O_2 Activation and Oxidative Dehydrogenation of Propane on Hexagonal Boron Nitride: Mechanism Revisited

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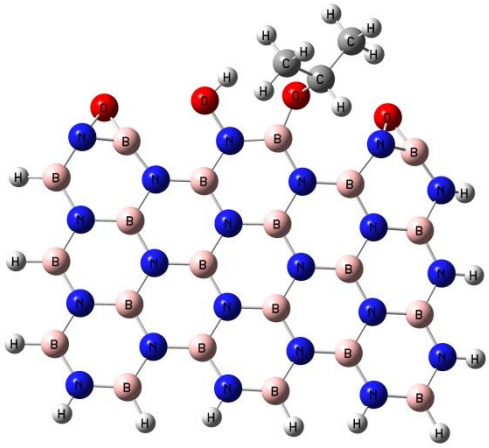
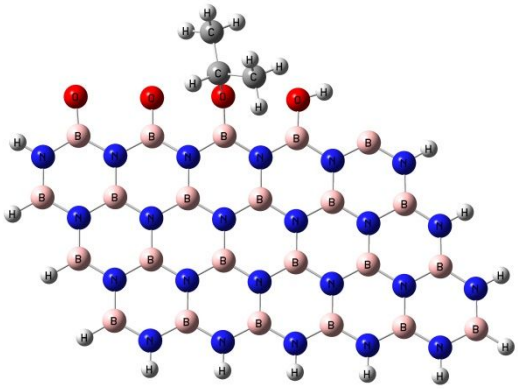


(a)



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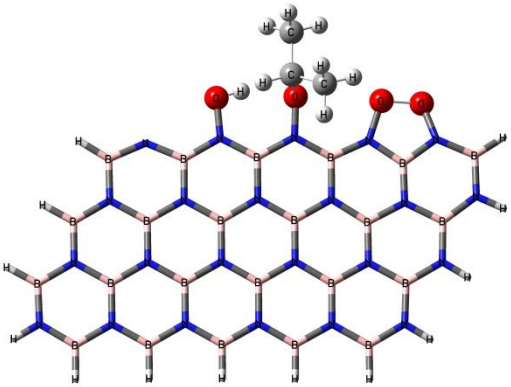

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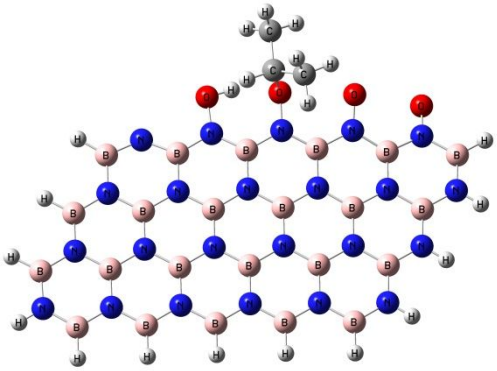

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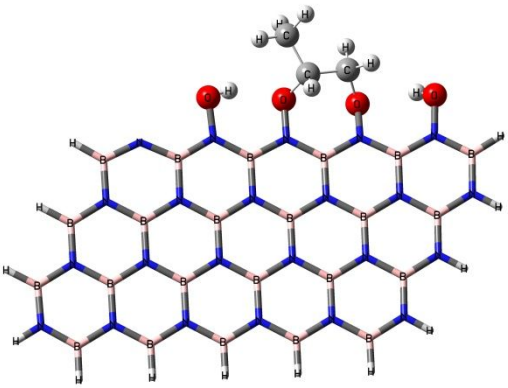

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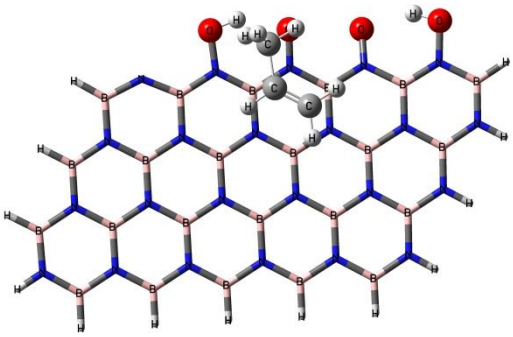

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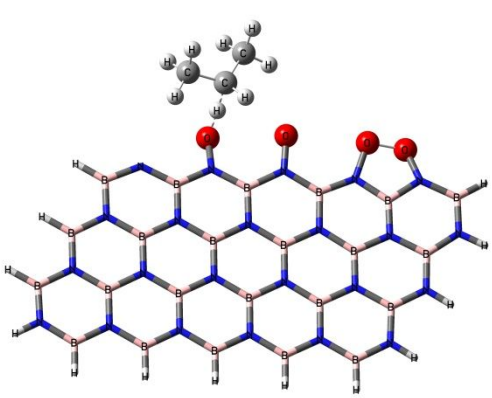

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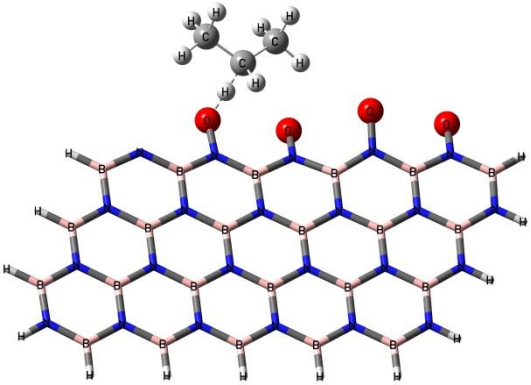

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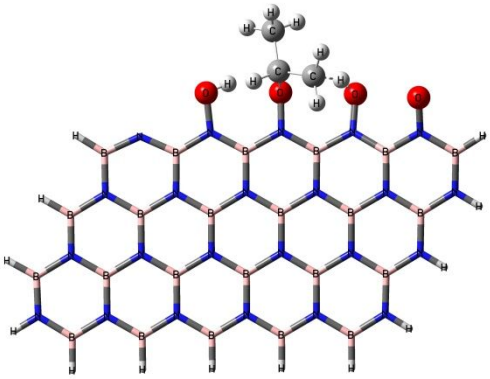
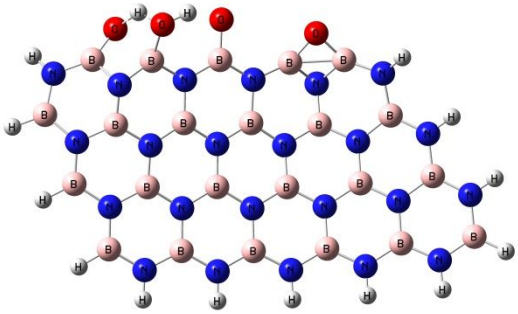


(i)



(j)

Figure S1. Optimized structures. (a) IM-arm-1a (b) IM-zig-B-1a (c) IM-zig-N-1 (d) IM-Zig-N-1a (e) IM-Zig-N-2 (f) IM-Zig-N-3 (g) TS3 (h) TS6 (i) TS9 (j) TS structure for formation B···OH_2 intermediate.

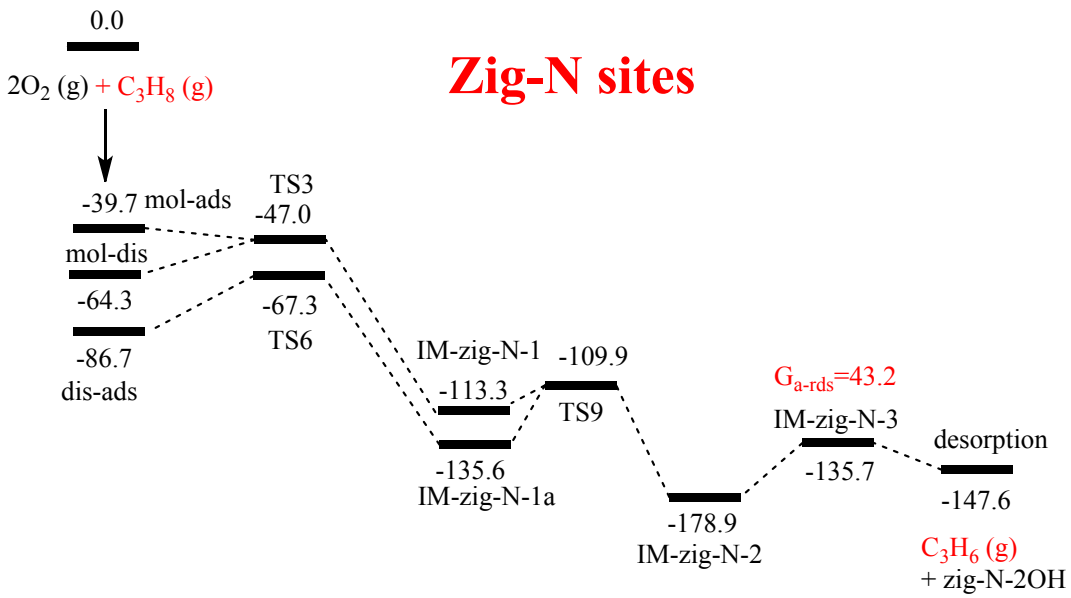
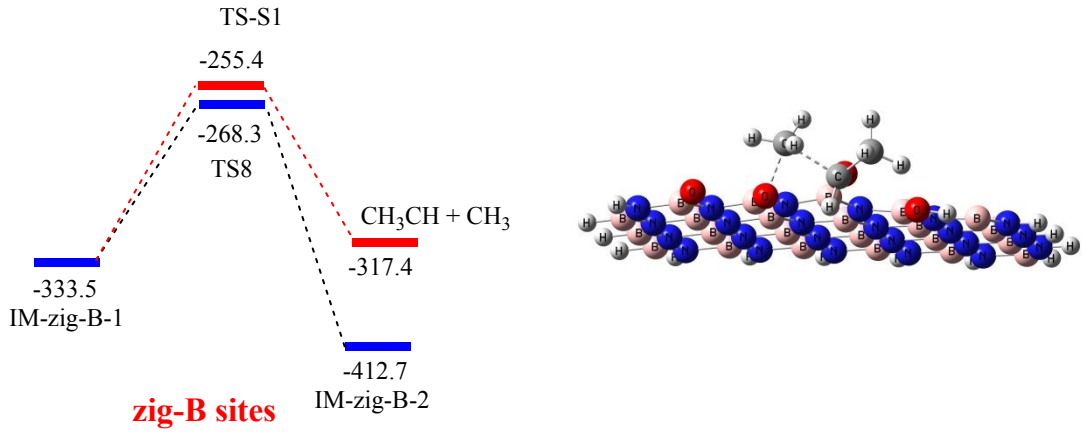


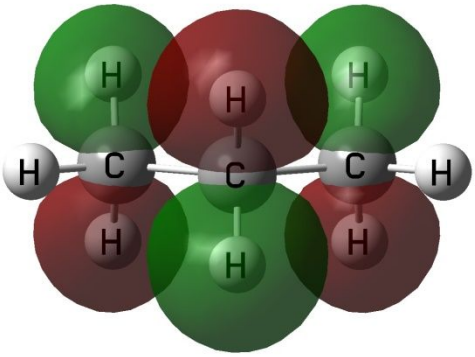
Figure S2. Free energy profile of ODHP reaction pathways on zig-N edge models at 763 K. (unit: kcal/mol)

On zig-N edge, the energy level of starting point is in the middle as compared with armchair and zig-B edge. It can be seen that the first dehydrogenation step is easily occurred whether the starting point is the molecular adsorption or dissociative adsorption (TS3 and TS6). The formed IM-zig-N-1 and IM-zig-N-1a can fast dehydrogenate into IM-zig-N-2 due to low activation free energy (e.g., ΔG_a = 25.7 kcal/mol for IM-zig-N-1a). Last, the IM-zig-N-2 breaks its two C-O bonds to form the IM-zig-N-3 ($\Delta G_{a\text{-}rds}$ = 43.2 kcal/mol) and finally the propene is produced by desorption (zig-N-2OH).

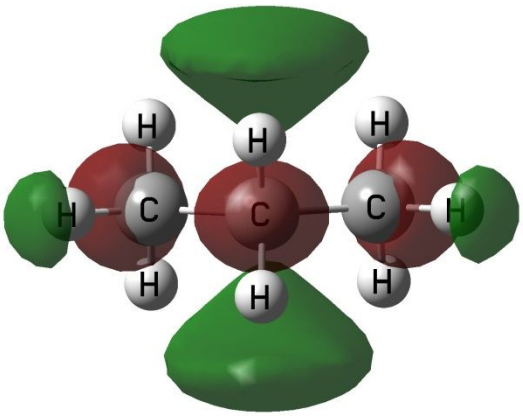


(a) (b)

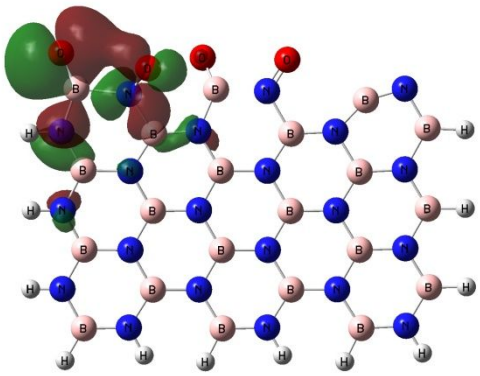
Figure S3. (a) Comparison of energy profile for the C-C bond break and 2nd dehydrogenation at zigzag B terminated edge. (b) Optimized structure of TS-S1



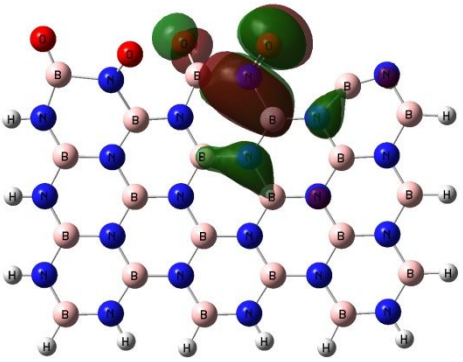
Propane HOMO



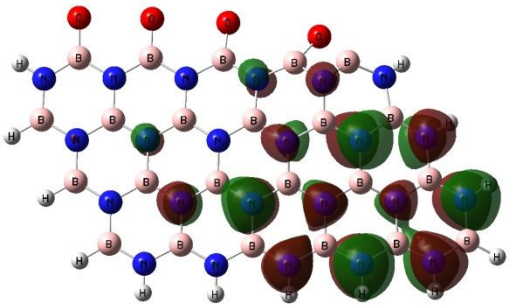
Propane LUMO



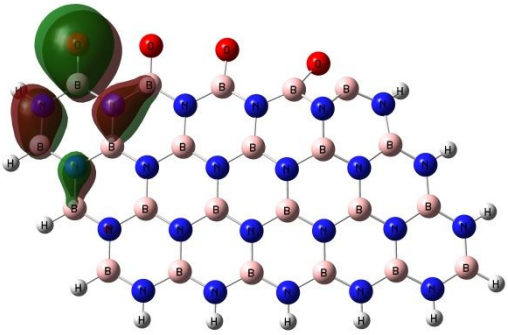
arm edge HOMO



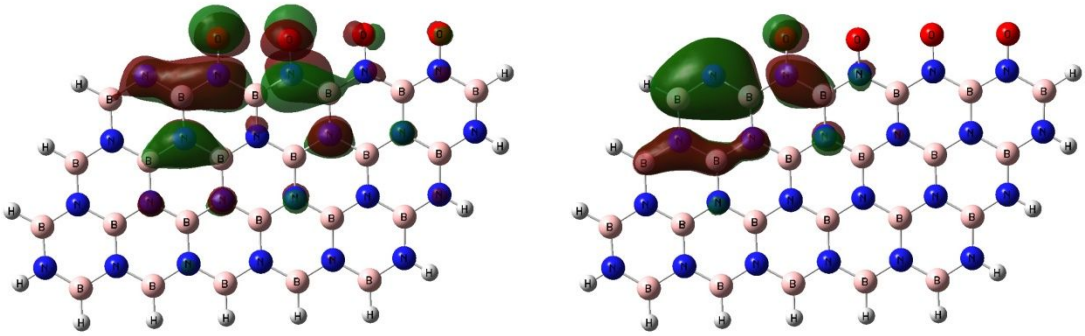
arm edge LUMO



Zig-B edge HOMO



Zig-B edge LUMO



Zig-N edge HOMO Zig-N edge LUMO

Figure S4. Frontier orbitals of propane, dissociative adsorption species on arm, zig-B, and zig-N edge models.

Table S1. NPA charge distributions of the involved atoms in different species.

species	O	H	C
O_2 and C_3H_8	0.000	0.188	-0.375
arm-4O	-0.109		
zig-B-4O	-0.855		
zig-N-4O	-0.209		
TS4	-0.271	0.372	-0.171
TS5	-0.567	0.260	-0.295
TS6	-0.403	0.329	-0.244

Routing Job for stationary points:

%chk=name.chk
%mem=xxGB
%nprocshared=xx
opt freq 6-311g(d,p) empiricaldispersion=gd3 m062x temperature=763

Title Card Required

Molecular specification

Routing Job for transition states search:

%chk=name.chk
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%nprocshared=xx
opt=(calcfc,ts,noeigentest) freq 6-311g(d,p) empiricaldispersion=gd3 m062x temperature=763

Title Card Required

Molecular specification

The optimized geometries of the crucial structure reported in the paper

IM-arm-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	6.987310	-2.808922	-0.361795
2	1	0	6.741827	-0.323852	-0.815754
3	1	0	6.480572	2.365772	-0.793353
4	1	0	-6.833074	1.363957	-1.343209
5	1	0	-6.838373	-1.135121	-0.640977
6	1	0	-6.763768	-3.595756	-0.234261
7	5	0	0.875878	-1.968818	0.177125
8	5	0	0.717421	0.535596	0.100951
9	5	0	-1.355218	-0.830585	0.000531
10	7	0	-0.569637	-2.043455	0.163905
11	7	0	1.526423	-0.676275	0.107775
12	7	0	-0.698881	0.440281	-0.057847
13	5	0	2.946615	-0.597360	-0.038773
14	5	0	-1.443100	1.672398	-0.294075
15	5	0	-1.235989	-3.322647	0.256047
16	5	0	3.137839	-3.079972	0.146830
17	5	0	2.672869	1.850820	-0.157912
18	5	0	0.539711	3.150504	0.440216
19	5	0	-3.561468	0.302216	-0.313753
20	5	0	-3.462675	-2.188036	-0.030204
21	5	0	1.012537	-4.440196	0.386819
22	5	0	4.956666	0.774856	-0.589293
23	5	0	5.193353	-1.682485	-0.267377
24	5	0	5.411673	-4.152644	0.015592
25	7	0	5.990314	-2.863959	-0.223455
26	7	0	4.003033	-4.223667	0.191959
27	7	0	5.766837	-0.374857	-0.561630
28	7	0	3.769280	-1.778913	-0.042629
29	7	0	1.690447	-3.172170	0.251328
30	7	0	-0.402152	-4.484320	0.401404
31	7	0	5.505822	2.145296	-0.933717
32	7	0	3.568101	0.713493	-0.254044
33	7	0	-2.689320	-3.402967	0.181780
34	7	0	-4.801282	-4.689317	0.141306
35	5	0	-3.385540	-4.659639	0.277468
36	5	0	4.476371	3.019080	-0.914050

37	5	0	-5.584581	-3.523384	-0.105113
38	5	0	-5.667337	-1.057325	-0.453206
39	7	0	3.190651	3.202677	-0.676664
40	7	0	1.347208	1.828926	0.190368
41	7	0	-2.799963	-0.909512	-0.101270
42	7	0	-4.906295	-2.255469	-0.189115
43	7	0	-0.785152	2.918423	-0.298389
44	7	0	-2.876353	1.570584	-0.453884
45	7	0	-5.020209	0.226907	-0.483311
46	5	0	-3.795193	2.639684	-0.618867
47	5	0	-5.779287	1.426260	-0.798995
48	7	0	-5.171854	2.678844	-0.348721
49	8	0	-1.715606	3.988068	-0.194511
50	8	0	-4.419610	3.544672	-1.421244
51	1	0	-5.270954	-5.578550	0.209795
52	1	0	-2.806617	-5.683928	0.468226
53	1	0	-0.843075	-5.386528	0.484401
54	1	0	1.619576	-5.461984	0.482625
55	1	0	3.588417	-5.130568	0.338607
56	1	0	6.092983	-5.126728	0.055783
57	8	0	1.355967	4.327887	-0.071505
58	8	0	2.184968	4.001765	-1.179226
59	6	0	-0.557568	2.515171	2.725827
60	6	0	0.390193	3.492285	2.024934
61	1	0	-0.603004	2.704781	3.803172
62	1	0	-1.574839	2.622098	2.332522
63	6	0	-0.038653	4.935551	2.326567
64	1	0	1.395167	3.352699	2.452054
65	1	0	-1.484527	4.593932	-0.905845
66	1	0	0.637450	5.657302	1.863164
67	1	0	-1.043968	5.123278	1.944213
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69	1	0	-0.254693	1.472293	2.586763

IM-arm-1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	1	0	-6.624888	2.736188	-1.158802
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6	1	0	-7.580320	-2.152549	-0.112831
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28	7	0	3.091964	-2.664391	-0.025584
29	7	0	0.758957	-3.528016	0.314436
30	7	0	-1.561064	-4.342524	0.554198
31	7	0	5.752199	0.650694	-0.965813
32	7	0	3.499657	-0.189589	-0.177501
33	7	0	-3.554428	-2.814634	0.266153
34	7	0	-5.888644	-3.633661	0.250040
35	5	0	-4.497310	-3.899166	0.375838
36	5	0	5.101121	1.867280	-0.757733
37	5	0	-6.411812	-2.331933	0.005213
38	5	0	-5.982963	0.092909	-0.336359
39	7	0	4.029429	2.202097	0.079142
40	7	0	1.572930	1.425018	-0.034341
41	7	0	-3.129691	-0.360097	-0.049213
42	7	0	-5.480847	-1.234595	-0.090759
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45	7	0	-5.080690	1.213652	-0.358022
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53	1	0	-2.185601	-5.119842	0.695934
54	1	0	0.196326	-5.727797	0.698141
55	1	0	2.130348	-5.876888	0.386813
56	1	0	4.557135	-6.480061	0.089256
57	8	0	1.723252	3.957811	0.122786
58	8	0	4.513267	3.006113	-1.193303
59	6	0	1.292947	4.865047	2.305690
60	6	0	2.354139	4.302086	1.370807
61	1	0	1.728668	5.102799	3.278554
62	1	0	0.866357	5.781058	1.888033
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66	1	0	4.165852	4.849712	0.362075
67	1	0	3.031609	6.192670	0.613195
68	1	0	3.980485	5.572881	1.979139
69	1	0	0.483110	4.146565	2.456867

IM-arm-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.746494	-4.576514	-0.623369
2	1	0	6.168164	-2.130544	-1.046622
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4	1	0	-6.740895	2.953313	-0.903208
5	1	0	-7.202759	0.576424	-0.414173
6	1	0	-7.721805	-1.817030	0.102683
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9	5	0	-1.797252	-0.462634	0.059058
10	7	0	-1.316139	-1.837709	0.190432
11	7	0	1.059952	-1.027717	0.007831
12	7	0	-0.829505	0.623419	0.032143
13	5	0	2.446538	-1.329060	-0.182159
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18	5	0	1.020783	2.785133	0.556467
19	5	0	-3.673300	1.188562	-0.275205
20	5	0	-4.167520	-1.259129	0.110139
21	5	0	-0.388382	-4.560924	0.432854
22	5	0	4.758769	-0.585075	-0.762833
23	5	0	4.314268	-3.012453	-0.471217
24	5	0	3.883271	-5.450952	-0.148876
25	7	0	4.776115	-4.361043	-0.440318
26	7	0	2.517864	-5.128187	0.087053
27	7	0	5.214213	-1.910425	-0.792710
28	7	0	2.930129	-2.693938	-0.198376
29	7	0	0.579674	-3.496941	0.220637
30	7	0	-1.763182	-4.250742	0.502505
31	7	0	5.748234	0.538169	-1.071365
32	7	0	3.406402	-0.212532	-0.407951
33	7	0	-3.707449	-2.634419	0.339454
34	7	0	-6.076047	-3.363318	0.445809
35	5	0	-4.691522	-3.680284	0.517856
36	5	0	5.050789	1.671760	-0.940846
37	5	0	-6.554041	-2.032138	0.178225
38	5	0	-6.033755	0.379564	-0.301392
39	7	0	3.881457	2.232845	-0.598147
40	7	0	1.557672	1.452614	0.130419
41	7	0	-3.201633	-0.187819	-0.014900
42	7	0	-5.585313	-0.984744	0.006502
43	7	0	-0.355385	3.011703	0.363678
44	7	0	-2.702762	2.272699	-0.342672
45	7	0	-5.084182	1.423832	-0.462944
46	5	0	-3.273411	3.572155	-0.837158
47	5	0	-5.548015	2.825631	-0.824269
48	7	0	-4.612368	3.829451	-1.043132
49	8	0	-0.826042	4.285955	0.828431
50	8	0	-2.286310	4.573867	-1.167277
51	1	0	-6.752943	-4.102201	0.574143
52	1	0	-4.366531	-4.811724	0.724964
53	1	0	-2.420434	-5.006109	0.639683
54	1	0	-0.041343	-5.697170	0.544009
55	1	0	1.875431	-5.885691	0.274612
56	1	0	4.279052	-6.572189	-0.116899
57	8	0	1.726251	3.753703	1.248007
58	8	0	3.478086	3.571451	-0.840870

59	6	0	3.803147	4.428733	0.308868
60	6	0	3.078012	4.002754	1.583034
61	1	0	4.890955	4.468338	0.438110
62	1	0	-1.327612	4.646895	0.023222
63	6	0	3.716341	2.892316	2.423267
64	1	0	3.058151	4.897960	2.215672
65	1	0	3.154312	2.802513	3.355300
66	1	0	3.708315	1.914065	1.941530
67	1	0	4.750706	3.152584	2.670737
68	1	0	3.420918	5.391513	-0.031443
69	1	0	-2.752846	5.336378	-1.550936

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	6.683596	-3.104582	-0.197628
2	1	0	6.659149	-0.590048	-0.242547
3	1	0	6.534677	2.061427	0.151509
4	1	0	-7.083482	1.884911	0.054217
5	1	0	-7.059120	-0.563430	0.264080
6	1	0	-7.087209	-3.044406	0.491976
7	5	0	0.595412	-1.919952	-0.278687
8	5	0	0.562911	0.575146	-0.450884
9	5	0	-1.578801	-0.634289	-0.210187
10	7	0	-0.839213	-1.895404	-0.198287
11	7	0	1.326788	-0.659857	-0.388047
12	7	0	-0.846906	0.616257	-0.334036
13	5	0	2.757252	-0.671089	-0.360930
14	5	0	-1.593131	1.892690	-0.268630
15	5	0	-1.578580	-3.138171	-0.060119
16	5	0	2.790833	-3.163387	-0.263532
17	5	0	2.681561	1.782873	-0.436348
18	5	0	0.619504	3.085343	-0.360069
19	5	0	-3.735065	0.659135	-0.147252
20	5	0	-3.731568	-1.853565	0.073697
21	5	0	0.593669	-4.402733	-0.149465
22	5	0	4.927732	0.603036	-0.301205
23	5	0	4.957655	-1.879926	-0.254936
24	5	0	5.001575	-4.372238	-0.219938
25	7	0	5.675744	-3.105382	-0.221562

26	7	0	3.582783	-4.359399	-0.241132
27	7	0	5.650208	-0.591678	-0.250166
28	7	0	3.512808	-1.890148	-0.294471
29	7	0	1.344409	-3.165834	-0.241525
30	7	0	-0.810119	-4.357729	-0.067701
31	7	0	5.609008	1.964848	-0.240520
32	7	0	3.494087	0.611797	-0.365987
33	7	0	-3.014924	-3.129952	0.085573
34	7	0	-5.177658	-4.282512	0.400543
35	5	0	-3.770431	-4.347578	0.254021
36	5	0	4.651574	2.902524	-0.309978
37	5	0	-5.904007	-3.046657	0.377328
38	5	0	-5.875044	-0.551600	0.150705
39	7	0	3.349035	3.153761	-0.388576
40	7	0	1.306462	1.828321	-0.596816
41	7	0	-2.998667	-0.617126	-0.077090
42	7	0	-5.166800	-1.831230	0.209833
43	7	0	-0.747286	3.086022	-0.121490
44	7	0	-3.004472	1.903990	-0.322210
45	7	0	-5.164320	0.654590	-0.048603
46	5	0	-3.883317	3.076961	-0.676642
47	5	0	-5.904279	1.972988	-0.173526
48	7	0	-5.245164	3.129274	-0.536084
49	8	0	-1.253571	4.294894	0.362698
50	8	0	-3.170611	4.164167	-1.263853
51	1	0	-5.691366	-5.141434	0.517849
52	1	0	-3.237936	-5.416105	0.275866
53	1	0	-1.308850	-5.229980	0.010360
54	1	0	1.143586	-5.460407	-0.134545
55	1	0	3.101302	-5.244854	-0.229830
56	1	0	5.619411	-5.387264	-0.197678
57	8	0	1.382650	4.282299	-0.266210
58	8	0	2.603530	4.153604	-0.979131
59	6	0	1.144794	3.266631	2.686066
60	6	0	1.033247	1.942954	2.673308
61	1	0	2.058355	3.751415	3.020799
62	1	0	-1.994135	4.499459	-0.267432
63	6	0	2.103737	0.982449	3.101961
64	1	0	0.094630	1.503053	2.338980
65	1	0	2.310151	0.243109	2.320464
66	1	0	3.030630	1.506631	3.347575
67	1	0	1.788655	0.418246	3.984189
68	1	0	0.328405	3.906876	2.366949
69	1	0	-3.855024	4.809658	-1.469841

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.663699	4.228851	-0.003326
2	1	0	-3.738231	5.819191	0.312321
3	1	0	7.066803	-2.953688	-0.453110
4	1	0	5.149107	-4.632126	-0.613667
5	5	0	1.543799	-0.424021	-0.115728
6	5	0	-0.822715	0.394380	-0.037437
7	5	0	1.082947	2.017517	0.122418
8	7	0	2.023915	0.930972	0.014223
9	7	0	0.120141	-0.698057	-0.104733
10	7	0	-0.339336	1.752565	0.078466
11	5	0	-0.358149	-2.065412	-0.167244
12	5	0	-1.271368	2.854056	0.149387
13	5	0	3.445964	1.193777	0.036149
14	5	0	1.993908	-2.859890	-0.415240
15	5	0	-2.737932	-1.229656	-0.112497
16	5	0	-3.181981	1.249498	-0.083119
17	5	0	0.633751	4.468084	0.363831
18	5	0	2.984588	3.640402	0.303541
19	5	0	3.916170	-1.250099	-0.244641
20	5	0	5.809893	0.380548	-0.066002
21	5	0	4.406849	-3.709506	-0.545751
22	5	0	6.288318	-2.061892	-0.349834
23	7	0	3.019006	-3.814185	-0.621750
24	7	0	4.876231	-2.335337	-0.380753
25	7	0	6.758141	-0.708422	-0.194191
26	7	0	0.594293	-3.113016	-0.363135
27	7	0	2.489485	-1.503678	-0.250797
28	7	0	4.389897	0.108294	-0.090459
29	7	0	6.281867	1.744141	0.087647
30	7	0	-1.779811	-2.284919	-0.049081
31	7	0	3.923899	2.555592	0.186158
32	5	0	5.340496	2.824996	0.211970
33	5	0	-5.109283	-0.316911	-0.389854

34	7	0	-4.193504	-1.438097	-0.187735
35	7	0	-2.254252	0.134413	-0.097938
36	7	0	1.567610	3.376657	0.267891
37	7	0	-4.611718	1.014586	-0.230181
38	7	0	-2.692485	2.598895	0.060631
39	7	0	-0.780243	4.211481	0.300139
40	5	0	-5.538607	2.138232	-0.212849
41	5	0	-3.619748	3.714684	0.105217
42	5	0	-1.709746	5.315972	0.369129
43	7	0	-5.021057	3.451106	-0.023744
44	7	0	-3.099036	5.039991	0.271782
45	1	0	8.964967	-1.316343	-0.270753
46	1	0	9.592638	1.108513	0.002817
47	1	0	-8.617405	0.393367	-0.887316
48	1	0	-7.589291	2.656714	-0.342317
49	5	0	8.176390	-0.433227	-0.167298
50	5	0	7.701647	2.013995	0.112439
51	7	0	8.602655	0.918101	-0.014820
52	7	0	-6.522018	-0.501664	-0.726149
53	7	0	-6.945822	1.880149	-0.376929
54	5	0	-7.474074	0.603744	-0.670696
55	8	0	0.256311	-4.468790	-0.532691
56	8	0	-2.211140	-3.617338	-0.022759
57	1	0	8.102485	3.126006	0.235497
58	1	0	5.728246	3.941019	0.334468
59	1	0	3.375617	4.754872	0.425829
60	1	0	1.030035	5.580690	0.488900
61	1	0	-1.318490	6.430367	0.499296
62	8	0	-4.709259	-2.615335	-0.005956
63	8	0	-6.956001	-1.641284	-1.176814
64	6	0	-3.003162	-3.453098	2.318166
65	6	0	-2.131980	-4.181299	1.309619
66	1	0	-2.741130	-2.395181	2.387392
67	1	0	-4.056731	-3.543332	2.055470
68	1	0	-2.839493	-3.895455	3.303372
69	6	0	-2.549643	-5.625691	1.118232
70	1	0	-0.688457	-4.457782	-0.744789
71	1	0	-1.079503	-4.128856	1.616892
72	1	0	-1.871647	-6.141325	0.435866
73	1	0	-2.535214	-6.148590	2.075527
74	1	0	-3.561777	-5.657740	0.710050

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.467950	4.374168	0.189123
2	1	0	-3.482163	5.938581	0.266013
3	1	0	7.053689	-3.190350	-0.037239
4	1	0	5.090623	-4.817729	-0.024620
5	5	0	1.607761	-0.474013	-0.055588
6	5	0	-0.728205	0.427909	-0.077686
7	5	0	1.224563	1.995236	0.009655
8	7	0	2.130977	0.872265	-0.021935
9	7	0	0.177824	-0.702125	-0.102757
10	7	0	-0.202791	1.773224	-0.004142
11	5	0	-0.344463	-2.056592	-0.141590
12	5	0	-1.106223	2.902762	0.056822
13	5	0	3.559373	1.092691	-0.010325
14	5	0	1.985580	-2.942025	-0.024056
15	5	0	-2.690411	-1.114302	-0.269920
16	5	0	-3.069856	1.347967	-0.037605
17	5	0	0.850457	4.468652	0.115727
18	5	0	3.175414	3.567552	0.052723
19	5	0	3.955047	-1.380541	-0.028967
20	5	0	5.897798	0.202222	-0.025458
21	5	0	4.374405	-3.872529	-0.004959
22	5	0	6.302052	-2.269832	-0.032967
23	7	0	2.984063	-3.943926	0.043159
24	7	0	4.883018	-2.502788	-0.022703
25	7	0	6.813017	-0.922486	-0.036853
26	7	0	0.578718	-3.146222	-0.059081
27	7	0	2.521964	-1.591168	-0.042807
28	7	0	4.470773	-0.028551	-0.024639
29	7	0	6.412409	1.559183	-0.015373
30	7	0	-1.766217	-2.211432	-0.291879
31	7	0	4.080625	2.447262	0.015516
32	5	0	5.503801	2.675049	0.008807
33	5	0	-5.046491	-0.202264	-0.167813
34	7	0	-4.115466	-1.292279	-0.312774
35	7	0	-2.161548	0.218980	-0.117544
36	7	0	1.752339	3.345766	0.058057
37	7	0	-4.501936	1.132629	-0.041902
38	7	0	-2.533740	2.686904	0.053957
39	7	0	-0.570060	4.251231	0.124627

40	5	0	-5.402825	2.270533	0.040482
41	5	0	-3.433561	3.822823	0.136134
42	5	0	-1.469017	5.382192	0.200624
43	7	0	-4.842162	3.584460	0.135806
44	7	0	-2.866930	5.141231	0.210960
45	1	0	9.000059	-1.601214	-0.057745
46	1	0	9.701930	0.818225	-0.050394
47	1	0	-8.553280	0.531163	-0.064283
48	1	0	-7.449545	2.814404	0.070138
49	5	0	8.238456	-0.688675	-0.046746
50	5	0	7.839057	1.787485	-0.025117
51	7	0	8.706639	0.657467	-0.042945
52	7	0	-6.471692	-0.363329	-0.173049
53	7	0	-6.816675	2.031673	0.012509
54	5	0	-7.384369	0.728128	-0.075930
55	8	0	0.188456	-4.493306	0.061128
56	8	0	-2.258250	-3.526495	-0.380640
57	1	0	8.273224	2.894052	-0.018577
58	1	0	5.925420	3.785614	0.023268
59	1	0	3.602228	4.675532	0.080151
60	1	0	1.282680	5.574585	0.157784
61	1	0	-1.042325	6.490626	0.253769
62	8	0	-4.609720	-2.511044	-0.815893
63	8	0	-7.044591	-1.648161	-0.107072
64	6	0	-4.598369	-3.540075	0.159254
65	6	0	-3.180897	-3.818375	0.675345
66	1	0	-4.975718	-4.412459	-0.380403
67	1	0	-5.280638	-3.295334	0.981037
68	6	0	-2.991081	-5.269629	1.068824
69	1	0	-0.653583	-4.541515	-0.409748
70	1	0	-2.940257	-3.162551	1.516302
71	1	0	-1.996056	-5.421331	1.488328
72	1	0	-3.737786	-5.562781	1.809956
73	1	0	-3.109069	-5.909582	0.190860
74	1	0	-6.660314	-2.119516	-0.855119

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	6.751115	3.002749	-0.362737

2	1	0	4.775846	4.587434	-0.546117
3	1	0	-5.791399	-4.570681	-0.064044
4	1	0	-3.821505	-6.130112	0.154592
5	5	0	-0.363551	-1.789789	0.044964
6	5	0	1.970393	-0.887023	0.002703
7	5	0	0.013321	0.700545	-0.140731
8	7	0	-0.888260	-0.435045	-0.049812
9	7	0	1.062062	-2.009472	0.089422
10	7	0	1.444309	0.458878	-0.125810
11	5	0	1.587112	-3.359083	0.212366
12	5	0	2.365204	1.565850	-0.229016
13	5	0	-2.315508	-0.226741	-0.082442
14	5	0	-0.742301	-4.279414	0.200806
15	5	0	3.926424	-2.452247	0.182386
16	5	0	4.318073	0.006472	-0.060967
17	5	0	0.406859	3.173582	-0.361630
18	5	0	-1.953221	2.280566	-0.147225
19	5	0	-2.680954	-2.732647	0.022607
20	5	0	-4.601825	-1.227301	-0.150056
21	5	0	-3.092403	-5.190378	0.139952
22	5	0	-5.053543	-3.638402	-0.065046
23	7	0	-1.684912	-5.367673	0.227788
24	7	0	-3.623980	-3.848172	0.033189
25	7	0	-5.572960	-2.294414	-0.165110
26	7	0	0.671482	-4.461563	0.271902
27	7	0	-1.260400	-2.931572	0.094292
28	7	0	-3.186136	-1.391808	-0.062453
29	7	0	-5.074032	0.094416	-0.240957
30	7	0	3.003673	-3.543574	0.267535
31	7	0	-2.850899	1.135051	-0.137132
32	5	0	-4.279857	1.258702	-0.252568
33	5	0	6.272183	-1.557668	0.125445
34	7	0	5.344567	-2.643345	0.227819
35	7	0	3.400743	-1.106025	0.042245
36	7	0	-0.516680	2.054037	-0.231155
37	7	0	5.747754	-0.214345	-0.023562
38	7	0	3.794169	1.350348	-0.203702
39	7	0	1.843290	2.912437	-0.360982
40	5	0	6.663825	0.901582	-0.135823
41	5	0	4.713114	2.464222	-0.317075
42	5	0	2.770283	3.987352	-0.477232
43	7	0	6.118750	2.220700	-0.283461
44	7	0	4.160910	3.792819	-0.460666
45	1	0	-7.805152	-2.795059	-0.302230

46	1	0	-8.386632	-0.368281	-0.481565
47	1	0	9.793636	-0.846964	0.082955
48	1	0	8.719595	1.420882	-0.174038
49	5	0	-6.980865	-1.937904	-0.286453
50	5	0	-6.419669	0.478022	-0.373533
51	7	0	-7.400985	-0.560023	-0.392205
52	7	0	7.696880	-1.745779	0.162609
53	7	0	8.077295	0.647943	-0.095537
54	5	0	8.617095	-0.663410	0.052742
55	8	0	-2.484657	3.533933	-0.094016
56	8	0	-0.036018	4.453565	-0.491825
57	1	0	-1.338358	-6.312085	0.300949
58	1	0	1.042401	-5.396544	0.349592
59	1	0	3.367704	-4.480120	0.357527
60	1	0	5.704347	-3.580514	0.328119
61	1	0	8.068056	-2.677230	0.266902
62	8	0	-5.127922	2.366134	-0.392287
63	8	0	-6.489958	1.866362	-0.463659
64	6	0	-3.931217	5.272558	0.600579
65	6	0	-3.132388	4.069104	1.059591
66	1	0	-4.670155	4.962339	-0.137994
67	1	0	-4.442024	5.740106	1.445134
68	1	0	-3.254396	5.999836	0.146036
69	6	0	-2.083629	4.424940	2.105034
70	1	0	-3.819074	3.319473	1.472779
71	1	0	0.708563	5.059473	-0.591414
72	1	0	-1.516766	3.538526	2.404435
73	1	0	-1.384223	5.151320	1.687974
74	1	0	-2.557165	4.844740	2.995561

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-6.782937	-3.109965	-0.478864
2	1	0	-4.792088	-4.682562	-0.420255
3	1	0	5.615269	4.579576	0.061023
4	1	0	3.667061	6.101047	0.422986
5	5	0	0.260271	1.745421	0.190402
6	5	0	-2.067835	0.827152	0.080873
7	5	0	-0.099764	-0.732152	0.086336

8	7	0	0.806281	0.401051	0.123858
9	7	0	-1.167697	1.953182	0.196374
10	7	0	-1.526437	-0.514089	0.024534
11	5	0	-1.709113	3.296333	0.299786
12	5	0	-2.430680	-1.641598	-0.074229
13	5	0	2.236138	0.208698	0.048558
14	5	0	0.617539	4.220548	0.388886
15	5	0	-4.038380	2.380847	0.117197
16	5	0	-4.396626	-0.087099	-0.108436
17	5	0	-0.477126	-3.223044	0.099129
18	5	0	1.870273	-2.236647	0.276636
19	5	0	2.579203	2.685789	0.147821
20	5	0	4.540925	1.170608	-0.224678
21	5	0	2.939387	5.161752	0.368431
22	5	0	4.884727	3.642402	0.021568
23	7	0	1.534764	5.324239	0.471049
24	7	0	3.471012	3.830100	0.188872
25	7	0	5.415777	2.328390	-0.207889
26	7	0	-0.798715	4.395096	0.427210
27	7	0	1.155685	2.879622	0.254059
28	7	0	3.120519	1.348882	-0.006358
29	7	0	5.069811	-0.158179	-0.471267
30	7	0	-3.127174	3.476113	0.268356
31	7	0	2.796155	-1.144198	0.033454
32	5	0	4.193212	-1.302661	-0.335859
33	5	0	-6.367146	1.467598	-0.103218
34	7	0	-5.456716	2.563305	0.050588
35	7	0	-3.497042	1.037678	0.029727
36	7	0	0.441071	-2.076236	0.144317
37	7	0	-5.826252	0.125834	-0.181183
38	7	0	-3.856564	-1.428260	-0.166459
39	7	0	-1.896222	-2.984719	-0.071109
40	5	0	-6.723764	-1.002472	-0.326219
41	5	0	-4.755553	-2.558032	-0.296411
42	5	0	-2.796468	-4.093903	-0.201721
43	7	0	-6.162797	-2.319733	-0.385502
44	7	0	-4.187018	-3.881176	-0.326497
45	1	0	7.557259	3.120499	-0.415579
46	1	0	8.302347	0.751411	-0.935636
47	1	0	-9.871440	0.729595	-0.390805
48	1	0	-8.768750	-1.536244	-0.503705
49	5	0	6.835653	2.176075	-0.447659
50	5	0	6.500805	-0.290303	-0.790312
51	7	0	7.323359	0.884049	-0.730264

52	7	0	-7.791681	1.646630	-0.180342
53	7	0	-8.138577	-0.756333	-0.400426
54	5	0	-8.694523	0.553804	-0.329467
55	8	0	2.291848	-3.485610	0.686644
56	8	0	-0.069295	-4.514045	0.189440
57	1	0	1.172173	6.258510	0.583162
58	1	0	-1.170930	5.329358	0.507009
59	1	0	-3.498893	4.411687	0.333336
60	1	0	-5.829360	3.498995	0.108552
61	1	0	-8.175017	2.577430	-0.127817
62	8	0	4.780363	-2.521417	-0.635493
63	8	0	7.111345	-1.450896	-1.146772
64	6	0	4.472509	-3.830414	-0.205163
65	6	0	3.616852	-3.843988	1.038660
66	1	0	5.424624	-4.332052	-0.010048
67	1	0	3.949826	-4.370005	-1.001555
68	6	0	3.560082	-5.221543	1.673034
69	1	0	4.012329	-3.110789	1.752952
70	1	0	0.874350	-4.566268	0.373969
71	1	0	2.857531	-5.214581	2.506387
72	1	0	3.219212	-5.959353	0.941846
73	1	0	4.541837	-5.521063	2.042172
74	1	0	6.468280	-2.168111	-1.171658
