
C	-1	-6.65218000	-1.32941400	-1.27689100
C	-1	-7.15343000	-0.03517400	-1.39938900
C	-1	-6.21839400	1.01699800	-1.49285700
C	-1	-4.88547300	-3.03172200	-1.07919400
C	-1	-0.97743700	-3.46708500	3.76941200
C	-1	-1.49894300	-3.03334500	1.40232200
H	0	-0.39955600	-3.88079800	5.81338600
C	0	5.72061400	-2.59078400	-2.33888100
H	-1	-7.33094400	-2.17690000	-1.17602900
H	-1	-1.23366700	-4.49990800	3.52939300
H	0	3.48785700	-2.31472000	-1.28851100
H	0	4.96273700	-4.28526500	-1.27071000
H	0	4.91321700	-2.56840100	-3.07916500
H	0	6.56069200	-3.14086200	-2.77268700
H	0	-4.73501800	5.85698900	0.08617600
H	-1	-6.57814800	2.03964100	-1.62616700
Mg	-1	1.55802500	3.33637000	-0.05933500
Mg	-1	-1.80119500	-0.15151900	0.33345400
Mg	0	1.00416100	0.60579600	1.04988900
O	0	2.14035900	1.41941100	-0.48902300
O	0	-0.00968500	-0.18510000	-0.61417400
O	-1	-0.35454600	-1.40861200	-2.42672000
O	-1	0.47660100	5.00723100	0.31193500
O	0	-0.17084100	2.33327200	0.51327200
O	-1	-2.30698000	1.77670400	0.49124200
O	0	-0.68102100	-0.24201900	2.02455900
O	-1	1.90952200	3.50706500	1.93721800
O	0	1.77520100	1.43129200	2.81179400
O	0	5.14744200	0.71766200	1.15927200
O	0	6.67897400	0.51497500	-0.58513000
C	-1	2.40468600	0.95329000	-1.69690700
C	-1	1.60592000	-0.03906200	-2.35104000
C	-1	1.98954000	-0.52497000	-3.61176600
C	-1	3.14528400	-0.09525000	-4.25824100

C	-1	3.93347200	0.87249500	-3.59770400
C	-1	3.57439200	1.38541400	-2.36436900
C	-1	0.35499600	-0.57257300	-1.77924500
C	-1	-0.85328900	5.17487700	0.23002100
C	-1	-1.78947600	4.09512400	0.28613900
C	-1	-3.16639000	4.37245600	0.23929400
C	-1	-3.66763900	5.66669500	0.11679600
C	-1	-2.73265500	6.71878400	0.02330500
C	-1	-4.85445000	0.78142500	-1.43900400
C	-1	-1.39973500	2.67006600	0.43695800
C	-1	-0.67605100	-1.16973300	2.95350600
C	-1	-1.09256800	-2.52529700	2.73414900
C	-1	-0.48997600	-3.13584500	5.03195000
C	-1	-0.13614600	-1.78630900	5.25448600
C	-1	-0.22755400	-0.83333600	4.25370600
C	-1	1.98684500	2.66845600	2.91849600
C	0	5.90800000	0.61136500	0.28258600
C	0	2.11035200	-2.42961400	0.87471900
C	0	3.36251600	-3.21310300	0.50984100
C	0	5.26369900	-3.24496700	-1.04243600
C	0	6.40227900	-3.30239700	-0.03074500
H	-1	1.32049300	-1.24088100	-4.09087700
H	-1	4.19615000	2.12886700	-1.86284500
H	-1	-3.84520500	3.52488700	0.34013300
H	-1	-4.13865500	1.60205100	-1.51223600
H	-1	0.21324400	-1.48692100	6.24509400
H	-1	0.05618300	0.20545600	4.43380000
H	0	1.55862400	-2.95059600	1.66138200
H	0	3.06631800	-4.22859300	0.19099900
H	0	1.44567700	-2.37507300	0.00506400
H	0	3.22681200	-0.74757800	0.80761900
H	0	3.98807700	-3.32966600	1.40293600
H	0	2.69398100	-1.07687300	2.29861100
H	0	6.03963400	-1.55999200	-2.15502400
H	0	7.23741400	-3.88143400	-0.43679800
H	0	6.09943900	-3.77680400	0.90709800
H	0	6.76422800	-2.29416200	0.19602100
N	0	2.40190400	-1.05838000	1.32424300
N	0	4.11877600	-2.49798700	-0.50989300
H	0	3.42664000	-0.48461900	-5.23031800
H	-1	4.86151100	1.21022500	-4.06437300
H	-1	-3.09235800	7.74151000	-0.10998200
O	-1	3.13119400	4.29317500	-0.91055600
H	0	3.05012200	5.16651100	-0.51219800
C	-1	-1.36866000	6.48329500	0.07718000
H	0	2.24296900	3.06946900	3.91176900

H	-1	-0.65291400	7.30383800	0.00392700
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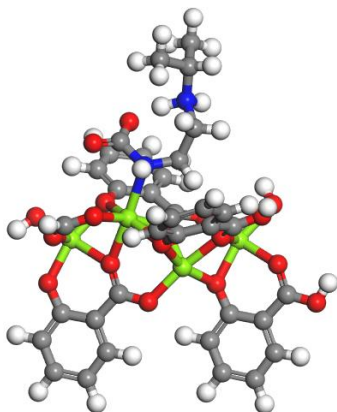
Mg-(C) TS<sub>1</sub>

-1 1

H	-8.12610400	-0.48496100	-1.37963300
Mg	-1.65223600	-2.49504700	-1.50131400
O	-0.95670800	-4.32263600	-1.89144200
O	-2.86256600	-0.90647800	-1.16897300
O	-3.27332100	-3.60018900	-0.90859400
O	-5.37668900	-4.34336000	-0.87949600
O	-1.30556200	-2.24013900	0.48708400
O	-1.29481900	-4.29264900	1.34791100
H	-0.14657500	-4.23597000	-2.40615700
C	-4.20197100	-0.84828400	-1.24583800
C	-5.04809700	-1.99758200	-1.15286000
C	-6.44310000	-1.83304900	-1.19743900
C	-7.04730900	-0.58715300	-1.35232000
C	-6.20030200	0.53351200	-1.48186200
C	-4.54438000	-3.38196000	-0.96520100
C	-0.58981900	-3.36493800	3.86516400
C	-1.15631000	-3.04171500	1.49075200
H	0.02915900	-3.67290800	5.91582100
C	5.59537900	-2.29070300	-2.63405900
H	-7.05107400	-2.72901700	-1.06807200
H	-0.76344600	-4.42136800	3.65589100
H	3.28275300	-2.29686900	-1.47259700
H	4.85022000	-4.06998400	-1.67614000
H	4.76221700	-2.18937300	-3.33531500
H	6.40686600	-2.81413100	-3.14485600
H	-5.10274800	5.52036300	-0.04974500
H	-6.64171000	1.51983100	-1.64100900
Mg	1.37171200	3.50852100	-0.16999700
Mg	-1.69445000	-0.22485800	0.34421500
Mg	1.17373600	0.66609300	1.03371500
O	2.09960100	1.64593500	-0.56358900

O	0.08704000	-0.13345000	-0.62192800
O	-0.16528600	-1.43973300	-2.39029300
O	0.16142700	5.09717700	0.16236300
O	-0.27159900	2.38606800	0.43026900
O	-2.35269600	1.66029600	0.45184000
O	-0.57576300	-0.17937000	2.03454200
O	1.71838600	3.76342900	1.81840000
O	1.69307900	1.72027400	2.77999600
O	4.50212100	1.12031800	1.97882800
O	5.16415800	0.08743600	0.00475000
C	2.39891000	1.15547300	-1.74663800
C	1.67917700	0.08415700	-2.36704300
C	2.09428600	-0.40499600	-3.61648800
C	3.20853500	0.09747000	-4.28305500
C	3.91968600	1.14367500	-3.65551600
C	3.52672600	1.66091800	-2.43429000
C	0.47803300	-0.53148200	-1.77153600
C	-1.17802200	5.15528400	0.08547800
C	-2.02414800	4.00598600	0.17845700
C	-3.41910700	4.17060700	0.13389700
C	-4.02331600	5.41650200	-0.02098400
C	-3.17635400	6.53708000	-0.15054600
C	-4.82158900	0.40965800	-1.43136500
C	-1.52043200	2.62160800	0.36611600
C	-0.47804900	-1.07488400	2.98337700
C	-0.78540600	-2.46515500	2.80491500
C	-0.12424200	-2.96001000	5.11440800
C	0.12113800	-1.58068600	5.29667000
C	-0.05153300	-0.66688000	4.27040800
C	1.86763900	2.96185300	2.82206900
C	4.68973900	0.51541100	0.99758600
C	2.24698000	-2.20694800	0.93137500
C	3.41293100	-3.06001800	0.43266600
C	5.20208500	-3.07294000	-1.39212800
C	6.34510600	-3.18977700	-0.39783500
H	1.48252900	-1.18553800	-4.07059000
H	4.08932900	2.46571000	-1.95833500
H	-4.02712600	3.27455100	0.26324500
H	-4.17440800	1.28261500	-1.53263400
H	0.45029100	-1.22627600	6.27598700
H	0.14873000	0.39600400	4.41941500
H	1.80243200	-2.77844000	1.76298300
H	3.10974100	-4.06993400	0.14054000
H	1.48031900	-2.20852100	0.14142300
H	4.25114400	-1.43684200	-0.47421000
H	4.19282400	-3.12249100	1.19382000

H	2.93275700	-0.86126500	2.24122200
H	5.94711400	-1.28831400	-2.37134300
H	7.21205700	-3.60809300	-0.91473200
H	6.11040500	-3.85199000	0.43803700
H	6.62683400	-2.20761100	-0.00626200
N	2.60651800	-0.84661900	1.27717000
N	4.01208600	-2.40189100	-0.76123700
H	3.51410100	-0.29444800	-5.24699400
H	4.81528800	1.54129100	-4.13810600
H	-3.61771700	7.52348600	-0.30967300
O	2.85866300	4.56383500	-1.05897600
H	2.71708700	5.43595400	-0.67512000
C	-1.79759700	6.41331400	-0.10002900
H	2.14318000	3.41531700	3.78926900
H	-1.15045900	7.28618300	-0.20131700
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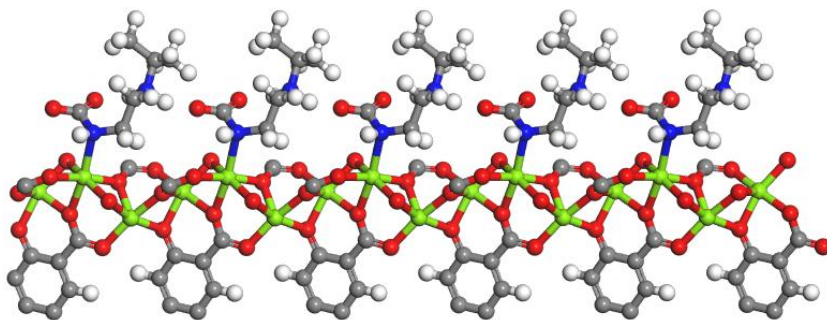
Mg-(D) Intermediate from Gaussian

-1 1

H	-7.59762900	-3.21179800	-0.66010300
Mg	-0.90187200	-2.76251900	-1.62497700
O	0.33821900	-4.20796800	-2.21564700
O	-2.54226400	-1.72317500	-1.05245700
O	-1.94004900	-4.39094300	-0.93868400
O	-3.62435700	-5.83949600	-0.73348300
O	-0.41876100	-2.45352600	0.32694900
O	0.42406300	-4.38789200	1.03533500
H	1.00024200	-3.82573200	-2.80232300
C	-3.81432900	-2.14716400	-0.97908400
C	-4.18167300	-3.52550100	-0.87562400
C	-5.53870700	-3.87106800	-0.75673300
C	-6.55792800	-2.92106700	-0.75723800
C	-6.18429500	-1.56815300	-0.89906100
C	-3.20263000	-4.64163500	-0.84141700
C	1.06900800	-3.33674900	3.51996400
C	0.12933900	-3.17479600	1.24971900

H	2.01215800	-3.45660800	5.46381100
C	7.38140800	-1.73253700	-1.65487900
H	-5.76999800	-4.92859000	-0.62528300
H	1.25416300	-4.37917100	3.25717100
H	4.90249500	-1.91001300	-1.51213000
H	6.61753600	-2.85065300	0.01715800
H	6.98052300	-2.41915000	-2.40701100
H	8.42521900	-2.00214600	-1.47848700
H	-6.74404100	3.43975800	0.75201600
H	-6.96156200	-0.80186500	-0.93969900
Mg	-0.04730300	3.88825400	-0.21202600
Mg	-1.50819800	-0.70871500	0.36895800
Mg	0.78211100	1.21955300	0.79972700
O	1.24494200	2.41369200	-0.80044000
O	0.00661600	0.03049400	-0.76457300
O	-0.00797100	-1.22076900	-2.59396500
O	-1.68768100	4.92769500	0.36051400
O	-1.09514600	2.23633400	0.48627200
O	-2.76977500	0.81137500	0.67948700
O	-0.23004800	-0.30130800	1.90349100
O	0.43580800	4.19724700	1.73989800
O	1.24002800	2.24971600	2.54618100
O	4.05026800	2.18469900	1.24882900
O	4.50881900	0.97205800	-0.58637700
C	1.53548900	2.10318300	-2.05215200
C	1.16755500	0.86202000	-2.66434100
C	1.56684600	0.58788300	-3.98271700
C	2.33834000	1.47416200	-4.72947100
C	2.70807700	2.68862500	-4.11103700
C	2.31584200	2.99767100	-2.82107900
C	0.34642300	-0.15912200	-1.98655300
C	-2.95975900	4.50360900	0.43386500
C	-3.32710300	3.12527200	0.53732700
C	-4.68412400	2.77980200	0.65623700
C	-5.70334500	3.72980200	0.65573200
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C	-4.85596300	-1.19062900	-1.00745800
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C	0.25333500	-1.13623400	2.79415500
C	0.43615100	-2.53894600	2.55301400
C	1.51591600	-2.82535900	4.73655500
C	1.27998100	-1.45519100	4.98742900
C	0.66772400	-0.63699300	4.05267400
C	0.98391000	3.47597700	2.66266900
C	3.89922300	1.22154000	0.50008700
C	2.89887900	-1.06652300	0.25136700

C	4.18180400	-1.88031800	0.40788300
C	6.60771700	-1.81796200	-0.34929200
C	7.16501900	-0.88109300	0.71045300
H	1.21750600	-0.34768500	-4.42132300
H	2.61382200	3.93765400	-2.35376000
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H	-4.57665100	-0.14127000	-1.11692100
H	1.58406700	-1.03264400	5.94763500
H	0.49736300	0.42261500	4.25326600
H	2.07534000	-1.64227200	0.67030100
H	3.98088700	-2.94857100	0.29956500
H	2.67698100	-0.93219000	-0.81091600
H	5.00945500	-0.39855100	-0.73140700
H	4.62506400	-1.71764500	1.39253400
H	2.90938500	0.16740300	1.91072300
H	7.35736300	-0.71561900	-2.05972100
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H	6.63900100	-0.96502400	1.66493800
H	7.11031000	0.15835500	0.37314500
N	2.87588100	0.24942800	0.89592600
N	5.17508000	-1.48014100	-0.62721900
H	2.64133800	1.24215300	-5.74445800
H	3.33711600	3.39373500	-4.65896500
H	-6.10697900	5.84900500	0.47327100
O	0.84660000	5.43000400	-1.18101500
H	0.45237000	6.18322400	-0.72785200
C	-4.00138200	5.46024100	0.40551200
H	1.21580300	3.96636800	3.62119300
H	-3.72208000	6.50950300	0.29603000
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Mg-(D) Intermediate from VASP

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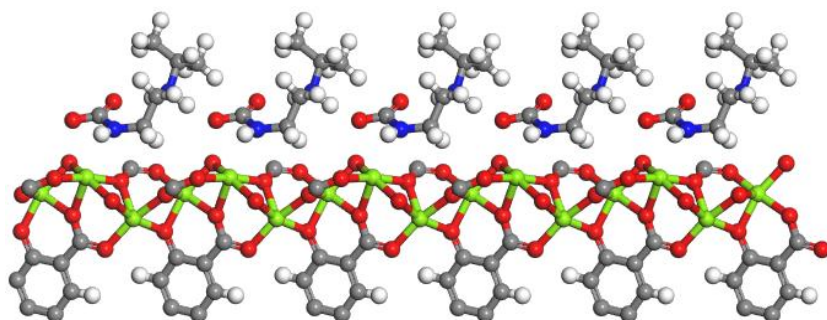
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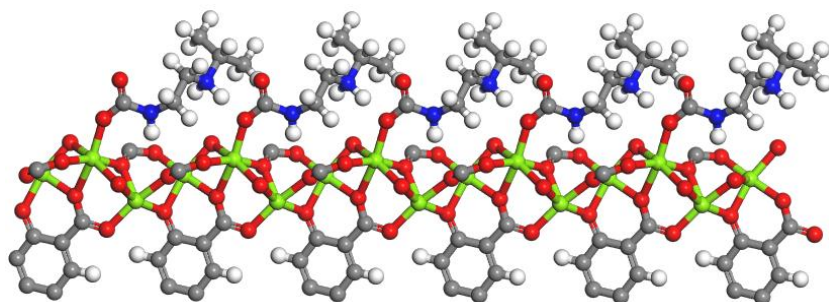
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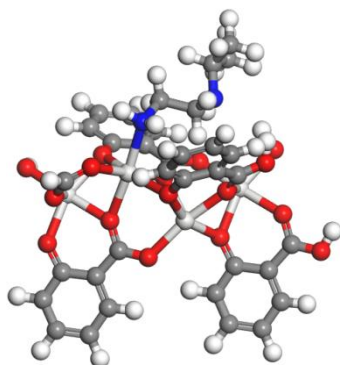
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0.4966372564135781	0.3638930324462777	0.8293105078307192
0.5053889031530403	0.3870977298524565	0.0277580764172285
0.4669480324587028	0.4200704480532096	0.0936700474289509
0.4185615501763849	0.4302440528284492	0.9743632642529434
0.4076190105037512	0.4043034531987644	0.7816485061587031
0.4452603120224481	0.3721147660595960	0.7112554961964932
0.5565701703827415	0.3819843543876758	0.1689771508927151
0.6685523881896387	0.8641073722197419	0.5755602027179805
0.6452987707053452	0.8948534651175422	0.4089205595368099

0.7197217003848451	0.9206923533749958	0.7223980332705295
0.4772427062666793	0.9404002404701757	0.1290562961108890
0.5720164065287321	0.0210172641427135	0.6974831694941628
0.5101111556280173	0.8989996132326965	0.8240017907490085
0.0709838086994168	0.5944006074838555	0.4611998183195070
0.9913037379366898	0.6215776172767065	0.0155959159487367
0.1228100920366018	0.6805361487211954	0.1442811051104016
0.3968202782688337	0.5255170327553245	0.7767582775710835
0.3648946807330233	0.4272008677172394	0.3405311784456870
0.3247851165087212	0.5064904481499255	0.4759659390187636
0.5638061422077740	0.6639033217584185	0.9603780818558150
0.6456002076205110	0.7415629776537713	0.7217191997302805
0.8934152204129830	0.5048908911387855	0.9208359786557381
0.9688938149477835	0.6089523339370118	0.3639396101627312
0.8385378921884268	0.5348360460568955	0.2328136147256075
0.5453243183934759	0.1058563182214769	0.5902561175775389
0.5896535409350392	0.0408110356351941	0.0394988572039381
0.6361429930091873	0.1602374735839618	0.9052761141879557
0.4786960078722160	0.4401934534430936	0.2427294717838464
0.3683122353756545	0.4094425953035241	0.6856170409568350
0.4365790721316785	0.3528047088173167	0.5613576761454979
0.5031787015084035	0.6737428402645307	0.7955610733675513
0.5598473209792587	0.7695336923718870	0.5668703955372862
0.5705880662996350	0.8240672377940754	0.7500604278303484
0.6571402856486159	0.7969325490271544	0.9250082796950565
0.4615891870391877	0.7085405131889360	0.0570009480059852
0.6967432600160350	0.8379209745158107	0.5134999858687692
0.6194300642284247	0.9240061397432413	0.4634783588719600
0.6056489792416357	0.8542165433911677	0.3076676670793148
0.6963954976286004	0.9318576736173441	0.3262289994187810
0.7684843836629369	0.9634995164260900	0.6448584776279347
0.7419060449663490	0.9012308272971197	0.8362689436034074
0.6893656278565032	0.9435544882799221	0.7928034309776422
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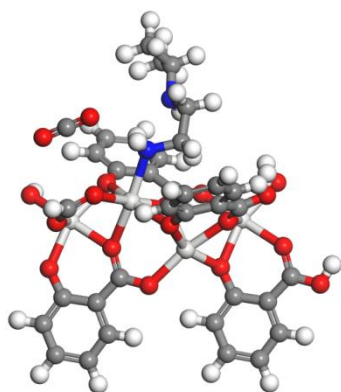
Sc-(A) i-2-MOF

-1 1

H	0	-1.96086300	7.81350600	-0.87055500
H	-1	0.28892900	6.72630400	-1.19598800
Sc	-1	-2.81679900	0.88617700	-1.34625300
H	0	-5.97637700	3.78603200	-0.40584000
O	-1	-4.69795400	-0.14646300	-1.76846600
O	-1	-1.41569800	2.55628700	-0.99813400
O	-1	-4.21790400	2.46446300	-0.76500300
O	-1	-5.24736700	4.42330600	-0.46957200
O	-1	-2.37895000	0.71278600	0.88138600
O	-1	-4.33798000	0.06351200	1.73625800
H	0	-4.46826800	-1.08265100	-1.67444100
C	-1	-1.61191300	3.88630900	-0.99084500
C	-1	-2.90227600	4.49738700	-0.85201200
C	-1	-2.97850300	5.90766300	-0.80854500
C	-1	-1.86523300	6.73449400	-0.91066900
C	-1	-0.60590700	6.11182900	-1.07840200
C	-1	-0.48649500	4.73235000	-1.11337800
C	-1	-4.16614300	3.77277000	-0.68711000
C	-1	-2.37322900	-0.35448500	3.03357800
C	-1	-3.18489600	-0.87040100	4.06945300
C	-1	-3.06482700	0.16238400	1.85363600
H	0	-3.32449200	-1.86123300	5.98756800
C	0	-3.41809600	-4.39046200	-1.17211800
C	0	-4.40929600	-4.98327600	-0.17779900
C	0	-4.01719000	-4.32398700	-2.57046800
H	-1	-3.96540000	6.33975500	-0.64606100
H	-1	-4.26259200	-0.81129600	3.91787700
H	0	-2.52997100	-2.58647700	-1.53197100
H	0	-5.30184900	-4.35122800	-0.11227400
H	0	-4.71512400	-5.98522100	-0.49419700
H	0	-4.90543500	-3.68207500	-2.57609600
H	0	-4.30910800	-5.31974300	-2.91680600
H	0	-3.29590700	-3.91628800	-3.28800400
N	0	-3.03233500	-3.03774800	-0.77104200
H	0	4.91552600	5.70452200	0.09724900
H	-1	7.16541400	4.61683200	-0.22583000
Sc	-1	4.05968200	-1.22329000	-0.37612100
Sc	-1	-0.32644600	1.34452600	0.52945300
Sc	0	1.27775500	-1.32934800	0.88756000
O	0	2.13037900	-2.27413700	-0.75161300
O	0	-0.02993200	-0.61697500	-0.52223100
O	-1	-1.53982000	-0.64287300	-2.20421300
O	-1	5.46069500	0.44685200	-0.02800900
O	0	2.67268100	0.36446800	0.16719000
O	-1	1.62911500	2.31382900	0.50058600
O	0	-0.09132700	-0.01447500	2.17725200



O	-1	4.49753700	-1.39667900	1.85153900
O	0	2.57429000	-2.14637700	2.75020600
C	-1	1.64613100	-2.55462800	-2.00945400
C	-1	0.38498800	-2.02843500	-2.45828900
C	-1	-0.06212900	-2.38792300	-3.75524700
C	-1	0.65171300	-3.22906700	-4.60063800
C	-1	1.87807700	-3.75340900	-4.12494600
C	-1	2.35882500	-3.41291000	-2.86526000
C	-1	-0.42869800	-1.08902600	-1.71500000
C	-1	5.26456800	1.77683700	-0.02068400
C	-1	3.97420700	2.38791900	0.11814800
C	-1	3.89798100	3.79819100	0.16160800
C	-1	5.01125100	4.62502200	0.05948700
C	-1	6.27057700	4.00235700	-0.10824600
C	-1	6.38998900	2.62287800	-0.14322400
C	-1	2.71037100	1.66329100	0.28309700
C	-1	-0.94297900	-0.48205800	3.15128100
H	0	4.35747400	-2.21037100	3.73994800
C	-1	-2.67154900	-1.47737000	5.21046100
C	-1	-1.26281500	-1.57039400	5.31714500
C	-1	-0.43102400	-1.09576700	4.31444200
C	-1	3.81165500	-1.94708400	2.82378800
C	0	-0.94055700	-3.74159600	0.48388800
C	0	-2.22957900	-2.91313400	0.43612800
H	0	-0.51174000	-2.95294500	2.34152800
H	-1	-0.98677200	-1.92346100	-4.09680500
H	-1	3.31828700	-3.80199300	-2.51383600
H	-1	2.91108400	4.23028300	0.32409300
H	-1	0.49009400	4.26038300	-1.24387000
H	-1	-0.81654300	-2.00754900	6.21206700
H	-1	0.65521300	-1.17389900	4.40674400
H	0	-0.45119200	-3.70487400	-0.49510700
H	0	-1.15915300	-4.79198800	0.71031700
H	0	-1.95286100	-1.85913400	0.53395200
H	0	-2.84268600	-3.15546000	1.31427100
H	0	0.66327100	-3.90271700	1.75927300
H	0	-2.54350900	-5.06493700	-1.21956600
H	0	-3.98048400	-5.07084300	0.82546000
N	0	-0.00333900	-3.18351000	1.48546400
H	0	0.27943500	-3.47353900	-5.59065100
H	-1	2.45643200	-4.43721300	-4.74816700
O	-1	5.33666400	-2.75235400	-1.23404300
H	0	5.30409700	-2.70119200	-2.19573800
H	-1	7.36657800	2.15091100	-0.27371400
H	-1	-4.67726900	-0.78972800	2.04893200



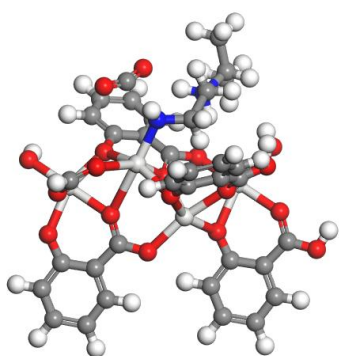
Sc-(B) Complex

-1 1

H	0	-8.31694300	1.83344700	-0.55607100
Sc	-1	-2.61723200	-2.12332100	-1.39227000
O	-1	-2.60026700	-4.24166200	-1.88720400
O	-1	-3.41693100	-0.11512500	-0.92936900
O	-1	-4.61958000	-2.64263800	-0.69944800
O	-1	-6.82384500	-2.65820000	-0.34656000
O	-1	-2.09535000	-1.87320500	0.80771900
O	-1	-2.40707500	-3.90729500	1.68426500
H	0	-1.76215900	-4.42581700	-2.32888200
C	-1	-4.68384800	0.33042700	-0.85856300
C	-1	-5.81640600	-0.53471100	-0.69588000
C	-1	-7.09864200	0.04902400	-0.58600200
C	-1	-7.31890600	1.41999900	-0.64656400
C	-1	-6.19136700	2.25284400	-0.84098800
C	-1	-5.75219900	-1.99364600	-0.57333800
C	-1	-1.12201900	-3.25388900	4.04433500
C	-1	-1.92627600	-2.72522300	1.79162200
H	0	-0.35378200	-3.78407800	5.99602600
C	0	4.33566500	-4.30252800	-2.95613500
H	-1	-7.93104300	-0.63067500	-0.40651700
H	-1	-1.66240800	-4.18995600	3.90089600
H	0	1.88304300	-4.91648400	0.23907100
H	0	2.39692300	-3.49264800	-1.64072600
H	0	3.64148100	-5.64358400	-1.43703100
H	0	3.40948800	-4.32366400	-3.54105900
H	0	5.02732300	-5.02731600	-3.39478300
H	0	-3.22908000	6.92227000	0.25371300
H	-1	-6.32653700	3.33262500	-0.92858300
Sc	-1	2.47119400	2.96537600	-0.58001300
Sc	-1	-1.74048600	0.25151200	0.48068900
Sc	0	1.35485300	0.43654200	0.69938500
O	0	2.48610000	0.79841900	-1.02364400
O	0	0.04554200	-0.34946400	-0.69145400
O	-1	-0.76048900	-1.59820300	-2.39205900

O	-1	1.67158100	4.97366000	-0.11701300
O	0	0.46479400	2.46312700	0.06241500
O	-1	-1.73538200	2.43044800	0.46582900
O	0	-0.40557700	-0.16141800	2.08592600
O	-1	2.99300000	3.21544500	1.61990900
O	0	2.76361900	1.17367500	2.54665500
O	0	5.94919500	1.06140400	1.70097800
O	0	5.22656400	-1.02299700	2.45140000
C	-1	2.46399900	0.23432400	-2.27504600
C	-1	1.39323100	-0.62278900	-2.69637600
C	-1	1.46353100	-1.20813800	-3.98093500
C	-1	2.53221700	-1.00831400	-4.84654900
C	-1	3.58469200	-0.17078700	-4.40250300
C	-1	3.54108400	0.43890100	-3.15938600
C	-1	0.20504500	-0.89753000	-1.90519000
C	-1	0.40470000	5.41909900	-0.04637300
C	-1	-0.72788800	4.55406500	0.11631100
C	-1	-2.01009100	5.13770300	0.22627900
C	-1	-2.23045400	6.50865800	0.16581900
C	-1	-1.10291500	7.34150300	-0.02860400
C	-1	-4.91587800	1.72187300	-0.93950500
C	-1	-0.66370300	3.09505700	0.23898100
C	-1	-0.41316000	-1.10563600	3.09172600
C	-1	-1.18030800	-2.32126800	2.98333300
C	-1	-0.37635700	-3.04670500	5.19996700
C	-1	0.34259900	-1.83042900	5.30040100
C	-1	0.32745000	-0.89783100	4.27495200
C	-1	3.16219800	2.36339600	2.60388500
C	0	5.58068300	0.02280700	2.07721700
C	0	1.64325300	-2.84418200	0.78921200
C	0	2.50256100	-4.00522400	0.30734500
C	0	4.07360100	-4.62669000	-1.49163200
C	0	5.37599800	-4.62294800	-0.69875500
H	-1	0.60862400	-1.80836600	-4.29290200
H	-1	4.35521600	1.08767300	-2.82640600
H	-1	-2.84249300	4.45800300	0.40586400
H	-1	-4.05093900	2.37241600	-1.08809000
H	-1	0.91182100	-1.61428100	6.20638000
H	-1	0.89276800	0.03395800	4.35698400
H	0	1.19579500	-3.06066600	1.76178000
H	0	0.82029500	-2.67566500	0.08626600
H	0	3.06957400	-1.62171200	0.08829200
H	0	3.28478900	-4.20611200	1.04845000
H	0	3.02391100	-1.63461400	1.70642500
H	0	4.77569600	-3.30392500	-3.05317900
N	0	2.42431400	-1.59587800	0.88369600

N	0	3.13279500	-3.64173400	-0.95347000
H	0	2.55580200	-1.47329900	-5.82689400
H	-1	4.45457600	-0.01077100	-5.04201100
H	-1	-1.23796700	8.42120600	-0.11619700
O	-1	4.32809700	3.49037500	-1.57975100
H	0	4.22114300	3.39467400	-2.53262000
C	-1	0.17259300	6.81043400	-0.12712200
H	0	3.65656500	2.73591200	3.51106500
H	-1	1.03763000	7.46099700	-0.27580600
H	0	-1.74896800	-4.59314900	1.86926400
H	0	-6.59449400	-3.60028600	-0.31564400
H	0	5.84249300	-3.63280900	-0.74569400
H	0	6.07500300	-5.35504700	-1.11473600
H	0	5.22212100	-4.87791700	0.35379200



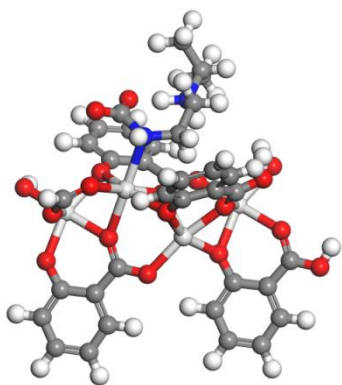
Sc-(C) TS<sub>1</sub>

-1 1

H	-3.27813900	7.41052400	-1.57788200
Sc	-3.00430000	0.43959600	-1.16206500
O	-4.69508200	-0.91437800	-1.36342700
O	-1.87562300	2.33841100	-1.07488700
O	-4.60698700	1.83216900	-0.66074900
O	-5.94171000	3.62006600	-0.58612000
O	-2.42018400	0.57277000	1.03241100
O	-4.19951800	-0.22621100	2.12733100
H	-4.52846700	-1.56697300	-2.05229300
C	-2.28538100	3.61076100	-1.22259600
C	-3.65371700	4.01951800	-1.08808300
C	-3.96159900	5.39253900	-1.21765100
C	-3.00604500	6.36501400	-1.48780800
C	-1.66736700	5.93535800	-1.64983600
C	-4.77189400	3.12907800	-0.76463500
C	-2.82776600	-0.42619800	4.52042500
C	-2.96474100	0.11339200	2.13477100
H	-2.72334000	-0.99348100	6.60577600
C	-3.11681700	-4.03041900	-3.07898800
H	-5.00025800	5.67794500	-1.05395400
H	-3.90394000	-0.58009200	4.43715600

H	-3.20093900	-3.54919300	0.86877100
H	-2.13929400	-2.57045000	-1.17952700
H	-4.09332700	-3.94409800	-1.16991600
H	-3.17188000	-2.95474400	-3.27263000
H	-3.96955000	-4.50962000	-3.56594500
H	3.87507300	6.56176700	-0.82639100
H	-0.89281300	6.66392100	-1.89715700
Sc	4.14833000	-0.40939600	-0.40995800
Sc	-0.52528500	1.49023000	0.47144800
Sc	1.21282600	-1.02234600	1.09240300
O	2.45168900	-1.64839500	-0.60678300
O	0.08126600	-0.28232600	-0.46960700
O	-1.49471600	-0.89026000	-1.98396600
O	5.27700600	1.48941900	-0.32278100
O	2.56453100	1.00740000	0.12656900
O	1.21091900	2.77107500	0.16598600
O	0.00894900	0.46683800	2.25695000
O	4.73234700	-0.27621000	1.78450700
O	3.00266500	-1.14692300	2.93034000
O	2.16524300	-4.45226600	1.07462900
O	0.36434400	-4.96735900	-0.29215600
C	1.91768100	-2.32242900	-1.71224400
C	0.57467300	-2.06245000	-2.14543300
C	0.11095400	-2.69471900	-3.32137100
C	0.88915800	-3.57279400	-4.06606400
C	2.20622600	-3.82581000	-3.61038000
C	2.70428700	-3.20739100	-2.47528400
C	-0.33780600	-1.14794100	-1.47883500
C	4.86724900	2.76176900	-0.47049100
C	3.49891200	3.17052600	-0.33597800
C	3.19103100	4.54354700	-0.46554500
C	4.14658400	5.51602200	-0.73570000
C	5.48526200	5.08636700	-0.89772900
C	-1.32134700	4.60081300	-1.51696300
C	2.38073500	2.28008600	-0.01252800
C	-0.71985700	0.11431100	3.38487900
C	-2.15451900	-0.02013100	3.34536700
C	-2.17538800	-0.68229500	5.72164200
C	-0.76954800	-0.51107900	5.74745500
C	-0.06908000	-0.13254600	4.61270300
C	4.18788900	-0.73560000	2.88687800
C	1.16338600	-4.52037500	0.45744100
C	-1.33603800	-2.59943500	1.33182500
C	-2.14606900	-3.66919600	0.60587600
C	-3.16173400	-4.33667000	-1.59235100
C	-3.04191000	-5.82377000	-1.30796800

H	-0.89370200	-2.43312700	-3.65428600
H	3.72325600	-3.40485500	-2.13291100
H	2.15237200	4.82895300	-0.30184800
H	-0.28516600	4.27812100	-1.64236800
H	-0.22467100	-0.66792700	6.68011500
H	1.01692000	-0.01179700	4.63925100
H	-1.76291400	-2.54999900	2.34131800
H	-1.57748100	-1.63565800	0.86667700
H	-1.14657200	-3.87338200	-1.18827200
H	-1.82788800	-4.67442300	0.88194500
H	0.34219800	-3.20336100	2.29520900
H	-2.19787200	-4.41208000	-3.53312600
H	-3.81341900	-6.35300300	-1.87233600
H	-3.18357000	-6.06248400	-0.25183500
H	-2.06750300	-6.20657900	-1.62845600
N	0.11412700	-2.76246400	1.40458100
N	-2.07977800	-3.56508500	-0.88297800
H	0.50556400	-4.03574800	-4.97083200
H	2.83959000	-4.53050400	-4.15211600
H	6.25981700	5.81492900	-1.14505100
O	5.65791500	-1.73925300	-1.23185800
H	5.41372000	-1.97096000	-2.13486200
C	5.83128200	3.75182200	-0.76485600
H	4.80726500	-0.72645300	3.79350100
H	6.86746400	3.42913000	-0.89026200
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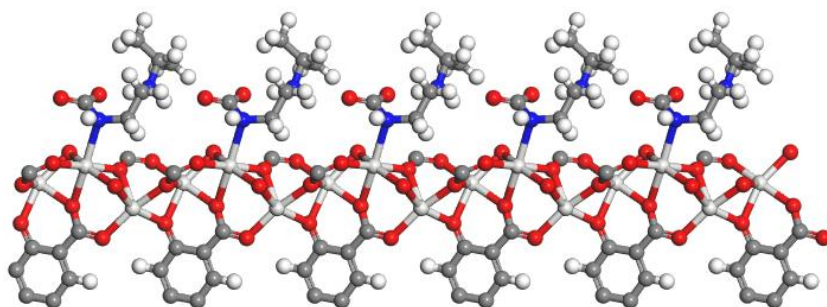
Sc-(D) Intermediate from Gaussian

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O	-3.38506200	-3.38635900	-1.69690300
O	-3.00840000	0.86535400	-1.06896900
O	-4.91498600	-1.17770500	-0.78793600
O	-7.04374700	-0.52530300	-0.62552300
O	-2.37823900	-1.04727000	0.88026300

O	-3.33140200	-2.82302400	1.85053600
H	-2.62449000	-3.82523200	-2.09743800
C	-4.08947600	1.66254300	-1.13497800
C	-5.43471300	1.17879800	-1.01730300
C	-6.49215400	2.11540100	-1.05419600
C	-6.29417400	3.48134800	-1.21780700
C	-4.96111600	3.93308000	-1.36548700
C	-5.81160800	-0.22068800	-0.80002400
C	-2.06496200	-2.37313600	4.26762700
C	-2.53134900	-1.82587100	1.92578000
H	-1.61397700	-2.93683700	6.30689700
C	0.96678400	-5.43762200	-2.91196400
H	-7.49767800	1.72318700	-0.90535200
H	-2.84692300	-3.12148200	4.13616400
H	-0.25816400	-4.80847400	0.87960500
H	0.32582900	-3.71281500	-1.20559000
H	0.14671500	-6.19025800	-1.07436400
H	0.04585500	-4.91859200	-3.19688400
H	0.97667800	-6.40582200	-3.41832300
H	-0.83046500	7.62088700	-0.30993400
H	-4.76604100	4.99445500	-1.53081800
Sc	3.49105100	2.12912700	-0.40519000
Sc	-1.39244800	0.84861900	0.45497100
Sc	1.63081500	0.14381000	0.92219900
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O	0.20892400	-0.33515900	-0.51884000
O	-0.81917700	-1.44022200	-2.20363000
O	3.29104300	4.31436900	-0.13737500
O	1.38639500	2.28418200	0.09634000
O	-0.74430400	2.92371300	0.30607100
O	-0.34302500	0.19713600	2.18599300
O	3.92111700	2.40169700	1.81184400
O	2.98463400	0.64277400	2.86097000
O	4.19933800	-2.25102100	1.57718200
O	3.20168400	-3.24761700	-0.16539100
C	2.78784100	-0.61559900	-1.92288900
C	1.54124400	-1.15856200	-2.38125700
C	1.51809900	-1.84511700	-3.61646400
C	2.65138800	-2.03640100	-4.39765000
C	3.87326800	-1.50485300	-3.91723300
C	3.93167500	-0.80602600	-2.72258700
C	0.27662500	-1.01033800	-1.67978300
C	2.20996800	5.11155900	-0.20338500
C	0.86473000	4.62781300	-0.08571000
C	-0.19271000	5.56441600	-0.12260200
C	0.00526900	6.93036200	-0.28621100

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C	-3.89534700	3.04958500	-1.32110900
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C	-0.69477600	-0.60976800	3.24879500
C	-1.77757900	-1.55617500	3.15008600
C	-1.36712200	-2.29403300	5.46798800
C	-0.32945900	-1.33378000	5.55480900
C	-0.00322500	-0.52630500	4.47631000
C	3.76809500	1.62314400	2.85737500
C	3.21409200	-2.60414200	0.92288700
C	0.65737500	-2.91614800	1.27045000
C	0.71229400	-4.33060900	0.72034600
C	1.04099400	-5.65173200	-1.40926000
C	2.28842200	-6.41601000	-0.99371000
H	0.54601800	-2.19647900	-3.96315900
H	4.87784200	-0.39534700	-2.36117300
H	-1.19823500	5.17220300	0.02624200
H	-2.86931400	3.40720000	-1.43466900
H	0.21874700	-1.21602600	6.49126500
H	0.80522900	0.20566900	4.54910100
H	0.16638800	-2.96973300	2.24356400
H	-0.00363700	-2.31555500	0.63777800
H	1.97739400	-3.80638300	-0.72922500
H	1.48213500	-4.92846800	1.21123800
H	2.10071200	-2.08148800	2.48227700
H	1.81719500	-4.84967700	-3.27126300
H	2.30935800	-7.37404000	-1.51862700
H	2.31028300	-6.62848000	0.07803100
H	3.19209100	-5.85825900	-1.25652100
N	1.92900400	-2.18074800	1.48452300
N	1.00398000	-4.31738400	-0.73429900
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H	4.79082800	-1.65771100	-4.48814400
H	1.53340300	8.44347000	-0.59922400
O	5.48026800	2.00879300	-1.27203400
H	5.39846500	1.85128700	-2.21935600
C	2.40409500	6.49860100	-0.38951400
H	4.33602800	1.87769100	3.76234100
H	3.43012900	6.85621600	-0.50307400
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Sc-(D) Intermediate from VASP

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Sc O C H N

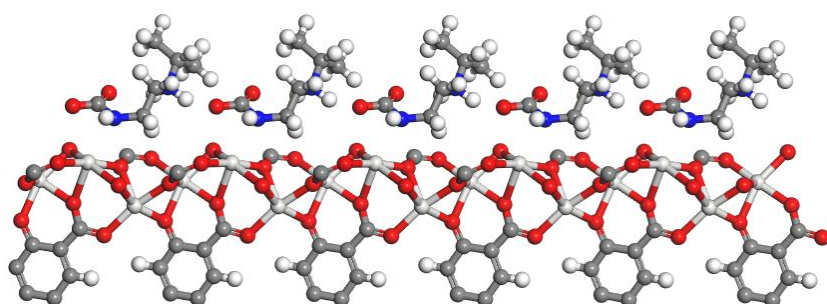
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Direct

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0.5913542535502287	0.2876705276413034	0.8861664856308025
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0.2713457585995371	0.6814787060778613	0.6123779413370158
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0.3203492841572952	0.5968004357766645	0.3086298474995104
0.3265528134620297	0.6451198228305088	0.9546325838289746
0.3821393139956442	0.6169543244485496	0.7401251385809786
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0.5741476729459976	0.8294298142665824	0.4307201774324980
0.7334381057504871	0.4409129270611203	0.4367189538912513
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0.7744373081517111	0.4211130159063643	0.0050273870365203
0.6412564966839298	0.2540526658475741	0.0986935866484089
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0.5773539968313557	0.2150062896656166	0.6658254976896529
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0.4737324589705594	0.9345533713913596	0.1497671465690260
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0.3392264372784481	0.5082676645723723	0.4820282471918489
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0.6214138617300122	0.1459143028345480	0.9239698709655286
0.4822282248389840	0.4378133575358021	0.2508352910287428
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0.4512016052972072	0.3687723958511455	0.5910666448422646
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0.5569047907814380	0.8087903269315575	0.9788014647999503
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0.5048592981489080	0.6707879507036907	0.4940844675052318
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Sc-(E) TS<sub>2</sub>

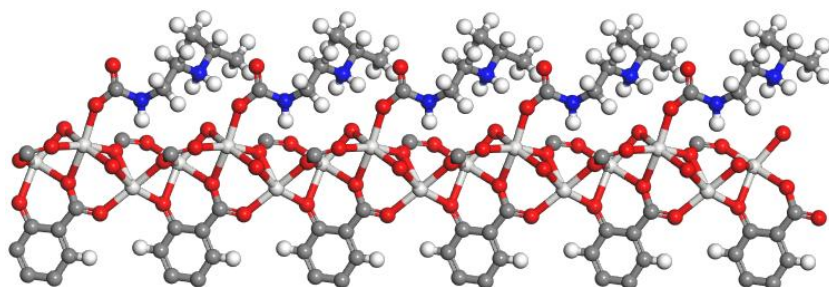
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Sc	O	C	H	N

## Direct

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Direct

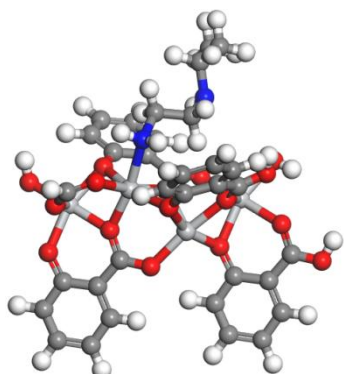
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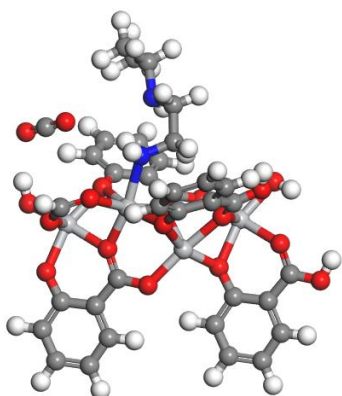
Ti-(A) i-2-MOF

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O	-4.04560700	2.45427700	-0.67384500
O	-5.09521100	4.42398300	-0.63716000
O	-2.34169400	0.68566500	0.71298200
O	-4.33717600	0.18653700	1.57654900
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C	-1.46751800	3.81932700	-1.08821300
C	-2.74258200	4.45963400	-0.98216500
C	-2.79387100	5.86875300	-1.02354600
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C	-2.41408300	-0.11849900	2.96564400
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H	-4.32124400	-0.47962000	3.85549900
H	-2.23695000	-3.24780500	-1.69010700
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Ti	1.21914300	-1.06541900	0.85561000
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O	-0.05412000	-0.49285500	-0.52337800
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C	1.54374200	-2.58534800	-1.87709000
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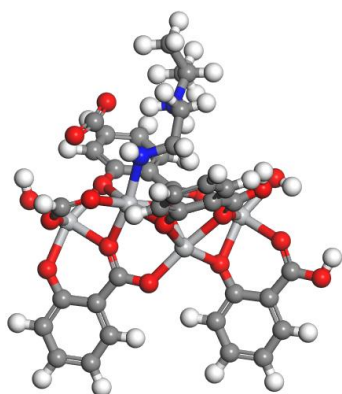
#### Ti-(B) Complex

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O	-1	-6.76266100	-2.36531800	-0.72032700
O	-1	-2.10475200	-1.86505800	0.52571400
O	-1	-2.64829300	-3.88907600	1.29819000
H	0	-3.38401600	-4.24320200	-1.57289100
C	-1	-4.49962300	0.54530700	-1.06407300
C	-1	-5.67103900	-0.27047800	-0.97482500
C	-1	-6.93203700	0.36082600	-0.96278000
C	-1	-7.08291500	1.74176800	-1.04182700
C	-1	-5.91289300	2.52651500	-1.15294100
C	-1	-5.65099600	-1.72724700	-0.83212300
C	-1	-1.61705200	-3.34981200	3.81591300
C	-1	-2.12784300	-2.73625300	1.49418900
H	0	-1.07322300	-3.94966200	5.82014600
C	0	4.99759500	-3.91707800	-2.29634700
H	-1	-7.80511700	-0.27949800	-0.83852200
H	-1	-2.16450600	-4.26609700	3.59164100

H	0	2.73742200	-3.30205200	-1.47400200
H	0	4.01417800	-5.40713200	-1.11238100
H	0	4.25543800	-3.92384800	-3.10231600
H	0	5.82054000	-4.57441500	-2.59110200
H	0	-2.95049100	6.84179200	0.28768800
H	-1	-5.99927600	3.61095300	-1.24474800
Ti	-1	2.52641100	2.70853500	-0.25120700
Ti	-1	-1.77874600	0.22592000	0.42960100
Ti	0	1.05009500	0.40232600	0.79862900
O	0	2.45939900	0.69842800	-0.76445200
O	0	-0.05715900	-0.29794500	-0.65425000
O	-1	-0.80601200	-1.36560000	-2.46994300
O	-1	1.86456500	4.67791200	0.26191800
O	0	0.58713300	2.29994000	0.26503700
O	-1	-1.64659300	2.27725900	0.59755300
O	0	-0.60461800	-0.26076200	2.07101900
O	-1	3.01131600	2.77752000	1.84359400
O	0	2.32167000	0.84230000	2.72743100
O	0	5.20202900	-0.64087200	1.31221500
O	0	6.23023600	0.96100900	-0.03172600
C	-1	2.54570900	0.12852800	-1.98704400
C	-1	1.45670600	-0.61700300	-2.53939900
C	-1	1.59960800	-1.17451300	-3.82466100
C	-1	2.76517700	-1.04356300	-4.57343600
C	-1	3.82940800	-0.30527900	-4.00718800
C	-1	3.71765000	0.27196100	-2.75329700
C	-1	0.17835900	-0.79829100	-1.86285000
C	-1	0.61644600	5.18788500	0.25380700
C	-1	-0.55497000	4.37209800	0.34305600
C	-1	-1.81589500	5.00347000	0.35511900
C	-1	-1.96677300	6.38441200	0.27607100
C	-1	-0.79675100	7.16915800	0.16495800
C	-1	-4.65607600	1.94246300	-1.16418400
C	-1	-0.53492800	2.91533100	0.48575700
C	-1	-0.72958300	-1.21682500	3.00279800
C	-1	-1.52149200	-2.39480500	2.78477400
C	-1	-0.98785900	-3.19297700	5.04803900
C	-1	-0.24313700	-2.00934100	5.25695200
C	-1	-0.11852400	-1.05137600	4.26270700
C	-1	2.98822700	1.90632500	2.81206900
C	0	5.71048000	0.16117700	0.63824900
C	0	1.35592400	-2.87807000	0.71250900
C	0	2.38646100	-3.95462500	0.40155700
C	0	4.38763900	-4.37429300	-0.97830800
C	0	5.43956500	-4.39163900	0.12529900
H	-1	0.73373900	-1.69121500	-4.23967700

H	-1	4.54371900	0.83866100	-2.31881900
H	-1	-2.68904800	4.36307900	0.47935800
H	-1	-3.75318900	2.55044100	-1.25178100
H	-1	0.23850700	-1.84259300	6.22219300
H	-1	0.46577700	-0.14277700	4.42384500
H	0	0.69728700	-3.19529400	1.52320800
H	0	1.86644700	-4.88961900	0.12827300
H	0	0.72885100	-2.70412900	-0.16891200
H	0	2.85978500	-1.55456600	0.53742300
H	0	2.96914300	-4.16684900	1.30550900
H	0	2.29135000	-1.64226800	2.05679800
H	0	5.38618900	-2.89714800	-2.20281800
H	0	6.27180600	-5.04481500	-0.15457700
H	0	5.03903200	-4.76003500	1.07423200
H	0	5.82935400	-3.38131600	0.28926100
N	0	1.99480900	-1.60235700	1.08267200
N	0	3.28682400	-3.47192300	-0.63416300
H	0	2.84718700	-1.48084900	-5.56308900
H	-1	4.76479400	-0.20111300	-4.55999200
H	-1	-0.88320800	8.25353000	0.07313100
O	-1	4.31005700	3.27697800	-1.15206200
H	0	5.05462200	2.71030000	-0.92220800
C	-1	0.46006600	6.58510600	0.15371500
H	0	3.54591000	2.13931800	3.72798400
H	-1	1.36288000	7.19301900	0.06609800
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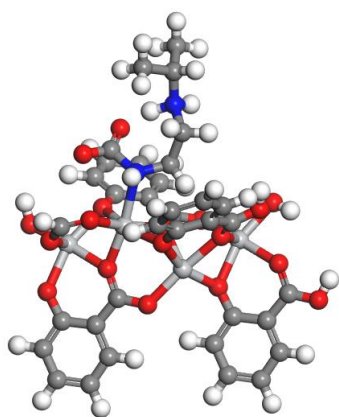


Ti-(C) TS<sub>1</sub>

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H		-7.93164500	1.94780400	-1.41387100
Ti		-2.31565700	-2.03159900	-1.41817000
O		-2.26468300	-4.08231600	-1.76124400
O		-3.05587300	-0.04975100	-1.09545100
O		-4.26975000	-2.48890800	-0.70749100
O		-6.50313200	-2.53014000	-0.68546600
O		-1.91355300	-1.77400000	0.67945700

O	-2.42482200	-3.74440000	1.59866000
H	-3.04531800	-4.35427400	-1.26450300
C	-4.31761200	0.41596900	-1.19063000
C	-5.46639100	-0.42823400	-1.07523900
C	-6.74543200	0.15957000	-1.16095200
C	-6.93484700	1.52349800	-1.36054200
C	-5.78568600	2.33493500	-1.49516200
C	-5.40779900	-1.86679600	-0.81057500
C	-1.50742700	-2.96531900	4.09758200
C	-1.94733400	-2.56265100	1.71596400
H	-1.02337000	-3.37905000	6.16352000
C	3.46328400	-4.50065800	-2.80315600
H	-7.60287300	-0.49704500	-1.01474700
H	-2.01795400	-3.91469700	3.93137700
H	1.88072200	-3.19845200	-1.21039300
H	2.46580000	-5.53438300	-1.20380400
H	2.54199600	-4.18570200	-3.30010100
H	3.81373600	-5.41694500	-3.28430000
H	-3.01229700	6.85081400	-0.31586100
H	-5.90123300	3.40463000	-1.68036400
Ti	2.60358200	2.87162700	-0.31183800
Ti	-1.64746000	0.31162400	0.42047000
Ti	1.20489600	0.55300600	0.88494000
O	2.59914800	0.86324800	-0.68470900
O	0.13309400	-0.24222900	-0.54675500
O	-0.51685000	-1.48029600	-2.29931800
O	1.86336500	4.85347400	0.01088000
O	0.65448500	2.43882000	0.16889700
O	-1.58389400	2.37308500	0.42086600
O	-0.53529500	0.00824600	2.13831700
O	3.00568500	3.12922500	1.78578900
O	2.30962400	1.27507900	2.82861400
O	4.65012800	-0.03568300	1.55866500
O	4.73656700	-1.76851800	0.01767000
C	2.76724800	0.15934700	-1.82401800
C	1.72320600	-0.66504200	-2.35051500
C	1.93196000	-1.32156800	-3.57873900
C	3.12083000	-1.21406700	-4.29385700
C	4.13981700	-0.39657500	-3.75380000
C	3.96277400	0.27805300	-2.55735900
C	0.42597700	-0.83239300	-1.70713000
C	0.60162600	5.31919400	-0.08429800
C	-0.54715200	4.47499000	0.03109300
C	-1.82612300	5.06286500	-0.05460400
C	-2.01553900	6.42679300	-0.25419500
C	-0.86637700	7.23823000	-0.38881400

C	-4.51228000	1.79412300	-1.41275200
C	-0.48856100	3.03642900	0.29575600
C	-0.65437900	-0.87827900	3.14104300
C	-1.40139900	-2.09594200	2.99424200
C	-0.93086000	-2.68655000	5.33389700
C	-0.23079300	-1.46557700	5.46947100
C	-0.09724700	-0.58924400	4.40366000
C	2.97190500	2.34057400	2.82229600
C	4.50202500	-0.92174900	0.80847600
C	1.43889300	-2.51327600	1.22227800
C	2.26807600	-3.70332100	0.75461400
C	3.24426100	-4.77419400	-1.32645500
C	4.51586400	-5.21640200	-0.62207100
H	1.09861600	-1.89927900	-3.97965700
H	4.75411000	0.90584400	-2.14265800
H	-2.68363400	4.40618000	0.09158500
H	-3.62549300	2.42253600	-1.51868100
H	0.20831100	-1.20385700	6.43392200
H	0.45273100	0.34850000	4.50894700
H	1.00476300	-2.82066600	2.18349600
H	1.68925800	-4.62976100	0.81395200
H	0.58887400	-2.41618400	0.53243100
H	3.37553000	-2.77477200	-0.69653200
H	3.17785400	-3.81121700	1.34789600
H	2.51742400	-1.15621900	2.25451400
H	4.21589000	-3.72173200	-2.95819900
H	4.91608100	-6.08992300	-1.14203900
H	4.34092700	-5.50269600	0.41718900
H	5.27530200	-4.42898400	-0.64949500
N	2.14605400	-1.24843200	1.31024300
N	2.68379100	-3.53997200	-0.67007800
H	3.25376700	-1.72913400	-5.23986300
H	5.09209100	-0.30725700	-4.27971600
H	-0.98199500	8.30785400	-0.57403300
O	4.40238800	3.42293000	-1.19298600
H	5.15467100	2.89733100	-0.89859800
C	0.40702900	6.69741800	-0.30640400
H	3.51708600	2.65791000	3.72140400
H	1.29374600	7.32576200	-0.41235000
H	-2.03640900	-4.35280500	2.23907200
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Ti-(D) Intermediate from Gaussian

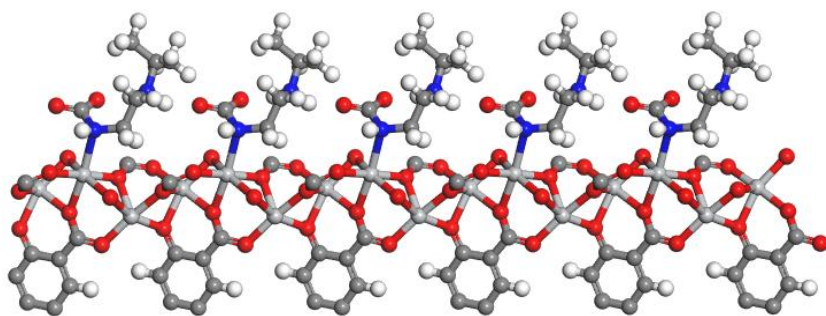
-1 1

H	-8.19568700	-1.74138500	-0.30600100
Ti	-1.51045000	-2.65956800	-1.66151100
O	-0.62805500	-4.40999000	-2.35659200
O	-2.97240500	-1.28574500	-0.91646700
O	-2.89702800	-4.03479000	-0.81366500
O	-4.83870900	-5.10345700	-0.53437000
O	-0.88388200	-2.45571800	0.38640100
O	-0.29878900	-4.52026400	1.00617600
H	-1.12503300	-5.06988500	-1.85853400
C	-4.30394700	-1.44762100	-0.77961100
C	-4.92204900	-2.73328000	-0.67608200
C	-6.32068500	-2.79644000	-0.50686900
C	-7.12305400	-1.66139800	-0.44442600
C	-6.49376400	-0.40253900	-0.57245300
C	-4.18995500	-4.00094100	-0.67224400
C	0.62570600	-3.65889600	3.47529400
C	-0.37638700	-3.26977900	1.26799700
H	1.61374900	-4.00572600	5.36651500
C	6.94622400	-3.21379200	-1.36532300
H	-6.75933000	-3.78539700	-0.37541900
H	0.56318800	-4.71487800	3.20963500
H	4.47813900	-2.89465800	-1.32346800
H	5.94004900	-3.97315800	0.37824500
H	6.44360400	-3.89898700	-2.05501500
H	7.91735200	-3.64556600	-1.11262500
H	-5.82124700	4.74068300	1.03217000
H	-7.09929600	0.50572300	-0.55542800
Ti	0.86514400	3.82235100	-0.31771500
Ti	-1.61363700	-0.46836400	0.46116600
Ti	0.90830400	1.14773800	0.59064900
O	1.71617500	2.06962800	-1.03093500
O	0.11190500	-0.08276200	-0.77363600
O	-0.33308300	-1.25613400	-2.64143000
O	-0.59681100	5.19617300	0.42732700



O	-0.55256700	2.50004000	0.35887500
O	-2.46311600	1.37846100	0.80942500
O	-0.14649100	-0.39831400	1.93854300
O	1.49171200	4.02620000	1.73019600
O	1.83376000	1.96823100	2.51764500
O	4.31334200	1.57081500	0.97289800
O	4.59763700	0.08799100	-0.68857800
C	1.92199400	1.65695900	-2.28344200
C	1.26912600	0.50095300	-2.81659600
C	1.51495500	0.14061400	-4.15557400
C	2.38148800	0.85491000	-4.97731900
C	3.01785000	1.99193000	-4.42912300
C	2.78610400	2.38601700	-3.12186400
C	0.32039500	-0.30895200	-2.06246400
C	-1.92835400	5.03429700	0.56418500
C	-2.54645400	3.74863700	0.66771300
C	-3.94505700	3.68557100	0.83694500
C	-4.74742700	4.82061200	0.89938700
C	-4.11813600	6.07947200	0.77136200
C	-5.12133100	-0.30021800	-0.73612500
C	-1.81436100	2.48097700	0.67155000
C	0.28304000	-1.33015400	2.79858600
C	0.13398000	-2.73368700	2.53369400
C	1.23783100	-3.27020300	4.66392200
C	1.34208500	-1.88429000	4.92397500
C	0.87840900	-0.94399100	4.01700900
C	1.99920700	3.21213900	2.61179200
C	4.01512300	0.56321900	0.33465700
C	2.62178400	-1.52899700	0.27546500
C	3.72603100	-2.54443800	0.55287500
C	6.13775800	-3.00497500	-0.09542000
C	6.83686900	-2.07668800	0.88490500
H	0.96212700	-0.71321600	-4.54838800
H	3.28253500	3.26325500	-2.70195700
H	-4.38373500	2.69652100	0.96837600
H	-4.63708100	0.67340200	-0.83653400
H	1.79078000	-1.54697900	5.86012100
H	0.96951300	0.12599200	4.21641400
H	1.69756100	-1.90035100	0.71443700
H	3.32911600	-3.56206100	0.53100200
H	2.44550500	-1.45170900	-0.80169000
H	4.84531100	-1.36239900	-0.68009600
H	4.16973900	-2.37663000	1.53679400
H	2.83446300	-0.16329600	1.81678200
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H	7.80988200	-2.49990200	1.14498900

H	6.27675300	-1.94800200	1.81478900
H	6.99715400	-1.09165600	0.43621100
N	2.83034600	-0.17490300	0.79676800
N	4.80320000	-2.43820300	-0.47034400
H	2.55295000	0.55485000	-6.00575200
H	3.71915600	2.56223900	-5.04093100
H	-4.72370300	6.98764000	0.78836600
O	2.04251000	5.22578500	-1.29763500
H	2.98854500	5.07207800	-1.19624100
C	-2.74570300	6.18179300	0.60768900
H	2.53296500	3.63891600	3.46961000
H	-2.26148700	7.15532100	0.50726000
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Ti-(D) Intermediate from VASP

1.00000000000000

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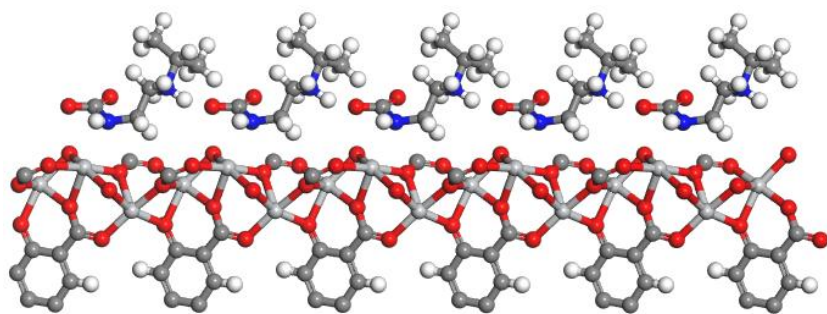
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Direct

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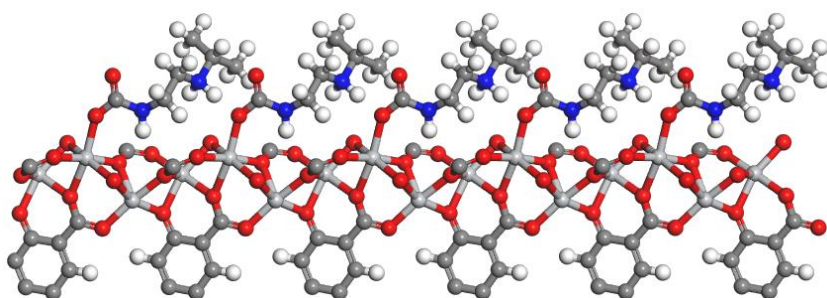
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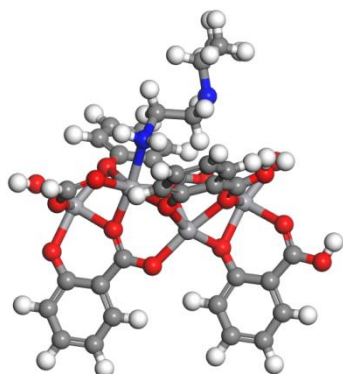
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0.4415973617696238	0.3727376762403338	0.7093786304556886
0.5516360264977322	0.3812224752268847	0.1501001489446665
0.6675109524340712	0.8546937578882918	0.6007819964986680
0.6462997008549323	0.8889979611733736	0.4465576394410249
0.7215835997766291	0.9092247800509128	0.7444533609695370
0.4884180262310096	0.9426156177097695	0.1278942187927328
0.5737620547501336	0.0259655622281159	0.6844497742231894
0.5097052151952397	0.9037311608129315	0.8097048909890745
0.0713083185040020	0.6044434741543370	0.4609020154486672
0.9915311051746443	0.6268106996310223	0.0033467911497027
0.1214164914903293	0.6808094119405084	0.1325775672632901
0.3919656892466961	0.5215992038057280	0.7830986005268485
0.3612988941389901	0.4235783157513566	0.3290419590470250
0.3218314362467467	0.5023095441884351	0.4619592602888503
0.5567284979695231	0.6557821270175026	0.9805632173137226
0.6406878951826585	0.7323461951726458	0.7545053241685125
0.8934828956301075	0.5152462539634257	0.9039127791283335
0.9730345884822214	0.6184959216908439	0.3638182933454388
0.8434728853242817	0.5438127137363438	0.2335243186367251
0.5526507870502542	0.1090170497949146	0.5729264569055204
0.5948151553804735	0.0425679170192197	0.0383865822829463

0.6378611752899701	0.1608301184620373	0.9042790252631434
0.4719827328872483	0.4356771136024804	0.2299243339658332
0.3653781135651144	0.4094829229053758	0.6879489104388696
0.4340547555068355	0.3550118453757065	0.5623507476668053
0.4969599988068438	0.6668300055839964	0.8252290302874528
0.5591718204045222	0.7606502044782530	0.5881947419608338
0.5683464776034413	0.8159322046213617	0.7629079236330725
0.6518175206329246	0.7899811582022949	0.9448775282696715
0.4584800244731468	0.7007406815189796	0.0846998432087460
0.6922280421059028	0.8269095058829592	0.5338766247872755
0.6252282194325218	0.9207818033590556	0.5067942677563053
0.6035387430373333	0.8499771242765206	0.3497081696758357
0.6971145013408560	0.9243741589808181	0.3632080330573402
0.7700402218637592	0.9523083729954251	0.6684073871515182
0.7437348953420440	0.8878016554842389	0.8472626604136480
0.6941361964360553	0.9325957962714924	0.8220131311543213
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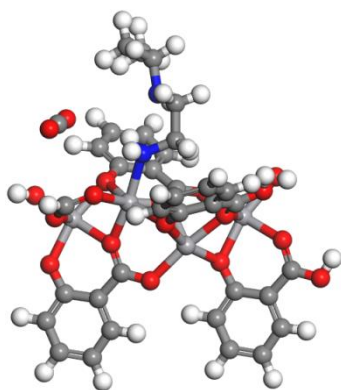
V-(A) i-2-MOF

-1 1

H	0	-1.65816000	7.69704100	-1.17790800
V	-1	-2.70072200	0.96198300	-1.48177000
O	-1	-4.48819100	-0.17560600	-1.78148800
O	-1	-1.23032700	2.43034900	-1.19971900
O	-1	-4.05224500	2.42742700	-0.87710200
O	-1	-5.03562200	4.42109800	-0.77305100
O	-1	-2.37981700	0.70747700	0.61790900
O	-1	-4.36362200	0.29162200	1.54425400
H	0	-4.97793400	-0.00931800	-0.96858700
C	-1	-1.40753800	3.76101700	-1.21051900
C	-1	-2.67891400	4.41073400	-1.09551300
C	-1	-2.72438800	5.81756900	-1.08902000
C	-1	-1.58808900	6.61543600	-1.19584000
C	-1	-0.34617000	5.95984800	-1.33481500
C	-1	-0.25965600	4.57835500	-1.34494700
C	-1	-3.98001500	3.72169600	-0.90414300
C	-1	-2.43960200	0.06245600	2.93755200

C	-1	-3.28956800	-0.26211200	4.01149900
C	-1	-3.10680000	0.38098400	1.64923700
H	0	-3.49465300	-0.94496000	6.05394300
C	0	-3.13965400	-5.06441500	-0.78902900
C	0	-3.62956600	-5.50764100	-2.16124400
H	-1	-3.70252200	6.27675900	-0.94637000
H	-1	0.56391900	6.55249400	-1.45137000
H	-1	-4.36250800	-0.21651200	3.82115100
H	0	-2.27136300	-3.45499600	-1.66989100
C	0	-4.18437600	-5.35515000	0.28141100
H	0	-2.23647900	-5.65506000	-0.55022800
H	0	-2.87552800	-5.31231500	-2.93217900
H	0	-4.54208300	-4.96567300	-2.43225900
H	0	-3.84689300	-6.57961600	-2.16903800
N	0	-2.85053900	-3.62949100	-0.85236000
H	0	4.88019100	5.50049100	0.03859000
V	-1	3.83630800	-1.23534800	-0.26140200
V	-1	-0.39508000	1.34167800	0.45650600
V	0	1.19507100	-1.09704300	0.89445800
O	0	2.05802200	-2.28901800	-0.58910100
O	0	-0.07932600	-0.49785700	-0.55708500
O	-1	-1.40184300	-0.46586600	-2.34074000
O	-1	5.30661900	0.23312700	0.02044700
O	0	2.54500200	0.24757600	0.27157400
O	-1	1.50134400	2.22398100	0.44731100
O	0	-0.15606300	0.20573500	2.12848200
O	-1	4.15706900	-1.48891600	1.83824800
O	0	2.16863000	-1.82853400	2.79299500
C	-1	1.56038400	-2.64881900	-1.78024300
C	-1	0.39065700	-2.04287000	-2.35200700
C	-1	-0.00205400	-2.40734200	-3.65244000
C	-1	0.68334700	-3.34183200	-4.42456000
C	-1	1.81770100	-3.94730700	-3.84388800
C	-1	2.23933200	-3.61218500	-2.56752700
C	-1	-0.40963900	-0.96671700	-1.71907200
C	-1	5.12952600	1.56388300	0.00984300
C	-1	3.85805000	2.21361400	0.12474900
C	-1	3.81267600	3.62043500	0.13134200
C	-1	4.94897500	4.41830200	0.02452200
C	-1	6.19079400	3.76272800	-0.11455300
C	-1	6.27730800	2.38123500	-0.12468500
C	-1	2.55696500	1.52467100	0.31601600
C	-1	-1.02010400	-0.07607600	3.10470300
H	0	3.93645900	-2.06910200	3.80909500
C	-1	-2.81527500	-0.69522200	5.24721300
C	-1	-1.41410800	-0.78474000	5.40863100

C	-1	-0.54727700	-0.48693000	4.37400800
C	-1	3.43037200	-1.81729400	2.86933600
C	0	-0.83608300	-3.63799700	0.67166200
C	0	-2.19368000	-3.03754800	0.30076300
H	0	-0.74237300	-2.41884100	2.31188800
H	-1	-0.85986900	-1.87962300	-4.06927100
H	-1	3.12770300	-4.07808400	-2.13522400
H	-1	2.83454100	4.07962200	0.27389200
H	-1	7.10098300	4.35536000	-0.23100800
H	-1	0.70299300	4.07549600	-1.45412600
H	-1	-1.00584000	-1.08774400	6.37528600
H	-1	0.53476900	-0.56183300	4.50069200
H	0	-0.23432600	-3.77425700	-0.23207800
H	0	-0.96970900	-4.62634300	1.12713900
H	0	-2.06297500	-1.97017700	0.09383200
H	0	-2.86261500	-3.09694700	1.16906100
H	0	0.60462500	-3.27846100	2.09046700
N	0	-0.10185800	-2.74469500	1.58766700
H	0	0.35946400	-3.58778700	-5.42949200
H	-1	2.36988000	-4.70374400	-4.40587700
O	-1	5.13510500	-2.66308200	-1.12037400
H	0	5.73880500	-2.93852000	-0.42219500
H	-1	7.24005700	1.87836300	-0.23376400
H	0	-4.75920500	-0.29184200	2.20322700
H	0	-5.79563000	3.82684400	-0.66847800
H	0	-4.43667700	-6.41984300	0.28458400
H	0	-5.09675900	-4.78179200	0.08393300
H	0	-3.83085400	-5.09970400	1.28506400

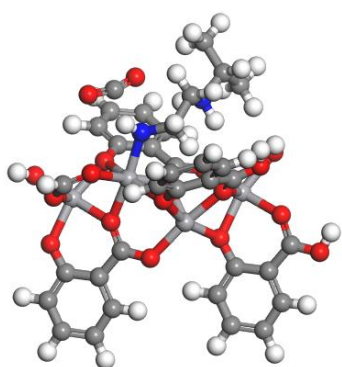


V-(B) Complex

-1	1			
H	0	-8.17665500	1.87920500	-0.45626200
V	-1	-2.65456200	-1.96703800	-1.49857200
O	-1	-2.52276300	-4.02720600	-1.97316200
O	-1	-3.27947400	-0.03040300	-0.97912200
O	-1	-4.48076700	-2.58090900	-0.68543500
O	-1	-6.68304900	-2.60345800	-0.35261200

O	-1	-2.01734800	-1.94587900	0.54290100
O	-1	-2.41485600	-3.97850600	1.36836200
H	0	-2.90585700	-4.44645100	-1.19499400
C	-1	-4.54560600	0.39258300	-0.85103800
C	-1	-5.67377400	-0.47348100	-0.67572500
C	-1	-6.95256900	0.09782300	-0.53671100
C	-1	-7.17870800	1.47161800	-0.57095500
C	-1	-6.05862500	2.30901700	-0.76107500
C	-1	-5.60843200	-1.95318900	-0.56230700
C	-1	-1.24146400	-3.40976300	3.78427200
C	-1	-1.93996400	-2.81324800	1.50818600
H	0	-0.53134000	-4.03385900	5.73095100
C	0	4.97322600	-3.74362600	-2.76255700
H	-1	-7.78031400	-0.58818500	-0.35651600
H	-1	-1.77499200	-4.33860600	3.57885400
H	0	2.74771900	-3.29254000	-1.76739400
H	0	4.24750800	-5.23599400	-1.40614000
H	0	4.16692200	-3.87527300	-3.49280400
H	0	5.82906700	-4.33736500	-3.09568400
H	0	-3.18384300	6.70074200	0.53752600
H	-1	-6.20131600	3.39017700	-0.82118700
V	-1	2.33796700	2.85381300	-0.50184200
V	-1	-1.74409200	0.13096900	0.50596000
V	0	1.18923100	0.46067000	0.63513000
O	0	2.40221900	0.86491100	-1.00704400
O	0	-0.09134500	-0.31878500	-0.74677100
O	-1	-0.91621900	-1.35592700	-2.52500500
O	-1	1.71338700	4.78974700	0.01787300
O	0	0.51780200	2.31160000	0.26385900
O	-1	-1.69011100	2.21649800	0.64407200
O	0	-0.43872900	-0.27134100	2.02449000
O	-1	2.97549900	2.87407500	1.53969300
O	0	2.50581400	0.86705900	2.40176700
O	0	5.44414800	-0.32715600	0.94036300
O	0	5.74475900	-0.04256900	3.23378800
C	-1	2.40265300	0.27763100	-2.20971200
C	-1	1.29818500	-0.48960800	-2.70842500
C	-1	1.35684500	-1.00732400	-4.01375900
C	-1	2.45037000	-0.81934300	-4.85490600
C	-1	3.52557400	-0.05255100	-4.35460200
C	-1	3.49878800	0.48239900	-3.08022900
C	-1	0.04977400	-0.74693800	-1.96175400
C	-1	0.44734100	5.21253700	0.14574600
C	-1	-0.68082700	4.34637300	0.32105700
C	-1	-1.95962200	4.91777700	0.46007300
C	-1	-2.18576200	6.29157300	0.42582900

C	-1	-1.06577800	7.12897100	0.23571700
C	-1	-4.78469600	1.78652200	-0.89707100
C	-1	-0.61580500	2.86716500	0.43430900
C	-1	-0.49114700	-1.22840600	2.95050900
C	-1	-1.25437000	-2.43412200	2.77092600
C	-1	-0.52898500	-3.26002300	4.97211800
C	-1	0.18783400	-2.05506800	5.14857200
C	-1	0.20399500	-1.07400300	4.17366100
C	-1	3.05348300	2.00501600	2.50470400
C	0	5.59107400	-0.18417000	2.08822000
C	0	1.58738400	-2.77385100	0.55022500
C	0	2.63456800	-3.81515800	0.17765300
C	0	4.53149900	-4.16753700	-1.36802400
H	-1	0.47868300	-1.54716200	-4.36886500
H	-1	4.33850400	1.06651800	-2.69904700
H	-1	-2.78737600	4.23177100	0.64016800
H	-1	-3.92198300	2.43748500	-1.05004000
H	-1	0.73345600	-1.89038500	6.08008800
H	-1	0.76371800	-0.14674300	4.31268600
H	0	1.05249400	-3.07133600	1.45466800
H	0	2.14379400	-4.78995400	0.01402200
H	0	0.84429300	-2.68860000	-0.24943700
H	0	2.98574900	-1.40244200	0.10686700
H	0	3.32578900	-3.94300000	1.01851000
H	0	2.61717300	-1.41848600	1.68941600
C	0	5.67589300	-4.01738300	-0.37170000
H	0	5.26243800	-2.68690200	-2.76380000
N	0	2.19884300	-1.45040800	0.76054800
N	0	3.38571300	-3.34384400	-0.97638900
H	0	2.46590800	-1.22916500	-5.85852900
H	-1	4.40861100	0.10274400	-4.97837000
H	-1	-1.20846900	8.21013000	0.17560500
O	-1	4.07681700	3.46423100	-1.52832600
H	0	4.68595500	3.77868400	-0.85184000
C	-1	0.20825000	6.60647600	0.09971300
H	0	3.60137500	2.27703100	3.41500000
H	-1	1.07096300	7.25744000	-0.05325600
H	0	-2.02100900	-4.62176300	1.96991200
H	0	-6.47540700	-3.55078700	-0.32156900
H	0	5.97979600	-2.96753300	-0.30097600
H	0	6.53816700	-4.60823200	-0.69552900
H	0	5.40217900	-4.36093700	0.63016800



V-(C) TS<sub>1</sub>

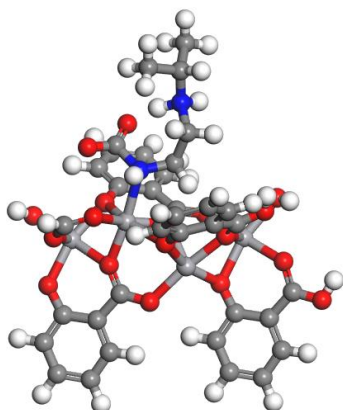
-1 1

H	0	-4.52771700	6.59845500	-1.42841200
V	-1	-2.96116800	-0.02823100	-1.34014700
O	-1	-4.23102300	-1.71147600	-1.54431400
O	-1	-2.14195100	1.89453600	-1.13517200
O	-1	-4.73897600	0.85374000	-0.68051700
O	-1	-6.39948900	2.33656100	-0.61011000
O	-1	-2.48833700	-0.08627200	0.74481800
O	-1	-4.14519700	-1.18323700	1.75621500
H	0	-4.40730800	-2.01564800	-0.64751100
C	-1	-2.80582600	3.05751300	-1.20939400
C	-1	-4.22558000	3.18877400	-1.06569400
C	-1	-4.80018400	4.47096600	-1.14861200
C	-1	-4.05384900	5.62480700	-1.37445600
C	-1	-2.65899600	5.47530100	-1.53033100
C	-1	-5.16312700	2.07567700	-0.76806900
C	-1	-2.91062400	-1.12645200	4.20758800
C	-1	-3.01599800	-0.61294900	1.80984200
H	0	-2.81216900	-1.72366900	6.28582700
C	0	-2.58492900	-4.42384400	-2.55147200
H	-1	-5.87603600	4.53879000	-0.98628500
H	-1	-3.92553000	-1.49526800	4.05400800
H	0	-1.84510600	-2.94536500	-0.69353300
H	0	-2.91897100	-5.12388300	-0.55012700
H	0	-3.20340900	-3.52695400	-2.40812500
H	0	-3.19281400	-5.20525300	-3.01517600
H	0	2.39963600	7.04339300	-0.43918900
H	-1	-2.04506700	6.35461500	-1.73656700
V	-1	3.96525200	0.41673900	-0.34793600
V	-1	-0.90128800	1.25750400	0.49067200
V	0	1.46500300	-0.47746500	0.91969800
O	0	2.69459300	-1.13944800	-0.62240500
O	0	0.04161300	-0.35445600	-0.50563700
O	-1	-1.24926400	-0.89071800	-2.22007400
O	-1	4.78435300	2.33902300	-0.14273100
O	0	2.22991500	1.33559600	0.26879500

O	-1	0.52677100	2.78071800	0.38205000
O	0	-0.20998400	0.35230700	2.18215400
O	-1	4.43788300	0.35780100	1.73708400
O	0	2.75078700	-0.67111200	2.78207200
O	0	3.23939800	-3.88793100	0.84143300
O	0	1.47910300	-4.64475000	-0.47002400
C	-1	2.31176400	-1.81015400	-1.71367100
C	-1	0.98105600	-1.73509300	-2.24349800
C	-1	0.69062100	-2.37467800	-3.46075500
C	-1	1.63838100	-3.09466500	-4.18328200
C	-1	2.94704300	-3.15055700	-3.65545300
C	-1	3.27296500	-2.52434600	-2.46682000
C	-1	-0.12772200	-0.98050800	-1.62404800
C	-1	4.12039100	3.50157900	-0.21722800
C	-1	2.70068300	3.63293600	-0.07343500
C	-1	2.12607900	4.91512800	-0.15635300
C	-1	2.87245600	6.06906000	-0.38220300
C	-1	4.26713300	5.91941600	-0.53806600
C	-1	-2.05555800	4.23268400	-1.45094700
C	-1	1.76311800	2.52027400	0.22396700
C	-1	-0.89161300	-0.15269000	3.21195000
C	-1	-2.26239400	-0.57046600	3.08985600
C	-1	-2.28914800	-1.28305600	5.44471700
C	-1	-0.95332300	-0.83596000	5.55827000
C	-1	-0.28006900	-0.28853000	4.48114500
C	-1	3.90949900	-0.17041900	2.80211100
C	0	2.25067600	-4.11552600	0.24990200
C	0	-0.46386700	-2.72849000	1.55277000
C	0	-1.07596200	-3.98335300	0.92955100
C	0	-2.07060100	-4.93084800	-1.21528400
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H	0	-0.64818200	-2.83413900	2.63094500
H	0	-2.05729400	-4.17265900	1.37371800
H	0	-1.08432100	-1.88944200	1.22645000
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H	0	1.49667600	-2.72953700	2.03386700
C	0	-1.21168800	-6.17606700	-1.33412700
H	0	-1.75623200	-4.19670600	-3.23049800
N	0	0.92050400	-2.40607800	1.26084300
N	0	-1.31182000	-3.81276400	-0.53719600



H	0	1.38507100	-3.57438100	-5.12204000
H	-1	3.71423100	-3.72013100	-4.18450900
H	-1	4.88119500	6.79877700	-0.74430700
O	-1	5.67721400	-0.44633200	-1.22793300
H	0	6.31436600	-0.55749000	-0.51445600
C	-1	4.87070400	4.67684600	-0.45868800
H	0	4.49641700	-0.16372800	3.73003900
H	-1	5.94898200	4.56499600	-0.58587700
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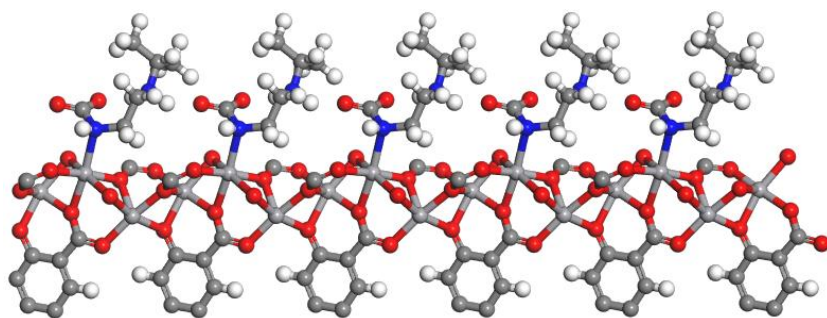
V-(D) Intermediate from Gaussian

-1 1

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O	-1	-2.96886500	-1.17771300	-0.98932900
O	-1	-2.94870400	-4.01074000	-0.90055900
O	-1	-4.91329600	-5.00263500	-0.55783900
O	-1	-0.94680800	-2.46802700	0.36148000
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H	0	-0.79146900	-4.99405400	-1.59717400
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C	-1	0.51344200	-3.68548000	3.46578000
C	-1	-0.46581800	-3.28486000	1.25113600
H	0	1.50168800	-4.08218100	5.34960400
C	0	6.84209300	-3.41580800	-1.31599800
H	-1	-6.76731200	-3.66131800	-0.38843700
H	-1	0.42134900	-4.73598700	3.18741500

H	0	4.37918200	-3.05433400	-1.29022800
H	0	5.82598300	-4.06374000	0.46652200
H	0	6.32781600	-4.12935700	-1.96727400
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Direct

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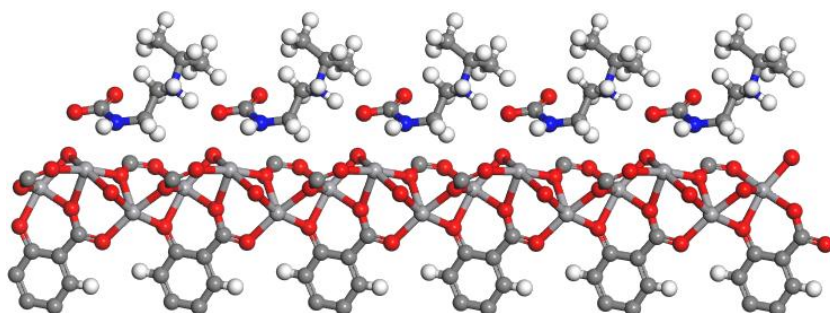
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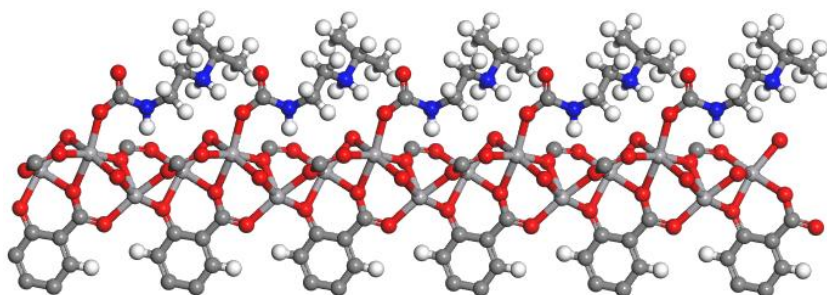
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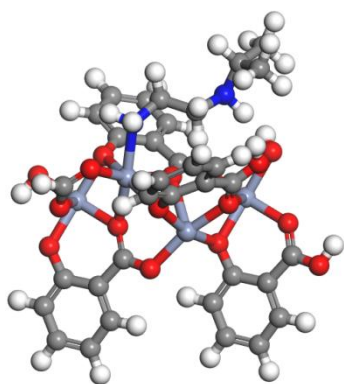
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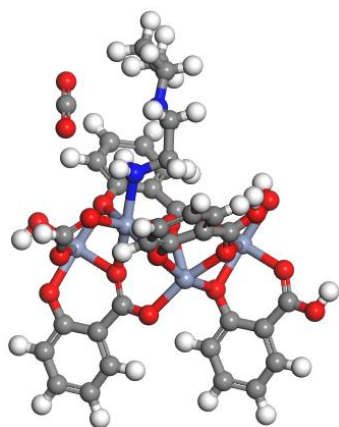
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H	0	-0.48725200	-3.64427600	-5.53352600
H	-1	0.90626700	-5.36231200	-4.37164400
H	-1	8.01705600	2.04379400	0.12756100
O	-1	4.09519700	-3.69905500	-1.28103400
H	0	5.03885300	-3.53300800	-1.17867100
H	-1	7.34906000	-0.34530600	-0.03937100
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H	0	-3.97041200	5.19119800	-0.50212900



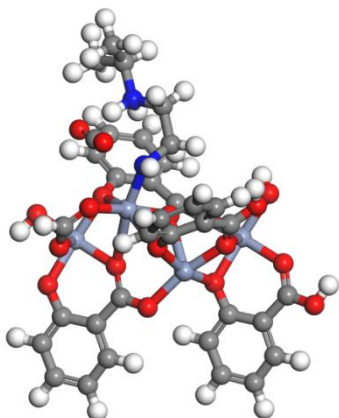
Cr-(B) Complex

-1 1

H	0	-8.14979800	-0.66185100	-1.20598400
Cr	-1	-1.68331600	-2.44211700	-1.82458300
O	-1	-0.54747900	-4.16361600	-1.91115800
O	-1	-2.87347700	-0.88391900	-1.19523600
O	-1	-3.25393700	-3.67590200	-1.49772200
O	-1	-5.19603100	-4.38636700	-0.69228700
O	-1	-1.62674700	-2.49457200	0.68234100
O	-1	-0.69011300	-4.43968100	1.20638800
H	0	0.15550400	-4.00359100	-2.55263800
C	-1	-4.22535200	-0.87965600	-1.24612000
C	-1	-5.01594100	-2.06028000	-1.13443400
C	-1	-6.41639100	-1.94989400	-1.09511200
C	-1	-7.06777600	-0.72359500	-1.22734100
C	-1	-6.27454300	0.42591500	-1.39918800
C	-1	-4.44865800	-3.42990500	-1.09030700
C	-1	-0.03052900	-3.61832400	3.74339100
C	-1	-0.93245400	-3.22194800	1.48534100
H	0	0.71516300	-3.96794700	5.74255400
C	0	6.11788900	-2.19793000	-2.40801000
H	-1	-6.98707600	-2.86598900	-0.94164300
H	-1	-0.06070800	-4.67224500	3.46661200
H	0	3.85383100	-3.69314000	0.56896700
H	0	3.89235500	-2.01107400	-1.26837600
H	0	5.50614800	-3.81589100	-1.14165300
H	0	5.27704800	-2.28576400	-3.10523100
H	0	6.96329800	-2.74851500	-2.83082300
H	0	-5.61419600	5.13912500	0.29717500
H	-1	-6.76492200	1.39047500	-1.54242000
Cr	-1	0.85293500	3.35743800	-0.32231300
Cr	-1	-1.93764200	-0.49277300	0.62402100
Cr	0	0.90690800	0.69519200	0.95798500
O	0	1.94822700	1.66389200	-0.45826200
O	0	0.20217400	-0.50569800	-0.51845000

O	-1	-0.21815100	-1.22605200	-2.57334500
O	-1	-0.33726700	4.91539600	0.30697700
O	0	-0.68949100	2.13168500	0.10089500
O	-1	-2.65980300	1.41286200	0.80993800
O	0	-0.62118700	-0.34723000	2.16716800
O	-1	0.90938600	3.30456700	2.18454600
O	0	1.80400000	1.34631000	2.79123900
O	0	5.33739000	1.31003500	0.98551000
O	0	6.93176800	1.04003900	-0.69235000
C	-1	2.39214500	1.16959500	-1.61072600
C	-1	1.70012600	0.14531900	-2.31854700
C	-1	2.14135200	-0.23028200	-3.59850200
C	-1	3.28186200	0.32414500	-4.17743500
C	-1	3.98267100	1.30087800	-3.44477100
C	-1	3.55192700	1.71797000	-2.19747000
C	-1	0.53695100	-0.58499200	-1.76849200
C	-1	-1.68914300	4.91957800	0.25615700
C	-1	-2.47971700	3.73903800	0.36777300
C	-1	-3.88014300	3.84943000	0.40713500
C	-1	-4.53152900	5.07573300	0.27492100
C	-1	-3.73833500	6.22515500	0.10304700
C	-1	-4.88979800	0.35542000	-1.40834700
C	-1	-1.91236200	2.36948900	0.41206400
C	-1	-0.31683800	-1.29118400	3.05014000
C	-1	-0.43095200	-2.68462900	2.77325800
C	-1	0.41897900	-3.23092000	5.00531700
C	-1	0.46204100	-1.85200300	5.28885200
C	-1	0.10350400	-0.90453500	4.34310900
C	-1	1.60381600	2.57768300	2.98767900
C	0	6.13010200	1.16657800	0.14330500
C	0	2.61300000	-1.97894800	0.91516400
C	0	3.97887800	-2.59829400	0.65654600
C	0	5.75466700	-2.74229100	-1.03347100
C	0	6.93532400	-2.63905800	-0.07556100
H	-1	1.54705400	-0.96715700	-4.13903500
H	-1	4.10863400	2.46259500	-1.62876200
H	-1	-4.45086800	2.93325000	0.56059500
H	-1	-4.28198300	1.25017000	-1.54427800
H	-1	0.77268900	-1.52703300	6.28312300
H	-1	0.13647800	0.16086700	4.57238600
H	0	2.17237100	-2.41504700	1.81566800
H	0	1.93835400	-2.21430200	0.08466900
H	0	3.31241100	-0.16306300	0.37998700
H	0	4.62802900	-2.42167100	1.52310400
H	0	3.07204700	-0.29434100	1.96962500
H	0	6.39201400	-1.14037000	-2.33817600

H	0	7.78791700	-3.20027900	-0.47010700
H	0	6.70199200	-3.04726200	0.91203000
H	0	7.24090700	-1.59504700	0.04598000
N	0	2.64947700	-0.51709600	1.07003700
N	0	4.59115700	-2.00760600	-0.52705100
H	0	3.61388700	0.01773200	-5.16329700
H	-1	4.89676900	1.72259800	-3.86669200
H	-1	-4.22867400	7.18980200	-0.04016300
O	-1	2.31803000	4.57315600	-1.07110200
H	0	1.96010200	5.46401100	-0.98943600
C	-1	-2.35358800	6.15465700	0.09388900
H	0	2.03187200	3.03736500	3.89420500
H	-1	-1.74573500	7.04949700	-0.04201900
H	0	-0.02611900	-4.82322000	1.79229500
H	0	-4.70993900	-5.22225300	-0.78202300



Cr-(C) TS<sub>1</sub>

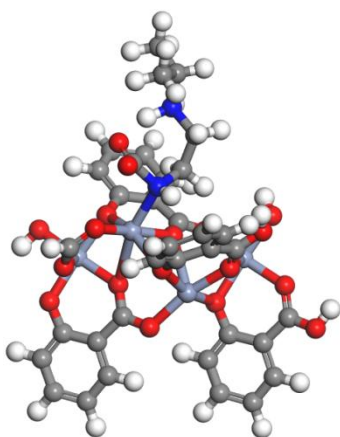
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H	0	-8.24874400	-0.17724100	-0.57671400
Cr	-1	-1.98651900	-2.25763900	-1.92747500
O	-1	-0.96762700	-4.02851000	-2.22240300
O	-1	-3.01752200	-0.68023000	-1.09716100
O	-1	-3.58909000	-3.42387600	-1.51809000
O	-1	-5.48447500	-4.07841900	-0.56714100
O	-1	-1.69540700	-2.46825200	0.55475500
O	-1	-0.82969600	-4.48922100	0.87346500
H	0	-0.31139400	-3.86533500	-2.91074700
C	-1	-4.36551300	-0.60082100	-1.01461300
C	-1	-5.21021700	-1.74230700	-0.89267400
C	-1	-6.59164200	-1.56012900	-0.70973800
C	-1	-7.17913100	-0.29503800	-0.70779500
C	-1	-6.33934600	0.81902300	-0.89152400
C	-1	-4.72312700	-3.14030500	-0.98198700
C	-1	0.11509400	-3.86294000	3.37570100
C	-1	-0.97214600	-3.27992800	1.24323900
H	0	1.02419800	-4.37508100	5.26957300
C	0	6.70429900	-0.35171100	-2.32348200



H	-1	-7.19824400	-2.45226900	-0.55294800
H	-1	-0.00337700	-4.89458000	3.04411500
H	0	4.22658900	-3.35617200	-1.18585900
H	0	4.27446300	-1.01525000	-1.83588600
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H	0	6.03275200	-0.12186600	-3.15497900
H	0	7.70071500	-0.53088500	-2.73369400
H	0	-5.24424900	5.37724000	0.99393500
H	-1	-6.78332700	1.81535200	-0.93112800
Cr	-1	1.01869100	3.29411400	-0.35639800
Cr	-1	-1.89181900	-0.45299300	0.64056000
Cr	0	1.30198600	0.32614500	0.81150200
O	0	2.00289800	1.53287000	-0.68146000
O	0	0.17723900	-0.51632500	-0.71293200
O	-1	-0.52995300	-1.07721600	-2.74662100
O	-1	-0.01231200	4.87152400	0.47391500
O	0	-0.57305000	2.14244300	0.09620000
O	-1	-2.47931200	1.47325000	1.00391100
O	0	-0.42604900	-0.47182800	2.05685900
O	-1	1.30975600	3.08341500	2.12580600
O	0	2.20550800	1.05659300	2.51800900
O	0	4.31559700	-0.95706000	3.06909200
O	0	4.97989400	0.33411600	1.25950400
C	-1	2.29667900	1.11195200	-1.91135300
C	-1	1.48149900	0.17155000	-2.60450700
C	-1	1.77628600	-0.14701100	-3.94081700
C	-1	2.88740100	0.38068900	-4.59677000
C	-1	3.71103700	1.27139300	-3.88248700
C	-1	3.42603900	1.63272300	-2.57731900
C	-1	0.33496800	-0.52863900	-1.98514100
C	-1	-1.36034800	4.95084600	0.55644000
C	-1	-2.20500700	3.80944700	0.67840200
C	-1	-3.58643100	3.99162200	0.86133900
C	-1	-4.17392000	5.25671500	0.86328200
C	-1	-3.33418300	6.37069000	0.67952800
C	-1	-4.96830800	0.67556700	-1.04069500
C	-1	-1.71791600	2.41144800	0.58908900
C	-1	-0.09793600	-1.48507800	2.84674600
C	-1	-0.31984300	-2.85092200	2.50393600
C	-1	0.70444000	-3.57896500	4.60721600
C	-1	0.85552300	-2.22452000	4.96262300
C	-1	0.46536400	-1.20258200	4.11177100
C	-1	2.03306500	2.27182600	2.81431500
C	0	4.45573200	-0.36341400	2.06610300
C	0	2.72166700	-2.20438900	-0.10439400
C	0	4.16759500	-2.54549600	-0.45403100

C	0	6.25338500	-1.58700800	-1.56334500
C	0	7.18178500	-1.93448300	-0.41264500
H	-1	1.09090800	-0.81626800	-4.46110700
H	-1	4.07713400	2.31004900	-2.02493100
H	-1	-4.19308000	3.09939900	1.01810400
H	-1	-4.32440600	1.54337100	-1.18491600
H	-1	1.27779500	-1.97879100	5.93832100
H	-1	0.58277200	-0.15664600	4.39652700
H	0	2.24203300	-3.16166900	0.15202900
H	0	2.23736000	-1.87029900	-1.03009000
H	0	4.84846300	-0.60341200	-0.35641000
H	0	4.73323800	-2.82907800	0.43553500
H	0	2.47529800	-1.69068300	1.82002100
H	0	6.76117500	0.52256300	-1.66699000
H	0	8.19394300	-2.05121600	-0.80677700
H	0	6.91123900	-2.87163300	0.07833500
H	0	7.20104600	-1.13407400	0.33355900
N	0	2.55350100	-1.20123400	0.93136600
N	0	4.84924100	-1.36070000	-1.06005400
H	0	3.10826300	0.11803200	-5.62558000
H	-1	4.60421500	1.66918900	-4.36770200
H	-1	-3.77811700	7.36710500	0.63994700
O	-1	2.47521100	4.47445100	-1.17556900
H	0	2.19116800	5.37494000	-0.98329800
C	-1	-1.96314300	6.22723400	0.53035700
H	0	2.52403900	2.64692300	3.72963000
H	-1	-1.31919600	7.09512300	0.38616100
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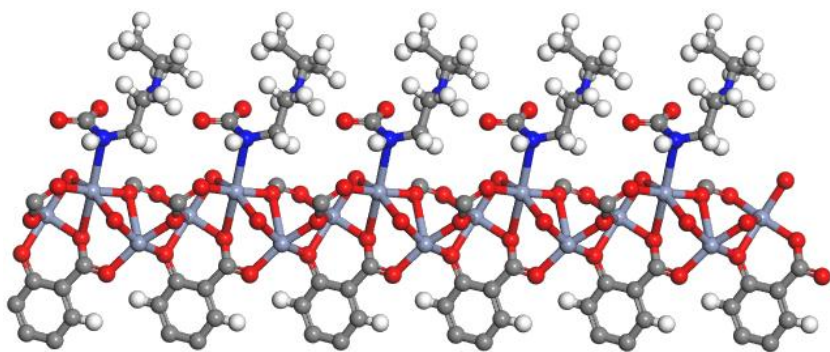


Cr-(D) Intermediate from Gaussian

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H	0	-7.73902400	-2.76253900	-0.42721100
Cr	-1	-1.16097100	-2.63674700	-1.86981800
O	-1	0.39153400	-3.96601400	-2.15944500
O	-1	-2.65236500	-1.48303300	-1.04199100

O	-1	-2.27044400	-4.26655500	-1.41294500
O	-1	-3.82083900	-5.50267500	-0.41620300
O	-1	-0.78232500	-2.68759400	0.60901500
O	-1	0.71866900	-4.29172700	0.93935700
H	0	0.95565200	-3.59361400	-2.84812700
C	-1	-3.94687000	-1.86103100	-0.93440000
C	-1	-4.35521900	-3.21778600	-0.77996400
C	-1	-5.71450700	-3.50832700	-0.57281500
C	-1	-6.69427100	-2.51553100	-0.57732700
C	-1	-6.28213500	-1.18747400	-0.79305200
C	-1	-3.42630100	-4.37125900	-0.85897000
C	-1	1.43053500	-3.33409400	3.41367100
C	-1	0.18160900	-3.19413700	1.29471300
H	0	2.48656000	-3.47134500	5.29526200
C	0	7.75922600	-0.51116600	-1.81220700
H	-1	-5.98238600	-4.54943000	-0.39168600
H	-1	1.66257800	-4.35165800	3.09905200
H	0	4.35949400	-2.67036400	-1.16183200
H	0	5.28492000	-0.75423900	-2.02826700
H	0	6.93116500	-2.37548600	-1.12644900
H	0	7.45724200	-0.66101700	-2.85337500
H	0	8.79931700	-0.83089600	-1.71641600
H	0	-6.76356200	3.50941400	1.00604700
H	-1	-7.03670800	-0.40010400	-0.83809000
Cr	-1	-0.18397200	3.63311300	-0.43598800
Cr	-1	-1.64592500	-0.85520000	0.67014900
Cr	0	1.07929000	0.98484000	0.75945000
O	0	1.33913500	2.28479900	-0.74018100
O	0	0.31184500	-0.25146600	-0.71773200
O	-1	-0.19925700	-1.05093400	-2.73369700
O	-1	-1.67536600	4.78682700	0.39183800
O	0	-1.28800600	2.01969000	0.06102200
O	-1	-2.84385600	0.76708800	1.01760400
O	0	-0.20722600	-0.34113100	2.03533500
O	-1	0.19465800	3.58216800	2.04282100
O	0	1.76740200	2.01555300	2.38731400
O	0	4.28277700	0.29673100	2.52707000
O	0	4.62095500	1.06631200	0.43506200
C	-1	1.73412600	1.97903700	-1.98450300
C	-1	1.27470400	0.80532900	-2.64833900
C	-1	1.64157600	0.57832100	-3.98549000
C	-1	2.50053900	1.43654200	-4.67029400
C	-1	2.98497500	2.56674100	-3.98479800
C	-1	2.61246700	2.83668600	-2.67957300
C	-1	0.44010000	-0.22791500	-1.99698800
C	-1	-2.96988400	4.40873300	0.49940800

C	-1	-3.37822000	3.05207500	0.65386500
C	-1	-4.73750700	2.76153300	0.86101400
C	-1	-5.71727100	3.75433000	0.85650300
C	-1	-5.30515200	5.08228900	0.64075500
C	-1	-4.94523100	-0.86331600	-0.96679000
C	-1	-2.44930200	1.89860100	0.57485900
C	-1	0.42064500	-1.17819900	2.85542400
C	-1	0.66792500	-2.54542600	2.53631400
C	-1	1.90612600	-2.84369800	4.62937000
C	-1	1.59619700	-1.51082200	4.96261100
C	-1	0.87267200	-0.69730800	4.10515100
C	-1	1.15860800	3.07572500	2.72854100
C	0	4.01282500	0.40704900	1.33371600
C	0	3.07978700	-1.09452100	-0.39384800
C	0	4.42554700	-1.81137500	-0.49121800
C	0	6.89496200	-1.31490700	-0.85468700
C	0	7.31463400	-1.12779000	0.59437600
H	-1	1.21519500	-0.29298300	-4.48286300
H	-1	3.00429000	3.70466600	-2.14956000
H	-1	-5.00540300	1.72033500	1.04212200
H	-1	-4.63386100	0.16770300	-1.13573600
H	-1	1.92396800	-1.11782100	5.92635300
H	-1	0.63417300	0.33242400	4.37277200
H	0	2.28346900	-1.83237000	-0.49954600
H	0	2.97788400	-0.40729900	-1.23673500
H	0	5.27170200	0.05064100	-0.54263600
H	0	4.76057700	-2.16870300	0.48525900
H	0	2.63889200	-1.01316200	1.59873900
H	0	7.71075300	0.55803200	-1.58232000
H	0	8.35651100	-1.43710400	0.70447100
H	0	6.71880000	-1.72712700	1.28712300
H	0	7.23170100	-0.07684200	0.88714500
N	0	2.83294100	-0.34517600	0.85383500
N	0	5.46742800	-0.88823000	-1.03236200
H	0	2.78293400	1.24230500	-5.69927500
H	-1	3.68493500	3.23261400	-4.49284300
H	-1	-6.05971000	5.86975400	0.59573700
O	-1	0.77772700	5.21882900	-1.29988900
H	0	0.20704600	5.97438400	-1.12134200
C	-1	-3.96824500	5.40644700	0.46701600
H	0	1.47689600	3.57111000	3.66012900
H	-1	-3.65686300	6.43756200	0.29809400
H	0	1.53281100	-4.47623700	1.42388600
H	0	-3.13483400	-6.16602200	-0.59633200



Cr-(D) Intermediate from VASP

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Cr  O  C  H  N
 6  20 48 32  2

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Direct

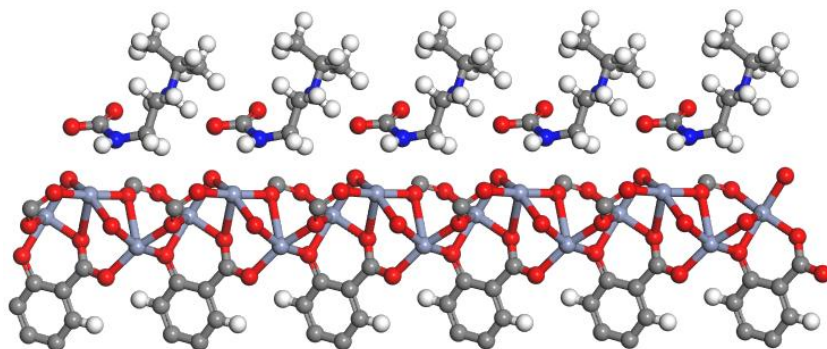
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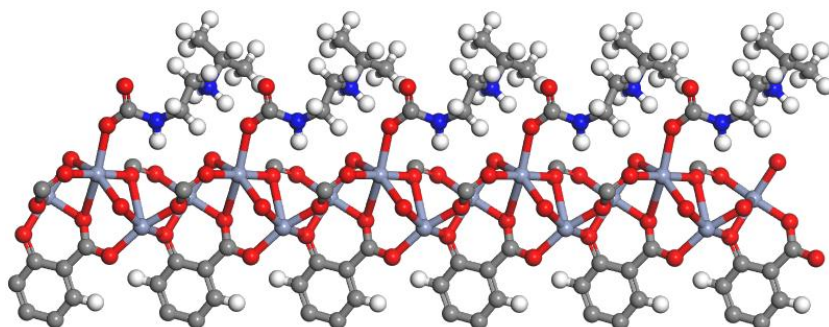
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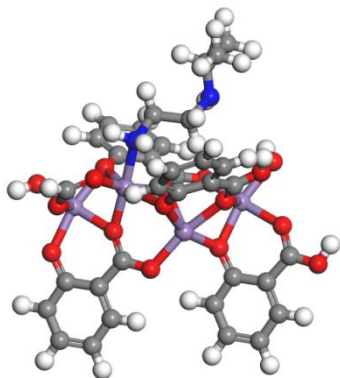
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0.0721227127680351	0.6148966251414336	0.6056603864680952
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0.0336760127623066	0.6372823697127288	0.9288916992353862
0.1056559115333329	0.6705605275049535	0.0002617214676164
0.2016319701614506	0.6576749167528106	0.5188840278106284
0.3284502577444997	0.5540083220806267	0.2058567509116145
0.3525862342196291	0.5606131537237857	0.9983261640108623
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0.3283166915897198	0.5011018208873423	0.3287171646483742
0.3505273710935839	0.6106141974384300	0.8500719676460591
0.5526602869060966	0.7264550868939210	0.2408943526515941
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0.5055277012459527	0.3883186061911346	0.0422663142552722
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0.3067546198603068	0.4939648294054066	0.4843834269997416
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0.4812075462436098	0.4459060607283050	0.2603323170739102
0.3654531916071093	0.4022959098297463	0.6847736698584228
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0.5115233916696411	0.6733750420957207	0.7561929865993875
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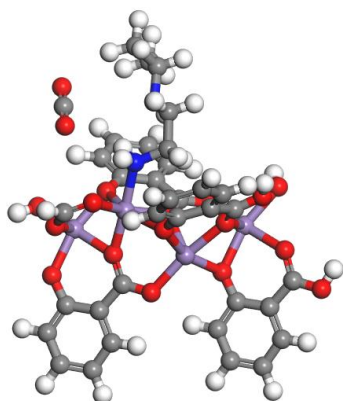
Mn-(A) i-2-MOF

-1 1

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H	1.46258000	6.47741200	-1.07696500
Mn	-2.49606400	1.35846400	-1.51827000
O	-4.37605000	0.49626700	-1.98314400
O	-0.88576900	2.62561200	-1.03338500
O	-3.69209200	3.00603200	-0.94515800
O	-4.36984500	5.08031700	-0.50354300
O	-2.31377600	0.98064400	0.63214200
O	-4.37414400	0.59384200	1.39382700
H	-4.20650800	-0.08124400	-2.73708400
C	-0.86725700	3.96830100	-0.98284000
C	-2.03710600	4.77655800	-0.83560800
C	-1.89605800	6.17292400	-0.74456100
C	-0.66151200	6.81400900	-0.81383500
C	0.48103800	6.00596700	-0.98976400
C	0.38247400	4.62710000	-1.07370200
C	-3.42634000	4.25226400	-0.74907400
C	-2.56373100	0.00543900	2.81730300
C	-3.49281300	-0.36588300	3.80401200
C	-3.11627600	0.56337100	1.55877100
H	-3.85551800	-1.25918900	5.73970700
C	-4.04064900	-4.43391400	-0.60754100
C	-4.81841300	-4.53371100	0.69906200
C	-4.94301600	-4.72729600	-1.79887700
H	-2.80627900	6.75068300	-0.58294700
H	-4.54625100	-0.19862000	3.57756700
H	-3.09158800	-3.02064200	-1.71321900
H	-3.25161700	-5.20750500	-0.58973100

H	-5.60615200	-3.77289900	0.72947100
H	-4.17697800	-4.39657900	1.57497400
H	-5.28462600	-5.51973800	0.78626500
H	-5.76472500	-4.00421400	-1.84173400
H	-5.36807200	-5.73255700	-1.72567800
H	-4.38675900	-4.66657600	-2.74108000
N	-3.48646700	-3.08869600	-0.77898800
H	5.53660600	4.90973100	0.50522700
H	7.58250000	3.49372300	0.17022800
Mn	3.62385600	-1.62522400	-0.27107700
Mn	-0.17623500	1.35343200	0.52826200
Mn	1.15699900	-1.38818400	0.68818900
O	1.81657100	-2.46080900	-0.77981900
O	-0.07034500	-0.43884300	-0.69634700
O	-1.38449000	-0.14131500	-2.51164600
O	5.23415200	-0.35807600	0.21380800
O	2.50432500	0.01470700	0.25914800
O	1.74998700	2.09667200	0.74363300
O	-0.23883200	-0.01420600	2.10002700
O	3.80614500	-2.00304400	1.87933500
O	1.75967000	-2.30533100	2.66459000
C	1.29249700	-2.65439000	-1.98795300
C	0.23236400	-1.88894900	-2.57143600
C	-0.14324000	-2.13264100	-3.90427000
C	0.45646400	-3.10941600	-4.69498500
C	1.48616500	-3.87223400	-4.10408600
C	1.89106600	-3.65193700	-2.79838300
C	-0.48338500	-0.78637600	-1.88212400
C	5.25266400	0.98461200	0.26435300
C	4.08281400	1.79287000	0.41158500
C	4.22377400	3.18927900	0.50261500
C	5.45840900	3.83032200	0.43335800
C	6.60095900	3.02227800	0.25743000
C	6.50239400	1.64341200	0.17349100
C	2.69358100	1.26857600	0.49812000
C	-1.17551200	-0.27777100	3.01612400
H	3.42801400	-2.83524000	3.73096900
C	-3.11802600	-0.97703300	4.99774200
C	-1.73855200	-1.19951000	5.20661400
C	-0.79682400	-0.86093800	4.25044000
C	3.00364500	-2.42031700	2.80596400
C	-1.21294000	-3.50596200	0.23080500
C	-2.48019100	-2.65464000	0.17676600
H	-0.64639600	-2.67251300	2.00635500
H	-0.91665700	-1.48745800	-4.32146100
H	2.70639300	-4.23539400	-2.36535200

H	3.31364200	3.76699500	0.66424600
H	1.27189600	4.00937800	-1.20944100
H	-1.40646000	-1.64101700	6.14879800
H	0.26672400	-1.04282100	4.41616500
H	-0.78447700	-3.59601800	-0.77131600
H	-1.46432600	-4.51900500	0.56834400
H	-2.20929200	-1.62393200	-0.07253500
H	-2.93018000	-2.61846100	1.17753300
H	0.45492300	-3.65314200	1.38904100
N	-0.19746000	-2.91930900	1.12421000
H	0.15125100	-3.26784800	-5.72324300
H	1.96763100	-4.66253900	-4.68435800
O	4.73543100	-3.12500400	-1.26445300
H	5.51929900	-3.28505200	-0.72727000
H	7.39181700	1.02569000	0.03775200
H	-4.85725900	0.10344000	2.06942000
H	-5.21308500	4.59842700	-0.50856400



#### Mn-(B) Complex

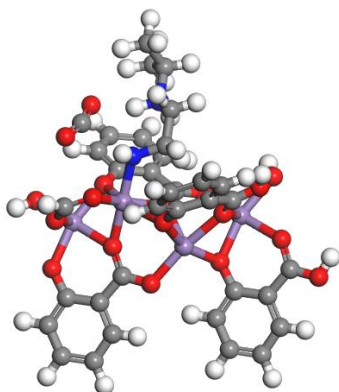
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H	0	-8.19833200	1.38938000	-1.15786700
Mn	-1	-2.35115200	-2.17444200	-1.60611600
O	-1	-2.08135200	-4.20847800	-2.00308400
O	-1	-3.19408600	-0.29576000	-1.14957400
O	-1	-4.28396900	-2.87983300	-0.99174800
O	-1	-6.50114600	-3.00324800	-0.77871000
O	-1	-1.97015200	-2.08953300	0.55042900
O	-1	-2.28723200	-4.13472700	1.38765100
H	0	-1.49812100	-4.27123900	-2.76893900
C	-1	-4.48368800	0.07877300	-1.16889200
C	-1	-5.57738400	-0.83385000	-1.05985800
C	-1	-6.88951800	-0.32879000	-1.05330600
C	-1	-7.17594900	1.02934300	-1.16813500
C	-1	-6.08682500	1.91549400	-1.30241800
C	-1	-5.43839400	-2.30880200	-0.92943400
C	-1	-1.36044300	-3.44423400	3.87166700
C	-1	-1.90688300	-2.93080600	1.52859400

H	0	-0.79536800	-3.95667300	5.89560900
C	0	5.32015100	-3.60041200	-2.17060600
H	-1	-7.69563200	-1.05046000	-0.92121500
H	-1	-1.79230700	-4.41985600	3.64533600
H	0	2.49496400	-4.39765600	0.59240600
H	0	3.15275500	-2.84603400	-1.20353500
H	0	4.31253100	-4.98140900	-0.87790400
H	0	4.52294000	-3.57005500	-2.92174600
H	0	6.06746300	-4.32667900	-2.50297500
H	0	-3.72712200	6.53581900	0.22318000
H	-1	-6.27776900	2.98404500	-1.42474900
Mn	-1	2.12023600	2.97150400	-0.22210800
Mn	-1	-1.83763500	0.08248400	0.43807600
Mn	0	1.16574300	0.66783300	0.76945000
O	0	2.40448500	1.01839500	-0.67306100
O	0	-0.02001600	-0.27258500	-0.67628200
O	-1	-0.58166300	-1.47632800	-2.50523200
O	-1	1.27754200	4.84921700	0.23504300
O	0	0.21049200	2.33443400	0.31467700
O	-1	-2.02960000	2.14161400	0.60570700
O	0	-0.63821700	-0.28906100	2.10173600
O	-1	2.50170300	3.05527500	1.93504900
O	0	2.07514200	1.05799700	2.78581800
O	0	5.35517200	0.17068600	1.02167300
O	0	6.79613500	-0.44788100	-0.70198900
C	-1	2.54588900	0.38048200	-1.82771400
C	-1	1.56845600	-0.45924900	-2.44596700
C	-1	1.82689700	-1.00140800	-3.71604800
C	-1	3.01522700	-0.77125800	-4.40329300
C	-1	3.97584200	0.05409900	-3.77847800
C	-1	3.74815200	0.61516000	-2.53517600
C	-1	0.26281900	-0.79475400	-1.83756000
C	-1	-0.01207200	5.22384600	0.21542400
C	-1	-1.10567000	4.31123900	0.32455900
C	-1	-2.41780400	4.81629800	0.33111000
C	-1	-2.70443300	6.17440300	0.21628100
C	-1	-1.61530800	7.06055300	0.08199800
C	-1	-4.78095700	1.45574600	-1.30434900
C	-1	-0.96687800	2.83625700	0.45498100
C	-1	-0.72410400	-1.22479600	3.04749200
C	-1	-1.35639800	-2.49395100	2.83698300
C	-1	-0.78653500	-3.20258800	5.11755800
C	-1	-0.20638200	-1.93157900	5.32791300
C	-1	-0.17835000	-0.97307600	4.32957400
C	-1	2.56503600	2.21219500	2.91362700
C	0	6.07102100	-0.14268300	0.15716500



C	0	1.81041700	-2.38842800	0.92294100
C	0	2.93550300	-3.39273300	0.72232700
C	0	4.77470500	-3.97860400	-0.80026700
C	0	5.89766700	-4.06430900	0.22637800
H	-1	1.03464700	-1.59748100	-4.17008100
H	-1	4.49866100	1.24879200	-2.05896500
H	-1	-3.22390400	4.09453000	0.46320300
H	-1	-3.94225400	2.14598000	-1.41053600
H	-1	0.22289500	-1.69793900	6.30462100
H	-1	0.27730200	0.00528000	4.49708300
H	0	1.20042300	-2.67476300	1.78235100
H	0	1.15122100	-2.39622100	0.04949500
H	0	3.13652700	-0.92620500	0.53392100
H	0	3.55354300	-3.43085100	1.62761600
H	0	2.64778700	-0.92507400	2.07572500
H	0	5.78980100	-2.61215800	-2.13293000
N	0	2.30573000	-1.01668400	1.12080600
N	0	3.76743100	-2.99004000	-0.40407800
H	0	3.18958900	-1.19685400	-5.38517100
H	-1	4.92844300	0.23804300	-4.28037400
H	-1	-1.80615500	8.12912000	-0.04023400
O	-1	3.88979400	3.66912600	-1.12082000
H	0	4.20935700	4.37089900	-0.54303300
C	-1	-0.30934200	6.60081900	0.08006700
H	0	3.02008600	2.52748700	3.86276600
H	-1	0.52937600	7.29095500	-0.02612000
H	0	-2.03731000	-4.69789900	2.12967700
H	0	-6.25350100	-3.94129500	-0.73382800
H	0	6.41680700	-3.10366400	0.30675300
H	0	6.62704200	-4.82150400	-0.07719800
H	0	5.53064300	-4.34063300	1.21893300

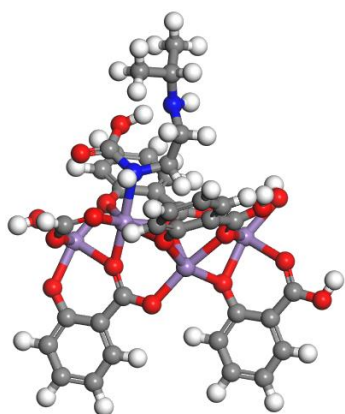


Mn-(C) TS<sub>1</sub>

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H	0	-8.05616100	1.66252000	-1.18261600
Mn	-1	-2.34577500	-2.12813500	-1.52094400
O	-1	-2.15250400	-4.18319200	-1.84864300

O	-1	-3.11734300	-0.20520900	-1.12728100
O	-1	-4.30119000	-2.74024000	-0.87868700
O	-1	-6.52066300	-2.77440700	-0.65690500
O	-1	-1.95461400	-1.98386200	0.63063600
O	-1	-2.34409300	-3.98614700	1.53795000
H	0	-1.57126300	-4.29516100	-2.61032100
C	-1	-4.39233600	0.21595000	-1.15660800
C	-1	-5.51850000	-0.65139600	-1.01410900
C	-1	-6.81106300	-0.09823300	-1.02211400
C	-1	-7.04775500	1.26485600	-1.18273700
C	-1	-5.92714800	2.10505900	-1.34956800
C	-1	-5.43356700	-2.12517200	-0.83361100
C	-1	-1.38406000	-3.24610800	3.99500000
C	-1	-1.91914200	-2.79308900	1.63686700
H	0	-0.83259800	-3.70940800	6.03448600
C	0	4.72973600	-3.78191900	-2.54102200
H	-1	-7.64278500	-0.78479700	-0.86368800
H	-1	-1.85242600	-4.21214200	3.80304500
H	0	2.07814600	-4.42286300	0.52901800
H	0	2.59219200	-2.94425300	-1.33933700
H	0	3.54785700	-5.12147600	-1.33890600
H	0	3.92235800	-3.52209100	-3.23170000
H	0	5.32026900	-4.58228300	-2.99279200
H	0	-3.39350900	6.68468100	0.01255800
H	-1	-6.07895300	3.17511600	-1.50789200
Mn	-1	2.31691900	2.89320200	-0.32323200
Mn	-1	-1.74248000	0.17665000	0.44378100
Mn	0	1.34688000	0.64719000	0.74989300
O	0	2.52667700	0.93465900	-0.73196900
O	0	0.05990800	-0.27342600	-0.66860400
O	-1	-0.55483600	-1.52701600	-2.44713100
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O	0	0.38462100	2.33998900	0.25523400
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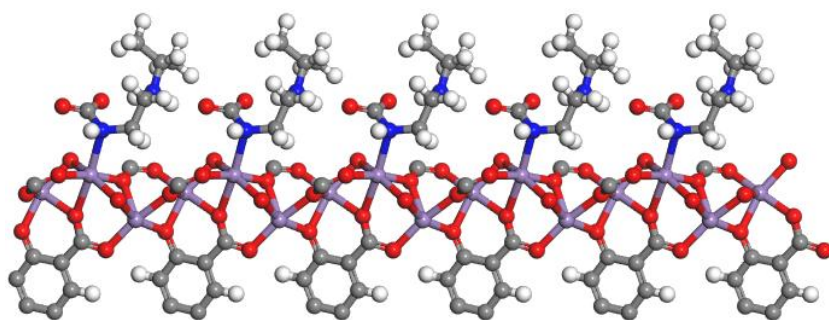
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Mn-(D) Intermediate from VASP

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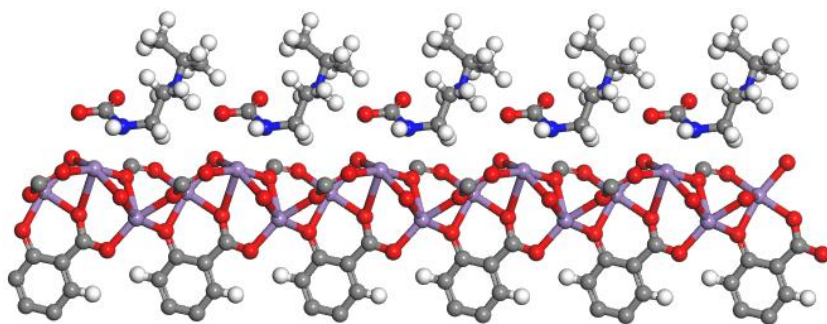
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Mn-(E) TS<sub>2</sub>

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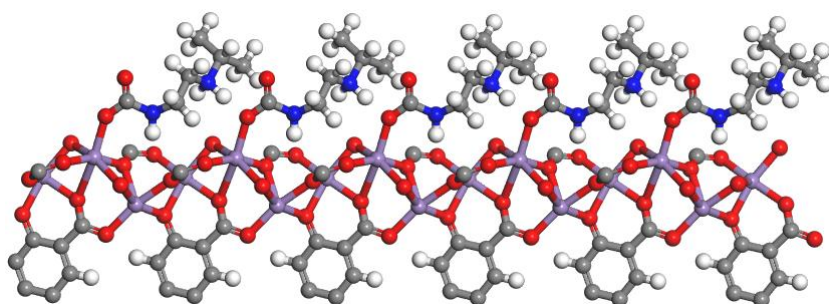
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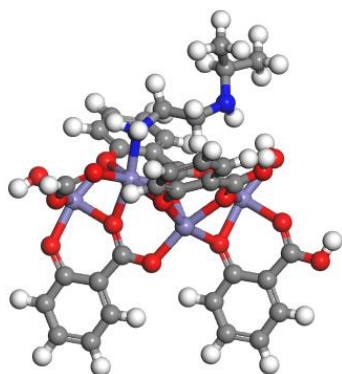
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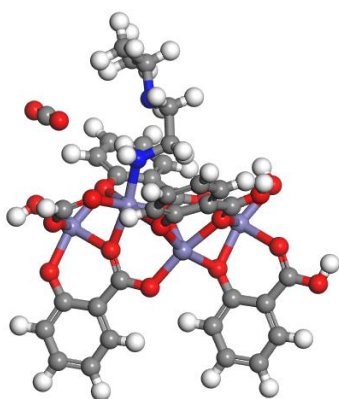
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H	0	3.55426000	-2.58678200	3.71934800
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C	-1	-1.52713300	-1.23474000	5.22547500
C	-1	-0.61972600	-0.88584500	4.24132600
C	-1	3.11642500	-2.27175700	2.76219000
C	0	-1.25618400	-3.44993900	0.12587700
C	0	-2.48588400	-2.67688000	0.59333300
H	0	-0.37861600	-3.13537800	1.94561600
H	-1	-0.81184800	-1.51790300	-4.33541000
H	-1	2.95171400	-4.11069100	-2.42422200
H	-1	3.06948800	3.85553400	0.68764600
H	-1	1.14138500	4.00159900	-1.17521100
H	-1	-1.15900500	-1.62889000	6.17499700
H	-1	0.45384900	-1.01136600	4.39008400
H	0	-1.02192600	-3.21758500	-0.91571700
H	0	-1.41852200	-4.53249800	0.19012400
H	0	-2.15888100	-1.64147200	0.69138600
H	0	-2.73857200	-3.02473700	1.60667600
H	0	0.62272000	-3.76574100	0.85510100
H	0	-3.31348900	-4.45205100	-1.36690900
N	0	-0.10303900	-3.06025700	0.96605600
H	0	0.32878200	-3.23842300	-5.75684300
H	-1	2.20775200	-4.55798800	-4.73962900
O	-1	4.82642800	-2.86311400	-1.28223200
H	0	5.72743900	-2.75177400	-0.95991100
H	-1	7.29878700	1.35435000	0.01836300
H	0	-4.76903100	-0.10065600	2.10690100
H	0	-5.36549700	4.16216700	-0.58249700



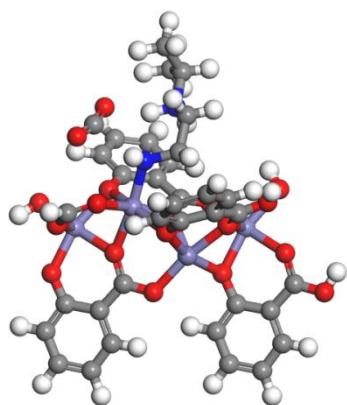
Fe-(B) Complex

-1 1				
H	0	-8.08413300	1.83657700	-0.96075700
Fe	-1	-2.46851500	-1.96503200	-1.59346900
O	-1	-2.28817700	-3.94274300	-2.08341000
O	-1	-3.17257500	-0.10060100	-1.09513900
O	-1	-4.34750600	-2.57679600	-0.97656400
O	-1	-6.57289700	-2.67178500	-0.83486800



O	-1	-2.01884200	-1.98001600	0.50278100
O	-1	-2.52046200	-4.00977400	1.28313500
H	0	-1.43551500	-4.07039400	-2.51459400
C	-1	-4.44086600	0.34221100	-1.08557700
C	-1	-5.57941600	-0.51563700	-0.99579800
C	-1	-6.86546900	0.04962300	-0.94433100
C	-1	-7.08292400	1.42359700	-1.00516800
C	-1	-5.95095000	2.25625500	-1.13739900
C	-1	-5.49386900	-1.99226500	-0.92739600
C	-1	-1.44401400	-3.47232700	3.76511800
C	-1	-2.02868600	-2.85111000	1.45626700
H	0	-0.84904800	-4.06317400	5.75882900
C	0	5.41033400	-3.47825100	-2.14304400
H	-1	-7.70340300	-0.63715800	-0.82106900
H	-1	-1.92539500	-4.42066800	3.52330300
H	0	3.04848100	-3.07383600	-1.40993000
H	0	4.43165000	-5.06646800	-1.08780700
H	0	4.70516400	-3.45222500	-2.98129100
H	0	6.26057800	-4.09953100	-2.43860700
H	0	-3.39339100	6.61271600	0.43949600
H	-1	-6.09103700	3.33557500	-1.22767900
Fe	-1	2.22262900	2.81023700	-0.19145400
Fe	-1	-1.77632400	0.08450700	0.45193500
Fe	0	1.08762600	0.31835200	0.79564700
O	0	2.38483100	0.83485300	-0.68225800
O	0	-0.07324700	-0.31533200	-0.66687800
O	-1	-0.72691100	-1.39025700	-2.51106900
O	-1	1.51859100	4.67467700	0.30689800
O	0	0.34970400	2.19992100	0.41094300
O	-1	-1.88172900	2.10349500	0.56717000
O	0	-0.59137600	-0.30636100	2.04917600
O	-1	2.67233400	2.79528300	1.90483000
O	0	2.13019900	0.78855400	2.69149700
O	0	5.46258800	-0.23053000	1.28758600
O	0	6.65190700	0.57573500	-0.54723400
C	-1	2.50196500	0.30713900	-1.91097300
C	-1	1.47069000	-0.46908200	-2.52344900
C	-1	1.66071200	-0.97492300	-3.82032700
C	-1	2.83868500	-0.77569200	-4.53445300
C	-1	3.85697300	-0.02259200	-3.90931700
C	-1	3.69431800	0.50857200	-2.64375700
C	-1	0.18207100	-0.76584700	-1.87034700
C	-1	0.25029900	5.11749300	0.31645200
C	-1	-0.88825000	4.25964500	0.40623900
C	-1	-2.17430500	4.82490400	0.45770000
C	-1	-2.39182800	6.19880700	0.39684400

C	-1	-1.25978500	7.03153500	0.26463400
C	-1	-4.66892700	1.73522300	-1.17723100
C	-1	-0.80276600	2.78294700	0.47462600
C	-1	-0.72251000	-1.26292200	2.98155700
C	-1	-1.42313000	-2.49251600	2.75856100
C	-1	-0.82790700	-3.28954400	5.00067200
C	-1	-0.18959600	-2.04969500	5.22943700
C	-1	-0.13900900	-1.06646600	4.25674100
C	-1	2.66244600	1.92408200	2.85820600
C	0	6.05469600	0.17542700	0.36922700
C	0	1.59105200	-2.70927500	0.72147200
C	0	2.71853600	-3.70313900	0.47739500
C	0	4.75311400	-4.02750900	-0.88373800
C	0	5.74625200	-4.06365500	0.27229600
H	-1	0.82694100	-1.51664600	-4.26846300
H	-1	4.48965700	1.08327800	-2.16694700
H	-1	-3.01223900	4.13812200	0.58096100
H	-1	-3.79894100	2.38563000	-1.27994400
H	-1	0.26742500	-1.86026800	6.20292800
H	-1	0.36123500	-0.11379900	4.43923800
H	0	0.95417400	-3.05009800	1.54044300
H	0	2.28736300	-4.69059400	0.23691900
H	0	0.96130700	-2.63840100	-0.17028500
H	0	2.95237300	-1.26286900	0.46403800
H	0	3.29519500	-3.82331100	1.40165000
H	0	2.44118300	-1.35973100	1.99763500
H	0	5.77014400	-2.45780400	-1.97201200
H	0	6.63861800	-4.62737100	-0.01588000
H	0	5.33091900	-4.54248900	1.16354700
H	0	6.05049800	-3.04679400	0.54216200
N	0	2.10823900	-1.36663500	1.03416000
N	0	3.59827000	-3.18697800	-0.56054700
H	0	2.96481700	-1.17556600	-5.53425600
H	-1	4.80511300	0.12527200	-4.43083900
H	-1	-1.39987200	8.11085600	0.17435200
O	-1	3.96425600	3.38502300	-1.10902900
H	0	4.16714900	4.24809800	-0.73232100
C	-1	0.02223800	6.51050300	0.22480100
H	0	3.10287600	2.19125200	3.82862700
H	-1	0.89215400	7.16084100	0.12206800
H	0	-2.38211000	-4.59790800	2.03528200
H	0	-6.34285500	-3.61534100	-0.81939700



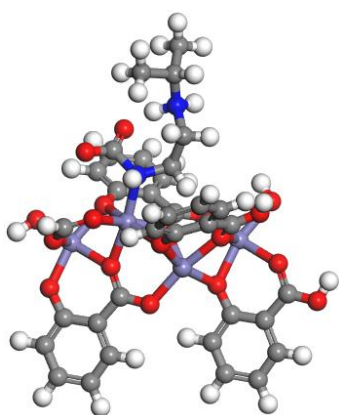
Fe-(C) TS<sub>1</sub>

-1 1

H	-8.05331100	1.24201800	-1.20905400
Fe	-2.15242200	-2.14828500	-1.48033900
O	-1.81061400	-4.13218000	-1.84260100
O	-3.00796900	-0.31684400	-1.11429200
O	-3.99588500	-2.86432500	-0.86849400
O	-6.21080600	-3.12123000	-0.77054300
O	-1.75928100	-2.00261300	0.62225800
O	-2.12740400	-4.01428800	1.51564600
H	-0.94514500	-4.21585300	-2.25888700
C	-4.30579900	0.02703900	-1.16031800
C	-5.37852500	-0.90874900	-1.04278500
C	-6.70440400	-0.44184600	-1.05498300
C	-7.02297900	0.90522000	-1.20569400
C	-5.95377200	1.81288200	-1.36417200
C	-5.18391000	-2.36765400	-0.88108300
C	-1.16143400	-3.24749200	3.98278100
C	-1.72908300	-2.81297300	1.62746500
H	-0.57781500	-3.66992000	6.02219200
C	4.71958000	-3.60619200	-2.61298200
H	-7.49125500	-1.18228700	-0.90798100
H	-1.56338900	-4.24281900	3.78961800
H	2.55446400	-2.96601300	-1.34654800
H	3.67266100	-5.05261000	-1.40987000
H	3.87741700	-3.39536000	-3.27839600
H	5.35546300	-4.35182600	-3.09578100
H	-3.77461500	6.44047900	-0.00415200
H	-6.17225200	2.87087000	-1.52428000
Fe	2.12659300	3.04877500	-0.27343500
Fe	-1.67161500	0.06763800	0.44888800
Fe	1.21176300	0.49625300	0.84532800
O	2.44236800	1.08483000	-0.66258900
O	0.09206000	-0.26682400	-0.60710800
O	-0.43505300	-1.49768900	-2.39297900
O	1.27104600	4.88021600	0.09261200

O	0.28643000	2.33529400	0.31971000
O	-1.93178900	2.07583000	0.43636100
O	-0.51082300	-0.13935900	2.09753300
O	2.51973500	3.19444700	1.82916200
O	2.09317200	1.21391100	2.75184900
O	4.74165400	0.30921400	1.77655900
O	5.06401000	-0.98233400	-0.12846200
C	2.63963400	0.47562600	-1.82781300
C	1.68649500	-0.41289700	-2.41373500
C	1.94877600	-0.97971600	-3.67222700
C	3.12713500	-0.73392100	-4.37104000
C	4.06872100	0.13145400	-3.77141900
C	3.83248800	0.72360900	-2.54494000
C	0.40682900	-0.76792900	-1.77221700
C	-0.02678300	5.22410000	0.04658600
C	-1.09950900	4.28831200	0.16412000
C	-2.42538900	4.75521400	0.15192000
C	-2.74402600	6.10220400	0.00119300
C	-1.67475600	7.00994200	-0.15726700
C	-4.63555300	1.39038600	-1.34319700
C	-0.90495700	2.82933000	0.32580400
C	-0.58757200	-1.04032800	3.07993200
C	-1.18738900	-2.33127800	2.91812200
C	-0.59420100	-2.94397200	5.21797700
C	-0.05741600	-1.64726200	5.38352300
C	-0.05493200	-0.72332800	4.35310000
C	2.54986900	2.38401100	2.83435100
C	4.74114400	-0.37424900	0.83042800
C	1.70177600	-2.40274600	1.04047600
C	2.67061900	-3.50867500	0.63434900
C	4.25896300	-4.13912700	-1.26688000
C	5.41727300	-4.41188300	-0.32249300
H	1.17048000	-1.60983300	-4.10428200
H	4.56948900	1.38526500	-2.08754800
H	-3.21224000	4.01477300	0.29892300
H	-3.81456600	2.09832300	-1.46672800
H	0.35777000	-1.36510300	6.35328800
H	0.36709100	0.27418600	4.48722300
H	1.22240300	-2.76215600	1.96494700
H	2.17709500	-4.47728300	0.51010900
H	0.89968000	-2.37703400	0.29022900
H	3.76015400	-2.23406100	-0.52134300
H	3.47660900	-3.60633800	1.36414800
H	2.64264000	-1.01692100	2.12014000
H	5.30057800	-2.68649600	-2.49332900
H	6.11676400	-5.08806600	-0.81988300

H	5.09794800	-4.89313100	0.60433000
H	5.95278200	-3.48956600	-0.07876900
N	2.31846300	-1.09519000	1.15791500
N	3.29859200	-3.14806300	-0.66726400
H	3.30901200	-1.18118600	-5.34195300
H	5.01666200	0.31997500	-4.27992200
H	-1.89323700	8.06793000	-0.31737700
O	3.84396300	3.69937000	-1.18607500
H	3.96872800	4.59974000	-0.86685200
C	-0.35653700	6.58744600	-0.13629200
H	2.95944300	2.75150800	3.78761000
H	0.46438700	7.29530700	-0.25984100
H	-1.97410400	-4.53704100	2.31173000
H	-5.91021500	-4.04130900	-0.68968900



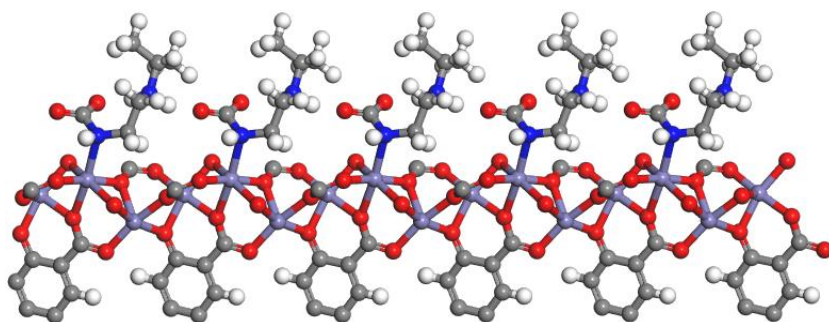
Fe-(D) Intermediate from Gaussian

-1 1

H	-8.07655900	-1.70709000	-0.21104600
Fe	-1.47635300	-2.58134200	-1.64660000
O	-0.50245900	-4.25350200	-2.30941100
O	-2.86585700	-1.24439100	-0.93810400
O	-2.80927800	-3.98709000	-0.91680100
O	-4.73298600	-5.06941400	-0.58605800
O	-0.82682600	-2.46362000	0.39324100
O	-0.29044700	-4.52862100	1.04788500
H	0.25774500	-3.97477000	-2.83256700
C	-4.18904600	-1.41440400	-0.77997900
C	-4.81527600	-2.69249300	-0.65924100
C	-6.20330000	-2.76230300	-0.44800600
C	-7.00838000	-1.62842200	-0.37763900
C	-6.38183600	-0.37438800	-0.54198100
C	-4.08163900	-3.97727700	-0.71869900
C	0.71888100	-3.65001000	3.45975800
C	-0.34213200	-3.27870000	1.27002600
H	1.73950600	-3.97912900	5.33797800
C	6.95780600	-3.16864000	-1.22798300
H	-6.63318500	-3.75441000	-0.30687000

H	0.67936000	-4.70491000	3.18556700
H	4.49064700	-2.90674100	-1.31820500
H	5.90103800	-3.82576100	0.52669200
H	6.50574900	-3.92298700	-1.87937400
H	7.93082000	-3.54541400	-0.90464600
H	-5.83804900	4.61055500	1.14956600
H	-6.99180800	0.53144500	-0.53161700
Fe	0.76310100	3.73571600	-0.28438100
Fe	-1.52487300	-0.50726900	0.48864500
Fe	0.99694000	0.99361200	0.59282800
O	1.70668100	2.06858600	-0.95583600
O	0.05162900	-0.06877600	-0.80102200
O	-0.28428700	-1.25999500	-2.66570000
O	-0.62640300	5.07266700	0.42411500
O	-0.56571100	2.33294700	0.42865000
O	-2.49353000	1.24764500	0.77616100
O	-0.08765700	-0.38693200	1.92046600
O	1.41262800	3.85343900	1.75546000
O	1.83256500	1.78996100	2.45455500
O	4.32274500	1.51395600	0.93480900
O	4.45534700	0.12038800	-0.82091700
C	1.91407900	1.67853000	-2.21922800
C	1.26620800	0.54457600	-2.79859100
C	1.50793800	0.21989600	-4.14396300
C	2.38677700	0.94720200	-4.94143000
C	3.03466100	2.05435900	-4.35028400
C	2.80245400	2.41477600	-3.03617500
C	0.32468000	-0.31729600	-2.05978100
C	-1.94959100	4.90265500	0.58224000
C	-2.57582200	3.62456600	0.70297900
C	-3.96384600	3.55475600	0.91421200
C	-4.76895800	4.68854300	0.98456100
C	-4.14238100	5.94267100	0.82024000
C	-5.01551200	-0.26720500	-0.73772100
C	-1.84221700	2.33968900	0.64350100
C	0.29892700	-1.32614100	2.79696200
C	0.19005800	-2.73101300	2.53812300
C	1.33007900	-3.25264900	4.64640400
C	1.37962000	-1.86659600	4.91733400
C	0.87965900	-0.93241500	4.02695500
C	1.89728900	3.03826600	2.63222500
C	3.93597400	0.58061000	0.24030500
C	2.54078600	-1.48247300	0.16216500
C	3.63739600	-2.48702200	0.50193500
C	6.09258300	-2.89008900	-0.01011100
C	6.72339900	-1.86979100	0.92381200

H	0.95186300	-0.62168400	-4.55867700
H	3.31331500	3.26783800	-2.58731700
H	-4.39373100	2.56264900	1.05535000
H	-4.53870500	0.70598500	-0.86425500
H	1.81590500	-1.52557000	5.85850000
H	0.92721500	0.13673400	4.24093200
H	1.58932500	-1.85567700	0.53041700
H	3.25022400	-3.50783400	0.47961600
H	2.44551800	-1.39606800	-0.92246900
H	4.77955200	-1.33698100	-0.74471800
H	4.03909100	-2.30403100	1.50131100
H	2.78468400	-0.16001000	1.72290100
H	7.12348700	-2.25595500	-1.80924300
H	7.68727500	-2.25047500	1.26944500
H	6.11216300	-1.67465600	1.80900000
H	6.89246300	-0.92242000	0.40304400
N	2.71123900	-0.12984700	0.70561400
N	4.75801900	-2.39338200	-0.47757500
H	2.55998700	0.67849500	-5.97745900
H	3.75370600	2.62673100	-4.94026100
H	-4.75235400	6.84850400	0.83060100
O	1.95516800	5.05706300	-1.30348100
H	1.79860100	5.90599000	-0.87580600
C	-2.77605700	6.04985300	0.62450000
H	2.33019900	3.44443200	3.55673200
H	-2.29928300	7.02295100	0.49794500
H	0.17142700	-5.01867200	1.73884800
H	-4.11135200	-5.81131700	-0.66763200



Fe-(D) Intermediate from VASP

1.00000000000000

21.2362935355011899	0.0310546435970045	-0.0047260941620644
-11.2626411671047446	19.1158319038748914	-0.0064664215974189
-0.0070686423974531	-0.0083177970588644	6.8392722185187287

Fe O C H N

6 20 48 32 2

Direct

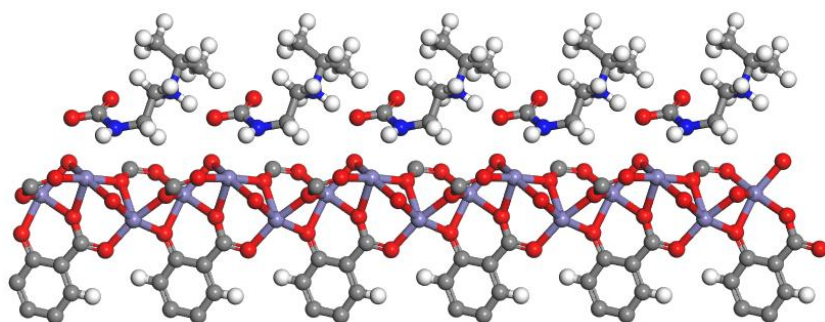
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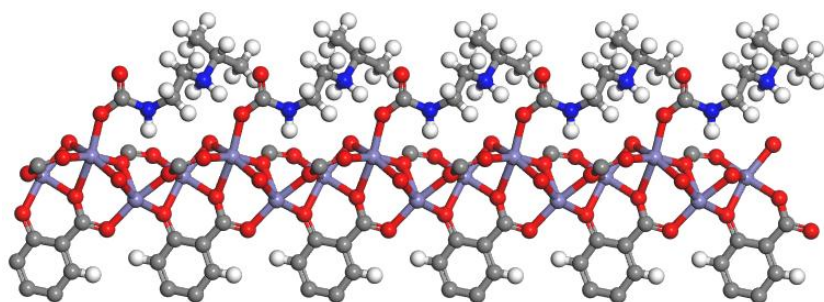
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Direct

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Direct

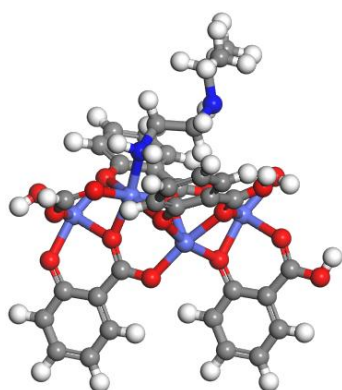
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0.8374146701631039	0.5403668665577938	0.2325027125298433
0.5504408387120158	0.1061880703910480	0.5896691900647453
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0.5002342845477640	0.6760752752072886	0.7956837853021074
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Co-(A) i-2-MOF

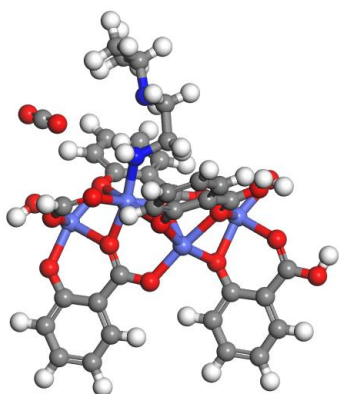
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O	-0.88999700	2.49859200	-1.06962500
O	-3.61072400	2.80910900	-0.83034900
O	-4.40043200	4.88751400	-0.67522900
O	-2.21011800	0.91102200	0.57169500
O	-4.25523600	0.70361300	1.42823500
H	-4.77097200	0.98845400	-1.26350600
C	-0.87827200	3.84268200	-1.07630100
C	-2.05280900	4.64144900	-0.94359700
C	-1.93246000	6.04148500	-0.90708800
C	-0.70392200	6.68892200	-1.01989600
C	0.44216600	5.88662400	-1.19994000
C	0.36114200	4.50470100	-1.23114400
C	-3.41767300	4.07964300	-0.80573600
C	-2.40826500	0.19487800	2.84331000
C	-3.30383700	-0.11601800	3.87872400
C	-2.99605000	0.64309400	1.56090300
H	-3.59318300	-0.88471200	5.87969100
C	-3.84375500	-4.60758700	-0.66578600
C	-4.74327100	-4.74654200	0.55640100
C	-4.58954300	-5.00110600	-1.93424600
H	-2.84552600	6.61490200	-0.74658400
H	-4.36640900	0.01545700	3.67173800
H	-2.90673500	-3.13781400	-1.70929000
H	-5.58886100	-4.05404300	0.48289000
H	-5.13399600	-5.76635200	0.62299800
H	-5.45761900	-4.34961300	-2.08116400
H	-4.93705200	-6.03658200	-1.87512000
H	-3.94479500	-4.91375600	-2.81592200
N	-3.39161500	-3.22262200	-0.81986300
H	5.39515600	4.91759100	0.21532100
H	7.44284800	3.51517800	-0.13289200
Co	3.57129700	-1.59666900	-0.26735500
Co	-0.21518600	1.33294600	0.44523800
Co	0.90894400	-1.28165800	0.88561500
O	1.81615200	-2.38757600	-0.66758800
O	-0.19670500	-0.53786800	-0.55801300
O	-1.38022800	-0.15085600	-2.40557100
O	5.13952600	-0.35421700	0.12941200
O	2.42256100	-0.06342100	0.36156300
O	1.62910900	2.03468900	0.52386000
O	-0.08978200	0.18321500	2.06811400
O	3.81939900	-1.94179300	1.77076800
O	1.78208300	-2.04040000	2.66662300
C	1.27997700	-2.66979700	-1.87028100



C	0.18988100	-1.94522100	-2.44887100
C	-0.24293000	-2.26039000	-3.74725500
C	0.32380300	-3.28585400	-4.50044500
C	1.36837600	-4.02256800	-3.90378000
C	1.83428600	-3.72427500	-2.63398800
C	-0.48349700	-0.80967000	-1.77835700
C	5.15125300	0.98985600	0.12287000
C	3.97673400	1.78861900	0.25548900
C	4.09708100	3.18865700	0.29199600
C	5.32561900	3.83609400	0.17918900
C	6.47170600	3.03379700	-0.00085600
C	6.39068300	1.65187300	-0.03206100
C	2.61186500	1.22682100	0.39334400
C	-1.00968100	-0.05298700	3.01619100
H	3.46102700	-2.55984800	3.70713800
C	-2.88305500	-0.63818100	5.09927000
C	-1.49490700	-0.82085400	5.28248400
C	-0.58513300	-0.53388800	4.27923500
C	3.03344200	-2.20969300	2.76002000
C	-1.21920100	-3.41795900	0.44096900
C	-2.53843000	-2.67911300	0.22192500
H	-0.90555800	-2.36412600	2.16644000
H	-1.02832000	-1.63480000	-4.17187500
H	2.66266700	-4.28691800	-2.19947300
H	3.18401600	3.76207400	0.45249900
H	1.25160100	3.88995700	-1.36951800
H	-1.13089600	-1.18968500	6.24388100
H	0.48613100	-0.67920000	4.42768600
H	-0.68776500	-3.53512900	-0.50626700
H	-1.40964300	-4.42173100	0.83634400
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H	-2.99759600	-5.30809300	-0.54505500
H	-4.21137900	-4.53891100	1.48995200
N	-0.33940400	-2.69531400	1.38345000
H	-0.02452100	-3.50801100	-5.50293300
H	1.81555800	-4.85243200	-4.45466200
O	4.64934100	-3.00367100	-1.20645200
H	5.53294300	-2.84866000	-0.85192200
H	7.28105300	1.03717200	-0.17045200
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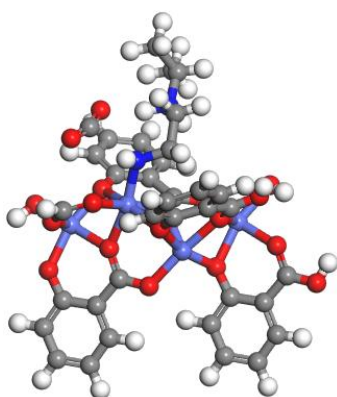
Co-(B) Complex

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H	0	-7.94175600	2.19207800	-0.89266200
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O	-1	-2.49152000	-3.77212400	-2.09026900
O	-1	-3.13427300	0.01911000	-1.05059300
O	-1	-4.40025400	-2.37932600	-0.89206700
O	-1	-6.62958800	-2.38531900	-0.75044200
O	-1	-2.01243300	-1.91580200	0.41358500
O	-1	-2.67521000	-3.89352500	1.21042800
H	0	-3.16416600	-4.08561100	-1.47702200
C	-1	-4.37774100	0.52815700	-1.03446300
C	-1	-5.55244500	-0.27470700	-0.93679100
C	-1	-6.81075100	0.34796200	-0.88166600
C	-1	-6.96165500	1.73192400	-0.94250700
C	-1	-5.79309900	2.50972500	-1.08386300
C	-1	-5.52285900	-1.75357600	-0.85303200
C	-1	-1.58905500	-3.40546700	3.70141100
C	-1	-2.11567800	-2.76842000	1.37754800
H	0	-1.02110400	-4.01786700	5.69752200
C	0	5.27585900	-3.56254200	-2.12728900
H	-1	-7.68001000	-0.29675500	-0.74996200
H	-1	-2.10819200	-4.33373500	3.46040500
H	0	2.90472500	-3.13025200	-1.43656700
H	0	4.24916800	-5.14867200	-1.11564300
H	0	4.58758500	-3.50846400	-2.97804700
H	0	6.11895000	-4.19624300	-2.41683000
H	0	-3.04166800	6.68629000	0.48512000
H	-1	-5.88353800	3.59440300	-1.17363600
Co	-1	2.37573000	2.63457800	-0.21405000
Co	-1	-1.76408300	0.13985900	0.41318300
Co	0	1.08511300	0.24280500	0.82970300
O	0	2.41350400	0.76255200	-0.72428900
O	0	-0.04351200	-0.38319400	-0.67152400
O	-1	-0.85837100	-1.28084500	-2.54121400
O	-1	1.76628000	4.51294800	0.32908300

O	0	0.51524700	2.11024400	0.46753500
O	-1	-1.72912500	2.10848800	0.62919500
O	0	-0.63269400	-0.26490200	2.00329100
O	-1	2.88805900	2.57802500	1.79320800
O	0	2.10703400	0.66314500	2.62807100
O	0	5.24428400	-0.39161400	1.38902800
O	0	6.54537400	0.47250900	-0.34048400
C	-1	2.47048700	0.21385500	-1.95054100
C	-1	1.39197500	-0.49194100	-2.56603200
C	-1	1.54723900	-1.00003500	-3.86595800
C	-1	2.73465600	-0.86439900	-4.58146400
C	-1	3.79674000	-0.17709300	-3.95516800
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C	-1	0.09109400	-0.71032800	-1.90494000
C	-1	0.52280100	5.02203500	0.34518100
C	-1	-0.65191100	4.21916300	0.44286700
C	-1	-1.91021300	4.84183000	0.49799400
C	-1	-2.06111700	6.22579200	0.43715500
C	-1	-0.89263100	7.00352800	0.29577700
C	-1	-4.53674100	1.92903800	-1.13148300
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C	-1	-0.27471400	-2.03685900	5.16766900
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C	-1	2.78488900	1.72552000	2.75729000
C	0	5.89085300	0.04448600	0.52260300
C	0	1.43235900	-2.75306300	0.69445100
C	0	2.52940000	-3.77702600	0.43652800
C	0	4.58423000	-4.11883500	-0.89002000
C	0	5.55298700	-4.18759100	0.28500500
H	-1	0.68253300	-1.48774100	-4.31699600
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H	-1	-2.77954200	4.19704700	0.62967900
H	-1	-3.63728300	2.53627300	-1.24245400
H	-1	0.19040400	-1.86844300	6.14120400
H	-1	0.36336400	-0.12793600	4.37307600
H	0	0.78630500	-3.08176000	1.51009300
H	0	2.06527600	-4.74122200	0.16738400
H	0	0.80744500	-2.63641100	-0.19388900
H	0	2.85682200	-1.35952500	0.45969700
H	0	3.09206200	-3.94102400	1.36229100
H	0	2.34041600	-1.45586900	1.99614500
H	0	5.65237600	-2.55256500	-1.93224100
H	0	6.44402500	-4.75700700	0.00419500

H	0	5.11523000	-4.67743600	1.15931500
H	0	5.86388700	-3.17946500	0.57871000
N	0	2.00964800	-1.43964800	1.03187500
N	0	3.43613200	-3.26332600	-0.57844700
H	0	2.83616600	-1.26438200	-5.58427700
H	-1	4.74966600	-0.08116000	-4.47988000
H	-1	-0.98307000	8.08820700	0.20600400
O	-1	4.04216100	3.21303500	-1.16155500
H	0	4.21740300	4.06069700	-0.73585700
C	-1	0.36372400	6.42284000	0.24815700
H	0	3.27474300	1.93747000	3.71521300
H	-1	1.26318300	7.03007500	0.13718700
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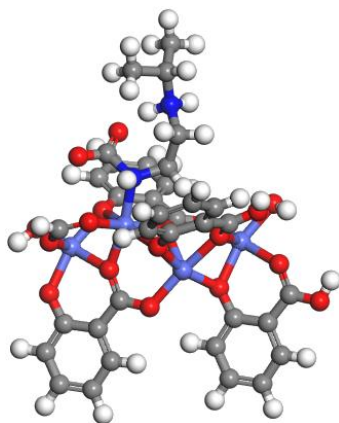
Co-(C) TS<sub>1</sub>

-1 1

H	0	-7.90847700	1.61721100	-1.28092200
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O	-1	-2.95383400	-0.19244700	-1.09060000
O	-1	-4.04828600	-2.65852200	-0.77288100
O	-1	-6.27522900	-2.82114400	-0.70728500
O	-1	-1.75474900	-1.91076400	0.56944500
O	-1	-2.30418700	-3.86097600	1.50775000
H	0	-2.64541400	-4.30885100	-1.14397900
C	-1	-4.23054200	0.22092600	-1.15996200
C	-1	-5.34703800	-0.65761500	-1.03477100
C	-1	-6.64830400	-0.12927800	-1.07543400
C	-1	-6.89640300	1.22970700	-1.25827800
C	-1	-5.78246300	2.07929700	-1.42505700
C	-1	-5.21389400	-2.11819700	-0.82520500
C	-1	-1.35732700	-3.09004300	3.98404700
C	-1	-1.83473000	-2.68695600	1.59802300
H	0	-0.82633000	-3.49270600	6.04291800
C	0	4.19674900	-4.11694800	-2.69296500
H	-1	-7.47321800	-0.82481200	-0.91933300

H	-1	-1.79779900	-4.07145200	3.80491400
H	0	2.27215400	-3.15684300	-1.28587000
H	0	3.25373300	-5.32846600	-1.18539600
H	0	3.28237800	-3.96149200	-3.27265800
H	0	4.74237800	-4.95079000	-3.14048400
H	0	-3.40581200	6.56653400	-0.12264000
H	-1	-5.94748100	3.14305400	-1.60932700
Co	-1	2.31420100	2.89116900	-0.29110800
Co	-1	-1.65605700	0.15084700	0.40356500
Co	0	1.20291000	0.44144300	0.90365300
O	0	2.49655600	0.99141500	-0.64405500
O	0	0.15450300	-0.35243400	-0.56326200
O	-1	-0.53170500	-1.43455500	-2.38744900
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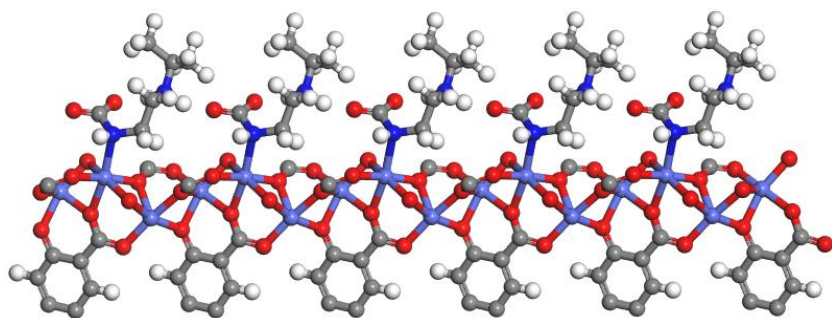
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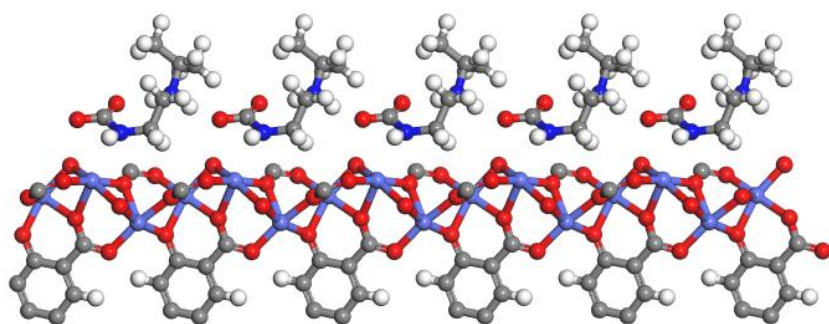
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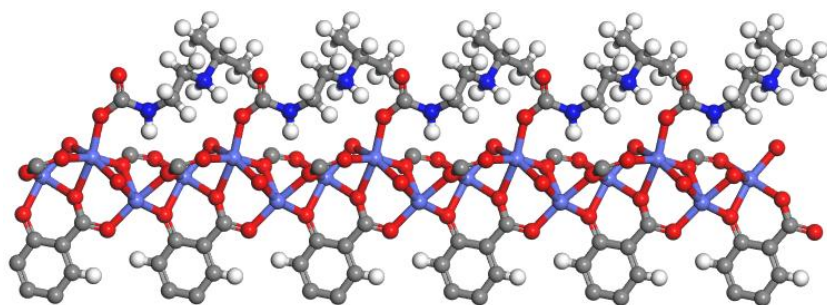
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Direct

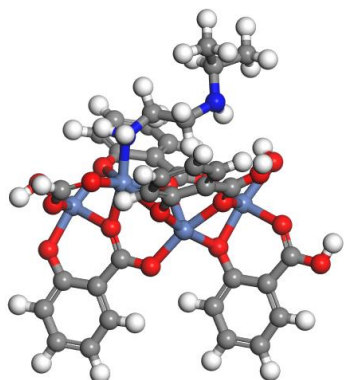
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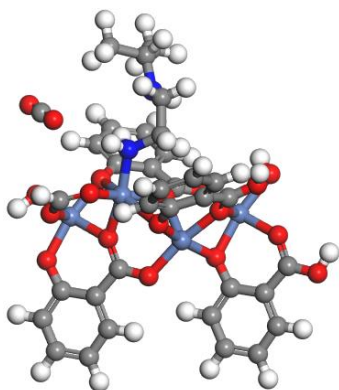
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C	-1	-0.63886900	-0.87235600	4.15351500
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C	0	-0.89060400	-3.52602700	0.12339400
C	0	-2.17820700	-2.85566200	0.58982300
H	0	-0.01591700	-3.23488800	1.96098500
H	-1	-0.75173300	-1.35096900	-4.34915100
H	-1	3.04850500	-3.91167900	-2.47643300
H	-1	2.80894600	3.90117600	0.78961400
H	-1	0.99287900	4.00724600	-1.12208900
H	-1	-1.17926900	-1.68950300	6.05729800

H	-1	0.43601600	-0.93470400	4.32761100
H	0	-0.66207100	-3.25115300	-0.90768600
H	0	-0.96871500	-4.61808200	0.16874500
H	0	-1.96077200	-1.78969600	0.66422800
H	0	-2.41033700	-3.20554800	1.60548200
H	0	1.01668600	-3.73492100	0.81993600
H	0	-2.89696200	-4.86437800	-1.19008300
N	0	0.23583400	-3.10030200	0.98130100
H	0	0.42689700	-3.02101000	-5.80172500
H	-1	2.32715500	-4.31949400	-4.80609300
H	-1	7.08720700	4.05171900	0.32913700
O	-1	4.84347000	-2.50096100	-1.30019700
H	0	5.69702000	-2.29884200	-0.89849100
H	-1	7.13220500	1.58419300	0.06842100
H	-1	-4.79735300	-0.16508000	2.03968900



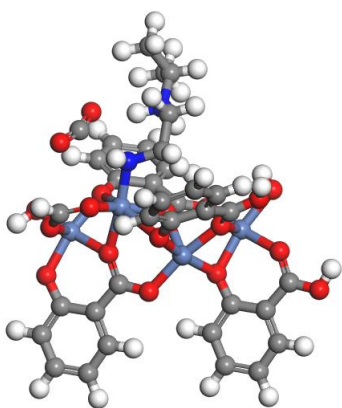
#### Ni-(B) Complex

-1 1

H	-7.83721600	2.32732900	-0.86365800
Ni	-2.60439400	-1.81772100	-1.49033500
O	-2.48906400	-3.78105200	-1.89461900
O	-3.06179400	0.06955200	-1.09623200
O	-4.41239100	-2.32709700	-0.90523200
O	-6.62734200	-2.27792300	-0.68333800
O	-2.12979200	-1.80189000	0.49088800
O	-2.69215300	-3.79461900	1.31717000
H	-1.71601200	-3.84633200	-2.46888800
C	-4.30410700	0.58620500	-1.05105100
C	-5.49814900	-0.18922900	-0.91512500
C	-6.74125200	0.46192000	-0.84116900
C	-6.86780000	1.84667800	-0.92454900
C	-5.68649300	2.59616700	-1.10151100
C	-5.51679800	-1.66979600	-0.82279700
C	-1.59450700	-3.25687700	3.77592900
C	-2.16265300	-2.65418900	1.46284100
H	-1.01101200	-3.84667300	5.77442300
C	4.43955600	-4.25421300	-2.44507800

H	-7.61974500	-0.16465300	-0.68489000
H	-2.12250400	-4.18418200	3.55248000
H	2.41171300	-3.55582800	-1.27886600
H	4.15823500	-5.28785900	-0.59098300
H	3.57003700	-4.71732100	-2.92451700
H	5.32861100	-4.81556800	-2.74580100
H	-2.87023000	6.71607400	0.33840200
H	-5.75626500	3.68030900	-1.21249000
Ni	2.36218300	2.57232500	-0.29028400
Ni	-1.73030400	0.14007200	0.43100900
Ni	1.21978000	0.27966300	0.90317700
O	2.43981500	0.71274700	-0.77726700
O	0.00998000	-0.51600400	-0.59554000
O	-0.91211200	-1.36294800	-2.44760500
O	1.90526000	4.45834500	0.10408900
O	0.57272600	2.07206700	0.37437000
O	-1.66013600	2.11037900	0.51662200
O	-0.77181800	-0.10300000	2.07142400
O	2.83755100	2.58662100	1.69101800
O	2.06294900	0.69897700	2.63754500
O	5.18375800	-0.34888700	1.65237700
O	6.49102900	0.23923500	-0.18486200
C	2.47186700	0.06982800	-1.92388500
C	1.36153500	-0.62598500	-2.50574100
C	1.48171700	-1.16883900	-3.79683800
C	2.65756700	-1.08678900	-4.53778700
C	3.74658700	-0.40922300	-3.94941900
C	3.65649500	0.15464400	-2.69117600
C	0.05879400	-0.81800700	-1.83243300
C	0.66314800	4.97467600	0.14888100
C	-0.53090600	4.19924100	0.28497300
C	-1.77399100	4.85038800	0.35889800
C	-1.90054500	6.23514300	0.27547800
C	-0.71916300	6.98469800	0.09854000
C	-4.44388500	1.98888100	-1.16487100
C	-0.54989900	2.71916800	0.37693500
C	-0.77903700	-1.09207900	2.95347500
C	-1.53591500	-2.29274000	2.75580100
C	-0.95734600	-3.08758700	5.00313200
C	-0.25675900	-1.87873800	5.20693100
C	-0.17442500	-0.91014700	4.22144800
C	2.80491300	1.73194600	2.66245900
C	5.83449800	-0.05091700	0.73213500
C	1.53625800	-2.66545200	1.10150700
C	2.54526500	-3.74369800	0.72868100
C	4.29497600	-4.24480100	-0.92968500

C	5.55214300	-3.68699900	-0.27087300
H	0.59672700	-1.64756400	-4.21742600
H	4.50942400	0.66268700	-2.23972700
H	-2.65248900	4.22381400	0.51514000
H	-3.53569000	2.57581200	-1.30698700
H	0.22116900	-1.70014900	6.17238600
H	0.36838200	0.02192400	4.38745300
H	1.12447200	-2.84571200	2.09601100
H	2.05320100	-4.72956200	0.76751000
H	0.70825000	-2.65632000	0.38741500
H	2.80870000	-1.36688500	0.26293700
H	3.34670900	-3.76063900	1.47676900
H	2.77133600	-1.23234800	1.88849200
H	4.53288300	-3.23006400	-2.82328100
H	6.41035400	-4.33737900	-0.46657100
H	5.44344800	-3.59933400	0.81456900
H	5.77493600	-2.69339300	-0.67508600
N	2.17535800	-1.33962500	1.06873200
N	3.12787300	-3.43465300	-0.56759500
H	2.73074000	-1.51662900	-5.53090300
H	4.69258700	-0.35423200	-4.49153300
H	-0.78900900	8.06877600	-0.01245900
O	4.05516400	3.02547600	-1.24764900
H	4.25137000	3.87752800	-0.83983600
C	0.52337200	6.37734700	0.03516400
H	3.41030900	1.89510800	3.56666100
H	1.43164000	6.96434200	-0.10693600
H	-2.55150600	-4.37484500	2.07487500
H	-6.46302800	-3.23536900	-0.66314700

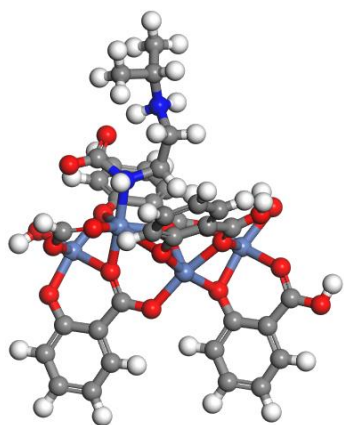


Ni-(C) TS<sub>1</sub>

-1 1			
H	-7.90551500	1.70516500	-1.07872000
Ni	-2.33554700	-2.01105500	-1.42772800
O	-2.04939400	-3.97267400	-1.74644700
O	-2.95600600	-0.15410100	-1.12263200
O	-4.10829000	-2.64532400	-0.85698300

O	-6.32424900	-2.77207100	-0.68056200
O	-1.90940500	-1.87557600	0.55993200
O	-2.32423300	-3.87319500	1.45848400
H	-1.26518600	-3.99335200	-2.30880200
C	-4.23741700	0.25857100	-1.12351600
C	-5.36621400	-0.60758900	-0.97826800
C	-6.66016800	-0.05990200	-0.95610100
C	-6.89858700	1.30497200	-1.10031300
C	-5.77939800	2.14257600	-1.28570500
C	-5.26475900	-2.07960400	-0.82390300
C	-1.33134000	-3.14678400	3.91327100
C	-1.89410600	-2.68763000	1.56617300
H	-0.74736800	-3.60471600	5.94586800
C	4.36919700	-3.90008000	-2.65904400
H	-7.48732200	-0.75070700	-0.79065800
H	-1.77577100	-4.12316200	3.71892100
H	2.42484100	-3.00108000	-1.23612300
H	3.40429100	-5.18008900	-1.22184600
H	3.46418900	-3.71043400	-3.24312500
H	4.91906700	-4.71283200	-3.13903500
H	-3.34631200	6.53845300	0.03248400
H	-5.93581500	3.21174500	-1.44369000
Ni	2.22309100	2.82276200	-0.31752400
Ni	-1.67023000	0.08891600	0.42592400
Ni	1.37001100	0.45865800	0.97535900
O	2.44689600	0.96793200	-0.74046700
O	0.13865200	-0.44634700	-0.54995600
O	-0.66506000	-1.45585700	-2.37018700
O	1.60320400	4.67851900	-0.01209700
O	0.46163100	2.20055500	0.31270800
O	-1.76483800	2.06005800	0.42963700
O	-0.72854400	-0.01129500	2.09344700
O	2.65012100	2.95677900	1.67029400
O	1.98949600	1.07366900	2.72729500
O	4.77744700	0.33983000	1.73048200
O	4.99783700	-1.11334700	-0.06472900
C	2.57627800	0.27409900	-1.84158100
C	1.54076800	-0.53483800	-2.41506900
C	1.73488800	-1.11756100	-3.67951200
C	2.91663300	-0.96779300	-4.40021300
C	3.93226600	-0.17853900	-3.81986500
C	3.76714500	0.42628700	-2.58854100
C	0.24322100	-0.80742200	-1.75976700
C	0.32202900	5.09087100	-0.01335200
C	-0.80678300	4.22471600	0.13206100
C	-2.10071900	4.77240100	0.15419800

C	-2.33914200	6.13727000	0.00994600
C	-1.21988400	6.97494700	-0.17542300
C	-4.48979800	1.63895100	-1.29914900
C	-0.70570400	2.75314900	0.28603400
C	-0.67861700	-0.95657700	3.01621100
C	-1.32912600	-2.22317600	2.85468800
C	-0.73861400	-2.87545300	5.14441500
C	-0.14500600	-1.60514600	5.31061400
C	-0.12029800	-0.67372300	4.28691300
C	2.66585000	2.14235700	2.67612800
C	4.69822100	-0.42716000	0.85055700
C	1.75388500	-2.33607100	1.19002700
C	2.68652800	-3.45907300	0.75951500
C	4.04688900	-4.29384200	-1.22817500
C	5.29327400	-4.54933000	-0.39832300
H	0.90228500	-1.68503100	-4.09668000
H	4.56467800	1.02152400	-2.14240800
H	-2.92787700	4.08159300	0.31960400
H	-3.63010500	2.29333400	-1.44819200
H	0.29430400	-1.34842200	6.27679800
H	0.33981200	0.30631200	4.42396800
H	1.29931800	-2.67140300	2.13314200
H	2.17027500	-4.42277400	0.73834300
H	0.93322200	-2.27487500	0.46655800
H	3.75979800	-2.32457100	-0.56569300
H	3.54700500	-3.53016300	1.42692400
H	2.69835800	-0.94658800	2.27581900
H	4.99123100	-3.00001200	-2.69161000
H	5.89658200	-5.30627700	-0.90490200
H	5.06308600	-4.92760800	0.59996000
H	5.89720800	-3.64187100	-0.30395700
N	2.41440700	-1.04218000	1.30351100
N	3.21196400	-3.20074300	-0.61194000
H	3.04715400	-1.42845600	-5.37356900
H	4.88268000	-0.06683500	-4.34528200
H	-1.37636900	8.04404500	-0.33342700
O	3.89441100	3.37639900	-1.25999600
H	4.01144000	4.25636600	-0.88249300
C	0.06964800	6.47125000	-0.18888200
H	3.26173700	2.40026100	3.56718000
H	0.92940800	7.12570400	-0.33791100
H	-2.15633000	-4.40445500	2.24580500
H	-6.08135700	-3.71061800	-0.61523100



Ni-(D) Intermediate from Gaussian

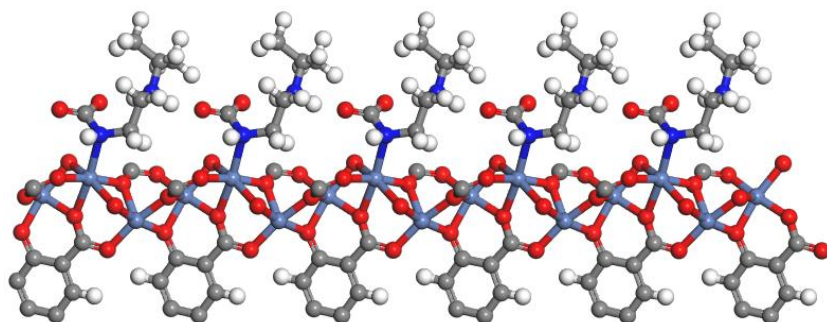
-1 1

H	-8.21308400	-0.03568700	0.02072100
Ni	-2.09930500	-2.26339900	-1.59656100
O	-1.45134500	-4.04738800	-2.25150000
O	-3.04911000	-0.65731200	-0.92971300
O	-3.58196700	-3.36293400	-0.91582400
O	-5.66292900	-4.02866700	-0.48680400
O	-1.40583400	-2.27906600	0.31905800
O	-1.23479100	-4.41378800	0.93846500
H	-0.75660000	-3.81528400	-2.87995900
C	-4.37318600	-0.56107200	-0.70638900
C	-5.25201900	-1.67975700	-0.55904800
C	-6.61362400	-1.45918300	-0.29044500
C	-7.15978800	-0.18175700	-0.18842600
C	-6.29037000	0.91212000	-0.37837200
C	-4.81322100	-3.09396500	-0.65082900
C	-0.04891600	-3.78435800	3.33366900
C	-1.05844300	-3.18307000	1.17596100
H	0.93180100	-4.34050500	5.18043100
C	6.59732800	-3.93393400	-1.20881800
H	-7.23627800	-2.34033000	-0.13344200
H	-0.29766700	-4.80604800	3.04578500
H	4.17299700	-3.35657300	-1.33931600
H	5.39288300	-4.55847100	0.46087500
H	6.07210500	-4.56417000	-1.93294500
H	7.49078700	-4.47167700	-0.88358400
H	-4.68415100	5.55815100	1.29890300
H	-6.69601800	1.92551600	-0.34634300
Ni	1.42861200	3.33157800	-0.32002200
Ni	-1.61909500	-0.31247400	0.46543800
Ni	1.32906300	0.85021300	0.67539100
O	1.98630200	1.62645300	-1.02884200
O	0.07072800	-0.26930500	-0.80625900
O	-0.75651400	-1.21804400	-2.64114000



O	0.47966800	4.93660500	0.34689200
O	-0.02765800	2.25210000	0.42440900
O	-2.13390500	1.56486600	0.78937000
O	-0.39561300	-0.39581600	1.94338300
O	2.12327800	3.31469100	1.59541300
O	1.93371400	1.25695600	2.48976000
O	4.47916100	1.10084500	0.98421100
O	4.58112600	-0.36364300	-0.71863700
C	2.07839500	1.14702100	-2.25616900
C	1.16439000	0.19462000	-2.81570200
C	1.27850500	-0.16453200	-4.16997400
C	2.27225300	0.34744400	-4.99985800
C	3.17241100	1.27534100	-4.43420800
C	3.07629400	1.66673500	-3.11253900
C	0.07519200	-0.45489200	-2.05469500
C	-0.84417000	5.03263800	0.56977300
C	-1.72299300	3.91393300	0.71727800
C	-3.08458500	4.13451400	0.98585000
C	-3.63075800	5.41193900	1.08782900
C	-2.76128500	6.50590000	0.89790900
C	-4.94107500	0.73191200	-0.63099000
C	-1.28471500	2.50011800	0.62523000
C	-0.03186900	-1.40817200	2.71623700
C	-0.41164600	-2.76220600	2.44076100
C	0.65718400	-3.53600400	4.50857500
C	0.98205100	-2.19237200	4.79630100
C	0.64479400	-1.16171800	3.93599000
C	2.47152900	2.40855600	2.45149300
C	4.06745500	0.17414100	0.29624600
C	2.40170200	-1.72835500	0.15985700
C	3.34466100	-2.88327700	0.47955600
C	5.72971200	-3.62373700	-0.00033400
C	6.45397400	-2.76313000	1.02181400
H	0.53264100	-0.85579700	-4.56382600
H	3.78692400	2.37291600	-2.68159300
H	-3.70724700	3.25336800	1.14281600
H	-4.27664600	1.58357500	-0.78167700
H	1.50184600	-1.96134500	5.72842300
H	0.89888100	-0.12570400	4.16635700
H	1.40675000	-1.98310600	0.52180300
H	2.81280500	-3.83380000	0.40681200
H	2.31625200	-1.59154800	-0.91954400
H	4.67865000	-1.88063400	-0.69735100
H	3.74247100	-2.80176400	1.49345200
H	2.84464300	-0.51565800	1.76856000
H	6.91891900	-3.01530100	-1.70997400

H	7.34569500	-3.29343100	1.36359500
H	5.84348400	-2.54895200	1.90292600
H	6.76759000	-1.81434400	0.57593600
N	2.76133900	-0.42960400	0.75349000
N	4.49080300	-2.91995100	-0.47286500
H	2.34638700	0.05375700	-6.04138000
H	3.98201600	1.67194000	-5.04990000
H	-3.16698600	7.51921400	0.92991600
O	2.77253900	4.37562600	-1.36496100
H	2.77222300	5.19725700	-0.85956000
C	-1.41204300	6.32560800	0.64527300
H	3.20535200	2.64926300	3.23462800
H	-0.74756200	7.17735400	0.49460200
H	-0.84351300	-4.98643500	1.60908600
H	-5.21657900	-4.88427800	-0.59959900



Ni-(D) Intermediate from VASP

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Ni	O	C	H	N
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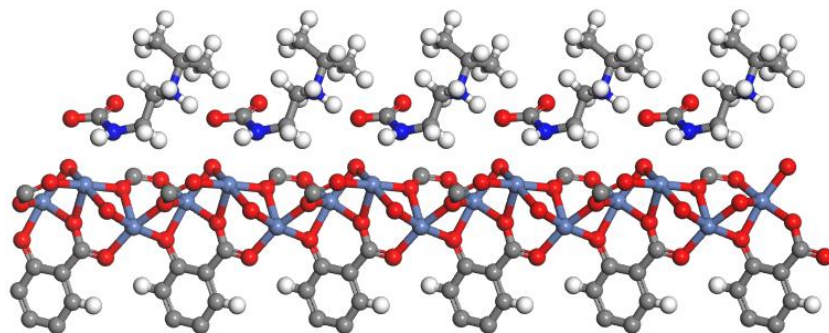
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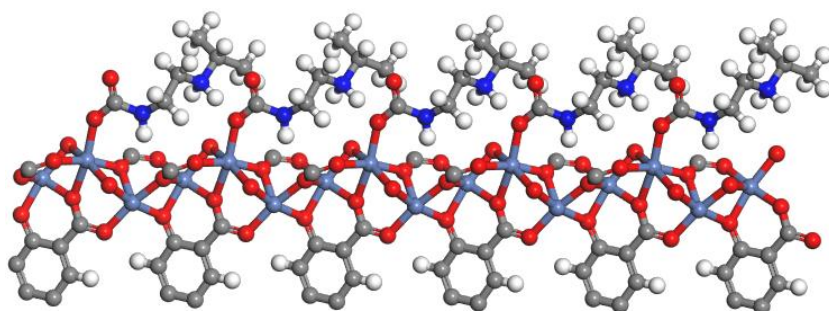
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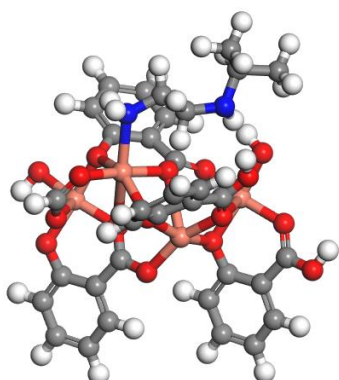
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0.3565480071244055	0.4616317190805608	0.2469714645911122
0.3334867388345484	0.5057943038384195	0.3241446327828323
0.3555612307410027	0.6152953758853656	0.8608831648055620
0.5400197890551268	0.7184200362661348	0.2676106637743407
0.5439859590106427	0.6978386576847317	0.9099109827662336
0.6172929881516936	0.7596982151006606	0.8226261002583070
0.7882866364403859	0.4819080246316081	0.4969199959880443
0.8055688972027903	0.4753653081259646	0.6995142114096794
0.8813289544853885	0.5174435661086161	0.7692035533559677
0.9408772989271381	0.5669985454571416	0.6494973476083483
0.9224693899046964	0.5749804646677112	0.4527098274079463
0.8486750519244106	0.5340043976042507	0.3786910025975422
0.7485048575065709	0.4249992467281928	0.8432966457755492
0.6246011972686053	0.2050993068663851	0.1665448547547030
0.5994371779639819	0.1883226158151534	0.3688512563124541
0.5703398336400562	0.1188268026412284	0.4401616410985076
0.5668959803550999	0.0651178909457354	0.3232546295246793
0.5948052753385917	0.0830794981466362	0.1270045352808881
0.6225956330619318	0.1506074624344733	0.0507541260985256
0.6009616247931935	0.2400922179584602	0.5112580549637916
0.4920912229372580	0.3579918533798117	0.8270779972690622
0.5013585382481579	0.3820418618284249	0.0282665019600703
0.4628193583694302	0.4158647039277785	0.0943437954508385
0.4136959084353977	0.4257981535549722	0.9729948282027853
0.4018422244527172	0.3985690977382122	0.7782400777413840
0.4395469932306713	0.3656145968623569	0.7075585170573138
0.5519131472743162	0.3762993005107290	0.1744595379518413
0.6717799446688251	0.8614299090631317	0.5774838148675250
0.6495030733046443	0.8930825182630772	0.4069994977492378
0.7258210064176801	0.9183761259374892	0.7239812409400007
0.4787119255507905	0.9411750271504684	0.1245757551271676
0.5776126545936519	0.0224878083367222	0.6994057136112023
0.5153894746702338	0.8994750938473726	0.8283107644583944
0.0712428540315196	0.5980632948490245	0.4541610097224557
0.9912755645557079	0.6283006439536407	0.0154199134369796
0.1244402669090138	0.6879610595449998	0.1457516028605892
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0.3569852685536454	0.4217315128801161	0.3430075510036444
0.3164004552052290	0.5020547005420539	0.4792991063821119
0.5573383640862070	0.6575242012596964	0.9578338009713933
0.6463935469362994	0.7390166105125212	0.7329795917055408
0.8926149415806900	0.5085110990135802	0.9216964471214519
0.9674724786418853	0.6149924503055803	0.3571005621415843
0.8351435785358802	0.5407173839874230	0.2263085827719089

0.5485294164579614	0.1077570196824744	0.5920408205005578
0.5953142912116748	0.0428218683934355	0.0335889056133798
0.6440655985459171	0.1638452608310814	0.8988017609929583
0.4749254975714275	0.4367037954377035	0.2452920402021163
0.3616239127517699	0.4031998263298964	0.6810946680756076
0.4301445639873215	0.3452056412837659	0.5562138616278858
0.5003655096443596	0.6741966977804376	0.7922164722392185
0.5596169786268826	0.7676779426650764	0.5740599632123204
0.5736601759218598	0.8251505220182072	0.7566919560821413
0.6556041206708243	0.7933907498644664	0.9414316511503575
0.4582158039371826	0.7064718770166575	0.0670106766338821
0.6257937644223781	0.9247570321237444	0.4614117949809603
0.6076562886901568	0.8520529878562481	0.3069464046714175
0.7012416231421912	0.9283398603326171	0.3199521224161017
0.6980664122712403	0.8328949663159534	0.5147591708537799
0.7757181890591895	0.9601364075112305	0.6431563549622750
0.7471903798785479	0.8977286392190033	0.8396844856469526
0.6973070622107671	0.9435575536171521	0.7959201144820203
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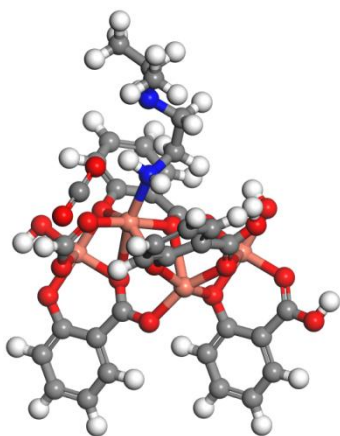
Cu-(A) i-2-MOF

-1 1

H	0	2.24719700	7.25984000	-0.27880800
Cu	-1	-1.43843600	1.95952300	-1.71625600
O	-1	-3.28530100	1.30387600	-2.01724600
O	-1	-0.68357800	0.37566400	-2.57516800
O	-1	0.32493700	2.41146100	-0.98943300
O	-1	-2.13319200	3.74619100	-1.47344300
O	-1	-2.26487600	5.65682500	-0.34393500
O	-1	-1.72387700	1.81432000	0.69010000
O	-1	-3.89029000	1.35555500	0.97407400
H	-1	-3.13544600	0.43492800	-2.40605900
C	-1	0.77068900	3.67779100	-0.88134700
C	-1	-0.09288800	4.78908100	-0.68609000
C	-1	0.45664800	6.05787200	-0.44015600
C	-1	1.83730100	6.27265600	-0.45901900

C	-1	2.67342100	5.18179600	-0.75299600
C	-1	2.16168900	3.91091900	-0.96429100
C	-1	-1.57022400	4.69825000	-0.82424200
C	-1	-2.40076000	0.47994800	2.58193700
C	-1	-3.46635700	0.29031300	3.47797700
C	-1	-2.67064400	1.25042800	1.34473400
C	0	-3.72996900	-1.99226200	0.59577200
H	0	-4.11108500	-0.46131800	5.40127300
C	0	-5.78544900	-1.71819900	-0.77834800
C	0	-6.55765400	-0.60674200	-1.47757800
H	-1	-0.23158000	6.87512200	-0.22293400
H	-1	-4.45505600	0.62954400	3.16822300
H	0	-4.21100300	-0.44070600	-0.62248200
H	0	-2.97805800	-1.36989200	1.09005100
H	0	-4.21674600	-2.56739400	1.39418300
C	0	-6.69542500	-2.53437600	0.13048700
H	0	-5.38945300	-2.39467600	-1.55773800
H	0	-5.88679500	0.00408700	-2.09203600
H	0	-7.02977700	0.05025800	-0.73855600
H	0	-7.33838500	-1.01924600	-2.12326100
N	0	-4.70090400	-1.09868900	-0.01364400
H	0	6.58899700	3.05148400	1.09340600
Cu	-1	2.90055100	-2.24901400	-0.34185100
Cu	-1	0.16230500	1.34930700	0.71225700
Cu	0	-0.05704700	-1.91828900	0.78966700
O	0	1.11202600	-2.82950100	-0.66526400
O	0	-0.65926900	-0.67700600	-0.62361900
O	-1	3.65992200	-3.83492400	-1.19637400
O	-1	4.66392400	-1.79707600	0.38487200
O	0	2.22563000	-0.46650600	-0.08900600
O	-1	2.07411200	1.44828700	1.03047000
O	0	-0.15548400	-0.11106100	1.98647700
O	-1	2.61511000	-2.39421700	2.06440500
O	0	0.44845600	-2.98694600	2.36696300
C	-1	0.67885900	-2.95398700	-1.93067700
C	-1	0.02681000	-1.87250600	-2.58779900
C	-1	-0.23870400	-1.94633200	-3.96524600
C	-1	0.03427500	-3.10037800	-4.70459800
C	-1	0.60107700	-4.19294900	-4.02876900
C	-1	0.92133700	-4.12907400	-2.68242400
C	-1	-0.45948900	-0.66338200	-1.87301900
C	-1	5.10967600	-0.53074600	0.49295700
C	-1	4.24609900	0.58054300	0.68831400
C	-1	4.79563600	1.84933500	0.93424900
C	-1	6.17630600	2.06421700	0.91538600
C	-1	7.01250700	0.97324000	0.62140900

C	-1	6.50077500	-0.29763700	0.41011400
C	-1	2.76876300	0.48971300	0.55016300
C	-1	-1.10727100	-0.03665800	2.89518700
H	0	1.90943600	-3.46593400	3.67153900
C	-1	-3.28121000	-0.32582700	4.71730600
C	-1	-1.97989600	-0.73869700	5.05944600
C	-1	-0.91575900	-0.59620100	4.18371700
C	-1	1.66834300	-2.95810900	2.71913900
C	0	-2.95425200	-2.94385600	-0.31315800
H	0	-1.99186100	-3.81725000	1.26571000
H	-1	-0.66032700	-1.06429900	-4.44730100
H	-1	1.37801700	-4.98409500	-2.18306900
H	-1	4.10740700	2.66658500	1.15137100
H	-1	3.74938200	5.34742600	-0.82409500
H	-1	2.81373300	3.06878800	-1.19420700
H	-1	-1.80965600	-1.17511600	6.04504600
H	-1	0.08953700	-0.91269000	4.46019000
H	0	-2.65138900	-2.41365200	-1.22192200
H	0	-3.57513800	-3.79750100	-0.61936400
H	0	-1.27189600	-4.09303100	-0.14905300
N	0	-1.73588100	-3.36621400	0.39001200
H	0	-0.18908400	-3.15113600	-5.76464300
H	-1	0.78520800	-5.11352700	-4.58313400
H	0	4.55665200	-3.77848000	-0.84068700
H	-1	8.08836900	1.13888900	0.55031000
H	-1	7.15272000	-1.13974900	0.18019800
H	-1	-4.56309200	0.79478200	1.37910100
H	0	-3.19988400	5.51990400	-0.56981000
H	0	-6.16724000	-3.37146600	0.59731600
H	0	-7.53029400	-2.94940900	-0.44225200
H	0	-7.10135500	-1.89965300	0.92596900

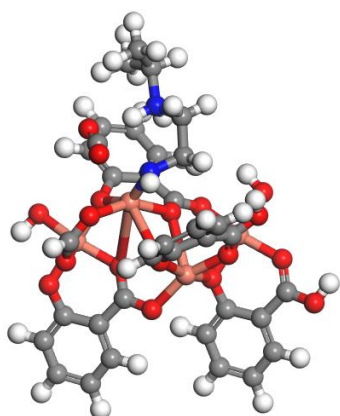


Cu-(B) Complex

-1	1			
H	0	7.67051200	-2.39010900	-0.94203200
Cu	-1	1.59706800	-2.59181400	1.68894400

O	-1	0.13617800	-3.86303600	2.17310400
O	-1	2.78940100	-1.34024000	0.73877900
O	-1	2.64529600	-4.13465500	1.19388300
O	-1	3.91104100	-5.28523600	-0.22279900
O	-1	0.88992800	-2.66655200	-0.65930800
O	-1	-0.67562200	-4.24304400	-0.60891800
H	0	-0.42264200	-3.31911800	2.74175800
C	-1	4.04414100	-1.66574200	0.37227600
C	-1	4.45091800	-2.99469400	0.06533500
C	-1	5.74232100	-3.22748300	-0.43413800
C	-1	6.67213000	-2.19354500	-0.56841000
C	-1	6.28484700	-0.90026500	-0.17567500
C	-1	3.60515400	-4.18207800	0.34415200
C	-1	-1.94729900	-3.24218800	-2.83830400
C	-1	-0.23379100	-3.13875500	-1.06354300
C	0	-7.09775400	-1.38321100	0.94168900
C	0	-8.04940200	-0.25760900	1.32439700
H	-1	5.99794100	-4.24791800	-0.72114900
H	-1	-2.12528800	-4.26086700	-2.49277000
H	0	-4.79530100	-2.58518100	2.01651200
H	0	-5.65888200	-0.35664800	1.92898000
H	0	-7.27776500	-2.23272800	1.62778800
H	0	-7.89465400	0.60845800	0.67155300
H	0	-7.88986400	0.06291300	2.35998300
H	0	-9.09042300	-0.57889200	1.22918300
H	0	6.31565400	3.62148000	-1.95649700
H	-1	7.01701400	-0.09306800	-0.22649000
Cu	-1	0.24034600	3.41737500	0.67270500
Cu	-1	1.50684100	-0.83733300	-0.73580700
Cu	0	-1.28796800	0.73962500	-0.25556200
O	0	-1.13343200	2.15158700	1.16684500
O	0	-0.25080200	-0.45499400	0.95064200
O	-1	0.81920400	-1.15578100	2.75758700
O	-1	1.43256000	4.66885800	-0.27755900
O	0	1.30251400	1.89291700	0.17448000
O	-1	2.55419600	0.72386200	-1.23913900
O	0	-0.11279700	-0.28289300	-1.73283300
O	-1	-0.46692300	3.34266600	-1.67562200
O	0	-2.20308700	1.87017100	-1.59357600
O	0	-3.94634400	1.88077700	-4.15001700
O	0	-4.95701500	0.67113800	-2.43356400
C	-1	-1.31696500	1.80620700	2.45552300
C	-1	-0.67118800	0.66766900	3.01197400
C	-1	-0.74061900	0.43451200	4.39493000
C	-1	-1.49622300	1.25596200	5.23379800
C	-1	-2.18844600	2.33642000	4.65760500

C	-1	-2.10730600	2.61136900	3.30472100
C	-1	0.00401100	-0.35859700	2.18552000
C	-1	2.68731000	4.34345600	-0.64396600
C	-1	3.09408500	3.01450300	-0.95100700
C	-1	4.38547800	2.78161500	-1.45047800
C	-1	5.31519700	3.81566200	-1.58474900
C	-1	4.92801400	5.10893200	-1.19201700
C	-1	5.00558400	-0.63382000	0.28646700
C	-1	2.24832300	1.82712100	-0.67219000
C	-1	-0.82176800	-1.10124100	-2.47983800
C	-1	-1.01781000	-2.46602100	-2.12792100
C	-1	-2.63615800	-2.73349100	-3.94187500
C	-1	-2.35895100	-1.41252100	-4.33955300
C	-1	-1.47281400	-0.61147000	-3.63663800
C	-1	-1.59062200	2.87031200	-2.07980700
C	0	-4.42709400	1.27957600	-3.27499400
C	0	-3.32017500	-1.30394400	1.09111600
C	0	-4.70455300	-1.93666100	1.12643500
H	0	-3.34533200	-3.34670600	-4.48556000
H	-1	-0.17900000	-0.40899400	4.79680900
H	-1	-2.66550500	3.43227400	2.85772200
H	-1	4.64110800	1.76128000	-1.73749000
H	-1	4.71275700	0.36986100	0.59327000
H	-1	-2.84778100	-1.01866800	-5.23161300
H	-1	-1.25864500	0.40846800	-3.95437100
H	0	-2.54671000	-2.07512400	1.15849400
H	0	-3.18997600	-0.65594100	1.96709300
H	0	-3.90735700	0.09325100	-0.23968700
H	0	-4.81607700	-2.58850000	0.25149100
H	0	-3.09790200	-1.11625300	-0.91766400
C	0	-7.37121200	-1.85775300	-0.48173600
N	0	-3.08722900	-0.49717000	-0.10902800
N	0	-5.72216300	-0.89781000	1.06979100
H	0	-1.55533900	1.06159100	6.29920200
H	-1	-2.82050500	2.95506300	5.29604100
H	-1	5.66018200	5.91612900	-1.24283100
O	-1	-0.53753000	4.85340500	1.74114400
H	0	-0.10780800	5.61315900	1.32737000
C	-1	3.64875200	5.37537800	-0.72987500
H	0	-2.09171000	3.36365800	-2.93351500
H	-1	3.35591400	6.37895900	-0.42306900
H	0	-1.59608800	-4.39664300	-0.85717800
H	0	3.33022900	-5.98813800	0.11272700
H	0	-6.71848600	-2.68548000	-0.77463200
H	0	-7.21513100	-1.03551500	-1.18822700
H	0	-8.40454900	-2.20614700	-0.57502400



Cu-(C) TS<sub>1</sub>

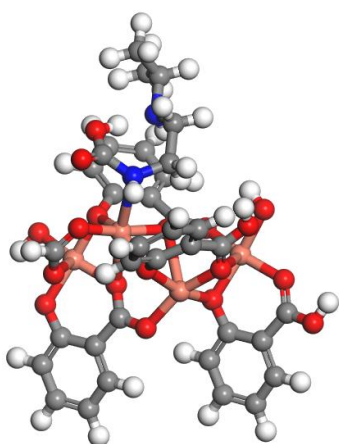
-1 1

H	0	-7.95093400	-1.37569400	-0.43264100
Cu	-1	-1.54697600	-2.39602200	-1.77401700
O	-1	-0.19820300	-3.85277200	-1.98212900
O	-1	-2.73380200	-0.99376600	-1.05550300
O	-1	-2.86846800	-3.78331100	-1.54254000
O	-1	-4.53860900	-4.75061300	-0.44362000
O	-1	-1.35372900	-2.55980300	0.66644300
O	-1	-0.03291200	-4.33211700	0.89635700
H	0	0.54917900	-3.38260200	-2.37107600
C	-1	-4.06868900	-1.14717700	-0.96100200
C	-1	-4.70132000	-2.40893900	-0.77743400
C	-1	-6.08691300	-2.46538900	-0.55794000
C	-1	-6.88006900	-1.31573500	-0.58991400
C	-1	-6.25347700	-0.08700400	-0.86229600
C	-1	-3.98016300	-3.69965400	-0.90801900
C	-1	0.87396100	-3.50607500	3.36305000
C	-1	-0.40940800	-3.17755600	1.27918900
C	0	5.94940100	-1.49516300	-1.76864700
C	0	6.05591100	-0.32337100	-2.72823400
H	-1	-6.52816900	-3.44168300	-0.35521900
H	-1	0.98336600	-4.54004700	3.03524900
H	0	4.28658700	-3.42553800	-0.72055000
H	0	3.89309500	-1.25710700	-1.70081800
H	0	5.86803300	-2.43053200	-2.33139800
H	0	6.12385500	0.62550000	-2.18670200
H	0	5.20047300	-0.27438100	-3.40814900
H	0	6.96045800	-0.43559700	-3.33023200
H	0	-6.05413700	4.40229900	0.98855600
H	-1	-6.86755600	0.81129500	-0.94138000
Cu	-1	0.35122200	3.37908200	-0.34967800
Cu	-1	-1.72683600	-0.66420700	0.66202400
Cu	0	1.70165700	0.43236100	0.64726300
O	0	1.61205900	1.93792400	-0.59043300
O	0	0.44588800	-0.54626800	-0.62238900

O	-1	-0.38394100	-1.07960600	-2.62461800
O	-1	-0.83550500	4.78134900	0.36883800
O	0	-1.00713500	2.01361100	-0.15400400
O	-1	-2.64031200	1.02450200	0.98072100
O	0	-0.42569300	-0.35490500	2.06860100
O	-1	0.54455800	3.21541100	2.09078200
O	0	2.14077600	1.59665300	2.27794700
O	0	4.76607500	0.08817400	3.03875000
O	0	5.09538200	0.86334900	0.87091800
C	-1	2.01572200	1.56976300	-1.81790500
C	-1	1.35384700	0.52687000	-2.52307000
C	-1	1.67473600	0.28349500	-3.86834300
C	-1	2.68812500	0.99436700	-4.51426300
C	-1	3.38324500	1.97350200	-3.78176700
C	-1	3.06264800	2.25981500	-2.46726900
C	-1	0.39398100	-0.39767900	-1.87812100
C	-1	-2.17039200	4.62793700	0.46333900
C	-1	-2.80302300	3.36617600	0.64690700
C	-1	-4.18871600	3.30971600	0.86639900
C	-1	-4.98167500	4.45939200	0.83453000
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C	-1	-4.88285200	0.00440900	-1.04689200
C	-1	-2.08196500	2.07545000	0.51631900
C	-1	0.13811900	-1.23428000	2.83708000
C	-1	0.22083400	-2.61376700	2.49794500
C	-1	1.38208200	-3.09184400	4.59646700
C	-1	1.20543800	-1.74479100	4.96271900
C	-1	0.59619000	-0.83359600	4.11444100
C	-1	1.48890000	2.59746000	2.70353200
C	0	4.78652700	0.38351400	1.90696100
C	0	2.93364400	-2.23594600	0.52908400
C	0	4.28732800	-2.51299400	-0.11787700
H	0	1.87193300	-3.79494900	5.26042600
H	-1	1.10165100	-0.47794600	-4.39770900
H	-1	3.62017800	2.99930600	-1.89499900
H	-1	-4.62987200	2.33343100	1.06912200
H	-1	-4.40354400	0.95916700	-1.26183100
H	-1	1.54801400	-1.41810000	5.94550900
H	-1	0.45752800	0.20647600	4.40764500
H	0	2.74666600	-3.09115700	1.19281700
H	0	2.16462700	-2.28801900	-0.25900900
H	0	4.63984700	-0.52302700	-0.43948800
H	0	5.06752500	-2.58046700	0.64185200
H	0	2.81729700	-1.14747200	2.21279000
C	0	7.12099800	-1.56674600	-0.80495900
N	0	2.89694600	-0.96337900	1.21907800



N	0	4.64661500	-1.37905800	-1.01817700
H	0	2.93776000	0.79310700	-5.55049000
H	-1	4.20883400	2.50033800	-4.26176400
H	-1	-4.96935900	6.58640000	0.48295800
O	-1	1.51435600	4.69550900	-1.20027700
H	0	1.11120500	5.50534200	-0.86284700
C	-1	-2.98446600	5.77963400	0.37744900
H	0	1.77855900	2.96327300	3.71107400
H	-1	-2.50534700	6.73427100	0.16250800
H	0	0.76673400	-4.61779500	1.35495400
H	0	-3.99794400	-5.52469000	-0.67221200
H	0	8.04500300	-1.60221000	-1.38672100
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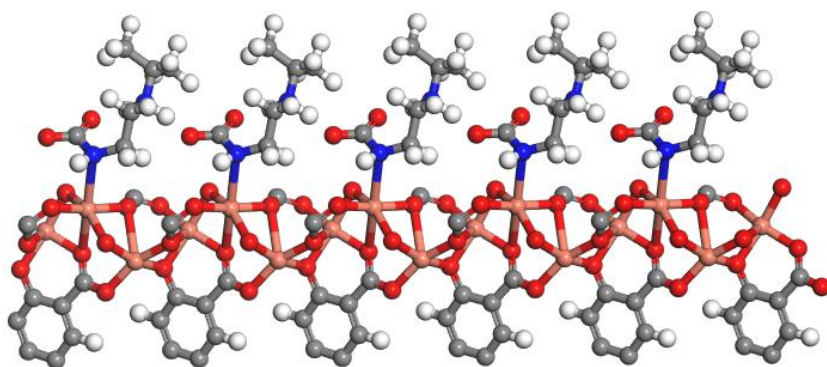


Cu-(D) Intermediate from Gaussian

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H	0	-7.77245700	-1.89172500	-0.64064200
Cu	-1	-1.27360900	-2.49933100	-1.75578000
O	-1	0.17593000	-3.86485300	-1.89268600
O	-1	-2.57481100	-1.16855400	-1.10244100
O	-1	-2.50612900	-3.96856400	-1.54038100
O	-1	-4.14345700	-5.02790400	-0.47732000
O	-1	-1.15110600	-2.60848500	0.69233100
O	-1	0.27708800	-4.28341300	0.99826500
H	0	0.89100200	-3.36340300	-2.30360700
C	-1	-3.89887000	-1.41012200	-1.04795500
C	-1	-4.45133500	-2.70849100	-0.86072400
C	-1	-5.83660300	-2.85471200	-0.68480600
C	-1	-6.70341100	-1.76203800	-0.76407000
C	-1	-6.15184800	-0.49846200	-1.03965900
C	-1	-3.64146300	-3.94959700	-0.94353700
C	-1	1.04400400	-3.35641600	3.47653300
C	-1	-0.18838400	-3.15062600	1.34676600
C	0	5.96047400	-1.42270600	-1.84548100
C	0	5.97122900	-0.48613100	-3.04314800

H	-1	-6.21802600	-3.85496500	-0.47778600
H	-1	1.23324200	-4.38613100	3.17216500
H	0	4.35089800	-3.16828000	-0.47892900
H	0	3.95261700	-1.07820800	-1.66651400
H	0	5.91916900	-2.46203500	-2.21097000
H	0	6.01482900	0.55803300	-2.71624200
H	0	5.07477600	-0.61082700	-3.65864300
H	0	6.84385600	-0.68709000	-3.67037300
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H	-1	-6.82179600	0.35479600	-1.15547900
Cu	-1	0.18669500	3.41512100	-0.38179000
Cu	-1	-1.65000300	-0.74264500	0.63986100
Cu	0	1.08423500	0.74725600	0.86742500
O	0	1.55229000	2.06579300	-0.55027800
O	0	0.50075000	-0.48821100	-0.57077100
O	-1	-0.17349000	-1.12175200	-2.59366900
O	-1	-1.11670100	4.74427000	0.27162500
O	0	-1.04572300	1.95897600	-0.14387400
O	-1	-2.68467200	0.88547100	0.89684900
O	0	-0.29270100	-0.29060000	1.99799300
O	-1	0.30788400	3.30515200	2.06645000
O	0	1.84245900	1.68167600	2.39657800
O	0	4.48807400	0.50734000	3.01988400
O	0	5.01004700	0.52958500	0.86523100
C	-1	2.01512100	1.69707500	-1.76165300
C	-1	1.44876900	0.59956600	-2.46639800
C	-1	1.82940600	0.35603400	-3.79625800
C	-1	2.81402900	1.12282500	-4.42284400
C	-1	3.41684300	2.15888400	-3.68701500
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C	-1	0.53053600	-0.37665400	-1.83542600
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C	-1	-4.37792100	3.05864600	0.68936400
C	-1	-5.24464300	4.15143200	0.61020200
C	-1	-4.69306700	5.41490700	0.33451500
C	-1	-4.78500900	-0.31773500	-1.18179600
C	-1	-2.18286700	1.96373800	0.43093100
C	-1	0.17563900	-1.14890700	2.88403800
C	-1	0.36181200	-2.52492000	2.57409700
C	-1	1.48191400	-2.88823100	4.71752200
C	-1	1.20332600	-1.55015100	5.05218800
C	-1	0.56305200	-0.69672900	4.16762200
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C	0	4.26284500	0.13251400	1.88132000
C	0	3.17853300	-1.87119400	0.72920500

C	0	4.45938400	-2.17113900	-0.02876600
H	0	2.00172600	-3.54307600	5.40685800
H	-1	1.32655400	-0.45107300	-4.32913300
H	-1	3.52193300	3.22993400	-1.81363800
H	-1	-4.75923500	2.05830400	0.89639100
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H	-1	0.34518400	0.33644300	4.43636100
H	0	2.99724900	-2.73880000	1.37003100
H	0	2.34456900	-1.81520700	0.02030600
H	0	4.84725000	-0.00048000	-0.01050800
H	0	5.30233300	-2.22226200	0.66734500
H	0	2.71185700	-0.87722300	2.48363900
C	0	7.22253200	-1.25363800	-1.00755700
N	-1	3.15224500	-0.67171600	1.59501800
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H	0	3.11082000	0.92060300	-5.44616000
H	-1	4.22107500	2.73205400	-4.15042400
H	-1	-5.36301500	6.26816500	0.21869500
O	-1	1.28501100	4.79160300	-1.21931600
H	0	0.81838300	5.58036100	-0.91394400
C	-1	-3.32622800	5.59563400	0.19237800
H	0	1.63810100	3.25299000	3.64101200
H	-1	-2.90513800	6.57670100	-0.02527700
H	0	1.06821600	-4.52846200	1.49318300
H	0	-3.54573100	-5.76897100	-0.67140000
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Cu-(D) Intermediate from VASP

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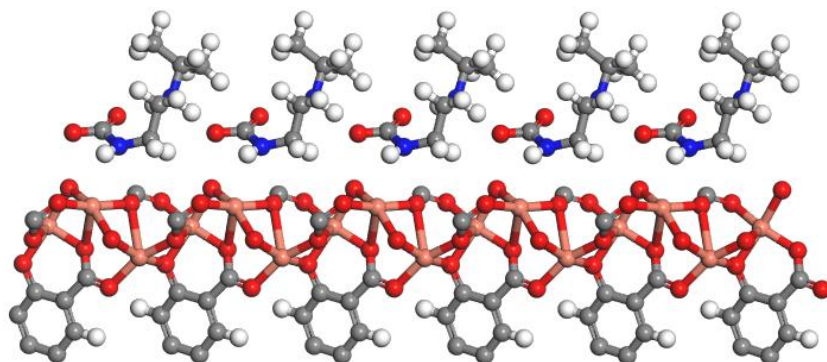
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0.3009547153977437	0.5904147801976052	0.3117087405529873
0.2952813990703547	0.6239493798058433	0.8775066948179884
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Cu-(E) TS<sub>2</sub>

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6 20 48 32 2

Direct

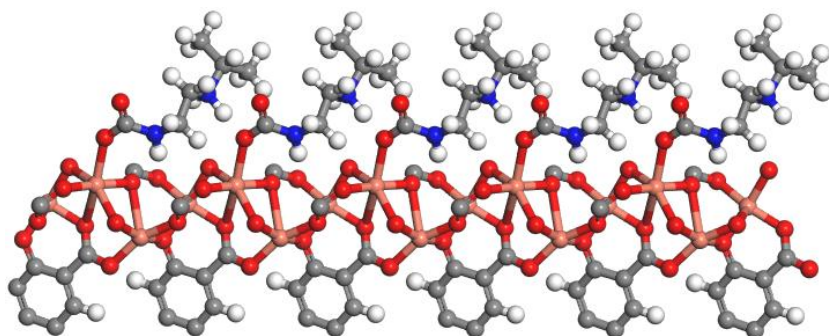
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Cu–(F) Product

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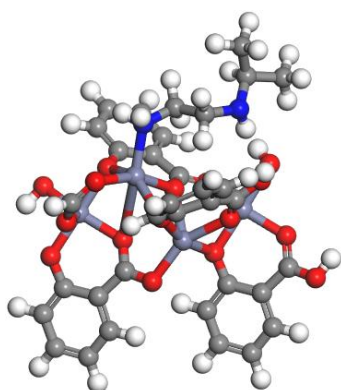
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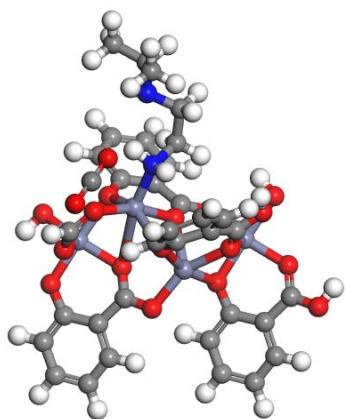
## Zn-(A) i-2-MOF

-1 1

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O	0.14734000	2.47715300	-1.01193100
O	-2.38891200	3.85450000	-1.29717500
O	-2.41809900	5.76185200	-0.17168100
O	-1.72531200	1.70952100	0.78220800
O	-3.85134100	1.33495900	1.38060100
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C	0.58368400	3.74937300	-0.92965300
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C	0.28797700	6.14209200	-0.51684600
C	1.65428000	6.37782800	-0.66843000
C	2.47768000	5.28346000	-0.98713000
C	1.96252500	4.00241000	-1.11341000
C	-1.75437600	4.79947900	-0.69070600
C	-2.18005800	0.50435600	2.82643600
C	-3.14145200	0.37756200	3.84428500
C	-2.60448500	1.21620700	1.58897900
C	-3.79184000	-2.00363500	0.67660700
H	-3.60034900	-0.30193800	5.84546100
C	-5.61246400	-1.89999100	-1.00504700
C	-6.46290100	-2.96023000	-0.31423600
C	-6.49157400	-0.85735900	-1.68665200
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H	-4.29800100	-0.41489500	-0.51824500
H	-3.16567200	-1.32141600	1.26176000
H	-4.31181300	-2.63197100	1.41387700
H	-5.02221700	-2.40753900	-1.79288900
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H	-5.85663800	-3.76014600	0.12310200
H	-7.14896600	-3.42256100	-1.03073300
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H	-7.06963400	-1.30319200	-2.50182500
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N	-4.75486800	-1.20410900	-0.04995300
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O	-0.02378000	-0.18868700	2.00990500
O	2.97576100	-2.48763700	1.84699600
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C	0.47125500	-2.90741700	-1.87889800
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C	-0.65487000	-0.59507400	-1.83935100
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C	4.98905000	1.94493400	0.54794200
C	6.35535300	2.18067000	0.39635700
C	7.17875200	1.08630200	0.07765700
C	6.66359700	-0.19474800	-0.04862200
C	2.94669700	0.60232100	0.37408100
C	-0.88502000	-0.05917700	3.01127800
H	2.45741500	-3.42317200	3.59652100
C	-2.84563400	-0.21378100	5.07293700
C	-1.52767300	-0.66110400	5.28270200
C	-0.56715200	-0.58236600	4.28576800
C	2.09651500	-2.98088500	2.65375100
C	-2.85648400	-2.89827400	-0.14062300
H	-2.02098300	-3.63146500	1.58819000
H	-1.20635400	-1.17203900	-4.30429700
H	1.22709400	-4.91007200	-2.14218800
H	4.30843700	2.76145500	0.79171400
H	2.60737400	3.16298300	-1.37301100
H	-1.26067400	-1.07862500	6.25530700
H	0.45096300	-0.93363300	4.45427000
H	-2.48487900	-2.35830200	-1.01427600
H	-3.38709000	-3.78580400	-0.50418500
H	-1.24561700	-4.11080400	0.25499200
N	-1.69260700	-3.30161000	0.68183700
H	-0.84929200	-3.30699300	-5.57565000
H	0.35355200	-5.17961500	-4.43988300
H	8.24365300	1.25582800	-0.09246200
H	4.51052500	-3.77518800	-1.24852700
H	7.30837400	-1.03410900	-0.30824000
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H	-3.36314400	5.61048300	-0.33989900
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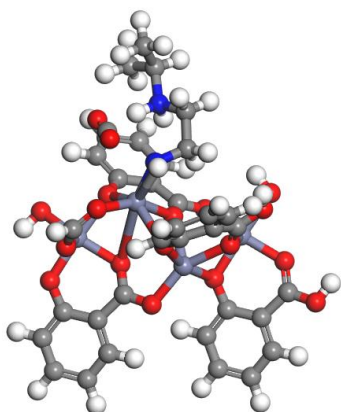
Zn-(B) Complex

-1 1

H	-7.96763600	-1.52611200	1.03385800
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O	-0.69885700	-4.22067500	-2.16718300
O	-3.00849900	-1.14593500	-0.74469600
O	-3.27189100	-3.99630100	-1.14795100
O	-4.72922000	-4.92713600	0.24002500
O	-1.15570500	-2.57870200	0.55242000
O	0.08327200	-4.42739800	0.78738600
H	-0.04508200	-3.78705300	-2.72683800
C	-4.28032300	-1.30089900	-0.32784900
C	-4.87005100	-2.56416900	-0.02359500
C	-6.17728900	-2.60996100	0.49059900
C	-6.95543600	-1.46430000	0.65100100
C	-6.38546800	-0.23078100	0.28494500
C	-4.23672500	-3.87788100	-0.30668900
C	1.28563100	-3.51970500	3.06338500
C	-0.20816600	-3.23768900	1.12628800
H	2.58577500	-3.79130700	4.77042800
C	7.87579400	-0.74482600	-1.21567500
H	-6.57196300	-3.59044000	0.75988000
H	1.27265000	-4.57450200	2.78652100
H	4.54328200	-2.97655000	-1.98453200
H	5.50118500	-0.79533500	-1.88573600
H	7.06558800	-2.70310700	-1.52714400
H	7.75055800	-0.42758100	-2.25690300
H	8.90605000	-1.08983700	-1.09182900
H	-5.75044800	4.55537100	1.94410000
H	-6.98988400	0.67573400	0.35552600
Zn	0.36133800	3.44829100	-0.61115600
Zn	-1.52888500	-0.48183100	0.52534600
Zn	1.47504900	0.54919000	0.22481800
O	1.55530200	1.82551800	-1.30842800
O	0.03951400	-0.44400900	-0.98538400

O	-0.84869000	-1.31721200	-2.82300900
O	-0.78982100	4.93320600	0.16653800
O	-1.05100200	2.08046400	-0.21221700
O	-2.51052200	1.15210400	1.15126800
O	0.13953800	-0.32862800	1.66830100
O	1.06294000	3.50044400	1.46369100
O	2.41426700	1.69635200	1.68204800
O	4.08577600	1.50613400	4.23356400
O	4.86808500	0.07390500	2.56995100
C	1.54251200	1.49563000	-2.60035500
C	0.76189200	0.41630000	-3.11362400
C	0.78780600	0.13562400	-4.49139300
C	1.59209000	0.84598000	-5.38024000
C	2.37552500	1.89267100	-4.85683000
C	2.34833400	2.21352900	-3.51169400
C	-0.04156900	-0.50152700	-2.27334600
C	-2.06162600	4.77834200	0.58340000
C	-2.65134800	3.51507200	0.88765500
C	-3.95859000	3.46927700	1.40185100
C	-4.73673800	4.61493800	1.56225300
C	-4.16680300	5.84836500	1.19618300
C	-5.08588400	-0.14672100	-0.18835100
C	-2.01806800	2.20126400	0.60456300
C	0.62850600	-1.23051800	2.50784800
C	0.55917500	-2.63206200	2.25101800
C	2.03104800	-3.08844000	4.16042200
C	2.01456600	-1.71122500	4.45725200
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C	2.01055400	2.84158100	2.03747400
C	4.45635800	0.79798900	3.38570300
C	3.12626900	-1.65780200	-1.03516700
C	4.48465400	-2.33986800	-1.08568600
C	6.89009500	-1.84636800	-0.85028300
C	7.11586100	-2.31752700	0.58217700
H	0.14268000	-0.66822800	-4.84804200
H	2.97229800	3.01415400	-3.11425200
H	-4.35326400	2.48879900	1.67113300
H	-4.65653800	0.81253200	-0.47718500
H	2.54941300	-1.35409700	5.33949700
H	1.32091200	0.25768800	3.89697600
H	2.31664700	-2.39166300	-1.05190600
H	2.99959900	-1.01485600	-1.91308300
H	3.89033200	-0.33476500	0.27767600
H	4.58116500	-3.00493100	-0.21995300
H	2.93485600	-1.42267600	0.98573400
H	7.72463900	0.12845700	-0.57178300

H	8.13686600	-2.69339200	0.69997000
H	6.43531200	-3.12593300	0.86554500
H	6.96705600	-1.48707300	1.28012900
N	2.99373800	-0.81633700	0.16871000
N	5.52886900	-1.32865400	-1.01981600
H	1.60782800	0.60564100	-6.43770800
H	3.03874900	2.44334900	-5.52675800
H	-4.77118600	6.75497300	1.26677900
O	1.30594600	4.76073000	-1.86782200
H	0.97360400	5.58102200	-1.48596200
C	-2.86718400	5.93251700	0.72290200
H	2.49808300	3.29413200	2.91526100
H	-2.43787300	6.89167900	0.43405300
H	-4.25608600	-5.70268400	-0.10438200
H	0.90995800	-4.72930200	1.18526000



Zn-(C) TS<sub>1</sub>

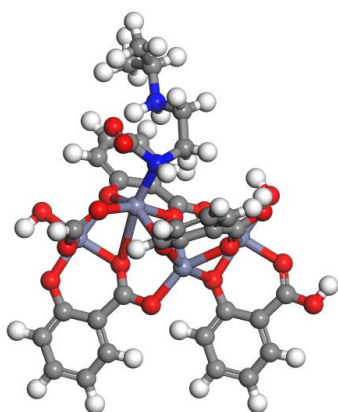
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O	-2.85416200	-0.90239300	-1.09757300
O	-3.30606300	-3.73274000	-1.47369100
O	-5.12817000	-4.45489900	-0.43679600
O	-1.50104100	-2.43394000	0.63204600
O	-0.54218400	-4.37520200	1.19777100
H	0.19848500	-3.90359900	-2.27163900
C	-4.19652800	-0.91832400	-0.98293800
C	-4.96499000	-2.10505000	-0.78967100
C	-6.35278000	-2.00431300	-0.59154500
C	-7.02680400	-0.78513300	-0.64697200
C	-6.26639500	0.37076000	-0.90411000
C	-4.42024600	-3.48407300	-0.88258200
C	0.19496700	-3.47050400	3.66513300
C	-0.78115000	-3.14830100	1.42756900
H	1.03451500	-3.77612600	5.63498700
C	6.11246700	-0.86944300	-2.73439000



H	-6.89573000	-2.92955800	-0.39470600
H	0.13867200	-4.53203900	3.42142500
H	3.95376600	-3.69914700	-0.73664600
H	3.83947800	-1.49753200	-1.72247100
H	5.68195500	-2.92873600	-2.28194900
H	5.28827400	-0.75575100	-3.44426500
H	7.01860500	-1.09527900	-3.30123500
H	-5.54511200	5.15463100	0.72639100
H	-6.77593000	1.33160500	-1.00013000
Zn	0.84406800	3.36192800	-0.31059600
Zn	-1.64378600	-0.31547600	0.46251000
Zn	1.54625700	0.31993700	0.86837500
O	1.94122900	1.59749100	-0.63801700
O	0.18149600	-0.50284200	-0.61759900
O	-0.37821100	-1.36862900	-2.58515000
O	-0.29758600	4.98358500	0.13856000
O	-0.76572100	2.16119900	-0.23241200
O	-2.57155400	1.43116900	0.79935600
O	-0.30782400	-0.25628200	1.97817600
O	1.05553500	3.45203800	1.86817900
O	2.13987300	1.55052000	2.45065200
O	4.70253800	-0.21152600	3.06061500
O	5.21301400	0.41967500	0.88201900
C	2.17151600	1.21894200	-1.89030900
C	1.42333400	0.19213400	-2.54115600
C	1.73423800	-0.15782300	-3.86727300
C	2.78777600	0.43018600	-4.56428700
C	3.53309500	1.42474500	-3.90198400
C	3.23246200	1.81317000	-2.60899000
C	0.36063200	-0.60470000	-1.88557000
C	-1.63991300	4.96774400	0.25321500
C	-2.40837300	3.78101800	0.44648300
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C	-3.70981900	6.25673800	0.33202300
C	-4.89146700	0.31081800	-1.06527700
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C	-0.23326400	-2.56101500	2.68277300
C	0.71027400	-3.05596800	4.89303600
C	0.76615400	-1.67008000	5.14061000
C	0.37574500	-0.74720200	4.18386200
C	1.77546600	2.73776700	2.66372000
C	4.80452900	0.01886400	1.91772000
C	2.71813700	-2.35968600	0.47522800
C	4.04668300	-2.79184400	-0.13342800

C	5.85573100	-1.99155200	-1.74407400
C	6.99223700	-2.16206900	-0.75099300
H	1.10942100	-0.91537100	-4.34191900
H	3.82715300	2.57149000	-2.09950200
H	-4.33911500	2.95651000	0.84144600
H	-4.31263300	1.21078100	-1.27251700
H	1.11903400	-1.32049400	6.11283600
H	0.42174500	0.32421000	4.38174700
H	2.38347200	-3.20702000	1.08926700
H	1.98373400	-2.28240200	-0.34086200
H	4.65146300	-0.85896100	-0.44720300
H	4.79397300	-2.95011400	0.64571600
H	2.75865000	-1.35510000	2.21488200
H	6.26251500	0.08559200	-2.22095800
H	7.91767100	-2.32116800	-1.30929200
H	6.85400000	-3.02336100	-0.09414400
H	7.11762700	-1.26356100	-0.13914200
N	2.81261000	-1.12050200	1.22976000
N	4.55965000	-1.71081800	-1.02500900
H	3.01926600	0.13812800	-5.58286400
H	4.38392700	1.87785700	-4.41451700
H	-4.21931500	7.21767400	0.23602300
O	2.17840400	4.51743900	-1.34899700
H	1.85485600	5.38215600	-1.07213100
C	-2.33485100	6.19688600	0.17087600
H	2.08493900	3.19791400	3.61843700
H	-1.75605700	7.09676000	-0.03638400
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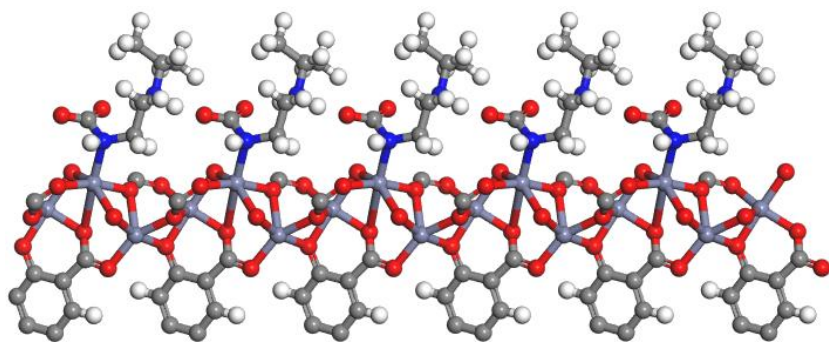


Zn-(D) Intermediate from Gaussian

-1 1			
H	-8.06462900	-0.83248200	-0.71498300
Zn	-1.62802500	-2.53971000	-1.57874800
O	-0.49033300	-4.24480900	-1.86763800
O	-2.80202100	-0.93370700	-1.15732400
O	-3.20772900	-3.76823500	-1.55405800

O	-5.04912400	-4.51627100	-0.57098200
O	-1.47907200	-2.45383800	0.60539100
O	-0.51231700	-4.38483600	1.19240400
H	0.31780100	-3.89809400	-2.26188100
C	-4.14677700	-0.96667400	-1.08061200
C	-4.90547400	-2.16346300	-0.91244800
C	-6.29944200	-2.08060300	-0.75322900
C	-6.98683200	-0.86971700	-0.82417000
C	-6.23400000	0.29634400	-1.05649400
C	-4.34113000	-3.53531200	-0.99388200
C	0.14372500	-3.47892400	3.68211900
C	-0.77298000	-3.16173600	1.41885700
H	0.93371700	-3.78021900	5.67281000
C	6.42526700	-0.71614500	-2.72450200
H	-6.83610500	-3.01314200	-0.57439600
H	0.10759000	-4.54029400	3.43391000
H	4.14782500	-3.49654200	-0.78009700
H	4.12476900	-1.33217700	-1.84638900
H	6.06846100	-2.76347100	-2.16927200
H	5.65233400	-0.68954300	-3.49835900
H	7.38094900	-0.93032600	-3.20843300
H	-5.61862500	5.08328900	0.60797600
H	-6.75260700	1.25108900	-1.16410900
Zn	0.81898100	3.37368400	-0.25433300
Zn	-1.64346800	-0.33678100	0.43791200
Zn	1.43054200	0.42669000	0.94571800
O	1.95196800	1.61997200	-0.54965600
O	0.22651100	-0.51077500	-0.58288000
O	-0.27954500	-1.36441100	-2.57584600
O	-0.35505200	4.97959700	0.16706900
O	-0.76502200	2.14417900	-0.20292800
O	-2.60211800	1.39712400	0.75343100
O	-0.32003000	-0.26669700	1.97379700
O	0.96789700	3.45946600	1.92978300
O	2.02891800	1.55532700	2.54285000
O	4.29668000	-0.52396900	3.02080700
O	4.75236400	0.06021000	0.89476800
C	2.21705900	1.25239900	-1.80208100
C	1.50039000	0.21845800	-2.47666700
C	1.85284800	-0.12337900	-3.79448200
C	2.91815200	0.47988800	-4.45985600
C	3.63203900	1.48151000	-3.77399100
C	3.29029900	1.86204600	-2.48888600
C	0.42970500	-0.59359900	-1.85355600
C	-1.69977100	4.94672000	0.24380100
C	-2.45846700	3.74993100	0.41196700

C	-3.85243500	3.83279200	0.57118500
C	-4.53982600	5.04367700	0.50024200
C	-3.78703100	6.20964900	0.26789800
C	-4.85443900	0.25399800	-1.17901600
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C	-0.14144000	-1.17048400	2.92668700
C	-0.26802600	-2.57169600	2.69066500
C	0.61904300	-3.06193800	4.92522900
C	0.65059800	-1.67626000	5.17821100
C	0.27576300	-0.75525500	4.21346300
C	1.67402800	2.75165800	2.74326900
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C	2.86991300	-2.19747200	0.33638900
C	4.23929300	-2.57230000	-0.20469200
C	6.14050400	-1.78463100	-1.68235500
C	7.19796800	-1.82196600	-0.59023300
H	1.25116000	-0.88711200	-4.28869700
H	3.86088500	2.62606600	-1.96069000
H	-4.38909900	2.90025200	0.75001600
H	-4.28130000	1.16173700	-1.36730600
H	0.97157500	-1.32542000	6.16098400
H	0.30277400	0.31600800	4.41560500
H	2.45873100	-3.10989700	0.77297300
H	2.21283700	-1.93831900	-0.49654600
H	4.80441500	-0.65434200	-0.42493100
H	4.95463600	-2.73788400	0.60235300
H	2.45231800	-1.55349800	2.23236700
H	6.49018900	0.27541500	-2.26537600
H	8.18134600	-1.91700400	-1.05654200
H	7.07546600	-2.67102600	0.08636100
H	7.18238100	-0.89952000	-0.00207400
N	2.80444000	-1.12735600	1.37858700
N	4.78846800	-1.51397300	-1.08979900
H	3.18246600	0.19277300	-5.47163900
H	4.49122700	1.94678700	-4.26105300
H	-4.30560000	7.16448400	0.16030400
O	2.16746100	4.54898400	-1.25143200
H	1.83626500	5.40827300	-0.96676000
C	-2.40743200	6.16739200	0.14539800
H	1.97851600	3.21163600	3.69713800
H	-1.83433100	7.07504200	-0.04291300
H	-4.57538400	-5.34196700	-0.76527700
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Zn-(D) Intermediate from VASP

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Direct

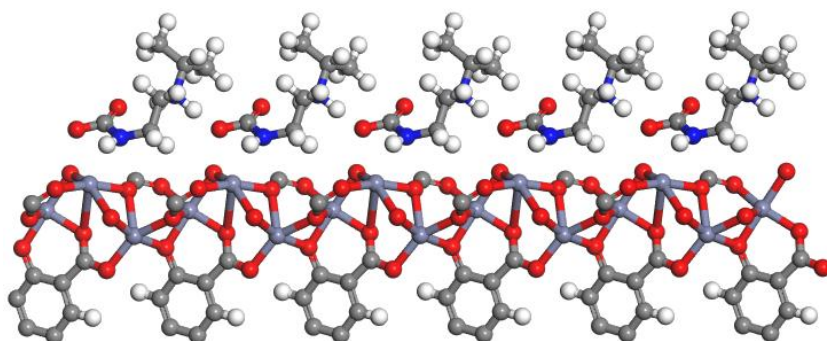
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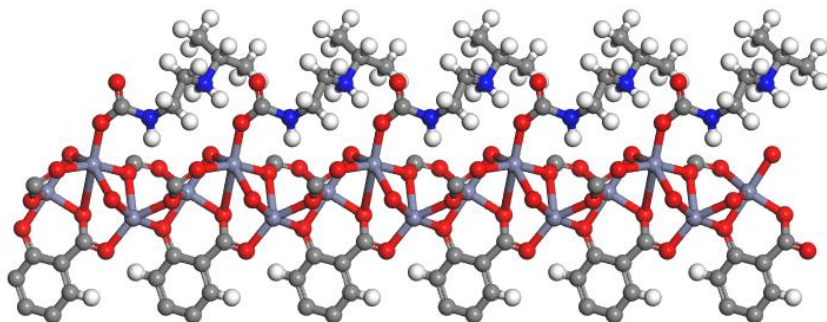
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Direct

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