

Effect of axial molecules and linkers length on CO₂ adsorption and selectivity of CAU-8: A combined DFT and GCMC simulations study

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Section S1: Computational Details

Lenard-Jones 6-12 terms of potential combined with Coulomb electrostatic potential

$$U(r_{ij}) = 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{r_{ij}}, \quad (1)$$

where ε_0 is the dielectric constant of vacuum, r_{ij} is the distance between atom i and atom j , q_i is the partial electric charge of atom i .

The parameters ε_{ij} and σ_{ij} are respectively the depth and the diameter of Lenard-Jones potential well, and these are totally determined via Lorentz-Berthelot mixing rules given as follows

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}, \sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j) \quad (2)$$

Table S1. LJ potential parameters for gases and frameworks in this work. The charges of gases are provided.

	E/k (K)	σ (Å)	q (e)
N_n2	93.980	3.572	0.000
C_co2	29.660	2.789	0.576
O_co2	82.960	3.011	-0.288
CH4_sp3	148.000	3.730	0.000

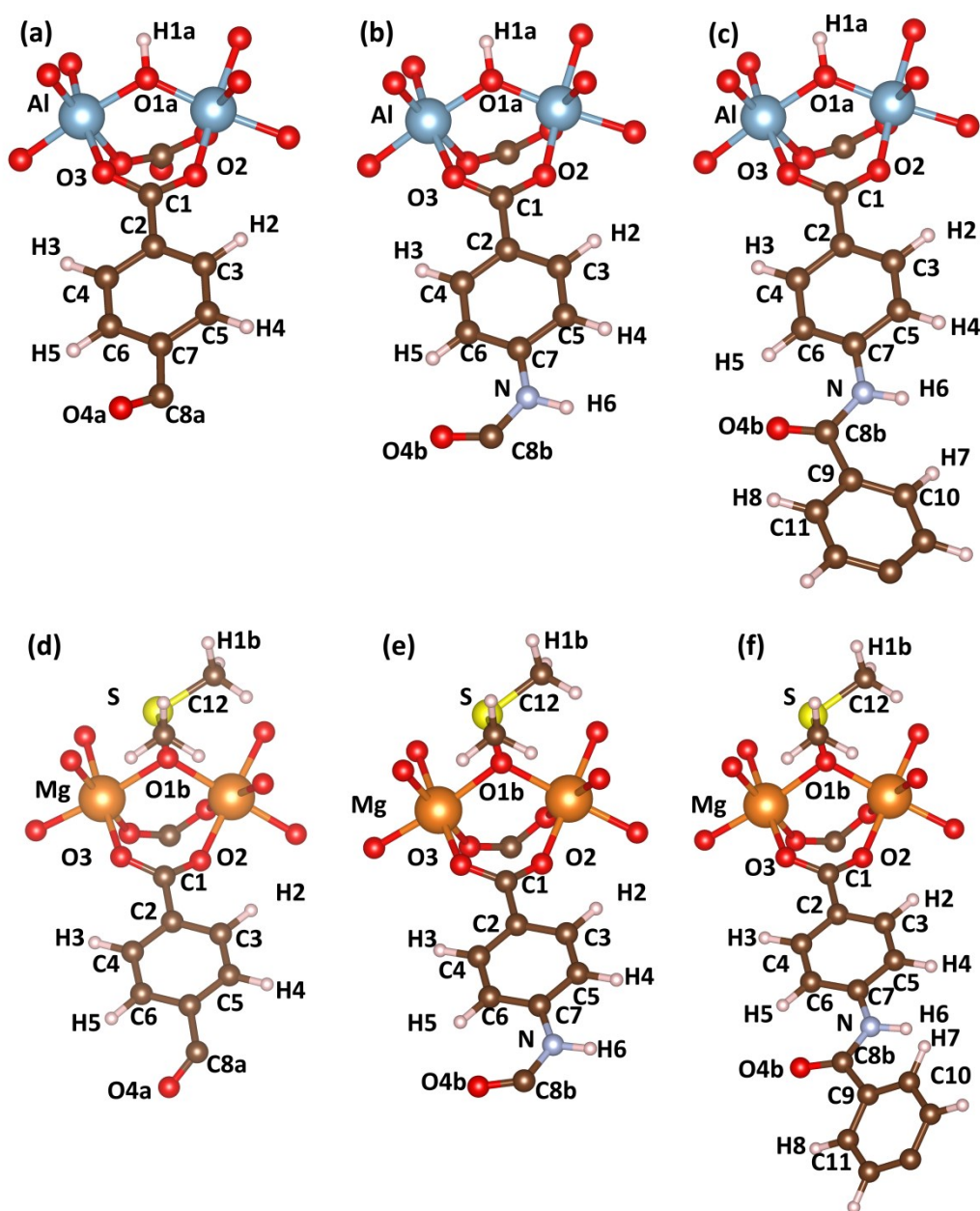


Figure S1. Atomic structure of unit framework of (a) CAU-8(Al), (b) **1a**, (c) **1b**, (d) CAU-8(Mg), (e) **2a**, and (f) **2b** with the labels used for force field sites.

Table S2. Lennard-Jones parameters used for six MOFs.

	E/k (K)	σ (Å)	Reference
Al	-	-	S1
Mg	-	-	-
O1a	93.00	3.02	S2
O1b	176.00	2.83	S3
O2, O3	55.00	2.80	S4
O4a	79.00	3.05	
O4b	79.00	3.05	
C1	20.00	3.85	S6
C2, C7, C9	21.00	3.88	S7
C3, C4, C5, C6, C10, C11	50.50	3.69	
C8a	40.00	3.82	S4
C8b	34.00	3.72	S5
C5	125.00	3.81	S3
N	111.00	3.34	S5
H_	-	-	-
S	2.14	3.47	S3

Table S3. CHELPG charge used for six MOFs.

	CAU-8(Al)	1a	1b	CAU-8(Mg)	2a	2b
Al	1.596	1.578	1.575	-	-	-
Mg	-	-	-	1.269	1.266	1.247
O1a	-0.804	-0.804	-0.810	-	-	-
O1b	-	-	-	-0.471	-0.474	-0.467
O2	-0.644	-0.712	-0.711	-0.729	-0.707	-0.703
O3	-0.672	-0.604	-0.604	-0.667	-0.694	-0.699
O4a	-0.410	-	-	-0.420	-	-
O4b	-	-0.471	-0.471	-	-0.477	-0.478
C1	0.740	0.727	0.718	0.748	0.748	0.740
C2	-0.076	-0.113	-0.110	-0.051	-0.095	-0.079
C3	-0.092	-0.007	-0.006	-0.099	-0.019	-0.033
C4	-0.061	-0.055	-0.047	-0.091	-0.071	-0.084
C5	-0.028	-0.317	-0.339	-0.042	-0.314	-0.319
C6	-0.106	-0.224	-0.242	-0.092	-0.226	-0.228
C7	0.005	0.429	0.457	0.007	0.423	0.427
C8a	0.359	-	-	0.354	-	-
C8b	-	0.483	0.568	-	0.482	0.572
C9	-	-	-0.047	-	-	-0.048
C10	-	-	-0.107	-	-	-0.108
C11	-	-	-0.058	-	-	-0.066
H1a	0.405	0.403	0.405	-	-	-
H1b	-	-	-	0.116	0.119	0.113
H2	0.113	0.097	0.095	0.112	0.097	0.099
H3	0.095	0.103	0.099	0.104	0.105	0.116
H4	0.040	0.159	0.156	0.038	0.153	0.148
H5	0.114	0.156	0.164	0.103	0.151	0.156
H6	-	0.300	0.290	-	0.301	0.288
H7	-	-	0.103	-	-	0.103
H8	-	-	0.096	-	-	0.096
N	-	-0.541	-0.588	-	-0.545	-0.580
S	-	-	-	0.290	0.298	0.286

Section S2: Reaction Mechanism

Al-H₂BPDC initial

0 1

Al	-4.92526900	0.37984600	-0.24735500
Al	-1.72185000	-0.02286900	0.34838300
O	-3.38947000	0.55361900	0.79843800
O	-5.00224100	2.26228700	-0.33639000
N	-5.86224800	3.06449900	-0.99390600
O	-5.72345400	4.25726800	-0.84613900
N	0.22102800	1.75053900	1.67443900
O	0.61349400	2.89481400	1.63257000
O	0.91628200	0.81297600	2.16961300
O	0.39442600	-1.56326600	2.61347300
H	0.47122300	-0.52449200	2.34419200
O	-6.74314700	2.53639200	-1.72018900
H	-6.67001100	0.92248900	-1.70179500
O	-5.91886700	0.20228400	1.34849900
O	-0.98883800	1.48398000	1.21672300
O	-1.72594800	-1.11280700	2.06286600
O	-7.75368100	-0.82758500	0.58251300
O	-3.80178000	0.38195600	-1.90752600
O	-1.69900700	0.88251800	-1.35121600
N	-2.71240200	0.99747600	-2.18336900
O	-2.56974400	1.63280700	-3.19696400
H	-3.46910000	1.20696500	1.51161400
N	-0.88674000	-1.93828800	2.55760100
O	-1.18686400	-3.01676700	2.98554000
N	-7.09977600	-0.39867500	1.57095100
O	-7.46644900	-0.49101100	2.72040300
O	-6.36063800	0.00440300	-1.40483000
H	-7.06994800	-0.38582900	-0.78908300
O	-0.07567700	-2.78183000	-0.95171500
C	0.56881200	-1.68821400	-0.61382800
O	-0.01894300	-0.68733200	-0.10500400
C	2.01265500	-1.66429900	-0.83110900
C	2.71395800	-2.85687600	-1.10963900
C	2.68578800	-0.42883600	-0.76370100
C	4.08950100	-2.81166500	-1.29136300
H	2.17286300	-3.80177700	-1.17258900
C	4.06762000	-0.40080300	-0.94367700
H	2.11828600	0.49817200	-0.63280600
C	4.78065800	-1.58890000	-1.18656500
H	4.65974800	-3.71235000	-1.52370300
H	4.59130300	0.55621000	-0.92205800
O	6.72041200	-2.42182800	-2.24936300
C	7.15061000	-0.61014200	-0.77435000
C	6.83950500	-0.05578800	0.48249800
C	8.37856100	-0.29556300	-1.38610100
C	7.73691000	0.80794100	1.10722100
H	5.90748200	-0.32229000	0.98390200
C	9.26607600	0.58368900	-0.77339900

H	8.61185000	-0.75846200	-2.34651600
C	8.94685900	1.13983900	0.47861500
H	7.52356500	1.24032800	2.08620700
H	10.21114200	0.84352800	-1.25084300
C	9.86011200	2.08135100	1.18954700
O	10.99954700	2.33291000	0.48628300
O	9.63137400	2.57995200	2.27654600
H	11.51327800	2.95229700	1.04157300
C	6.26259300	-1.59916800	-1.46000400
N	-3.58643400	-2.31141800	-0.36503200
O	-4.63241300	-1.62253500	-0.22547600
O	-3.58751400	-3.51548400	-0.43725700
O	-2.41135500	-1.67696200	-0.46662700
O	0.95289400	2.21263800	-1.24997700
H	0.07597000	1.95828300	-1.59063200
H	0.76853000	2.98088000	-0.68442300
H	-1.05811500	-2.62614900	-0.79439800

Al-H₂BPDC TS

0 1

Al	3.33515800	-1.14208900	0.38265100
Al	1.16691000	1.39659300	0.14827000
O	2.84174800	0.69154500	0.30499200
O	2.86487300	-1.12575800	2.23112700
N	3.26892600	-1.95412400	3.20705900
O	3.08686900	-1.59674300	4.34999000
N	1.46146300	3.66869200	2.05591000
O	2.16586700	4.23814800	2.84717800
O	0.49857900	4.28915200	1.42295200
O	0.85521100	5.03509900	-1.09861500
H	0.87666200	4.91697900	-0.08764200
O	3.79288900	-3.05228600	2.88324400
H	3.76747000	-3.26222300	1.27787400
O	5.09861900	-0.61702400	0.78633800
O	1.62258000	2.39885900	1.81028700
O	1.88459700	3.10296300	-0.73266200
O	6.11635000	-2.21958700	-0.38759200
O	1.34692300	-1.59944100	0.13072200
O	0.19744700	0.05058500	1.08178700
N	0.39727700	-1.24511100	0.91236000
O	-0.34642200	-2.02741400	1.44270100
H	3.46354200	1.20285600	0.85170200
N	1.33848900	3.85584400	-1.59149600
O	1.24174400	3.66121500	-2.76284400
N	6.20943100	-1.11661400	0.20980600
O	7.22953900	-0.47633800	0.31859500
O	3.71231500	-3.00309400	0.29941700

H	4.65924800	-2.98502600	-0.04537900
O	0.98574200	-0.75342000	-3.20973300
C	0.35823900	-0.21026200	-2.23716400
O	0.84015100	0.77665800	-1.58519200
C	-0.97212600	-0.77733100	-1.91057000
C	-1.16997500	-2.16773900	-2.00771500
C	-2.01691500	0.06153000	-1.48840600
C	-2.39457800	-2.71368300	-1.63898800
H	-0.34599800	-2.80080600	-2.33879600
C	-3.25137100	-0.48906200	-1.14694600
H	-1.86167800	1.14117400	-1.46658200
C	-3.44132800	-1.88109900	-1.20387600
H	-2.57186000	-3.79022300	-1.67230000
H	-4.07505800	0.15563800	-0.83417000
O	-4.91041500	-3.72659300	-0.87600600
C	-5.83840100	-1.60951900	-0.30504900
C	-5.95951100	-1.35665800	1.07114600
C	-6.75565700	-1.04606600	-1.20542800
C	-6.98986500	-0.54353300	1.54008700
H	-5.24836900	-1.80230000	1.77027700
C	-7.78942600	-0.23491100	-0.73451500
H	-6.66275100	-1.24924400	-2.27470900
C	-7.90765200	0.02251000	0.64089500
H	-7.10780000	-0.33276000	2.60458200
H	-8.50962800	0.20181400	-1.42699000
C	-8.98427400	0.88655400	1.20081000
O	-9.82414500	1.36538600	0.23872100
O	-9.11865100	1.15195000	2.38185400
H	-10.48117700	1.90640400	0.71965500
C	-4.74196400	-2.51709500	-0.80725300
N	3.92433000	-0.21102200	-2.27956900
O	3.37006500	-1.15692700	-1.55234300
O	4.95895700	0.33160200	-1.95888300
O	3.30669700	0.07673500	-3.35827900
O	-0.55914400	2.34728700	0.20215600
H	-1.21535200	1.78148600	0.65026700
H	-0.38141500	3.17961400	0.77330000
H	2.02477600	-0.39788800	-3.28299600

Al-H₂BPDC final

0 1

Al	3.16146900	-0.90355700	0.47631500
Al	2.12872900	2.14143000	0.05565100
O	3.25482100	0.77832100	-0.36737300
O	4.91750300	-0.51135200	1.11035500

N	5.60128100	-1.00912600	2.15793800
O	6.66734900	-0.49541100	2.41547800
N	3.64493400	4.46697800	-0.97332100
O	4.66922700	4.87523100	-1.45358600
O	2.52044100	5.11285700	-1.08749000
O	0.65978100	4.28366100	-2.79576500
H	1.48869800	4.64818700	-2.33503600
O	5.09986000	-1.96506700	2.80338600
H	3.72939500	-2.47579000	2.12557600
O	3.72507700	-1.68494100	-1.14219700
O	3.63215300	3.35078100	-0.29167500
O	1.70246200	2.51024400	-1.95119000
O	3.79675700	-3.85286800	-0.59550000
O	2.45900400	-0.01408100	2.19110500
N	2.60178100	1.14352200	2.70772400
O	2.45121400	2.20438400	1.92828900
O	2.82200000	1.31182300	3.87961600
H	4.16892000	1.01343000	-0.60142200
N	0.64587900	2.95364400	-2.47900400
O	-0.33317600	2.33116900	-2.76224600
N	4.11340800	-2.94353900	-1.40920900
O	4.72654600	-3.12965800	-2.43458600
O	2.96892700	-2.50666900	1.45589200
H	3.18518300	-3.23740200	0.79093900
O	1.28715200	-1.04315100	-0.02884900
C	0.36443300	-0.16091600	0.01040700
O	0.58830600	1.10054500	0.12534400
C	-1.04584900	-0.59705800	-0.06487100
C	-1.37990200	-1.94258300	0.18151600
C	-2.05161300	0.33456900	-0.37637700
C	-2.70883900	-2.34682700	0.10794100
H	-0.59824500	-2.65734300	0.44470400
C	-3.38196100	-0.07400200	-0.43594700
H	-1.77514900	1.36863500	-0.58338500
C	-3.72214700	-1.41706100	-0.18622100
H	-2.98855400	-3.38837700	0.27453000
H	-4.15948300	0.64387700	-0.70233100
O	-5.32514600	-3.07958400	-0.70187200
C	-6.28166300	-1.02721400	0.00916200
C	-6.18782800	0.00084000	0.96686800
C	-7.51850800	-1.28654900	-0.60950100
C	-7.30882000	0.76466700	1.28577200
H	-5.24336700	0.18135300	1.48339000
C	-8.63398200	-0.51054500	-0.30831300
H	-7.57684400	-2.10893200	-1.32468900
C	-8.53192300	0.52150100	0.64196700

H	-7.26464800	1.55752100	2.03442500
H	-9.59041200	-0.69733300	-0.79725100
C	-9.69124600	1.38354200	1.01192500
O	-10.82586200	1.05118700	0.33480000
O	-9.65002200	2.28955100	1.82495000
H	-11.50859600	1.67279500	0.65622500
C	-5.13115000	-1.92879000	-0.31979700
N	0.84481200	-4.41382000	-1.33230200
O	0.78341300	-4.42149500	-0.10947500
O	0.77150000	-5.32478000	-2.11371100
O	1.02130700	-3.13643300	-1.94560900
O	0.99007400	3.70237700	0.37481300
H	0.82735300	3.84577500	1.32392700
H	1.49448900	4.49108300	-0.01785200
H	1.09465300	-2.50801600	-1.18048800

Al-H₂ODA initial

0 1

Al	-6.28671300	0.24687200	-0.55325200
Al	-3.19517000	-0.04312800	0.51438300
O	-4.98546700	0.17008500	0.78142800
O	-6.64860400	2.01659000	-0.00540100
N	-7.51536100	2.91859300	-0.50424500
O	-7.59481800	3.98088200	0.06991700
N	-1.81511800	1.29852800	2.74462100
O	-1.61677700	2.40953800	3.18426000
O	-1.06426800	0.31603300	3.02097100
O	-1.24659300	-2.09893400	2.50288100
H	-1.29986100	-1.03409900	2.62519800
O	-8.17840600	2.61416900	-1.52906600
H	-7.84767900	1.12149000	-2.05491500
O	-7.48536000	-0.58816900	0.64555300
O	-2.87290000	1.10730200	1.97734600
O	-3.29847700	-1.68061300	1.71759400
O	-8.97944800	-1.43972300	-0.78811500
O	-4.93279000	0.96236100	-1.84602600
O	-3.05515400	1.42238300	-0.73102600
N	-3.92792300	1.73671400	-1.66354900
O	-3.73202800	2.70933000	-2.34752700
H	-5.27460300	0.52933300	1.63538700
N	-2.42411400	-2.54652900	2.05628900
O	-2.60609000	-3.73048000	2.01188600
N	-8.57059000	-1.33990700	0.40023700
O	-9.09626400	-1.88059400	1.34688900
O	-7.44433200	0.19241300	-2.03690900

H	-8.16883300	-0.46206900	-1.75149100
O	-0.93639300	-1.97968700	-1.26035100
C	-0.54101300	-1.00681500	-0.46487400
O	-1.36514600	-0.32706600	0.22431600
C	0.88229000	-0.73920700	-0.38698400
C	1.81794500	-1.63610500	-0.94501900
C	1.32503100	0.43883700	0.25474900
C	3.17900400	-1.38695300	-0.84927700
H	1.46590000	-2.53922200	-1.44504200
C	2.68326400	0.69806900	0.33624400
H	0.59805400	1.17027900	0.62059400
C	3.62087500	-0.21154700	-0.20014800
H	3.91175600	-2.07622000	-1.26350200
H	3.03264800	1.61802500	0.81118500
N	4.97087600	0.10296300	-0.06971100
H	5.23029700	0.97119800	0.41419000
O	6.09738000	-1.65849200	-1.10595700
C	7.35504800	0.17563300	-0.10434800
O	7.30325300	1.24529800	0.50642900
N	8.45492800	-0.50312100	-0.52551600
H	8.21739200	-1.37276100	-1.01335200
C	9.81170100	-0.17724100	-0.38123500
C	10.75466200	-1.07288100	-0.92264100
C	10.24305100	0.99245300	0.27476600
C	12.11474800	-0.80718400	-0.81223400
H	10.41120500	-1.97820700	-1.43023700
H	9.50673900	1.67795100	0.68937400
C	11.60752900	1.24553600	0.37797400
C	12.55350100	0.35756800	-0.15900900
H	12.84626700	-1.49873200	-1.23040400
H	11.96926200	2.14396100	0.88106700
C	13.99260300	0.69441200	-0.00994500
O	14.42329100	1.68926900	0.54672600
O	14.81141500	-0.24349200	-0.57200400
H	15.71806000	0.08462100	-0.41177300
N	-4.53565300	-2.07743500	-1.29719500
O	-5.68848200	-1.58591500	-1.15379700
O	-4.33476300	-3.16939700	-1.76934400
O	-3.47791400	-1.34414800	-0.93537100
O	-0.71885800	2.88888100	0.38419200
H	-1.13376000	3.35242500	1.13070200
H	-1.46828500	2.67434800	-0.20089700
H	-1.94049600	-1.99259200	-1.26097000
C	6.07026900	-0.58951500	-0.49840200

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Al	-3.80471400	1.90415900	-0.02596000
Al	-3.16008600	-1.32109100	0.57458300
O	-4.23539100	0.14088600	0.49294300
O	-3.34238200	2.31228400	1.79052700
N	-2.53761100	3.26492200	2.27990500
O	-2.36276700	3.28521700	3.47947500
N	-4.42308300	-2.68767000	2.90474700
O	-5.26011700	-2.65049500	3.76698100
O	-3.99870500	-3.84125600	2.41893000
O	-4.86287400	-4.70308100	0.13558400
H	-4.71127900	-4.36332500	1.09730900
O	-2.00401400	4.08059600	1.47707700
H	-2.63245200	3.93425300	0.01267000
O	-5.61884400	2.33537200	0.23963300
O	-3.88216600	-1.60863000	2.43584100
O	-4.70929200	-2.49658700	0.03502600
O	-5.63648900	4.47487500	-0.40480700
O	-1.83135300	1.28281100	-0.18367800
O	-1.63561400	-0.41401900	1.24760200
N	-1.13529300	0.68425600	0.70701000
O	-0.03856200	1.05208400	1.03906800
H	-5.20269500	0.02568300	0.47468000
N	-4.75649400	-3.58377600	-0.62555000
O	-4.75656500	-3.69512500	-1.81036400
N	-6.26498800	3.49644100	0.08174300
O	-7.42898300	3.53469200	0.41382800
O	-3.22960900	3.56235600	-0.71850900
H	-4.08354400	4.10878800	-0.71948000
O	-2.01438700	-0.51404200	-3.18638000
C	-1.69562300	-0.99375500	-2.03466000
O	-2.58447700	-1.41174100	-1.21485100
C	-0.25726700	-1.03095300	-1.72807700
C	0.58745500	-0.03454700	-2.25336400
C	0.28560000	-2.03259200	-0.90222800
C	1.93743800	0.00122300	-1.92618900
H	0.16015100	0.73733100	-2.89404800
C	1.63839000	-2.02345100	-0.59359500
H	-0.35366600	-2.84189700	-0.54892100
C	2.47227400	-0.99581800	-1.08409200
H	2.58789000	0.78831800	-2.30182600
H	2.06694600	-2.81353300	0.02794500
N	3.81433600	-1.01732500	-0.70845400
H	4.14157400	-1.75876000	-0.07788100
O	4.75854100	0.83176800	-1.77320600
C	6.13229500	-0.59336200	-0.34862900

O	6.17434600	-1.59223900	0.37374900
N	7.13964800	0.26265000	-0.66380100
H	6.83295900	1.01615100	-1.28778600
C	8.48181300	0.24762800	-0.25667000
C	9.31591600	1.27761400	-0.73398100
C	9.00238600	-0.74580700	0.59581700
C	10.65614700	1.31839300	-0.36689500
H	8.90336500	2.04542000	-1.39384100
C	10.34541200	-0.69181600	0.95595900
H	8.34933500	-1.53644000	0.95962200
C	11.18336200	0.33110500	0.48352900
H	11.30347800	2.11435100	-0.73518100
H	10.77437300	-1.44733600	1.61650000
C	12.60549200	0.32412100	0.91227700
O	13.10564900	-0.49731900	1.66095400
O	13.32082400	1.35514500	0.37269300
H	14.22557800	1.24666900	0.72619400
N	-4.84929400	0.45888700	-2.32167800
O	-3.96297700	1.32578000	-1.88823100
O	-5.93606000	0.31595200	-1.78571600
O	-4.49859800	-0.21940900	-3.33627100
O	-2.11562400	-2.95647300	0.97880100
H	-2.71547800	-3.48369900	1.62539000
H	-1.32725300	-2.67187900	1.47844600
H	-3.07026800	-0.36221600	-3.28619300
C	4.82137100	-0.15492800	-1.04198800

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Al	3.94708800	-1.44690600	0.26365800
Al	4.11562000	1.78614700	0.32575400
O	4.63559900	0.18861800	-0.36878600
O	5.74953800	-1.82559700	0.77186500
N	6.24169800	-2.69266500	1.67502500
O	7.43215500	-2.64571500	1.89462800
N	6.34867300	3.52838600	-0.54594800
O	7.42907000	3.60226200	-1.06993200
O	5.54658800	4.55057800	-0.46625300
O	3.43092400	4.72938500	-2.06902100
H	4.35612100	4.69136700	-1.65143400
O	5.44863300	-3.49213200	2.23584100
H	3.96017900	-3.35513000	1.63517100
O	4.11832100	-2.12872400	-1.48619700
O	5.94736900	2.40419700	-0.01244300
O	3.77615100	2.58921000	-1.57229700

O	3.37745600	-4.22336800	-1.23015200
O	3.71046700	-0.63624400	2.13847000
O	4.52207200	1.44546000	2.15251900
N	4.29159800	0.30085300	2.77897100
O	4.59880700	0.20389800	3.93972300
H	5.56278900	0.10572200	-0.64975500
N	2.93779400	3.46067900	-1.92945100
O	1.78571300	3.28744100	-2.19239800
N	3.98706100	-3.38327300	-1.94618000
O	4.44467500	-3.62539400	-3.03939500
O	3.21342500	-3.00130800	1.04788300
H	3.10663200	-3.64723600	0.27721900
O	2.14477100	-0.81761300	-0.07474700
C	1.61671100	0.32474300	0.16417400
O	2.30732400	1.38488100	0.41212700
C	0.15372400	0.44977400	0.17114700
C	-0.65814100	-0.69707300	0.25815400
C	-0.44886200	1.72158200	0.10508600
C	-2.04404700	-0.59094400	0.26879100
H	-0.19513300	-1.68154700	0.34417500
C	-1.83003000	1.83797200	0.10202300
H	0.18168900	2.60839800	0.03988500
C	-2.64054700	0.68414200	0.18193500
H	-2.67436300	-1.47469300	0.34456700
H	-2.29932700	2.82257500	0.03457100
N	-4.02328700	0.86619800	0.17523100
H	-4.39584900	1.82088900	0.11331600
O	-4.90852000	-1.28809100	0.31723200
C	-6.39699400	0.63827800	0.19257200
O	-6.49087400	1.86573700	0.11753800
N	-7.39629300	-0.28177600	0.24789400
H	-7.04097700	-1.24191800	0.30624000
C	-8.78532700	-0.09021100	0.23456700
C	-9.59957500	-1.23802300	0.29984700
C	-9.37165300	1.18869100	0.15954600
H	-9.13652800	-2.22666400	0.35721100
C	-10.75885600	1.29740500	0.15145800
H	-8.73369100	2.06869700	0.10899000
C	-11.57705600	0.15801600	0.21644500
H	-11.61592900	-2.00136000	0.34098800
H	-11.23917700	2.27574200	0.09399900
C	-13.04930600	0.35251600	0.20327700
O	-13.61150800	1.43221000	0.14062600
O	-13.73492900	-0.82721500	0.27009300
H	-14.67816800	-0.57168200	0.25379100
C	-10.98421700	-1.11441800	0.29077800

N	0.40893000	-3.51758300	-1.76825900
O	0.39807900	-3.71017800	-0.55920600
O	-0.04149100	-4.18958300	-2.65895000
O	1.03670700	-2.31597200	-2.21008700
O	3.66238400	3.58909400	0.94666200
H	4.40961200	4.18885300	0.61226500
H	3.60642800	3.63082200	1.91773900
H	1.37589200	-1.89411700	-1.37615600
C	-5.02079900	-0.06599700	0.23705700

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Al	-7.80092000	0.42039400	-0.49303800
Al	-4.69806800	-0.00304400	0.49430800
O	-6.45605900	0.37065400	0.79889500
O	-8.01197800	2.25589500	-0.10370600
N	-8.83781100	3.16865800	-0.64952300
O	-8.81900400	4.28147900	-0.17414100
N	-3.13868900	1.43586700	2.53890000
O	-2.84122100	2.56601100	2.85874100
O	-2.45258500	0.42987000	2.88826300
O	-2.83021300	-2.00426800	2.61427800
H	-2.80097400	-0.93315400	2.63218500
O	-9.56626900	2.82131000	-1.61454800
H	-9.35900600	1.26774900	-2.01361200
O	-9.00960600	-0.20374000	0.81960000
O	-4.23642600	1.25399500	1.82814100
O	-6.45300200	0.90845600	-1.89283800
O	-10.61049600	-1.08004600	-0.47707600
O	-4.87504400	-1.50616200	1.85719900
O	-4.50328800	1.32539000	-0.89034200
N	-5.38737000	1.61690400	-1.81912200
O	-5.14866100	2.50328900	-2.60004400
H	-6.68243000	0.83379900	1.62117400
N	-4.05437700	-2.40049300	2.25061000
O	-4.32365800	-3.56596200	2.32795200
N	-10.15069300	-0.89767900	0.68256500
O	-10.67491200	-1.30872600	1.69317200
O	-9.01958800	0.31755500	-1.92477600
H	-9.77478800	-0.25476800	-1.55501100
O	-2.65656500	-2.28061200	-1.13133000
C	-2.16122500	-1.25979300	-0.45998700
O	-2.91012500	-0.45063600	0.17574000
C	-0.72363000	-1.09037100	-0.45510800
C	0.12926100	-2.10105900	-0.94789700

C	-0.17532600	0.11071600	0.04878500
C	1.50689400	-1.94344300	-0.92323800
H	-0.30128000	-3.02225700	-1.34267600
C	1.19829300	0.27675200	0.05861300
H	-0.83441500	0.92596100	0.36222800
C	2.05665800	-0.74418100	-0.41202800
H	2.17286900	-2.71722400	-1.29630600
H	1.62355900	1.21429900	0.42721400
N	3.42715700	-0.50456800	-0.34310200
H	3.68656900	0.41114800	0.01755700
O	4.32110200	-2.36863300	-1.37537000
C	9.84308700	0.71410000	0.23487200
O	9.98154300	1.79026000	0.81071100
N	10.89104200	-0.08566400	-0.18741300
H	10.63647000	-1.00556100	-0.53892700
C	12.27223900	0.14989600	-0.09717200
C	13.12937100	-0.87469300	-0.54998400
C	12.82054800	1.34660200	0.40722400
C	14.50873400	-0.71440200	-0.50183300
H	12.70249200	-1.80249200	-0.94253800
C	14.20393300	1.49415900	0.44856200
H	12.15567500	2.13032200	0.76169800
C	15.06134500	0.47695200	-0.00023500
H	15.16768800	-1.50906700	-0.85211100
H	14.65024600	2.41197800	0.83558800
C	16.52481400	0.70727300	0.07601100
O	17.05468000	1.71928400	0.50196800
O	17.24930700	-0.35468000	-0.39066800
H	18.18280100	-0.08394000	-0.28861800
N	-6.25712800	-2.09079000	-1.06208600
O	-6.15729900	-3.23619800	-1.42792100
O	-7.36434200	-1.49932300	-0.93339700
O	-5.13506200	-1.41056400	-0.80952000
O	-2.02462200	2.71987900	-0.00343600
H	-2.38799400	3.26655000	0.71319100
H	-2.80576500	2.49676000	-0.54206700
H	-3.65716200	-2.21482400	-1.10367400
C	5.84442900	-0.74993500	-0.49790300
C	6.11964800	0.16877900	0.53188500
C	6.89992300	-1.21819200	-1.29696600
C	7.42001300	0.62047500	0.74448700
H	5.33031600	0.51157600	1.20638300
C	8.20007500	-0.76560900	-1.08346100
H	6.67163800	-1.93478800	-2.08746500
C	8.47579400	0.15151200	-0.05320900
H	7.65002500	1.34074800	1.53115000

H	8.99139000	-1.10669800	-1.75614200
C	4.48031500	-1.30513300	-0.78574100

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Al	5.29344400	-1.84771700	0.13785600
Al	4.38205500	1.32572600	0.67187300
O	5.60364300	-0.02483100	0.57864200
O	4.67325500	-2.11048900	1.92671200
N	4.60620500	-3.24843900	2.63206800
O	4.46541800	-3.15229000	3.83206700
N	5.43343800	2.65161100	3.13908800
O	6.24971300	2.63744800	4.02300500
O	4.86283800	3.76559000	2.75193400
O	5.69711400	4.95302200	0.53027100
H	5.58165200	4.56446700	1.46435900
O	4.67396200	-4.34366900	2.01395100
H	4.73119600	-4.10506700	0.41164900
O	7.06019900	-2.24101400	0.66789200
O	5.07280100	1.55236300	2.54252800
O	5.80977600	2.74890300	0.29555700
O	7.46501400	-3.76944100	-0.90715600
O	3.32871500	-1.34645000	-0.20169600
O	2.86776100	0.30738700	1.21413100
N	2.52478300	-0.84130100	0.65456900
O	1.46034700	-1.33031400	0.92866900
H	6.32594600	0.01655300	1.22943100
N	5.70169200	3.86279800	-0.29522900
O	5.64488100	4.05444800	-1.46944800
N	7.92951200	-2.99582500	-0.03095700
O	9.10324700	-2.89237400	0.24300200
O	4.88819500	-3.60773100	-0.45708600
H	5.79336800	-3.89995100	-0.79098200
O	3.69006200	0.43102800	-3.12999900
C	3.21008200	0.91567000	-2.04081000
O	3.97148200	1.41714200	-1.14065800
C	1.74909700	0.87760000	-1.89258100
C	1.01227900	-0.15550000	-2.50168700
C	1.07143500	1.84708300	-1.12975300
C	-0.36230900	-0.25769700	-2.32495800
H	1.54209200	-0.90490700	-3.09063100
C	-0.30439400	1.77204500	-0.97186300
H	1.62862200	2.68420200	-0.70790000
C	-1.03691700	0.71017200	-1.54971500
H	-0.92799700	-1.07630800	-2.76246800

H	-0.83132400	2.54322100	-0.40300500
N	-2.41419100	0.68631900	-1.32511800
H	-2.76485300	1.40972500	-0.70164700
O	-3.06171600	-1.26087800	-2.38741500
C	-8.87544900	0.78636100	-0.20489000
O	-9.19780300	1.94438600	0.05349700
N	-9.74765400	-0.28349300	-0.14863600
H	-9.36650700	-1.19510300	-0.38519000
C	-11.10931500	-0.29551800	0.19256700
C	-11.76400400	-1.54495900	0.16588600
C	-11.83026000	0.86157600	0.55178100
C	-13.11124900	-1.64452300	0.49027400
H	-11.20441300	-2.44295200	-0.11306600
C	-13.17934700	0.74722200	0.87443000
H	-11.32160200	1.82199300	0.57061200
C	-13.83495600	-0.49401800	0.84933000
H	-13.61259900	-2.61228200	0.46815300
H	-13.75660900	1.62996900	1.15535500
C	-15.27425700	-0.53582300	1.20585500
O	-15.94680600	0.43010300	1.52393000
O	-15.79504100	-1.79879100	1.14304300
H	-16.73336600	-1.69473800	1.39570200
N	6.50476900	-0.58645100	-2.13684700
O	5.53892800	-1.38267800	-1.71614900
O	7.63184000	-0.65555800	-1.69365600
O	6.17382900	0.23281500	-3.04940100
O	3.19562400	2.84837400	1.09211500
H	2.35388400	2.48111000	1.42146300
H	3.66654200	3.34287600	1.85781200
H	4.76175200	0.33671700	-3.09674200
C	-4.76164300	0.04728800	-1.33415200
C	-5.23806600	1.33653900	-1.03666000
C	-5.65535300	-1.03469400	-1.29292500
C	-6.57030200	1.53046600	-0.68046500
H	-4.58719200	2.21108700	-1.12227600
C	-6.98520300	-0.83913400	-0.92815600
H	-5.27995200	-2.02493100	-1.55547200
C	-7.46132900	0.44667300	-0.61173300
H	-6.96255000	2.52316700	-0.45437000
H	-7.63418400	-1.71846000	-0.90126800
C	-3.35045500	-0.25567300	-1.74724600

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Al	5.55742800	-1.28975300	0.23182400
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Al	5.39796000	1.94160600	0.14086600
O	6.04053200	0.37242400	-0.51330900
O	7.41661600	-1.46052600	0.64243600
N	8.04717600	-2.22536000	1.55158300
O	9.23705600	-2.04688600	1.69430600
N	7.39542500	3.85094800	-0.93508600
O	8.43303000	4.00493100	-1.52428900
O	6.50022300	4.79288500	-0.85268100
O	4.29710600	4.68565200	-2.33607600
H	5.24169700	4.75774600	-1.96878300
O	7.37522600	-3.07101300	2.19641500
H	5.84790200	-3.11595000	1.68325900
O	5.69915500	-2.03735600	-1.49386000
O	7.13828400	2.72070000	-0.33127300
O	4.87818100	2.61463900	-1.76975700
O	5.19455900	-4.18040600	-1.10037800
O	5.34896000	-0.41500600	2.08251200
O	5.93728500	1.73667700	1.95361700
N	5.85978400	0.60857800	2.64482700
O	6.23410500	0.60478300	3.78996100
H	6.95666300	0.36748600	-0.83925900
N	3.94095800	3.38231400	-2.11747000
O	2.80016800	3.08574000	-2.31118200
N	5.66902800	-3.31961300	-1.89018800
O	6.08102200	-3.56823900	-3.00014200
O	5.03647000	-2.86909400	1.12838000
H	4.95275600	-3.56041000	0.39528700
O	3.68628100	-0.86136800	-0.02008800
C	3.05617300	0.23426600	0.19302800
O	3.64839500	1.37013600	0.34848300
C	1.59265300	0.21325700	0.27733400
C	0.90580700	-0.99965900	0.47569200
C	0.85804800	1.41122900	0.17329000
C	-0.48121900	-1.03450100	0.55892300
H	1.47052500	-1.92640600	0.59136600
C	-0.52523900	1.38584100	0.24033800
H	1.38801100	2.35180700	0.02210700
C	-1.21383800	0.16520000	0.43078300
H	-1.01133100	-1.97069700	0.71493300
H	-1.09267600	2.31571600	0.14319200
N	-2.60733900	0.22323200	0.49379900
H	-3.00851600	1.14651400	0.34690300
O	-3.19664900	-2.00315000	0.67456500
C	-9.13816500	0.68779500	0.86624200
O	-9.47844700	1.63957300	1.56461700
N	-10.00916800	-0.06263600	0.09485500

H	-9.58070100	-0.74548700	-0.52530800
C	-11.40237800	0.05487900	-0.02981800
C	-12.04106400	-0.81124000	-0.94181000
C	-12.16963900	0.97677700	0.71106200
C	-13.41859800	-0.76205500	-1.11658200
H	-11.44494900	-1.52799200	-1.51454300
C	-13.54863100	1.01459800	0.52665500
H	-11.67174600	1.64611700	1.40818300
C	-14.18882600	0.15532800	-0.38064900
H	-13.90793500	-1.43310500	-1.82274900
H	-14.16205500	1.72069600	1.08926400
C	-15.66183800	0.25521500	-0.52294900
O	-16.37512500	1.03246100	0.08842300
O	-16.16395400	-0.63383500	-1.43292900
H	-17.12761700	-0.47122200	-1.43476400
N	2.14137400	-3.80426700	-1.47308500
O	2.22592700	-3.93639200	-0.25908400
O	1.70960400	-4.56216000	-2.30211300
O	2.61173200	-2.56863600	-2.00756800
O	4.80049900	3.72066900	0.70783200
H	4.79698300	3.80152800	1.67810000
H	5.46506900	4.37299600	0.30456600
H	2.95319700	-2.07226400	-1.21652700
C	-4.95572600	-0.38546300	0.68846500
C	-5.37611800	0.89563400	1.09083400
C	-5.92292400	-1.35324300	0.37312000
C	-6.73229000	1.20948200	1.14046900
H	-4.65309400	1.64898400	1.41548700
C	-7.27850600	-1.03388200	0.40818600
H	-5.58187300	-2.35721400	0.11546300
C	-7.69756600	0.25811000	0.77428100
H	-7.07889100	2.18786900	1.47707000
H	-8.00689000	-1.81909400	0.18897400
C	-3.51931100	-0.82118300	0.62704500

Mg-H₂BPDC initial

0 1			
Mg	4.51733000	-0.09304800	-0.18397200
O	2.96060000	1.36450000	-0.35604400
O	4.97070100	0.69323200	1.76611800
O	3.93709900	-0.88369800	-2.04519400
O	5.73377700	1.27604700	-1.11530500
O	0.18704600	1.83706600	0.88504100
O	0.59663800	1.64298700	-2.06203600
O	7.32700600	2.07600900	0.20532100

O	-0.44536600	1.25935200	-3.95448300
O	-2.38275400	0.79384300	2.20443000
O	3.34235100	-1.55066800	0.73805800
O	1.47904800	-0.54809700	1.35147900
N	2.34057600	-1.47263500	1.54570400
N	2.86234800	-1.50106400	-2.32163800
O	2.83263000	-2.42616400	-3.11950400
O	2.21903700	-2.27376300	2.46221400
N	-0.50605300	1.49387800	-2.76110700
O	-1.60894600	1.61537600	-2.13969300
N	6.58604400	2.20500700	-0.82465300
O	6.66965800	3.19307100	-1.54268300
O	6.06868100	-1.39841400	-0.00506200
Mg	1.08102800	0.43673700	-0.45054400
O	-0.68049500	-0.61581000	-0.55667400
C	-2.71805500	-1.70006400	-1.12840300
C	-3.37369000	-2.66854700	-1.91288500
C	-3.43724300	-0.92063100	-0.20647800
C	-4.74443900	-2.85296000	-1.77162200
H	-2.79935000	-3.26480000	-2.62284700
C	-4.81492300	-1.09913100	-0.08640500
H	-2.91869700	-0.19236900	0.42551200
C	-5.48105400	-2.05680700	-0.87362000
H	-5.27632700	-3.61169300	-2.34806500
H	-5.36737200	-0.50190900	0.64123700
C	-1.26613700	-1.46643200	-1.25557400
O	-7.37797900	-3.47486600	-0.92044700
C	-7.88414500	-1.22689600	-0.35604600
C	-9.09376500	-1.57142600	0.27501400
C	-7.63447900	0.11876600	-0.68689600
C	-10.02293200	-0.58944400	0.60436800
H	-9.28020100	-2.62439300	0.49357800
C	-8.57360500	1.10111100	-0.37772300
H	-6.71596300	0.39221400	-1.20880000
C	-9.76501000	0.75456200	0.27803000
H	-10.95399500	-0.85006600	1.10833000
H	-8.40608700	2.14842000	-0.63456000
C	-10.72502100	1.84916000	0.59587600
O	-10.55612800	3.02449500	0.32436300
O	-11.84106500	1.39692300	1.23716700
H	-12.38634500	2.19391500	1.38905300
O	1.76367400	-1.13612400	-1.72284600
C	-6.94929800	-2.33796600	-0.73051200
O	-0.63868900	-2.21261200	-2.15269600
H	0.33349400	-1.94826100	-2.14183900
S	3.46349900	2.81476200	-0.78573500

C	2.05985900	3.91474400	-0.45944400
H	1.18418500	3.58610300	-1.03251700
H	1.87612300	3.88874600	0.62164600
H	2.38574400	4.92114900	-0.75919400
C	3.43851500	2.80984000	-2.59757900
H	2.45316100	2.46109000	-2.93476100
H	3.66142300	3.83521100	-2.92448900
H	4.25338700	2.14063900	-2.89514300
S	6.31432000	-2.92372700	0.11534900
C	4.98857400	-3.76339100	-0.81606700
H	4.01845200	-3.51173000	-0.37040500
H	5.04714100	-3.40657600	-1.85214600
H	5.18713600	-4.84366400	-0.77351200
C	5.78697200	-3.39468700	1.79670700
H	4.74331200	-3.09138800	1.95200800
H	5.91874400	-4.48139600	1.89921400
H	6.45316400	-2.86981900	2.49306600
N	-0.71698900	2.69031500	1.03109700
O	-0.81362300	3.42167200	1.98572900
N	5.90294000	0.20954000	2.46627800
O	7.15758000	0.45814700	2.07904300
H	7.11806900	1.07812700	1.19859700
O	5.74529700	-0.45347100	3.46469300
S	-2.00060700	-0.00985900	3.45130100
C	-1.42484800	-1.65591400	2.87346300
H	-2.30148500	-2.16906200	2.45778900
H	-0.65390400	-1.50904100	2.10670000
H	-1.02479500	-2.21732700	3.72932900
C	-0.35702200	0.58980700	4.00879100
H	-0.07259200	0.03013300	4.91134100
H	0.37849400	0.45271600	3.20621900
H	-0.48179600	1.65419900	4.24376800
O	-1.62734600	2.85895500	0.05276100
H	-1.46786400	2.20640100	-0.75731000

Mg-H₂BPDC TS

0 1

Mg	-4.30882600	-0.19377400	-0.18946600
O	-2.82160600	-1.60747900	0.35249100
O	-5.25788600	-0.65392100	1.70752500
O	-2.70642700	0.07583000	-1.58550400
O	-5.28469000	-1.77386100	-1.02352600
O	-0.14596400	-1.20695300	1.53266400
O	-0.45943100	-2.37067800	-1.18938500
O	-7.44376600	-1.49266000	-0.58949300

O	0.77100500	-2.55401300	-2.99968000
O	2.38985600	0.13336100	2.10310900
O	-3.45634600	1.40116900	0.88151800
O	-1.26099300	1.18193700	0.76278600
N	-2.28455700	1.91750400	0.97746400
N	-2.89009600	1.00135000	-2.52933100
O	-3.89381400	0.93088500	-3.22158900
O	-2.15283600	3.10021400	1.28272200
N	0.70499000	-2.46572900	-1.78998900
O	1.74069100	-2.48373100	-1.04670900
N	-6.52150900	-2.09512900	-1.23808900
O	-6.78566100	-2.97457100	-2.04171100
O	-5.72366300	1.11174900	-0.78437500
Mg	-1.06612300	-0.60595600	-0.31504900
O	0.55730800	0.24886400	-1.19544400
C	2.57424300	1.50991300	-1.32245300
C	3.20115100	2.71012200	-1.71613100
C	3.30408600	0.51275300	-0.65562300
C	4.54640000	2.90803300	-1.43213600
H	2.61817000	3.47769900	-2.22603000
C	4.65896500	0.71024600	-0.39140700
H	2.80074200	-0.39289800	-0.32162000
C	5.29095800	1.90409400	-0.78022400
H	5.05054700	3.83916200	-1.69606600
H	5.21123100	-0.05158300	0.16004800
C	1.12934400	1.30269800	-1.53956700
O	7.05696500	3.37249300	-0.20571000
C	7.71786400	1.09785500	-0.33697600
C	8.84715000	1.29412600	0.47918500
C	7.60753600	-0.08420000	-1.09391000
C	9.83192700	0.31521700	0.56911400
H	8.92662500	2.23074800	1.03381100
C	8.60349400	-1.05648000	-1.02223100
H	6.75355700	-0.23034000	-1.75737600
C	9.71274300	-0.86735500	-0.18352700
H	10.69996800	0.45588000	1.21368000
H	8.54450500	-1.97532000	-1.60805400
C	10.73748000	-1.94840400	-0.13559100
O	10.68634100	-2.98498900	-0.77325300
O	11.76512400	-1.65824000	0.71319100
H	12.36371500	-2.42924600	0.65977600
O	-2.04501700	1.92040000	-2.63089600
C	6.71779300	2.21093000	-0.42580900
O	0.49182500	2.31443200	-2.10307500
H	-0.47953300	2.06659300	-2.21303000
S	-3.26262400	-3.11707400	0.54520600

C	-1.84347400	-3.88768700	1.36983100
H	-0.95397400	-3.77892700	0.73723900
H	-1.72175100	-3.39119900	2.34036500
H	-2.09779000	-4.94589900	1.52285400
C	-3.11474100	-3.91449700	-1.07974500
H	-2.14213400	-3.64991900	-1.51658600
H	-3.21282400	-4.99654300	-0.90861400
H	-3.95608400	-3.53941500	-1.67383200
S	-6.17768600	2.59210300	-0.78180800
C	-4.75124500	3.58687400	-1.33087400
H	-3.92390400	3.48512400	-0.61706000
H	-4.47414400	3.21894900	-2.32712400
H	-5.08545900	4.63204200	-1.39842700
C	-6.19600900	3.13006000	0.96126400
H	-5.21607200	2.91475000	1.40762300
H	-6.42101800	4.20591100	0.97754900
H	-6.99912300	2.57244700	1.45850300
N	0.61336000	-1.99157300	2.13439600
O	0.59886800	-2.17595400	3.33030600
N	-6.26737600	-0.06289000	2.16654900
O	-7.37179100	-0.02625300	1.39874200
H	-7.21616100	-0.64103000	0.51945400
O	-6.32628400	0.48075600	3.24438300
S	2.20159000	1.35473600	3.00298400
C	1.75502900	2.77189400	1.92053100
H	2.60846900	2.93810900	1.25095400
H	0.84612700	2.53197300	1.35171800
H	1.59737400	3.65770800	2.55251800
C	0.54817100	1.19601600	3.78908100
H	-0.20202500	1.04591900	3.00199700
H	0.59278000	0.31562300	4.44176100
H	0.34438000	2.10239500	4.37662100
O	1.48495700	-2.73251100	1.42558800
H	1.45173200	-2.49636800	0.38821900

Mg-H₂BPDC final

0 1

Mg	-2.77286300	-0.99504900	0.21536000
O	-2.38841900	0.86291500	1.24448700
O	-4.89652700	-0.48496300	0.39891600
O	-0.69014200	-4.62912600	-0.44571000
O	-2.83555900	-1.77421200	2.10921800
O	-2.52602700	3.78780200	0.60911900
O	0.02984200	2.59364900	1.63653600
O	-4.73654600	-2.85450100	2.47445600

O	2.19539100	2.87958700	1.75766400
O	-0.13964700	3.49300900	-1.04123500
O	-2.91071100	-0.23685800	-1.72743100
O	-2.61609900	1.94800200	-1.64238000
N	-2.82323800	0.88949400	-2.32715300
N	-0.75952900	-4.73637400	0.78140100
O	-1.02155900	-5.72075700	1.42883800
O	-2.93612400	0.94446500	-3.55280300
N	1.07616300	3.30812800	1.59558700
O	0.92657500	4.61146600	1.40481500
N	-3.68930300	-2.29255600	2.93242100
O	-3.46927300	-2.23705100	4.13597600
O	-3.25214000	-2.80408000	-0.58018900
Mg	-1.33586900	2.19412000	-0.00401500
O	-0.14758100	0.65057500	-0.60784500
C	1.54262400	-1.00150400	-0.55231100
C	1.86172200	-2.35812700	-0.74213100
C	2.56281300	-0.03548600	-0.57051600
C	3.18469200	-2.73741900	-0.95256300
H	1.07004800	-3.10965300	-0.74464200
C	3.89149700	-0.42321400	-0.73719100
H	2.29671200	1.01377200	-0.43519900
C	4.21476700	-1.78005200	-0.92771500
H	3.44982000	-3.77955100	-1.13966900
H	4.67943600	0.33207500	-0.74493100
C	0.12967300	-0.55329900	-0.34797300
O	5.80825600	-3.22787900	-1.91693600
C	6.77411000	-1.50566100	-0.60361400
C	8.01407400	-1.58096900	-1.26428700
C	6.68492500	-0.82299600	0.62460100
C	9.13740800	-0.95572200	-0.73147100
H	8.06810700	-2.14394700	-2.19779600
C	7.81346800	-0.21444700	1.17107400
H	5.73697200	-0.79241600	1.16447200
C	9.04032200	-0.26742900	0.49161700
H	10.09642700	-0.99835100	-1.24845900
H	7.77061600	0.30953700	2.12743000
C	10.20864400	0.41447900	1.11700800
O	10.17831100	1.01685700	2.17530900
O	11.34435900	0.29669800	0.37095500
H	12.03119100	0.77456600	0.87648300
O	-0.48077600	-3.59455500	1.53118200
C	5.61459400	-2.24537900	-1.20340700
O	-0.73625200	-1.40863100	0.06847400
H	-0.49289600	-2.82004400	0.87334500
S	-2.74486600	0.84168500	2.79491300

C	-2.78808900	2.58360000	3.29721000
H	-1.83017400	3.07234800	3.08702200
H	-3.59446600	3.06055000	2.72829900
H	-3.02181300	2.58196100	4.37180500
C	-1.20715600	0.33834700	3.61519400
H	-0.38428100	0.95555000	3.23292000
H	-1.35584800	0.46621100	4.69648500
H	-1.08544000	-0.72466400	3.38070000
S	-3.25652800	-3.57074100	-1.92687100
C	-1.84078200	-2.97221800	-2.91051700
H	-1.93612300	-1.89029500	-3.06008700
H	-0.94437700	-3.22773700	-2.33570500
H	-1.85126700	-3.52101300	-3.86299800
C	-4.57990500	-2.79938800	-2.91915800
H	-4.38269400	-1.72284600	-3.00274400
H	-4.59662200	-3.28506900	-3.90514200
H	-5.52289300	-2.98994400	-2.39188500
N	-2.35909300	5.05161100	0.45333500
O	-3.25280800	5.75336800	0.00235300
N	-5.80992900	-1.17795000	-0.11599800
O	-5.99479400	-2.41897600	0.36795800
H	-5.31811900	-2.55121700	1.18661800
O	-6.53791000	-0.82103300	-1.01299100
S	-0.00302100	4.12218200	-2.44753600
C	-0.03748700	2.74284200	-3.64317200
H	0.72262200	2.02808900	-3.30257600
H	-1.03208100	2.27864400	-3.67175300
H	0.23960900	3.14913700	-4.62642400
C	-1.62559800	4.84862800	-2.84851400
H	-1.58994800	5.19852900	-3.89014000
H	-2.39859800	4.08173200	-2.70413900
H	-1.77822500	5.69907900	-2.17194500
O	-1.23589900	5.58444800	0.79782000
H	-0.11718800	4.85037200	1.14380900

Mg-H₂ODA initial

0 1

Mg	-5.58391600	0.62865200	-0.26707800
O	-4.39740800	-1.14278500	-0.44488500
O	-6.28975900	-0.09855100	1.63172000
O	-4.75052700	1.33340200	-2.06361500
O	-7.03868500	-0.39085500	-1.30034500
O	-1.86480700	-2.28921100	0.87748900
O	-2.08527000	-1.89369000	-2.06804600
O	-8.82881900	-0.84519100	-0.07098800

O	-0.91232700	-1.70145400	-3.91220000
O	0.80815600	-1.91278600	2.40754600
O	-4.15586400	1.74755000	0.76532800
O	-2.62119800	0.30704800	1.41393000
N	-3.24932800	1.40187600	1.61472000
N	-3.54913000	1.69459900	-2.26667800
O	-3.26930900	2.61885200	-3.01585700
O	-2.99610500	2.11513400	2.57601700
N	-0.95037600	-1.97282100	-2.72566700
O	0.07412700	-2.34927500	-2.07317600
N	-8.09447500	-1.10530000	-1.08099100
O	-8.37435400	-2.01922500	-1.84601300
O	-6.80898100	2.24572400	-0.08799400
Mg	-2.35174900	-0.66729800	-0.42044800
O	-0.40068400	-0.04639400	-0.38854700
C	1.85790800	0.56197900	-0.79741800
C	2.77047100	1.37409700	-1.49546200
C	2.32932900	-0.39669300	0.12006300
C	4.13969700	1.24512700	-1.28780100
H	2.39620900	2.10875300	-2.20940300
C	3.69389200	-0.52868900	0.33440300
H	1.62617700	-1.02088400	0.68030000
C	4.60779400	0.28510300	-0.36624500
H	4.85519400	1.86594700	-1.82300300
H	4.05894000	-1.27229600	1.04789300
C	0.40970900	0.67165300	-1.01212700
N	5.96962700	0.09620100	-0.10798600
H	6.23992100	-0.62667500	0.56831300
O	7.06215400	1.64899900	-1.46461000
C	8.35259500	0.16512400	-0.02837900
O	8.33850400	-0.73988600	0.80803900
N	9.43205800	0.80407500	-0.55782500
H	9.16101300	1.52268700	-1.23773000
C	10.79545200	0.61045600	-0.30177800
C	11.71068500	1.42217500	-1.00136400
C	11.26428900	-0.35174500	0.61502600
C	13.07713500	1.27836700	-0.79103600
H	11.33912600	2.16590700	-1.71125800
C	12.63467100	-0.48474900	0.81568800
H	10.54932600	-0.97395000	1.14962100
C	13.55252600	0.32091700	0.12215000
H	13.78595700	1.90563500	-1.33182600
H	13.02361000	-1.22236100	1.51986600
C	14.99900600	0.12221500	0.38796600
O	15.46324000	-0.69138100	1.16830700
O	15.78892600	0.96258100	-0.34615200

H	16.70345500	0.73676600	-0.08581200
O	-2.59575000	1.06158600	-1.64558600
C	7.04970300	0.73943500	-0.63294300
O	0.02125100	1.57585600	-1.90320300
H	-0.98214700	1.54064700	-1.95365200
S	-5.19645500	-2.42166100	-0.96010700
C	-4.09595100	-3.82511600	-0.63461300
H	-3.14364800	-3.68410600	-1.16040200
H	-3.95937500	-3.88037300	0.45234200
H	-4.62801500	-4.71875200	-0.99124900
C	-5.08769400	-2.35503800	-2.76768500
H	-4.03434900	-2.22906200	-3.05203200
H	-5.52294300	-3.28888700	-3.15036700
H	-5.71406500	-1.50588400	-3.06266200
S	-6.70578600	3.78162600	0.09023400
C	-5.17979600	4.32698600	-0.74900400
H	-4.31505000	3.84617600	-0.27560100
H	-5.26573300	4.02732200	-1.80115200
H	-5.13099400	5.42208000	-0.66742800
C	-6.16777000	4.06110200	1.81061100
H	-5.22901600	3.52190100	1.99354400
H	-6.05417700	5.14494900	1.95619500
H	-6.96881200	3.67891200	2.45594500
N	-1.16996500	-3.32178300	1.01287200
O	-1.28136700	-4.10056700	1.92757400
N	-7.11670300	0.56179500	2.31935000
O	-8.37647400	0.62285100	1.87731200
H	-8.44033900	0.04204900	0.97179900
O	-6.85642100	1.13492800	3.35148800
S	0.52016300	-1.07434900	3.65678600
C	0.35696400	0.67092700	3.10719900
H	1.35292600	0.99176100	2.77593900
H	-0.36407400	0.71311100	2.28139100
H	0.01935400	1.28464700	3.95396200
C	-1.24889700	-1.31608100	4.08404100
H	-1.47092000	-0.72824300	4.98619100
H	-1.87869900	-1.00534400	3.24116100
H	-1.37158600	-2.38732700	4.28679100
O	-0.26240300	-3.63354400	0.06770200
H	-0.24704800	-2.93471300	-0.72016800

Mg-H₂ODA TS

0 1

Mg	5.33416900	-0.22820900	-0.32299400
O	4.13432400	0.84607900	1.11662100

O	6.31007700	-1.00899600	1.50880300
O	3.77335700	0.71110000	-1.40587600
O	6.57195500	1.38615900	-0.25392400
O	1.16572000	0.44591300	1.91978600
O	2.05810500	2.86991100	0.53847800
O	8.64590700	0.60434500	-0.09214100
O	1.17923500	4.41034500	-0.75645900
O	-1.48077300	-0.97481300	2.36637600
O	4.18786500	-1.96733100	-0.18060200
O	2.11361100	-1.24408900	0.05467900
N	2.92658500	-2.20167000	-0.18317700
N	3.75266300	0.85591400	-2.73271000
O	4.63946600	0.29668700	-3.37625400
O	2.51155400	-3.33601400	-0.40883300
N	1.02756100	3.52853700	0.06481100
O	-0.12478800	3.20374300	0.51224800
N	7.85440000	1.58608300	-0.28194100
O	8.27918400	2.71544400	-0.47391600
O	6.60019900	-1.29642000	-1.47493200
Mg	2.27803400	0.85063200	0.12010900
O	0.78071200	0.94001100	-1.19652100
C	-1.55889800	0.79202700	-1.66462100
C	-2.58693300	0.95759100	-2.61256200
C	-1.88278700	0.43283600	-0.34371000
C	-3.91842000	0.77603400	-2.25547900
H	-2.33255900	1.23784900	-3.63534600
C	-3.20633300	0.24160800	0.02257700
H	-1.10833000	0.27104800	0.40564300
C	-4.23314500	0.41808300	-0.92665500
H	-4.72081000	0.90650500	-2.97863500
H	-3.42482400	-0.05332800	1.05217400
C	-0.15180700	0.99581800	-2.01641300
N	-5.54849700	0.21994300	-0.49530000
H	-5.70263400	-0.02788200	0.48855100
O	-6.86176300	0.58752600	-2.38817300
C	-7.91421900	-0.00264300	-0.27302800
O	-7.76368000	-0.28845800	0.91599300
N	-9.07736100	0.09154400	-0.97482400
H	-8.91837100	0.34607500	-1.95559600
C	-10.39533600	-0.10790600	-0.54460900
C	-11.42208900	0.05560700	-1.49593600
C	-10.71346500	-0.45959400	0.78253300
C	-12.75054900	-0.12933800	-1.13118900
H	-11.16717700	0.32918800	-2.52323000
C	-12.04745800	-0.64169500	1.13357400
H	-9.91332000	-0.58256900	1.50969900

C	-13.07583600	-0.48096600	0.19061800
H	-13.54554700	-0.00299200	-1.86628100
H	-12.32056100	-0.91423400	2.15452600
C	-14.47508600	-0.69203700	0.63784800
O	-14.81101200	-0.99821400	1.76912200
O	-15.38234900	-0.50579600	-0.36778500
H	-16.25197800	-0.67058000	0.04661200
O	2.86566900	1.56445400	-3.22977600
C	-6.71330900	0.30870100	-1.19686700
O	0.10257200	1.25776200	-3.29671800
H	1.08704800	1.39288400	-3.35941600
S	4.86312800	1.81229400	2.13557200
C	3.57529300	2.18849700	3.35708500
H	2.74309700	2.70027400	2.85654700
H	3.26053700	1.23559900	3.80031000
H	4.02974200	2.82765100	4.12684200
C	4.98148700	3.44038600	1.33733200
H	4.00171200	3.70287200	0.91540500
H	5.30133300	4.14654000	2.11780200
H	5.75155600	3.34264200	0.56293800
S	6.71545800	-2.60469000	-2.29290600
C	5.11148000	-2.89973200	-3.11383900
H	4.33584800	-3.09138200	-2.36232900
H	4.89137000	-1.99450900	-3.69324700
H	5.24526400	-3.76255200	-3.78191900
C	6.61895100	-3.96330000	-1.07879300
H	5.70546500	-3.83391800	-0.48295100
H	6.61017500	-4.91392500	-1.63060600
H	7.51875700	-3.89894400	-0.45469700
N	0.60684900	0.96324300	2.91352200
O	0.68677800	0.53743800	4.04225900
N	7.19839600	-1.89323100	1.54859000
O	8.32957500	-1.67404500	0.84972300
H	8.27688200	-0.69329200	0.42018700
O	7.12574300	-2.93248300	2.16296400
S	-1.17714400	-2.47544800	2.31002500
C	-0.88630800	-2.91082900	0.54912000
H	-1.82792000	-2.71801800	0.01938700
H	-0.07231800	-2.29505100	0.14479100
H	-0.62821300	-3.97744900	0.48827900
C	0.56242600	-2.69778800	2.85257700
H	1.20265900	-2.03440300	2.25815400
H	0.59948500	-2.41543500	3.91172600
H	0.84135200	-3.75300800	2.72365500
O	-0.12162500	2.07596900	2.73505300
H	-0.05231400	2.42024400	1.72083300

Mg-H₂ODA final

0 1

Mg	3.30852200	-1.54103800	-0.01291100
O	3.83165800	0.23859100	-1.11552400
O	5.46898800	-1.88639200	0.15389300
O	-0.07457000	-4.06956700	0.32952100
O	3.35237300	-2.42884200	-1.86098900
O	4.98947600	2.91985200	-0.50102500
O	2.35754100	2.73523200	-1.92437000
O	4.72773400	-4.16694600	-1.89688300
O	0.52243300	3.82312000	-2.40911900
O	2.44490800	3.68205000	0.74077000
O	3.43986500	-0.74668900	1.91736100
O	4.02434800	1.37440400	1.75414400
N	3.70972300	0.37009400	2.47865400
N	0.13962900	-4.28065100	-0.86735500
O	0.10675300	-5.33584400	-1.45335200
O	3.66188000	0.46980800	3.70597900
N	1.68002400	3.79736600	-2.06092000
O	2.29506000	4.95366000	-1.84872800
N	4.05491100	-3.28755800	-2.52671400
O	4.05428800	-3.24098100	-3.75078000
O	2.94471600	-3.33457000	0.87617900
Mg	3.18994600	1.95604300	-0.07619500
O	1.42801600	1.02547800	0.32950000
C	-0.73639700	0.12753200	0.03393600
C	-1.58062100	-0.98925400	0.15148400
C	-1.30681600	1.40749300	-0.09560200
C	-2.96665900	-0.84726000	0.14448900
H	-1.15081100	-1.98560100	0.26867800
C	-2.68660600	1.56144000	-0.12361400
H	-0.64750100	2.27110500	-0.19232600
C	-3.52757400	0.43635400	-0.00076400
H	-3.62237600	-1.70981400	0.24592100
H	-3.12661500	2.55469500	-0.24630800
C	0.74739900	-0.00328200	0.05317300
N	-4.91043500	0.65472200	-0.02995200
H	-5.25097900	1.61572800	-0.14410700
O	-5.85639200	-1.46418600	0.21381400
C	-7.28919600	0.49058400	-0.02124800
O	-7.36182400	1.71388200	-0.15611500
N	-8.30815500	-0.40737500	0.07011600
H	-7.96695400	-1.36883700	0.17793100
C	-9.69178600	-0.19187400	0.03567400

C	-10.52907100	-1.31972600	0.14854500
C	-10.25438200	1.09251000	-0.10539700
C	-11.91089300	-1.17129000	0.12159300
H	-10.08493600	-2.31277700	0.25674400
C	-11.63907500	1.22630900	-0.13064100
H	-9.59887700	1.95668900	-0.19259500
C	-12.47964300	0.10678600	-0.01843100
H	-12.55953300	-2.04310900	0.20841200
H	-12.10013000	2.20962000	-0.23902500
C	-13.94699500	0.32683300	-0.05349200
O	-14.49043100	1.41176900	-0.17180600
O	-14.65591300	-0.83611100	0.06312100
H	-15.59340800	-0.56246300	0.02613300
O	0.43342800	-3.17441200	-1.66063700
C	-5.93012100	-0.24220700	0.06998300
O	1.27539100	-1.15221700	-0.19761000
H	0.63998400	-2.41353400	-1.01606700
S	4.37367200	-0.03319800	-2.58583700
C	5.15980900	1.51882900	-3.09806400
H	4.44518400	2.34845100	-3.05662200
H	5.99395400	1.69662600	-2.40958800
H	5.53078000	1.34661700	-4.11889800
C	2.89784100	0.02419500	-3.63899700
H	2.33342000	0.93665200	-3.40856300
H	3.23928500	-0.00171200	-4.68321400
H	2.33964900	-0.88968100	-3.40854100
S	2.44361700	-3.93660100	2.21300300
C	1.23050900	-2.77416800	2.92552400
H	1.71047500	-1.80103100	3.08229600
H	0.41126800	-2.71295100	2.20134600
H	0.87442400	-3.21366500	3.86817100
C	3.78893900	-3.64277600	3.41104500
H	4.00777400	-2.56776500	3.44689600
H	3.46486200	-4.02262200	4.39037200
H	4.65752500	-4.21198400	3.05727600
N	5.32213400	4.15505600	-0.39377600
O	6.36771700	4.48015600	0.15010000
N	5.95703200	-2.83281000	0.82118000
O	5.72778600	-4.08342600	0.38384300
H	5.18256300	-4.01055300	-0.53449800
O	6.61784800	-2.71221700	1.82685200
S	2.39252400	4.43797700	2.08854200
C	1.74698000	3.25918600	3.32409700
H	0.81088800	2.86592200	2.90734200
H	2.46894500	2.45191000	3.50479300
H	1.54226700	3.82323000	4.24535500

C	4.10742500	4.53240500	2.69850900
H	4.08131100	4.95205100	3.71430100
H	4.53938800	3.52249600	2.68856100
H	4.65461900	5.20733600	2.02833900
O	4.54321100	5.06120500	-0.88147000
H	3.29219800	4.78998400	-1.41335500

Mg-H₂TDA initial

0 1

Mg	-6.95410500	0.50635400	-0.10351400
O	-5.68795700	-1.18268700	-0.45166900
O	-7.52944900	-0.38072400	1.77254400
O	-6.24901000	1.36667000	-1.88608300
O	-8.40376600	-0.52214500	-1.13576000
O	-3.03689300	-2.27207300	0.67348500
O	-3.42356200	-1.70240400	-2.22642200
O	-10.10553100	-1.15414700	0.13980100
O	-2.35398000	-1.32795800	-4.10511000
O	-0.30408200	-1.86334800	2.11768300
O	-5.53712100	1.63032700	0.93822200
O	-3.90156800	0.23480200	1.41581500
N	-4.57426800	1.27790200	1.72026400
N	-5.07951200	1.80824700	-2.11715000
O	-4.88661900	2.79383000	-2.81381600
O	-4.31204800	1.93744200	2.71691900
N	-2.32004200	-1.67797500	-2.93927200
O	-1.24704900	-2.04219700	-2.36195700
N	-9.40821600	-1.30719300	-0.91733000
O	-9.67620900	-2.18450600	-1.72819500
O	-8.24962400	2.03979600	0.23946000
Mg	-3.67011400	-0.59806900	-0.49185500
O	-1.75738100	0.12291900	-0.50721200
C	0.44478100	0.88311300	-0.96160300
C	1.28542600	1.79273700	-1.62892600
C	1.00645500	-0.11398000	-0.14049600
C	2.66765800	1.72554900	-1.48753900
H	0.84423600	2.55877500	-2.26791200
C	2.38319000	-0.18570400	0.00602300
H	0.36373900	-0.81598700	0.39927100
C	3.22827600	0.72531600	-0.66432300
H	3.32433500	2.42841900	-1.99397800
H	2.81301600	-0.96267200	0.64530500
C	-1.01302500	0.92784300	-1.10867700
N	4.60728900	0.57049100	-0.47733500
H	4.86969500	-0.18399800	0.15273900

O	5.48928400	2.38114900	-1.60973100
C	11.03258300	-0.42820200	0.36554100
O	11.19021800	-1.44598300	1.03509800
N	12.07042000	0.34454100	-0.13134700
H	11.80351800	1.08711800	-0.77316900
C	13.45296000	0.17995500	0.03994500
C	14.29750800	1.08306600	-0.63951600
C	14.01713000	-0.82343200	0.85425900
C	15.67808100	0.99123000	-0.51360800
H	13.85892100	1.86209600	-1.27026200
C	15.40149900	-0.90305300	0.97239000
H	13.36221200	-1.52177800	1.36941400
C	16.24607600	-0.00683200	0.29758300
H	16.32638900	1.69097700	-1.04137300
H	15.85908000	-1.67238800	1.59702500
C	17.71091300	-0.15480800	0.47205000
O	18.25503400	-1.00064700	1.16171800
O	18.42241400	0.77574500	-0.23506600
H	19.35828500	0.57367200	-0.03932000
O	-4.06520400	1.19160800	-1.58323700
O	-1.48958700	1.87038400	-1.91405100
H	-2.49011200	1.78199100	-1.92522900
S	-6.44454100	-2.46739100	-1.01389900
C	-5.25919800	-3.82727000	-0.83296800
H	-4.34283500	-3.60240800	-1.39245400
H	-5.06544100	-3.94339800	0.24041800
H	-5.76259500	-4.72395800	-1.22209800
C	-6.42817900	-2.28053600	-2.81637000
H	-5.39765500	-2.08139700	-3.13982200
H	-6.83473100	-3.21006600	-3.23904900
H	-7.10986200	-1.44877600	-3.02585700
S	-8.21552800	3.56412100	0.51621600
C	-6.76137900	4.24419100	-0.35174400
H	-5.85126900	3.78092400	0.04852800
H	-6.88285500	4.00989400	-1.41690900
H	-6.76432800	5.33265800	-0.19838800
C	-7.60997800	3.75918400	2.22572800
H	-6.63770200	3.25982500	2.32926700
H	-7.54391700	4.83570700	2.43913400
H	-8.35873300	3.29348600	2.87894200
N	-2.28244400	-3.27056900	0.70865500
O	-2.30749500	-4.11100700	1.57395400
N	-8.35510900	0.18789700	2.53905300
O	-9.63620800	0.20916000	2.15882300
H	-9.71402700	-0.31515100	1.22044400
O	-8.07523700	0.70626800	3.59479900

S	-0.58135800	-1.10301700	3.41839400
C	-0.86438200	0.65445300	2.96544000
H	0.09756300	1.04936500	2.61437200
H	-1.61834800	0.69399300	2.16947500
H	-1.20363200	1.20478900	3.85404800
C	-2.31319100	-1.46543000	3.90836200
H	-2.52514800	-0.93604600	4.84834400
H	-2.99736600	-1.14943200	3.11106600
H	-2.36787500	-2.55056200	4.06075700
O	-1.40664800	-3.46991100	-0.29508200
H	-1.46889400	-2.72450300	-1.03768200
C	7.01920000	0.85317400	-0.59380800
C	8.06079900	1.79432400	-0.61244800
C	7.31388400	-0.48660300	-0.28148100
C	9.36509500	1.41048400	-0.30855400
H	7.81667700	2.82728500	-0.86556700
C	8.61817200	-0.87013100	0.02329200
H	6.53572300	-1.25402000	-0.31106800
C	9.65985100	0.07076300	0.00356400
H	10.14446800	2.17672700	-0.27878500
H	8.86159400	-1.90295600	0.27755900
C	5.64758600	1.35337600	-0.95583900

Mg-H₂ODA TS

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Mg	-6.59852000	0.15977000	-0.12122000
O	-5.22052000	0.14744000	1.54510000
O	-7.32407000	2.00289000	0.88154000
O	-5.18115000	-1.36580000	-0.50861000
O	-7.81182000	-0.93510000	1.09186000
O	-2.16106000	0.71915000	1.61996000
O	-3.23228000	-1.95086000	2.16933000
O	-9.84754000	-0.05765000	0.93591000
O	-2.53510000	-4.02956000	2.04610000
O	0.53292000	1.95233000	0.82383000
O	-5.45848000	1.49454000	-1.25264000
O	-3.36907000	0.96801000	-0.76363000
N	-4.20224000	1.61561000	-1.48552000
N	-5.33544000	-2.31269000	-1.43732000
O	-6.32171000	-2.22921000	-2.16825000
O	-3.81210000	2.34794000	-2.39112000
N	-2.27493000	-2.84527000	2.11340000
O	-1.07263000	-2.41170000	2.14203000
N	-9.08584000	-1.00009000	1.33278000
O	-9.52905000	-1.95657000	1.95067000

O	-8.01524000	0.35723000	-1.54507000
Mg	-3.50570000	-0.62700000	0.59712000
O	-2.18014000	-1.61952000	-0.51002000
C	0.08306000	-1.96026000	-1.19274000
C	0.99590000	-2.73903000	-1.92961000
C	0.55946000	-0.88890000	-0.41487000
C	2.35969000	-2.46889000	-1.89198000
H	0.62636000	-3.57041000	-2.53120000
C	1.91447000	-0.60540000	-0.37491000
H	-0.12280000	-0.24855000	0.14307000
C	2.82948000	-1.39505000	-1.10352000
H	3.07225000	-3.07206000	-2.44902000
H	2.24558000	0.24878000	0.22262000
C	-1.35228000	-2.23935000	-1.20159000
N	4.18152000	-1.04777000	-1.00443000
H	4.37672000	-0.29263000	-0.35096000
O	5.22170000	-2.64983000	-2.30271000
C	10.45788000	0.79146000	-0.49778000
O	10.57936000	2.01277000	-0.54936000
N	11.48572000	-0.07914000	-0.17130000
H	11.22023000	-1.05298000	-0.04599000
C	12.82859000	0.20867000	0.11442000
C	13.65499000	-0.87483000	0.47998000
C	13.37345000	1.50714000	0.04204000
C	14.99869000	-0.67286000	0.76964000
H	13.23177000	-1.88232000	0.53430000
C	14.72124000	1.69486000	0.33365000
H	12.73061000	2.33962000	-0.23314000
C	15.54745000	0.61966000	0.69860000
H	15.63296000	-1.51330000	1.05221000
H	15.16331000	2.69163000	0.28427000
C	16.97314000	0.89799000	0.99533000
O	17.49933000	1.99717000	0.94960000
O	17.66989000	-0.22892000	1.33701000
H	18.58024000	0.08382000	1.50571000
O	-4.50052000	-3.22638000	-1.48781000
O	-1.75984000	-3.22175000	-2.00307000
H	-2.74301000	-3.29493000	-1.86830000
S	-5.81006000	0.09894000	3.01231000
C	-4.37399000	0.47388000	4.05621000
H	-3.61359000	-0.30501000	3.91453000
H	-4.00481000	1.46266000	3.75707000
H	-4.72342000	0.50347000	5.09763000
C	-6.02454000	-1.65266000	3.44662000
H	-5.10840000	-2.19941000	3.18450000
H	-6.23171000	-1.68169000	4.52659000

H	-6.89212000	-2.00309000	2.87514000
S	-8.24683000	0.85000000	-2.99315000
C	-6.77119000	0.41606000	-3.97651000
H	-5.89903000	0.96253000	-3.59760000
H	-6.63851000	-0.66787000	-3.87163000
H	-6.98930000	0.67976000	-5.02125000
C	-7.98925000	2.65605000	-2.95404000
H	-7.00085000	2.85840000	-2.52007000
H	-8.06423000	3.03379000	-3.98357000
H	-8.79264000	3.07945000	-2.33871000
N	-1.48028000	0.88703000	2.65739000
O	-1.41509000	1.92594000	3.27259000
N	-8.20007000	2.78228000	0.43718000
O	-9.41450000	2.26586000	0.16317000
H	-9.41706000	1.23545000	0.45730000
O	-8.04749000	3.96425000	0.23097000
S	0.18717000	3.08214000	-0.15219000
C	-0.33234000	2.30601000	-1.73385000
H	0.53811000	1.75705000	-2.11503000
H	-1.17812000	1.62971000	-1.55460000
H	-0.61953000	3.10047000	-2.43689000
C	-1.47437000	3.71062000	0.30928000
H	-2.17127000	2.86453000	0.35152000
H	-1.37145000	4.17183000	1.29904000
H	-1.78868000	4.45640000	-0.43433000
O	-0.78050000	-0.15028000	3.14208000
H	-0.98492000	-1.04659000	2.58434000
C	6.59633000	-0.98112000	-1.28469000
C	7.75448000	-1.75316000	-1.46873000
C	6.72711000	0.36127000	-0.88401000
C	9.01234000	-1.21364000	-1.20929000
H	7.63738000	-2.77543000	-1.83196000
C	7.98623000	0.90557000	-0.64059000
H	5.85197000	1.01092000	-0.79803000
C	9.14071000	0.11812000	-0.77446000
H	9.89607000	-1.83034000	-1.39390000
H	8.10786000	1.95179000	-0.35549000
C	5.28405000	-1.64805000	-1.59454000

Mg-H₂ODA final

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Mg	4.72951300	-1.42559400	-0.05731600
O	5.04849900	0.40928800	-1.14990300
O	6.91667100	-1.57346400	0.05099900
O	1.59680100	-4.25694400	0.28959900

O	4.81078500	-2.28421500	-1.91830300
O	5.95814700	3.19649600	-0.53774400
O	3.30736000	2.75217700	-1.86773200
O	6.34822800	-3.87760300	-2.02272800
O	1.35460500	3.65684600	-2.26057300
O	3.42619000	3.69164200	0.80016500
O	4.84568400	-0.65238000	1.88321800
O	5.23937600	1.51282900	1.72863200
N	5.03057400	0.47869500	2.44958200
N	1.78149200	-4.40802100	-0.92098400
O	1.81553000	-5.44156200	-1.54456700
O	5.00344800	0.56355700	3.67892000
N	2.52485900	3.74384300	-1.96645000
O	3.03300000	4.95350600	-1.77597400
N	5.57703500	-3.05711400	-2.61798300
O	5.54070000	-2.98826800	-3.84062900
O	4.55937300	-3.25973300	0.80667400
Mg	4.28886400	2.04378300	-0.06132400
O	2.64093300	0.94903100	0.40358900
C	0.55583000	-0.12504100	0.12785100
C	-0.19168500	-1.30935100	0.23813900
C	-0.12417600	1.10358400	0.03326200
C	-1.58498200	-1.28683100	0.25920200
H	0.32118500	-2.26869500	0.32834200
C	-1.51146000	1.13828900	0.03009000
H	0.45613100	2.02242800	-0.06029900
C	-2.25820000	-0.05402400	0.14577900
H	-2.16247000	-2.20197600	0.36505200
H	-2.03184400	2.09550700	-0.07003100
C	2.04341400	-0.12809700	0.11505100
N	-3.65532600	0.06192800	0.12740900
H	-4.00547400	1.01416400	0.05492300
O	-4.35427200	-2.10144400	0.53844700
C	-10.16530500	0.78039000	-0.14565200
O	-10.42217400	1.96028300	-0.37201400
N	-11.12322600	-0.21012700	0.00134100
H	-10.77186000	-1.16286100	0.06027000
C	-12.52129000	-0.09665900	-0.02893400
C	-13.26607700	-1.28960500	0.08303700
C	-13.19436900	1.13600100	-0.15384300
C	-14.65505800	-1.25958400	0.07034900
H	-12.74303900	-2.24559600	0.18092500
C	-14.58594600	1.15153900	-0.16373900
H	-12.61564300	2.05152600	-0.24795300
C	-15.33148900	-0.03324200	-0.05313900
H	-15.22613000	-2.18422800	0.15624100

H	-15.12708300	2.09457200	-0.26008300
C	-16.81095100	0.06313400	-0.07213900
O	-17.44666000	1.09851400	-0.17679300
O	-17.41974900	-1.15670500	0.04251900
H	-18.37667600	-0.96013500	0.01656200
O	1.94980600	-3.25406300	-1.68246500
O	2.66462900	-1.22020700	-0.17599000
H	2.11282700	-2.50015000	-1.01667700
S	5.55679500	0.20838800	-2.64364800
C	6.16162200	1.83763400	-3.16223700
H	5.37009100	2.59078800	-3.07942400
H	7.00107900	2.09075100	-2.50447000
H	6.50644800	1.71556400	-4.19932700
C	4.04220800	0.12768400	-3.63904200
H	3.39902600	0.97640300	-3.37404100
H	4.34343000	0.14715400	-4.69569900
H	3.58736600	-0.83992700	-3.40087200
S	4.13042800	-3.92282100	2.13968000
C	2.82945800	-2.88143700	2.88313000
H	3.22453400	-1.87217200	3.04828900
H	1.99952400	-2.88209700	2.16855500
H	2.52461100	-3.36299400	3.82316800
C	5.46145800	-3.52825600	3.32471700
H	5.58584300	-2.43875500	3.37288500
H	5.18643700	-3.94836600	4.30259900
H	6.37152100	-4.01356600	2.95064100
N	6.15149400	4.45854600	-0.40410200
O	7.13958300	4.88706800	0.17477100
N	7.50121000	-2.47968800	0.69612500
O	7.38529700	-3.73924800	0.24006400
H	6.81694500	-3.70346900	-0.66577000
O	8.16195200	-2.31312600	1.69527300
S	3.29772000	4.38037400	2.17877800
C	2.76233500	3.09417600	3.35932300
H	1.88896900	2.61059200	2.90304300
H	3.56748400	2.36869700	3.53512400
H	2.47258800	3.59941800	4.29173900
C	4.99507100	4.60964000	2.80143700
H	4.92791900	4.99516200	3.82887400
H	5.51556100	3.64314300	2.76293500
H	5.48296900	5.34871700	2.15323600
O	5.29638200	5.28199300	-0.90953500
H	4.06451900	4.89006100	-1.38752500
C	-6.03255600	-0.44204700	0.16620000
C	-7.02551300	-1.22548200	0.77539900
C	-6.41265400	0.70927200	-0.54749800

C	-8.36661900	-0.85747300	0.69057700
H	-6.71487400	-2.12087600	1.31621400
C	-7.75358600	1.07790400	-0.63125500
H	-5.66990700	1.30944500	-1.08001500
C	-8.74647900	0.29448300	-0.02197400
H	-9.11048500	-1.45840300	1.22063900
H	-8.06396500	1.97340700	-1.17200500
C	-4.61382300	-0.92612400	0.29302800

Section S3: Electronic structure

The total DOS of all MOFs and the partial DOS of ions surrounding the Fermi energy E_F are examined, as displayed in Figure S1. The valence and conduction band of these MOFs shows mainly orbitals contributions from linkers. PDOS of Al, Mg metal; and OH, DMSO axial molecules in these MOFs reveal that their orbitals occupy below -1.00 eV; i.e they do not affect on the physical properties of these MOFs. The band gap of these MOFs are from 2.25 eV to 2.58 eV as shown in Figure S2, indicating that these belong to the semiconductor. The band structure of these MOFs are flat and featureless which have also been witnessed in that of IRMOF-1 series, which could be explained by the weak orbital hybridizations.

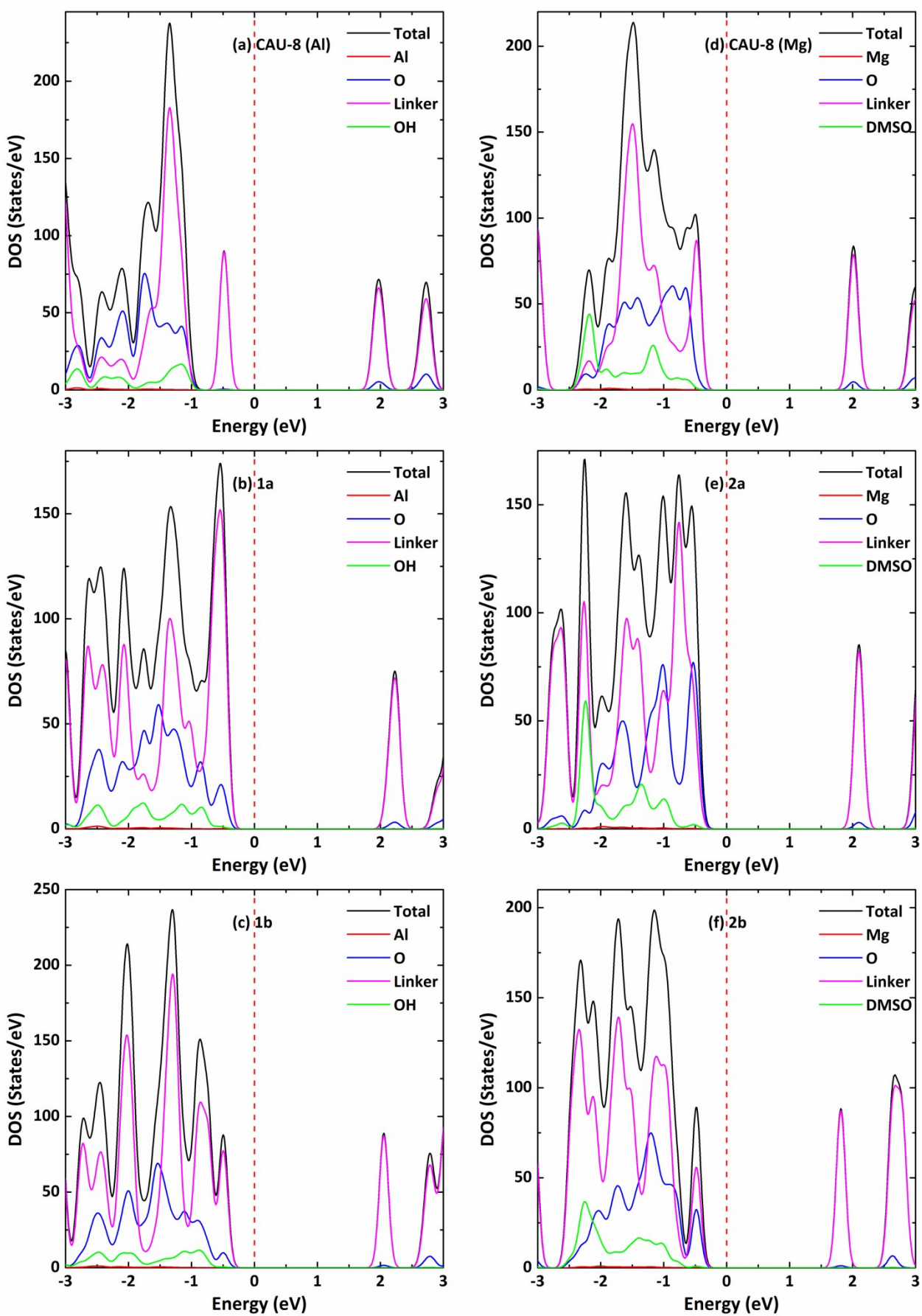


Figure S2. Total density of states and projected density of states for of (a) CAU-8(Al), (b) **1a**, (c) **1b**, (d) CAU-8(Mg), (e) **2a**, and (f) **2b**. Fermi level is set to zero.

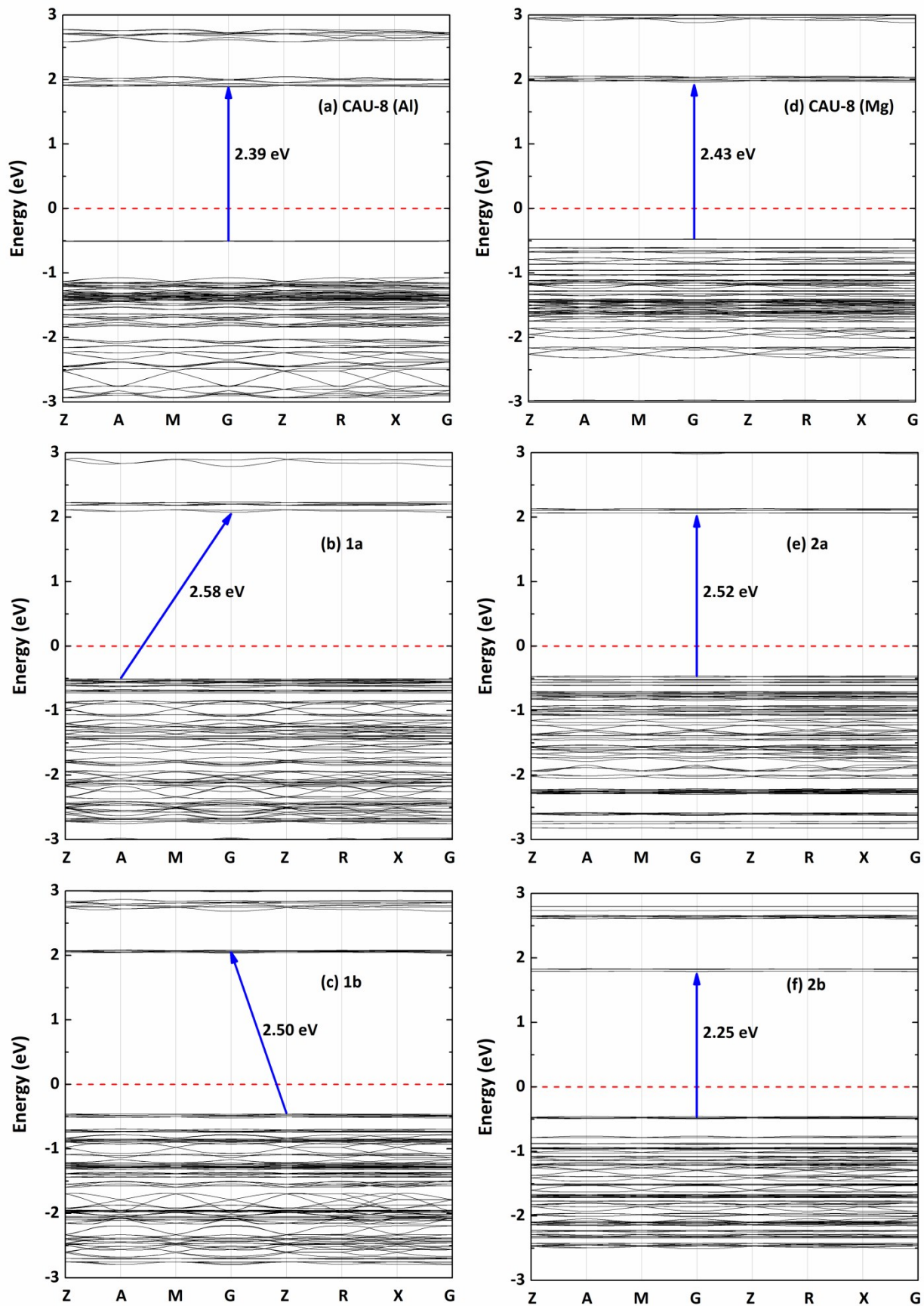


Figure S3. Band structures of (a) CAU-8(Al), (b) **1a**, (c) **1b**, (d) CAU-8(Mg), (e) **2a**, and (f) **2b**.

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