

## Supporting Information for:

### A theoretical study on $\pi$ -stacking and ferromagnetism of perylene diimide radical anion dimer

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Section 1:

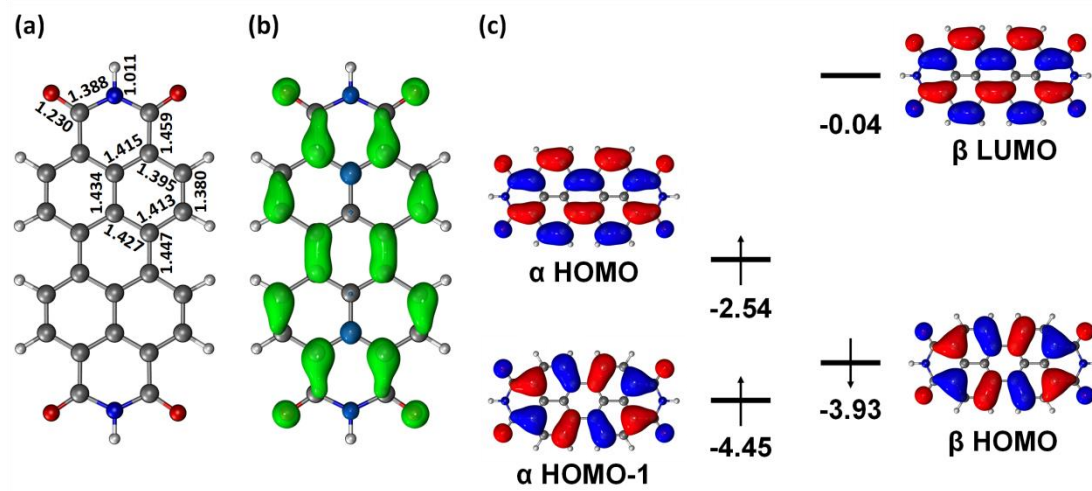


Fig. S1: (a) Optimized structure (Å), (b) spin density distribution maps (isovalue=0.002 a.u.), and (c) KS orbitals (eV, isovalue=0.020 a.u.) of PDI<sup>-</sup> at UM05-2X/6-31+G(d) theoretical level.

**Section 2:**

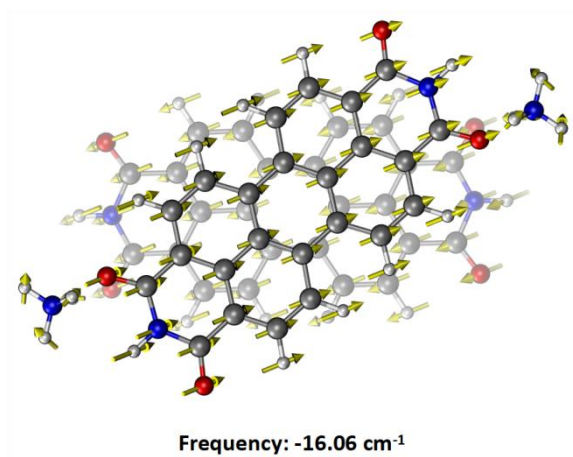


Fig. S2: Vibrational mode of the imaginary frequency of pimer 2.

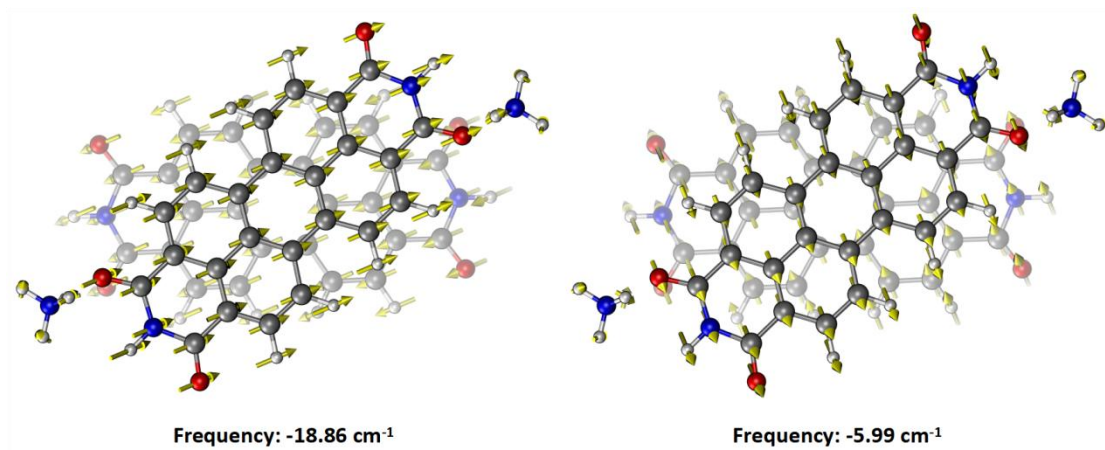


Fig. S3: Vibrational mode of the imaginary frequency of pimer 13.

### Section 3:

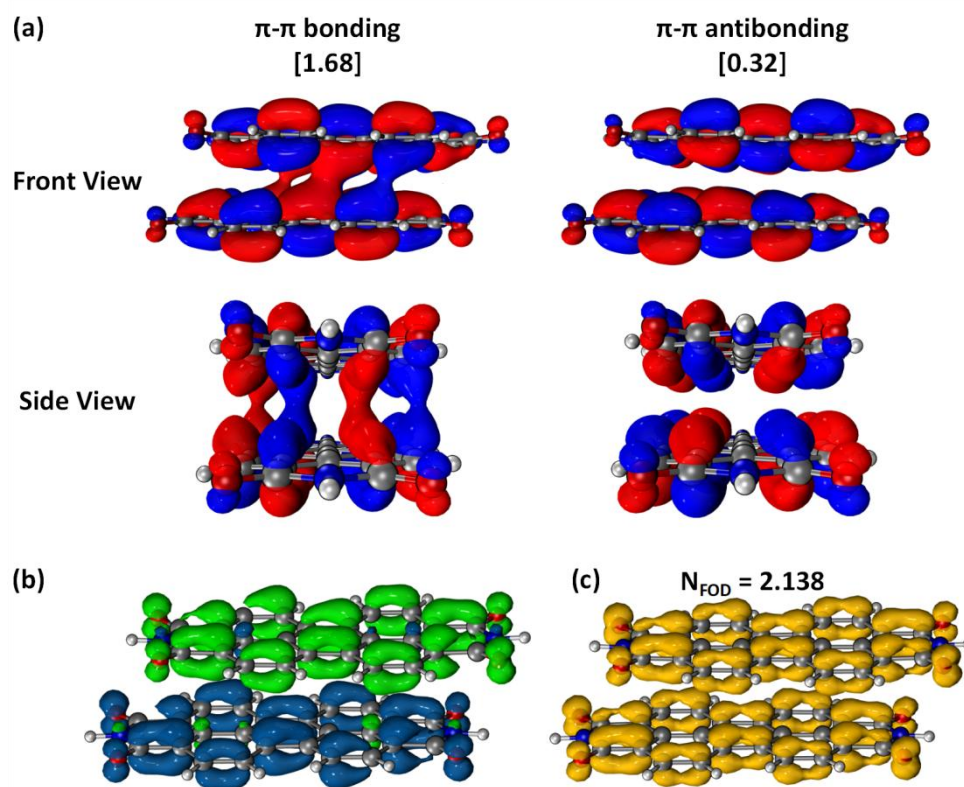


Fig. S4: (a) SS-CASSCF/jul-cc-pV(D+d)Z molecular orbitals included in the active space (6e, 6o, values in square brackets are occupation numbers, isovalue=0.020 a.u.), (b) U-DFT spin density representation (isovalue=0.002 a.u.), and (c) FOD (isovalue=0.002 a.u.) and  $N_{\text{FOD}}$  for pimer 1. Ammoniums are omitted for clarity.

#### Section 4:

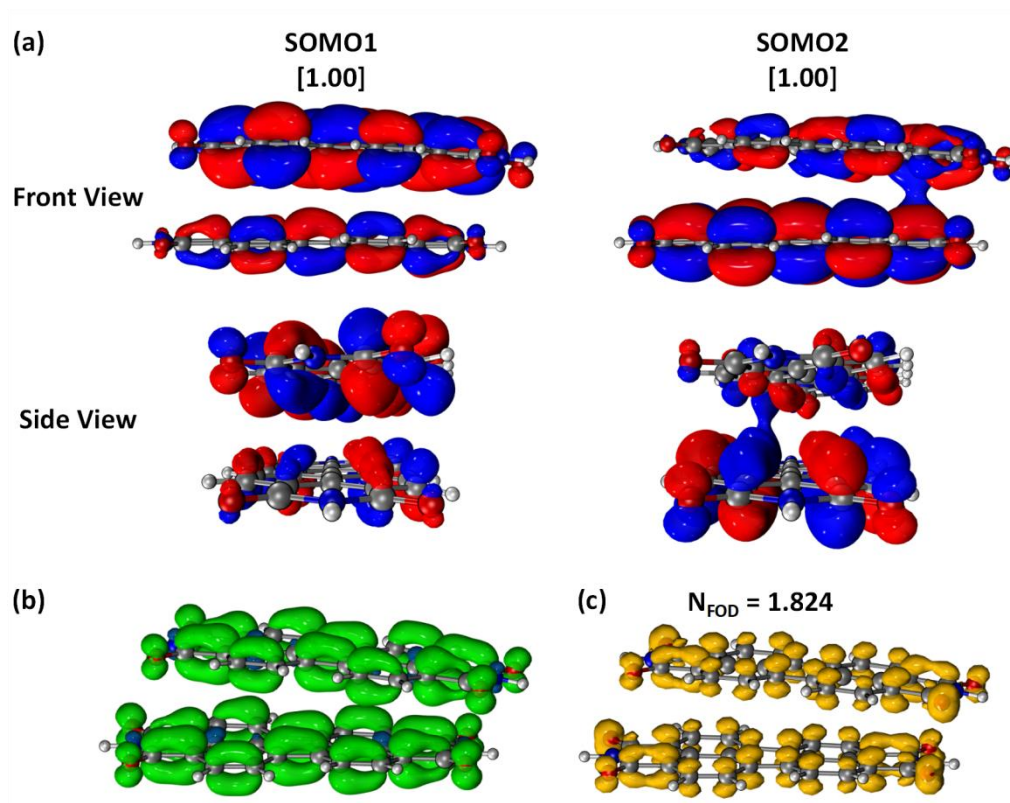


Fig. S5: (a) SS-CASSCF/jul-cc-pV(D+d)Z molecular orbitals included in the active space (6e, 6o, values in square brackets are occupation numbers, isovalue=0.020 a.u.), (b) U-DFT spin density representation (isovalue=0.002 a.u.), and (c) FOD (isovalue=0.002 a.u.) and  $N_{\text{FOD}}$  for pimer 12. Ammoniums are omitted for clarity.

Section 5:

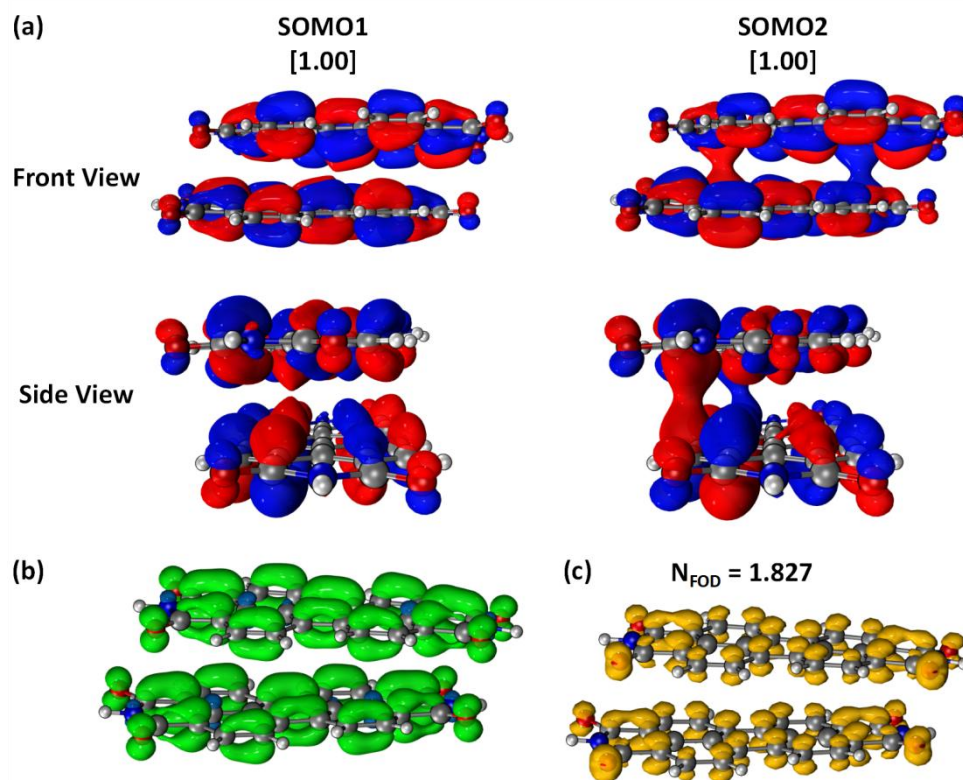


Fig. S6: (a) SS-CASSCF/jul-cc-pV(D+d)Z molecular orbitals included in the active space (6e, 6o, values in square brackets are occupation numbers, isovalue=0.020 a.u.), (b) U-DFT spin density representation (isovalue=0.002 a.u.), and (c) FOD (isovalue=0.002 a.u.) and  $N_{\text{FOD}}$  for pimer **12-1**. Ammoniums are omitted for clarity.

## Section 6:

In addition to the total energy differences between pimers discussed in the text, the differences in Gibbs free energy between them are also listed in Table S1. The Gibbs free energy is given as:

$$G = E_{\text{elec}} + G_{\text{corr}}$$

where  $E_{\text{elec}}$  is the single-point energy calculated at B2GP-PLYP-D4/jul-cc-pV(D+d)Z level on geometries optimized at UM05-2X/6-31+G(d) level and  $G_{\text{corr}}$  is the thermal correction to Gibbs free energy at 298.15 K and 1 atm state evaluated by vibrational frequency calculation on the optimized structures. In order to better deal with low vibrational frequencies, Grimme's entropy interpolation between harmonic and free-rotor approximations was applied<sup>1,2</sup>.

Table S1: Gibbs free energy difference between the pimers

Pimer	$\Delta G$ (kcal/mol)
1	0.2
1-1	0.0
1-2	+20.9
3	+5.9
3-1	+3.3
4	+2.9
5	+9.4
5-1	+10.0
6	+5.6
7	+19.1
8	+23.7
9	+21.9
10	+29.6
11	+23.9
12	+2.8
12-1	+2.3
12-2	+5.7
12-3	+20.2
12-4	+20.0
14	+5.7
14-1	+4.9
15	+7.8
16	+13.5
16-1	+10.4
17	+6.3
18	+5.8
19	+22.2

<b>20</b>	+26.2
<b>21</b>	+23.9
<b>22</b>	+27.6
<b>23</b>	+23.7

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### **Section 7:**

#### References

- 1 S. Grimme, *Chem. Eur. J.*, 2012, **18**, 9955-9964.
- 2 T. Lu and Q. Chen, *Comput. Theor. Chem.*, 2021, **1200**, 113249.



## Section 8:

Cartesian coordinates of different pimers on LS state PES

Cartesian coordinates of pimer 1

C	-0.614888	-0.059038	1.690875
C	-2.035894	0.078608	1.790921
C	0.201867	1.110448	1.734553
C	-0.417636	2.373691	1.856537
C	-0.045175	-1.358253	1.556735
C	-2.604097	1.362877	1.919047
C	-2.854237	-1.080013	1.77325
C	1.63699	0.969259	1.66553
C	-1.78848	2.496429	1.943602
H	0.177808	3.27383	1.872346
C	-0.902363	-2.483505	1.550646
C	1.390564	-1.494776	1.447565
C	-4.047378	1.523134	2.031316
C	-4.28363	-0.945476	1.905981
C	-2.268587	-2.345935	1.659215
C	2.499056	2.084587	1.782034
C	2.207287	-0.327	1.503482
H	-2.261605	3.46567	2.035267
H	-0.492305	-3.478481	1.471202
C	2.010487	-2.752682	1.290764
O	-4.642409	2.583524	2.15784
N	-4.774685	0.326531	2.00352
O	-5.090277	-1.906028	1.963337
H	-2.908321	-3.218899	1.673638
H	2.092061	3.066706	1.966701
C	3.866358	1.94716	1.7033
C	3.628506	-0.463132	1.408625
H	1.41374	-3.649814	1.232564
C	3.382377	-2.877429	1.205628
C	4.450512	0.693221	1.483692
H	4.505871	2.808009	1.853967
C	4.196752	-1.745933	1.263107
H	3.854173	-3.843559	1.082859
C	5.884447	0.555884	1.395177
C	5.647469	-1.908465	1.217319
N	6.374953	-0.710373	1.267485
O	6.700155	1.51278	1.429176
O	6.248378	-2.967151	1.150673
H	-5.775583	0.423031	2.117737
H	7.381923	-0.808536	1.238032

N	-6.296234	-3.492201	0.242937
H	-5.815543	-4.319553	-0.098865
H	-5.712017	-2.976588	0.958844
H	-6.466978	-2.782538	-0.541642
H	-7.18354	-3.759013	0.663203
C	0.61426	0.058783	-1.691251
C	2.035231	-0.079136	-1.791305
C	-0.202708	-1.110548	-1.734898
C	0.41654	-2.37393	-1.856623
C	0.04479	1.358108	-1.557047
C	2.603186	-1.363539	-1.919315
C	2.853793	1.079314	-1.773551
C	-1.637815	-0.969069	-1.666082
C	1.787372	-2.496937	-1.943674
H	-0.179091	-3.273953	-1.872106
C	0.902167	2.483179	-1.55111
C	-1.390927	1.494865	-1.447577
C	4.046466	-1.52409	-2.031333
C	4.283289	0.944485	-1.905633
C	2.268397	2.345322	-1.65959
C	-2.500094	-2.084137	-1.783362
C	-2.207866	0.32725	-1.503663
H	2.260323	-3.466285	-2.035107
H	0.492304	3.478243	-1.47172
C	-2.010596	2.752822	-1.290366
O	4.641274	-2.584625	-2.157712
N	4.774027	-0.327672	-2.003364
O	5.090192	1.904737	-1.961834
H	2.90831	3.218155	-1.673899
H	-2.093281	-3.066182	-1.968841
C	-3.867385	-1.946447	-1.704673
C	-3.629052	0.46362	-1.408729
H	-1.413677	3.649831	-1.231995
C	-3.382472	2.877797	-1.205041
C	-4.45129	-0.69253	-1.48429
H	-4.507068	-2.807014	-1.856229
C	-4.197051	1.746488	-1.262786
H	-3.854082	3.843979	-1.081961
C	-5.885254	-0.554947	-1.395784
C	-5.647764	1.909299	-1.216973
N	-6.375493	0.711419	-1.267708
O	-6.701068	-1.511653	-1.429933
O	-6.248397	2.968118	-1.149991
H	5.774976	-0.424434	-2.116882

H	-7.382442	0.80975	-1.238145
N	6.298739	3.492864	-0.244048
H	6.467969	2.782231	0.540349
H	7.186595	3.757841	-0.664298
H	5.713365	2.978867	-0.959664
H	5.819967	4.321129	0.098251

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.790385	0.683944	0.614702

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Cartesian coordinates of pimer **1-1**

C	-0.632606	-0.026851	-1.690156
C	-2.046701	0.170726	-1.787884
C	0.232251	1.104378	-1.718915
C	-0.329844	2.392945	-1.825242
C	-0.117876	-1.353828	-1.572949
C	-2.558222	1.479176	-1.889722
C	-2.916366	-0.952976	-1.795587
C	1.667046	0.903352	-1.644291
C	-1.695789	2.576404	-1.901627
H	0.305741	3.264897	-1.842242
C	-1.024896	-2.441826	-1.589414
C	1.304903	-1.550342	-1.468262
C	-3.995603	1.704306	-1.987832
C	-4.335623	-0.753099	-1.929962
C	-2.381722	-2.244457	-1.704266
C	2.573156	1.981084	-1.709063
C	2.176174	-0.418674	-1.503584
H	-2.126166	3.566558	-1.979055
H	-0.660163	-3.455275	-1.520511
C	1.872116	-2.841525	-1.357349
O	-4.542638	2.792983	-2.074526
N	-4.772539	0.540121	-1.995126
O	-5.190489	-1.672304	-2.014606
H	-3.053834	-3.092446	-1.740573
H	2.210918	2.990651	-1.826021
C	3.938162	1.783821	-1.632169
C	3.589634	-0.615436	-1.41053
H	1.237714	-3.714449	-1.359537
C	3.23392	-3.025433	-1.272841
C	4.453707	0.497464	-1.477564
H	4.630569	2.61419	-1.676734

C	4.107659	-1.931433	-1.271649
H	3.644762	-4.027347	-1.248072
C	5.902697	0.308745	-1.431734
C	5.534625	-2.13388	-1.187759
N	6.319167	-1.020558	-1.272094
O	6.742	1.187776	-1.524941
O	6.090363	-3.251618	-1.043997
H	-5.769661	0.680686	-2.097499
H	7.320488	-1.165175	-1.242166
N	-6.108714	-3.530713	-0.430197
H	-5.533983	-4.333773	-0.191855
H	-5.611556	-2.882814	-1.115826
H	-6.308781	-2.925891	0.425785
H	-6.985209	-3.843561	-0.841296
C	0.663847	0.096216	1.690833
C	2.089752	0.011489	1.779376
C	-0.11445	-1.09869	1.769868
C	0.549976	-2.334097	1.967624
C	0.05042	1.371993	1.533322
C	2.71004	-1.252171	1.973206
C	2.860952	1.186681	1.687996
C	-1.548821	-1.012324	1.674096
C	1.920029	-2.404561	2.072883
H	-0.015676	-3.2495	2.050187
C	0.867123	2.518307	1.450845
C	-1.396176	1.461177	1.46911
C	4.142055	-1.330195	2.097698
C	4.315263	1.123783	1.7729
C	2.242686	2.426408	1.519141
C	-2.37106	-2.160968	1.750878
C	-2.168432	0.266319	1.52428
H	2.403887	-3.356656	2.250538
H	0.425283	3.494754	1.325277
C	-2.060687	2.699122	1.356111
O	4.790834	-2.381494	2.336301
N	4.836477	-0.16019	1.970117
O	5.075699	2.076941	1.700793
H	2.868614	3.306934	1.451584
H	-1.930224	-3.135409	1.894039
C	-3.742862	-2.071567	1.675333
C	-3.593586	0.352558	1.442423
H	-1.497411	3.618666	1.321875
C	-3.438282	2.777375	1.292344
C	-4.373277	-0.834331	1.497229

H	-4.35094	-2.959791	1.795941
C	-4.209669	1.616297	1.328925
H	-3.944744	3.72928	1.201022
C	-5.81264	-0.749515	1.425107
C	-5.667089	1.724854	1.293756
N	-6.350502	0.50113	1.331636
O	-6.588017	-1.73812	1.442062
O	-6.306197	2.761565	1.242452
H	5.842743	-0.213472	2.065452
H	-7.360553	0.562618	1.309756
N	5.282774	-4.606828	1.066858
H	5.589799	-4.192242	0.132888
H	4.551923	-5.301535	0.943342
H	4.939658	-3.774253	1.63807
H	6.08248	-5.026675	1.535178

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.790332	0.683572	0.614387

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Cartesian coordinates of pimer 1-2

C	0.287562	-0.001772	-1.70545
C	1.715743	-0.001094	-1.837227
C	-0.409181	1.240282	-1.649832
C	0.331109	2.448838	-1.730669
C	-0.407716	-1.244518	-1.64677
C	2.408956	1.231952	-1.913678
C	2.410325	-1.233546	-1.911532
C	-1.848988	1.241783	-1.528125
C	1.69429	2.447426	-1.861
H	-0.181187	3.398176	-1.699789
C	0.333839	-2.452401	-1.725959
C	-1.847416	-1.247423	-1.524023
C	3.826185	1.23375	-2.082813
C	3.827459	-1.233985	-2.080792
C	1.696954	-2.449703	-1.856825
C	-2.593642	2.435319	-1.469108
C	-2.542086	-0.003158	-1.461821
H	2.242934	3.376466	-1.944439
H	-0.177449	-3.402239	-1.69382
C	-2.590444	-2.44172	-1.460085
O	4.559829	2.251161	-2.203714
N	4.432618	0.000081	-2.146836

O	4.562261	-2.25086	-2.200231
H	2.246453	-3.37833	-1.939249
H	-2.09599	3.391816	-1.514419
C	-3.975119	2.426271	-1.346058
C	-3.963547	-0.003865	-1.332829
H	-2.091458	-3.397719	-1.501019
C	-3.971928	-2.434041	-1.337181
C	-4.662932	1.224118	-1.274357
H	-4.54065	3.347306	-1.291367
C	-4.661322	-1.232541	-1.27021
H	-4.536266	-3.355594	-1.279034
C	-6.133145	1.241235	-1.168197
C	-6.131565	-1.251368	-1.164595
N	-6.737145	-0.00528	-1.079652
O	-6.808623	2.256228	-1.167301
O	-6.805739	-2.267198	-1.161044
H	5.432549	0.000464	-2.300547
H	-7.748337	-0.0059	-1.038426
N	5.567131	-4.037531	-0.564343
H	4.982272	-4.814143	-0.268471
H	5.045519	-3.400697	-1.238014
H	5.842077	-3.42055	0.263594
H	6.403031	-4.394547	-1.021374
C	-0.895563	0.003815	1.751596
C	-2.318847	0.005075	1.865515
C	-0.201322	-1.241493	1.699521
C	-0.94555	-2.435204	1.758548
C	-0.199522	1.247929	1.69542
C	-3.018992	-1.221088	1.926847
C	-3.017164	1.23247	1.922202
C	1.240194	-1.238974	1.596466
C	-2.327814	-2.422485	1.870781
H	-0.449223	-3.392455	1.708931
C	-0.942026	2.442959	1.749401
C	1.242008	1.243044	1.593555
C	-4.485793	-1.238868	2.044619
C	-4.483909	1.25286	2.039873
C	-2.324296	2.432682	1.861439
C	1.986512	-2.445184	1.59908
C	1.938289	0.001464	1.532898
H	-2.894384	-3.3439	1.912431
H	-0.444249	3.399242	1.695841
C	1.990115	2.44819	1.594701
O	-5.154541	-2.257168	2.124897

N	-5.095494	0.007538	2.068914
O	-5.15103	2.272503	2.116397
H	-2.889572	3.355051	1.899287
H	1.477923	-3.391873	1.696964
C	3.353325	-2.444191	1.516901
C	3.369851	0.000344	1.436198
H	1.482878	3.395722	1.691468
C	3.356924	2.445097	1.513038
C	4.06859	-1.231906	1.407268
H	3.903187	-3.373674	1.59015
C	4.07047	1.231592	1.405284
H	3.9081	3.373854	1.585527
C	5.496621	-1.234169	1.324778
C	5.498388	1.231511	1.323024
N	6.107636	-0.00176	1.299953
O	6.232519	-2.255067	1.267456
O	6.236042	2.251328	1.264507
H	-6.103572	0.008467	2.161804
H	7.118761	-0.002482	1.253324
N	5.573621	4.033352	-0.566892
H	5.048519	3.400277	-1.240773
H	4.992947	4.812522	-0.269488
H	5.846714	3.413786	0.260448
H	6.410873	4.386873	-1.024184

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
-2773.758754		0.683482	0.616038

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Cartesian coordinates of pimer 2

O	-1.800731	0.202157	-6.133552
N	-1.720441	-1.892075	-5.274689
H	-1.784893	-2.25519	-6.215779
C	1.715791	0.481889	-1.336562
C	-1.749695	-0.045089	-3.760062
C	1.716388	0.968772	-2.681983
C	1.700929	1.414189	-0.257344
C	-1.759203	-0.532839	-5.113216
C	-1.764201	1.331756	-3.505169
H	-1.785799	2.017525	-4.342449
C	1.659329	2.79538	-0.549188
C	-1.667972	-2.872675	-4.277138
C	1.722306	-0.925282	-1.102335

C	-1.716388	-0.968772	-2.681983
C	1.680082	2.359699	-2.917762
C	1.749695	0.045089	-3.760062
C	1.722306	0.925282	1.102335
C	-1.745641	1.802431	-2.210722
C	1.647109	3.257488	-1.847194
H	1.62686	3.518731	0.250851
O	-1.624096	-4.051235	-4.607606
C	-1.680082	-2.359699	-2.917762
C	1.745641	-1.802431	-2.210722
C	1.700929	-1.414189	0.257344
C	-1.715791	-0.481889	-1.336562
C	1.667972	2.872675	-4.277138
C	1.759203	0.532839	-5.113216
C	1.764201	-1.331756	-3.505169
C	1.745641	1.802431	2.210722
C	1.715791	-0.481889	1.336562
H	-1.746847	2.870752	-2.060211
C	-1.722306	0.925282	-1.102335
H	1.614262	4.317358	-2.064741
C	-1.647109	-3.257488	-1.847194
H	1.746847	-2.870752	-2.060211
C	1.659329	-2.79538	0.549188
C	-1.700929	-1.414189	-0.257344
O	1.624096	4.051235	-4.607606
N	1.720441	1.892075	-5.274689
O	1.800731	-0.202157	-6.133552
H	1.785799	-2.017525	-4.342449
H	1.746847	2.870752	2.060211
C	1.764201	1.331756	3.505169
C	1.716388	-0.968772	2.681983
C	-1.700929	1.414189	0.257344
H	-1.614262	-4.317358	-2.064741
C	-1.659329	-2.79538	-0.549188
H	1.62686	-3.518731	-0.250851
C	1.647109	-3.257488	1.847194
C	-1.722306	-0.925282	1.102335
C	1.749695	-0.045089	3.760062
H	1.785799	2.017525	4.342449
C	1.680082	-2.359699	2.917762
C	-1.659329	2.79538	0.549188
C	-1.715791	0.481889	1.336562
H	-1.62686	-3.518731	0.250851
H	1.614262	-4.317358	2.064741



C	-1.745641	-1.802431	2.210722
C	1.759203	-0.532839	5.113216
C	1.667972	-2.872675	4.277138
H	-1.62686	3.518731	-0.250851
C	-1.647109	3.257488	1.847194
C	-1.716388	0.968772	2.681983
H	-1.746847	-2.870752	2.060211
C	-1.764201	-1.331756	3.505169
N	1.720441	-1.892075	5.274689
O	1.800731	0.202157	6.133552
O	1.624096	-4.051235	4.607606
C	-1.680082	2.359699	2.917762
H	-1.614262	4.317358	2.064741
C	-1.749695	0.045089	3.760062
H	-1.785799	-2.017525	4.342449
C	-1.667972	2.872675	4.277138
C	-1.759203	0.532839	5.113216
N	-1.720441	1.892075	5.274689
O	-1.624096	4.051235	4.607606
O	-1.800731	-0.202157	6.133552
H	1.784893	2.25519	-6.215779
H	1.784893	-2.25519	6.215779
H	-1.784893	2.25519	6.215779
N	0	0	8.02933
H	-0.007229	0.830237	8.61629
H	-0.844282	-0.022729	7.37082
H	0.844282	0.022729	7.37082
H	0.007229	-0.830237	8.61629
N	0	0	-8.02933
H	-0.007229	-0.830237	-8.61629
H	-0.844282	0.022729	-7.37082
H	0.844282	-0.022729	-7.37082
H	0.007229	0.830237	-8.61629

Cartesian coordinates of pimer 3

O	6.784099	2.449589	-0.066423
N	6.383906	0.562535	1.116221
H	7.375308	0.367452	1.058731
C	0.559236	-1.710105	-1.067724
C	4.53545	1.97976	0.569959
C	1.970778	-1.940381	-1.038729
C	0.060372	-0.477337	-1.58229
C	5.9516	1.711676	0.517594

C	4.023905	3.196314	0.094239
H	4.717418	3.961133	-0.236666
C	0.980687	0.486769	-2.048867
C	5.591628	-0.472442	1.618003
C	-0.320237	-2.713105	-0.561898
C	3.654837	1.006195	1.106892
C	2.857058	-0.939195	-1.515736
C	2.468663	-3.152909	-0.5196
C	-1.366864	-0.244095	-1.610319
C	2.66875	3.440189	0.101936
C	2.3398	0.258479	-2.013319
H	0.631705	1.43453	-2.428985
O	6.124134	-1.506171	1.996451
C	4.155372	-0.209525	1.618061
C	0.231006	-3.911242	-0.058152
C	-1.746474	-2.476544	-0.58006
C	2.244975	1.249196	1.105998
C	4.285708	-1.156768	-1.449432
C	3.908766	-3.398789	-0.465138
C	1.593956	-4.127923	-0.040859
C	-1.91822	0.95406	-2.11152
C	-2.244877	-1.249193	-1.105873
H	2.319359	4.399	-0.249275
C	1.746629	2.476752	0.580625
H	3.020602	1.026838	-2.355087
C	3.280215	-1.177458	2.1174
H	-0.412085	-4.689551	0.32348
C	-2.66849	-3.439768	-0.100768
C	1.366921	0.244003	1.610183
O	5.154187	-0.333925	-1.823314
N	4.704234	-2.357777	-0.949646
O	4.434068	-4.417584	-0.045797
H	2.011935	-5.048057	0.346473
H	-1.275152	1.735277	-2.487419
C	-3.28024	1.177161	-2.117874
C	-3.654756	-1.006292	-1.106867
C	0.320405	2.713315	0.562342
H	3.694777	-2.103082	2.497147
C	1.918191	-0.954237	2.111216
H	-2.31899	-4.398296	0.251108
C	-4.023656	-3.196012	-0.093152
C	-0.060338	0.477268	1.582081
C	-4.155392	0.209222	-1.618457
H	-3.694816	2.102699	-2.497813

C	-4.535285	-1.979755	-0.569599
C	-0.230792	3.911509	0.058684
C	-0.559125	1.710198	1.067853
H	1.275081	-1.735382	2.487187
H	-4.717134	-3.960642	0.238234
C	-0.980704	-0.48705	2.048076
C	-5.591595	0.472032	-1.618409
C	-5.951381	-1.711703	-0.517273
H	0.412358	4.689807	-0.322874
C	-1.593741	4.128201	0.041288
C	-1.970658	1.940504	1.038753
H	-0.63182	-1.435102	2.427562
C	-2.339826	-0.25871	2.012487
N	-6.383789	-0.562795	-1.116079
O	-6.124292	1.505628	-1.997038
O	-6.783923	-2.449612	0.066959
C	-2.468491	3.153113	0.519798
H	-2.011713	5.048356	-0.346002
C	-2.856983	0.939195	1.515412
H	-3.020702	-1.027302	2.353607
C	-3.908626	3.398916	0.465045
C	-4.285652	1.156736	1.448936
N	-4.70414	2.357765	0.949035
O	-4.433815	4.417825	0.045813
O	-5.154055	0.333808	1.822611
H	5.703361	-2.496849	-0.860101
H	-7.375188	-0.367686	-1.058617
H	-5.703264	2.496682	0.859191
N	-5.795618	-2.139534	2.526895
H	-5.056484	-2.795588	2.767133
H	-5.393564	-1.177906	2.3344
H	-6.269324	-2.438396	1.624651
H	-6.474008	-2.085129	3.28316
N	5.793729	2.139918	-2.526523
H	5.392563	1.177886	-2.333416
H	6.470893	2.085966	-3.283933
H	5.053771	2.795506	-2.765572
H	6.268613	2.439265	-1.625413

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.783415	0.685292	0.616838

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Cartesian coordinates of pimer 3-1

O	6.622427	-2.788631	0.174875
N	6.394841	-0.838162	-0.95089
H	7.392569	-0.707877	-0.842563
C	0.653125	1.805398	0.991388
C	4.441126	-2.158254	-0.547931
C	2.077511	1.897534	1.072933
C	-0.0027	0.620461	1.447236
C	5.865254	-1.980255	-0.418808
C	3.834976	-3.359002	-0.146624
H	4.46614	-4.18267	0.167877
C	0.786925	-0.445158	1.936592
C	5.692537	0.256559	-1.459624
C	-0.083261	2.892813	0.442055
C	3.645993	-1.112698	-1.085212
C	2.827499	0.800335	1.5758
C	2.724239	3.071928	0.63777
C	-1.442069	0.54332	1.394804
C	2.468685	-3.511414	-0.206272
C	2.161281	-0.355198	1.993304
H	0.322384	-1.367114	2.251887
O	6.30362	1.263828	-1.784026
C	4.242641	0.084074	-1.53302
C	0.609749	4.048909	0.032777
C	-1.527191	2.785135	0.322378
C	2.225507	-1.263905	-1.151168
C	4.269178	0.880317	1.616615
C	4.181481	3.183228	0.705537
C	1.984914	4.1395	0.133324
C	-2.149597	-0.574044	1.894216
C	-2.181583	1.62227	0.819708
H	2.045758	-4.46185	0.081775
C	1.626879	-2.467869	-0.670441
H	2.739787	-1.198701	2.347454
C	3.453021	1.119048	-2.037209
H	0.070438	4.897254	-0.35973
C	-2.298564	3.800444	-0.275843
C	1.436404	-0.197428	-1.669968
O	5.030365	-0.033721	2.014565
N	4.835793	2.052276	1.197863
O	4.829653	4.163556	0.377899
H	2.513772	5.03018	-0.180248
H	-1.617306	-1.397221	2.346348
C	-3.522166	-0.655393	1.80826

C	-3.604766	1.52365	0.716646
C	0.193364	-2.595508	-0.678062
H	3.939588	2.0299	-2.363229
C	2.080233	0.979311	-2.103148
H	-1.82406	4.684126	-0.673907
C	-3.670795	3.691273	-0.385121
C	-0.005574	-0.345598	-1.722015
C	-4.269412	0.367613	1.211883
H	-4.032909	-1.523462	2.205876
C	-4.330383	2.566332	0.107145
C	-0.45694	-3.742799	-0.158073
C	-0.600122	-1.538835	-1.218603
H	1.502576	1.810497	-2.477982
H	-4.260529	4.469695	-0.85148
C	-0.838573	0.663275	-2.248814
C	-5.705527	0.271592	1.098564
C	-5.783679	2.48404	-0.010468
H	0.121994	-4.551542	0.261218
C	-1.827247	-3.86005	-0.164481
C	-2.023776	-1.670901	-1.236022
H	-0.411774	1.573754	-2.640788
C	-2.212159	0.526561	-2.267984
N	-6.351692	1.328833	0.533916
O	-6.400864	-0.703398	1.484024
O	-6.507868	3.331181	-0.507457
C	-2.624555	-2.837394	-0.695662
H	-2.312891	-4.740322	0.235955
C	-2.813953	-0.626417	-1.761013
H	-2.846913	1.31378	-2.655049
C	-4.057201	-2.950582	-0.659843
C	-4.266265	-0.728677	-1.746719
N	-4.768781	-1.923462	-1.213062
O	-4.673688	-3.923535	-0.147451
O	-5.053105	0.117321	-2.150624
H	5.847212	2.09895	1.193903
H	-7.354884	1.247838	0.431975
H	-5.777968	-1.995139	-1.212379
N	-6.348344	-3.315323	1.789459
H	-5.725648	-3.653239	0.985861
H	-6.004687	-3.67881	2.674542
H	-6.311616	-2.251951	1.775402
H	-7.308564	-3.620855	1.649841
N	5.469471	-2.57467	2.576563
H	5.135945	-1.579217	2.422419

H	6.085806	-2.610945	3.385066
H	4.678207	-3.19948	2.709315
H	5.997434	-2.840077	1.694544

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.786836	0.68464	0.616086

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Cartesian coordinates of pimer 4

C	-0.688345	1.655879	-1.110353
C	-2.113705	1.646033	-1.230477
C	0.058498	0.531172	-1.573652
C	-0.636179	-0.564973	-2.131617
C	-0.04609	2.778036	-0.51217
C	-2.759891	0.522283	-1.789131
C	-2.861426	2.754614	-0.758096
C	1.499028	0.542383	-1.44975
C	-2.011817	-0.571303	-2.233165
H	-0.097587	-1.436193	-2.472238
C	-0.836744	3.866671	-0.073328
C	1.392848	2.778633	-0.367244
C	-4.211518	0.477722	-1.869935
C	-4.297688	2.729971	-0.831211
C	-2.207807	3.856454	-0.19297
C	2.293934	-0.533253	-1.905606
C	2.141887	1.662095	-0.843705
H	-2.538915	-1.426539	-2.63732
H	-0.36936	4.736524	0.361542
C	2.078233	3.850727	0.242397
O	-4.883418	-0.452046	-2.298896
N	-4.864882	1.627118	-1.402398
O	-5.040135	3.650528	-0.394971
H	-2.801784	4.696479	0.142481
H	1.833383	-1.392667	-2.368437
C	3.663961	-0.529095	-1.758061
C	3.564056	1.657309	-0.68504
H	1.535047	4.707341	0.61036
C	3.448935	3.834456	0.396034
C	4.319151	0.543825	-1.143528
H	4.243949	-1.368156	-2.121149
C	4.198117	2.749403	-0.058927
H	3.970678	4.655075	0.870935
C	5.754273	0.539807	-0.972573

C	5.64633	2.762434	0.114605
N	6.308062	1.639301	-0.391613
O	6.523569	-0.390758	-1.322792
O	6.296933	3.659649	0.626674
H	-5.874202	1.600286	-1.468179
H	7.310302	1.626498	-0.254787
N	-6.651567	3.018054	1.583634
H	-7.628874	3.260658	1.439569
H	-6.05529	3.361153	0.763013
H	-6.324554	3.432903	2.452301
H	-6.549279	1.961635	1.603197
C	0.688679	-1.65794	1.110517
C	2.114152	-1.649025	1.22934
C	-0.056934	-0.53249	1.573996
C	0.638918	0.56296	2.131787
C	0.045091	-2.779969	0.513462
C	2.761603	-0.525683	1.78743
C	2.860673	-2.758141	0.756352
C	-1.49754	-0.54219	1.450271
C	2.01465	0.56827	2.232365
H	0.101217	1.43442	2.473193
C	0.834613	-3.869107	0.073936
C	-1.394032	-2.779786	0.370152
C	4.213332	-0.48212	1.867077
C	4.297053	-2.734553	0.828133
C	2.205832	-3.85963	0.192009
C	-2.291052	0.535112	1.904432
C	-2.141715	-1.661953	0.845667
H	2.542637	1.423022	2.636391
H	0.36628	-4.738689	-0.360453
C	-2.080883	-3.852203	-0.23724
O	4.886212	0.447003	2.295923
N	4.865508	-1.631838	1.398697
O	5.038573	-3.655296	0.391055
H	2.799004	-4.699969	-0.144083
H	-1.829412	1.394863	2.365549
C	-3.661114	0.532563	1.756636
C	-3.563884	-1.655799	0.687322
H	-1.538816	-4.710067	-0.603938
C	-3.451677	-3.834757	-0.39026
C	-4.317448	-0.540616	1.143977
H	-4.240344	1.373117	2.117531
C	-4.199464	-2.748089	0.063037
H	-3.974461	-4.655639	-0.863559

C	-5.752614	-0.534468	0.972492
C	-5.647717	-2.759385	-0.1105
N	-6.307949	-1.634222	0.393339
O	-6.519755	0.398374	1.320482
O	-6.299584	-3.656675	-0.620801
H	5.874837	-1.606188	1.464879
H	-7.310126	-1.620305	0.256209
N	6.645453	-3.008604	-1.588471
H	6.317235	-3.417361	-2.459565
H	6.54139	-1.951254	-1.600059
H	6.052414	-3.359491	-0.769462
H	7.623707	-3.250062	-1.448927

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.786246	0.68394	0.614954

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Cartesian coordinates of pimer 5

O	-7.499518	1.525898	-0.776014
N	-7.286294	-0.700956	-0.452064
H	-8.279297	-0.72109	-0.257374
C	0.350941	0.492614	1.557824
C	-5.351743	0.531774	-1.10704
C	-1.0639	0.436241	1.755747
C	0.949772	1.71659	1.144898
C	-6.748121	0.506606	-0.790541
C	-4.742176	1.700695	-1.597121
H	-5.362266	2.557959	-1.830558
C	0.126589	2.847036	0.953165
C	-6.61374	-1.922453	-0.307629
C	1.132011	-0.681695	1.776708
C	-4.573012	-0.644011	-0.924681
C	-1.845652	1.599777	1.548422
C	-1.664779	-0.776785	2.156964
C	2.379622	1.769531	0.927377
C	-3.391273	1.746698	-1.832749
C	-1.237837	2.792968	1.156714
H	0.55886	3.786501	0.644974
O	-7.250064	-2.921467	-0.006799
C	-5.174135	-1.852015	-0.521563
C	0.479224	-1.868864	2.177074
C	2.558362	-0.625432	1.579025
C	-3.159007	-0.594714	-1.14686



C	-3.280359	1.552845	1.756986
C	-3.107526	-0.849439	2.362627
C	-0.886603	-1.914499	2.369705
C	3.029165	2.952347	0.509956
C	3.158959	0.59501	1.146764
H	-2.969194	2.657591	-2.22799
C	-2.55809	0.625544	-1.579179
H	-1.856645	3.668592	1.011273
C	-4.392577	-2.993085	-0.314448
H	1.045535	-2.773712	2.335703
C	3.391835	-1.746355	1.83254
C	-2.379966	-1.769414	-0.927367
O	-4.03131	2.540377	1.620089
N	-3.799996	0.347281	2.140742
O	-3.727143	-1.842112	2.712457
H	-1.381707	-2.827182	2.675822
H	2.460642	3.850262	0.324014
C	4.391911	2.993742	0.314498
C	4.572936	0.644677	0.924545
C	-1.131729	0.681438	-1.776841
H	-4.884306	-3.899025	0.013952
C	-3.029835	-2.952056	-0.509886
H	2.970007	-2.657368	2.227778
C	4.742725	-1.699998	1.596832
C	-0.950103	-1.716835	-1.144819
C	5.173749	1.852873	0.521513
H	4.883397	3.899842	-0.013823
C	5.351966	-0.53092	1.106771
C	-0.478634	1.868426	-2.177313
C	-0.350952	-0.493032	-1.557809
H	-2.461539	-3.850093	-0.323851
H	5.363037	-2.557126	1.830181
C	-0.127181	-2.847463	-0.952938
C	6.613335	1.923681	0.307511
C	6.748364	-0.505414	0.790175
H	-1.044728	2.773375	-2.336114
C	0.887205	1.913727	-2.369838
C	1.063924	-0.436995	-1.755611
H	-0.55969	-3.7868	-0.644697
C	1.237271	-2.79372	-1.156342
N	7.286195	0.702345	0.45175
O	7.24937	2.922887	0.006718
O	7.499954	-1.524474	0.775477
C	1.66511	0.775852	-2.156876

H	1.382556	2.826258	-2.676007
C	1.8454	-1.600687	-1.548082
H	1.855871	-3.669461	-1.010733
C	3.107896	0.848187	-2.362307
C	3.280134	-1.55405	-1.756343
N	3.800087	-0.34867	-2.140195
O	3.727766	1.84062	-2.712366
O	4.030846	-2.541752	-1.619047
H	-4.799754	0.29317	2.28448
H	8.27918	0.722754	0.257002
H	4.79988	-0.294727	-2.283736
N	6.406796	-3.406698	-0.647999
H	6.176532	-4.2475	-0.124111
H	5.521665	-3.0055	-1.044716
H	6.880121	-2.670411	0.004351
H	7.04006	-3.651735	-1.405631
N	-6.406402	3.407336	0.647371
H	-7.039791	3.652533	1.404844
H	-6.879843	2.671003	-0.005315
H	-6.175677	4.248098	0.123632
H	-5.521676	3.005815	1.044349

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$E_{elec}$ (a.u.)	ZPE (a.u.)	$G_{corr}$ (a.u.)	
	-2773.775663	0.683885	0.614638

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Cartesian coordinates of pimer 5-1

O	7.383139	-2.518799	0.760856
N	7.289982	-0.261013	0.608986
H	8.28452	-0.27419	0.421785
C	-0.340174	-0.167726	-1.638437
C	5.244437	-1.472722	0.985394
C	1.078273	-0.143442	-1.813049
C	-1.009337	-1.420651	-1.552148
C	6.689252	-1.513974	0.791839
C	4.530909	-2.670558	1.08336
H	5.075932	-3.601446	1.001107
C	-0.252984	-2.605856	-1.651149
C	6.680609	0.960438	0.624978
C	-1.054838	1.065884	-1.550935
C	4.572422	-0.238072	1.062828
C	1.789659	-1.359038	-1.89747
C	1.753338	1.101125	-1.900482

C	-2.446471	-1.446106	-1.359569
C	3.164598	-2.65725	1.263083
C	1.117824	-2.577293	-1.824491
H	-0.739776	-3.567288	-1.59467
O	7.37413	1.982252	0.341269
C	5.283063	0.987541	0.931083
C	-0.331774	2.278275	-1.638092
C	-2.481671	1.042174	-1.370648
C	3.155671	-0.213863	1.267356
C	3.240252	-1.351192	-2.071289
C	3.189458	1.132077	-2.085646
C	1.035357	2.296341	-1.81745
C	-3.164677	-2.657139	-1.262862
C	-3.155803	-0.213772	-1.267309
H	2.648762	-3.603185	1.319546
C	2.446352	-1.446206	1.359639
H	1.694228	-3.490404	-1.89962
C	4.602914	2.207132	1.102569
H	-0.846804	3.223543	-1.561065
C	-3.249478	2.236071	-1.322885
C	2.481507	1.04206	1.370647
O	3.950941	-2.340047	-2.156706
N	3.820676	-0.080653	-2.154497
O	3.851236	2.185757	-2.196516
H	1.574924	3.231758	-1.88662
H	-2.648793	-3.603061	-1.319103
C	-4.531026	-2.670466	-1.083216
C	-4.572553	-0.237985	-1.062806
C	1.009207	-1.420798	1.552052
H	5.171423	3.129476	1.102558
C	3.249271	2.236019	1.32259
H	-2.773047	3.19324	-1.468147
C	-4.603166	2.207135	-1.102984
C	1.05472	1.065725	1.551085
C	-5.244576	-1.472671	-0.985379
H	-5.076014	-3.601371	-1.000962
C	-5.283219	0.987573	-0.931228
C	0.252839	-2.606037	1.650826
C	0.34003	-0.167895	1.638425
H	2.772765	3.193201	1.467508
H	-5.171758	3.12943	-1.10344
C	0.331678	2.278117	1.638565
C	-6.689362	-1.513942	-0.791892
C	-6.680875	0.960489	-0.625041

H	0.739621	-3.567459	1.594172
C	-1.117959	-2.577486	1.824099
C	-1.078426	-0.143611	1.813018
H	0.846733	3.223403	1.561918
C	-1.035437	2.296164	1.818001
N	-7.290246	-0.260961	-0.609383
O	-7.383238	-2.51878	-0.760952
O	-7.374141	1.982222	-0.340972
C	-1.789814	-1.359233	1.897253
H	-1.694379	-3.4906	1.899065
C	-1.75346	1.10094	1.900736
H	-1.57496	3.231582	1.887528
C	-3.240329	-1.351415	2.071167
C	-3.189532	1.13188	2.086266
N	-3.820764	-0.080807	2.154753
O	-3.951124	-2.34021	2.156413
O	-3.85121	2.185575	2.198024
H	4.824842	-0.079974	-2.275149
H	-8.284695	-0.2742	-0.421745
H	-4.82488	-0.080208	2.275805
N	-6.190187	3.363544	1.514779
H	-5.923991	4.302107	1.227426
H	-5.321538	2.835441	1.781767
H	-6.698135	2.846753	0.696704
H	-6.811108	3.427677	2.318133
N	6.192536	3.362085	-1.51603
H	6.814024	3.425344	-2.318994
H	6.699708	2.845259	-0.696977
H	5.323737	2.834498	-1.783029
H	5.926625	4.300985	-1.229508

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.775367	0.683773	0.615279

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Cartesian coordinates of pimer **6**

O	-1.719153	-5.460582	-1.247383
N	-3.469667	-4.083896	-1.553295
H	-4.058908	-4.905731	-1.521807
C	1.076871	-1.695385	1.872141
C	-1.282444	-3.115962	-1.490495
C	1.866695	-2.887799	1.930037
C	1.729202	-0.42875	1.839625

C	-2.123298	-4.288069	-1.419272
C	0.10681	-3.230329	-1.382516
H	0.547753	-4.211287	-1.262516
C	3.140644	-0.386427	1.870926
C	-4.138184	-2.869261	-1.736357
C	-0.345346	-1.798881	1.832617
C	-1.875622	-1.836199	-1.650618
C	3.273131	-2.790857	1.965798
C	1.223435	-4.155175	1.9377
C	0.933054	0.775599	1.753542
C	0.910222	-2.11219	-1.413798
C	3.894803	-1.538366	1.937016
H	3.657829	0.559789	1.833549
O	-5.356966	-2.867769	-1.836859
C	-3.275051	-1.695881	-1.777388
C	-0.939705	-3.080547	1.918731
C	-1.138441	-0.601007	1.697087
C	-1.045099	-0.67089	-1.679811
C	4.092964	-3.993793	2.030826
C	2.020372	-5.351402	1.927746
C	-0.178087	-4.22445	1.965444
C	1.523963	2.058587	1.736154
C	-0.48538	0.667918	1.664043
H	1.975905	-2.247862	-1.30992
C	0.366954	-0.815146	-1.556343
H	4.976047	-1.499694	1.96496
C	-3.846922	-0.431529	-1.923065
H	-2.014137	-3.179902	1.94963
C	-2.54334	-0.648873	1.567266
C	-1.650084	0.614704	-1.820524
O	5.314194	-4.028781	2.085018
N	3.374249	-5.194199	2.008809
O	1.562477	-6.523242	1.838818
H	-0.659837	-5.190637	2.048404
H	2.595115	2.16688	1.806375
C	0.761186	3.201095	1.618634
C	-1.27096	1.854506	1.522871
C	1.205481	0.362287	-1.574868
H	-4.923263	-0.357784	-2.008959
C	-3.053652	0.697316	-1.939232
H	-3.059697	-1.596658	1.559791
C	-3.291922	0.498418	1.409112
C	-0.811611	1.791588	-1.833198
C	-0.630064	3.119774	1.506662

H	1.228448	4.177418	1.605716
C	-2.672536	1.749517	1.388188
C	2.609902	0.276116	-1.458561
C	0.601489	1.647503	-1.713117
H	-3.541152	1.656032	-2.029781
H	-4.366184	0.451336	1.286563
C	-1.354613	3.091897	-1.971852
C	-1.419846	4.318347	1.363109
C	-3.480995	2.942645	1.191114
H	3.090474	-0.682359	-1.338261
C	3.403763	1.401888	-1.482882
C	1.433655	2.812675	-1.733145
H	-2.420421	3.226466	-2.077521
C	-0.551445	4.208785	-1.989043
N	-2.771075	4.147143	1.224689
O	-0.951985	5.480294	1.365733
O	-4.690938	2.970703	1.00401
C	2.83215	2.669979	-1.624832
H	4.480396	1.328937	-1.39731
C	0.840793	4.09792	-1.862263
H	-0.992313	5.18789	-2.130057
C	3.696809	3.84061	-1.653776
C	1.679385	5.265513	-1.876167
N	3.02616	5.060336	-1.791088
O	4.917118	3.836098	-1.564048
O	1.269144	6.45564	-1.962672
H	3.93088	-6.039243	2.023002
H	-3.336231	4.981579	1.142905
H	3.613828	5.883804	-1.816603
N	-0.470041	7.487653	-0.326738
H	0.018418	8.213106	0.193316
H	0.205302	7.053452	-1.05082
H	-0.76629	6.727168	0.337539
H	-1.278016	7.894593	-0.790454
N	-0.151964	-7.238946	-0.006865
H	-0.84378	-7.876069	0.382065
H	-0.659273	-6.443726	-0.469185
H	0.503876	-6.89769	0.776498
H	0.394595	-7.738281	-0.704983

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.781073	0.683953	0.613982

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Cartesian coordinates of pimer 7

C	-0.177424	1.620445	-0.68065
C	-0.083857	1.68692	-2.107295
C	1.0065	1.768221	0.098344
C	2.237716	1.992215	-0.559416
C	-1.448375	1.402442	-0.073558
C	1.164346	1.898986	-2.716112
C	-1.264188	1.535484	-2.891967
C	0.914333	1.704719	1.543317
C	2.319031	2.048131	-1.931495
H	3.144799	2.118131	0.011769
C	-2.597929	1.273262	-0.899404
C	-1.542223	1.341373	1.365447
C	1.279511	1.965334	-4.161862
C	-1.151501	1.591272	-4.28776
C	-2.514282	1.326552	-2.264511
C	2.048378	1.838018	2.367552
C	-0.356954	1.490924	2.149594
H	3.262538	2.216604	-2.43415
H	-3.568744	1.1189	-0.454705
C	-2.769291	1.128816	2.023705
O	2.296133	2.171758	-4.808
N	0.062949	1.787552	-4.851304
O	-2.210162	1.495065	-5.053629
H	-3.397804	1.220324	-2.879034
H	3.021357	2.007489	1.9333
C	1.954878	1.763706	3.747466
C	-0.44906	1.414874	3.572036
H	-3.67969	1.011108	1.457153
C	-2.852644	1.073741	3.404892
C	0.72461	1.542866	4.355482
H	2.832655	1.862798	4.372759
C	-1.70821	1.208063	4.180654
H	-3.79868	0.910833	3.904559
C	0.643473	1.462596	5.814133
C	-1.827908	1.17321	5.641525
N	-0.618077	1.266386	6.336871
O	1.612232	1.540624	6.572676
O	-2.871278	1.077568	6.262375
H	0.145791	1.848855	-5.85788
H	-0.701767	1.304095	7.344759
N	-1.900702	1.150982	-7.650991
H	-1.144538	1.486151	-8.238014
H	-2.013224	1.433198	-6.065573

H	-2.769822	1.457187	-8.076177
H	-1.889723	0.129415	-7.65395
C	0.177509	-1.620052	0.680748
C	0.084391	-1.68662	2.107416
C	-1.006631	-1.767959	-0.0979
C	-2.237584	-1.992324	0.560211
C	1.44825	-1.401876	0.07328
C	-1.163568	-1.899142	2.716592
C	1.26489	-1.53486	2.891751
C	-0.914904	-1.704282	-1.542901
C	-2.318446	-2.048497	1.932314
H	-3.144802	-2.118446	-0.010712
C	2.597957	-1.272089	0.898812
C	1.541756	-1.341287	-1.365771
C	-1.278287	-1.965636	4.162369
C	1.152628	-1.590666	4.287593
C	2.514709	-1.325355	2.263946
C	-2.049223	-1.837231	-2.36681
C	0.356257	-1.490795	-2.149566
H	-3.261745	-2.217337	2.435236
H	3.568558	-1.117176	0.453833
C	2.768735	-1.12933	-2.024395
O	-2.294612	-2.172581	4.808804
N	-0.061589	-1.787423	4.851475
O	2.211441	-1.493923	5.053148
H	3.398351	-1.218668	2.878217
H	-3.022154	-2.006236	-1.93227
C	-1.956077	-1.763128	-3.746762
C	0.448028	-1.415123	-3.572051
H	3.679335	-1.011906	-1.458105
C	2.85177	-1.074728	-3.405615
C	-0.725888	-1.54291	-4.355154
H	-2.834071	-1.861957	-4.371793
C	1.707081	-1.208859	-4.181044
H	3.79774	-0.912345	-3.905575
C	-0.645136	-1.463125	-5.813854
C	1.826413	-1.17455	-5.641959
N	0.616395	-1.267528	-6.336983
O	-1.614071	-1.541102	-6.572134
O	2.869669	-1.079406	-6.263097
H	-0.144129	-1.848776	5.858072
H	0.69986	-1.305858	-7.344868
N	1.90274	-1.150853	7.65053
H	2.773075	-1.455295	8.074508



H	1.889382	-0.129324	7.654182
H	2.014802	-1.432341	6.065241
H	1.148021	-1.488286	8.238107

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.760391	0.68359	0.614864

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Cartesian coordinates of pimer **8**

O	-6.757641	2.560285	0.120271
N	-6.391553	0.659459	-1.05454
H	-7.379866	0.456873	-0.972204
C	-0.56723	-1.789347	1.031837
C	-4.51933	2.081843	-0.533586
C	-1.980618	-2.007418	0.986238
C	-0.059354	-0.559643	1.552528
C	-5.958336	1.821036	-0.455165
C	-4.012298	3.287128	-0.058294
H	-4.705225	4.033629	0.310556
C	-0.981267	0.412008	2.023489
C	-5.599888	-0.381048	-1.529256
C	0.304942	-2.798085	0.535505
C	-3.648127	1.108776	-1.073353
C	-2.871315	-0.991361	1.457315
C	-2.476978	-3.211328	0.459091
C	1.364072	-0.335672	1.587078
C	-2.649806	3.53125	-0.076822
C	-2.335212	0.209968	1.974056
H	-0.623304	1.351391	2.416137
O	-6.1184	-1.439207	-1.855203
C	-4.158916	-0.113181	-1.570562
C	-0.244586	-3.992292	0.023703
C	1.739474	-2.572761	0.56152
C	-2.240658	1.346827	-1.082787
C	-4.255514	-1.220371	1.342521
C	-3.914455	-3.446508	0.367823
C	-1.605469	-4.197946	-0.012937
C	1.92618	0.857984	2.084988
C	2.2407	-1.346913	1.082713
H	-2.298564	4.483403	0.2897
C	-1.73954	2.572558	-0.561195
H	-2.998539	0.990631	2.318886
C	-3.293506	-1.076994	-2.079634

H	0.399069	-4.773923	-0.349478
C	2.649676	-3.531868	0.077818
C	-1.363936	0.335802	-1.587412
O	-5.223491	-0.408106	1.684971
N	-4.701781	-2.393157	0.840257
O	-4.447165	-4.452005	-0.071164
H	-2.029188	-5.112025	-0.407539
H	1.291409	1.642513	2.468304
C	3.29377	1.077186	2.078654
C	3.648193	-1.108994	1.073181
C	-0.305035	2.79813	-0.535399
H	-3.711027	-2.002936	-2.455933
C	-1.925917	-0.857754	-2.085682
H	2.298337	-4.484212	-0.288123
C	4.012205	-3.287971	0.059403
C	0.05948	0.559849	-1.552699
C	4.159083	0.113184	1.56977
H	3.71137	2.003251	2.454567
C	4.519316	-2.082448	0.534015
C	0.244374	3.992456	-0.023762
C	0.567239	1.789507	-1.031809
H	-1.291056	-1.642163	-2.4691
H	4.705139	-4.034754	-0.308871
C	0.981476	-0.411627	-2.023855
C	5.600031	0.38105	1.527954
C	5.958363	-1.821856	0.455492
H	-0.399357	4.774122	0.349211
C	1.605241	4.198239	0.012886
C	1.980609	2.007693	-0.986166
H	0.623582	-1.35089	-2.416858
C	2.335407	-0.209513	-1.974319
N	6.391616	-0.659742	1.053821
O	6.118578	1.439463	1.853092
O	6.757632	-2.561664	-0.11923
C	2.476848	3.21165	-0.459009
H	2.028861	5.11241	0.407377
C	2.871411	0.991736	-1.457271
H	2.998788	-0.989962	-2.319535
C	3.914303	3.446892	-0.367567
C	4.25557	1.220827	-1.342289
N	4.701738	2.393608	-0.839961
O	4.446909	4.452401	0.071526
O	5.223681	0.408602	-1.684647
H	-5.701053	-2.501853	0.708041

H	7.379957	-0.457312	0.971444
H	5.700961	2.502172	-0.707206
N	5.329392	-1.971648	-2.720811
H	4.571994	-2.639856	-2.811373
H	5.035641	-0.524576	-2.10785
H	6.004311	-2.366926	-2.063127
H	5.78178	-1.889939	-3.625526
N	-5.329816	1.971285	2.722128
H	-5.035529	0.524872	2.108965
H	-5.787266	1.888412	3.624204
H	-4.572317	2.638601	2.818146
H	-6.000952	2.368169	2.061524

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.751565	0.6825	0.613378

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Cartesian coordinates of pimer **9**

C	-0.688592	-1.76579	0.981953
C	-2.117864	-1.760182	1.047746
C	0.03614	-0.67744	1.545921
C	-0.678034	0.374998	2.162178
C	-0.022682	-2.845585	0.329209
C	-2.783771	-0.684243	1.661436
C	-2.850328	-2.829595	0.453825
C	1.484116	-0.667813	1.453724
C	-2.052985	0.376511	2.217331
H	-0.150511	1.215365	2.587195
C	-0.799651	-3.893864	-0.23522
C	1.416621	-2.842613	0.243483
C	-4.234837	-0.632245	1.676371
C	-4.252097	-2.771723	0.467781
C	-2.167309	-3.891566	-0.180822
C	2.256833	0.386623	1.975831
C	2.146314	-1.747045	0.799478
H	-2.59654	1.197734	2.667062
H	-0.312882	-4.72073	-0.728492
C	2.129918	-3.879711	-0.390517
O	-4.931709	0.262067	2.140124
N	-4.867365	-1.737142	1.082022
O	-4.975939	-3.705863	-0.0952
H	-2.741157	-4.694004	-0.623899
H	1.782248	1.216287	2.477363

C	3.635087	0.412507	1.837473
C	3.56765	-1.720391	0.669448
H	1.607665	-4.726873	-0.807176
C	3.508779	-3.846707	-0.505046
C	4.297439	-0.618979	1.179873
H	4.213507	1.239502	2.230242
C	4.232273	-2.777599	0.009623
H	4.048327	-4.644369	-0.99877
C	5.745557	-0.551883	0.984914
C	5.690087	-2.762219	-0.135437
N	6.329844	-1.648286	0.408406
O	6.439586	0.423754	1.299982
O	6.350947	-3.637643	-0.668487
H	-5.875511	-1.660978	1.039271
H	7.329294	-1.605602	0.258585
N	-7.451257	-3.053291	-0.613466
H	-8.172267	-3.072148	0.099557
H	-5.984943	-3.457024	-0.223003
H	-7.748656	-3.669876	-1.362667
H	-7.385357	-2.106666	-0.990664
C	0.688481	1.766198	-0.98173
C	2.117765	1.760888	-1.047237
C	-0.035899	0.677686	-1.545831
C	0.678615	-0.374587	-2.161974
C	0.022208	2.845817	-0.329053
C	2.784029	0.685113	-1.660836
C	2.849879	2.830369	-0.453025
C	-1.483885	0.667704	-1.453834
C	2.053576	-0.375784	-2.216897
H	0.151362	-1.215114	-2.587007
C	0.798833	3.894347	0.235374
C	-1.417096	2.84239	-0.243347
C	4.235106	0.633332	-1.675318
C	4.251663	2.772497	-0.466202
C	2.166508	3.892272	0.181354
C	-2.256255	-0.386859	-1.976186
C	-2.146433	1.746679	-0.799517
H	2.597395	-1.196892	-2.666522
H	0.311779	4.721231	0.728336
C	-2.130736	3.87914	0.390844
O	4.932257	-0.260771	-2.139065
N	4.867292	1.738073	-1.080321
O	4.975156	3.706475	0.097492
H	2.740099	4.694854	0.624503

H	-1.781393	-1.216262	-2.477883
C	-3.634514	-0.413141	-1.837976
C	-3.567773	1.719612	-0.669617
H	-1.60875	4.726318	0.807806
C	-3.509595	3.845723	0.505269
C	-4.297199	0.61809	-1.180312
H	-4.212703	-1.240204	-2.230936
C	-4.232757	2.77652	-0.009678
H	-4.049398	4.643119	0.999144
C	-5.74536	0.550671	-0.985815
C	-5.690575	2.760714	0.135217
N	-6.329983	1.646724	-0.408997
O	-6.439068	-0.424972	-1.301566
O	-6.351782	3.635917	0.668189
H	5.875393	1.661694	-1.036654
H	-7.329492	1.603943	-0.259606
N	7.450168	3.054005	0.616892
H	7.746744	3.670459	1.366534
H	7.384852	2.107135	0.993555
H	5.984116	3.457599	0.225926
H	8.171473	3.07378	-0.095805

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.753948	0.682658	0.612889

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Cartesian coordinates of pimer **10**

O	7.810394	2.011309	-0.60875
N	7.527634	0.105681	0.577295
H	8.523357	-0.05923	0.495371
C	-0.611483	-1.28477	-1.188906
C	5.63166	1.558863	0.246761
C	0.802072	-1.497786	-1.250364
C	-1.154215	-0.052768	-1.663791
C	7.055622	1.29036	0.037038
C	5.086916	2.753887	-0.208423
H	5.742067	3.477764	-0.675597
C	-0.276374	0.927082	-2.19808
C	6.794663	-0.8921	1.218203
C	-1.441563	-2.300958	-0.63922
C	4.80877	0.586584	0.861249
C	1.642083	-0.475723	-1.783307
C	1.347525	-2.702662	-0.774909

C	-2.574457	0.176125	-1.572163
C	3.732814	3.004953	-0.065319
C	1.077431	0.731559	-2.254905
H	-0.667599	1.867311	-2.553841
O	7.359704	-1.900238	1.612893
C	5.356062	-0.633856	1.330397
C	-0.849931	-3.508164	-0.20251
C	-2.867873	-2.063228	-0.521774
C	3.40802	0.831111	0.991854
C	3.026968	-0.694188	-1.80865
C	2.784233	-2.924026	-0.803351
C	0.509964	-3.70558	-0.263257
C	-3.168763	1.375981	-2.013826
C	-3.408034	-0.831029	-0.991975
H	3.349623	3.944725	-0.431691
C	2.867778	2.063255	0.521606
H	1.730721	1.499165	-2.647352
C	4.531506	-1.596885	1.902159
H	-1.463669	-4.302756	0.193475
C	-3.732994	-3.004953	0.064979
C	2.574509	-0.176066	1.572099
O	3.841616	0.214329	-2.285563
N	3.528729	-1.859839	-1.342849
O	3.376431	-3.919871	-0.414312
H	0.96081	-4.628622	0.077372
H	-2.56504	2.160635	-2.442744
C	-4.531363	1.597092	-1.902146
C	-4.808773	-0.586426	-0.861388
C	1.441477	2.300971	0.639197
H	4.97251	-2.526125	2.238311
C	3.1689	-1.375837	2.013882
H	-3.349894	-3.94482	0.431201
C	-5.087082	-2.75381	0.208082
C	1.154244	0.052725	1.663671
C	-5.355991	0.634064	-1.330491
H	-4.972303	2.526387	-2.238228
C	-5.63173	-1.55869	-0.246966
C	0.849803	3.508223	0.202671
C	0.61145	1.28473	1.188867
H	2.565246	-2.16046	2.442952
H	-5.742293	-3.4777	0.675153
C	0.276442	-0.927231	2.197826
C	-6.794592	0.89236	-1.218376
C	-7.055658	-1.290076	-0.037181

H	1.463515	4.302886	-0.193212
C	-0.510091	3.705618	0.263537
C	-0.80211	1.497706	1.250415
H	0.667699	-1.867514	2.553407
C	-1.077371	-0.73176	2.254685
N	-7.527592	-0.105326	-0.577328
O	-7.359602	1.900443	-1.613228
O	-7.810445	-2.010998	0.608634
C	-1.347608	2.702628	0.77512
H	-0.960968	4.628707	-0.076924
C	-1.642074	0.475568	1.783278
H	-1.730632	-1.499452	2.647014
C	-2.78431	2.923973	0.803713
C	-3.026986	0.693981	1.80874
N	-3.528765	1.859692	1.343098
O	-3.376562	3.919872	0.414888
O	-3.84155	-0.214585	2.285628
H	4.530686	-1.999007	-1.308046
H	-8.523307	0.059634	-0.495407
H	-4.530712	1.998915	1.308409
N	-6.453428	0.318464	2.515473
H	-6.899855	-0.593617	2.43369
H	-4.83274	0.044443	2.295716
H	-6.957508	0.936712	1.88643
H	-6.616007	0.651184	3.460805
N	6.453769	-0.319337	-2.514998
H	6.957947	-0.937232	-1.885692
H	6.899789	0.592958	-2.433336
H	6.616766	-0.652205	-3.460202
H	4.832583	-0.045054	-2.295915

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.74117	0.682664	0.612431

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Cartesian coordinates of pimer **11**

O	7.37779	1.335594	1.004284
N	7.423211	-0.7828	0.218743
H	8.416152	-0.670017	0.058411
C	-0.465086	1.468181	-1.045591
C	5.33714	0.099674	1.028379
C	0.957451	1.57237	-1.15703
C	-1.197072	2.513674	-0.409908

C	6.764521	0.287805	0.771031
C	4.613522	1.091347	1.681762
H	5.131775	1.973203	2.036817
C	-0.489529	3.639037	0.096901
C	6.874171	-1.99707	-0.198987
C	-1.115171	0.308803	-1.557172
C	4.690879	-1.0854	0.596482
C	1.622267	2.710639	-0.613078
C	1.685217	0.544052	-1.782329
C	-2.62935	2.400968	-0.285697
C	3.247928	0.956334	1.872448
C	0.872097	3.736988	0.008942
H	-1.026686	4.441143	0.578842
O	7.597972	-2.850587	-0.683914
C	5.42637	-2.124158	-0.013819
C	-0.341555	-0.695382	-2.176506
C	-2.552082	0.179822	-1.407404
C	3.281238	-1.222422	0.77191
C	3.019886	2.781246	-0.711063
C	3.132891	0.631715	-1.899356
C	1.026618	-0.585278	-2.287085
C	-3.411901	3.40989	0.309508
C	-3.281487	1.224545	-0.769361
H	2.72461	1.751457	2.380854
C	2.551948	-0.177808	1.410243
H	1.391956	4.59755	0.407892
C	4.781562	-3.274893	-0.450342
H	-0.812459	-1.586919	-2.561206
C	-3.247959	-0.954462	-1.86939
C	2.62901	-2.398717	0.288062
O	3.685039	3.793617	-0.215852
N	3.692787	1.797859	-1.353548
O	3.874573	-0.192232	-2.414854
H	1.61831	-1.362147	-2.753829
H	-2.951088	4.316461	0.669873
C	-4.782046	3.277397	0.451947
C	-4.691156	1.087547	-0.594148
C	1.115029	-0.306659	1.559952
H	5.373086	-4.055496	-0.910324
C	3.411431	-3.407408	-0.307702
H	-2.724525	-1.749774	-2.377386
C	-4.613589	-1.089459	-1.678889
C	1.196768	-2.511493	0.412603
C	-5.426754	2.126486	0.015733



H	-5.373691	4.058173	0.91148
C	-5.337334	-0.097629	-1.025895
C	0.341472	0.697638	2.179168
C	0.464862	-1.465986	1.048358
H	2.950524	-4.313772	-0.66847
H	-5.131784	-1.971424	-2.033767
C	0.489178	-3.636943	-0.093942
C	-6.874568	1.999461	0.200663
C	-6.764791	-0.2857	-0.768812
H	0.812402	1.589244	2.563673
C	-1.026709	0.587632	2.289759
C	-0.957676	-1.570091	1.159847
H	1.02629	-4.439213	-0.575662
C	-0.872438	-3.734881	-0.005849
N	-7.423507	0.785028	-0.216797
O	-7.598525	2.853126	0.685093
O	-7.378089	-1.333434	-1.002162
C	-1.685376	-0.541714	1.785126
H	-1.61834	1.364592	2.756427
C	-1.622556	-2.708397	0.616028
H	-1.392305	-4.595555	-0.404546
C	-3.133061	-0.629251	1.902139
C	-3.020145	-2.778866	0.714041
N	-3.69302	-1.795403	1.3564
O	-3.874695	0.194795	2.417542
O	-3.685345	-3.791333	0.218936
H	4.703512	1.826267	-1.39088
H	-8.416524	0.672434	-0.056802
H	-4.703771	-1.823579	1.393335
N	-6.298803	-3.752074	0.282874
H	-6.727998	-2.969919	-0.221755
H	-4.728537	-3.721213	0.290377
H	-6.743043	-3.811763	1.193744
H	-6.544281	-4.601492	-0.217297
N	6.297952	3.754888	-0.278638
H	6.742425	3.814666	-1.189367
H	6.72703	2.972517	0.22584
H	6.543337	4.604202	0.221754
H	4.728559	3.723476	-0.286739

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.751747	0.683025	0.613895

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Cartesian coordinates of different pimers on HS state PES

Cartesian coordinates of pimer **12**

C	0.694109	0.857586	1.602286
C	2.09495	0.63332	1.792604
C	-0.227739	-0.176666	1.940467
C	0.267542	-1.381975	2.482946
C	0.247331	2.107466	1.082101
C	2.538625	-0.595185	2.323609
C	3.021566	1.654338	1.454735
C	-1.6382	0.035463	1.711011
C	1.618242	-1.585307	2.672046
H	-0.410477	-2.177658	2.750709
C	1.20582	3.106857	0.798045
C	-1.165046	2.322281	0.861014
C	3.96147	-0.844263	2.519443
C	4.435264	1.418647	1.622051
C	2.552787	2.884316	0.980915
C	-2.595752	-0.960575	2.005553
C	-2.083766	1.275252	1.165614
H	1.994523	-2.51281	3.083837
H	0.891128	4.07458	0.4386
C	-1.663956	3.532625	0.332894
O	4.450154	-1.864392	2.980436
N	4.801982	0.206264	2.131017
O	5.338517	2.245483	1.340669
H	3.263069	3.677381	0.783502
H	-2.28653	-1.906291	2.422435
C	-3.933962	-0.769999	1.745968
C	-3.47887	1.471897	0.909702
H	-0.991219	4.343687	0.098999
C	-3.010364	3.715232	0.094
C	-4.399998	0.426378	1.188111
H	-4.638852	-1.555463	1.984881
C	-3.923149	2.696002	0.371243
H	-3.387377	4.644151	-0.313976
C	-5.798765	0.608824	0.882126
C	-5.341065	2.911581	0.100442
N	-6.17142	1.830941	0.412078
O	-6.689357	-0.269769	1.023284
O	-5.831564	3.936189	-0.348166
H	5.79358	0.041172	2.252354
H	-7.145598	1.945916	0.16437
N	5.796847	3.555926	-0.888663

H	5.055962	4.13477	-1.27431
H	5.506898	3.131291	0.046722
H	6.003999	2.723837	-1.526195
H	6.639471	4.112045	-0.763525
C	-0.671029	-1.175154	-1.395631
C	-2.096115	-1.276064	-1.473196
C	-0.032589	0.021766	-1.837556
C	-0.831731	1.095682	-2.286382
C	0.080943	-2.265343	-0.869013
C	-2.845427	-0.17913	-1.949344
C	-2.737062	-2.468565	-1.048115
C	1.409392	0.100958	-1.8149
C	-2.205951	1.000116	-2.33939
H	-0.374645	2.030358	-2.574524
C	-0.60582	-3.43158	-0.458549
C	1.51857	-2.15081	-0.766767
C	-4.296929	-0.249615	-1.990864
C	-4.172391	-2.553097	-1.073859
C	-1.977453	-3.531733	-0.546258
C	2.102632	1.208074	-2.356536
C	2.16056	-0.977715	-1.262154
H	-2.813877	1.832816	-2.668882
H	-0.055402	-4.27799	-0.077152
C	2.310959	-3.16846	-0.193555
O	-5.054241	0.649861	-2.333083
N	-4.840571	-1.475066	-1.588747
O	-4.832718	-3.535713	-0.644819
H	-2.489432	-4.431826	-0.231597
H	1.555975	2.007997	-2.832064
C	3.477596	1.276834	-2.333694
C	3.588332	-0.88901	-1.214802
H	1.846728	-4.048096	0.225552
C	3.685922	-3.07014	-0.13709
C	4.237843	0.256291	-1.748214
H	3.988123	2.105911	-2.808553
C	4.334868	-1.948918	-0.658337
H	4.287012	-3.848982	0.313213
C	5.677346	0.337585	-1.722801
C	5.792879	-1.8913	-0.637412
N	6.343657	-0.726664	-1.187979
O	6.345214	1.313009	-2.151692
O	6.538765	-2.751654	-0.196516
H	-5.849982	-1.517843	-1.634515
H	7.354453	-0.675255	-1.184236

N	-6.828561	-2.901317	0.973759
H	-6.73404	-1.840552	1.076287
H	-7.755125	-3.125593	0.618183
H	-6.07498	-3.233196	0.287998
H	-6.699597	-3.357648	1.873664

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$E_{\text{elec}}$ (a.u.)	ZPE (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.785559	0.683945	0.614008

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Cartesian coordinates of pimer **12-1**

C	0.700471	0.047765	-1.783616
C	2.108726	0.282718	-1.874592
C	-0.193642	1.15985	-1.731978
C	0.343334	2.468775	-1.799431
C	0.21985	-1.292072	-1.735223
C	2.594546	1.614648	-1.945905
C	2.996186	-0.814125	-1.871659
C	-1.606881	0.920421	-1.597746
C	1.697103	2.690154	-1.907047
H	-0.312266	3.325596	-1.770214
C	1.149711	-2.351069	-1.722867
C	-1.209721	-1.531994	-1.685271
C	4.008727	1.855168	-2.002491
C	4.433188	-0.590453	-1.919055
C	2.508727	-2.118615	-1.781155
C	-2.537714	1.98016	-1.49061
C	-2.095657	-0.422671	-1.582786
H	2.092823	3.696076	-1.960459
H	0.8103	-3.372367	-1.640086
C	-1.748578	-2.833389	-1.73666
O	4.535267	2.99992	-2.015083
N	4.817668	0.749812	-2.033947
O	5.300622	-1.452583	-1.866617
H	3.219263	-2.93461	-1.750026
H	-2.19903	3.004551	-1.50148
C	-3.885321	1.742413	-1.347067
C	-3.501595	-0.661392	-1.46433
H	-1.098194	-3.686361	-1.857895
C	-3.108515	-3.054408	-1.64572
C	-4.392482	0.436802	-1.316559
H	-4.56821	2.57852	-1.274625
C	-3.988593	-1.983417	-1.49265

H	-3.51856	-4.055305	-1.685108
C	-5.801379	0.19012	-1.132967
C	-5.42125	-2.244351	-1.37249
N	-6.215651	-1.104992	-1.211581
O	-6.667168	1.078282	-0.91167
O	-5.948597	-3.344331	-1.410849
H	5.817091	0.891418	-2.093155
H	-7.198945	-1.279929	-1.049462
N	6.596779	3.357042	-0.404257
H	7.4934	3.446814	-0.876549
H	5.802216	3.262829	-1.120577
H	6.59758	2.47078	0.200067
H	6.443528	4.180016	0.173377
C	-0.700484	0.050617	1.783307
C	-2.108712	0.285775	1.874147
C	-0.219948	-1.289297	1.736393
C	-1.14988	-2.348247	1.725309
C	0.193702	1.162579	1.730353
C	-2.996233	-0.811006	1.872535
C	-2.594429	1.617823	1.944052
C	1.209604	-1.52938	1.686665
C	-2.508863	-2.115634	1.783464
H	-0.810551	-3.369662	1.643684
C	-0.343191	2.471618	1.796149
C	1.606938	0.922907	1.596552
C	-4.433201	-0.587169	1.919823
C	-4.008572	1.858506	2.000432
C	-1.69693	2.69322	1.903681
C	1.748357	-2.830745	1.739505
C	2.095622	-0.420227	1.583001
H	-3.219455	-2.931615	1.753332
H	0.312429	3.328376	1.765646
C	2.537869	1.982473	1.48862
O	-5.300707	-1.449296	1.868392
N	-4.817582	0.753246	2.0333
O	-4.53497	3.003373	2.011756
H	-2.092567	3.699237	1.955903
H	1.097911	-3.683534	1.861679
C	3.108289	-3.051968	1.648882
C	3.501549	-0.659175	1.464948
H	2.199308	3.006909	1.498683
C	3.885472	1.744486	1.345507
C	3.988441	-1.981209	1.494731
H	3.518245	-4.052855	1.689347

C	4.39253	0.438815	1.316212
H	4.568418	2.580488	1.272415
C	5.421073	-2.242371	1.374943
C	5.801456	0.191869	1.133191
N	6.215604	-1.10319	1.213183
O	5.948344	-3.342341	1.414218
O	6.667388	1.079731	0.911236
H	-5.816999	0.894941	2.092407
H	7.198919	-1.278392	1.051459
N	-6.596785	3.357113	0.401066
H	-6.597419	2.470209	-0.202252
H	-7.493369	3.447241	0.873356
H	-5.801921	3.264115	1.117471
H	-6.443806	4.179467	-0.177532

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
-2773.785604		0.683332	0.613349

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Cartesian coordinates of pimer **12-2**

C	0.58272	0.829035	1.573213
C	1.990855	0.648458	1.749374
C	-0.305744	-0.210826	1.96867
C	0.224418	-1.374627	2.559505
C	0.095363	2.049264	1.010575
C	2.472414	-0.541918	2.330266
C	2.888274	1.674065	1.347891
C	-1.730715	-0.044778	1.751215
C	1.584264	-1.536105	2.737727
H	-0.431762	-2.167367	2.884321
C	1.029228	3.04438	0.638332
C	-1.322181	2.234558	0.842208
C	3.906062	-0.745493	2.518075
C	4.309384	1.488714	1.519288
C	2.384058	2.85985	0.805078
C	-2.652635	-1.064085	2.062678
C	-2.212417	1.175918	1.198034
H	1.988547	-2.4326	3.18977
H	0.689497	3.977583	0.215447
C	-1.86651	3.439332	0.330319
O	4.424542	-1.732265	3.015049
N	4.71356	0.309752	2.079078
O	5.185717	2.329503	1.20366

H	3.075452	3.647327	0.532662
H	-2.308585	-2.008432	2.455109
C	-4.007051	-0.903383	1.849889
C	-3.618389	1.341242	0.990915
H	-1.218697	4.271975	0.101155
C	-3.219496	3.594429	0.133946
C	-4.500235	0.292939	1.324479
H	-4.707672	-1.697664	2.074765
C	-4.111474	2.554407	0.439452
H	-3.61957	4.535186	-0.225451
C	-5.936545	0.442227	1.108898
C	-5.521462	2.709127	0.206568
N	-6.33112	1.685562	0.610052
O	-6.781713	-0.416416	1.317669
O	-6.042554	3.703842	-0.366664
H	5.709866	0.179703	2.20374
H	-7.321153	1.791507	0.429372
N	5.800088	3.556991	-1.047714
H	5.113	4.156564	-1.495525
H	5.436693	3.178754	-0.125073
H	6.012724	2.689119	-1.648675
H	6.657728	4.078879	-0.883285
C	-0.68896	-1.121414	-1.414545
C	-2.114277	-1.215042	-1.495931
C	-0.03464	0.05938	-1.881658
C	-0.827732	1.129871	-2.354787
C	0.051732	-2.207821	-0.868973
C	-2.865413	-0.120322	-2.000756
C	-2.758593	-2.393379	-1.068989
C	1.402684	0.125324	-1.864809
C	-2.200513	1.039518	-2.409813
H	-0.362412	2.056125	-2.657325
C	-0.640581	-3.363113	-0.455392
C	1.494351	-2.098521	-0.757867
C	-4.306894	-0.203335	-2.049364
C	-4.214721	-2.499074	-1.122607
C	-2.015615	-3.456227	-0.558544
C	2.109203	1.208561	-2.442472
C	2.145708	-0.945664	-1.280347
H	-2.778249	1.881223	-2.766333
H	-0.099017	-4.209619	-0.061465
C	2.273179	-3.105811	-0.152854
O	-5.06623	0.712665	-2.446752
N	-4.871631	-1.374615	-1.630842

O	-4.86631	-3.467619	-0.765248
H	-2.542256	-4.347749	-0.243065
H	1.57096	1.995412	-2.949072
C	3.483138	1.266634	-2.417407
C	3.573566	-0.866156	-1.230418
H	1.798439	-3.968585	0.288971
C	3.649285	-3.017249	-0.093083
C	4.235197	0.259492	-1.794116
H	4.002455	2.074293	-2.919158
C	4.308315	-1.915653	-0.642013
H	4.242348	-3.788309	0.380695
C	5.671194	0.329634	-1.763284
C	5.767756	-1.869088	-0.617281
N	6.32854	-0.723755	-1.195974
O	6.352853	1.288647	-2.216067
O	6.504482	-2.723466	-0.151084
H	-5.883531	-1.420199	-1.622275
H	7.339664	-0.679654	-1.190661
N	-5.290285	3.315299	-2.86789
H	-5.597115	3.637429	-1.896854
H	-4.481163	3.844023	-3.182153
H	-5.060436	2.281928	-2.77562
H	-6.054961	3.432832	-3.528734

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.779924	0.683829	0.613065

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Cartesian coordinates of pimer **12-3**

C	-0.698737	-0.18969	1.829154
C	-2.076538	0.19335	1.939715
C	0.295997	0.819307	1.682376
C	-0.103715	2.180184	1.652979
C	-0.351023	-1.571594	1.876961
C	-2.423775	1.564176	1.901647
C	-3.069955	-0.806325	2.101441
C	1.686211	0.432734	1.568589
C	-1.419772	2.545097	1.76106
H	0.636226	2.95665	1.534056
C	-1.374859	-2.529822	2.100035
C	1.029605	-1.962925	1.719623
C	-3.794363	1.951261	2.026021
C	-4.439205	-0.425304	2.190537



C	-2.688689	-2.161974	2.211143
C	2.71769	1.380108	1.433092
C	2.026188	-0.952564	1.576674
H	-1.714091	3.585731	1.741063
H	-1.120283	-3.572608	2.214783
C	1.426663	-3.313616	1.685817
O	-4.219169	3.134757	2.046327
N	-4.70411	0.923925	2.147919
O	-5.426477	-1.205663	2.313696
H	-3.44587	-2.903592	2.432413
H	2.493748	2.435768	1.425002
C	4.042705	0.996777	1.27648
C	3.391682	-1.337963	1.421117
H	0.692577	-4.100486	1.771879
C	2.75621	-3.677667	1.53041
C	4.387661	-0.347296	1.262012
H	4.824178	1.735573	1.147447
C	3.739633	-2.707404	1.402439
H	3.052414	-4.718353	1.504936
C	5.79163	-0.73503	1.036243
C	5.144684	-3.120074	1.237772
N	6.061253	-2.087787	1.127846
O	6.684001	0.063487	0.789385
O	5.513225	-4.283701	1.21289
H	-5.676174	1.183204	2.252944
H	7.013855	-2.3634	0.927117
N	-5.869951	-3.253506	0.767014
H	-5.106026	-3.916328	0.665243
H	-5.612695	-2.47581	1.472003
H	-6.060105	-2.758444	-0.153391
H	-6.707187	-3.739928	1.078468
C	0.750032	0.598494	-1.781277
C	2.174577	0.611827	-1.862399
C	0.068333	-0.650617	-1.688661
C	0.827971	-1.835357	-1.677186
C	0.0407	1.835926	-1.776083
C	2.889682	-0.606054	-1.845315
C	2.864373	1.843475	-1.935619
C	-1.375511	-0.660582	-1.604009
C	2.212708	-1.81371	-1.755202
H	0.343078	-2.795146	-1.584458
C	0.774529	3.035402	-1.848499
C	-1.399823	1.820876	-1.685649
C	4.362406	-0.603347	-1.856868

C	4.337222	1.875462	-1.954688
C	2.159845	3.037991	-1.927748
C	-2.110227	-1.873102	-1.56337
C	-2.085268	0.575145	-1.59169
H	2.787619	-2.730328	-1.724758
H	0.266877	3.987846	-1.835923
C	-2.159187	3.020152	-1.714853
O	5.041593	-1.616831	-1.776883
N	4.963801	0.640134	-1.944176
O	4.9927	2.905824	-1.967902
H	2.715594	3.96557	-1.975565
H	-1.591526	-2.818416	-1.606228
C	-3.478422	-1.881582	-1.502452
C	-3.517776	0.563842	-1.505069
H	-1.661123	3.970151	-1.833563
C	-3.524623	3.007617	-1.627929
C	-4.205355	-0.672302	-1.453189
H	-4.021228	-2.817809	-1.53418
C	-4.230456	1.790142	-1.500163
H	-4.082333	3.931348	-1.712754
C	-5.635502	-0.686624	-1.394129
C	-5.65428	1.777941	-1.40787
N	-6.255194	0.542211	-1.385468
O	-6.360515	-1.713254	-1.339973
O	-6.403154	2.794177	-1.336382
H	5.97349	0.65309	-1.85415
H	-7.266195	0.533323	-1.337559
N	-5.740991	4.602543	0.438044
H	-5.13896	4.042868	1.10604
H	-5.216928	5.40214	0.092281
H	-6.01301	3.939633	-0.367405
H	-6.576977	4.929932	0.915999

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.756246	0.682805	0.612551

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Cartesian coordinates of pimer **12-4**

C	-0.942523	1.410953	1.341236
C	-2.344249	1.676243	1.309323
C	-0.034242	2.4053	0.871378
C	-0.554729	3.620572	0.386828
C	-0.481972	0.150988	1.824952

C	-2.815809	2.913772	0.815101
C	-3.255076	0.690765	1.749901
C	1.382815	2.131721	0.895547
C	-1.919494	3.869427	0.360441
H	0.106423	4.388375	0.014906
C	-1.431165	-0.795836	2.253417
C	0.939335	-0.115586	1.85401
C	-4.261926	3.177078	0.715881
C	-4.706112	0.924709	1.656017
C	-2.792216	-0.530663	2.21763
C	2.334041	3.097878	0.474264
C	1.847695	0.873925	1.377631
H	-2.310505	4.80378	-0.021221
H	-1.115759	-1.76718	2.60255
C	1.458711	-1.328543	2.374359
O	-4.73367	4.204178	0.253208
N	-5.088501	2.165421	1.1765
O	-5.546925	0.089655	1.957014
H	-3.514046	-1.274142	2.530398
H	2.004489	4.072834	0.149675
C	3.677492	2.839763	0.49581
C	3.257557	0.606792	1.403731
H	0.788097	-2.074971	2.771391
C	2.805767	-1.572299	2.41839
C	4.167325	1.59023	0.937752
H	4.383114	3.614195	0.224298
C	3.726362	-0.624879	1.920244
H	3.182905	-2.478415	2.875502
C	5.568493	1.321481	0.959423
C	5.133358	-0.882935	1.971986
N	5.951777	0.11545	1.495157
O	6.47894	2.084188	0.525641
O	5.674044	-1.935005	2.40037
H	-6.08155	2.294463	1.018553
H	6.946667	-0.068184	1.526445
N	4.921217	-4.105759	1.06945
H	5.657447	-4.806964	1.041272
H	5.198461	-3.314856	1.722211
H	4.804066	-3.655312	0.094238
H	4.051589	-4.533314	1.376487
C	0.347676	-1.01132	-1.516756
C	1.769947	-0.921317	-1.679143
C	-0.223943	-2.217142	-1.014719
C	0.626788	-3.323876	-0.754605

C	-0.466259	0.103756	-1.867734
C	2.58419	-2.033771	-1.344817
C	2.339412	0.270687	-2.184876
C	-1.649829	-2.293303	-0.802842
C	1.983467	-3.237892	-0.915344
H	0.202803	-4.26872	-0.449856
C	0.153376	1.275575	-2.373219
C	-1.901353	0.01388	-1.701149
C	3.997937	-1.934029	-1.483558
C	3.75539	0.360114	-2.360659
C	1.511801	1.359616	-2.530063
C	-2.264386	-3.42822	-0.239217
C	-2.465536	-1.178537	-1.158441
H	2.607157	-4.109193	-0.760143
H	-0.447232	2.133088	-2.634679
C	-2.762122	1.073727	-2.041244
O	4.84278	-2.831386	-1.201186
N	4.482683	-0.747371	-1.983018
O	4.369538	1.348927	-2.836621
H	1.97476	2.256776	-2.918316
H	-1.670521	-4.278847	0.05945
C	-3.635574	-3.488676	-0.037738
C	-3.875625	-1.252794	-0.95052
H	-2.366969	1.988254	-2.456122
C	-4.132042	0.995642	-1.830638
C	-4.445001	-2.418539	-0.390388
H	-4.099629	-4.364712	0.396663
C	-4.694047	-0.149242	-1.283649
H	-4.780661	1.828684	-2.072522
C	-5.898679	-2.507178	-0.165415
C	-6.142393	-0.190162	-1.013518
N	-6.631946	-1.398857	-0.554963
O	-6.454374	-3.482949	0.31376
O	-6.890185	0.762652	-1.180508
H	5.484534	-0.704889	-2.115768
H	-7.616697	-1.417848	-0.323417
N	6.149449	3.071436	-1.876481
H	6.298212	2.768783	-0.852436
H	7.029971	3.027134	-2.38357
H	5.453619	2.392747	-2.297839
H	5.779511	4.016998	-1.9281

$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.756484	0.68278	0.612438

Cartesian coordinates of pimer **13**

O	0.159382	-6.134098	-1.817481
N	-1.929206	-5.261316	-1.742935
H	-2.29785	-6.200043	-1.811192
C	0.49121	-1.333209	1.719012
C	-0.07175	-3.759298	-1.761751
C	0.987785	-2.67513	1.725856
C	1.415953	-0.247478	1.70122
C	-0.568881	-5.108997	-1.776328
C	1.306906	-3.51405	-1.771131
H	1.986699	-4.356136	-1.793832
C	2.799107	-0.529585	1.65972
C	-2.903029	-4.257011	-1.689263
C	-0.917401	-1.108828	1.723178
C	-0.987774	-2.675119	-1.726135
C	2.380444	-2.901409	1.693238
C	0.071762	-3.759305	1.761699
C	0.917401	1.108828	1.723178
C	1.786961	-2.223167	-1.748042
C	3.27035	-1.824514	1.653606
H	3.516786	0.275366	1.623506
O	-4.084016	-4.579376	-1.649838
C	-2.380444	-2.901385	-1.693406
C	-1.786961	-2.223227	1.747374
C	-1.415953	0.247478	1.70122
C	-0.491215	-1.333219	-1.719505
C	2.90303	-4.25708	1.689414
C	0.568851	-5.108998	1.776824
C	-1.306895	-3.514088	1.770785
C	1.786961	2.223227	1.747374
C	-0.49121	1.333209	1.719012
H	2.8563	-2.079912	-1.747261
C	0.917381	-1.108813	-1.723752
H	4.331786	-2.034524	1.621952
C	-3.270308	-1.824437	-1.653749
H	-2.856299	-2.080089	1.746225
C	-2.799107	0.529585	1.65972
C	-1.415912	-0.247453	-1.701724
O	4.084038	-4.579408	1.650088

N	1.929232	-5.261324	1.743361
O	-0.159317	-6.13411	1.818459
H	-1.986655	-4.356204	1.793531
H	2.856299	2.080089	1.746225
C	1.306895	3.514088	1.770785
C	-0.987785	2.67513	1.725856
C	1.415912	0.247453	-1.701724
H	-4.331753	-2.034374	-1.621907
C	-2.799057	-0.529514	-1.65995
H	-3.516786	-0.275366	1.623506
C	-3.27035	1.824514	1.653606
C	-0.917381	1.108813	-1.723752
C	-0.071762	3.759305	1.761699
H	1.986655	4.356204	1.793531
C	-2.380444	2.901409	1.693238
C	2.799057	0.529514	-1.65995
C	0.491215	1.333219	-1.719505
H	-3.516675	0.275501	-1.623512
H	-4.331786	2.034524	1.621952
C	-1.786961	2.223167	-1.748042
C	-0.568851	5.108998	1.776824
C	-2.90303	4.25708	1.689414
H	3.516675	-0.275501	-1.623512
C	3.270308	1.824437	-1.653749
C	0.987774	2.675119	-1.726135
H	-2.8563	2.079912	-1.747261
C	-1.306906	3.51405	-1.771131
N	-1.929232	5.261324	1.743361
O	0.159317	6.13411	1.818459
O	-4.084038	4.579408	1.650088
C	2.380444	2.901385	-1.693406
H	4.331753	2.034374	-1.621907
C	0.07175	3.759298	-1.761751
H	-1.986699	4.356136	-1.793832
C	2.903029	4.257011	-1.689263
C	0.568881	5.108997	-1.776328
N	1.929206	5.261316	-1.742935
O	4.084016	4.579376	-1.649838
O	-0.159382	6.134098	-1.817481
H	2.297851	-6.200011	1.812324
H	-2.297851	6.200011	1.812324
H	2.29785	6.200043	-1.811192
N	-0.00134	8.019375	0.000391
H	0.827783	8.607784	0.013647

H	-0.002222	7.363142	-0.845039
H	0.001596	7.362499	0.845315
H	-0.832692	8.60466	-0.012445
N	0.00134	-8.019375	0.000391
H	-0.827783	-8.607784	0.013647
H	0.002222	-7.363142	-0.845039
H	-0.001596	-7.362499	0.845315
H	0.832692	-8.60466	-0.012445

Cartesian coordinates of pimer **14**

O	-6.586124	2.495802	-0.187991
N	-6.207863	0.560888	-1.293975
H	-7.209037	0.412797	-1.289452
C	-0.760512	-1.527713	1.185549
C	-4.330147	1.92161	-0.714339
C	-2.176625	-1.734386	1.170089
C	-0.233703	-0.321356	1.731209
C	-5.75485	1.708326	-0.709961
C	-3.788219	3.119729	-0.227089
H	-4.461244	3.909437	0.086568
C	-1.131272	0.638626	2.248113
C	-5.441029	-0.48349	-1.822009
C	0.096647	-2.534452	0.647923
C	-3.469454	0.91988	-1.236222
C	-3.03738	-0.738119	1.698123
C	-2.701519	-2.928	0.630897
C	1.197614	-0.110338	1.742311
C	-2.426222	3.321212	-0.209954
C	-2.493607	0.432303	2.233349
H	-0.758725	1.563814	2.660396
O	-6.003264	-1.47458	-2.263162
C	-3.997649	-0.271264	-1.776093
C	-0.483106	-3.698825	0.098561
C	1.525832	-2.335622	0.681901
C	-2.052868	1.123833	-1.218048
C	-4.470058	-0.937146	1.66048
C	-4.142169	-3.156521	0.603924
C	-1.849598	-3.89384	0.096793
C	1.775498	1.068966	2.259258
C	2.052891	-1.123881	1.21808
H	-2.054016	4.269978	0.145419
C	-1.525826	2.33554	-0.681774
H	-3.155788	1.185764	2.638469

C	-3.142087	-1.25664	-2.275509
H	0.140657	-4.469246	-0.328666
C	2.426214	-3.321347	0.210165
C	-1.197579	0.110351	-1.742377
O	-5.319355	-0.118528	2.082604
N	-4.91382	-2.112652	1.126584
O	-4.694157	-4.158241	0.177612
H	-2.28803	-4.791827	-0.319203
H	1.150282	1.860048	2.643412
C	3.142139	1.256687	2.275294
C	3.46948	-0.919944	1.236234
C	-0.096646	2.534402	-0.647816
H	-3.578466	-2.166866	-2.667441
C	-1.775449	-1.068903	-2.259452
H	2.053995	-4.270135	-0.145136
C	3.788215	-3.119883	0.227291
C	0.233735	0.321387	-1.731255
C	3.997691	0.271251	1.775983
H	3.578531	2.166953	2.66712
C	4.330159	-1.921731	0.71444
C	0.48309	3.698758	-0.0984
C	0.760527	1.52772	-1.185529
H	-1.150224	-1.859935	-2.643696
H	4.461233	-3.909628	-0.08629
C	1.131317	-0.63856	-2.248199
C	5.441074	0.483474	1.821849
C	5.754876	-1.708469	0.710033
H	-0.140681	4.469129	0.328905
C	1.849576	3.89381	-0.096658
C	2.176636	1.734422	-1.170079
H	0.758788	-1.56376	-2.660472
C	2.493647	-0.432212	-2.23344
N	6.207897	-0.560971	1.293952
O	6.003313	1.474628	2.262862
O	6.586126	-2.495979	0.188115
C	2.70151	2.928019	-0.63083
H	2.287995	4.791782	0.319386
C	3.037406	0.738199	-1.698173
H	3.155829	-1.185652	-2.638591
C	4.142154	3.156566	-0.603854
C	4.470076	0.93726	-1.660539
N	4.91382	2.112736	-1.126592
O	4.694131	4.1583	-0.177572
O	5.319404	0.118652	-2.082655



H	-5.916217	-2.247911	1.082978
H	7.209071	-0.412885	1.289394
H	5.916215	2.247999	-1.082938
N	5.890405	-2.452568	-2.358049
H	5.160482	-3.106679	-2.62782
H	5.523495	-1.459203	-2.347979
H	6.216727	-2.64322	-1.358656
H	6.674341	-2.52028	-3.002973
N	-5.890732	2.452711	2.358064
H	-5.523562	1.459491	2.348195
H	-6.674834	2.520281	3.002797
H	-5.161059	3.107072	2.627902
H	-6.216904	2.643073	1.358497

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.781053	0.684392	0.614184

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Cartesian coordinates of pimer **14-1**

O	-6.559385	-2.708093	-0.059651
N	-6.305148	-0.757208	1.056975
H	-7.307401	-0.633801	0.989096
C	-0.741221	1.714053	-1.048784
C	-4.361477	-2.079049	0.618122
C	-2.167137	1.776144	-1.154746
C	-0.048556	0.5634	-1.53589
C	-5.787977	-1.89888	0.51425
C	-3.764033	-3.275355	0.196926
H	-4.399729	-4.094393	-0.119943
C	-0.805511	-0.499959	-2.083491
C	-5.597706	0.309809	1.621835
C	-0.039512	2.80046	-0.452828
C	-3.556713	-1.044085	1.164968
C	-2.879611	0.687952	-1.726224
C	-2.849372	2.919315	-0.690239
C	1.389131	0.516015	-1.455423
C	-2.397264	-3.436938	0.248343
C	-2.177766	-0.436295	-2.176014
H	-0.312114	-1.3965	-2.427198
O	-6.208737	1.285852	2.026399
C	-4.145844	0.139477	1.655361
C	-0.771365	3.912694	0.010667
C	1.405495	2.73692	-0.340314

C	-2.136755	-1.20467	1.219181
C	-4.317954	0.748428	-1.81937
C	-4.302653	3.00833	-0.797502
C	-2.145742	3.973814	-0.111402
C	2.131802	-0.581789	-1.952102
C	2.095941	1.603831	-0.856811
H	-1.98248	-4.386658	-0.05385
C	-1.547488	-2.409287	0.726057
H	-2.728878	-1.267623	-2.596522
C	-3.346934	1.156745	2.178649
H	-0.262574	4.752438	0.458453
C	2.146685	3.764428	0.276626
C	-1.339291	-0.156759	1.760488
O	-5.05081	-0.15088	-2.298605
N	-4.91933	1.884315	-1.355246
O	-4.983611	3.960745	-0.452796
H	-2.702523	4.834255	0.236683
H	1.625599	-1.41886	-2.408248
C	3.504472	-0.625014	-1.85963
C	3.522798	1.548209	-0.756386
C	-0.116341	-2.549199	0.728507
H	-3.827362	2.05978	2.533745
C	-1.974025	1.010887	2.228618
H	1.646439	4.627649	0.687782
C	3.522518	3.701352	0.375234
C	0.102936	-0.317431	1.806063
C	4.224251	0.41958	-1.264511
H	4.039323	-1.480029	-2.253949
C	4.2174	2.608631	-0.141312
C	0.524452	-3.687363	0.180444
C	0.687629	-1.505198	1.280917
H	-1.390681	1.828208	2.623734
H	4.08839	4.493134	0.848605
C	0.944715	0.679513	2.338002
C	5.660442	0.367025	-1.151914
C	5.673638	2.576904	-0.037284
H	-0.060499	-4.481569	-0.257887
C	1.895188	-3.81597	0.183157
C	2.110032	-1.646337	1.286623
H	0.525852	1.589018	2.740663
C	2.318398	0.539543	2.338434
N	6.276243	1.445305	-0.591302
O	6.386717	-0.587229	-1.537313
O	6.371033	3.446327	0.460752

C	2.701996	-2.813753	0.734684
H	2.372204	-4.69135	-0.238115
C	2.908665	-0.609548	1.811482
H	2.960069	1.321685	2.723858
C	4.132229	-2.929269	0.675912
C	4.361716	-0.71172	1.766535
N	4.854281	-1.905386	1.227421
O	4.74304	-3.890589	0.138108
O	5.154306	0.14048	2.143149
H	-5.928923	1.925385	-1.414844
H	7.281351	1.393335	-0.489706
H	5.863218	-1.975633	1.206065
N	6.378929	-3.192148	-1.821596
H	7.34964	-3.470844	-1.6989
H	5.780489	-3.564015	-1.019732
H	6.312953	-2.12532	-1.795981
H	6.03608	-3.553641	-2.707945
N	-5.54174	-2.724037	-2.518817
H	-5.187395	-1.723276	-2.492635
H	-6.225541	-2.822424	-3.265659
H	-4.773452	-3.374536	-2.659676
H	-6.000821	-2.890743	-1.573764

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.781721	0.684221	0.61353

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Cartesian coordinates of pimer **15**

C	-0.571596	-1.82562	1.060304
C	-1.99818	-1.845646	1.173031
C	0.149943	-0.691714	1.53945
C	-0.56934	0.384768	2.104145
C	0.097389	-2.926263	0.448991
C	-2.668415	-0.743428	1.744682
C	-2.722625	-2.959589	0.674274
C	1.589144	-0.664726	1.408586
C	-1.944562	0.36224	2.200269
H	-0.050674	1.265495	2.451176
C	-0.671554	-4.016299	-0.025613
C	1.535254	-2.894619	0.311006
C	-4.12061	-0.729022	1.820766
C	-4.156959	-2.954952	0.723312
C	-2.043544	-4.03175	0.080946

C	2.357278	0.432566	1.858359
C	2.258242	-1.762982	0.792877
H	-2.490592	1.202866	2.610276
H	-0.186659	-4.86476	-0.482867
C	2.246713	-3.942634	-0.310609
O	-4.814342	0.177329	2.265129
N	-4.748481	-1.87656	1.320243
O	-4.884713	-3.8641	0.237574
H	-2.62001	-4.870612	-0.286554
H	1.877001	1.279991	2.323399
C	3.725694	0.466886	1.699598
C	3.679161	-1.719604	0.628022
H	1.725057	-4.810571	-0.68319
C	3.617306	-3.892468	-0.465345
C	4.406892	-0.587933	1.083819
H	4.283336	1.325757	2.051286
C	4.339984	-2.793002	-0.0039
H	4.157363	-4.696799	-0.947459
C	5.836627	-0.531598	0.880961
C	5.786804	-2.763456	-0.189106
N	6.419353	-1.619106	0.303367
O	6.575342	0.432948	1.201198
O	6.457271	-3.641922	-0.709382
H	-5.758427	-1.864734	1.379748
H	7.417475	-1.57102	0.145875
N	-6.623556	-3.05621	-1.557288
H	-7.585666	-3.330824	-1.37313
H	-5.968598	-3.455925	-0.803737
H	-6.346755	-3.399452	-2.473652
H	-6.547496	-1.999275	-1.515439
C	0.571558	1.825613	-1.060408
C	1.998141	1.845582	-1.173143
C	-0.150028	0.691744	-1.539566
C	0.569204	-0.384735	-2.104334
C	-0.097383	2.926282	-0.449093
C	2.66833	0.743342	-1.744793
C	2.722631	2.95952	-0.674432
C	-1.589224	0.664788	-1.40864
C	1.944429	-0.362266	-2.200454
H	0.050492	-1.265403	-2.451445
C	0.6716	4.016322	0.025443
C	-1.535243	2.894661	-0.311035
C	4.120536	0.728848	-1.820832
C	4.156944	2.954829	-0.723498

C	2.043586	4.03173	-0.081146
C	-2.357404	-0.432456	-1.858448
C	-2.258272	1.763026	-0.792848
H	2.490424	-1.202879	-2.61053
H	0.18674	4.864815	0.482673
C	-2.246657	3.9427	0.310592
O	4.81423	-0.177445	-2.265356
N	4.748442	1.876369	-1.320308
O	4.884719	3.864042	-0.237859
H	2.620078	4.870596	0.286306
H	-1.87717	-1.279845	-2.323597
C	-3.725809	-0.466757	-1.699602
C	-3.679175	1.719638	-0.627851
H	-1.724983	4.810686	0.683032
C	-3.61723	3.892492	0.46552
C	-4.406959	0.588008	-1.083672
H	-4.283482	-1.32558	-2.051348
C	-4.339937	2.792994	0.004198
H	-4.15725	4.696823	0.947676
C	-5.836654	0.531624	-0.880583
C	-5.786725	2.763352	0.189717
N	-6.419309	1.618999	-0.302683
O	-6.575422	-0.432878	-1.200869
O	-6.457114	3.641739	0.71022
H	5.75839	1.8645	-1.379785
H	-7.417386	1.570812	-0.144942
N	6.623973	3.056568	1.556492
H	6.347679	3.400236	2.472845
H	6.547805	1.999664	1.515128
H	5.968722	3.456101	0.802981
H	7.586036	3.330962	1.371754

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.77755	0.6841	0.613997

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Cartesian coordinates of pimer **16**

O	-7.694666	1.733317	0.323292
N	-7.405384	-0.316187	-0.601107
H	-8.378452	-0.506345	-0.397321
C	0.535748	-0.878923	1.485781
C	-5.571309	1.21465	-0.620157
C	-0.87169	-1.110772	1.593294

C	1.045359	0.434223	1.70255
C	-6.938356	0.928679	-0.285562
C	-5.057835	2.51545	-0.489046
H	-5.740992	3.327402	-0.266385
C	0.145462	1.469373	2.031012
C	-6.663503	-1.398149	-1.092983
C	1.398716	-1.967666	1.156159
C	-4.720649	0.157666	-1.036768
C	-1.734724	-0.037055	1.926716
C	-1.386744	-2.405448	1.363929
C	2.466872	0.674856	1.566588
C	-3.721686	2.766312	-0.694376
C	-1.210815	1.238322	2.140661
H	0.505741	2.474198	2.186988
O	-7.227667	-2.458949	-1.314745
C	-5.236681	-1.136345	-1.257177
C	0.833247	-3.245043	0.950051
C	2.813769	-1.727462	1.018787
C	-3.322664	0.407342	-1.213279
C	-3.162178	-0.266219	2.041523
C	-2.820875	-2.654436	1.454497
C	-0.527037	-3.457809	1.048774
C	3.030182	1.954869	1.759233
C	3.322999	-0.408287	1.212683
H	-3.372747	3.784572	-0.613722
C	-2.81447	1.726903	-1.019322
H	-1.89051	2.045497	2.380751
C	-4.381669	-2.180795	-1.619582
H	1.46225	-4.085796	0.699947
C	3.72008	-2.767422	0.69315
C	-2.465689	-0.67516	-1.567077
O	-3.984187	0.614371	2.366752
N	-3.596184	-1.538131	1.786338
O	-3.368702	-3.732397	1.275695
H	-0.954013	-4.439188	0.885547
H	2.401141	2.795351	2.009185
C	4.384055	2.178943	1.619418
C	4.721197	-0.159687	1.036169
C	-1.399494	1.968011	-1.155749
H	-4.800876	-3.168054	-1.76089
C	-3.027973	-1.955678	-1.759361
H	3.370291	-3.785335	0.611802
C	5.056491	-2.517593	0.488035
C	-1.044404	-0.433378	-1.703223

C	5.238223	1.133904	1.256724
H	4.804079	3.165811	1.761055
C	5.57106	-1.217296	0.619543
C	-0.834819	3.245485	-0.948051
C	-0.535742	0.880012	-1.485758
H	-2.398239	-2.795766	-2.008881
H	5.738962	-3.330042	0.265074
C	-0.143789	-1.467659	-2.032516
C	6.665335	1.394517	1.092855
C	6.938644	-0.932614	0.285524
H	-1.464355	4.08549	-0.696768
C	0.525377	3.459134	-1.046108
C	0.871556	1.11283	-1.592839
H	-0.503449	-2.47255	-2.189499
C	1.212282	-1.235549	-2.142241
N	7.406542	0.311939	0.601474
O	7.230168	2.45501	1.314453
O	7.694422	-1.737855	-0.322879
C	1.385784	2.407602	-1.362132
H	0.951754	4.440559	-0.881579
C	1.735317	0.040029	-1.927246
H	1.892515	-2.04198	-2.383272
C	2.819771	2.657531	-1.452197
C	3.162545	0.270413	-2.042451
N	3.595814	1.542109	-1.785478
O	3.366958	3.735544	-1.271809
O	3.985079	-0.60886	-2.370041
H	-4.592359	-1.707943	1.836711
H	8.379879	0.501243	0.398178
H	4.591844	1.712753	-1.836031
N	6.157812	-2.227938	-2.446477
H	5.745061	-3.157764	-2.461628
H	5.381728	-1.531937	-2.350549
H	6.829439	-2.139387	-1.618023
H	6.655179	-2.06465	-3.319186
N	-6.16239	2.227685	2.446009
H	-6.661348	2.064404	3.317793
H	-6.832664	2.136589	1.6157
H	-5.751372	3.158244	2.46102
H	-5.384863	1.533144	2.352176

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)
-2773.769632	0.685365	0.615125

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Cartesian coordinates of pimer **16-1**

O	7.531523	-2.075777	0.799767
N	7.448272	-0.18391	-0.446609
H	8.427032	-0.041359	-0.231641
C	-0.516432	1.325795	1.226211
C	5.491676	-1.54891	-0.307917
C	0.899444	1.498225	1.329962
C	-1.097683	0.076923	1.605577
C	6.866977	-1.32255	0.038412
C	4.864711	-2.766209	0.004649
H	5.46836	-3.581703	0.387015
C	-0.25417	-0.945749	2.096411
C	6.815026	0.864148	-1.125679
C	-1.316393	2.39739	0.736353
C	4.745302	-0.505606	-0.916301
C	1.701246	0.442286	1.835896
C	1.484619	2.715991	0.923533
C	-2.516615	-0.112716	1.457821
C	3.51937	-2.941361	-0.220089
C	1.107135	-0.764937	2.212149
H	-0.665118	-1.903916	2.373966
O	7.471164	1.831299	-1.480325
C	5.375147	0.69391	-1.308262
C	-0.685069	3.599413	0.358734
C	-2.751324	2.215588	0.617058
C	3.337578	-0.666842	-1.109895
C	3.13243	0.616443	1.955719
C	2.931656	2.898447	0.999128
C	0.685815	3.753064	0.443898
C	-3.1444	-1.336018	1.800956
C	-3.321404	0.955062	0.954793
H	3.083017	-3.901939	0.008235
C	2.713126	-1.900332	-0.74618
H	1.74067	-1.561912	2.57934
C	4.624063	1.733502	-1.860449
H	-1.26795	4.424653	-0.020766
C	-3.598784	3.245454	0.161512
C	2.586106	0.415193	-1.649341
O	3.903776	-0.241105	2.435764
N	3.639061	1.811661	1.521319
O	3.539788	3.902188	0.658287
H	1.165131	4.676203	0.143842
H	-2.565276	-2.145954	2.216884
C	-4.489932	-1.532461	1.607213



C	-4.727241	0.754341	0.779169
C	1.292292	-2.051223	-0.916874
H	5.129468	2.648979	-2.137879
C	3.258841	1.59917	-2.015412
H	-3.193145	4.213828	-0.088153
C	-4.957825	3.053091	0.021483
C	1.14829	0.275293	-1.788939
C	-5.296258	-0.518881	1.064396
H	-4.943817	-2.470705	1.90016
C	-5.530208	1.815257	0.318896
C	0.618255	-3.248212	-0.577624
C	0.528456	-0.952558	-1.418278
H	2.710599	2.436455	-2.418801
H	-5.602678	3.847635	-0.329959
C	0.346849	1.329889	-2.265783
C	-6.685806	-0.74877	0.791939
C	-6.965552	1.626642	0.138043
H	1.171701	-4.097777	-0.20758
C	-0.749435	-3.369163	-0.700395
C	-0.890308	-1.082838	-1.539809
H	0.792038	2.274716	-2.535706
C	-1.024177	1.200044	-2.373631
N	-7.422804	0.326323	0.387376
O	-7.262662	-1.870343	0.884217
O	-7.76322	2.482003	-0.215047
C	-1.519535	-2.301141	-1.171028
H	-1.250385	-4.291264	-0.435443
C	-1.648999	0.006996	-2.016931
H	-1.638822	2.019445	-2.724148
C	-2.95382	-2.430364	-1.275172
C	-3.099445	-0.102318	-2.132061
N	-3.629901	-1.337987	-1.746256
O	-3.587572	-3.468662	-0.972661
O	-3.855187	0.770173	-2.531147
H	4.642319	1.934253	1.567958
H	-8.408016	0.16835	0.218504
H	-4.636787	-1.398871	-1.813708
N	-6.084057	-3.978842	-0.117019
H	-5.127164	-3.72645	-0.49479
H	-5.978826	-4.718459	0.573738
H	-6.55168	-3.11348	0.341991
H	-6.672794	-4.319984	-0.873518
N	5.883067	-2.021253	2.904742
H	6.360472	-1.741726	3.758958

H	6.589805	-2.14988	2.114559
H	5.381488	-2.891384	3.066485
H	5.182437	-1.288281	2.641591

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
-2773.773881		0.684685	0.614556

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Cartesian coordinates of pimer **17**

O	7.416276	1.395796	0.824182
N	7.390924	-0.756206	0.140573
H	8.375086	-0.65461	-0.072213
C	-0.46606	1.30012	-1.205221
C	5.368178	0.173294	1.002497
C	0.956274	1.364864	-1.34563
C	-1.162356	2.39117	-0.608428
C	6.758872	0.329533	0.672305
C	4.671336	1.187385	1.675546
H	5.211197	2.053574	2.036204
C	-0.421908	3.513878	-0.174184
C	6.823201	-1.993414	-0.193715
C	-1.156416	0.134723	-1.655322
C	4.690254	-1.020927	0.633888
C	1.655193	2.508007	-0.878781
C	1.646885	0.284016	-1.936004
C	-2.59743	2.309126	-0.438537
C	3.321464	1.078588	1.910481
C	0.950479	3.56867	-0.3005
H	-0.92551	4.353284	0.280239
O	7.536371	-2.869316	-0.659714
C	5.388181	-2.093043	0.044644
C	-0.417397	-0.917231	-2.237521
C	-2.585698	0.05131	-1.479553
C	3.280776	-1.128869	0.855925
C	3.093431	2.565074	-0.994478
C	3.094268	0.330453	-2.08217
C	0.95242	-0.843894	-2.375286
C	-3.344268	3.354344	0.144506
C	-3.280771	1.12879	-0.855807
H	2.826754	1.884519	2.429878
C	2.585695	-0.051175	1.479301
H	1.50415	4.432737	0.043249
C	4.70732	-3.252584	-0.330679

H	-0.913421	-1.816989	-2.566402
C	-3.321514	-1.078185	-1.911375
C	2.597445	-2.309361	0.439085
O	3.79272	3.526699	-0.593446
N	3.698	1.494325	-1.592373
O	3.797325	-0.53483	-2.584374
H	1.517494	-1.659035	-2.809307
H	-2.854819	4.263028	0.459883
C	-4.707226	3.251866	0.332051
C	-4.690253	1.020767	-0.633805
C	1.156447	-0.134646	1.655329
H	5.272467	-4.058038	-0.780793
C	3.344351	-3.354966	-0.143181
H	-2.826812	-1.883814	-2.431251
C	-4.67141	-1.187015	-1.676605
C	1.162319	-2.391182	0.608622
C	-5.388143	2.09259	-0.043981
H	-5.27231	4.057021	0.782776
C	-5.368222	-0.173228	-1.003052
C	0.4175	0.91726	2.237706
C	0.466057	-1.300044	1.205296
H	2.854956	-4.263922	-0.45786
H	-5.211343	-2.052938	-2.0378
C	0.421791	-3.513734	0.174115
C	-6.82318	1.992899	0.194298
C	-6.758946	-0.329562	-0.67303
H	0.913578	1.816938	2.566724
C	-0.952305	0.843935	2.375571
C	-0.956285	-1.364701	1.345637
H	0.925339	-4.353055	-0.280526
C	-0.950616	-3.568401	0.300286
N	-7.390954	0.755915	-0.14068
O	-7.536321	2.868628	0.660671
O	-7.416429	-1.395676	-0.825608
C	-1.646836	-0.283862	1.936098
H	-1.517329	1.659018	2.809762
C	-1.65527	-2.507748	0.878653
H	-1.504348	-4.43234	-0.043683
C	-3.094208	-0.33026	2.082323
C	-3.09352	-2.564742	0.994348
N	-3.698039	-1.493924	1.592144
O	-3.79714	0.534683	2.585281
O	-3.792876	-3.526308	0.593308
H	4.705132	1.506258	-1.678715

H	-8.375155	0.654277	0.071901
H	-4.705109	-1.506118	1.679156
N	-6.347421	-3.719982	-0.176174
H	-6.763678	-2.775579	-0.483423
H	-5.350029	-3.595184	0.173675
H	-6.923189	-4.119127	0.56185
H	-6.339234	-4.361426	-0.966226
N	6.347587	3.720219	0.175141
H	6.9231	4.119383	-0.563064
H	6.763768	2.775668	0.482171
H	6.339772	4.361609	0.965254
H	5.349983	3.595701	-0.174281

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.780052	0.684007	0.614101

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Cartesian coordinates of pimer **18**

O	4.36626	-5.427238	-0.520703
C	4.294762	-4.217957	-0.689414
N	5.458667	-3.445574	-0.611943
C	3.077013	-3.461688	-0.953217
H	6.307606	-3.951949	-0.395227
C	5.569819	-2.092088	-0.757278
C	1.850687	-4.1325	-1.009169
C	3.134547	-2.067358	-1.154529
O	6.701808	-1.565243	-0.573703
C	4.373912	-1.373515	-1.096351
H	1.843048	-5.204334	-0.859352
C	0.684677	-3.436086	-1.2431
C	1.928705	-1.339304	-1.411422
H	6.879103	-0.2844	0.268071
C	4.414785	0.001366	-1.377578
H	-0.243012	-3.986999	-1.262141
C	0.686472	-2.037258	-1.439755
C	1.993444	0.070199	-1.62289
N	7.099354	0.546064	0.920817
H	5.371118	0.507949	-1.412363
C	3.260864	0.700433	-1.639736
C	-0.53756	-1.29356	-1.646796
C	0.772344	0.816106	-1.802267
H	7.486076	0.190773	1.792413
H	6.249676	1.126769	1.131469

H	7.792643	1.146549	0.47938
H	3.340448	1.75484	-1.8565
C	-1.79851	-1.928572	-1.671893
C	-0.474941	0.121749	-1.806522
C	0.771915	2.221033	-1.941883
H	-1.873282	-2.998009	-1.550213
C	-2.964332	-1.209414	-1.834767
C	-1.686994	0.864929	-1.960633
H	1.699168	2.772869	-1.919779
C	-0.4023	2.931746	-2.073568
C	-2.929299	0.180336	-1.975532
H	-3.92358	-1.710766	-1.849925
C	-1.63167	2.270756	-2.08413
H	-0.394961	4.01083	-2.156152
C	-4.155352	0.928461	-2.12693
C	-2.857947	3.046114	-2.190028
N	-4.032769	2.287625	-2.228752
O	-5.296825	0.417831	-2.177631
O	-2.937045	4.266665	-2.245344
H	-4.883979	2.818673	-2.354776
H	-6.661274	0.270852	-1.288948
N	-7.474174	0.107282	-0.644368
H	-7.908975	0.992829	-0.398628
H	-8.160872	-0.485915	-1.104538
H	-7.104719	-0.395794	0.241133
O	-6.586229	-1.242677	1.386875
C	-5.376391	-1.583291	1.504636
C	-4.255271	-0.684975	1.476587
N	-5.102803	-2.909864	1.67407
C	-2.938861	-1.206324	1.598734
C	-4.442629	0.699307	1.345535
C	-3.847037	-3.51381	1.791514
H	-5.896437	-3.536867	1.707862
C	-1.818391	-0.315726	1.568456
C	-2.721191	-2.591322	1.750259
C	-3.368735	1.558076	1.309177
H	-5.450324	1.093462	1.300134
O	-3.776511	-4.729375	1.91135
C	-0.501406	-0.848728	1.696187
C	-2.037812	1.084106	1.411707
C	-1.421692	-3.095214	1.859155
H	-3.561881	2.615595	1.211782
C	0.630611	0.049321	1.675138
C	-0.338724	-2.244282	1.833055

C	-0.905677	1.980293	1.369449
H	-1.290663	-4.164481	1.965181
C	0.411154	1.446331	1.501778
C	1.955497	-0.422258	1.818665
H	0.647884	-2.675323	1.904514
C	-1.061907	3.37213	1.194207
C	1.53503	2.330991	1.445786
C	3.03263	0.433337	1.764093
H	2.147318	-1.474506	1.961855
C	0.025597	4.2198	1.147163
H	-2.043957	3.802737	1.071083
C	2.847645	1.804983	1.564989
C	1.321391	3.715384	1.265845
H	4.037447	0.044649	1.864934
H	-0.103223	5.284625	1.002523
C	3.984077	2.688684	1.450751
C	2.454651	4.628756	1.184855
O	5.18394	2.333164	1.490492
N	3.709646	4.018453	1.280834
O	2.389874	5.84046	1.034246
H	4.504045	4.641761	1.216944

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.779723	0.684096	0.613034

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Cartesian coordinates of pimer **19**

C	0.718432	0.807744	1.608154
C	2.113647	0.534025	1.779211
C	-0.231011	-0.194165	1.951944
C	0.22374	-1.416565	2.492777
C	0.306363	2.076985	1.100062
C	2.515786	-0.703716	2.305122
C	3.079553	1.527083	1.419174
C	-1.641557	0.060387	1.726488
C	1.56429	-1.666317	2.669208
H	-0.481148	-2.184708	2.771149
C	1.29951	3.054982	0.822946
C	-1.09434	2.337079	0.886643
C	3.928273	-1.011661	2.480502
C	4.439791	1.20719	1.553628
C	2.634444	2.794203	0.97165
C	-2.623498	-0.905948	2.008553

C	-2.046426	1.314871	1.187345
H	1.915649	-2.603481	3.080659
H	1.007979	4.039644	0.490905
C	-1.562269	3.561583	0.366113
O	4.389184	-2.046574	2.936548
N	4.79514	0.00401	2.059866
O	5.459394	1.97592	1.260413
H	3.35679	3.5715	0.76558
H	-2.346062	-1.864553	2.418535
C	-3.961935	-0.677656	1.734914
C	-3.43064	1.551151	0.928253
H	-0.869353	4.35571	0.133468
C	-2.907932	3.783556	0.12804
C	-4.377186	0.530593	1.187475
H	-4.70062	-1.442333	1.940703
C	-3.84506	2.791496	0.395531
H	-3.256224	4.726043	-0.27439
C	-5.786255	0.733796	0.843662
C	-5.263497	3.042657	0.117506
N	-6.127091	1.989038	0.414591
O	-6.648618	-0.149459	0.922429
O	-5.709497	4.085247	-0.33141
H	5.784576	-0.20054	2.138148
H	-7.090735	2.124365	0.137147
N	5.580795	3.768288	-0.599504
H	4.835913	4.363906	-0.942677
H	5.329658	2.743511	0.556013
H	5.877629	3.151559	-1.36002
H	6.366159	4.36307	-0.355882
C	-0.675505	-1.206355	-1.385057
C	-2.101096	-1.325103	-1.413763
C	-0.072235	-0.005551	-1.85216
C	-0.89759	1.049128	-2.299617
C	0.108838	-2.281876	-0.869042
C	-2.877966	-0.249842	-1.876642
C	-2.718031	-2.520811	-0.937652
C	1.37428	0.10795	-1.847938
C	-2.268306	0.935119	-2.311902
H	-0.461515	1.982247	-2.622447
C	-0.553358	-3.454677	-0.413631
C	1.542547	-2.147923	-0.810132
C	-4.328306	-0.325587	-1.846911
C	-4.116168	-2.578756	-0.896867
C	-1.917112	-3.576559	-0.441608

C	2.031471	1.237454	-2.367684
C	2.153856	-0.957631	-1.313845
H	-2.89907	1.751716	-2.638061
H	0.023072	-4.28434	-0.03399
C	2.369019	-3.151055	-0.26439
O	-5.108284	0.559047	-2.176682
N	-4.842842	-1.539503	-1.373222
O	-4.749142	-3.616462	-0.402152
H	-2.398826	-4.476897	-0.084762
H	1.464087	2.043913	-2.805994
C	3.412153	1.341659	-2.352133
C	3.576206	-0.834603	-1.280854
H	1.936031	-4.048729	0.149236
C	3.746594	-3.017711	-0.222072
C	4.190675	0.329434	-1.80336
H	3.904464	2.204952	-2.781493
C	4.358182	-1.87787	-0.732509
H	4.369402	-3.785598	0.217449
C	5.647904	0.465103	-1.783107
C	5.819047	-1.763845	-0.691795
N	6.340638	-0.588218	-1.234168
O	6.258618	1.447142	-2.212219
O	6.575985	-2.600322	-0.227324
H	-5.851776	-1.553138	-1.291591
H	7.349438	-0.505946	-1.221722
N	-7.159691	-2.996302	0.432556
H	-7.113496	-2.038624	0.789033
H	-7.946368	-3.055014	-0.205802
H	-5.737145	-3.403353	-0.141157
H	-7.362193	-3.61304	1.212914

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.75278	0.6828	0.612269

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Cartesian coordinates of pimer **20**

O	-6.818624	-2.50751	-0.241011
N	-6.452814	-0.653904	1.007155
H	-7.436322	-0.434086	0.91223
C	-0.493077	1.864856	-1.039351
C	-4.590823	-2.088261	0.482958
C	-1.906296	2.091044	-0.987316
C	0.006671	0.643362	-1.584597



C	-6.023714	-1.801835	0.380381
C	-4.091177	-3.281226	-0.028036
H	-4.786688	-4.004377	-0.436347
C	-0.922599	-0.321825	-2.055459
C	-5.656854	0.357257	1.536742
C	0.386848	2.857555	-0.523075
C	-3.715413	-1.141675	1.062427
C	-2.803706	1.085959	-1.470162
C	-2.394013	3.288605	-0.4398
C	1.428107	0.407858	-1.618133
C	-2.731569	-3.542606	0.00265
C	-2.274895	-0.114883	-1.998132
H	-0.570661	-1.263031	-2.449383
O	-6.16823	1.407834	1.895613
C	-4.220245	0.06824	1.593705
C	-0.155032	4.046787	0.011402
C	1.816363	2.614632	-0.536301
C	-2.310596	-1.396612	1.081615
C	-4.185037	1.322045	-1.349069
C	-3.827002	3.528432	-0.334713
C	-1.513494	4.260064	0.051779
C	1.983321	-0.777926	-2.142147
C	2.310601	1.396653	-1.081591
H	-2.386494	-4.485199	-0.393266
C	-1.816392	-2.614599	0.536315
H	-2.943342	-0.891399	-2.342753
C	-3.349036	1.010199	2.131187
H	0.493583	4.817657	0.397964
C	2.731528	3.542754	-0.002816
C	-1.428069	-0.407863	1.618197
O	-5.162382	0.520191	-1.692704
N	-4.621671	2.483683	-0.816974
O	-4.356217	4.526701	0.12659
H	-1.931079	5.169549	0.463263
H	1.344715	-1.545045	-2.553175
C	3.34912	-1.010138	-2.131135
C	3.715433	1.141788	-1.062461
C	-0.386894	-2.857632	0.523218
H	-3.760188	1.931546	2.525271
C	-1.983241	0.77794	2.1422
H	2.386439	4.485411	0.392936
C	4.09115	3.281444	0.027824
C	-0.006638	-0.643417	1.584668
C	4.220304	-0.068129	-1.593691

H	3.760304	-1.931475	-2.525207
C	4.59082	2.088456	-0.483094
C	0.154932	-4.046991	-0.01103
C	0.493069	-1.864919	1.039402
H	-1.344612	1.545062	2.553185
H	4.786658	4.004649	0.436042
C	0.922665	0.321702	2.055611
C	5.656918	-0.357105	-1.536703
C	6.023716	1.802083	-0.380506
H	-0.493722	-4.817966	-0.397318
C	1.513388	-4.2603	-0.051441
C	1.906282	-2.091134	0.987318
H	0.570751	1.262823	2.449758
C	2.274957	0.114758	1.998189
N	6.452837	0.654057	-1.007084
O	6.168327	-1.407669	-1.895589
O	6.818597	2.507866	0.240802
C	2.393953	-3.288755	0.439887
H	1.930933	-5.169887	-0.462741
C	2.803728	-1.086034	1.470062
H	2.943434	0.891203	2.342921
C	3.82693	-3.528634	0.334801
C	4.185044	-1.322134	1.348872
N	4.621636	-2.48377	0.816751
O	4.356116	-4.527026	-0.126275
O	5.162423	-0.520265	1.692394
H	-5.620414	2.59661	-0.683626
H	7.436363	0.434305	-0.912204
H	5.620372	-2.596723	0.683369
N	5.289248	1.83795	2.78739
H	4.54128	2.518193	2.866388
H	4.982867	0.402289	2.136769
H	5.992315	2.235238	2.161427
H	5.710039	1.73112	3.704652
N	-5.289268	-1.837967	-2.787584
H	-4.982821	-0.402335	-2.137242
H	-5.710771	-1.730996	-3.704504
H	-4.541217	-2.518032	-2.867298
H	-5.9918	-2.235467	-2.16116

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.745488	0.682296	0.611223

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Cartesian coordinates of pimer **21**

C	-0.650239	-1.857328	0.980807
C	-2.079828	-1.845981	1.041251
C	0.075641	-0.761055	1.52633
C	-0.636527	0.305182	2.119393
C	0.015691	-2.95117	0.349489
C	-2.743749	-0.75784	1.633694
C	-2.815571	-2.921904	0.459819
C	1.524093	-0.752247	1.42803
C	-2.0119	0.312227	2.169759
H	-0.10766	1.152399	2.528973
C	-0.764222	-4.002181	-0.208841
C	1.453142	-2.95385	0.268484
C	-4.195725	-0.699211	1.638179
C	-4.213353	-2.854664	0.461787
C	-2.131253	-3.992707	-0.162802
C	2.297171	0.317085	1.915864
C	2.185005	-1.846238	0.798249
H	-2.55434	1.143547	2.602073
H	-0.27883	-4.835098	-0.693193
C	2.166684	-4.005997	-0.341425
O	-4.889675	0.210417	2.076656
N	-4.8292	-1.807025	1.057872
O	-4.943294	-3.787539	-0.100707
H	-2.705955	-4.796886	-0.601661
H	1.824245	1.160469	2.395833
C	3.675451	0.341396	1.768627
C	3.605816	-1.822764	0.664095
H	1.643723	-4.862954	-0.736566
C	3.546109	-3.978562	-0.454764
C	4.336279	-0.707088	1.139712
H	4.253008	1.182833	2.130857
C	4.270492	-2.897902	0.032996
H	4.084258	-4.789052	-0.928649
C	5.780732	-0.633108	0.91446
C	5.727216	-2.881583	-0.123242
N	6.366743	-1.7467	0.374127
O	6.46851	0.36146	1.177277
O	6.386159	-3.771134	-0.635436
H	-5.835152	-1.716937	0.991768
H	7.362284	-1.697778	0.20159
N	-7.403742	-3.075234	-0.656107
H	-8.133494	-3.115154	0.047208
H	-5.941241	-3.520293	-0.24556

H	-7.695514	-3.664402	-1.429153
H	-7.334334	-2.116018	-0.998417
C	0.650456	1.858069	-0.981013
C	2.080077	1.847219	-1.040698
C	-0.074742	0.761559	-1.526969
C	0.638084	-0.304116	-2.120236
C	-0.016198	2.951654	-0.350016
C	2.744684	0.759464	-1.633084
C	2.81514	2.923228	-0.458565
C	-1.5232	0.751922	-1.428847
C	2.013485	-0.310611	-2.170011
H	0.109726	-1.151311	-2.530517
C	0.763052	4.002755	0.209063
C	-1.453709	2.953944	-0.269994
C	4.196675	0.70126	-1.636662
C	4.212946	2.856419	-0.459626
C	2.130115	3.99367	0.163909
C	-2.295543	-0.31812	-1.91626
C	-2.184848	1.845785	-0.799604
H	2.556424	-1.141526	-2.602475
H	0.277106	4.835334	0.693442
C	-2.168005	4.00619	0.338862
O	4.891154	-0.208004	-2.075078
N	4.829464	1.809015	-1.055509
O	4.942249	3.789413	0.10348
H	2.704324	4.797859	0.603394
H	-1.822032	-1.16153	-2.395607
C	-3.673826	-0.343217	-1.769173
C	-3.605678	1.821635	-0.665845
H	-1.645618	4.863727	0.733504
C	-3.547465	3.978169	0.451656
C	-4.335367	0.705237	-1.140965
H	-4.250831	-1.185235	-2.130928
C	-4.271124	2.896794	-0.035601
H	-4.0862	4.788726	0.924761
C	-5.779794	0.630466	-0.915891
C	-5.727877	2.879733	0.120261
N	-6.366623	1.744139	-0.37656
O	-6.466722	-0.364924	-1.177809
O	-6.387508	3.769239	0.631639
H	5.835439	1.719308	-0.989227
H	-7.362177	1.694789	-0.204232
N	7.400174	3.075452	0.665306
H	7.688375	3.660568	1.442754

H	7.330355	2.114301	1.00214
H	5.939917	3.521637	0.25094
H	8.132546	3.120016	-0.035002

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.749567	0.682766	0.6117

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Cartesian coordinates of pimer **22**

O	7.788604	2.014555	-0.549034
N	7.52438	0.072489	0.581049
H	8.520523	-0.084054	0.488622
C	-0.604376	-1.18708	-1.260265
C	5.619191	1.524567	0.308772
C	0.810626	-1.387458	-1.331005
C	-1.159063	0.049776	-1.708374
C	7.042564	1.270292	0.081435
C	5.064508	2.72864	-0.108428
H	5.71272	3.470855	-0.55612
C	-0.290872	1.04437	-2.233157
C	6.802658	-0.944789	1.204891
C	-1.424647	-2.222456	-0.731712
C	4.805363	0.529083	0.898731
C	1.640946	-0.349253	-1.848044
C	1.366772	-2.598465	-0.88388
C	-2.579798	0.266779	-1.602418
C	3.708906	2.965432	0.045557
C	1.063466	0.860056	-2.300192
H	-0.691925	1.985495	-2.575325
O	7.377847	-1.95617	1.57512
C	5.362985	-0.699582	1.331299
C	-0.821802	-3.431614	-0.319265
C	-2.852866	-2.000427	-0.606983
C	3.40342	0.760261	1.042375
C	3.027041	-0.555373	-1.879049
C	2.80525	-2.808048	-0.921114
C	0.539935	-3.617079	-0.388466
C	-3.18529	1.473258	-2.010479
C	-3.403364	-0.759935	-1.042267
H	3.317946	3.912954	-0.291426
C	2.852684	2.000541	0.606804
H	1.708732	1.638485	-2.684603
C	4.548178	-1.682417	1.883975

H	-1.42737	-4.237964	0.065364
C	-3.70934	-2.965442	-0.046356
C	2.580084	-0.266386	1.603006
O	3.834344	0.367731	-2.340753
N	3.540035	-1.725474	-1.434988
O	3.405345	-3.808225	-0.556276
H	0.999431	-4.542632	-0.066712
H	-2.588752	2.273439	-2.420319
C	-4.547598	1.683276	-1.883025
C	-4.805308	-0.528641	-0.898824
C	1.424471	2.222476	0.731845
H	4.997329	-2.617468	2.191582
C	3.185858	-1.472536	2.011603
H	-3.31857	-3.91314	0.290357
C	-5.064981	-2.728609	0.107271
C	1.159296	-0.049664	1.708833
C	-5.362665	0.700276	-1.331015
H	-4.996567	2.618519	-2.190317
C	-5.619411	-1.52428	-0.309504
C	0.821439	3.431562	0.319454
C	0.604394	1.187059	1.260613
H	2.589558	-2.272534	2.422145
H	-5.713386	-3.47097	0.554444
C	0.291259	-1.044429	2.233555
C	-6.80239	0.945474	-1.205201
C	-7.042915	-1.270086	-0.082765
H	1.426857	4.237964	-0.065293
C	-0.540302	3.616908	0.388901
C	-0.810632	1.387248	1.331443
H	0.692452	-1.985543	2.575591
C	-1.063109	-0.860338	2.300577
N	-7.524454	-0.072036	-0.582102
O	-7.377369	1.957024	-1.575289
O	-7.789312	-2.014694	0.546828
C	-1.366966	2.598196	0.884404
H	-0.99994	4.542427	0.06725
C	-1.640783	0.348912	1.848504
H	-1.708259	-1.638917	2.684882
C	-2.805465	2.807634	0.921841
C	-3.026907	0.55476	1.879375
N	-3.540081	1.72485	1.435477
O	-3.405685	3.807879	0.557389
O	-3.834099	-0.368446	2.34114
H	4.543079	-1.857745	-1.407742

H	-8.520679	0.084392	-0.490347
H	-4.54314	1.85706	1.408528
N	-6.451954	0.142534	2.570388
H	-6.897417	-0.762557	2.426847
H	-4.826979	-0.116915	2.353296
H	-6.953302	0.799113	1.979072
H	-6.620981	0.41497	3.533668
N	6.452004	-0.143559	-2.571292
H	6.952996	-0.801825	-1.981558
H	6.898024	0.760911	-2.42552
H	6.620891	-0.413878	-3.535198
H	4.827182	0.115993	-2.353536

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.742575	0.682441	0.610692

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Cartesian coordinates of pimer **23**

O	7.456541	1.410601	0.984445
N	7.494852	-0.713778	0.211251
H	8.486529	-0.603094	0.041715
C	-0.543672	1.378137	-1.109478
C	5.418439	0.173639	1.03971
C	0.878748	1.47667	-1.22912
C	-1.267037	2.422678	-0.458932
C	6.842581	0.360217	0.76523
C	4.70361	1.166811	1.704064
H	5.227197	2.048245	2.05173
C	-0.549692	3.533132	0.0631
C	6.940021	-1.928683	-0.19772
C	-1.203879	0.230517	-1.631812
C	4.765691	-1.008995	0.614952
C	1.551866	2.607896	-0.680178
C	1.597127	0.453129	-1.872113
C	-2.697108	2.316278	-0.324353
C	3.343249	1.028622	1.918358
C	0.812362	3.626365	-0.03551
H	-1.078276	4.328112	0.565874
O	7.65842	-2.785607	-0.685407
C	5.49378	-2.050522	-0.002542
C	-0.440256	-0.766525	-2.278493
C	-2.63853	0.103487	-1.463043
C	3.357305	-1.143839	0.806878

C	2.949394	2.67207	-0.781805
C	3.045157	0.529366	-1.986382
C	0.926479	-0.661008	-2.396643
C	-3.471053	3.324829	0.283677
C	-3.3573	1.143815	-0.806843
H	2.825988	1.825884	2.429842
C	2.638534	-0.103488	1.463041
H	1.339522	4.477267	0.374461
C	4.840564	-3.197361	-0.436662
H	-0.919973	-1.645142	-2.681343
C	-3.343258	-1.028579	-1.918453
C	2.697122	-2.316342	0.324472
O	3.619821	3.676754	-0.280998
N	3.615982	1.680894	-1.417829
O	3.780655	-0.291411	-2.51503
H	1.510921	-1.433025	-2.880406
H	-3.004189	4.228725	0.642853
C	-4.840548	3.197273	0.436815
C	-4.765695	1.008985	-0.614958
C	1.203891	-0.230538	1.631859
H	5.425146	-3.97921	-0.903338
C	3.471074	-3.32493	-0.283485
H	-2.826	-1.825821	-2.429972
C	-4.703627	-1.166752	-1.704209
C	1.26705	-2.422732	0.459038
C	-5.493778	2.050484	0.002586
H	-5.425126	3.979096	0.903542
C	-5.418455	-0.173612	-1.039802
C	0.440273	0.766508	2.278539
C	0.543686	-1.378175	1.109561
H	3.004221	-4.228867	-0.642573
H	-5.227222	-2.048151	-2.05195
C	0.549703	-3.533183	-0.062996
C	-6.940033	1.928672	0.197697
C	-6.84261	-0.360174	-0.765383
H	0.919992	1.645129	2.681377
C	-0.926461	0.660991	2.396696
C	-0.878734	-1.476703	1.229201
H	1.078285	-4.32816	-0.565777
C	-0.812353	-3.626401	0.035592
N	-7.494875	0.713801	-0.211351
O	-7.658425	2.785585	0.685414
O	-7.456592	-1.410524	-0.984695
C	-1.597111	-0.453149	1.872176



H	-1.510903	1.433015	2.880449
C	-1.551855	-2.607923	0.68025
H	-1.339517	-4.477292	-0.374396
C	-3.045141	-0.529374	1.986434
C	-2.949387	-2.672057	0.781814
N	-3.615974	-1.680863	1.417809
O	-3.780646	0.291452	2.514995
O	-3.619827	-3.676704	0.280939
H	4.627182	1.699209	-1.450773
H	-8.486564	0.603133	-0.041879
H	-4.627177	-1.699144	1.450698
N	-6.228874	-3.703078	0.41255
H	-6.701165	-2.974341	-0.131987
H	-4.663463	-3.620266	0.37463
H	-6.648367	-3.715107	1.337001
H	-6.455301	-4.593599	-0.020781
N	6.228843	3.703207	-0.412697
H	6.648346	3.715278	-1.337142
H	6.701111	2.974428	0.131802
H	6.455287	4.593697	0.020691
H	4.66347	3.620406	-0.374756

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$E_{\text{elec}}$ (a.u.)	$ZPE$ (a.u.)	$G_{\text{corr}}$ (a.u.)	
	-2773.750635	0.682796	0.612414

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Cartesian coordinates of NH<sub>4</sub>PDI tetramers in LS and HS state

LS state

C	2.681768	-0.104257	-0.152554
C	3.821717	0.756025	-0.093688
C	2.16684	-0.488667	-1.422823
C	2.816676	-0.039175	-2.588867
C	2.074568	-0.545093	1.062004
C	4.431498	1.18062	-1.288872
C	4.315392	1.188668	1.166384
C	0.978171	-1.316971	-1.482945
C	3.932511	0.77133	-2.523663
H	2.449905	-0.330463	-3.560548
C	2.595766	-0.076787	2.291604
C	0.929209	-1.413119	1.002527
C	5.613355	2.037522	-1.255633
C	5.463519	2.060741	1.225339
C	3.677359	0.771001	2.338547
C	0.382326	-1.673661	-2.709795
C	0.393246	-1.778154	-0.270541
H	4.42809	1.127446	-3.416659
H	2.125186	-0.359993	3.220449
C	0.296212	-1.89656	2.172826
O	6.251392	2.410755	-2.220639
N	6.009682	2.434892	0.03263
O	5.990576	2.496917	2.278184
H	4.020135	1.163189	3.287412
H	0.803858	-1.324024	-3.639116
C	-0.749758	-2.46101	-2.758177
C	-0.768641	-2.608283	-0.330243
H	0.676683	-1.622725	3.145001
C	-0.824867	-2.688935	2.107587
C	-1.326617	-2.936095	-1.579491
H	-1.20545	-2.741581	-3.69803
C	-1.362092	-3.077394	0.872891
H	-1.339324	-2.984551	3.013771
C	-2.543548	-3.738955	-1.66091
C	-2.542171	-3.896392	0.817639
N	-3.05385	-4.153944	-0.418952
O	-3.118356	-4.063405	-2.683286
O	-3.110164	-4.400618	1.826555
H	6.841689	3.008449	0.073557
H	-3.892414	-4.717844	-0.458089
N	6.662967	1.156451	4.37149

H	6.000682	0.459739	4.699861
H	6.249442	1.709319	3.527256
H	7.544767	0.677592	3.990302
H	6.903845	1.793891	5.125862
C	3.446154	-3.703933	-0.47583
C	2.300288	-4.5151	-0.748367
C	3.864775	-3.516283	0.876851
C	3.152344	-4.178317	1.90508
C	4.145467	-3.10116	-1.559811
C	1.608033	-5.144945	0.319776
C	1.87087	-4.683794	-2.077741
C	5.001865	-2.678514	1.151186
C	2.064283	-4.97358	1.630693
H	3.461344	-4.071039	2.933393
C	3.680726	-3.310393	-2.872534
C	5.30696	-2.276808	-1.284808
C	0.453483	-5.964544	0.042007
C	0.681549	-5.473432	-2.381307
C	2.561863	-4.077863	-3.124427
C	5.476016	-2.467525	2.467976
C	5.698359	-2.061566	0.066132
H	1.555675	-5.493262	2.43235
H	4.190513	-2.856794	-3.707951
C	6.05316	-1.673393	-2.31666
O	-0.211677	-6.592611	0.899413
N	0.074965	-6.06483	-1.266918
O	0.208721	-5.64433	-3.490719
H	2.195897	-4.228238	-4.131331
H	5.001355	-2.966354	3.298768
C	6.562593	-1.664603	2.722536
C	6.820208	-1.218697	0.339002
H	5.781454	-1.833133	-3.348104
C	7.137782	-0.864173	-2.046466
C	7.224757	-0.999034	1.682463
H	6.952147	-1.574964	3.72929
C	7.52331	-0.624809	-0.728247
H	7.697774	-0.386388	-2.83868
C	8.346295	-0.138884	1.964719
C	8.683465	0.22618	-0.469958
N	8.992351	0.396296	0.887552
O	8.743553	0.155807	3.11898
O	9.366779	0.777664	-1.312689
H	-0.747836	-6.619668	-1.461142
H	9.785888	0.990652	1.084653

N	-1.360275	-5.801967	3.102122
H	-2.13511	-5.155882	2.672314
H	-0.802143	-5.301757	3.787135
H	-0.754639	-6.109897	2.272659
H	-1.783268	-6.620482	3.532351
C	-3.446779	3.703687	-0.475932
C	-2.300951	4.514905	-0.748459
C	-4.146164	3.101033	-1.559925
C	-3.68161	3.310559	-2.872667
C	-3.865283	3.515861	0.876758
C	-1.8717	4.683905	-2.077872
C	-1.608512	5.144484	0.319725
C	-5.307518	2.2765	-1.284937
C	-2.562858	4.078197	-3.124581
H	-4.191457	2.857078	-3.70811
C	-3.152633	4.177554	1.90503
C	-5.002427	2.678156	1.151051
C	-0.68253	5.473793	-2.381429
C	-0.453918	5.964156	0.042011
C	-2.06453	4.972806	1.630673
C	-6.053652	1.673047	-2.316789
C	-5.698838	2.061142	0.065988
H	-2.197079	4.228855	-4.131517
H	-3.461365	4.069941	2.933393
C	-5.476658	2.467237	2.467841
O	-0.210061	5.645244	-3.490929
N	-0.075625	6.064745	-1.266985
O	0.211257	6.592016	0.899476
H	-1.555575	5.492113	2.432369
H	-5.782063	1.832985	-3.348227
C	-7.138053	0.863561	-2.046606
C	-6.820549	1.218098	0.338846
H	-5.002181	2.96628	3.298616
C	-6.563131	1.664164	2.722404
C	-7.523481	0.624038	-0.728396
H	-7.697954	0.385683	-2.838812
C	-7.225129	0.99843	1.682302
H	-6.952721	1.574503	3.729159
C	-8.683332	-0.227348	-0.470114
C	-8.346512	0.13812	1.964544
N	-8.992311	-0.397375	0.887384
O	-9.366283	-0.779283	-1.31283
O	-8.743886	-0.156399	3.118843
H	0.74708	6.619723	-1.461245

H	-9.785661	-0.99196	1.084501
N	1.361552	5.802291	3.102431
H	0.804006	5.302492	3.78823
H	0.755293	6.109521	2.273514
H	2.136468	5.155932	2.67224
H	1.784593	6.621257	3.531755
C	-2.681447	0.104814	-0.152224
C	-3.821279	-0.755594	-0.093394
C	-2.074449	0.545916	1.062323
C	-2.595989	0.078079	2.29194
C	-2.166433	0.489112	-1.422483
C	-4.31511	-1.188033	1.166669
C	-4.430764	-1.180531	-1.288588
C	-0.92895	1.413751	1.002831
C	-3.677558	-0.769768	2.338873
H	-2.12589	0.361903	3.220842
C	-2.816049	0.039364	-2.588537
C	-0.977834	1.317484	-1.482624
C	-5.463171	-2.060239	1.225591
C	-5.612428	-2.037678	-1.255384
C	-3.931713	-0.77136	-2.523351
C	-0.295853	1.897083	2.173144
C	-0.392889	1.778642	-0.27023
H	-4.020728	-1.161413	3.28783
H	-2.449208	0.330627	-3.560196
C	-0.382011	1.674191	-2.70949
O	-5.990398	-2.496201	2.278413
N	-6.008969	-2.434816	0.032867
O	-6.250062	-2.411392	-2.22046
H	-4.427112	-1.127686	-3.416354
H	-0.676329	1.623231	3.145312
C	0.825354	2.689251	2.10797
C	0.769116	2.608658	-0.329914
H	-0.80365	1.32471	-3.638821
C	0.750107	2.461452	-2.757894
C	1.362659	3.07769	0.873238
H	1.339777	2.98481	3.01418
C	1.327088	2.936474	-1.579189
H	1.205777	2.742098	-3.697746
C	2.542664	3.896744	0.817908
C	2.544058	3.739268	-1.660648
N	3.054325	4.15433	-0.418674
O	3.110594	4.40127	1.826794
O	3.119043	4.063484	-2.683018

H	-6.840848	-3.008548	0.073712
H	3.892936	4.718181	-0.45783
N	-6.663799	-1.156836	4.372128
H	-7.545426	-0.678031	3.990327
H	-6.002175	-0.460158	4.701916
H	-6.249208	-1.708796	3.527891
H	-6.905255	-1.79509	5.125618

HS state

C	-2.438077	0.404859	0.376262
C	-3.560544	-0.407421	0.723752
C	-1.643129	0.979682	1.414001
C	-2.029879	0.77266	2.76036
C	-2.13172	0.61931	-0.998442
C	-3.87393	-0.627533	2.089235
C	-4.339502	-0.98976	-0.297318
C	-0.47759	1.744728	1.064902
C	-3.112093	-0.011026	3.088074
H	-1.477312	1.246281	3.557558
C	-2.956971	0.035864	-1.978233
C	-0.972895	1.41958	-1.349008
C	-4.996933	-1.454526	2.445908
C	-5.470275	-1.846018	0.037102
C	-4.034407	-0.757284	-1.637808
C	0.40524	2.251218	2.048876
C	-0.166399	1.965158	-0.311689
H	-3.395157	-0.168512	4.120653
H	-2.752757	0.189552	-3.026324
C	-0.599598	1.64212	-2.688521
O	-5.356422	-1.692598	3.623427
N	-5.714033	-1.987981	1.405424
O	-6.189307	-2.428689	-0.761723
H	-4.654032	-1.214959	-2.397864
H	0.237132	2.027009	3.09046
C	1.522266	2.975927	1.713139
C	0.998273	2.72033	-0.65618
H	-1.195478	1.235683	-3.490903
C	0.533902	2.357978	-3.012227
C	1.82584	3.253157	0.371377
H	2.213717	3.28216	2.48672
C	1.336872	2.898864	-2.009232
H	0.83135	2.509547	-4.041305
C	3.017017	3.964995	0.016988

C	2.583113	3.563113	-2.383083
N	3.315511	4.076026	-1.303904
O	3.821006	4.492302	0.848814
O	3.015842	3.676417	-3.51499
H	-6.447195	-2.64511	1.629857
H	4.212769	4.483028	-1.535605
N	-8.009584	-1.145747	3.88418
H	-8.572797	-1.950724	4.146596
H	-6.993509	-1.419143	3.853149
H	-8.354502	-0.771738	2.832856
H	-8.137849	-0.424291	4.588608
C	-3.241072	3.996328	-0.352802
C	-2.052581	4.786536	-0.297448
C	-3.769328	3.621937	-1.621451
C	-3.114967	4.061061	-2.78677
C	-3.8619	3.581631	0.864875
C	-1.417035	5.174953	-1.49578
C	-1.510997	5.152733	0.959385
C	-4.943317	2.77046	-1.676651
C	-1.958303	4.814707	-2.725387
H	-3.497829	3.794348	-3.759508
C	-3.287055	3.984188	2.0921
C	-5.028337	2.742068	0.807503
C	-0.173957	5.939855	-1.460084
C	-0.283635	5.9112	1.027185
C	-2.141436	4.746326	2.137372
C	-5.498072	2.347738	-2.901449
C	-5.534849	2.325071	-0.461754
H	-1.442488	5.127219	-3.62355
H	-3.728095	3.669462	3.024822
C	-5.692849	2.304397	1.979079
O	0.4672	6.309456	-2.428668
N	0.282755	6.254747	-0.174119
O	0.263017	6.254903	2.094987
H	-1.700419	5.035573	3.081606
H	-5.074919	2.684664	-3.834949
C	-6.576837	1.49216	-2.944888
C	-6.652564	1.433375	-0.515309
H	-5.357822	2.640825	2.94756
C	-6.757369	1.441547	1.923087
C	-7.152571	1.021365	-1.763602
H	-6.996889	1.160369	-3.884846
C	-7.240203	0.96186	0.693643
H	-7.248086	1.143212	2.839419

C	-8.28127	0.10051	-1.844474
C	-8.311001	0.017649	0.629353
N	-8.770842	-0.323031	-0.602622
O	-8.805818	-0.301702	-2.867363
O	-8.884559	-0.529011	1.625152
H	1.132701	6.800151	-0.152315
H	-9.50885	-1.012373	-0.638659
N	2.864478	5.885538	2.722756
H	3.293109	5.196451	1.919869
H	3.409087	6.742761	2.769817
H	1.866035	6.107539	2.471946
H	2.882326	5.435163	3.633874
C	3.241966	-3.996904	-0.351163
C	2.053474	-4.78712	-0.295933
C	3.861723	-3.580791	0.866586
C	3.285989	-3.982196	2.093777
C	3.771251	-3.623865	-1.619777
C	1.510888	-5.151998	0.960859
C	1.418974	-5.176912	-1.494353
C	5.027986	-2.740967	0.809265
C	2.140413	-4.744395	2.138929
H	3.726257	-3.666459	3.026522
C	3.118007	-4.064493	-2.785171
C	4.945072	-2.772143	-1.674934
C	0.283559	-5.910454	1.028443
C	0.175916	-5.941833	-1.458861
C	1.961366	-4.818169	-2.723916
C	5.691268	-2.301642	1.980915
C	5.535454	-2.325232	-0.46003
H	1.698682	-5.032695	3.083113
H	3.501801	-3.799012	-3.757881
C	5.500636	-2.350483	-2.899727
O	-0.263685	-6.253368	2.096253
N	-0.282044	-6.255028	-0.172894
O	-0.464242	-6.312839	-2.427556
H	1.446429	-5.131877	-3.622165
H	5.355425	-2.63695	2.949502
C	6.755475	-1.438395	1.924861
C	6.652876	-1.433167	-0.513625
H	5.078324	-2.688491	-3.833217
C	6.579115	-1.494531	-2.943198
C	7.239262	-0.960018	0.695295
H	7.245099	-1.138614	2.841308
C	7.153735	-1.022295	-1.761952



H	6.999767	-1.163538	-3.883169
C	8.3097	-0.01538	0.630851
C	8.28209	-0.101019	-1.842892
N	8.770482	0.324059	-0.6011
O	8.88212	0.532705	1.626507
O	8.807232	0.300387	-2.865787
H	-1.131911	-6.800558	-0.151228
H	9.508104	1.013807	-0.637287
N	-2.864036	-5.885573	2.725319
H	-3.408623	-6.742804	2.77251
H	-1.865687	-6.107288	2.473124
H	-3.293359	-5.196426	1.924003
H	-2.880753	-5.435671	3.636696
C	2.437653	-0.404856	0.377652
C	3.559789	0.408122	0.724616
C	2.132089	-0.621276	-0.996923
C	2.95782	-0.039111	-1.977091
C	1.642296	-0.978459	1.415762
C	4.339169	0.989204	-0.296844
C	3.872407	0.630174	2.089978
C	0.973503	-1.422096	-1.347003
C	4.034873	0.754771	-1.637189
H	2.754445	-0.194591	-3.025085
C	2.028353	-0.769583	2.762041
C	0.477008	-1.744111	1.067097
C	5.469685	1.846005	0.036981
C	4.994985	1.457948	2.446096
C	3.110199	0.014816	3.089261
C	0.600831	-1.646352	-2.686402
C	0.16647	-1.966286	-0.309357
H	4.654883	1.211441	-2.397537
H	1.475432	-1.242171	3.559608
C	-0.406184	-2.24949	2.051307
O	6.189242	2.42747	-0.762257
N	5.712508	1.990123	1.405249
O	5.353808	1.697785	3.623484
H	3.392662	0.173797	4.121778
H	1.19712	-1.240998	-3.489027
C	-0.532639	-2.362449	-3.009722
C	-0.998141	-2.721729	-0.653432
H	-0.238439	-2.024143	3.092704
C	-1.523188	-2.974438	1.715941
C	-1.336187	-2.901877	-2.006423
H	-0.829633	-2.515261	-4.038745

C	-1.826288	-3.253056	0.374394
H	-2.21502	-3.27979	2.489542
C	-2.582575	-3.566047	-2.379991
C	-3.01777	-3.964751	0.020431
N	-3.315644	-4.077397	-1.300519
O	-3.014904	-3.680435	-3.511939
O	-3.822231	-4.490451	0.852657
H	6.445539	2.647585	1.629134
H	-4.213202	-4.483836	-1.532074
N	8.006929	1.151002	3.885003
H	8.351726	0.776195	2.833954
H	8.570374	1.956008	4.146835
H	6.990916	1.424589	3.85386
H	8.135075	0.429978	4.589897