Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Aggregation Induced Emission and Mechanochromism in Tetraphenylethene Substituted Pyrazabole

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Thermogravimetric analysis

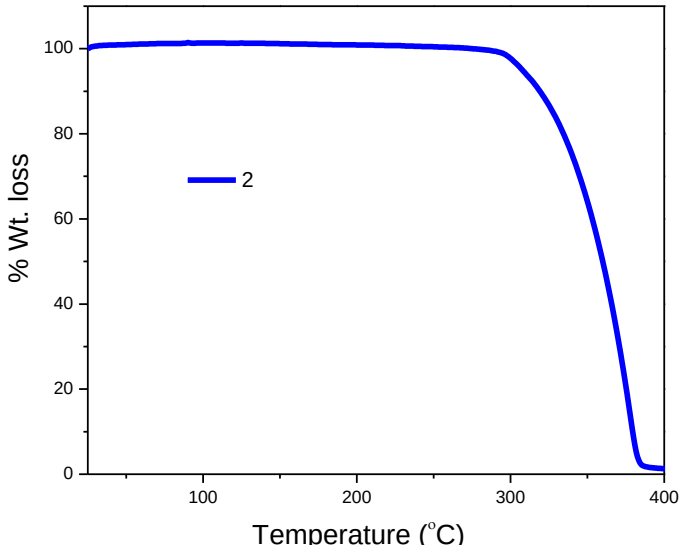


Fig. S1 Thermogravimetric analysis of **2**, measured at a heating rate of 10 °C/ min under nitrogen atmosphere.

Aggregation induced emission

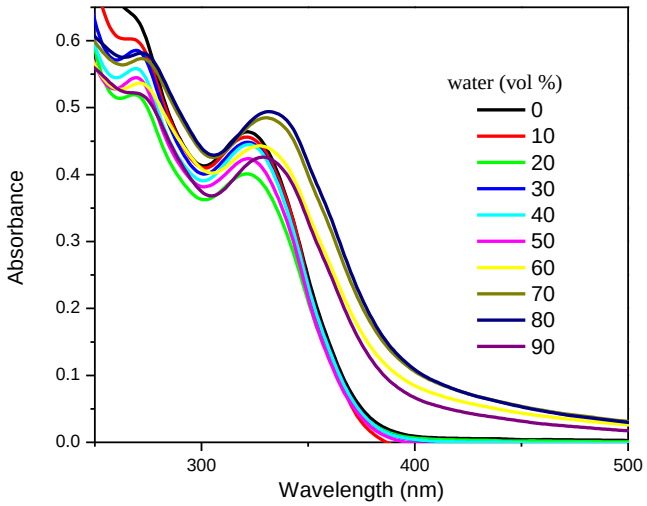


Fig. S2 UV-vis absorption spectra of **2** in THF–water mixtures with different water fractions.

Mechanochromism

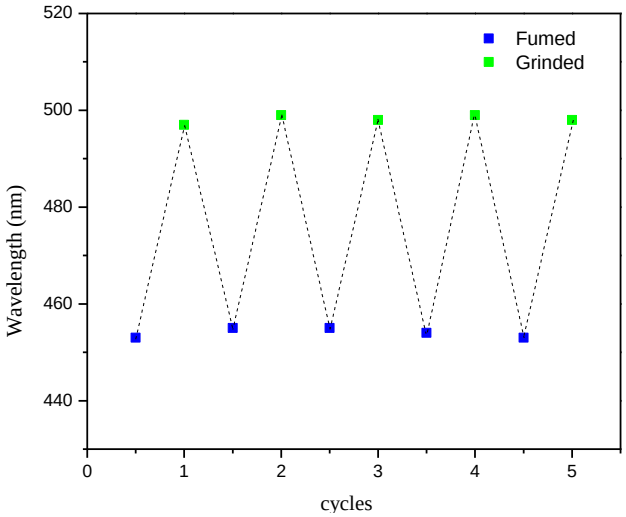


Fig. S3 Repeated switching of the solid-state fluorescence of **2** by repeated grinding and fuming cycles.

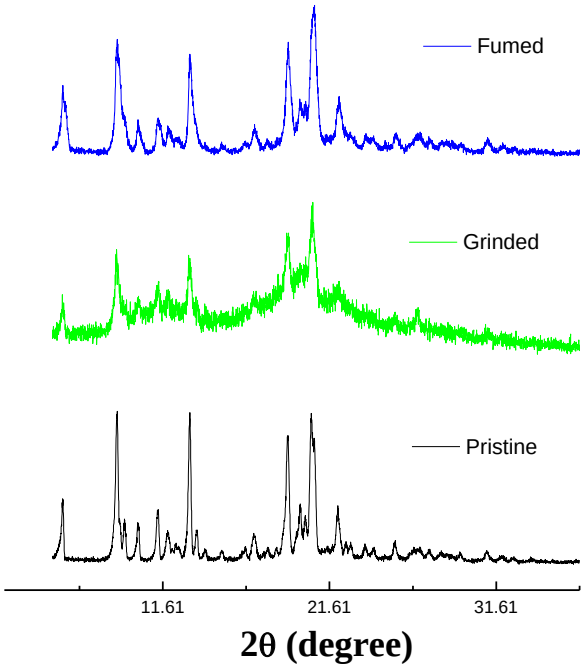
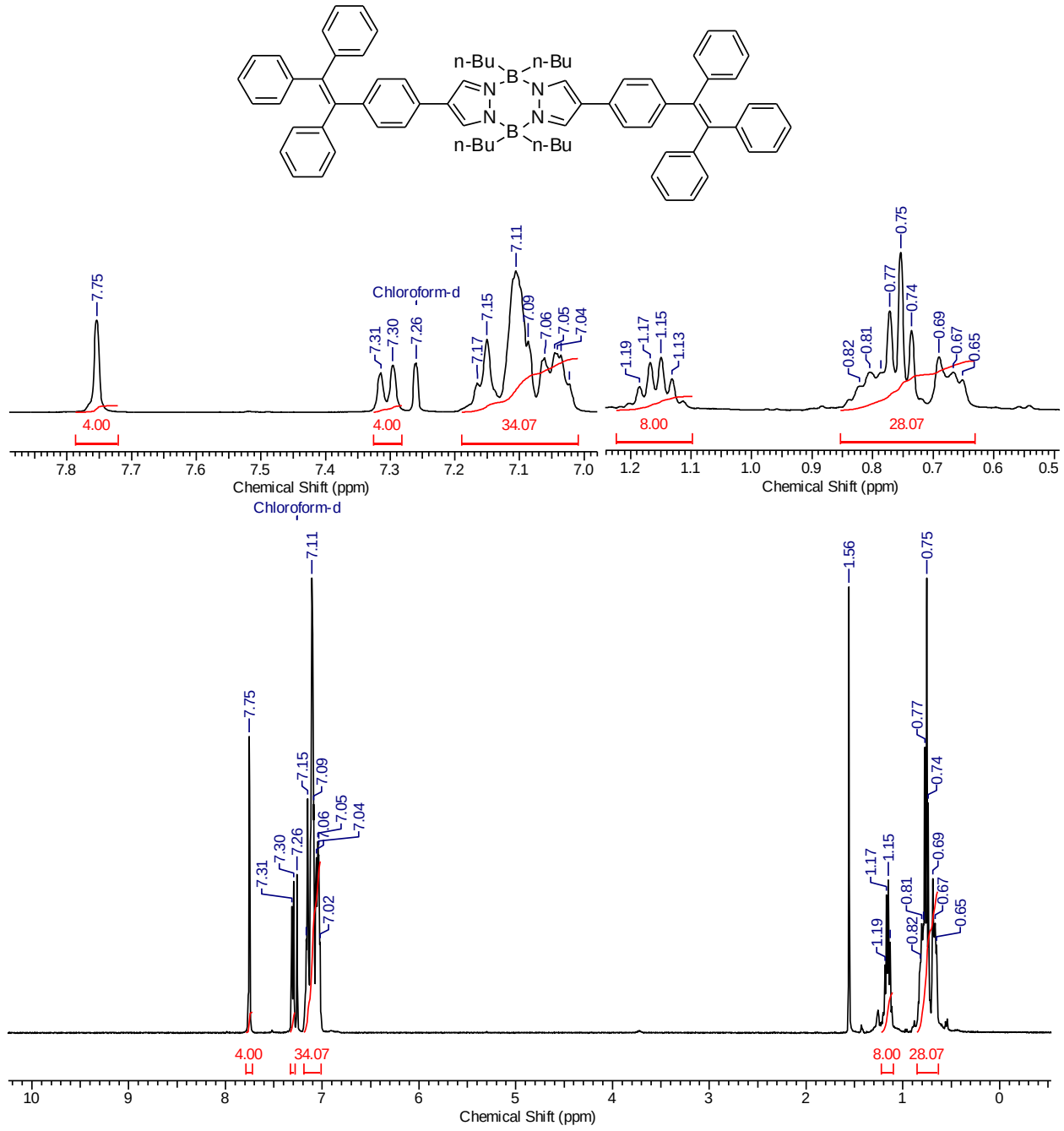
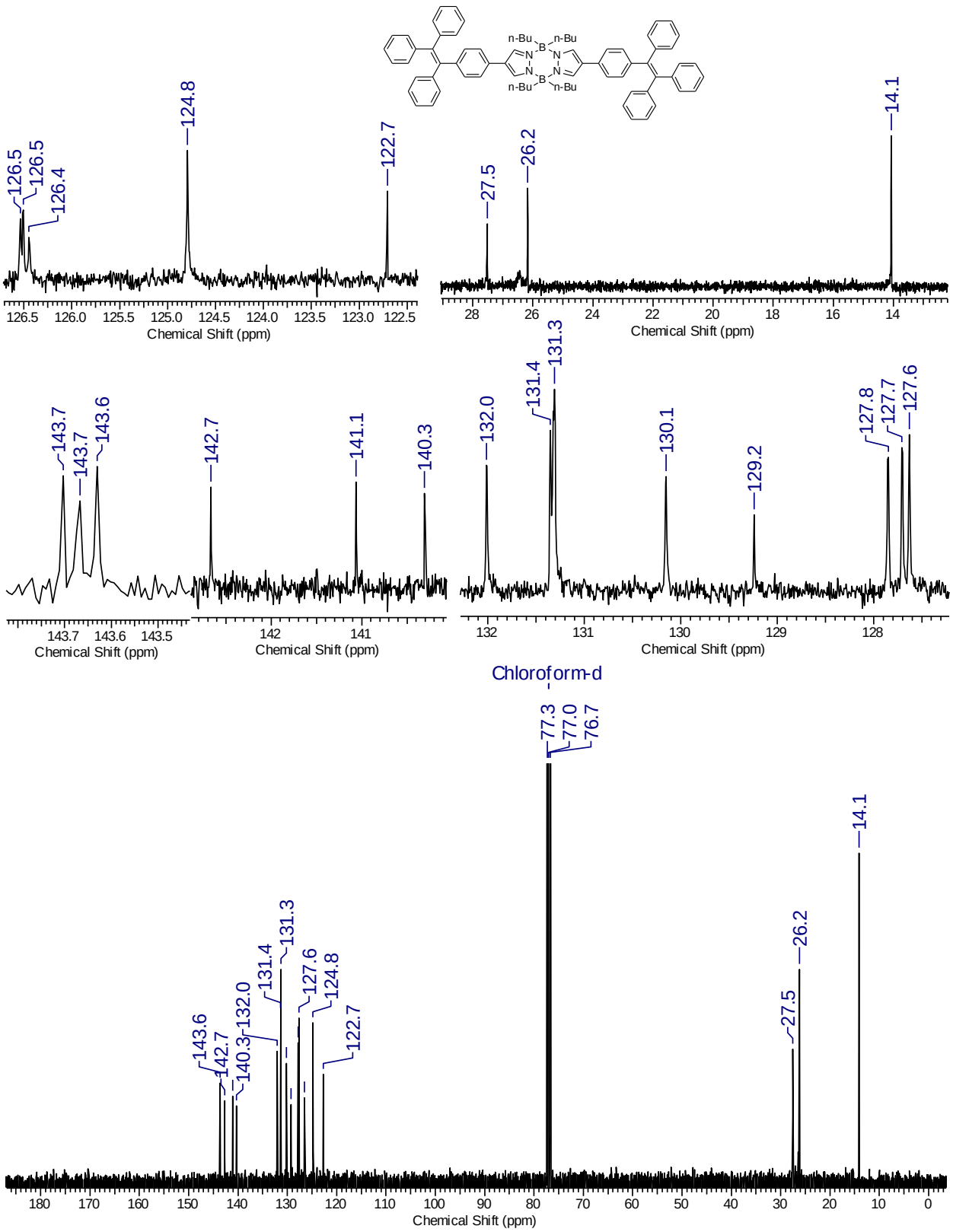


Fig. S4 PXRD curves of **2** in Synthesized, Grinded and Fumed form.


n-Bu
n-Bu
B
N
N
N
N
B
n-Bu
n-Bu
Chloroform-d
7.75
7.31
7.30
7.26
7.17
7.15
7.11
7.09
7.06
7.05
7.04
1.19
1.17
1.15
1.13
0.82
0.81
0.77
0.75
0.74
0.69
0.67
0.65
4.00
4.00
34.07
8.00
28.07
Chemical Shift (ppm)
Chemical Shift (ppm)
Chloroform-d
7.75
7.31
7.30
7.26
7.15
7.11
7.09
7.06
7.05
7.04
7.02
1.56
1.19
1.17
1.15
0.82
0.81
0.77
0.75
0.74
0.69
0.67
0.65
4.00
34.07
8.00
28.07
Chemical Shift (ppm)


n-Bu
n-Bu
n-Bu
n-Bu
126.5
126.5
126.4
124.8
122.7
27.5
26.2
14.1
Chemical Shift (ppm)
143.7
143.7
143.6
142.7
141.1
140.3
132.0
131.4
131.3
130.1
129.2
127.8
127.7
127.6
Chemical Shift (ppm)
Chloroform-d
77.3
77.0
76.7
143.6
142.7
140.3
132.0
131.4
131.3
127.6
124.8
122.7
27.5
26.2
14.1
Chemical Shift (ppm)

DFT calculation data of pyrazabole 2:

Calculation method: B3LYP/6-31+G(d) with Gaussian 09

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.059331	-1.238970	0.768272
2	7	0	-1.238054	-0.336104	0.566346
3	7	0	-1.296843	0.785685	-0.197011
4	6	0	0.134963	-1.765437	2.304686
5	1	0	-0.686927	-2.480964	2.462684
6	1	0	1.043388	-2.377054	2.428343
7	6	0	0.110395	-0.696518	3.412036
8	1	0	-0.828727	-0.126393	3.354685
9	1	0	0.910428	0.033973	3.225621
10	6	0	0.273385	-1.236051	4.844424
11	1	0	1.219204	-1.793333	4.914843
12	1	0	0.369917	-0.385949	5.534293
13	6	0	-0.877060	-2.130702	5.320832
14	1	0	-1.835872	-1.598395	5.271044
15	1	0	-0.728320	-2.448156	6.359537
16	1	0	-0.967780	-3.036046	4.710195
17	6	0	-0.021525	-2.422585	-0.360259
18	1	0	-0.967257	-2.965537	-0.198346
19	1	0	-0.118734	-1.968829	-1.360236
20	6	0	1.115373	-3.456565	-0.402967
21	1	0	1.222734	-3.938731	0.580375
22	1	0	2.074246	-2.955423	-0.602045
23	6	0	0.911340	-4.547080	-1.465158
24	1	0	-0.039430	-5.064442	-1.271843
25	1	0	0.801492	-4.071692	-2.450332
26	6	0	2.049736	-5.571605	-1.515468
27	1	0	3.008158	-5.088396	-1.743682
28	1	0	1.871530	-6.334528	-2.282494
29	1	0	2.162433	-6.087685	-0.553581
30	6	0	-2.590981	1.086363	-0.401690
31	1	0	-2.858444	1.971905	-0.957054
32	6	0	-2.495113	-0.730491	0.830418
33	1	0	-2.669720	-1.638930	1.386858
34	6	0	-3.409286	0.146887	0.237063
35	5	0	-0.063240	1.741577	-0.503104
36	7	0	1.233325	0.835934	-0.306681
37	7	0	1.291945	-0.282453	0.461979
38	6	0	-0.141288	2.272198	-2.037991
39	1	0	0.681178	2.987122	-2.195654
40	1	0	-1.049093	2.885467	-2.158117

41	6	0	-0.120395	1.206300	-3.148343
42	1	0	0.818288	0.635073	-3.094662
43	1	0	-0.920703	0.476067	-2.962189
44	6	0	-0.286066	1.749884	-4.578884
45	1	0	-1.231787	2.307740	-4.645847
46	1	0	-0.384481	0.901717	-5.270869
47	6	0	0.863769	2.645364	-5.055210
48	1	0	1.822532	2.112658	-5.008550
49	1	0	0.713198	2.965476	-6.092837
50	1	0	0.955993	3.549133	-4.442491
51	6	0	0.021226	2.921847	0.628336
52	1	0	0.966885	3.464671	0.465672
53	1	0	0.120300	2.465378	1.626891
54	6	0	-1.115184	3.956168	0.676285
55	1	0	-1.223836	4.441551	-0.305351
56	1	0	-2.073920	3.454589	0.875234
57	6	0	-0.909066	5.043196	1.741634
58	1	0	0.041808	5.560446	1.548589
59	1	0	-0.798197	4.564599	2.725129
60	6	0	-2.046687	6.068324	1.796711
61	1	0	-3.005143	5.585387	2.025304
62	1	0	-1.866623	6.828918	2.565582
63	1	0	-2.160534	6.587336	0.836532
64	6	0	2.585828	-0.584878	0.664601
65	1	0	2.854253	-1.469123	1.221646
66	6	0	2.490758	1.226064	-0.576713
67	1	0	2.666376	2.131364	-1.138033
68	6	0	3.404225	0.349234	0.018461
69	6	0	-4.876251	0.092922	0.274623
70	6	0	-5.551776	-0.523827	1.341102
71	6	0	-5.650585	0.662115	-0.749861
72	6	0	-6.941093	-0.571676	1.377769
73	1	0	-4.982741	-0.949334	2.163597
74	6	0	-7.039754	0.609169	-0.714022
75	1	0	-5.158967	1.138642	-1.593916
76	6	0	-7.718022	-0.020109	0.343673
77	1	0	-7.436400	-1.041068	2.222859
78	1	0	-7.612081	1.055740	-1.520800
79	6	0	-9.209811	-0.051447	0.408538
80	6	0	-9.985920	-0.429055	-0.651296
81	6	0	-9.785924	0.361932	1.725283
82	6	0	-11.465056	-0.215309	-0.685399
83	6	0	-9.422950	-1.091438	-1.867626
84	6	0	-9.329896	1.525442	2.369833
85	6	0	-10.749757	-0.423869	2.379634
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87	6	0	-12.029224	1.037040	-0.388566
88	6	0	-9.781340	-0.647518	-3.152841
89	6	0	-8.572449	-2.205303	-1.764110
90	6	0	-9.843046	1.907374	3.608390
91	1	0	-8.569963	2.135309	1.889288
92	6	0	-11.254761	-0.048714	3.623658

93	1	0	-11.101313	-1.335097	1.905888
94	6	0	-13.706169	-1.061505	-1.130281
95	1	0	-11.907943	-2.225935	-1.327135
96	6	0	-13.407334	1.235720	-0.457150
97	1	0	-11.378257	1.857927	-0.104348
98	6	0	-9.279943	-1.273332	-4.293046
99	1	0	-10.455111	0.198821	-3.253281
100	6	0	-8.080529	-2.839241	-2.904080
101	1	0	-8.300265	-2.574541	-0.780203
102	6	0	-10.808103	1.121099	4.241270
103	1	0	-9.485002	2.818008	4.081749
104	1	0	-11.996417	-0.674694	4.113078
105	6	0	-14.252626	0.186157	-0.822194
106	1	0	-14.354441	-1.884485	-1.420114
107	1	0	-13.820861	2.214497	-0.228118
108	6	0	-8.427143	-2.372750	-4.173577
109	1	0	-9.560038	-0.904668	-5.276494
110	1	0	-7.428262	-3.702417	-2.799660
111	1	0	-11.203333	1.413821	5.210388
112	1	0	-15.327099	0.341040	-0.873350
113	1	0	-8.041932	-2.866005	-5.062027
114	6	0	4.871375	0.388972	-0.026628
115	6	0	5.549970	0.968434	-1.111570
116	6	0	5.642559	-0.151259	1.016045
117	6	0	6.939788	1.003655	-1.151202
118	1	0	4.982584	1.379192	-1.942725
119	6	0	7.031726	-0.131821	0.966138
120	1	0	5.147550	-0.571249	1.887711
121	6	0	7.714248	0.434965	-0.124358
122	1	0	7.437667	1.463511	-1.999929
123	1	0	7.600911	-0.553504	1.788217
124	6	0	9.205516	0.488531	-0.173315
125	6	0	9.992872	-0.592393	0.111498
126	6	0	9.771408	1.816550	-0.564319
127	6	0	11.468378	-0.482273	0.323772
128	6	0	9.447114	-1.979293	0.230794
129	6	0	9.310826	2.997606	0.043854
130	6	0	10.729788	1.926794	-1.585946
131	6	0	12.348898	-1.382132	-0.302775
132	6	0	12.011434	0.478096	1.194278
133	6	0	9.802189	-2.795825	1.319228
134	6	0	8.616757	-2.524162	-0.763452
135	6	0	9.814333	4.241591	-0.333402
136	1	0	8.555642	2.934470	0.822522
137	6	0	11.224983	3.171470	-1.971975
138	1	0	11.084734	1.026917	-2.078686
139	6	0	13.724602	-1.303128	-0.092623
140	1	0	11.947125	-2.145264	-0.963402
141	6	0	13.386084	0.550065	1.413947
142	1	0	11.346494	1.169188	1.702658
143	6	0	9.316073	-4.097835	1.427178
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147	6	0	10.773824	4.333950	-1.343904
148	1	0	9.453319	5.140450	0.159820
149	1	0	11.962350	3.232746	-2.768193
150	6	0	14.249665	-0.336161	0.767262
151	1	0	14.386982	-2.001282	-0.597985
152	1	0	13.782421	1.298043	2.095773
153	6	0	8.482545	-4.621152	0.436405
154	1	0	9.593095	-4.706310	2.284261
155	1	0	7.503543	-4.232153	-1.446184
156	1	0	11.161376	5.303978	-1.643774
157	1	0	15.321488	-0.278762	0.937534
158	1	0	8.109629	-5.638832	0.515814

Total Energy (HF) = - 3135.7078462 Hartree