

Electronic Supplementary Information

A zinc-containing porphyrin aluminum MOF in sorption of diethyl sulfide vapor: mechanistic experimental and computational study

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Materials and methods

Construction of hemi-spherical gas flow spectroscopic mini-chamber for *in situ* time-dependent ATR-FTIR spectroscopy in controlled atmosphere

The hemispherical body of the spectroscopic mini-chamber was fabricated from a template: transparent acrylic dome (plastic hemisphere) 1" diameter (from Supremetech), Figure S1. First, the through hole was drilled at the center of the top of the template, to accommodate pushing the screw of the ATR assembly. Then, the template was inverted, its internal volume was filled with liquid colorless transparent epoxy mixed with hardener (Dr. Resin brand), then stainless steel sapphire anvil (Specac product GS10531) was placed inside epoxy with hardener with its tip up. The epoxy with hardener was leveled to edges of the template, to make the empty internal volume of the spectroscopic mini-chamber of only few cubic millimeters. The epoxy was allowed to solidify for 24 hours. Then, two holes were drilled through the front and rear sides of the obtained spectroscopic mini-chamber, and two pieces of soft silicone tubing (1/16" ID x 1/8" OD) were inserted to the holes, to make gas inlet port (item 4 in Figure 3) and gas outlet port (item 5 in Figure 3). Gas inlet port and gas outlet port can be used interchangeably. To ensure gas tightness between the spectroscopic mini-chamber and the ATR baseplate, flat adhesive mini O-ring was cut from soft silicone adhesive sheet 1 mm thick (hardness 50 Durometer), this O-ring was placed between the spectroscopic mini-chamber and the ATR baseplate, and the ATR bridge assembly was locked.



Figure S1. Template for making spectroscopic mini-chamber: transparent hollow hemisphere.

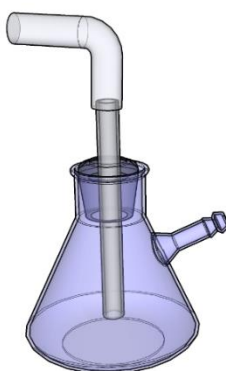


Figure S2. The in-flow setup for generation of flow of DES vapor in dried air.

Results and Discussion

Table S1. Brief description of cluster Al-TCPPZn in DFT computations.

#	Name of group	Total charge
12	Al(+3)	+36
10	HCO ₂ (-1)	-10
19	OH(-)	-19
2	TCPPZn(-2)	-4
2	OC ₂ -C ₆ H ₄ -CO ₂ (-2)	-4
4	HOC-C ₆ H ₄ -COH	0
		Net charge: -1

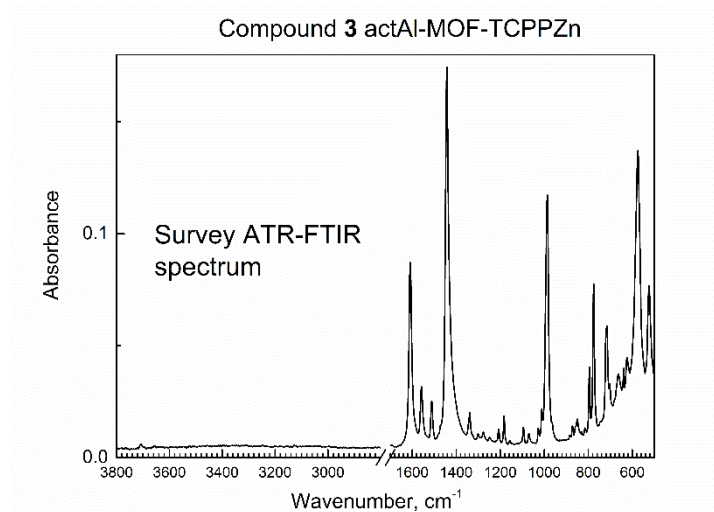


Figure S3. The *in situ* ATR-FTIR survey spectrum of sorbent compound **3** actAl-MOF-TCPPZn.

Table S2. Major IR peaks of sorbent compound **3**.

Wavenumber, cm ⁻¹	Peak Assignment
3708 w	$\nu(\text{O-H})$ free
1608	def(phenyl)
1557	$\nu_{\text{asym}}(\text{COO}^-)$
1511	$\nu_{\text{asym}}(\text{COO}^-)$
1442	$\nu_{\text{sym}}(\text{COO}^-)$
986	def(μ -OH) free

ν = stretch; def = deformation; w = weak; μ = the O-H group connected to Al atom in MOF.

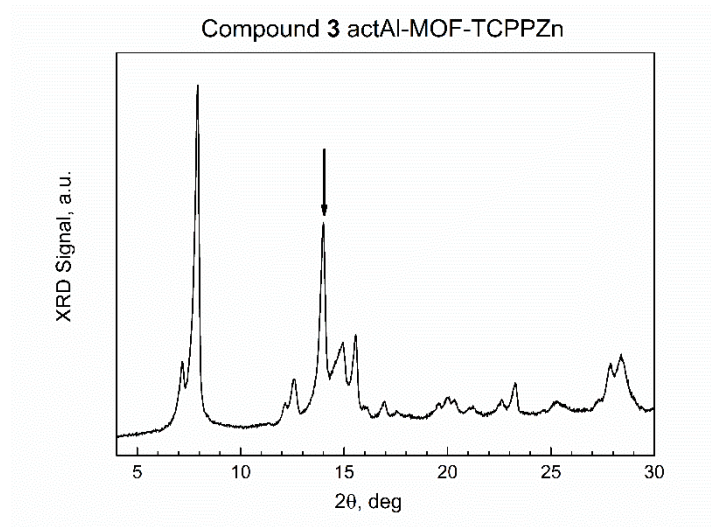


Figure S4. Powder XRD of compound **3**.

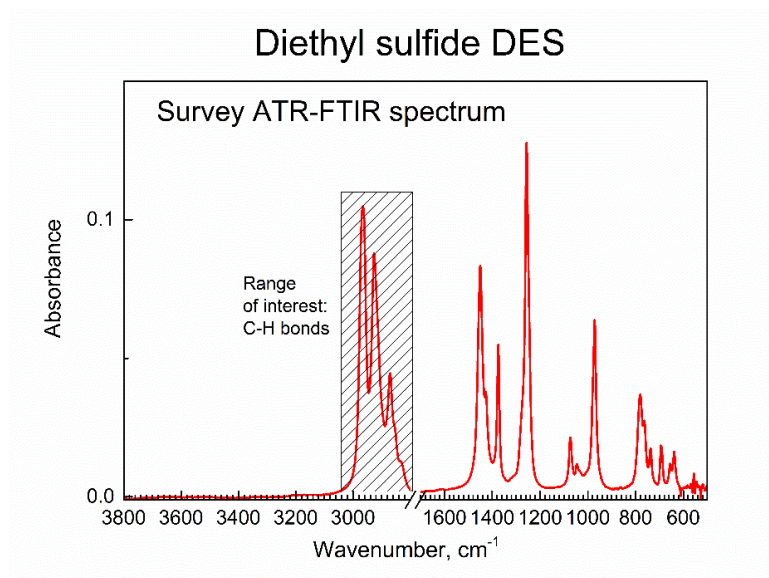


Figure S5. The survey ATR-FTIR spectrum of DES.

Table S3. Assignments of major ATR-FTIR peaks of DES (a) (b).

Wavenumber, cm^{-1}	Literature ¹ wavenumber, cm^{-1}	Assignment
2965	2970	CH_2 asymm. str.
2926	2929	CH_3 str., CH_2 sym. str.
2870	2871	CH_3 sym. str.
1450	1451	CH_3 def.
1427	1427	CH_2 sciss.
1257	1258	CH_2 wag.
1047 w	1046	CH_3 rock.
971	972	C-C str.
693	694	S-C str.

(a) str. = stretch; asymm. = asymmetric; sym. = symmetric; def. = deformation; sciss. = scission; wag. = wagging; rock. = rocking; w = weak.

(b) S.D. Christesen, Vibrational spectra and assignments of diethyl sulfide, 2-chlorodiethyl sulfide and 2, 2'-dichlorodiethyl sulfide, *J. Raman Spectrosc.*, 1991, **22**, 459-465.

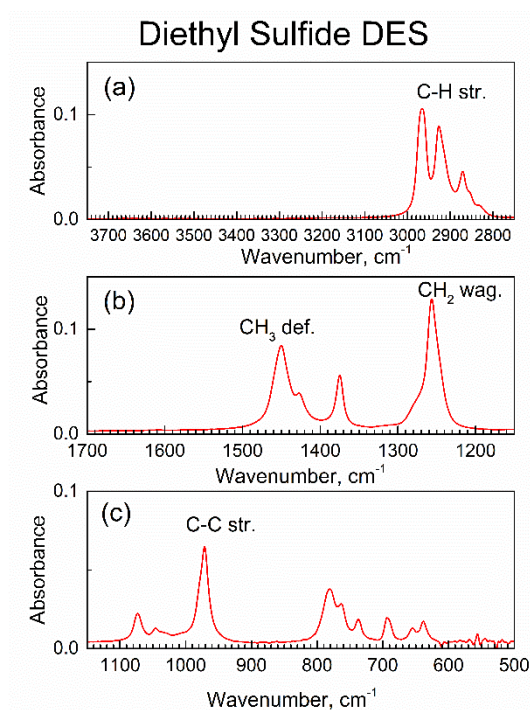
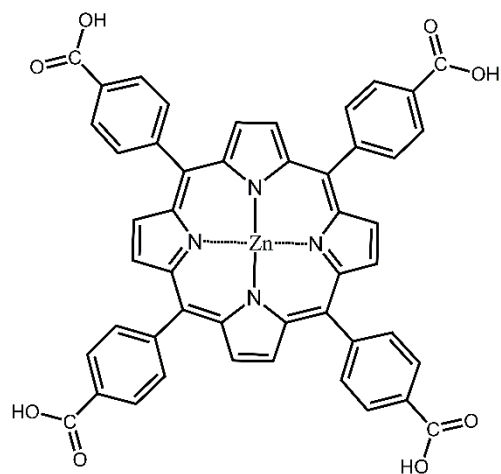


Figure S6. ATR-FTIR spectra of DES: a) high wavenumbers, b) the mid-IR, c) low wavenumbers.



zinc meso-tetra(4-carboxyphenyl) porphine, ZnTCPP

Figure S7. Molecular structure of model compound Zn(II) meso-tetra(4-carboxyphenyl) porphine (ZnTCPP) as model of linker in Al-MOF compound **3**.

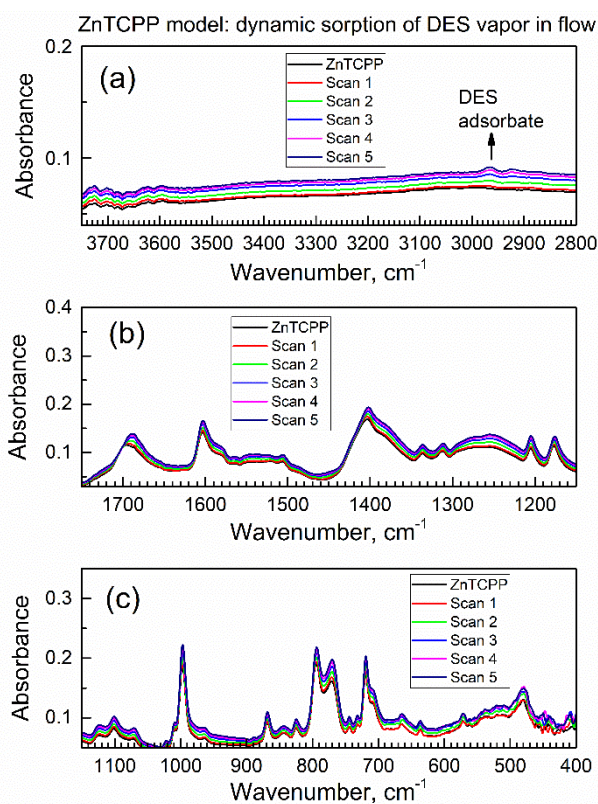


Figure S8. The early sequence (0-9.6 min) of *in situ* time-dependent ATR-FTIR spectra of ZnTCPP model compound in flow of DES vapor. a) high wavenumbers, b) mid-IR, c) low wavenumbers.

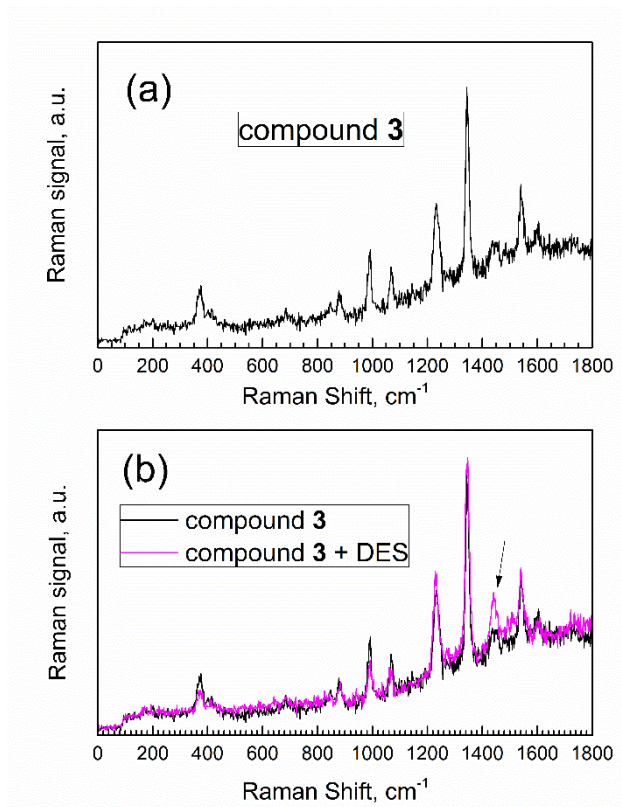


Figure S9. Raman spectra of a) compound 3; b) compound 3 with added DES.

Table S4. Cartesian Coordinates of Species on the Al-TCPP(Zn) PES

DES al-linker11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-0.000000	0.000000	0.565368
2	6	0	-0.000000	1.398952	-0.622444
3	1	0	-0.886329	1.319023	-1.262240
4	1	0	0.886329	1.319023	-1.262240
5	6	0	-0.000000	-1.398952	-0.622444
6	1	0	-0.886329	-1.319023	-1.262240
7	1	0	0.886329	-1.319023	-1.262240
8	6	0	0.000000	-2.727524	0.130226
9	1	0	-0.886349	-2.820246	0.766348
10	1	0	0.000000	-3.563675	-0.577854
11	1	0	0.886349	-2.820246	0.766348
12	6	0	0.000000	2.727524	0.130226
13	1	0	0.000000	3.563675	-0.577854
14	1	0	-0.886349	2.820246	0.766348
15	1	0	0.886349	2.820246	0.766348

Al-TCPPZn zn5aa

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-3.611665	10.447542	-0.246606
2	8	0	-0.561673	9.239894	1.509227
3	8	0	-1.886007	8.559423	-0.927024
4	8	0	2.102210	9.515126	1.794966
5	8	0	-2.998531	8.292853	1.547584
6	8	0	0.965639	9.678243	-0.703691
7	8	0	-2.267274	11.019477	1.983999
8	8	0	-0.291787	7.210664	-0.103958
9	8	0	-0.840103	11.045900	-0.558413
10	8	0	1.030225	7.017490	2.170299
11	1	0	-0.395160	9.959820	2.137911
12	1	0	-3.176280	7.154601	-2.796877
13	1	0	-3.205546	5.487904	-4.660766
14	1	0	-2.840368	5.943008	2.357315
15	1	0	-0.934130	-2.022047	-2.652671

16	1	0	0.836691	4.401284	-3.736565
17	1	0	0.833487	5.989799	-1.820698
18	1	0	-0.429377	5.714931	3.629674
19	1	0	-4.424468	-2.168163	-5.140872
20	13	0	0.884461	8.376837	0.791681
21	13	0	-2.072451	9.979286	0.512203
22	6	0	-2.306396	6.539673	-3.005102
23	6	0	-2.315749	5.616677	-4.051217
24	6	0	-3.417697	6.110215	3.260776
25	6	0	-1.942051	-2.379691	-2.836786
26	6	0	-0.042722	4.994501	-3.522971
27	6	0	-0.040153	5.882971	-2.455718
28	6	0	0.298026	4.952978	3.886325
29	6	0	-3.901113	-2.475699	-4.241104
30	6	0	-1.182905	6.647125	-2.179694
31	6	0	-1.191573	4.816205	-4.301940
32	6	0	-3.794795	7.427138	3.580500
33	6	0	-2.596930	-1.999915	-4.016924
34	6	0	-1.139050	7.546697	-0.989324
35	6	0	3.359066	9.500559	1.907094
36	6	0	-3.382504	8.529553	2.684439
37	6	0	0.291787	10.712948	-0.982937
38	8	0	-8.325959	-5.176498	-1.258121
39	8	0	-5.636541	-6.522344	0.880724
40	8	0	-6.768727	-7.545071	-1.450884
41	8	0	-3.120393	-6.178460	1.965551
42	8	0	-8.141217	-6.686007	0.952225
43	8	0	-3.659156	-5.360320	-0.484167
44	8	0	-6.784206	-4.141347	0.925514
45	8	0	-4.551116	-7.948565	-1.191880
46	8	0	-5.680294	-5.021768	-1.416656
47	8	0	-4.186026	-8.658602	1.466673
48	1	0	-6.102894	-7.145959	1.459934
49	1	0	-3.542108	-4.171810	3.248737
50	1	0	-2.017077	-3.605899	-1.061649
51	1	0	-5.530412	-2.242615	1.923033
52	1	0	-5.519854	-3.705271	-3.517517
53	13	0	-3.933903	-7.014588	0.422337
54	13	0	-7.056200	-5.989322	-0.319235
55	6	0	-2.548937	-4.080740	3.674419
56	6	0	-2.547953	-3.261949	-1.942593
57	6	0	-6.123079	-2.184987	2.829770
58	6	0	-4.517136	-3.333532	-3.338008
59	6	0	-1.590841	-5.052801	3.356825
60	6	0	-3.833867	-3.756107	-2.192643
61	6	0	-5.693516	-8.136375	-1.703822

62	6	0	-1.940940	-6.176592	2.420234
63	6	0	-4.449083	-4.779446	-1.291268
64	8	0	2.277790	7.591488	-0.160105
65	8	0	5.636541	6.522344	0.880724
66	8	0	3.659156	5.360320	-0.484167
67	8	0	8.141217	6.686007	0.952225
68	8	0	3.120393	6.178460	1.965551
69	8	0	6.768727	7.545071	-1.450884
70	8	0	4.186026	8.658602	1.466673
71	8	0	5.680294	5.021768	-1.416656
72	8	0	4.551116	7.948565	-1.191880
73	8	0	6.784206	4.141347	0.925514
74	1	0	2.396276	8.078503	-0.988985
75	1	0	6.102894	7.145959	1.459934
76	1	0	2.017077	3.605899	-1.061649
77	1	0	0.934130	2.022047	-2.652671
78	1	0	3.542108	4.171810	3.248737
79	1	0	3.205546	-5.487904	-4.660766
80	1	0	4.424468	2.168163	-5.140872
81	1	0	5.519854	3.705271	-3.517517
82	1	0	5.530412	2.242615	1.923033
83	1	0	-0.836691	-4.401284	-3.736565
84	13	0	7.056200	5.989322	-0.319235
85	13	0	3.933903	7.014588	0.422337
86	6	0	2.547953	3.261949	-1.942593
87	6	0	1.942051	2.379691	-2.836786
88	6	0	2.548937	4.080740	3.674419
89	6	0	2.315749	-5.616677	-4.051217
90	6	0	3.901113	2.475699	-4.241104
91	6	0	4.517136	3.333532	-3.338008
92	6	0	6.123079	2.184987	2.829770
93	6	0	0.042722	-4.994501	-3.522971
94	6	0	3.833867	3.756107	-2.192643
95	6	0	2.596930	1.999915	-4.016924
96	6	0	1.590841	5.052801	3.356825
97	6	0	1.191573	-4.816205	-4.301940
98	6	0	4.449083	4.779446	-1.291268
99	6	0	1.940940	6.176592	2.420234
100	6	0	5.693516	8.136375	-1.703822
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102	8	0	0.561673	-9.239894	1.509227
103	8	0	-0.965639	-9.678243	-0.703691
104	8	0	2.998531	-8.292853	1.547584
105	8	0	-2.102210	-9.515126	1.794966
106	8	0	1.886007	-8.559423	-0.927024
107	8	0	-1.030225	-7.017490	2.170299

108	8	0	0.840103	-11.045900	-0.558413
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110	8	0	2.267274	-11.019477	1.983999
111	1	0	-2.396276	-8.078503	-0.988985
112	1	0	0.395160	-9.959820	2.137911
113	1	0	2.840368	-5.943008	2.357315
114	1	0	3.176280	-7.154601	-2.796877
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117	13	0	2.072451	-9.979286	0.512203
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119	6	0	3.417697	-6.110215	3.260776
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121	6	0	-0.298026	-4.952978	3.886325
122	6	0	0.040153	-5.882971	-2.455718
123	6	0	3.794795	-7.427138	3.580500
124	6	0	1.182905	-6.647125	-2.179694
125	6	0	-0.291787	-10.712948	-0.982937
126	6	0	3.382504	-8.529553	2.684439
127	6	0	-3.359066	-9.500559	1.907094
128	6	0	1.139050	-7.546697	-0.989324
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132	8	0	-3.800813	2.756805	8.678923
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135	8	0	-1.682864	1.951081	8.801816
136	8	0	-5.502581	0.614221	5.871395
137	8	0	-0.654930	1.685074	6.289549
138	8	0	-4.744014	0.090762	8.509389
139	1	0	-2.916695	1.456405	5.780203
140	1	0	-2.953877	-2.264102	4.767376
141	1	0	-3.481414	4.051449	3.891222
142	1	0	-5.101991	-0.487451	3.681553
143	1	0	-1.034001	3.802684	5.131769
144	13	0	-4.721770	1.655719	7.383023
145	13	0	-1.566072	0.508887	7.484942
146	6	0	-2.219570	-3.021079	4.513277
147	6	0	-3.771695	5.074219	4.104862
148	6	0	-5.891827	-1.221941	3.793350
149	6	0	-0.035275	3.889596	4.717727
150	6	0	-6.691619	-1.190550	4.954675
151	6	0	0.922821	2.915067	5.037202
152	6	0	-6.419072	-0.208570	5.987928
153	6	0	-2.608829	2.743624	9.102718

154	6	0	-3.825063	-0.673508	8.920607
155	6	0	0.561674	1.776539	5.925553
156	8	0	3.117009	-1.066819	6.642077
157	8	0	0.000000	-0.000000	8.325182
158	8	0	4.485268	-3.111049	6.004286
159	8	0	2.591686	0.603803	8.689961
160	8	0	3.800813	-2.756805	8.678923
161	8	0	1.475748	0.963312	6.257355
162	8	0	4.744014	-0.090762	8.509389
163	8	0	0.654930	-1.685074	6.289549
164	8	0	5.502581	-0.614221	5.871395
165	8	0	1.682864	-1.951081	8.801816
166	1	0	2.916695	-1.456405	5.780203
167	1	0	0.000000	-0.000000	9.290008
168	1	0	3.481414	-4.051449	3.891222
169	1	0	2.953877	2.264102	4.767376
170	1	0	1.034001	-3.802684	5.131769
171	1	0	5.101991	0.487451	3.681553
172	13	0	1.566072	-0.508887	7.484942
173	13	0	4.721770	-1.655719	7.383023
174	6	0	3.771695	-5.074219	4.104862
175	6	0	2.219570	3.021079	4.513277
176	6	0	0.035275	-3.889596	4.717727
177	6	0	5.891827	1.221941	3.793350
178	6	0	-0.922821	-2.915067	5.037202
179	6	0	6.691619	1.190550	4.954675
180	6	0	-0.561674	-1.776539	5.925553
181	6	0	3.825063	0.673508	8.920607
182	6	0	2.608829	-2.743624	9.102718
183	6	0	6.419072	0.208570	5.987928
184	6	0	-4.528535	7.702340	4.740161
185	6	0	-4.531450	5.344409	5.262238
186	6	0	7.144755	3.131611	3.022119
187	6	0	7.713738	2.133351	5.144060
188	6	0	-4.916654	6.658621	5.572314
189	6	0	7.933078	3.109666	4.178592
190	1	0	-4.797381	8.728483	4.973261
191	1	0	-5.501411	6.850841	6.467770
192	1	0	8.709960	3.857252	4.310150
193	1	0	8.317779	2.099802	6.046794
194	6	0	-4.895530	4.269738	6.164632
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196	1	0	-5.548395	4.477534	7.021994
197	1	0	8.037026	5.029360	2.206311
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199	6	0	-7.144755	-3.131611	3.022119

200	6	0	4.531450	-5.344409	5.262238
201	6	0	4.528535	-7.702340	4.740161
202	1	0	-8.317779	-2.099802	6.046794
203	1	0	4.797381	-8.728483	4.973261
204	6	0	-7.933078	-3.109666	4.178592
205	6	0	4.916654	-6.658621	5.572314
206	1	0	5.501411	-6.850841	6.467770
207	1	0	-8.709960	-3.857252	4.310150
208	6	0	4.895530	-4.269738	6.164632
209	6	0	-7.364993	-4.179648	2.001167
210	1	0	5.548395	-4.477534	7.021994
211	1	0	-8.037026	-5.029360	2.206311
212	1	0	-7.024079	-0.209098	6.904333
213	1	0	3.373206	-9.573178	3.038079
214	1	0	7.024079	0.209098	6.904333
215	1	0	-3.373206	9.573178	3.038079
216	1	0	3.791641	10.339468	2.474263
217	1	0	-0.763821	-11.405350	-1.698176
218	1	0	-5.740368	-8.920240	-2.476233
219	1	0	0.763821	11.405350	-1.698176
220	1	0	5.740368	8.920240	-2.476233
221	1	0	-2.356506	3.526076	9.833412
222	1	0	4.147578	1.500158	9.569434
223	1	0	2.356506	-3.526076	9.833412
224	1	0	-4.147578	-1.500158	9.569434
225	1	0	-3.791641	-10.339468	2.474263
226	8	0	6.326540	-2.248524	7.827203
227	8	0	3.611665	-10.447542	-0.246606
228	8	0	8.325959	5.176498	-1.258121
229	1	0	2.896420	-11.716985	1.752788
230	1	0	-9.038622	-6.701097	0.591586
231	1	0	9.038622	6.701097	0.591586
232	1	0	-2.896420	11.716985	1.752788
233	1	0	-6.424602	2.391451	8.776731
234	1	0	-7.958315	-4.647656	-1.976833
235	1	0	-3.731022	10.021138	-1.104335
236	1	0	7.958315	4.647656	-1.976833
237	1	0	6.424602	-2.391451	8.776731
238	1	0	3.731022	-10.021138	-1.104335
239	7	0	-1.199159	3.176461	-7.717562
240	7	0	-1.436365	1.255376	-5.571027
241	7	0	-1.518930	-0.916641	-7.476670
242	7	0	-1.444345	1.020390	-9.625634
243	6	0	-1.102744	3.918149	-8.867756
244	6	0	-0.931912	5.314807	-8.538665
245	6	0	-0.942507	5.405362	-7.177664

246	6	0	-1.119303	4.060669	-6.671837
247	6	0	-1.221867	3.719914	-5.318718
248	6	0	-1.391796	2.414845	-4.827234
249	6	0	-1.658909	2.109522	-3.438875
250	6	0	-1.898909	0.770532	-3.364057
251	6	0	-1.750090	0.236234	-4.700498
252	6	0	-1.979426	-1.108382	-5.046891
253	6	0	-1.836008	-1.640179	-6.337888
254	6	0	-2.097852	-3.014633	-6.701863
255	6	0	-2.000937	-3.099326	-8.060336
256	6	0	-1.690027	-1.781724	-8.545506
257	6	0	-1.695954	-1.408606	-9.884459
258	6	0	-1.596769	-0.113467	-10.383201
259	6	0	-1.645360	0.233227	-11.785805
260	6	0	-1.509263	1.587492	-11.863122
261	6	0	-1.378654	2.072420	-10.507958
262	6	0	-1.197924	3.407154	-10.159314
263	1	0	-0.832836	6.115170	-9.261205
264	1	0	-0.847516	6.288965	-6.562772
265	1	0	-1.696538	2.836939	-2.641265
266	1	0	-2.167375	0.195717	-2.490799
267	1	0	-2.329686	-3.807721	-6.007238
268	1	0	-2.135264	-3.972989	-8.683481
269	1	0	-1.826883	-2.205228	-10.609165
270	1	0	-1.756271	-0.478956	-12.592902
271	1	0	-1.498477	2.212044	-12.747588
272	1	0	-1.136800	4.122279	-10.974723
273	7	0	1.199159	-3.176461	-7.717562
274	7	0	1.436365	-1.255376	-5.571027
275	7	0	1.518930	0.916641	-7.476670
276	7	0	1.444345	-1.020390	-9.625634
277	6	0	1.102744	-3.918149	-8.867756
278	6	0	0.931912	-5.314807	-8.538665
279	6	0	0.942507	-5.405362	-7.177664
280	6	0	1.119303	-4.060669	-6.671837
281	6	0	1.221867	-3.719914	-5.318718
282	6	0	1.391796	-2.414845	-4.827234
283	6	0	1.658909	-2.109522	-3.438875
284	6	0	1.898909	-0.770532	-3.364057
285	6	0	1.750090	-0.236234	-4.700498
286	6	0	1.979426	1.108382	-5.046891
287	6	0	1.836008	1.640179	-6.337888
288	6	0	2.097852	3.014633	-6.701863
289	6	0	2.000937	3.099326	-8.060336
290	6	0	1.690027	1.781724	-8.545506
291	6	0	1.695954	1.408606	-9.884459

292	6	0	1.596769	0.113467	-10.383201
293	6	0	1.645360	-0.233227	-11.785805
294	6	0	1.509263	-1.587492	-11.863122
295	6	0	1.378654	-2.072420	-10.507958
296	6	0	1.197924	-3.407154	-10.159314
297	1	0	0.832836	-6.115170	-9.261205
298	1	0	0.847516	-6.288965	-6.562772
299	1	0	1.696538	-2.836939	-2.641265
300	1	0	2.167375	-0.195717	-2.490799
301	1	0	2.329686	3.807721	-6.007238
302	1	0	2.135264	3.972989	-8.683481
303	1	0	1.826883	2.205228	-10.609165
304	1	0	1.756271	0.478956	-12.592902
305	1	0	1.498477	-2.212044	-12.747588
306	1	0	1.136800	-4.122279	-10.974723
307	30	0	1.136877	-1.132946	-7.591768
308	30	0	-1.136877	1.132946	-7.591768

2DES@Al-TCPPZn zn7a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-6.965431	7.126482	-1.467357
2	8	0	-4.108333	7.855453	0.767272
3	8	0	-4.409914	6.382851	-1.531998
4	8	0	-2.225666	9.628071	1.348557
5	8	0	-5.728395	5.795369	0.715338
6	8	0	-2.684916	8.946219	-1.302305
7	8	0	-6.533238	8.531286	0.780771
8	8	0	-2.419864	6.230305	-0.490163
9	8	0	-4.931282	9.086269	-1.585033
10	8	0	-1.739227	6.982030	1.917125
11	1	0	-4.442296	8.567239	1.335932
12	1	0	-4.547328	4.913544	-3.506378
13	1	0	-3.802620	3.085604	-5.023776
14	1	0	-4.766786	3.746920	1.702732
15	1	0	-0.193124	-4.376238	-3.509707
16	1	0	-0.536623	2.214936	-2.382812
17	1	0	-1.268019	4.079331	-0.891585
18	1	0	-2.567546	4.991744	3.010481
19	1	0	-4.326396	-4.741088	-4.583907
20	13	0	-2.328984	7.946761	0.348628
21	13	0	-5.583815	7.631483	-0.469080

22	6	0	-3.674142	4.316358	-3.269033
23	6	0	-3.253898	3.296132	-4.111554
24	6	0	-5.438906	3.713814	2.553480
25	6	0	-1.164730	-4.820695	-3.340672
26	6	0	-1.425610	2.791328	-2.620209
27	6	0	-1.832971	3.831686	-1.784035
28	6	0	-1.619151	4.666850	3.423705
29	6	0	-3.491039	-5.038451	-3.956602
30	6	0	-2.942721	4.618583	-2.116332
31	6	0	-2.103506	2.540442	-3.822133
32	6	0	-6.350037	4.770624	2.732029
33	6	0	-2.241708	-4.428895	-4.143901
34	6	0	-3.300025	5.827928	-1.311434
35	6	0	-1.239181	10.268006	1.800722
36	6	0	-6.351502	5.885974	1.764158
37	6	0	-3.742996	9.398132	-1.830410
38	8	0	-5.766134	-9.622276	-0.351280
39	8	0	-2.537546	-9.147403	1.456765
40	8	0	-3.200830	-10.820417	-0.625321
41	8	0	-0.484748	-7.327900	2.132736
42	8	0	-4.623940	-10.459442	1.911260
43	8	0	-1.848585	-7.179667	-0.087891
44	8	0	-4.684245	-7.646252	1.408701
45	8	0	-1.149347	-9.860525	-0.773811
46	8	0	-3.649591	-8.161578	-0.999299
47	8	0	0.009593	-9.999577	1.712406
48	1	0	-2.542751	-9.896034	2.073378
49	1	0	-1.632126	-5.656311	3.482643
50	1	0	-0.513358	-6.037931	-1.681567
51	1	0	-4.044185	-5.322018	2.073456
52	1	0	-4.629427	-6.468479	-2.799239
53	13	0	-0.941566	-8.607633	0.747021
54	13	0	-4.175879	-9.506365	0.438846
55	6	0	-0.761378	-5.044520	3.690033
56	6	0	-1.339437	-5.747639	-2.322714
57	6	0	-4.623940	-5.324522	2.990890
58	6	0	-3.665653	-5.994835	-2.956761
59	6	0	0.479783	-5.446021	3.180673
60	6	0	-2.598753	-6.328768	-2.117701
61	6	0	-2.027219	-10.728553	-1.056107
62	6	0	0.584957	-6.687521	2.341526
63	6	0	-2.733026	-7.298301	-0.992321
64	8	0	-0.575249	8.109579	-0.214207
65	8	0	2.537546	9.147403	1.456765
66	8	0	1.848585	7.179667	-0.087891
67	8	0	4.623940	10.459442	1.911260

68	8	0	0.484748	7.327900	2.132736
69	8	0	3.200830	10.820417	-0.625321
70	8	0	-0.009593	9.999577	1.712406
71	8	0	3.649591	8.161578	-0.999299
72	8	0	1.149347	9.860525	-0.773811
73	8	0	4.684245	7.646252	1.408701
74	1	0	-0.570867	8.587837	-1.056617
75	1	0	2.542751	9.896034	2.073378
76	1	0	0.513358	6.037931	-1.681567
77	1	0	0.193124	4.376238	-3.509707
78	1	0	1.632126	5.656311	3.482643
79	1	0	3.802620	-3.085604	-5.023776
80	1	0	4.326396	4.741088	-4.583907
81	1	0	4.629427	6.468479	-2.799239
82	1	0	4.044185	5.322018	2.073456
83	1	0	0.536623	-2.214936	-2.382812
84	13	0	4.175879	9.506365	0.438846
85	13	0	0.941566	8.607633	0.747021
86	6	0	1.339437	5.747639	-2.322714
87	6	0	1.164730	4.820695	-3.340672
88	6	0	0.761378	5.044520	3.690033
89	6	0	3.253898	-3.296132	-4.111554
90	6	0	3.491039	5.038451	-3.956602
91	6	0	3.665653	5.994835	-2.956761
92	6	0	4.623940	5.324522	2.990890
93	6	0	1.425610	-2.791328	-2.620209
94	6	0	2.598753	6.328768	-2.117701
95	6	0	2.241708	4.428895	-4.143901
96	6	0	-0.479783	5.446021	3.180673
97	6	0	2.103506	-2.540442	-3.822133
98	6	0	2.733026	7.298301	-0.992321
99	6	0	-0.584957	6.687521	2.341526
100	6	0	2.027219	10.728553	-1.056107
101	8	0	0.575249	-8.109579	-0.214207
102	8	0	4.108333	-7.855453	0.767272
103	8	0	2.684916	-8.946219	-1.302305
104	8	0	5.728395	-5.795369	0.715338
105	8	0	2.225666	-9.628071	1.348557
106	8	0	4.409914	-6.382851	-1.531998
107	8	0	1.739227	-6.982030	1.917125
108	8	0	4.931282	-9.086269	-1.585033
109	8	0	2.419864	-6.230305	-0.490163
110	8	0	6.533238	-8.531286	0.780771
111	1	0	0.570867	-8.587837	-1.056617
112	1	0	4.442296	-8.567239	1.335932
113	1	0	4.766786	-3.746920	1.702732

114	1	0	4.547328	-4.913544	-3.506378
115	1	0	2.567546	-4.991744	3.010481
116	1	0	1.268019	-4.079331	-0.891585
117	13	0	5.583815	-7.631483	-0.469080
118	13	0	2.328984	-7.946761	0.348628
119	6	0	5.438906	-3.713814	2.553480
120	6	0	3.674142	-4.316358	-3.269033
121	6	0	1.619151	-4.666850	3.423705
122	6	0	1.832971	-3.831686	-1.784035
123	6	0	6.350037	-4.770624	2.732029
124	6	0	2.942721	-4.618583	-2.116332
125	6	0	3.742996	-9.398132	-1.830410
126	6	0	6.351502	-5.885974	1.764158
127	6	0	1.239181	-10.268006	1.800722
128	6	0	3.300025	-5.827928	-1.311434
129	8	0	-3.262250	-0.361853	6.179745
130	8	0	-6.666220	-0.723969	7.343791
131	8	0	-0.996678	-1.532786	5.893286
132	8	0	-4.639462	0.977610	8.042742
133	8	0	-2.095205	-1.516437	8.371790
134	8	0	-5.454539	0.666012	5.394060
135	8	0	-2.387409	1.171186	8.237326
136	8	0	-5.099133	-2.013879	5.543810
137	8	0	-1.232914	1.245964	5.804967
138	8	0	-4.335812	-1.830262	8.209405
139	1	0	-3.148575	-0.598266	5.245516
140	1	0	-1.817343	-3.553945	4.838798
141	1	0	-4.705374	1.858527	3.370966
142	1	0	-4.283865	-3.253265	3.485094
143	1	0	-2.395546	2.897807	4.392666
144	13	0	-4.959660	-0.550047	6.901255
145	13	0	-1.641142	-0.159646	7.040047
146	6	0	-0.862267	-3.880273	4.443393
147	6	0	-5.410769	2.676288	3.464403
148	6	0	-4.761233	-4.187671	3.767584
149	6	0	-1.521833	3.505845	4.184279
150	6	0	-5.536307	-4.248079	4.945243
151	6	0	-0.280086	3.107039	4.699236
152	6	0	-5.682551	-3.078488	5.788421
153	6	0	-3.574611	1.518895	8.456343
154	6	0	-3.178842	-2.083096	8.653991
155	6	0	-0.168541	1.872991	5.524278
156	8	0	3.262250	0.361853	6.179745
157	8	0	-0.000000	0.000000	7.884392
158	8	0	5.454539	-0.666012	5.394060
159	8	0	2.095205	1.516437	8.371790

160	8	0	4.639462	-0.977610	8.042742
161	8	0	0.996678	1.532786	5.893286
162	8	0	4.335812	1.830262	8.209405
163	8	0	1.232914	-1.245964	5.804967
164	8	0	5.099133	2.013879	5.543810
165	8	0	2.387409	-1.171186	8.237326
166	1	0	3.148575	0.598266	5.245516
167	1	0	-0.000000	0.000000	8.849081
168	1	0	4.705374	-1.858527	3.370966
169	1	0	1.817343	3.553945	4.838798
170	1	0	2.395546	-2.897807	4.392666
171	1	0	4.283865	3.253265	3.485094
172	13	0	1.641142	0.159646	7.040047
173	13	0	4.959660	0.550047	6.901255
174	6	0	5.410769	-2.676288	3.464403
175	6	0	0.862267	3.880273	4.443393
176	6	0	1.521833	-3.505845	4.184279
177	6	0	4.761233	4.187671	3.767584
178	6	0	0.280086	-3.107039	4.699236
179	6	0	5.536307	4.248079	4.945243
180	6	0	0.168541	-1.872991	5.524278
181	6	0	3.178842	2.083096	8.653991
182	6	0	3.574611	-1.518895	8.456343
183	6	0	5.682551	3.078488	5.788421
184	6	0	-7.228229	4.786115	3.821197
185	6	0	-6.308918	2.678631	4.551263
186	6	0	5.231635	6.526708	3.397226
187	6	0	6.146139	5.447343	5.346770
188	6	0	-7.217027	3.732411	4.728767
189	6	0	5.976111	6.593317	4.580446
190	1	0	-7.913537	5.619652	3.944625
191	1	0	-7.896708	3.721497	5.576469
192	1	0	6.423630	7.536382	4.880427
193	1	0	6.734642	5.471902	6.259959
194	6	0	-6.256065	1.599418	5.520479
195	6	0	5.068019	7.736570	2.566991
196	1	0	-6.923344	1.611215	6.392122
197	1	0	5.262226	8.739265	2.980466
198	6	0	-6.146139	-5.447343	5.346770
199	6	0	-5.231635	-6.526708	3.397226
200	6	0	6.308918	-2.678631	4.551263
201	6	0	7.228229	-4.786115	3.821197
202	1	0	-6.734642	-5.471902	6.259959
203	1	0	7.913537	-5.619652	3.944625
204	6	0	-5.976111	-6.593317	4.580446
205	6	0	7.217027	-3.732411	4.728767

206	1	0	7.896708	-3.721497	5.576469
207	1	0	-6.423630	-7.536382	4.880427
208	6	0	6.256065	-1.599418	5.520479
209	6	0	-5.068019	-7.736570	2.566991
210	1	0	6.923344	-1.611215	6.392122
211	1	0	-5.262226	-8.739265	2.980466
212	1	0	-6.319224	-3.134881	6.680823
213	1	0	6.884889	-6.825463	1.980366
214	1	0	6.319224	3.134881	6.680823
215	1	0	-6.884889	6.825463	1.980366
216	1	0	-1.482988	11.188235	2.353850
217	1	0	3.591486	-10.160670	-2.610712
218	1	0	-1.714632	-11.497847	-1.780270
219	1	0	-3.591486	10.160670	-2.610712
220	1	0	1.714632	11.497847	-1.780270
221	1	0	-3.707329	2.402767	9.096846
222	1	0	3.120271	2.901059	9.387117
223	1	0	3.707329	-2.402767	9.096846
224	1	0	-3.120271	-2.901059	9.387117
225	1	0	1.482988	-11.188235	2.353850
226	8	0	6.666220	0.723969	7.343791
227	8	0	6.965431	-7.126482	-1.467357
228	8	0	5.766134	9.622276	-0.351280
229	1	0	7.386237	-8.763352	0.388463
230	1	0	-5.412051	-10.973081	1.685854
231	1	0	5.412051	10.973081	1.685854
232	1	0	-7.386237	8.763352	0.388463
233	1	0	-6.804180	-0.737997	8.298918
234	1	0	-5.773684	-9.177377	-1.207851
235	1	0	-6.692968	6.571864	-2.208590
236	1	0	5.773684	9.177377	-1.207851
237	1	0	6.804180	0.737997	8.298918
238	1	0	6.692968	-6.571864	-2.208590
239	7	0	-1.249881	1.252703	-7.264610
240	7	0	-1.677752	-0.889702	-5.368280
241	7	0	-1.934515	-2.785158	-7.537492
242	7	0	-1.649271	-0.619496	-9.430242
243	6	0	-1.200105	2.143865	-8.325308
244	6	0	-1.183998	3.492555	-7.827268
245	6	0	-1.309809	3.421088	-6.470757
246	6	0	-1.392017	2.020338	-6.119585
247	6	0	-1.668263	1.529150	-4.833143
248	6	0	-1.746707	0.166866	-4.490044
249	6	0	-1.999748	-0.329869	-3.154606
250	6	0	-2.065634	-1.688928	-3.239390
251	6	0	-1.890822	-2.035054	-4.633378

252	6	0	-2.042307	-3.336482	-5.141051
253	6	0	-2.050176	-3.674560	-6.499671
254	6	0	-2.197591	-5.018115	-7.018932
255	6	0	-2.184312	-4.917506	-8.379034
256	6	0	-2.025861	-3.516960	-8.694860
257	6	0	-2.001046	-2.987445	-9.982245
258	6	0	-1.848585	-1.647094	-10.320996
259	6	0	-1.858303	-1.133671	-11.672017
260	6	0	-1.653497	0.211152	-11.583667
261	6	0	-1.517654	0.522650	-10.178413
262	6	0	-1.293983	1.797440	-9.667868
263	1	0	-1.095002	4.378526	-8.441019
264	1	0	-1.345069	4.241107	-5.769775
265	1	0	-2.126214	0.284761	-2.275588
266	1	0	-2.257706	-2.396592	-2.446289
267	1	0	-2.299846	-5.907555	-6.414200
268	1	0	-2.282334	-5.711247	-9.108917
269	1	0	-2.119396	-3.689792	-10.802408
270	1	0	-2.004931	-1.733822	-12.561217
271	1	0	-1.585849	0.935454	-12.384717
272	1	0	-1.224788	2.609141	-10.384245
273	7	0	1.249881	-1.252703	-7.264610
274	7	0	1.677752	0.889702	-5.368280
275	7	0	1.934515	2.785158	-7.537492
276	7	0	1.649271	0.619496	-9.430242
277	6	0	1.200105	-2.143865	-8.325308
278	6	0	1.183998	-3.492555	-7.827268
279	6	0	1.309809	-3.421088	-6.470757
280	6	0	1.392017	-2.020338	-6.119585
281	6	0	1.668263	-1.529150	-4.833143
282	6	0	1.746707	-0.166866	-4.490044
283	6	0	1.999748	0.329869	-3.154606
284	6	0	2.065634	1.688928	-3.239390
285	6	0	1.890822	2.035054	-4.633378
286	6	0	2.042307	3.336482	-5.141051
287	6	0	2.050176	3.674560	-6.499671
288	6	0	2.197591	5.018115	-7.018932
289	6	0	2.184312	4.917506	-8.379034
290	6	0	2.025861	3.516960	-8.694860
291	6	0	2.001046	2.987445	-9.982245
292	6	0	1.848585	1.647094	-10.320996
293	6	0	1.858303	1.133671	-11.672017
294	6	0	1.653497	-0.211152	-11.583667
295	6	0	1.517654	-0.522650	-10.178413
296	6	0	1.293983	-1.797440	-9.667868
297	1	0	1.095002	-4.378526	-8.441019

298	1	0	1.345069	-4.241107	-5.769775
299	1	0	2.126214	-0.284761	-2.275588
300	1	0	2.257706	2.396592	-2.446289
301	1	0	2.299846	5.907555	-6.414200
302	1	0	2.282334	5.711247	-9.108917
303	1	0	2.119396	3.689792	-10.802408
304	1	0	2.004931	1.733822	-12.561217
305	1	0	1.585849	-0.935454	-12.384717
306	1	0	1.224788	-2.609141	-10.384245
307	16	0	-2.516863	-1.051554	2.622428
308	16	0	2.516863	1.051554	2.622428
309	6	0	1.150119	1.730431	1.590823
310	1	0	0.731351	0.903834	1.008333
311	1	0	0.382845	2.042193	2.302131
312	6	0	-1.150119	-1.730431	1.590823
313	1	0	-0.731351	-0.903834	1.008333
314	1	0	-0.382845	-2.042193	2.302131
315	6	0	3.424944	0.051578	1.373901
316	1	0	3.616843	0.677386	0.496201
317	1	0	4.398178	-0.151332	1.832841
318	6	0	-3.424944	-0.051578	1.373901
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321	6	0	2.726332	-1.248743	0.978358
322	1	0	3.332969	-1.808929	0.256488
323	1	0	2.542249	-1.884692	1.850493
324	1	0	1.759067	-1.056664	0.502955
325	6	0	-2.726332	1.248743	0.978358
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328	1	0	-2.542249	1.884692	1.850493
329	6	0	1.563149	2.892545	0.691660
330	1	0	1.890052	3.752388	1.282754
331	1	0	2.375349	2.612878	0.012347
332	1	0	0.715482	3.217578	0.076836
333	6	0	-1.563149	-2.892545	0.691660
334	1	0	-1.890052	-3.752388	1.282754
335	1	0	-2.375349	-2.612878	0.012347
336	1	0	-0.715482	-3.217578	0.076836
337	30	0	-1.377518	-0.822600	-7.395535
338	30	0	1.377518	0.822600	-7.395535
