Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Phenothiazine-Based Small-Molecule Organic Solar Cells with Power Conversion Efficiency Over 7% and Open Circuit Voltage of About 1.0 V Using Solvent Vapor Annealing

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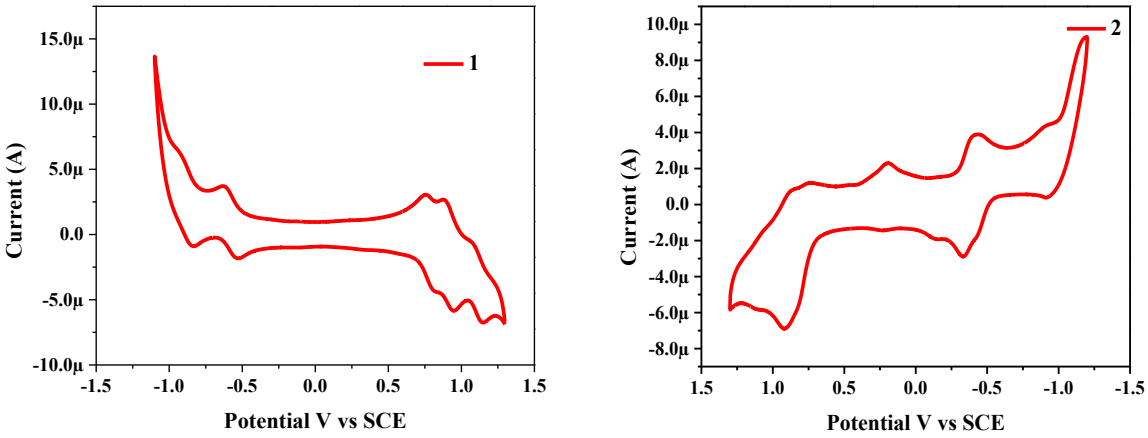

Figure S1. Cyclic voltammograms of phenothiazine **1** and **2** in 0.1 M solution of Bu_4NPF_6 in dichloromethane at 25 °C.

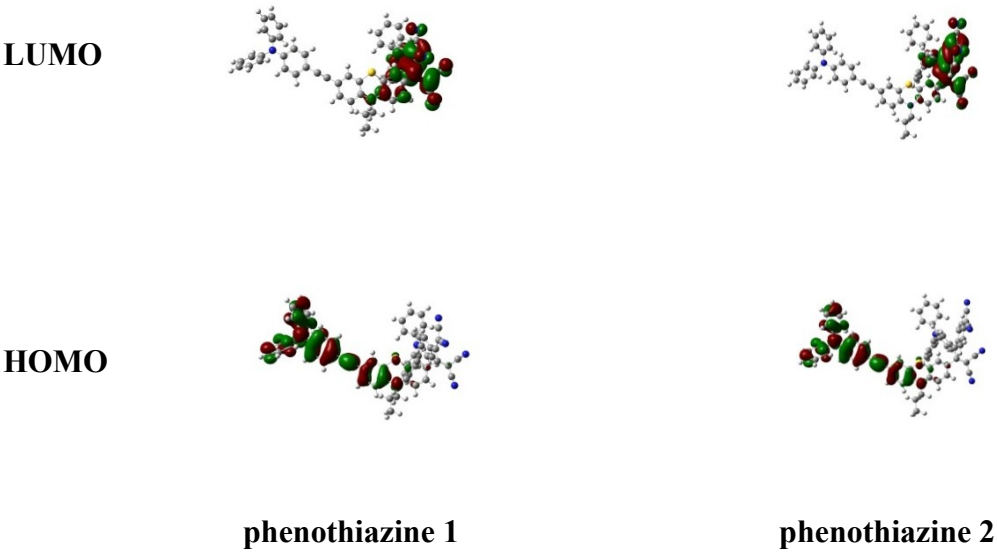

Figure S2. The molecular orbitals of phenothiazine **1** and **2** estimated from DFT calculation.

TD-DFT Calculation data

Phenothiazines **1** and **2**

Calculation method: B3LYP/6-31G (d, p) level

Excitation energies and oscillator strengths:

Phenothiazine **1**

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Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      1.6422 eV  755.00 nm  f=0.0943
<S**2>=0.000
     234 -> 237        0.10204
     236 -> 237        0.69833
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3130.51875155
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      2.0188 eV  614.16 nm  f=0.1172
<S**2>=0.000
     234 -> 237        0.27330
     235 -> 237        0.63517
     235 -> 238        0.11284

 Excited State   3:      Singlet-A      2.0909 eV  592.98 nm  f=0.0786
<S**2>=0.000
     234 -> 237        0.62963
     235 -> 237       -0.26197
     236 -> 237       -0.10754
     236 -> 238       -0.10739

 Excited State   4:      Singlet-A      2.1409 eV  579.13 nm  f=0.1507
<S**2>=0.000
     234 -> 238        0.10107
     235 -> 238       -0.10121
     236 -> 238        0.68102

 Excited State   5:      Singlet-A      2.5461 eV  486.96 nm  f=0.25
60  <S**2>=0.000
     234 -> 238       -0.29003
     235 -> 238        0.61549
     236 -> 238        0.13818
```

```
 Excited State   6:      Singlet-A      2.6256 eV  472.21 nm  f=0.4432
<S**2>=0.000
     234 -> 238        0.61820
     235 -> 237       -0.11964
     235 -> 238        0.29885

 Excited State   7:      Singlet-A      2.8325 eV  437.72 nm  f=0.0273
<S**2>=0.000
     232 -> 237        0.19532
     233 -> 237        0.66978

 Excited State   8:      Singlet-A      3.0746 eV  403.25 nm  f=1.1589
<S**2>=0.000
     232 -> 237        0.43668
     233 -> 237       -0.14497
     236 -> 239        0.51820

 Excited State   9:      Singlet-A      3.1643 eV  391.82 nm  f=0.3501
<S**2>=0.000
     232 -> 237        0.48937
     232 -> 238       -0.11128
     233 -> 237       -0.12755
     236 -> 239       -0.45515

 Excited State  10:      Singlet-A      3.3544 eV  369.62 nm  f=0.0204
<S**2>=0.000
     232 -> 238        0.18303
     233 -> 238        0.67099

 Excited State  11:      Singlet-A      3.4178 eV  362.76 nm  f=0.0395
<S**2>=0.000
     226 -> 237       -0.19199
     229 -> 237        0.66499

 Excited State  12:      Singlet-A      3.5259 eV  351.64 nm  f=0.0023
<S**2>=0.000
     221 -> 237       -0.27491
     228 -> 237        0.62627
     231 -> 237       -0.11316

 Excited State  13:      Singlet-A      3.5568 eV  348.59 nm  f=0.0059
<S**2>=0.000
     228 -> 237        0.11004
     230 -> 237       -0.12825
     231 -> 237        0.62039
     232 -> 238        0.20788

 Excited State  14:      Singlet-A      3.5801 eV  346.31 nm  f=0.0101
<S**2>=0.000
     230 -> 237        0.64051
     232 -> 238        0.20508
     234 -> 239        0.14129
```

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 Excited State  15:      Singlet-A      3.5851 eV  345.84 nm  f=0.0448
<S**2>=0.000
     230 -> 237       -0.26293
     231 -> 237       -0.27834
     232 -> 238        0.39246
     234 -> 239        0.31846
     235 -> 239       -0.17856

 Excited State  16:      Singlet-A      3.6078 eV  343.66 nm  f=0.0113
<S**2>=0.000
     226 -> 237        0.63843
     229 -> 237        0.21011
     229 -> 238       -0.14096

 Excited State  17:      Singlet-A      3.6848 eV  336.48 nm  f=0.1112
<S**2>=0.000
     224 -> 237        0.10436
     231 -> 237        0.11116
     232 -> 238       -0.38499
     233 -> 238        0.12243
     234 -> 239        0.39363
     235 -> 239       -0.28018
     236 -> 240        0.12134

 Excited State  18:      Singlet-A      3.7485 eV  330.76 nm  f=0.0896
<S**2>=0.000
     220 -> 237        0.12388
     221 -> 237        0.12783
     234 -> 239       -0.18681
     234 -> 240        0.17583
     235 -> 239        0.12481
     236 -> 240        0.55320
     236 -> 241       -0.17274

 Excited State  19:      Singlet-A      3.7631 eV  329.47 nm  f=0.0131
<S**2>=0.000
     220 -> 237       -0.10797
     221 -> 237        0.60594
     228 -> 237        0.27829
     236 -> 240       -0.11855

 Excited State  20:      Singlet-A      3.8088 eV  325.52 nm  f=0.0047
<S**2>=0.000
     220 -> 237       -0.15501
     234 -> 239        0.35522
     235 -> 239        0.56902
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   20
LETran=     370.
```

Phenothiazine **2**

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Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      2.1586 eV  574.38 nm  f=1.1792
<S**2>=0.000
     253 -> 257       -0.10658
     255 -> 257        0.68315
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3359.86521827
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      2.5415 eV  487.85 nm  f=0.1726
<S**2>=0.000
     252 -> 257       -0.10661
     254 -> 257       -0.46141
     254 -> 258        0.13073
     256 -> 257        0.47877

 Excited State   3:      Singlet-A      3.0381 eV  408.10 nm  f=0.3223
<S**2>=0.000
     253 -> 257        0.36204
     254 -> 257       -0.11472
     254 -> 258        0.26273
     255 -> 258        0.31081
     256 -> 257       -0.29448
     256 -> 258       -0.22427

 Excited State   4:      Singlet-A      3.0824 eV  402.24 nm  f=0.0984
<S**2>=0.000
     252 -> 257        0.13260
     253 -> 257        0.36973
     254 -> 257        0.36047
     255 -> 258        0.13379
     256 -> 257        0.40508

 Excited State   5:      Singlet-A      3.1733 eV  390.71 nm  f=0.5182
<S**2>=0.000
     253 -> 257       -0.30163
     253 -> 258       -0.11642
     254 -> 258       -0.14823
     255 -> 258        0.57605

 Excited State   6:      Singlet-A      3.2423 eV  382.40 nm  f=0.4781
<S**2>=0.000
     252 -> 257        0.10607
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     253 -> 257       -0.32001
     254 -> 257        0.27506
     254 -> 258        0.36376
     256 -> 257        0.10217
     256 -> 258       -0.31430
     256 -> 259       -0.15959

 Excited State   7:      Singlet-A      3.6440 eV  340.24 nm  f=0.3984
<S**2>=0.000
     240 -> 257       -0.12763
     251 -> 257        0.52614
     251 -> 258       -0.13416
     252 -> 257        0.20562
     252 -> 258       -0.11187
     254 -> 258       -0.11610
     256 -> 259       -0.22629

 Excited State   8:      Singlet-A      3.6974 eV  335.33 nm  f=0.8672
<S**2>=0.000
     251 -> 257        0.23971
     254 -> 258        0.19774
     256 -> 259        0.56146

 Excited State   9:      Singlet-A      3.8967 eV  318.18 nm  f=0.0105
<S**2>=0.000
     238 -> 257        0.56958
     241 -> 257        0.31566
     247 -> 257        0.15516

 Excited State  10:      Singlet-A      3.9593 eV  313.14 nm  f=0.0630
<S**2>=0.000
     237 -> 257        0.10884
     241 -> 257       -0.13184
     242 -> 257        0.14168
     243 -> 257        0.11540
     244 -> 257        0.17778
     247 -> 257       -0.11716
     251 -> 257       -0.15082
     252 -> 257        0.41903
     252 -> 258       -0.14917
     253 -> 258        0.12097
     254 -> 257       -0.21919
     254 -> 258       -0.10491
     256 -> 258       -0.21031

 Excited State  11:      Singlet-A      4.0092 eV  309.25 nm  f=0.0765
<S**2>=0.000
     238 -> 257        0.29944
     241 -> 257       -0.29005
     247 -> 257       -0.20843
     253 -> 258        0.31297
     254 -> 258        0.11948
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     256 -> 258        0.29104

 Excited State  12:      Singlet-A      4.0415 eV  306.78 nm  f=0.0430
<S**2>=0.000
     238 -> 257       -0.21446
     241 -> 257        0.32376
     247 -> 257        0.19926
     251 -> 258       -0.10905
     253 -> 258        0.40176
     256 -> 258        0.21098

 Excited State  13:      Singlet-A      4.0858 eV  303.45 nm  f=0.0164
<S**2>=0.000
     252 -> 257        0.28561
     252 -> 258        0.13498
     253 -> 258       -0.33357
     254 -> 258        0.22857
     254 -> 259        0.14976
     256 -> 258        0.37716

 Excited State  14:      Singlet-A      4.2502 eV  291.71 nm  f=0.0082
<S**2>=0.000
     240 -> 258        0.11513
     251 -> 258       -0.26308
     252 -> 257       -0.21844
     252 -> 258       -0.17870
     254 -> 259        0.28404
     254 -> 260        0.15463
     254 -> 261       -0.19043
     254 -> 262       -0.16984
     254 -> 263       -0.10580
     256 -> 260       -0.10095
     256 -> 261        0.12205
     256 -> 262        0.11091
     256 -> 263        0.10460

 Excited State  15:      Singlet-A      4.3345 eV  286.04 nm  f=0.2874
<S**2>=0.000
     240 -> 257        0.14273
     242 -> 257        0.17589
     248 -> 257        0.19069
     251 -> 257        0.10305
     251 -> 258        0.36465
     254 -> 259        0.29910
     254 -> 263       -0.11676

 Excited State  16:      Singlet-A      4.4049 eV  281.47 nm  f=0.0459
<S**2>=0.000
     236 -> 257        0.13151
     237 -> 257        0.10199
     240 -> 257        0.22502
     241 -> 257        0.11698
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     242 -> 257        0.34770
     248 -> 257        0.33260
     251 -> 258       -0.20532
     253 -> 258       -0.14290
     254 -> 259       -0.15794

 Excited State  17:      Singlet-A      4.4101 eV  281.14 nm  f=0.0274
<S**2>=0.000
     254 -> 265        0.21993
     256 -> 265        0.60938
     256 -> 273       -0.12490

 Excited State  18:      Singlet-A      4.4967 eV  275.72 nm  f=0.0497
<S**2>=0.000
     251 -> 259        0.14747
     254 -> 259        0.15764
     254 -> 263        0.38536
     254 -> 266        0.13519
     254 -> 268       -0.12644
     256 -> 263       -0.35271
     256 -> 266       -0.14136
     256 -> 268        0.15295

 Excited State  19:      Singlet-A      4.5385 eV  273.18 nm  f=0.1069
<S**2>=0.000
     241 -> 257        0.11011
     255 -> 260        0.37819
     255 -> 261        0.42901
     255 -> 262       -0.18206

 Excited State  20:      Singlet-A      4.5440 eV  272.85 nm  f=0.1447
<S**2>=0.000
     241 -> 257       -0.10283
     248 -> 257       -0.14191
     253 -> 262        0.11306
     255 -> 260        0.39969
     255 -> 261       -0.22396
     255 -> 262        0.38212
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   20
LETran=     370.
```

Theoretical calculation:

Calculation method: B3LYP/6-31G** for C, H, N, S with Gaussian 09.

1

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.743780	-3.265752	-1.614756
2	6	0	-0.478754	-2.776898	-1.111978
3	6	0	-1.690141	-3.286560	-1.564680
4	6	0	-1.731668	-4.331546	-2.506941
5	6	0	-0.512730	-4.840679	-2.981127
6	6	0	0.700206	-4.309346	-2.557902
7	6	0	-4.004235	-5.023558	-1.992958
8	6	0	-4.198578	-4.053974	-0.981848
9	6	0	-5.200683	-4.204010	-0.036022
10	1	0	-5.312764	-3.436098	0.720884
11	6	0	-6.098862	-5.293011	-0.076858
12	6	0	-5.891818	-6.263835	-1.077067
13	6	0	-4.860880	-6.141365	-1.995798
14	1	0	-0.473644	-1.982006	-0.374130
15	1	0	-0.506476	-5.659989	-3.690212
16	1	0	1.628720	-4.711167	-2.948591
17	1	0	-6.508191	-7.152145	-1.116980
18	1	0	-4.707342	-6.941712	-2.709312
19	7	0	-2.978346	-4.860812	-2.931374
20	16	0	-3.221927	-2.565005	-1.006658
21	6	0	-3.065095	-5.534183	-4.235435
22	1	0	-2.443896	-6.441791	-4.259984
23	1	0	-4.098174	-5.860870	-4.359004
24	6	0	-7.165351	-5.387865	0.922159
25	6	0	-6.923668	-4.707571	2.245229
26	6	0	-8.355221	-6.062222	0.764855
27	6	0	-5.987700	-5.354486	3.158314
28	6	0	-7.587016	-3.518673	2.469068
29	6	0	-8.785313	-6.681693	-0.453356
30	6	0	-9.286982	-6.199624	1.847208
31	6	0	-5.774780	-6.750286	3.080109
32	6	0	-5.245356	-4.648463	4.133101
33	6	0	-8.392585	-2.908564	1.451687
34	6	0	-7.555800	-2.790658	3.701552
35	7	0	-9.177165	-7.200259	-1.419023
36	7	0	-10.053615	-6.352352	2.709345
37	6	0	-4.913274	-7.407726	3.937877

38	1	0	-6.327391	-7.338375	2.355947
39	1	0	-5.322375	-3.571237	4.203777
40	6	0	-4.368611	-5.294619	4.983484
41	7	0	-9.035721	-2.378357	0.639119
42	7	0	-7.564940	-2.166862	4.684529
43	6	0	-4.188445	-6.694847	4.918513
44	1	0	-4.806633	-8.483239	3.866572
45	1	0	-3.798444	-4.714323	5.698676
46	7	0	-3.316779	-7.348530	5.790082
47	6	0	-2.715314	-8.597651	5.435144
48	6	0	-3.000753	-6.794131	7.071759
49	6	0	-2.765061	-9.676248	6.328024
50	6	0	-2.049630	-8.743423	4.209946
51	6	0	-1.663964	-6.699422	7.480537
52	6	0	-4.021084	-6.368273	7.933646
53	1	0	-3.279080	-9.559577	7.276313
54	6	0	-2.155435	-10.884824	5.996167
55	6	0	-1.455810	-9.960538	3.879879
56	1	0	-1.998970	-7.903030	3.525311
57	1	0	-0.876899	-7.031383	6.811570
58	6	0	-1.354687	-6.183631	8.737794
59	6	0	-3.701306	-5.838665	9.182620
60	1	0	-5.056812	-6.453056	7.621675
61	1	0	-2.200387	-11.714941	6.694710
62	6	0	-1.502920	-11.034460	4.770902
63	1	0	-0.941779	-10.063197	2.928836
64	1	0	-0.315634	-6.113614	9.045398
65	6	0	-2.369437	-5.747070	9.591575
66	1	0	-4.498585	-5.509533	9.842097
67	1	0	-1.033245	-11.978709	4.513715
68	1	0	-2.124920	-5.340450	10.567879
69	6	0	1.980018	-2.721049	-1.172420
70	6	0	3.036168	-2.250483	-0.790998
71	6	0	4.267096	-1.698418	-0.343113
72	6	0	5.498859	-2.148135	-0.861432
73	6	0	4.294171	-0.682549	0.634610
74	6	0	6.700238	-1.613982	-0.419247
75	1	0	5.502804	-2.935832	-1.607861
76	1	0	3.357764	-0.313342	1.040064
77	6	0	5.493581	-0.137926	1.068962
78	6	0	6.720512	-0.595748	0.552537
79	1	0	7.635772	-1.984977	-0.822597
80	1	0	5.488597	0.652051	1.811606
81	7	0	7.942851	-0.046429	0.999590
82	6	0	9.034822	0.113341	0.098509
83	6	0	8.099845	0.350570	2.358969
84	6	0	10.333656	-0.246241	0.489518
85	6	0	8.828834	0.640324	-1.186067
86	6	0	8.713565	1.572736	2.673092
87	6	0	7.653542	-0.478009	3.400104
88	1	0	10.496952	-0.656842	1.480268
89	6	0	11.402812	-0.074862	-0.387533

90	6	0	9.901620	0.790965	-2.062397
91	1	0	7.828144	0.928996	-1.489934
92	1	0	9.056855	2.217707	1.871153
93	6	0	8.881218	1.951641	4.003523
94	6	0	7.809316	-0.082170	4.726989
95	1	0	7.187189	-1.428284	3.162321
96	1	0	12.402314	-0.357694	-0.070068
97	6	0	11.194281	0.439072	-1.668829
98	1	0	9.726127	1.200396	-3.053030
99	1	0	9.358009	2.900742	4.230702
100	6	0	8.426833	1.131029	5.037681
101	1	0	7.458592	-0.734228	5.521738
102	1	0	12.028719	0.565074	-2.351661
103	1	0	8.552860	1.432819	6.072790
104	6	0	-2.719306	-4.609245	-5.410845
105	1	0	-1.702914	-4.219061	-5.301585
106	1	0	-3.390717	-3.744017	-5.375271
107	6	0	-2.855846	-5.333232	-6.753695
108	1	0	-3.875091	-5.704027	-6.908872
109	1	0	-2.618759	-4.661079	-7.583111
110	1	0	-2.176713	-6.190979	-6.818575

E(HF)=-3130.5534345

2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.514067	-2.801216	-0.788522
2	6	0	-1.416225	-2.594539	0.070840
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4	6	0	0.035672	-3.896690	-1.388913
5	6	0	-1.049927	-4.071754	-2.261137
6	6	0	-2.303096	-3.550352	-1.961073
7	6	0	2.455216	-3.658659	-1.393330
8	6	0	2.502013	-2.873831	-0.217686
9	6	0	3.616488	-2.103520	0.078154
10	1	0	3.615340	-1.515088	0.989288
11	6	0	4.761888	-2.115396	-0.746299
12	6	0	4.703026	-2.882069	-1.925871
13	6	0	3.571977	-3.616407	-2.250043
14	1	0	-1.547803	-2.010073	0.974953
15	1	0	-0.919645	-4.623100	-3.184770
16	1	0	-3.129843	-3.710717	-2.644444
17	1	0	5.527389	-2.872909	-2.627282
18	1	0	3.551459	-4.145203	-3.195173
19	7	0	1.319434	-4.427451	-1.677766

20	16	0	1.163543	-2.980521	0.952456
21	6	0	1.430063	-5.597623	-2.560807
22	1	0	1.075557	-5.368887	-3.576812
23	1	0	2.491198	-5.833807	-2.647786
24	6	0	5.935150	-1.326948	-0.353051
25	6	0	5.703940	-0.082749	0.449329
26	6	0	7.234808	-1.648305	-0.689761
27	6	0	4.968885	0.983842	-0.226942
28	6	0	7.625824	-2.860439	-1.347022
29	6	0	8.329663	-0.767603	-0.399747
30	6	0	5.113121	1.191941	-1.618193
31	6	0	4.056445	1.826714	0.450638
32	7	0	7.991548	-3.835027	-1.868710
33	7	0	9.245396	-0.075268	-0.207407
34	6	0	4.437982	2.200759	-2.280912
35	1	0	5.808561	0.576870	-2.179906
36	1	0	3.847800	1.651438	1.500452
37	6	0	3.363963	2.828480	-0.205144
38	6	0	3.549020	3.051344	-1.587287
39	1	0	4.606356	2.352213	-3.340510
40	1	0	2.649796	3.432571	0.341948
41	7	0	2.863560	4.075337	-2.247739
42	6	0	2.555867	3.977134	-3.640599
43	6	0	2.452699	5.252536	-1.547051
44	6	0	2.841528	5.048318	-4.498036
45	6	0	1.945431	2.824002	-4.154257
46	6	0	1.139755	5.724663	-1.679130
47	6	0	3.362686	5.955017	-0.743989
48	1	0	3.312900	5.940018	-4.098390
49	6	0	2.518843	4.963820	-5.851150
50	6	0	1.640103	2.742598	-5.511741
51	1	0	1.711117	2.000717	-3.487327
52	1	0	0.437396	5.180741	-2.301991
53	6	0	0.745906	6.884873	-1.014805
54	6	0	2.955449	7.105483	-0.070976
55	1	0	4.383331	5.597874	-0.653866
56	1	0	2.745419	5.799121	-6.506946
57	6	0	1.921679	3.811195	-6.365231
58	1	0	1.166328	1.845564	-5.899227
59	1	0	-0.273879	7.241843	-1.123331
60	6	0	1.648063	7.577221	-0.204854
61	1	0	3.668080	7.642074	0.548165
62	1	0	1.676010	3.747112	-7.420619
63	1	0	1.336237	8.477429	0.315362
64	6	0	-3.792392	-2.262618	-0.478179
65	6	0	-4.888086	-1.803868	-0.210939
66	6	0	-6.167493	-1.269167	0.101641
67	6	0	-7.281784	-1.518015	-0.725824
68	6	0	-6.362772	-0.473662	1.249472
69	6	0	-8.529484	-0.992004	-0.425093
70	1	0	-7.153053	-2.119701	-1.619715
71	1	0	-5.521917	-0.277724	1.906863

72	6	0	-7.612215	0.042951	1.559135
73	6	0	-8.719667	-0.203699	0.725678
74	1	0	-9.368741	-1.186013	-1.083524
75	1	0	-7.740890	0.640250	2.454801
76	7	0	-9.990948	0.327319	1.036683
77	6	0	-11.173502	-0.411953	0.744356
78	6	0	-10.107060	1.611369	1.643357
79	6	0	-12.279356	0.224151	0.160011
80	6	0	-11.252003	-1.780696	1.045207
81	6	0	-10.988147	1.809654	2.717267
82	6	0	-9.351666	2.695103	1.169485
83	1	0	-12.221733	1.281278	-0.076715
84	6	0	-13.440683	-0.496759	-0.110841
85	6	0	-12.411158	-2.497009	0.753998
86	1	0	-10.403241	-2.275135	1.505827
87	1	0	-11.571263	0.973713	3.088919
88	6	0	-11.112592	3.069927	3.298611
89	6	0	-9.469566	3.947369	1.769087
90	1	0	-8.676564	2.548899	0.332858
91	1	0	-14.288436	0.009747	-0.563078
92	6	0	-13.512942	-1.860631	0.178869
93	1	0	-12.456829	-3.555589	0.992939
94	1	0	-11.798738	3.207613	4.129248
95	6	0	-10.352184	4.144335	2.832988
96	1	0	-8.878209	4.776409	1.391188
97	1	0	-14.417013	-2.420458	-0.039473
98	1	0	-10.446702	5.123056	3.292955
99	6	0	0.715071	-6.836664	-2.003814
100	1	0	-0.349714	-6.629125	-1.860924
101	1	0	1.126296	-7.051913	-1.011140
102	6	0	0.888719	-8.047888	-2.925076
103	1	0	1.945746	-8.303599	-3.058349
104	1	0	0.385926	-8.926136	-2.510561
105	1	0	0.464119	-7.862077	-3.918199
106	6	0	6.162270	-0.013586	1.766643
107	6	0	6.262418	1.235050	2.491783
108	6	0	6.569077	-1.198786	2.492597
109	6	0	6.670351	1.287338	3.787206
110	1	0	6.065539	2.159713	1.963681
111	6	0	6.952114	-1.153885	3.795712
112	1	0	6.522214	-2.159844	1.993143
113	6	0	7.009014	0.092053	4.517504
114	1	0	6.772542	2.245513	4.285741
115	1	0	7.215413	-2.068413	4.316486
116	6	0	7.391752	0.141992	5.860528
117	6	0	7.438835	1.373235	6.575049
118	6	0	7.744078	-1.035348	6.580450
119	7	0	8.024694	-2.009646	7.156100
120	7	0	7.467679	2.390920	7.143386

E(HF) = -3361.58356984