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

Supporting Information

A Combined Theoretical and Experimental Study of Small Anthracene-Water Clusters

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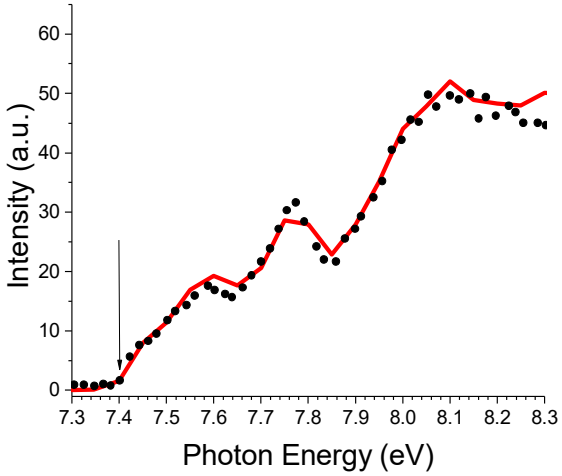

Figure S1: Experimental photoionization efficiency curve of anthracene (red solid line), and previous experimental photoionization efficiency values (black dots).[1] The arrow shows the onset of ionization which is 7.4 eV.

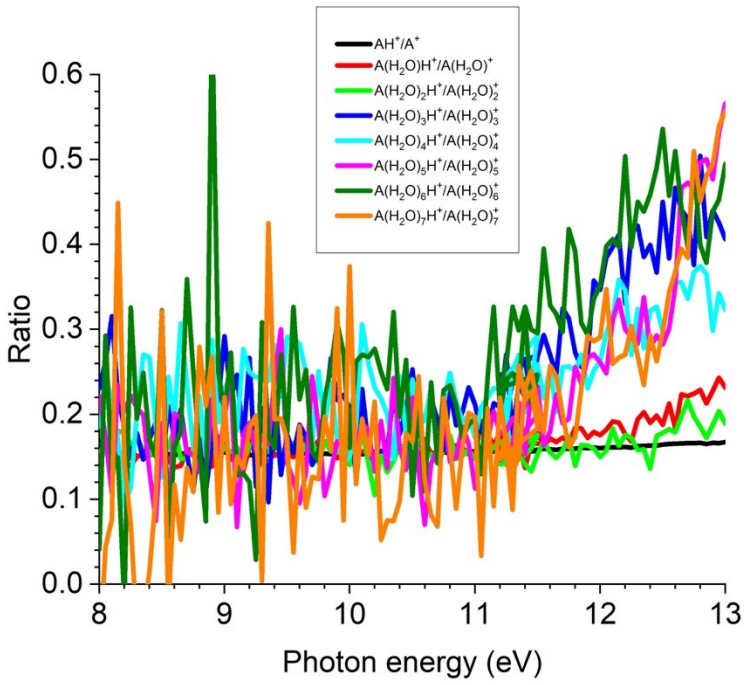

Figure S2: The intensity ratios of AH^+/A, and $A(H_2O)_nH^+/A(H2O)_n^+$ for n=1 to 7 at different photon energies. The flat baseline below 11.2 eV represents the 15% contribution of ^{13}C in anthracene.

Method benchmark

For the calculations reported in the manuscript, we have chosen to use ωB97X-V functional.[2] The validity of this functional was recently assessed in naphthalene water clusters.[3] To further check the functional validity for the dimer structures, we have compared binding energies (BE) obtained with ωB97X-V functional, to those obtained from restricted MP2[4] and CCSD(T)[5] with MP2 geometries. All calculations were performed using the cc-pVDZ basis set.[6] CCSD(T) calculations employed the RI approximation for the treatment of the two-electron integrals.[7] The results of our benchmark are presented in TableS1. There is a very good agreement for between BE calculated in ωB97X-V and those calculated using CCSD(T) in the case of the not covalently bonded isomers (B and C). For the covalently-bonded structures CCSD(T) BEs are lower than those obtained using both ωB97X-V and MP2 methods. However, the general trend in stability, which is important for the results presented in this manuscript does not change.

Table TS1: Binding energies calculated with different methods using a cc-pVDZ basis set.

Structure	ωB97X-V	MP2	CCSD(T)
A	-22.9	-22.3	-18.4
B	-12.5	-18.0	-11.8
C	-12.3	-18.8	-11.3
D	-7.1	-7.4	-4.9

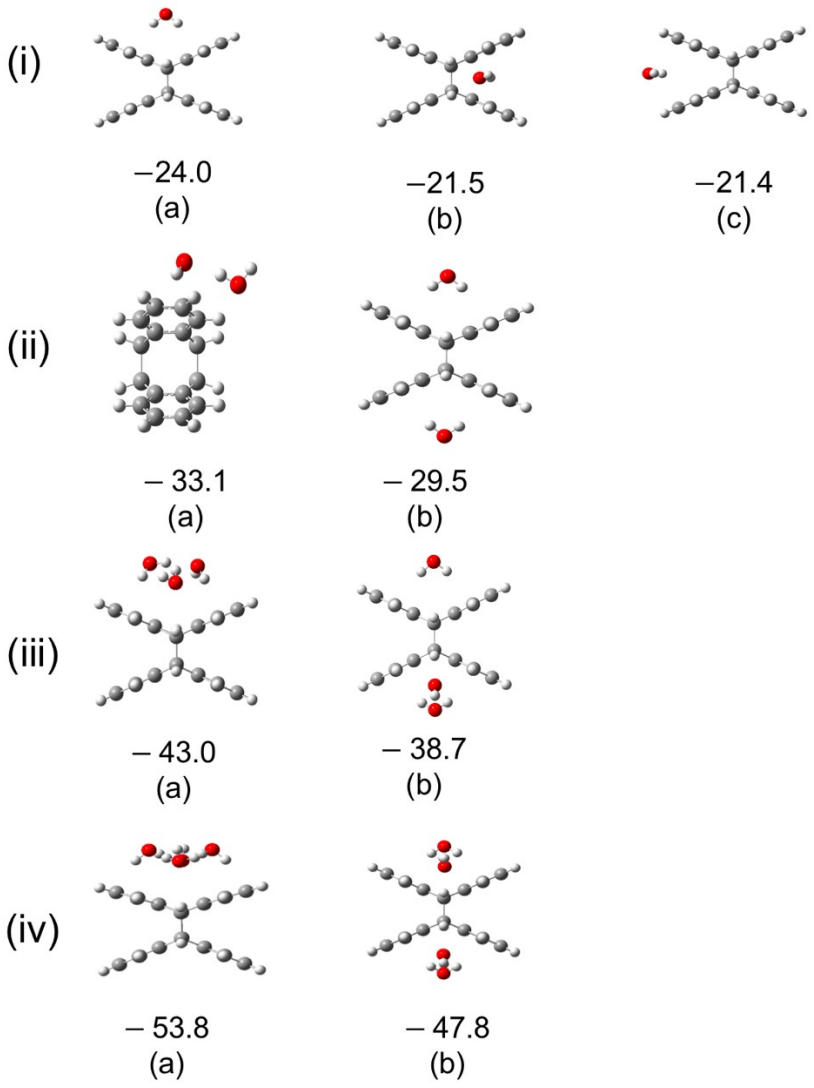

Figure S3: Neutral clusters of two anthracene molecules with one (Panel (i)), two (Panel(ii)), three (Panel(iii)) and four (Panel (iv)) water molecules, and their BEs calculated via: $E_{BE} = E_{complex} - E_{water} - 2 \times E_{anthracene}$.

Table TS2: Experimental and calculated ionization energies (IE) of anthracene-water (A_2W_n) bonded clusters in eV. A_2W_n-cluster nomenclature (a to c) follows the indexing utilized in Figure S2. We observe that these bonded systems all exhibit values of IEs significantly higher than the experimental values, and in fact were not expected to form under the experimental conditions.

species	**experimental**	**calculated**		
	IE (eV)	a	b	c
A_2W	7.2	7.7	8.0	7.9
A_2W_2	7.2	7.9	8.2	-
A_2W_3	7.3	7.9	7.2	-
A_2W_4	7.3	7.8	7.0	-

Table TS3: Calculated ionization energies for clusters of anthracene with water using EOM-IP-CCSD) with the cc-pVDZ basis set.

species	A	AW		AW_2		AW_3			A_2		A_2W	
isomer		top	side	top	side	top	side	split	sandwich	cross	top	inside
HOMO	7.4	7.7	7.5	7.8	7.5	7.6	7.3	7.5	6.9	7.3	7.1	7.2
	8.5	8.8	8.7	8.9	8.6	8.8	8.4	8.7	7.5	7.3	7.7	7.6
	9.3	9.6	9.4	9.7	9.4	9.5	9.2	9.4	8.1	8.4	8.3	8.6
	10.4	10.7	10.5	10.7	10.5	10.6	10.3	10.4	8.7	8.4	8.9	8.7
	10.7	10.9	10.7	10.9	10.8	10.9	10.5	10.7	8.7	8.8	8.9	9.1
	11.3	11.5	11.3	11.0	11.3	11.4	11.1	11.0	9.3	9.4	9.5	9.4
	11.5	11.6	11.6	11.6	11.5	11.5	11.3	11.1	9.8	10.1	10.0	10.2
	12.3	11.7	11.9	11.8	11.5	11.6	11.7	11.3	10.0	10.1	10.2	10.4
	11.9	12.1	12.4	11.9	12.0	11.7	11.8	11.4	10.5	10.3	10.5	10.5
	12.9	12.6	12.6	12.3	12.2	11.9	12.0	11.9	10.7	10.5	10.8	10.7
				12.7	12.5	12.1	12.2	12.0	11.0	11.0	10.9	10.8
				13.0	13.0	12.6	12.3	12.4	11.0	11.1	11.1	11.2
						13.1	12.8	12.9	11.7	11.3	11.2	11.3
						13.2	13.0	12.9	11.2	11.3	11.3	11.4
									11.2	11.7	11.5	11.4
									11.6	12.1	11.7	11.7
									11.6	11.7	11.8	11.8
									12.3	12.1	11.8	12.1
									12.6	12.6	12.5	12.4
									12.6	12.7	12.6	12.8
									12.6	12.7	12.7	12.9
									12.8	12.9	12.8	13.0
									12.8	12.9	12.9	13.1

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Cartesian coordinates of all structures in this manuscript, organized in the following order:

Section 1: NEUTRAL STRUCTURES
1.i) Neutral Anthracene monomer
1.ii) Neutral Anthracene plus water clusters in the "on-top" configuration
1.iii) Neutral Anthracene plus water clusters in the "side" configuration

1.iv) Neutral Anthracene dimers
1.v) Neutral Anthracene dimer plus water clusters
- Not Bonded Anthracenes: Anthracene not bonded structures (corresponding to structures presented on the manuscript in Figures 4 and 5)
- Bonded Anthracenes Structures: corresponding to the structures presented here in the SI, Figure S3)

Section 2: IONIZED STRUCTURES
2.i) Ionized Anthracene monomer
2.ii) Ionized Anthracene plus water clusters in the "on-top" configuration
2.iii) Ionized Neutral Anthracene plus water clusters in the "side" configuration

2.iv) Ionized Anthracene dimers
2.v) Ionized Anthracene dimer plus water clusters

Section 1: NEUTRAL STRUCTURES

1) <u>Neutral Anthracene Monomer</u>

1.i)

Ant

C	-2.433741	1.419304	0.000000
C	-3.623253	0.765511	0.000000
C	-3.664362	-0.663251	0.000000
C	-2.514556	-1.384668	0.000000
C	-1.196891	0.695546	0.000000
C	0.038275	1.341804	0.000000
C	-1.238090	-0.733479	0.000000
C	-0.041902	-1.449282	0.000000
C	1.234345	0.626150	0.000000
C	2.510792	1.277438	0.000000

C	1.193071	-0.803040	0.000000
C	2.430019	-1.526578	0.000000
C	3.619492	-0.872636	0.000000
C	3.660694	0.556117	0.000000
H	-2.398581	2.504607	0.000000
H	-4.553397	1.323640	0.000000
H	-4.624996	-1.167183	0.000000
H	-2.542348	-2.470141	0.000000
H	0.069257	2.428376	0.000000
H	-0.072727	-2.535825	0.000000
H	2.538164	2.362924	0.000000
H	2.395184	-2.611851	0.000000
H	4.549468	-1.431095	0.000000
H	4.621283	1.060072	0.000000

1.ii) “on- top” isomers

AntW

A

0 1

O	0.000000	-0.000001	-3.003148
C	-0.714849	-3.643558	0.306396
C	0.714849	-3.643558	0.306396
C	1.403413	-2.473810	0.319475
C	0.715368	-1.216327	0.332540
C	-1.403413	-2.473810	0.319475
C	-0.715368	-1.216327	0.332540
C	1.397197	0.000000	0.334366
C	0.715368	1.216327	0.332540
C	-1.397197	0.000000	0.334366
C	-0.715368	1.216327	0.332540
C	1.403413	2.473810	0.319475
C	0.714848	3.643559	0.306397
C	-0.714848	3.643559	0.306397
C	-1.403413	2.473810	0.319475
H	0.000000	-0.757863	-2.410686
H	0.000000	0.757862	-2.410688
H	-1.246427	-4.589064	0.294424
H	1.246427	-4.589064	0.294424
H	2.489117	-2.469753	0.317467
H	-2.489117	-2.469753	0.317467
H	2.484037	-0.000000	0.327825
H	-2.484037	-0.000000	0.327825
H	2.489117	2.469753	0.317467
H	1.246427	4.589064	0.294425
H	-1.246427	4.589064	0.294425
H	-2.489117	2.469753	0.317467

AntW2

B

0 1

O	1.629455	0.815180	2.888091
O	-1.252801	1.342926	3.042997
C	-3.170155	2.307771	-0.592486
C	-4.367161	1.672320	-0.521455
C	-4.427507	0.253233	-0.362581
C	-3.288568	-0.479924	-0.280028
C	-1.943392	1.571427	-0.509294
C	-0.699240	2.199411	-0.566740
C	-2.003996	0.151029	-0.349261
C	-0.817651	-0.575348	-0.253896
C	0.485834	1.472692	-0.471497
C	1.771266	2.105566	-0.519017
C	0.424575	0.053123	-0.311455
C	1.652498	-0.679730	-0.202138
C	2.852673	-0.042606	-0.250662
C	2.913096	1.377602	-0.413801
H	1.956477	1.717113	2.826072
H	1.902414	0.396955	2.062769
H	-3.120580	3.385982	-0.708281
H	-5.289815	2.239309	-0.581251
H	-5.394930	-0.233529	-0.304075
H	-3.330350	-1.557267	-0.153950
H	-0.654186	3.279135	-0.681242
H	-0.863417	-1.653318	-0.124573
H	1.812502	3.183522	-0.643432
H	1.603813	-1.757637	-0.080550
H	3.774522	-0.608574	-0.169023

H	3.880245	1.867056	-0.454304
H	-1.566357	1.334925	2.134715
H	-0.325148	1.068986	2.989786

AntW3

C

0 1

O	-1.064514	-0.680671	2.600040
O	1.751712	-0.689969	2.666646
O	0.420130	1.704262	3.222693
C	-3.060987	1.833931	0.009263
C	-4.246882	1.228779	-0.253917
C	-4.281430	-0.096508	-0.789209
C	-3.129616	-0.768882	-1.041038
C	-1.820568	1.160636	-0.241987
C	-0.589985	1.754272	0.032269
C	-1.855061	-0.167537	-0.775265
C	-0.655390	-0.840933	-1.005452
C	0.608662	1.083544	-0.204911
C	1.878234	1.683425	0.078781
C	0.575567	-0.245032	-0.731360
C	1.816631	-0.927569	-0.951214
C	3.002074	-0.323585	-0.672007
C	3.033777	1.007663	-0.149601
H	-1.510329	-0.680252	1.747264
H	-0.888853	0.253946	2.799217
H	0.831910	-0.992641	2.558609
H	2.138647	-0.726116	1.785592
H	-3.029301	2.839031	0.418401
H	-5.179506	1.746598	-0.057804
H	-5.239770	-0.562530	-0.991600
H	-3.153199	-1.776028	-1.446076
H	-0.561954	2.752719	0.458698
H	-0.680641	-1.851663	-1.404575
H	1.893070	2.686088	0.493710
H	1.790513	-1.938283	-1.347249
H	3.935237	-0.849298	-0.844741
H	3.990186	1.469320	0.070572
H	0.518912	1.961857	4.142543
H	1.089649	1.007580	3.073393

AntW4

D

0 1

O	-1.297867	1.742449	-0.340615
O	-3.376982	-0.013620	-0.667969
O	-1.640963	-2.157497	-0.357833
O	0.444259	-0.398063	-0.074447
C	-3.460674	1.105509	-3.984030
C	-4.590071	0.356104	-4.082006
C	-4.519962	-1.071667	-4.022036
C	-3.323016	-1.695223	-3.867478
C	-0.875449	-1.557972	-3.565887
C	-2.109441	-0.941114	-3.758367
C	-2.179380	0.485872	-3.814472
C	-1.013677	1.233681	-3.665427
C	1.417353	1.373851	-3.249824
C	0.218147	0.617430	-3.457549
C	0.289578	-0.809875	-3.413240
C	1.560024	-1.427758	-3.169056
C	2.674542	-0.675272	-2.972274
C	2.601560	0.752846	-3.012675
H	-5.555036	0.836370	-4.204423
H	-3.510468	2.189477	-4.021241
H	-5.433092	-1.652155	-4.098366
H	-3.265047	-2.777724	-3.811242
H	-0.826486	-2.641165	-3.501712
H	-1.070262	2.318381	-3.679620
H	1.355153	2.457361	-3.273044
H	1.609866	-2.511793	-3.132682
H	3.629433	-1.153631	-2.781873
H	3.501390	1.335677	-2.848087
H	-1.474859	2.248785	0.455921
H	-2.104502	1.201016	-0.492754
H	-3.796865	-0.035244	-1.533958
H	-2.877200	-0.852198	-0.591973
H	-1.709195	-2.652145	0.462411
H	-0.828759	-1.610287	-0.267899
H	1.094191	-0.405082	-0.784682

H	-0.053001	0.440164	-0.172055

1.iii) side isomers

AntW1

E
0 1

O	0.092771	-4.660971	-0.346066
C	4.850239	0.813144	-0.513417
C	4.849628	-0.616252	-0.515167
C	3.678422	-1.302682	-0.500359
C	3.680411	1.501893	-0.497007
C	-1.262847	-1.307270	-0.434299
C	-2.433640	-0.619577	-0.418075
C	-2.435747	0.809967	-0.416449
C	-1.267309	1.501224	-0.431104
C	1.206823	1.497780	-0.463989
C	-0.008992	0.815664	-0.448574
C	-0.008087	-0.613998	-0.450147
C	1.206792	-1.298545	-0.467132
C	2.421514	-0.614356	-0.482650
C	2.422451	0.815523	-0.481008
H	3.677923	2.587836	-0.495770
H	5.796174	1.344267	-0.525490
H	5.795083	-1.148158	-0.528655
H	3.671429	-2.388559	-0.501890
H	0.072174	-5.146674	0.482881
H	0.062187	-5.332472	-1.032726
H	-1.247465	-2.392798	-0.435583
H	-3.379281	-1.151451	-0.406349
H	-3.382390	1.340028	-0.403393
H	-1.266344	2.587174	-0.429934
H	1.207142	2.584872	-0.462785
H	1.198977	-2.385140	-0.467568

AntW2

F
0 1

O	-0.003296	-3.785274	-2.043375
O	0.551090	-4.883957	0.554809
C	4.826659	0.398083	-0.820125
C	4.928251	-0.763935	0.006461
C	3.811435	-1.423484	0.406460
C	3.612860	0.856597	-1.218905
C	-1.110163	-1.870196	0.394529
C	-2.323896	-1.437637	-0.038365
C	-2.427574	-0.282779	-0.876206
C	-1.314143	0.395374	-1.254956
C	1.149427	0.631314	-1.223219
C	-0.012782	-0.032491	-0.831918
C	0.090122	-1.185000	0.008377
C	1.349172	-1.631902	0.410019
C	2.510231	-0.970926	0.010419
C	2.408872	0.188861	-0.820733
H	-0.722455	-3.211212	-1.753271
H	0.742560	-3.187268	-2.159260
H	3.532990	1.738437	-1.847435
H	5.731378	0.911759	-1.127462
H	5.908381	-1.114242	0.311877
H	3.881061	-2.307041	1.033487
H	0.515141	-5.841533	0.605755
H	0.385040	-4.664851	-0.377076
H	-1.018974	-2.750008	1.024366
H	-3.226298	-1.963505	0.255448
H	-3.406614	0.047855	-1.206225
H	-1.390245	1.272773	-1.890211
H	1.071959	1.509504	-1.859143
H	1.421518	-2.524002	1.025994

AntW3

G
0 1

O	-0.712881	-4.179120	-2.514281
O	1.724936	-4.991887	-1.331853
O	0.783981	-5.302379	1.305794

C	4.669955	-0.203399	-1.096252
C	4.823059	-1.156474	-0.041916
C	3.739892	-1.793947	0.471380
C	3.441267	0.075265	-1.601933
C	-1.127867	-2.623934	0.439100
C	-2.356738	-2.375329	-0.088985
C	-2.516095	-1.411678	-1.135206
C	-1.440881	-0.739251	-1.622851
C	0.998957	-0.320664	-1.599521
C	-0.126231	-0.976776	-1.101193
C	0.029277	-1.928485	-0.045764
C	1.299333	-2.179115	0.471601
C	2.424587	-1.528696	-0.033978
C	2.272207	-0.579022	-1.093137
H	-0.711636	-3.428018	-3.114632
H	-1.188421	-3.864334	-1.734012
H	0.932639	-4.733498	-1.837179
H	2.267300	-4.198123	-1.295398
H	3.323619	0.798644	-2.403165
H	5.547843	0.297030	-1.490788
H	5.814224	-1.364680	0.346382
H	3.847693	-2.517529	1.273806
H	0.890510	-6.207927	1.604598
H	1.121923	-5.289887	0.390179
H	-0.988528	-3.366847	1.218273
H	-3.227268	-2.906126	0.281861
H	-3.505786	-1.223502	-1.537772
H	-1.560052	-0.007266	-2.416457
H	0.882258	0.404068	-2.401353
H	1.409856	-2.915612	1.262391

AntW4

H
0 1

O	-1.234507	-5.136594	-0.987826
O	0.419040	-4.635359	-3.115227
O	2.618036	-5.017825	-1.467658
O	0.965097	-5.568105	0.648349
C	4.152962	-1.672513	-1.688425
C	4.378457	-2.021511	-0.319420
C	3.330796	-2.192388	0.528497
C	2.888374	-1.505849	-2.156625
C	-1.546965	-2.393889	1.280713
C	-2.811665	-2.310615	0.790932
C	-3.037239	-1.949208	-0.574797
C	-1.989614	-1.686684	-1.398982
C	0.450168	-1.550644	-1.761308
C	-0.640462	-1.770144	-0.923102
C	-0.415039	-2.128315	0.442746
C	0.891236	-2.245700	0.912107
C	1.981757	-2.031903	0.072375
C	1.756468	-1.679694	-1.294951
H	-1.774428	-4.413265	-0.653429
H	-0.550765	-5.297225	-0.305286
H	-0.258627	-4.766491	-2.414971
H	0.246947	-5.317820	-3.768592
H	1.932771	-4.845327	-2.145924
H	3.147174	-4.215150	-1.419127
H	2.711888	-1.248758	-3.196507
H	5.002175	-1.544811	-2.351186
H	5.395305	-2.152055	0.035057
H	3.496863	-2.465884	1.565934
H	1.131912	-6.479527	0.900736
H	1.640023	-5.358786	-0.035760
H	-1.370344	-2.674605	2.314449
H	-3.660815	-2.520226	1.432583
H	-4.054086	-1.890138	-0.947908
H	-2.156119	-1.420794	-2.438347
H	0.278820	-1.306312	-2.805711
H	1.062913	-2.540396	1.943371

1.iv) <u>Anthracene Dimers</u>

Ant2

A
0 1

C	4.208381	0.414425	1.573693
C	3.406275	0.155259	0.457069
C	3.310434	1.098978	-0.564571
C	4.016184	2.303321	-0.470689
C	4.909574	1.614243	1.671373
C	5.790270	1.970292	2.857476
C	4.812243	2.565750	0.642188
C	5.597307	3.854833	0.819675
C	7.093503	2.532174	2.313564
C	8.346696	2.155264	2.791591
C	6.995966	3.483888	1.284372
C	8.153015	4.044452	0.747863
C	9.410059	3.666508	1.232071
C	9.506831	2.722569	2.253443
H	4.286228	-0.326172	2.376993
H	2.859140	-0.789238	0.385729
H	2.687840	0.898427	-1.441307
H	3.943574	3.046282	-1.272319
H	6.007662	1.053619	3.427632
H	5.668652	4.365156	-0.153511
H	8.419863	1.412667	3.593542
H	8.074501	4.785374	-0.055098
H	10.314793	4.109580	0.805897
H	10.487744	2.421674	2.632616
C	6.648087	4.537571	5.155712
C	7.353832	5.741926	5.249579
C	7.258019	6.685602	4.227899
C	6.455947	6.426398	3.111264
C	5.852089	4.275086	4.042820
C	5.067085	2.985953	3.865292
C	5.754756	5.226566	3.013611
C	4.874094	4.870498	1.827498
C	3.668410	3.356855	3.400586
C	2.511362	2.796313	3.937092
C	3.570894	4.308537	2.371362
C	2.317699	4.685394	1.893260
C	1.157565	4.118102	2.431408
C	1.254321	3.174219	3.452837
H	6.720737	3.794632	5.957359
H	7.976347	5.942545	6.126352
H	7.805190	7.630086	4.299185
H	6.378068	7.166971	2.307945
H	4.995738	2.475632	4.838480
H	4.656664	5.787153	1.257329
H	2.589843	2.055396	4.740060
H	2.244566	5.427992	1.091308
H	0.176661	4.418927	2.052148
H	0.349576	2.731205	3.879041

B
0 1

C	-15.004161	0.108011	-0.115449
C	-14.546618	0.207719	1.167426
C	-14.185506	1.483371	1.725067
C	-14.325350	2.656737	0.909742
C	-14.823821	2.511466	-0.431587
C	-15.145537	1.281361	-0.929847
C	-13.660071	1.604002	3.017273
C	-13.933741	3.899155	1.422739
C	-13.386249	4.016283	2.705943
C	-13.246081	2.842899	3.521256
C	-12.638677	2.971431	4.818532
H	-12.528997	2.071681	5.432468
C	-12.191750	4.181736	5.266079
C	-12.332282	5.354790	4.451044
C	-12.915010	5.274632	3.218734
H	-13.531398	0.704727	3.629981
H	-15.269330	-0.868639	-0.531240
H	-14.431221	-0.684033	1.791910
H	-14.924443	3.410213	-1.048604
H	-15.517127	1.181625	-1.954059
H	-14.019579	4.791444	0.792385
H	-11.725199	4.266548	6.252089
H	-11.970855	6.316223	4.827989

H	-13.020600	6.164606	2.589940
C	-11.425130	4.955405	-1.623619
C	-11.512353	3.598341	-1.497154
C	-11.060867	2.938209	-0.301932
C	-10.501936	3.732124	0.755386
C	-10.416513	5.156740	0.578924
C	-10.867613	5.749200	-0.565954
C	-11.192822	1.555450	-0.125952
C	-10.098586	3.108071	1.942293
C	-10.252376	1.729042	2.127090
C	-10.811383	0.934981	1.069574
C	-11.004841	-0.472921	1.290428
H	-11.437651	-1.070973	0.482075
C	-10.674949	-1.046266	2.484999
C	-10.115505	-0.252534	3.542055
C	-9.906298	1.085221	3.365855
H	-11.641204	0.953130	-0.923984
H	-11.777590	5.447570	-2.534993
H	-11.941576	2.987320	-2.297808
H	-9.994498	5.756776	1.391559
H	-10.804145	6.834756	-0.686502
H	-9.692347	3.716680	2.757975
H	-10.832074	-2.117260	2.644210
H	-9.854537	-0.730486	4.491019
H	-9.485160	1.697207	4.169990

C
0 1

C	2.311349	0.348671	12.951806
C	3.292425	0.974938	13.666060
C	3.460996	2.396561	13.577978
C	2.645428	3.139362	12.773460
C	1.429003	1.096292	12.097196
C	0.413592	0.480055	11.354505
C	1.602475	2.518150	12.003214
C	0.756557	3.256781	11.165988
C	-0.437005	1.220303	10.523720
C	-1.485728	0.601477	9.757610
C	-0.260610	2.641757	10.425752
C	-1.135594	3.389776	9.563200
C	-2.121008	2.767100	8.853727
C	-2.298561	1.347653	8.953690
H	2.178075	-0.736034	13.018758
H	3.955930	0.395005	14.314486
H	4.249909	2.880766	14.161061
H	2.773151	4.223850	12.696247
H	0.280452	-0.605375	11.427467
H	0.895764	4.340730	11.085787
H	-1.619116	-0.482610	9.835546
H	-0.988441	4.471700	9.483470
H	-2.773188	3.345159	8.193098
H	-3.090978	0.865510	8.373416
C	-0.232030	1.411493	6.215961
C	-1.023575	2.213239	5.445064
C	-0.800028	3.629732	5.404489
C	0.210811	4.191773	6.130208
C	0.839756	1.964225	6.999127
C	1.657680	1.165240	7.807372
C	1.069331	3.380683	6.951464
C	2.113071	3.930677	7.706041
C	2.700545	1.714844	8.563996
C	3.542433	0.906285	9.403795
C	2.936255	3.129827	8.508641
C	4.011240	3.680964	9.289071
C	4.791373	2.878379	10.071026
C	4.552548	1.466093	10.131447
H	-0.403469	0.331193	6.258570
H	-1.836409	1.781141	4.853891
H	-1.444709	4.257132	4.781796
H	0.388148	5.271734	6.097530
H	1.473569	0.086060	7.853974
H	2.290630	5.011489	7.667354
H	3.349463	-0.170362	9.452490
H	4.189173	4.760468	9.243479
H	5.602302	3.309497	10.665470
H	5.178595	0.842017	10.775292

D
0 1

C	-9.587536	-2.184216	-0.965870
C	-8.215311	-2.190397	-0.683582
C	-7.550374	-1.001706	-0.384945
C	-8.262133	0.213327	-0.373679
C	-9.626798	0.216344	-0.660502
C	-10.293115	-0.980440	-0.954281
C	-6.062333	-0.928606	-0.080936
C	-7.469845	1.472642	-0.058193
C	-6.202239	1.426451	-0.899785
C	-5.490503	0.213085	-0.909577
C	-4.342109	0.091473	-1.691710
H	-3.795490	-0.849632	-1.704016
C	-3.891319	1.170908	-2.461457
C	-4.598058	2.374305	-2.451788
C	-5.754913	2.497694	-1.672536
H	-5.584875	-1.864625	-0.388296
H	-10.097304	-3.115255	-1.200761
H	-7.662202	-3.127920	-0.700623
H	-10.176983	1.155872	-0.661332
H	-11.356396	-0.966914	-1.180682
H	-8.059579	2.348586	-0.347325
H	-2.994948	1.067819	-3.067780
H	-4.256447	3.214231	-3.051491
H	-6.311256	3.433417	-1.671666
C	-7.040637	-0.683606	2.329050
C	-5.761565	-0.763839	1.509137
C	-4.951580	0.485466	1.818018
C	-5.671188	1.720108	1.827903
C	-7.160776	1.633549	1.530845
C	-7.713630	0.470872	2.339481
C	-3.610092	0.470116	2.115199
C	-5.022047	2.891220	2.137271
C	-3.629886	2.907010	2.442156
C	-2.908610	1.669604	2.430677
C	-1.521776	1.681115	2.737538
H	-0.974954	0.740183	2.730236
C	-0.871992	2.860783	3.039461
C	-1.585309	4.084510	3.050998
C	-2.934556	4.103918	2.760447
H	-3.060009	-0.470160	2.117708
H	-7.388575	-1.562959	2.865476
H	-5.183308	-1.644625	1.804490
H	-7.641082	2.566051	1.842422
H	-8.645904	0.593590	2.885379
H	-5.570803	3.832080	2.154646
H	0.190504	2.853833	3.269593
H	-1.065518	5.009141	3.289013
H	-3.484653	5.042787	2.768131

1.v) Neutral Anthracene Plus Water Clusters

Ant2W

Not Bonded Anthracenes:

A
0 1

C	-8.625322	-2.404924	0.412506
C	-7.278939	-2.415149	0.187178
C	-6.527717	-1.188757	0.153804
C	-7.222606	0.050503	0.362032
C	-8.640626	0.016143	0.600296
C	-9.319186	-1.167744	0.624151
C	-5.145208	-1.169184	-0.070043
C	-6.502976	1.251498	0.331542
C	-5.121470	1.272149	0.101881
C	-4.425972	0.032579	-0.100984
C	-3.006192	0.067195	-0.326982
H	-2.478841	-0.879936	-0.480583
C	-2.329597	1.253023	-0.352297
C	-3.025336	2.491638	-0.155488
C	-4.372717	2.498936	0.064530
H	-4.614543	-2.115158	-0.227211
H	-9.185839	-3.344147	0.438110
H	-6.746184	-3.358184	0.026111
H	-9.163918	0.963021	0.768144
H	-10.396320	-1.181567	0.812984

H	-7.032377	2.196601	0.496333
H	-1.249850	1.266351	-0.527993
H	-2.466679	3.431816	-0.183065
H	-4.908545	3.440429	0.222042
C	-9.591456	-2.364936	4.098216
C	-8.248860	-2.381963	3.849226
C	-7.493483	-1.159968	3.793997
C	-8.177286	0.085226	4.004671
C	-9.592946	0.061054	4.256724
C	-10.275430	-1.121218	4.303425
C	-6.112347	-1.150555	3.557287
C	-7.447988	1.281561	3.976110
C	-6.066092	1.289802	3.749066
C	-5.382438	0.044380	3.531586
C	-3.962960	0.066397	3.296641
H	-3.449646	-0.884321	3.121047
C	-3.273791	1.243647	3.285469
C	-3.955920	2.486037	3.507612
C	-5.302015	2.509163	3.730141
H	-5.591277	-2.099664	3.391113
H	-10.154786	-3.301499	4.143206
H	-7.721535	-3.327127	3.686684
H	-10.110399	1.011829	4.419493
H	-11.350923	-1.127345	4.503231
H	-7.968528	2.229995	4.148172
H	-2.196541	1.249190	3.097861
H	-3.385514	3.419318	3.491544
H	-5.825519	3.455581	3.899838
O	-6.721402	-0.343121	6.929502
H	-6.192231	-0.026466	6.184012
H	-7.492199	-0.718620	6.482518

B

0 1

C	-9.255512	-1.595604	0.634764
C	-7.929566	-1.910421	0.552352
C	-6.939809	-0.887740	0.351246
C	-7.371792	0.475932	0.232742
C	-8.780673	0.765789	0.304901
C	-9.687890	-0.235595	0.504819
C	-5.571167	-1.180525	0.284129
C	-6.413780	1.484153	0.053953
C	-5.045785	1.191094	-0.007307
C	-4.613971	-0.172771	0.112468
C	-3.204566	-0.456157	0.064356
H	-2.878000	-1.497292	0.157325
C	-2.291944	0.547120	-0.098113
C	-2.724565	1.908179	-0.227989
C	-4.053977	2.217142	-0.183231
H	-5.242131	-2.222059	0.376262
H	-9.997006	-2.381477	0.804682
H	-7.595883	-2.948389	0.651030
H	-9.104957	1.806819	0.209522
H	-10.755363	-0.003982	0.566252
H	-6.747341	2.523386	-0.030067
H	-1.222895	0.317821	-0.135210
H	-1.979606	2.697788	-0.363462
H	-4.389665	3.255039	-0.278591
C	-8.860635	-3.031960	4.074421
C	-7.549958	-2.693721	3.893524
C	-7.146042	-1.315515	3.828279
C	-8.146127	-0.295494	3.962724
C	-9.515738	-0.692547	4.142501
C	-9.861181	-2.013118	4.197795
C	-5.810386	-0.941939	3.632213
C	-7.761240	1.052678	3.923721
C	-6.422297	1.424401	3.737737
C	-5.426455	0.402764	3.573788
C	-4.059949	0.793878	3.355857
H	-3.307776	0.010475	3.220480
C	-3.707296	2.111148	3.305541
C	-4.697587	3.132883	3.486643
C	-6.005973	2.802949	3.700766
H	-5.047202	-1.719642	3.515970
H	-9.156044	-4.084040	4.125235
H	-6.781119	-3.467352	3.796236
H	-10.276934	0.088669	4.235172
H	-10.906936	-2.302051	4.338253
H	-8.524603	1.830448	4.046305

H	-2.666693	2.395803	3.127179
H	-4.393430	4.183888	3.462745
H	-6.763148	3.578802	3.851901
O	-8.359335	3.674610	1.705224
H	-8.127012	2.766015	1.948823
H	-7.492511	4.101229	1.659478

C
0 1

C	-8.157999	1.610486	-1.168782
C	-7.937330	0.411931	-0.552949
C	-6.597296	-0.036972	-0.279603
C	-5.493568	0.804277	-0.649399
C	-5.770393	2.056228	-1.303646
C	-7.056218	2.442841	-1.555869
C	-6.347152	-1.270102	0.337898
C	-4.186923	0.386194	-0.359094
C	-3.935464	-0.847005	0.258691
C	-5.040164	-1.699229	0.599900
C	-4.769400	-2.972605	1.212609
H	-5.617436	-3.615302	1.468824
C	-3.488719	-3.367490	1.473403
C	-2.385917	-2.509056	1.147884
C	-2.601567	-1.293362	0.563410
H	-7.197071	-1.882880	0.651670
H	-9.179771	1.944643	-1.370407
H	-8.768644	-0.230467	-0.247395
H	-4.928127	2.691512	-1.597814
H	-7.254456	3.395439	-2.056487
H	-3.343917	1.031808	-0.630550
H	-3.295231	-4.339556	1.936632
H	-1.366402	-2.839280	1.367294
H	-1.761022	-0.639778	0.308679
C	-5.201312	-2.266045	4.973775
C	-5.093816	-1.220591	4.102460
C	-6.132689	-0.230150	4.011504
C	-7.280694	-0.347043	4.868276
C	-7.352333	-1.462318	5.775631
C	-6.351114	-2.389967	5.822442
C	-6.061415	0.831013	3.100207
C	-8.300294	0.611572	4.783265
C	-8.228729	1.675634	3.872944
C	-7.084709	1.784354	3.009361
C	-7.029924	2.865778	2.063103
H	-6.164281	2.931777	1.397555
C	-8.045211	3.773706	1.981159
C	-9.187208	3.666718	2.842504
C	-9.276683	2.655044	3.755095
H	-5.197629	0.906311	2.429626
H	-4.410615	-3.020055	5.025335
H	-4.221627	-1.123389	3.448338
H	-8.227982	-1.551654	6.426451
H	-6.419554	-3.235891	6.512482
H	-9.177599	0.520550	5.432944
H	-7.997656	4.585193	1.249077
H	-9.991312	4.403938	2.761123
H	-10.148831	2.568532	4.411002
O	-9.043309	-1.179063	2.075467
H	-8.706500	-0.273245	2.155271
H	-8.694418	-1.592538	2.878263

Ant2W2

A
0 1

C	-9.049257	-2.411889	0.148508
C	-7.834967	-2.123333	0.700267
C	-7.071881	-0.993092	0.244382
C	-7.610092	-0.170108	-0.803666
C	-8.895164	-0.507420	-1.355105
C	-9.588052	-1.590368	-0.895875
C	-5.828574	-0.668250	0.803772
C	-6.879440	0.941404	-1.246750
C	-5.634633	1.262889	-0.692346
C	-5.097104	0.438999	0.355860
C	-3.829547	0.797335	0.939277
H	-3.431356	0.176744	1.749078
C	-3.146833	1.899137	0.505744
C	-3.677559	2.716099	-0.548659

C	-4.877449	2.407869	-1.126995
H	-5.428338	-1.282192	1.618403
H	-9.625379	-3.268548	0.510007
H	-7.428732	-2.734237	1.511958
H	-9.305904	0.124852	-2.148159
H	-10.565487	-1.835975	-1.320908
H	-7.294259	1.573178	-2.039403
H	-2.190338	2.166086	0.964187
H	-3.110506	3.587568	-0.889255
H	-5.283782	3.025676	-1.934547
C	-8.964505	-2.855221	4.123282
C	-7.620699	-2.934162	4.358426
C	-6.795207	-1.757141	4.296374
C	-7.414592	-0.497907	3.990983
C	-8.828207	-0.459861	3.722386
C	-9.575917	-1.600738	3.792684
C	-5.411924	-1.803010	4.521369
C	-6.632142	0.665378	3.960735
C	-5.255965	0.624123	4.224553
C	-4.627896	-0.641491	4.487861
C	-3.207085	-0.672278	4.714532
H	-2.729758	-1.638505	4.907407
C	-2.469587	0.477880	4.699199
C	-3.100924	1.743734	4.461726
C	-4.445837	1.815066	4.233329
H	-4.935141	-2.765050	4.740814
H	-9.583975	-3.755532	4.181198
H	-7.150495	-3.891723	4.605190
H	-9.267922	0.499862	3.434250
H	-10.649528	-1.566028	3.586030
H	-7.113690	1.614615	3.708556
H	-1.390847	0.440475	4.877565
H	-2.495505	2.654970	4.465164
H	-4.930389	2.775699	4.033489
O	-8.639300	2.102841	1.732884
H	-7.827079	2.644171	1.750264
H	-8.354768	1.315297	1.245388
O	-6.055025	3.298599	1.861956
H	-5.509841	2.494958	1.843434
H	-5.746672	3.774947	1.076932

B

0 1

C	-15.317639	0.841582	-0.111954
C	-14.849110	0.967111	1.166804
C	-14.263551	2.206431	1.611637
C	-14.175955	3.303419	0.690417
C	-14.682796	3.127257	-0.644302
C	-15.232340	1.938906	-1.033497
C	-13.743429	2.346302	2.907508
C	-13.567239	4.496570	1.099782
C	-13.033093	4.635137	2.386615
C	-13.126261	3.538537	3.308771
C	-12.535918	3.679674	4.613115
H	-12.604912	2.835359	5.306508
C	-11.889573	4.829067	4.967681
C	-11.796688	5.925218	4.045467
C	-12.353491	5.832964	2.802113
H	-13.787691	1.493606	3.594804
H	-15.755274	-0.104466	-0.445683
H	-14.896407	0.140644	1.884256
H	-14.606089	3.965112	-1.344871
H	-15.611080	1.814981	-2.052464
H	-13.474535	5.324944	0.388458
H	-11.437678	4.923337	5.959634
H	-11.275107	6.837982	4.348555
H	-12.280247	6.662958	2.092017
C	-10.727157	4.778262	-1.861431
C	-11.105265	3.486527	-1.628592
C	-10.846050	2.858627	-0.361105
C	-10.165481	3.610600	0.654784
C	-9.769660	4.962457	0.364981
C	-10.046845	5.529970	-0.846086
C	-11.281988	1.558571	-0.076011
C	-9.949659	3.028871	1.910347
C	-10.415352	1.741999	2.205426
C	-11.097507	0.990409	1.189978
C	-11.630892	-0.302229	1.527045
H	-12.161387	-0.863931	0.751596

C	-11.517556	-0.797308	2.793688
C	-10.831435	-0.048502	3.807167
C	-10.287799	1.170273	3.519212
H	-11.824198	0.993853	-0.842961
H	-10.936978	5.248047	-2.826992
H	-11.627173	2.908568	-2.398289
H	-9.252918	5.531234	1.144864
H	-9.748025	6.562074	-1.052176
H	-9.450280	3.611286	2.692842
H	-11.958916	-1.764388	3.049344
H	-10.749620	-0.464015	4.815805
H	-9.769429	1.749160	4.290408
O	-14.946784	-0.391926	4.178825
H	-15.356329	-1.239525	4.393186
H	-15.706790	0.221091	4.095303
O	-16.846319	1.619089	3.608889
H	-16.852628	1.560467	2.640353
H	-16.274457	2.388147	3.760449

C
0 1

O	5.074849	6.589780	3.432336
C	4.183926	0.117271	2.859971
C	2.971066	0.410197	2.306963
C	2.816665	1.563087	1.467793
C	3.876715	2.385929	1.217329
C	5.329025	0.952450	2.613318
C	6.585208	0.673832	3.166045
C	5.171458	2.111348	1.780240
C	6.273181	2.943813	1.546559
C	7.690630	1.499211	2.923101
C	8.986661	1.222429	3.480568
C	7.529877	2.662698	2.097010
C	8.669349	3.509583	1.867268
C	9.883626	3.214894	2.417972
C	10.046067	2.048792	3.237329
H	5.406516	7.436958	3.109378
H	5.011912	6.717181	4.402088
H	4.306082	-0.756261	3.508639
H	2.104756	-0.225610	2.510933
H	1.835362	1.783804	1.037190
H	3.760566	3.272100	0.585011
H	6.704601	-0.206971	3.806938
H	6.146294	3.838894	0.927574
H	9.103615	0.334507	4.110149
H	8.540103	4.397633	1.240109
H	10.743912	3.865320	2.233513
H	11.027642	1.827108	3.666735
O	4.973429	6.474233	6.251738
C	7.113200	2.038082	6.702973
C	8.177311	2.849668	6.432210
C	8.035731	3.964731	5.540762
C	6.834053	4.229799	4.946190
C	5.825849	2.288211	6.111248
C	4.713525	1.478673	6.377848
C	5.683227	3.406495	5.222560
C	4.432860	3.674193	4.644473
C	3.461722	1.747393	5.809245
C	2.308820	0.930055	6.077614
C	3.317566	2.874768	4.931514
C	2.024728	3.149734	4.364706
C	0.951422	2.355746	4.650097
C	1.098231	1.222879	5.517810
H	7.219989	1.183831	7.379675
H	9.151406	2.649513	6.888505
H	8.907377	4.587393	5.318455
H	6.706497	5.068213	4.253054
H	4.822891	0.622115	7.052851
H	4.335028	4.523828	3.959420
H	2.422656	0.068452	6.743582
H	1.926610	4.008641	3.693355
H	-0.027945	2.574568	4.214477
H	0.227978	0.595328	5.732173
H	5.808064	6.004787	6.410442
H	4.322165	5.759421	6.331463

D
0 1

C	-14.942585	0.098788	-0.321933

C	-14.582053	0.210935	0.990364
C	-14.228984	1.487631	1.550823
C	-14.274060	2.647696	0.705654
C	-14.675779	2.490404	-0.666527
C	-14.991315	1.259236	-1.165260
C	-13.803915	1.621182	2.878815
C	-13.889563	3.890131	1.224021
C	-13.441857	4.019799	2.544548
C	-13.397962	2.860004	3.390837
C	-12.905243	3.003973	4.734872
H	-12.874167	2.117445	5.375736
C	-12.477942	4.215879	5.198700
C	-12.524373	5.376075	4.352840
C	-12.994685	5.280721	3.073366
H	-13.754622	0.733658	3.519051
H	-15.202172	-0.878443	-0.739472
H	-14.541438	-0.671065	1.637347
H	-14.706734	3.379331	-1.304494
H	-15.287554	1.148565	-2.212498
H	-13.906238	4.772193	0.574135
H	-12.103341	4.312895	6.221807
H	-12.184293	6.339269	4.744310
H	-13.032773	6.160477	2.423198
C	-11.250557	4.883086	-1.866082
C	-11.354504	3.533747	-1.683324
C	-10.994725	2.930596	-0.428176
C	-10.505471	3.773025	0.627478
C	-10.396500	5.187566	0.389803
C	-10.763393	5.724851	-0.810879
C	-11.144421	1.557129	-0.196704
C	-10.185608	3.204454	1.867585
C	-10.359714	1.835941	2.106335
C	-10.851276	0.993837	1.051068
C	-11.053784	-0.404965	1.320598
H	-11.429406	-1.041267	0.513146
C	-10.795936	-0.922808	2.557342
C	-10.305463	-0.081005	3.611683
C	-10.089763	1.249009	3.391817
H	-11.531220	0.916843	-0.996737
H	-11.533337	5.332228	-2.822542
H	-11.726608	2.886351	-2.483650
H	-10.022631	5.824088	1.198165
H	-10.683247	6.802739	-0.979003
H	-9.827430	3.848849	2.677797
H	-10.957144	-1.987051	2.752615
H	-10.101490	-0.516438	4.594255
H	-9.720065	1.897547	4.192186
O	-16.073913	4.388393	4.476968
H	-15.913488	3.784592	3.739224
H	-15.180267	4.695715	4.683213
O	-7.727540	1.672143	-0.049708
H	-8.224484	1.107075	0.557253
H	-8.344739	2.403341	-0.191206

E

0 1

C	-8.673041	-2.481063	0.821900
C	-7.320729	-2.507701	0.640279
C	-6.561182	-1.286718	0.585664
C	-7.255277	-0.036365	0.723812
C	-8.680787	-0.054102	0.917831
C	-9.365915	-1.233043	0.964040
C	-5.172571	-1.283067	0.401914
C	-6.528185	1.159416	0.668059
C	-5.140489	1.163860	0.473874
C	-4.446373	-0.086248	0.341137
C	-3.024484	-0.067227	0.127369
H	-2.499427	-1.021884	0.022776
C	-2.345422	1.114846	0.041827
C	-3.039894	2.363999	0.167197
C	-4.388791	2.386080	0.380621
H	-4.643935	-2.236142	0.290037
H	-9.240376	-3.415423	0.864511
H	-6.789244	-3.458540	0.530468
H	-9.202987	0.901029	1.033090
H	-10.448298	-1.235018	1.119716
H	-7.056576	2.113039	0.775165
H	-1.265158	1.117006	-0.130046
H	-2.479118	3.300082	0.091157

H -4.923991 3.335303 0.481997
C -9.760119 -2.261265 4.465015
C -8.409822 -2.287775 4.265400
C -7.652781 -1.068270 4.180112
C -8.343520 0.184482 4.311320
C -9.767430 0.169408 4.515936
C -10.451119 -1.010515 4.588869
C -6.265664 -1.066940 3.983182
C -7.614264 1.379509 4.249312
C -6.226611 1.380332 4.059575
C -5.536131 0.127892 3.920464
C -4.110218 0.141880 3.727083
H -3.590795 -0.814597 3.610396
C -3.421608 1.319149 3.683115
C -4.111032 2.568795 3.826123
C -5.463574 2.598962 4.006724
H -5.738998 -2.021599 3.877102
H -10.324811 -3.195560 4.533384
H -7.877407 -3.238723 4.165169
H -10.290386 1.125775 4.617038
H -11.533052 -1.009417 4.750158
H -8.139846 2.334122 4.361573
H -2.338923 1.318063 3.529273
H -3.541024 3.501612 3.786219
H -5.992214 3.551066 4.118582
O -5.323451 0.600782 -2.708331
H -4.624402 1.012459 -2.182047
H -5.908343 0.246582 -2.024169
O -6.657183 -0.038550 7.254879
H -6.054228 0.112430 6.513730
H -7.475772 -0.280841 6.801019

F
0 1

C -8.367762 -3.477406 -1.138110
C -7.006764 -3.395428 -1.047733
C -6.344653 -2.117702 -1.045624
C -7.145472 -0.928030 -1.120723
C -8.575607 -1.056477 -1.215477
C -9.165107 -2.288383 -1.229936
C -4.949178 -2.001097 -0.973997
C -6.519558 0.325719 -1.098688
C -5.124779 0.440793 -1.037875
C -4.320388 -0.748288 -0.981526
C -2.888576 -0.611020 -0.931908
H -2.277580 -1.518788 -0.896014
C -2.303147 0.623452 -0.937017
C -3.106760 1.810443 -0.985193
C -4.468154 1.720508 -1.030759
H -4.336934 -2.908439 -0.923754
H -8.858485 -4.455195 -1.146283
H -6.395675 -4.301526 -0.984598
H -9.169563 -0.139861 -1.266394
H -10.252874 -2.376837 -1.306255
H -7.143838 1.224287 -1.110893
H -1.213295 0.713971 -0.905498
H -2.619612 2.789637 -0.981488
H -5.087397 2.622418 -1.064963
C -9.632696 -1.498829 2.549932
C -8.312247 -1.449393 2.203316
C -7.473729 -0.371448 2.658425
C -8.049757 0.652188 3.488940
C -9.442988 0.555970 3.838307
C -10.206741 -0.481034 3.384166
C -6.119549 -0.289754 2.307092
C -7.245553 1.714421 3.924647
C -5.891600 1.798047 3.570860
C -5.315895 0.771708 2.745565
C -3.923596 0.862434 2.395804
H -3.494091 0.086820 1.754580
C -3.159308 1.901030 2.843281
C -3.732072 2.923702 3.669694
C -5.051069 2.875987 4.019385
H -5.683913 -1.065168 1.667539
H -10.262222 -2.317588 2.189794
H -7.872985 -2.220870 1.562860
H -9.877433 1.335270 4.471688
H -11.265156 -0.541871 3.652794

H	-7.682356	2.490896	4.561436
H	-2.102713	1.962006	2.567033
H	-3.101764	3.746547	4.019008
H	-5.491275	3.653862	4.650853
O	-9.048272	1.650672	0.543258
H	-9.365543	0.834395	0.958668
H	-8.323396	1.905235	1.132778
O	-5.827265	-0.848458	5.705287
H	-5.233027	-0.255119	5.226037
H	-6.571658	-0.924746	5.092588

Ant2W3

A

0 1

C	3.433543	6.128434	18.352067
C	2.298443	6.202830	19.105509
C	1.677235	7.470761	19.359692
C	2.212870	8.619979	18.854901
C	4.027309	7.314613	17.792866
C	5.179220	7.266076	16.996250
C	3.408738	8.586148	18.054323
C	3.972813	9.748684	17.514485
C	5.744449	8.430405	16.458116
C	6.924769	8.395915	15.636248
C	5.130988	9.699316	16.728034
C	5.719448	10.888218	16.172990
C	6.847330	10.816904	15.405990
C	7.459467	9.548123	15.129928
H	3.916697	5.164696	18.162139
H	1.861355	5.295334	19.531238
H	0.768571	7.508341	19.967595
H	1.741019	9.589409	19.044731
H	5.652323	6.298297	16.796569
H	3.483827	10.713478	17.679709
H	7.391877	7.426834	15.434023
H	5.224662	11.845560	16.358446
H	7.283077	11.726040	14.981772
H	8.359719	9.509396	14.509303
C	8.445698	7.245522	18.893888
C	8.965418	8.404887	18.394169
C	8.334416	9.663559	18.665909
C	7.204552	9.717140	19.429874
C	7.257731	7.259940	19.705140
C	6.699352	6.085891	20.227427
C	6.628155	8.520429	19.981095
C	5.471341	8.548555	20.770461
C	5.542581	6.114815	21.016948
C	4.953821	4.917153	21.553426
C	4.916946	7.376020	21.298869
C	3.733553	7.392874	22.115541
C	3.206512	6.235014	22.610847
C	3.825769	4.974056	22.320867
H	8.925165	6.282976	18.687098
H	9.868101	8.381270	17.776385
H	8.757977	10.579791	18.245065
H	6.712700	10.673885	19.633025
H	7.180572	5.123955	20.016302
H	4.986997	9.509642	20.976581
H	5.432257	3.957082	21.334238
H	3.261284	8.357493	22.327059
H	2.306362	6.260820	23.231991
H	3.388784	4.056136	22.725109
O	2.808312	11.106661	14.956498
O	2.448559	8.318966	14.876713
H	3.496672	10.738370	14.349174
H	2.193558	11.547892	14.353551
H	2.749628	7.899378	15.695857
H	2.342541	9.261263	15.126309
O	4.394085	9.525896	13.385765
H	5.262149	9.353015	13.779937
H	3.809158	8.844430	13.789892

B

0 1

C	-0.252274	7.787739	13.112286
C	-1.601819	7.637566	13.257499
C	-2.509400	8.578075	12.666307

C	-2.037477	9.644011	11.955545
C	0.282650	8.894257	12.362628
C	1.663799	9.070050	12.193373
C	-0.623840	9.843457	11.779821
C	-0.108404	10.931390	11.062866
C	2.178572	10.166500	11.485740
C	3.596186	10.367445	11.330226
C	1.271143	11.117916	10.906622
C	1.815153	12.235558	10.182709
C	3.164934	12.392717	10.052516
C	4.069345	11.445371	10.637886
H	0.454079	7.094108	13.578758
H	-2.001774	6.796189	13.831061
H	-3.586787	8.436434	12.793572
H	-2.727113	10.365967	11.506837
H	2.351383	8.336950	12.624556
H	-0.800391	11.654458	10.616810
H	4.273290	9.646108	11.798363
H	1.122931	12.957542	9.738139
H	3.566567	13.247620	9.500705
H	5.147096	11.594960	10.525507
C	8.300629	7.646199	15.830051
C	9.059802	8.711281	15.438668
C	8.556275	10.048977	15.560178
C	7.309379	10.275319	16.067898
C	6.980145	7.841077	16.368808
C	6.170398	6.766471	16.763427
C	6.475550	9.181744	16.490932
C	5.185523	9.386551	16.997976
C	4.883155	6.973333	17.275393
C	4.037570	5.880017	17.678667
C	4.378799	8.312494	17.391636
C	3.044876	8.512611	17.892981
C	2.273090	7.450934	18.268134
C	2.779525	6.110914	18.161451
H	8.681221	6.624164	15.737882
H	10.060909	8.550309	15.028772
H	9.181061	10.887894	15.241300
H	6.918074	11.293145	16.159106
H	6.553173	5.744370	16.669897
H	4.785040	10.403122	17.058947
H	4.425368	4.859889	17.595136
H	2.659260	9.534017	17.943843
H	1.259653	7.612583	18.645746
H	2.148335	5.272925	18.471141
O	2.785719	9.879983	15.060455
O	2.574808	7.119481	14.823722
H	3.597235	9.615946	14.571832
H	2.233748	10.282806	14.372470
H	2.592619	6.630420	15.659951
H	2.408339	8.052556	15.091805
O	4.748398	8.396417	13.750076
H	5.591908	8.290240	14.213266
H	4.174227	7.684522	14.112673

C
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C	4.814542	-1.233998	2.212603
C	3.708002	-1.740239	1.591247
C	3.269569	-1.207207	0.333548
C	3.947229	-0.179859	-0.259048
C	5.563033	-0.157931	1.620554
C	6.700484	0.383953	2.233454
C	5.113872	0.383046	0.368592
C	5.815596	1.450906	-0.205470
C	7.405442	1.448436	1.655468
C	8.566847	2.023561	2.277899
C	6.945999	1.999722	0.412736
C	7.662032	3.108332	-0.158443
C	8.760809	3.628941	0.463412
C	9.220500	3.076474	1.704046
H	5.152803	-1.639681	3.171644
H	3.148794	-2.561306	2.049835
H	2.383514	-1.631283	-0.148812
H	3.616290	0.248414	-1.210731
H	7.040171	-0.026710	3.191254
H	5.452956	1.870527	-1.148740
H	8.910809	1.604868	3.228902
H	7.307277	3.522563	-1.108164

H	9.298763	4.472745	0.020593
H	10.098280	3.509368	2.192547
O	4.303149	4.213387	6.591906
O	5.155528	1.524847	6.671312
C	7.017658	3.583558	4.977185
C	8.038515	4.484219	5.112194
C	8.208401	5.543729	4.161359
C	7.349177	5.671299	3.107034
C	6.082098	3.699350	3.887139
C	5.012334	2.802063	3.739463
C	6.252410	4.758107	2.934400
C	5.341092	4.881998	1.876046
C	4.098439	2.935646	2.685853
C	2.993067	2.027814	2.529990
C	4.264509	3.998453	1.734388
C	3.304646	4.121399	0.668286
C	2.256714	3.247517	0.564287
C	2.101839	2.177635	1.507669
H	3.931140	4.193864	5.695647
H	5.170505	4.621657	6.441564
H	6.867915	2.772014	5.698122
H	8.741754	4.395205	5.945860
H	9.034232	6.250349	4.286375
H	7.478440	6.475868	2.375874
H	4.885986	1.996873	4.472247
H	5.473181	5.691682	1.149483
H	2.890355	1.206620	3.246535
H	3.419255	4.944278	-0.046585
H	1.526713	3.356507	-0.244540
H	1.270320	1.477234	1.392049
H	5.004329	1.082670	7.516162
H	4.775954	2.419565	6.798806
O	3.388386	2.336686	-2.408178
H	3.398723	2.693424	-1.505689
H	3.933076	2.963721	-2.903815

D
0 1

O	8.974225	-0.647710	-0.234639
C	4.173643	0.060635	2.295127
C	2.997298	0.209481	1.619243
C	2.922719	1.052456	0.461330
C	4.029449	1.716949	0.018159
C	5.363410	0.739148	1.856807
C	6.584256	0.607526	2.531509
C	5.290368	1.581687	0.695901
C	6.441808	2.251697	0.261978
C	7.735658	1.275407	2.095930
C	8.998056	1.140348	2.772595
C	7.663822	2.115650	0.932561
C	8.857771	2.782597	0.486252
C	10.040192	2.623917	1.151403
C	10.110732	1.789535	2.317800
H	4.229335	-0.566409	3.190335
H	2.095840	-0.304351	1.965656
H	1.966266	1.170027	-0.056043
H	3.976054	2.371495	-0.857757
H	6.639844	-0.035140	3.417121
H	6.384947	2.896428	-0.622012
H	9.049434	0.497115	3.656661
H	8.797567	3.420336	-0.401358
H	10.942435	3.132077	0.798699
H	11.067081	1.672540	2.835845
H	8.057722	-0.367304	-0.107601
H	9.462859	0.047378	0.227756
O	2.833796	4.513436	6.155369
O	3.497185	1.773953	6.175471
C	6.980241	4.057913	3.798197
C	8.062834	4.755020	3.345998
C	7.937864	5.636109	2.221338
C	6.736343	5.792583	1.591977
C	5.695986	4.193932	3.164757
C	4.574931	3.479237	3.609302
C	5.570191	5.079918	2.041628
C	4.323001	5.222495	1.419320
C	3.325686	3.629351	2.987295
C	2.163965	2.909417	3.445083
C	3.196062	4.522218	1.870464
C	1.905823	4.668609	1.251433

C	0.822660	3.981548	1.720280
C	0.953303	3.089508	2.836762
H	2.046423	4.477434	5.589705
H	3.517014	4.809949	5.532765
H	7.070445	3.373599	4.648003
H	9.036375	4.634282	3.829148
H	8.818201	6.181789	1.868867
H	6.637803	6.466202	0.734392
H	4.661701	2.792710	4.460100
H	4.224876	5.902701	0.565459
H	2.285065	2.214375	4.282210
H	1.808980	5.348676	0.398733
H	-0.154619	4.107030	1.244729
H	0.075507	2.538802	3.188757
H	3.903561	1.477975	6.999830
H	3.268379	2.711402	6.347485

E

0 1

O	3.599812	1.649642	1.239912
C	5.542979	-2.716735	0.178817
C	5.492693	-3.705039	-0.761412
C	6.027618	-3.485888	-2.074061
C	6.593452	-2.286880	-2.399518
C	6.130820	-1.439333	-0.123189
C	6.192298	-0.410807	0.826509
C	6.666147	-1.220152	-1.437462
C	7.237096	0.021550	-1.745920
C	6.766298	0.831233	0.515140
C	6.828390	1.898530	1.481048
C	7.299323	1.053254	-0.800518
C	7.877006	2.336164	-1.101905
C	7.916186	3.323919	-0.160063
C	7.382835	3.103268	1.153719
H	4.313120	1.460160	0.609619
H	3.697346	2.597319	1.423514
H	5.137596	-2.878129	1.182640
H	5.043855	-4.672714	-0.519405
H	5.978755	-4.289742	-2.814050
H	7.002717	-2.116155	-3.400200
H	5.768047	-0.561898	1.825752
H	7.642459	0.189112	-2.749776
H	6.417968	1.716169	2.478471
H	8.285260	2.502377	-2.103975
H	8.358511	4.295242	-0.400162
H	7.426062	3.906285	1.894701
O	4.915252	5.872341	6.825554
C	7.667779	3.346900	4.965645
C	8.882091	3.967955	5.028985
C	9.025094	5.329475	4.600848
C	7.950608	6.023217	4.121912
C	6.511021	4.041031	4.465016
C	5.260117	3.415172	4.371353
C	6.655454	5.403483	4.030674
C	5.541619	6.081671	3.518616
C	4.148795	4.096027	3.852650
C	2.860251	3.461205	3.739569
C	4.291879	5.457898	3.415563
C	3.139214	6.136477	2.884790
C	1.934949	5.500484	2.790022
C	1.793730	4.138927	3.220831
H	7.551488	2.306814	5.286068
H	9.755896	3.429631	5.406576
H	10.005594	5.809823	4.662102
H	8.055480	7.063027	3.797086
H	5.147683	2.366228	4.665548
H	5.649773	7.121837	3.194039
H	2.774545	2.418388	4.057535
H	3.250110	7.175099	2.558206
H	1.066380	6.026336	2.383610
H	0.821260	3.646660	3.131096
H	5.800718	5.538256	6.628658
H	4.373878	5.401722	6.176546
O	4.387624	0.427241	3.612809
H	4.040781	0.805118	2.773321
H	3.806692	-0.326167	3.782098

Ant2W4

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C 5.381528 11.685318 16.593012
C 6.210149 12.386497 15.762899
C 6.584246 11.845388 14.486706
C 6.117930 10.624838 14.087728
C 4.865386 10.398787 16.207126
C 3.989454 9.679125 17.026861
C 5.243965 9.856675 14.933453
C 4.732475 8.616946 14.533733
C 3.471313 8.442813 16.624934
C 2.536224 7.713066 17.437146
C 3.853412 7.899294 15.352654
C 3.295188 6.637265 14.945426
C 2.410784 5.970324 15.747458
C 2.020566 6.520272 17.015208
H 5.094958 12.090849 17.568562
H 6.603836 13.359355 16.070942
H 7.247936 12.421570 13.835074
H 6.391006 10.212894 13.110990
H 3.679852 10.106284 17.985540
H 4.991683 8.222196 13.546605
H 2.242707 8.140648 18.400969
H 3.588380 6.226653 13.973901
H 1.988189 5.014041 15.424168
H 1.305826 5.975776 17.639167
C 5.646816 7.445964 19.557681
C 5.203660 6.239961 19.095486
C 5.622010 5.753246 17.813417
C 6.472692 6.490027 17.040563
C 6.539260 8.254146 18.771290
C 6.995773 9.503101 19.212909
C 6.964472 7.764207 17.490690
C 7.832263 8.542909 16.714357
C 7.859433 10.283322 18.433883
C 8.322974 11.574326 18.867535
C 8.293095 9.789016 17.157387
C 9.182098 10.598474 16.368649
C 9.603157 11.817927 16.815414
C 9.161751 12.316167 18.086065
H 5.328254 7.822332 20.535311
H 4.518988 5.637084 19.699306
H 5.245129 4.791104 17.454818
H 6.790715 6.127432 16.057727
H 6.667526 9.879582 20.188484
H 8.150858 8.171543 15.734022
H 7.988016 11.949969 19.840098
H 9.507852 10.216296 15.396100
H 10.278959 12.425203 16.205898
H 9.506592 13.296874 18.427096
O 2.986673 12.131854 14.164201
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H 2.465407 11.870124 14.962958
H 2.170498 10.256869 11.920371
H 2.901217 10.716821 13.188329
O 0.901246 9.038353 14.589467
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B
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C 4.733175 6.221133 17.148955
C 5.657078 5.784440 16.140270
C 6.385218 6.695805 15.427612
C 5.322655 8.542431 16.683044
C 5.146863 9.911779 16.908271
C 6.242238 8.106972 15.670065
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H	3.862993	7.892241	18.168684
H	4.154029	5.477502	17.703782
H	5.771060	4.714407	15.943797
H	7.083815	6.369134	14.651062
H	4.416404	10.243920	17.651408
H	7.609320	8.728773	14.120271
H	4.948130	12.602735	17.126566
H	8.124346	11.080434	13.568407
H	7.745554	13.497511	13.952750
H	6.156580	14.260036	15.738568
C	-0.355729	9.003961	13.819972
C	-0.936681	10.014128	14.534702
C	-0.630560	11.384838	14.236282
C	0.242705	11.694559	13.232692
C	0.571581	9.290190	12.757579
C	1.209966	8.272134	12.040929
C	0.872939	10.661007	12.456342
C	1.797875	10.955501	11.448675
C	2.137184	8.566685	11.035540
C	2.836282	7.531929	10.322025
C	2.436422	9.937619	10.732119
C	3.419153	10.222815	9.720179
C	4.061219	9.211691	9.061525
C	3.765030	7.840664	9.369218
H	-0.577798	7.957168	14.049498
H	-1.636762	9.784157	15.343144
H	-1.099189	12.179347	14.823964
H	0.489184	12.736778	13.008107
H	1.012841	7.227978	12.299926
H	2.057935	11.998543	11.247098
H	2.615117	6.489354	10.570086
H	3.648661	11.269391	9.497669
H	4.810003	9.440612	8.297690
H	4.294675	7.045151	8.837378
O	3.383861	7.688617	14.086028
O	2.576582	10.014179	15.283978
H	3.948317	7.120410	14.630863
H	4.020386	8.119403	13.460443
H	1.617958	10.053999	15.151290
H	2.824346	9.120111	14.935766
O	4.030284	11.448515	13.458194
O	5.103707	9.118592	12.502738
H	4.637207	11.988815	13.985563
H	3.451021	11.017655	14.136861
H	4.874827	9.096406	11.561810
H	4.798489	10.014189	12.797133

C
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O	7.510841	3.291058	-1.018826
O	2.815165	5.556725	2.056604
C	4.011541	-0.122885	3.793245
C	2.823028	0.061881	3.148642
C	2.745755	0.911292	1.995210
C	3.859263	1.544251	1.524186
C	5.210962	0.518904	3.325010
C	6.445123	0.346733	3.963898
C	5.134134	1.364195	2.165877
C	6.291460	2.000968	1.696219
C	7.606204	0.976270	3.495321
C	8.882026	0.799363	4.134406
C	7.527851	1.819144	2.335461
C	8.726558	2.460402	1.856130
C	9.920255	2.258811	2.491806
C	9.999983	1.416137	3.650492
H	7.359396	3.550305	-1.936300
H	7.695309	2.329856	-1.070497
H	4.072735	-0.757475	4.683535
H	1.915697	-0.423643	3.518635
H	1.779413	1.062264	1.505545
H	3.802048	2.212564	0.659389
H	6.504478	-0.294137	4.851025
H	6.244353	2.637352	0.804541
H	8.937111	0.160291	5.021461
H	8.651961	3.096653	0.967700
H	10.826939	2.747022	2.121361
H	10.965473	1.272410	4.144427
H	3.315016	6.167213	1.499985
H	2.729870	6.030078	2.910221

O	2.588623	6.426343	4.733487
O	8.017552	0.543315	-0.652109
C	7.061532	2.789587	6.826175
C	8.157397	3.416122	6.305553
C	8.052306	4.193213	5.105015
C	6.851742	4.317572	4.467747
C	5.778229	2.898284	6.186450
C	4.636519	2.264519	6.694846
C	5.671467	3.678681	4.985550
C	4.429693	3.791356	4.344820
C	3.391867	2.382970	6.062930
C	2.209187	1.744550	6.576609
C	3.285760	3.165244	4.863670
C	2.002393	3.286777	4.220217
C	0.900328	2.677543	4.751912
C	1.006273	1.890029	5.946875
H	3.375224	5.987503	5.094973
H	1.878039	5.826008	5.008914
H	7.139756	2.193815	7.741528
H	9.129917	3.323346	6.798078
H	8.945428	4.673193	4.695087
H	6.766084	4.895561	3.541728
H	4.718458	1.669433	7.611775
H	4.334321	4.376466	3.422347
H	2.294074	1.142203	7.487170
H	1.946264	3.863890	3.292059
H	-0.071273	2.771562	4.257230
H	0.113236	1.403056	6.349967
H	7.258809	0.359621	-0.075190
H	8.740384	0.634133	-0.011045

D

0 1

O	3.161847	1.176518	1.257396
C	5.682625	-2.732098	0.544431
C	5.633147	-3.813836	-0.286522
C	5.889717	-3.663691	-1.690246
C	6.185768	-2.438150	-2.213473
C	5.989944	-1.422192	0.033099
C	6.040577	-0.298441	0.868966
C	6.246156	-1.271813	-1.372873
C	6.541662	-0.001058	-1.882393
C	6.332726	0.974110	0.353150
C	6.361546	2.139142	1.200262
C	6.588382	1.127056	-1.051454
C	6.873888	2.442342	-1.559384
C	6.892611	3.525026	-0.726766
C	6.628300	3.372943	0.674922
H	3.391049	0.413725	0.704582
H	3.806689	1.844370	0.970925
H	5.490275	-2.837678	1.616745
H	5.398605	-4.804732	0.112673
H	5.846501	-4.542605	-2.339931
H	6.382330	-2.320784	-3.283902
H	5.836725	-0.401729	1.940866
H	6.736258	0.114317	-2.954438
H	6.143209	2.002771	2.264412
H	7.072108	2.557143	-2.629898
H	7.107774	4.520701	-1.125767
H	6.643421	4.253447	1.324718
O	2.817901	4.244340	5.985027
O	3.484864	1.536984	5.986124
C	7.765309	4.076518	5.646438
C	8.842712	4.790668	6.084826
C	9.023656	6.154847	5.680242
C	8.124096	6.756522	4.848253
C	6.791533	4.674746	4.772848
C	5.678010	3.960083	4.309354
C	6.976544	6.038755	4.361247
C	6.040831	6.629435	3.500459
C	4.747318	4.555184	3.444195
C	3.616189	3.819633	2.942324
C	4.930425	5.916818	3.028757
C	3.966649	6.497160	2.129849
C	2.906914	5.767710	1.672045
C	2.729607	4.402707	2.081523
H	2.316818	4.399624	5.169034
H	3.670088	4.662695	5.783085
H	7.624084	3.032936	5.944366

H	9.578972	4.325622	6.746422
H	9.893414	6.710048	6.042725
H	8.261212	7.796328	4.535408
H	5.524982	2.918251	4.612519
H	6.183332	7.669739	3.187786
H	3.511024	2.776229	3.245942
H	4.105607	7.536634	1.816059
H	2.186582	6.218840	0.983550
H	1.892791	3.818228	1.687698
H	3.977304	1.415773	6.808682
H	3.193361	2.474114	6.021099
O	4.714156	0.677119	3.645558
H	4.038130	0.730375	2.944142
H	4.225138	0.859774	4.473656

Bonded Anthracenes Structures:

Ant2W

A
0 1

C	4.223156	0.458150	1.604202
C	3.452616	0.185719	0.468327
C	3.359603	1.130377	-0.553421
C	4.036373	2.350122	-0.440328
C	4.898735	1.671681	1.719993
C	5.769161	2.029823	2.913116
C	4.802900	2.625370	0.690914
C	5.576132	3.920698	0.877357
C	7.071848	2.593799	2.370470
C	8.325631	2.199440	2.833544
C	6.974741	3.548814	1.342638
C	8.133679	4.093089	0.791671
C	9.391161	3.694655	1.259194
C	9.487038	2.748987	2.279577
H	4.305712	-0.287460	2.401676
H	2.931283	-0.771575	0.380378
H	2.764981	0.917633	-1.446426
H	3.971477	3.091086	-1.244337
H	5.989709	1.111671	3.479073
H	5.648864	4.432526	-0.094902
H	8.397180	1.448216	3.626838
H	8.056099	4.830174	-0.014507
H	10.296640	4.120730	0.818265
H	10.468143	2.428721	2.641401
C	6.622663	4.591393	5.210380
C	7.328077	5.795873	5.304404
C	7.227265	6.742821	4.286151
C	6.422023	6.486006	3.171417
C	5.822687	4.331564	4.099441
C	5.040710	3.040823	3.919469
C	5.722395	5.285217	3.072755
C	4.844839	4.928618	1.884874
C	3.642015	3.404092	3.449379
C	2.486177	2.833768	3.978457
C	3.543179	4.356749	2.421374
C	2.290026	4.725958	1.937036
C	1.131111	4.149657	2.468140
C	1.229208	3.204334	3.488315
H	6.699059	3.846473	6.009852
H	7.953871	5.994721	6.179086
H	7.772642	7.688153	4.358974
H	6.340405	7.228803	2.370564
H	4.969687	2.528839	4.891727
H	4.624888	5.845165	1.315698
H	2.565659	2.091787	4.780404
H	2.216549	5.470034	1.136512
H	0.150109	4.445102	2.084877
H	0.325353	2.754283	3.908920
O	7.335687	0.565270	-0.292150
H	7.699545	1.319691	0.191604
H	6.383236	0.684603	-0.172778

B
0 1

C	4.147521	0.383981	1.570541
C	3.330554	0.073719	0.478523
C	3.188377	0.987284	-0.564630
C	3.857854	2.214627	-0.514500
C	4.815964	1.604971	1.623581
C	5.712336	2.011650	2.781787
C	4.667088	2.528886	0.575630
C	5.411249	3.846935	0.710827
C	6.983657	2.605929	2.197389
C	8.259837	2.287846	2.658605
C	6.831127	3.535668	1.153991
C	7.956078	4.133154	0.589348
C	9.235471	3.819877	1.062782
C	9.388676	2.897224	2.097291
H	4.260489	-0.331787	2.391595
H	2.811256	-0.888136	0.442392
H	2.555669	0.745419	-1.423129
H	3.745212	2.933943	-1.332916
H	5.972452	1.113846	3.364205
H	5.443722	4.342173	-0.272323
H	8.378034	1.554543	3.464605
H	7.836194	4.854365	-0.226568
H	10.114068	4.296725	0.618409
H	10.383890	2.662175	2.482548
C	6.552906	4.650078	4.997095
C	7.227801	5.875875	5.043700
C	7.064844	6.796892	4.009324
C	6.233371	6.490106	2.925923
C	5.727660	4.340612	3.917978
C	4.981328	3.023783	3.789674
C	5.569099	5.266788	2.873042
C	4.673436	4.855381	1.716741
C	3.559917	3.337701	3.353243
C	2.435958	2.755547	3.935124
C	3.405007	4.258539	2.303135
C	2.128616	4.579211	1.845961
C	1.002317	3.988495	2.428139
C	1.155639	3.078931	3.473248
H	6.674596	3.928572	5.813171
H	7.895862	6.097991	5.879325
H	7.582273	7.760281	4.046081
H	6.105507	7.212323	2.112344
H	4.953750	2.532742	4.775142
H	4.410381	5.751256	1.133180
H	2.557854	2.043032	4.757990
H	2.009963	5.294435	1.025058
H	0.002932	4.243690	2.064672
H	0.276745	2.619161	3.934093
O	10.027601	4.512226	4.714667
H	9.634703	4.982066	3.964372
H	9.350542	3.842441	4.882530

C
0 1

C	4.158260	0.412867	1.503177
C	3.364718	0.186340	0.373278
C	3.293414	1.149720	-0.631996
C	4.015656	2.341729	-0.508724
C	4.875257	1.600506	1.630650
C	5.749233	1.919845	2.831730
C	4.803043	2.571294	0.617407
C	5.606107	3.845115	0.826926
C	7.067284	2.459680	2.298926
C	8.313347	2.008824	2.733951
C	6.994451	3.441226	1.295114
C	8.164658	3.978264	0.763403
C	9.413597	3.541068	1.218783
C	9.487227	2.552685	2.198649
H	4.217601	-0.342284	2.294211
H	2.804598	-0.748532	0.278522
H	2.677321	0.974307	-1.518730
H	3.962769	3.100172	-1.297403
H	5.944295	0.999575	3.401024
H	5.695979	4.371232	-0.136375
H	8.364236	1.219822	3.491603
H	8.103331	4.742778	-0.018764
H	10.328451	3.966005	0.795690
H	10.461325	2.192864	2.543296
C	6.554666	4.473254	5.221150

C	7.259397	5.675739	5.352591
C	7.217266	6.622477	4.330661
C	6.458961	6.373115	3.181280
C	5.818784	4.210849	4.065919
C	5.029829	2.929142	3.849979
C	5.758416	5.176614	3.046302
C	4.889063	4.852324	1.842916
C	3.643231	3.329885	3.375437
C	2.471926	2.778507	3.890141
C	3.570718	4.301914	2.363319
C	2.329022	4.708380	1.879775
C	1.154546	4.150011	2.396009
C	1.226152	3.185778	3.400461
H	6.569556	3.731471	6.026340
H	7.833819	5.875004	6.262239
H	7.763804	7.564738	4.430503
H	6.409708	7.122694	2.384035
H	4.952525	2.392812	4.806639
H	4.692150	5.782423	1.287081
H	2.532087	2.021656	4.679562
H	2.275927	5.466781	1.091047
H	0.182359	4.473700	2.013014
H	0.310015	2.749516	3.809148
O	7.090882	1.237827	5.680670
H	7.623092	1.982079	5.360266
H	7.533729	0.978842	6.500235

Ant2W2

A
0 1

C	-8.749749	-2.659666	-3.802413
C	-7.490510	-2.636229	-3.193456
C	-6.888703	-1.421409	-2.871354
C	-7.550114	-0.216422	-3.162317
C	-8.802695	-0.242423	-3.771715
C	-9.405515	-1.463670	-4.091657
C	-5.531707	-1.317853	-2.196076
C	-6.840795	1.069036	-2.771657
C	-5.391254	0.955878	-3.212149
C	-4.730287	-0.249213	-2.920434
C	-3.394565	-0.411099	-3.283052
H	-2.881326	-1.350802	-3.052600
C	-2.710541	0.621331	-3.933699
C	-3.367407	1.816214	-4.225174
C	-4.709102	1.980665	-3.864855
H	-5.010022	-2.282584	-2.292054
H	-9.216347	-3.616585	-4.053693
H	-6.972897	-3.574025	-2.965058
H	-9.315170	0.698792	-3.998587
H	-10.388658	-1.477960	-4.571014
H	-7.311143	1.912222	-3.301221
H	-1.662127	0.488014	-4.215829
H	-2.837107	2.624093	-4.737705
H	-5.227612	2.918202	-4.093335
C	-9.092734	-1.723905	0.926070
C	-7.763793	-1.904897	0.524598
C	-7.102995	-0.895821	-0.177913
C	-7.768413	0.308513	-0.469431
C	-9.091511	0.483841	-0.065453
C	-9.756998	-0.533584	0.627746
C	-5.657281	-1.018482	-0.629700
C	-6.969538	1.374360	-1.204572
C	-5.615676	1.476812	-0.518543
C	-4.956672	0.268796	-0.228058
C	-3.726736	0.286919	0.431591
H	-3.251350	-0.662170	0.698279
C	-3.144879	1.507675	0.794565
C	-3.794097	2.707078	0.498893
C	-5.031704	2.689488	-0.154091
H	-5.191682	-1.854924	-0.092238
H	-9.606581	-2.514484	1.480832
H	-7.215573	-2.813615	0.791705
H	-9.608161	1.422917	-0.291384
H	-10.794232	-0.389389	0.943794
H	-7.490941	2.339594	-1.107065
H	-2.183671	1.518785	1.316886
H	-3.342434	3.661252	0.785430
H	-5.547627	3.629524	-0.377644

O	-4.773683	-2.507651	1.966582
H	-5.199090	-1.712580	2.355118
H	-4.549797	-3.045494	2.736639
O	-6.044882	-0.121753	2.777888
H	-5.509267	0.506894	2.267099
H	-6.852865	-0.194696	2.243981

B
0 1

C	-8.820637	-2.350293	-0.455211
C	-7.548912	-2.385379	0.127274
C	-6.980221	-1.221209	0.641340
C	-7.687871	-0.008060	0.573076
C	-8.954884	0.023310	-0.007172
C	-9.523031	-1.147286	-0.522144
C	-5.599814	-1.179038	1.275333
C	-7.000835	1.223475	1.140208
C	-5.571946	1.228822	0.622339
C	-4.864774	0.015548	0.690589
C	-3.554439	-0.050263	0.219165
H	-3.008743	-0.998572	0.264318
C	-2.941353	1.086922	-0.318743
C	-3.642402	2.290765	-0.384694
C	-4.958170	2.359767	0.086542
H	-5.056139	-2.097325	1.004898
H	-9.258072	-3.265243	-0.864482
H	-6.992363	-3.327288	0.173966
H	-9.500687	0.970741	-0.066262
H	-10.513856	-1.114948	-0.983851
H	-7.517272	2.121307	0.767318
H	-1.915787	1.027403	-0.693765
H	-3.169007	3.179323	-0.811710
H	-5.513548	3.301627	0.027841
C	-9.025416	-2.195226	4.398337
C	-7.709684	-2.264314	3.926969
C	-7.095851	-1.133348	3.391222
C	-7.802910	0.079999	3.323139
C	-9.113180	0.145867	3.794649
C	-9.726328	-0.991289	4.332523
C	-5.666914	-1.128083	2.873445
C	-7.067812	1.274507	2.738337
C	-5.687420	1.316598	3.372375
C	-4.979835	0.103402	3.440662
C	-3.712881	0.071901	4.021094
H	-3.167222	-0.875605	4.080332
C	-3.144704	1.242463	4.536136
C	-3.847005	2.445508	4.469058
C	-5.118662	2.480696	3.886460
H	-5.150582	-2.025981	3.246332
H	-9.498861	-3.083770	4.825326
H	-7.154350	-3.206205	3.985606
H	-9.658814	1.094214	3.749591
H	-10.751860	-0.931699	4.707629
H	-7.611406	2.192842	3.008766
H	-2.153955	1.210041	4.997997
H	-3.409530	3.360435	4.878340
H	-5.675057	3.422685	3.839611
O	-6.138934	-0.097053	-2.436121
H	-5.494603	0.285764	-1.824679
H	-6.812051	-0.445449	-1.835123
O	-6.521122	0.176579	6.450433
H	-5.848552	0.522841	5.847586
H	-7.166161	-0.208122	5.840927

Ant2W3

A
0 1

C	2.211242	6.838833	13.126923
C	1.129064	6.303918	13.832616
C	1.206768	6.152330	15.218695
C	2.373443	6.525298	15.897102
C	3.374782	7.209766	13.799698
C	4.601225	7.752575	13.088242
C	3.460534	7.041882	15.191420
C	4.784161	7.398398	15.845612
C	5.152991	8.910230	13.900843
C	5.595483	10.100155	13.323176

C	5.242462	8.735034	15.291203
C	5.765433	9.754653	16.088781
C	6.213715	10.945351	15.504787
C	6.129563	11.115974	14.121635
H	2.145698	6.985754	12.044524
H	0.217031	6.019200	13.300379
H	0.358437	5.743543	15.775277
H	2.441359	6.398073	16.982945
H	4.292247	8.133537	12.104606
H	4.635907	7.490651	16.932994
H	5.508264	10.237011	12.241033
H	5.834021	9.614774	17.173082
H	6.622686	11.741643	16.133227
H	6.469346	12.049121	13.663597
C	8.129086	7.444983	12.808072
C	9.316985	7.760228	13.476639
C	9.406933	7.582910	14.856488
C	8.308881	7.089851	15.569577
C	7.032211	6.958318	13.516101
C	5.704793	6.610982	12.861504
C	7.123148	6.779086	14.907051
C	5.886268	6.253379	15.617659
C	5.260925	5.265961	13.412728
C	4.774772	4.234901	12.611551
C	5.349125	5.086916	14.803916
C	4.948626	3.880124	15.373609
C	4.456498	2.848345	14.566956
C	4.370053	3.025570	13.186852
H	8.055872	7.583458	11.724005
H	10.174469	8.141812	12.914837
H	10.335160	7.824534	15.382299
H	8.377439	6.948085	16.653620
H	5.854005	6.521316	11.774257
H	6.176430	5.888034	16.615121
H	4.707881	4.376802	11.527496
H	5.019329	3.742531	16.458022
H	4.144591	1.902893	15.020027
H	3.989973	2.219810	12.552183
O	2.449704	9.980394	12.306953
O	2.851435	11.249864	14.813112
H	1.755761	9.667310	12.940720
H	1.956146	10.558348	11.708142
H	3.658047	10.937718	15.250138
H	2.991275	10.993037	13.878874
O	0.780752	9.528687	14.418716
H	0.987225	8.670197	14.818743
H	1.413343	10.151775	14.844082

B

0 1

O	7.331096	0.379464	-0.169170
C	4.191409	0.418265	1.658113
C	3.427460	0.111848	0.526542
C	3.365639	1.011414	-0.537656
C	4.066147	2.221001	-0.470513
C	4.892411	1.620929	1.727338
C	5.755067	2.013957	2.914428
C	4.825967	2.529934	0.656871
C	5.620577	3.817468	0.797309
C	7.073395	2.537291	2.369287
C	8.314532	2.153670	2.874051
C	7.006289	3.447115	1.299152
C	8.180461	3.954966	0.744810
C	9.424884	3.565177	1.252610
C	9.491135	2.666510	2.317140
H	7.703744	1.173478	0.238996
H	6.381015	0.559003	-0.139105
H	4.250591	-0.291649	2.489491
H	2.887376	-0.837737	0.474645
H	2.776929	0.770651	-1.427336
H	4.024068	2.927200	-1.306557
H	5.952977	1.117543	3.521452
H	5.714894	4.287211	-0.194064
H	8.364434	1.440131	3.702904
H	8.124972	4.657194	-0.093821
H	10.343073	3.960928	0.809468
H	10.461988	2.354449	2.712230
O	3.427877	5.460533	5.897456
O	4.194359	2.935162	6.873487

C	6.563834	4.671916	5.148256
C	7.258104	5.885767	5.220798
C	7.205274	6.785631	4.155493
C	6.450120	6.479442	3.017658
C	5.820812	4.360484	4.008240
C	5.030703	3.070253	3.869473
C	5.757269	5.272052	2.939674
C	4.894576	4.877614	1.750658
C	3.646341	3.446443	3.368921
C	2.474573	2.951021	3.943500
C	3.574775	4.354808	2.297911
C	2.330949	4.745472	1.803516
C	1.156709	4.239159	2.372154
C	1.228275	3.347793	3.443464
H	2.935574	5.179318	5.109020
H	4.278371	5.747184	5.526763
H	6.559783	3.974903	5.992448
H	7.835937	6.130065	6.116987
H	7.743980	7.735917	4.212299
H	6.398088	7.190994	2.186473
H	4.933267	2.609291	4.860909
H	4.697038	5.773629	1.141647
H	2.547281	2.286186	4.810173
H	2.275549	5.454386	0.970301
H	0.183736	4.551832	1.982284
H	0.311091	2.962430	3.898391
H	3.971247	2.835687	7.807556
H	3.881039	3.839089	6.652279

Ant2W4

A
0 1

C	6.381367	11.452395	13.695865
C	6.478511	12.137447	12.480821
C	6.073349	11.514500	11.295109
C	5.574348	10.209122	11.329896
C	5.912811	10.138354	13.726041
C	5.910041	9.293347	14.985722
C	5.506486	9.514757	12.538217
C	5.097738	8.056851	12.627787
C	4.636739	8.470879	15.040223
C	3.930701	8.245590	16.222263
C	4.225650	7.850689	13.851894
C	3.109942	7.012673	13.855292
C	2.420640	6.763150	15.046104
C	2.831842	7.381306	16.232109
H	6.687630	11.937853	14.627999
H	6.866636	13.160279	12.458943
H	6.143353	12.048375	10.342591
H	5.246014	9.719842	10.407312
H	5.941270	9.958635	15.861052
H	4.519150	7.794005	11.730063
H	4.251671	8.739439	17.145021
H	2.787681	6.539047	12.922441
H	1.559023	6.088681	15.048441
H	2.292901	7.192122	17.165375
C	6.907401	6.131844	16.304887
C	6.561029	4.776156	16.311787
C	6.154233	4.156541	15.131217
C	6.093181	4.892038	13.942419
C	6.844022	6.867915	15.123777
C	7.206287	8.343158	15.040107
C	6.432218	6.243249	13.933241
C	6.391267	7.103600	12.679517
C	8.105478	8.512462	13.824603
C	9.293231	9.240069	13.849238
C	7.694490	7.887212	12.633997
C	8.477309	8.000480	11.487201
C	9.667039	8.736433	11.514007
C	10.074718	9.355898	12.694282
H	7.229968	6.620074	17.230927
H	6.614442	4.204222	17.242718
H	5.887278	3.095753	15.130881
H	5.776477	4.406868	13.012775
H	7.770759	8.623761	15.943055
H	6.339393	6.446188	11.797573
H	9.612722	9.723936	14.778607
H	8.155904	7.510829	10.561538

H	10.277103	8.820325	10.609925
H	11.006652	9.928015	12.721323
O	3.217526	12.170954	12.763593
O	2.325652	9.752894	11.980869
H	4.120707	12.298843	12.435825
H	3.354124	12.022878	13.730210
H	1.602657	9.972285	11.375917
H	2.726352	10.642235	12.180700
O	1.442915	9.853038	14.587264
O	3.438531	11.460758	15.411958
H	1.569306	8.966168	14.957366
H	1.674424	9.728963	13.635712
H	2.976536	12.105425	15.966753
H	2.724498	10.801305	15.195716

B

0 1

C	6.381367	11.452395	13.695865
C	6.478511	12.137447	12.480821
C	6.073349	11.514500	11.295109
C	5.574348	10.209122	11.329896
C	5.912811	10.138354	13.726041
C	5.910041	9.293347	14.985722
C	5.506486	9.514757	12.538217
C	5.097738	8.056851	12.627787
C	4.636739	8.470879	15.040223
C	3.930701	8.245590	16.222263
C	4.225650	7.850689	13.851894
C	3.109942	7.012673	13.855292
C	2.420640	6.763150	15.046104
C	2.831842	7.381306	16.232109
H	6.687630	11.937853	14.627999
H	6.866636	13.160279	12.458943
H	6.143353	12.048375	10.342591
H	5.246014	9.719842	10.407312
H	5.941270	9.958635	15.861052
H	4.519150	7.794005	11.730063
H	4.251671	8.739439	17.145021
H	2.787681	6.539047	12.922441
H	1.559023	6.088681	15.048441
H	2.292901	7.192122	17.165375
C	6.907401	6.131844	16.304887
C	6.561029	4.776156	16.311787
C	6.154233	4.156541	15.131217
C	6.093181	4.892038	13.942419
C	6.844022	6.867915	15.123777
C	7.206287	8.343158	15.040107
C	6.432218	6.243249	13.933241
C	6.391267	7.103600	12.679517
C	8.105478	8.512462	13.824603
C	9.293231	9.240069	13.849238
C	7.694490	7.887212	12.633997
C	8.477309	8.000480	11.487201
C	9.667039	8.736433	11.514007
C	10.074718	9.355898	12.694282
H	7.229968	6.620074	17.230927
H	6.614442	4.204222	17.242718
H	5.887278	3.095753	15.130881
H	5.776477	4.406868	13.012775
H	7.770759	8.623761	15.943055
H	6.339393	6.446188	11.797573
H	9.612722	9.723936	14.778607
H	8.155904	7.510829	10.561538
H	10.277103	8.820325	10.609925
H	11.006652	9.928015	12.721323
O	3.217526	12.170954	12.763593
O	2.325652	9.752894	11.980869
H	4.120707	12.298843	12.435825
H	3.354124	12.022878	13.730210
H	1.602657	9.972285	11.375917
H	2.726352	10.642235	12.180700
O	1.442915	9.853038	14.587264
O	3.438531	11.460758	15.411958
H	1.569306	8.966168	14.957366
H	1.674424	9.728963	13.635712
H	2.976536	12.105425	15.966753
H	2.724498	10.801305	15.195716

Section 2: IONIZED STRUCTURES

2.i) Ionized Anthracene Monomer

Ant

0 1

C	-2.417715	1.419127	0.000000
C	-3.628982	0.751314	0.000000
C	-3.669369	-0.649052	0.000000
C	-2.498462	-1.385375	0.000000
C	-1.209667	0.695970	0.000000
C	0.038384	1.345085	0.000000
C	-1.250877	-0.732755	0.000000
C	-0.042115	-1.452362	0.000000
C	1.247149	0.625485	0.000000
C	2.494741	1.278083	0.000000
C	1.205934	-0.803247	0.000000
C	2.413964	-1.526424	0.000000
C	3.625246	-0.858626	0.000000
C	3.665640	0.541734	0.000000
H	-2.390505	2.503734	0.000000
H	-4.555184	1.314336	0.000000
H	-4.626418	-1.157864	0.000000
H	-2.533422	-2.469768	0.000000
H	0.069481	2.431281	0.000000
H	-0.073196	-2.538559	0.000000
H	2.529744	2.362475	0.000000
H	2.386696	-2.611029	0.000000
H	4.551442	-1.421657	0.000000
H	4.622686	1.050554	0.000000

2.ii) “on- top” isomers

AntW
A
0 1

C	-0.700601	-3.649147	0.327018
C	0.700601	-3.649147	0.327018
C	1.403431	-2.457700	0.334351
C	0.715178	-1.228836	0.341584
C	-1.403431	-2.457700	0.334351
C	-0.715178	-1.228836	0.341584
C	1.400563	0.000000	0.342836
C	0.715178	1.228836	0.341584
C	-1.400563	0.000000	0.342836
C	-0.715178	1.228836	0.341584
C	1.403431	2.457700	0.334351
C	0.700601	3.649148	0.327019
C	-0.700601	3.649148	0.327019
C	-1.403431	2.457700	0.334351
H	-1.236586	-4.591238	0.320460
H	1.236586	-4.591238	0.320460
H	2.488399	-2.461460	0.332946
H	-2.488399	-2.461460	0.332946
H	2.487175	0.000000	0.339709
H	-2.487175	0.000000	0.339709
H	2.488399	2.461460	0.332947
H	1.236586	4.591238	0.320461
H	-1.236586	4.591238	0.320461
H	-2.488399	2.461460	0.332947
O	0.000000	-0.000001	-3.121176
H	0.000000	-0.767707	-2.544142
H	0.000000	0.767706	-2.544144

AntW2
B
0 1

O	1.932307	1.323013	3.136570
O	-0.812965	1.024203	2.360605
C	-3.238737	2.285497	-0.623718
C	-4.458237	1.633999	-0.602608
C	-4.516199	0.236128	-0.526699

C	-3.354225	-0.511362	-0.472374
C	-2.041220	1.549522	-0.569007
C	-0.786143	2.183605	-0.578767
C	-2.099837	0.125994	-0.491267
C	-0.900298	-0.604995	-0.427038
C	0.414230	1.451998	-0.525509
C	1.668290	2.089179	-0.542839
C	0.355611	0.028323	-0.447206
C	1.553171	-0.707561	-0.385532
C	2.771969	-0.055718	-0.403268
C	2.829425	1.341605	-0.483983
H	2.193724	2.148351	3.556251
H	2.357877	0.631733	3.652836
H	-3.197839	3.368133	-0.680619
H	-5.377881	2.206200	-0.646297
H	-5.479422	-0.261247	-0.511225
H	-3.401767	-1.593747	-0.413671
H	-0.744075	3.268176	-0.628785
H	-0.945045	-1.688572	-0.360135
H	1.715731	3.171688	-0.602851
H	1.510949	-1.790146	-0.325942
H	3.691411	-0.628042	-0.355967
H	3.792586	1.838670	-0.500657
H	-1.379852	1.025720	3.136085
H	0.090580	1.116983	2.703057

AntW3

C
0 1

O	-1.276201	-0.861083	2.381881
O	1.504648	-0.563149	2.446509
O	-0.120799	1.638674	2.992945
C	-2.890455	1.877426	0.099427
C	-4.111191	1.264199	-0.109909
C	-4.173324	-0.028815	-0.647148
C	-3.015884	-0.710219	-0.973183
C	-1.696831	1.207071	-0.224970
C	-0.439513	1.800895	-0.008303
C	-1.760055	-0.110810	-0.767587
C	-0.561867	-0.786100	-1.066029
C	0.756694	1.126788	-0.310099
C	2.011257	1.720386	-0.082464
C	0.694482	-0.195172	-0.846033
C	1.891755	-0.875137	-1.137239
C	3.111172	-0.265733	-0.908031
C	3.171610	1.030378	-0.380602
H	-1.877838	-1.341495	2.957076
H	-1.221966	0.043550	2.734776
H	0.645281	-1.019430	2.456334
H	2.095970	-1.082071	2.998313
H	-2.842476	2.877785	0.516863
H	-5.027844	1.785166	0.141720
H	-5.137758	-0.497032	-0.807250
H	-3.068091	-1.712651	-1.385235
H	-0.391135	2.798281	0.416725
H	-0.609232	-1.792672	-1.472274
H	2.057399	2.722340	0.331452
H	1.848460	-1.880798	-1.542434
H	4.029813	-0.793863	-1.136815
H	4.136433	1.492447	-0.204659
H	-0.073206	2.120971	3.823114
H	0.667615	1.066026	2.962815

AntW4

D
0 1

C	-3.423718	1.159720	-3.989951
C	-4.582811	0.428622	-4.165138
C	-4.548679	-0.972152	-4.149306
C	-3.355522	-1.642746	-3.957974
C	-0.929451	-1.577110	-3.580463
C	-2.159054	-0.923581	-3.783575
C	-2.194188	0.502908	-3.800129
C	-0.998139	1.220005	-3.614173
C	1.427091	1.287142	-3.238401
C	0.233420	0.566408	-3.424347
C	0.268675	-0.860059	-3.406912

C	1.496801	-1.515011	-3.203264
C	2.655122	-0.782292	-3.028814
C	2.620708	0.618134	-3.046580
H	-5.526215	0.941184	-4.315196
H	-3.451347	2.244336	-3.997454
H	-5.466739	-1.531784	-4.288499
H	-3.330650	-2.727357	-3.940300
H	-0.906328	-2.662008	-3.548989
H	-1.026898	2.305376	-3.609200
H	1.399851	2.371676	-3.246833
H	1.524317	-2.599357	-3.184293
H	3.598923	-1.292923	-2.876301
H	3.538242	1.178398	-2.907085
H	-1.668184	2.521366	-0.032016
H	-2.237875	1.190559	-0.600285
H	-4.071010	-0.346656	-0.143743
H	-2.747186	-1.011906	-0.613939
H	-1.294613	-2.872400	0.027078
H	-0.599877	-1.533539	-0.353200
H	1.010032	0.002102	0.621075
H	-0.111399	0.662562	-0.229590
O	-1.466402	1.795664	-0.628925
O	-3.319720	-0.226583	-0.730378
O	-1.327950	-2.143581	-0.598539
O	0.474016	-0.119631	-0.166820

2.iii) side isomers

AntW

E
0 1

O	0.179511	-4.456598	-0.371469
C	4.847716	0.769728	-0.520711
C	4.845394	-0.631579	-0.499606
C	3.652671	-1.330350	-0.471995
C	3.658373	1.474353	-0.514194
C	-1.253973	-1.329611	-0.401710
C	-2.446324	-0.626736	-0.395327
C	-2.448173	0.773907	-0.416406
C	-1.258319	1.479153	-0.443901
C	1.199892	1.476348	-0.478935
C	-0.028838	0.792889	-0.451130
C	-0.028555	-0.636233	-0.429618
C	1.197241	-1.326910	-0.436792
C	2.426133	-0.639619	-0.464746
C	2.428618	0.788953	-0.486254
H	3.664459	2.559202	-0.530534
H	5.790603	1.303989	-0.542345
H	5.786457	-1.169384	-0.505063
H	3.650645	-2.415202	-0.455743
H	0.118445	-5.018675	0.407119
H	0.116559	-5.061175	-1.117366
H	-1.241272	-2.414816	-0.385694
H	-3.388218	-1.162859	-0.373852
H	-3.390786	1.309184	-0.411071
H	-1.264899	2.564018	-0.460038
H	1.201732	2.562881	-0.495174
H	1.182944	-2.414384	-0.420148

AntW2

F
0 1

O	0.565204	-6.405581	-1.777455
O	0.284788	-4.513622	0.298052
C	4.843815	0.612101	-0.620140
C	4.863158	-0.772068	-0.399518
C	3.681436	-1.474744	-0.258459
C	3.644655	1.294552	-0.703277
C	-1.219786	-1.540563	-0.159147
C	-2.424454	-0.864717	-0.253602
C	-2.450774	0.517325	-0.480083
C	-1.273918	1.232287	-0.613789
C	1.185049	1.265905	-0.651679
C	-0.032247	0.574165	-0.521785
C	-0.007671	-0.836198	-0.290934

C	1.228349	-1.502758	-0.200753
C	2.445363	-0.806589	-0.338189
C	2.425352	0.603277	-0.566096
H	-0.164956	-6.751958	-2.298063
H	1.259698	-7.068181	-1.830419
H	3.634905	2.365746	-0.876986
H	5.778785	1.149895	-0.727822
H	5.811984	-1.292668	-0.339358
H	3.693084	-2.546050	-0.088625
H	0.183978	-5.000608	1.120280
H	0.362267	-5.193684	-0.393703
H	-1.182892	-2.612085	0.012251
H	-3.356801	-1.408531	-0.152068
H	-3.402909	1.030349	-0.552515
H	-1.300689	2.302365	-0.791146
H	1.169371	2.338684	-0.823758
H	1.227561	-2.576733	-0.021097

AntW3

G
0 1

O	-0.985468	-8.148383	-2.339239
O	1.164683	-6.525824	-1.544378
O	1.052917	-4.826019	0.615777
C	4.683060	0.863439	-0.793906
C	4.939714	-0.463389	-0.421207
C	3.896712	-1.342412	-0.197628
C	3.384923	1.313090	-0.943057
C	-0.919102	-2.243974	-0.036465
C	-2.221911	-1.797136	-0.180778
C	-2.485081	-0.472069	-0.550329
C	-1.448636	0.415561	-0.778738
C	0.967288	0.865172	-0.862587
C	-0.112585	-0.007209	-0.640000
C	0.153300	-1.359598	-0.261875
C	1.485082	-1.790500	-0.118921
C	2.564380	-0.912171	-0.341930
C	2.302915	0.439484	-0.721128
H	-1.283290	-8.220574	-3.250239
H	-1.254694	-8.964614	-1.908870
H	0.428790	-7.100499	-1.818337
H	1.968194	-6.981138	-1.806532
H	3.190662	2.340978	-1.231129
H	5.511312	1.541336	-0.965704
H	5.963945	-0.799614	-0.308187
H	4.091901	-2.370052	0.090518
H	1.128907	-5.343626	1.421103
H	1.093967	-5.473479	-0.116850
H	-0.696918	-3.268217	0.248134
H	-3.047240	-2.477965	-0.006379
H	-3.511150	-0.139182	-0.658115
H	-1.658043	1.441072	-1.064749
H	0.767791	1.893946	-1.150167
H	1.666608	-2.824933	0.169628

AntW4

H
0 1

O	-0.320316	-7.371178	0.840508
O	0.196616	-9.429205	-1.188006
O	0.850150	-7.044616	-2.771093
O	0.224247	-5.090331	-0.786172
C	4.452396	0.248984	-0.021727
C	4.547105	-1.149855	-0.013221
C	3.418154	-1.928918	-0.182578
C	3.231021	0.870101	-0.199238
C	-1.416001	-2.276540	-0.902879
C	-2.643905	-1.659933	-1.078696
C	-2.747200	-0.263213	-1.083944
C	-1.624832	0.528111	-0.914665
C	0.802257	0.701505	-0.557150
C	-0.361632	-0.067099	-0.732226
C	-0.259604	-1.492727	-0.725561
C	0.996939	-2.098726	-0.541778
C	2.160894	-1.323288	-0.365474
C	2.064238	0.101221	-0.373917
H	-0.190980	-7.618640	1.759016

H	-0.106867	-8.153305	0.312895
H	-0.575176	-9.977791	-1.362585
H	0.942283	-10.036814	-1.144844
H	0.570213	-7.886799	-2.385369
H	0.679390	-7.109994	-3.713691
H	3.162564	1.952947	-0.205051
H	5.346474	0.847161	0.112306
H	5.513271	-1.620768	0.126922
H	3.486255	-3.011800	-0.177717
H	0.037033	-5.751087	-0.099808
H	0.439891	-5.630675	-1.563948
H	-1.312239	-3.358164	-0.901221
H	-3.534542	-2.262892	-1.214340
H	-3.716407	0.202280	-1.222834
H	-1.710487	1.609773	-0.920892
H	0.728445	1.785661	-0.562986
H	1.048860	-3.187899	-0.541254

2.iv) Ionized Anthracene dimers

Ant

A
1 2

C	-6.447056	-3.811959	1.310013
C	-5.566789	-2.747028	1.289173
C	-5.957235	-1.494991	0.730019
C	-7.286726	-1.349682	0.207102
C	-8.171860	-2.465160	0.256785
C	-7.757768	-3.669376	0.791952
C	-5.084181	-0.396718	0.697723
C	-7.680750	-0.112473	-0.332298
C	-6.798792	0.987006	-0.382921
C	-5.471892	0.841516	0.137224
C	-4.579036	1.953471	0.085747
H	-3.561638	1.834374	0.471174
C	-4.991610	3.151057	-0.446399
C	-6.312458	3.299031	-0.960178
C	-7.192405	2.245361	-0.933689
H	-4.068247	-0.508949	1.091562
H	-6.130538	-4.774522	1.721264
H	-4.551714	-2.857247	1.683070
H	-9.182508	-2.358431	-0.148863
H	-8.441941	-4.522049	0.810550
H	-8.689992	-0.006197	-0.744444
H	-4.302709	3.998993	-0.486417
H	-6.618648	4.258389	-1.385169
H	-8.203724	2.354174	-1.336932
C	-9.931221	-1.055739	2.852767
C	-8.883475	-1.758990	3.414519
C	-7.604156	-1.151811	3.573992
C	-7.417740	0.200723	3.129952
C	-8.515885	0.893165	2.540320
C	-9.746486	0.278150	2.412910
C	-6.520011	-1.842741	4.143787
C	-6.157433	0.801766	3.272351
C	-5.072994	0.116465	3.865726
C	-5.257622	-1.234450	4.305044
C	-4.153546	-1.929929	4.887403
H	-4.296433	-2.959740	5.228377
C	-2.934292	-1.312625	5.020585
C	-2.754102	0.033035	4.588194
C	-3.796169	0.732564	4.029246
H	-6.665186	-2.871112	4.491423
H	-10.912781	-1.526693	2.751620
H	-9.027936	-2.788025	3.757119
H	-8.373761	1.926817	2.209947
H	-10.588150	0.824876	1.978655
H	-6.017492	1.836197	2.940177
H	-2.094227	-1.849339	5.468906
H	-1.778377	0.510008	4.712999
H	-3.663500	1.770134	3.707246

B
1 2

C	2.311899	0.448719	12.558526
C	3.284528	1.066145	13.318009
C	3.400140	2.478007	13.323759
C	2.544931	3.254254	12.566352
C	1.400981	1.221063	11.781680
C	0.382868	0.621555	11.016845
C	1.521426	2.650472	11.785287
C	0.613865	3.419132	11.024449
C	-0.542360	1.390757	10.285003
C	-1.605008	0.787724	9.548382
C	-0.424907	2.822054	10.293653
C	-1.377504	3.598125	9.562504
C	-2.389097	2.985762	8.864863
C	-2.501875	1.566189	8.854560
H	2.217259	-0.641511	12.558569
H	3.967786	0.465862	13.924660
H	4.171834	2.953807	13.935025
H	2.633523	4.344844	12.574739
H	0.286201	-0.469897	11.017537
H	0.698895	4.511342	11.038843
H	-1.700799	-0.302472	9.551795
H	-1.292386	4.689150	9.575833
H	-3.118478	3.587261	8.315980
H	-3.319433	1.096319	8.300986
C	-0.086231	1.213382	6.426004
C	-0.938299	2.012624	5.690604
C	-0.813230	3.423494	5.730598
C	0.165876	4.016564	6.500971
C	0.942749	1.792238	7.219722
C	1.845251	0.999639	7.961087
C	1.073363	3.220132	7.257058
C	2.097604	3.794390	8.033712
C	2.887205	1.571754	8.706729
C	3.829938	0.771649	9.424964
C	3.017085	3.001581	8.746431
C	4.084216	3.578953	9.497314
C	4.969469	2.778006	10.179875
C	4.842334	1.359832	10.141870
H	-0.179758	0.123730	6.390896
H	-1.715420	1.557144	5.070829
H	-1.494113	4.042740	5.140494
H	0.267661	5.105916	6.525662
H	1.750835	-0.091293	7.922406
H	2.202822	4.884821	8.057643
H	3.735233	-0.318049	9.386406
H	4.191451	4.667962	9.515970
H	5.788494	3.228920	10.746946
H	5.562757	0.740605	10.682763

C
1 2

C	4.195470	0.423578	1.596841
C	3.384938	0.183003	0.494163
C	3.288147	1.136352	-0.537919
C	4.001946	2.326046	-0.462139
C	4.903497	1.628839	1.695004
C	5.788550	1.962848	2.874542
C	4.805215	2.589874	0.655499
C	5.593224	3.870967	0.811042
C	7.076491	2.542226	2.333913
C	8.337505	2.165896	2.815753
C	6.978040	3.503115	1.294139
C	8.142489	4.067788	0.756682
C	9.386004	3.702145	1.257454
C	9.483712	2.749086	2.289660
H	4.281211	-0.322802	2.392302
H	2.826582	-0.753951	0.420460
H	2.655449	0.933128	-1.405942
H	3.937489	3.061590	-1.269647
H	6.012214	1.040883	3.431042
H	5.671579	4.367951	-0.167010
H	8.413511	1.415524	3.608511
H	8.066984	4.798732	-0.054036
H	10.294398	4.147887	0.843726
H	10.467203	2.461445	2.670545
C	6.662009	4.515232	5.147521
C	7.375533	5.705108	5.223489
C	7.278844	6.658363	4.191377
C	6.468621	6.417563	3.088498

C	5.859067	4.251228	4.029719
C	5.071428	2.969940	3.873997
C	5.760823	5.212184	2.990234
C	4.876105	4.878045	1.810480
C	3.686606	3.337458	3.390671
C	2.522143	2.772614	3.927941
C	3.588167	4.298356	2.350800
C	2.327149	4.674417	1.868684
C	1.180993	4.090967	2.394523
C	1.278691	3.137973	3.426864
H	6.726440	3.779734	5.955077
H	8.007936	5.908475	6.091693
H	7.837027	7.595413	4.265152
H	6.382934	7.163869	2.292958
H	4.993022	2.472873	4.852002
H	4.652319	5.799994	1.254001
H	2.597595	2.041756	4.738738
H	2.251183	5.424742	1.075882
H	0.197511	4.378324	2.013403
H	0.370289	2.692100	3.840434

2.v) Ionized Anthracene dimer plus water clusters

AntW

A
1 2

C	-6.777231	2.341732	-0.960071
C	-7.305933	1.195134	-0.378013
C	-6.437883	0.184235	0.100410
C	-5.018906	0.349543	-0.025076
C	-4.512305	1.529829	-0.615008
C	-5.384420	2.510227	-1.075196
C	-6.950714	-0.985511	0.706696
C	-4.161995	-0.667166	0.456767
C	-4.670756	-1.849142	1.044572
C	-6.088228	-2.007479	1.175529
C	-6.600779	-3.181803	1.771245
H	-7.683690	-3.298518	1.873283
C	-5.738169	-4.176878	2.213298
C	-4.344856	-4.024872	2.077993
C	-3.814572	-2.875646	1.507653
H	-8.038903	-1.085670	0.809360
H	-7.448135	3.121547	-1.330152
H	-8.385350	1.051517	-0.263588
H	-3.430587	1.663810	-0.709552
H	-4.984766	3.418521	-1.534170
H	-3.078100	-0.541785	0.363318
H	-6.141646	-5.086300	2.666156
H	-3.677407	-4.816782	2.427543
H	-2.731590	-2.755186	1.410735
C	-3.099770	0.090525	3.769667
C	-3.875032	1.096842	3.263904
C	-5.309109	1.047112	3.369694
C	-5.914046	-0.086101	4.011917
C	-5.063528	-1.126331	4.525971
C	-3.704543	-1.039744	4.412110
C	-6.126242	2.070791	2.871261
C	-7.309735	-0.143028	4.129057
C	-8.126100	0.883610	3.635760
C	-7.521206	2.014448	2.989106
C	-8.371605	3.059837	2.483976
H	-7.905834	3.921350	1.994720
C	-9.727913	2.992473	2.627393
C	-10.332740	1.873311	3.294721
C	-9.559281	0.853233	3.778312
H	-5.664061	2.938596	2.386962
H	-2.009275	0.150252	3.703662
H	-3.416115	1.970575	2.789040
H	-5.528248	-1.982869	5.024959
H	-3.067001	-1.828169	4.822618
H	-7.770972	-1.000391	4.632082
H	-10.363520	3.799340	2.252683
H	-11.418178	1.853804	3.432187
H	-10.015510	0.005812	4.300457
O	-9.943411	-0.208741	0.698224
H	-10.151893	0.293771	1.504758
H	-10.805847	-0.393218	0.300623

B

1 2

C	-8.917512	-2.191271	0.503254
C	-7.548966	-2.289422	0.292358
C	-6.743630	-1.125159	0.290757
C	-7.361483	0.151531	0.511432
C	-8.761171	0.221578	0.725481
C	-9.524415	-0.936957	0.714866
C	-5.349475	-1.184910	0.073712
C	-6.566622	1.315752	0.514332
C	-5.171839	1.255130	0.268619
C	-4.551339	-0.018068	0.048697
C	-3.157823	-0.074071	-0.196508
H	-2.680722	-1.044380	-0.363010
C	-2.407402	1.092265	-0.236726
C	-3.019519	2.343407	-0.029142
C	-4.381953	2.425970	0.227380
H	-4.876070	-2.158748	-0.093161
H	-9.531940	-3.095446	0.502622
H	-7.083828	-3.265515	0.125547
H	-9.211773	1.203392	0.902244
H	-10.603205	-0.879939	0.879080
H	-7.053139	2.282172	0.694827
H	-1.333723	1.041549	-0.435505
H	-2.416305	3.254245	-0.067954
H	-4.858071	3.395902	0.395330
C	-9.342096	-2.499790	4.041298
C	-7.986442	-2.434470	3.859145
C	-7.313996	-1.169031	3.795568
C	-8.089399	0.033561	3.923002
C	-9.510444	-0.076976	4.102677
C	-10.116181	-1.302841	4.162181
C	-5.923025	-1.073689	3.625934
C	-7.439973	1.274111	3.872413
C	-6.049407	1.369399	3.711327
C	-5.273474	0.165375	3.588359
C	-3.845477	0.274851	3.443632
H	-3.256286	-0.644359	3.361842
C	-3.235446	1.495717	3.430509
C	-4.010881	2.697152	3.554590
C	-5.369136	2.635942	3.689724
H	-5.330265	-1.992164	3.546656
H	-9.841235	-3.470800	4.106419
H	-7.391068	-3.349634	3.778152
H	-10.098630	0.840255	4.209205
H	-11.196459	-1.375414	4.316324
H	-8.029664	2.191411	3.979145
H	-2.148199	1.566999	3.335136
H	-3.501747	3.665468	3.556640
H	-5.960650	3.550817	3.799015
O	-8.842804	3.469243	1.091639
H	-9.087512	3.971079	1.882431
H	-9.269628	3.960295	0.373849

C

1 2

C	-8.664984	-2.520096	0.346180
C	-7.303439	-2.478547	0.235226
C	-6.604238	-1.222398	0.241893
C	-7.363919	-0.007881	0.361707
C	-8.795671	-0.096875	0.478909
C	-9.424058	-1.308621	0.469408
C	-5.208884	-1.147545	0.108545
C	-6.695341	1.221590	0.345178
C	-5.299930	1.297574	0.198817
C	-4.540370	0.084578	0.077813
C	-3.115751	0.174566	-0.079259
H	-2.539545	-0.750654	-0.182362
C	-2.491301	1.392306	-0.124121
C	-3.249389	2.599383	-0.010872
C	-4.608910	2.553045	0.150812
H	-4.631809	-2.073005	-0.000568
H	-9.188518	-3.480431	0.322624
H	-6.724338	-3.400899	0.122094
H	-9.372577	0.830377	0.558574
H	-10.513865	-1.364113	0.544387
H	-7.275794	2.148415	0.419548
H	-1.407869	1.449347	-0.262010

H	-2.735639	3.563492	-0.065221
H	-5.192196	3.476567	0.225796
C	-9.639516	-2.248893	3.920483
C	-8.269265	-2.321289	3.704754
C	-7.489410	-1.143944	3.679711
C	-8.126759	0.124202	3.870189
C	-9.526375	0.170126	4.074123
C	-10.268539	-1.002225	4.101860
C	-6.088242	-1.187672	3.484468
C	-7.339904	1.296362	3.858847
C	-5.940080	1.250585	3.675520
C	-5.302364	-0.019329	3.488815
C	-3.896886	-0.068624	3.317021
H	-3.410760	-1.037833	3.170235
C	-3.147548	1.095884	3.331065
C	-3.777623	2.345842	3.508382
C	-5.151204	2.425489	3.681207
H	-5.600929	-2.158718	3.346460
H	-10.235360	-3.165154	3.946679
H	-7.782513	-3.289866	3.559236
H	-10.015982	1.137882	4.218493
H	-11.348177	-0.959699	4.268001
H	-7.825981	2.266703	4.007554
H	-2.064032	1.049779	3.197137
H	-3.175203	3.258072	3.512683
H	-5.635338	3.396441	3.822734
O	-6.330252	-0.218975	6.397979
H	-5.577743	0.095084	6.919384
H	-6.916154	-0.596896	7.069271

D

1 2

C	4.131549	0.466502	1.587363
C	3.292503	0.265180	0.501899
C	3.202616	1.235704	-0.522939
C	3.952676	2.400297	-0.454243
C	4.873030	1.653895	1.688578
C	5.791878	1.953085	2.851881
C	4.782162	2.632820	0.653348
C	5.618514	3.885435	0.807843
C	7.084145	2.499487	2.287721
C	8.337816	2.071385	2.739198
C	6.998774	3.467083	1.264505
C	8.168163	3.997286	0.708602
C	9.411956	3.576371	1.172205
C	9.496300	2.611873	2.187084
H	4.215162	-0.290795	2.372218
H	2.704797	-0.653667	0.426643
H	2.546767	1.056726	-1.379175
H	3.897126	3.143555	-1.255050
H	6.003133	1.032644	3.411923
H	5.694542	4.388235	-0.167544
H	8.388531	1.317486	3.529785
H	8.101906	4.741813	-0.090929
H	10.324979	3.992666	0.738451
H	10.476299	2.278779	2.539427
C	6.605879	4.503436	5.188809
C	7.292815	5.708922	5.306960
C	7.212012	6.670883	4.289469
C	6.441386	6.427199	3.155490
C	5.840516	4.246055	4.045704
C	5.079151	2.953369	3.857759
C	5.755520	5.214818	3.023838
C	4.906092	4.887274	1.815739
C	3.699599	3.300493	3.343905
C	2.527762	2.712968	3.845603
C	3.610155	4.279356	2.308781
C	2.353702	4.644224	1.801911
C	1.208375	4.030047	2.286351
C	1.295878	3.060905	3.312373
H	6.659744	3.743693	5.973500
H	7.892069	5.911140	6.198878
H	7.748926	7.617778	4.390529
H	6.369556	7.182114	2.366277
H	5.002698	2.435950	4.823067
H	4.682433	5.813394	1.265963
H	2.595493	1.976140	4.651275
H	2.285522	5.406636	1.020278
H	0.228971	4.303400	1.884676

H	0.382791	2.595477	3.693116
O	7.046068	1.223037	5.722547
H	7.911484	1.562212	5.994772
H	6.887870	0.497868	6.344704

E

1 2

C	4.219761	0.442415	1.544750
C	3.452983	0.174957	0.408954
C	3.348033	1.130721	-0.607084
C	4.009881	2.353741	-0.487178
C	4.871883	1.670584	1.675063
C	5.720593	2.011401	2.882882
C	4.765617	2.630851	0.654578
C	5.503902	3.941093	0.839216
C	7.000014	2.649311	2.397424
C	8.265076	2.335809	2.931735
C	6.893420	3.618697	1.330166
C	8.052528	4.214880	0.815956
C	9.281719	3.902795	1.367246
C	9.387479	2.961597	2.435621
H	4.313955	-0.310257	2.333919
H	2.938734	-0.785045	0.311785
H	2.750954	0.919143	-1.498039
H	3.936337	3.099377	-1.285390
H	5.972573	1.087590	3.423717
H	5.579027	4.457183	-0.129154
H	8.342476	1.597487	3.734074
H	7.976038	4.934308	-0.003492
H	10.190042	4.376740	0.984658
H	10.374067	2.732854	2.847777
C	6.699372	4.488285	5.145796
C	7.461709	5.650249	5.204609
C	7.365692	6.611188	4.182995
C	6.505474	6.408446	3.107854
C	5.853459	4.260209	4.052107
C	5.007133	3.005825	3.904556
C	5.753618	5.230392	3.024604
C	4.804518	4.933262	1.874509
C	3.618721	3.405657	3.455586
C	2.461388	2.842487	3.998203
C	3.516990	4.372426	2.438825
C	2.258708	4.765956	1.977364
C	1.105971	4.199781	2.522562
C	1.207218	3.238254	3.532571
H	6.757558	3.748269	5.950268
H	8.125236	5.826005	6.055597
H	7.955943	7.529479	4.244041
H	6.415370	7.166895	2.323841
H	4.945343	2.493507	4.875967
H	4.591347	5.868074	1.335344
H	2.540717	2.093063	4.792229
H	2.179319	5.522117	1.189701
H	0.122563	4.513655	2.163005
H	0.303008	2.800156	3.963072
O	7.374495	0.893476	0.242179
H	8.079571	0.366927	-0.160168
H	6.564393	0.529970	-0.146803

F

1 2

C	4.109496	0.434103	1.646762
C	3.249344	0.171160	0.591006
C	3.098571	1.106070	-0.460017
C	3.808836	2.297021	-0.447405
C	4.810463	1.648390	1.690560
C	5.752529	2.015888	2.817533
C	4.658526	2.592453	0.629595
C	5.453558	3.877484	0.724238
C	7.010127	2.593665	2.205676
C	8.290408	2.241104	2.644471
C	6.859656	3.526534	1.158512
C	7.993073	4.090760	0.563297
C	9.265169	3.745042	1.015833
C	9.415406	2.821570	2.059926
H	4.239911	-0.296726	2.450239
H	2.693238	-0.769600	0.559443
H	2.427499	0.877619	-1.292311
H	3.706460	3.012096	-1.268877

H	6.006665	1.107414	3.383142
H	5.486592	4.352652	-0.267119
H	8.406056	1.505756	3.447685
H	7.877498	4.805176	-0.257924
H	10.149448	4.190957	0.552732
H	10.413713	2.566389	2.422016
C	6.525801	4.671263	5.054190
C	7.175622	5.903407	5.115786
C	7.021429	6.830201	4.075285
C	6.225337	6.521372	2.973962
C	5.735604	4.348703	3.946204
C	5.024094	3.019864	3.813532
C	5.585218	5.279786	2.897613
C	4.724397	4.881049	1.719557
C	3.617998	3.290977	3.321440
C	2.484121	2.674041	3.870751
C	3.466124	4.234435	2.259092
C	2.183939	4.534688	1.773982
C	1.076520	3.891389	2.305485
C	1.227096	2.957952	3.358136
H	6.632098	3.952583	5.873597
H	7.815893	6.142522	5.967636
H	7.524522	7.799269	4.130924
H	6.099329	7.248786	2.165777
H	4.971629	2.535331	4.799557
H	4.449473	5.779868	1.148429
H	2.598289	1.966316	4.697046
H	2.066211	5.270261	0.972908
H	0.077343	4.114145	1.921731
H	0.342444	2.470427	3.776439
O	9.909103	4.595865	4.547195
H	9.459855	5.005899	3.794415
H	9.285648	3.899797	4.795256

Ant2W

A
1 2

C	-6.463765	-3.802138	1.232743
C	-5.563483	-2.768463	1.253585
C	-5.910748	-1.482757	0.717205
C	-7.225183	-1.291559	0.170820
C	-8.142009	-2.395837	0.178179
C	-7.771634	-3.612389	0.688779
C	-5.003371	-0.415283	0.709733
C	-7.569050	-0.043620	-0.370146
C	-6.650823	1.016891	-0.403064
C	-5.340300	0.827916	0.149859
C	-4.394110	1.908228	0.078135
H	-3.386335	1.746011	0.475835
C	-4.729855	3.093955	-0.518176
C	-6.041679	3.285681	-1.068814
C	-6.970034	2.282051	-1.008882
H	-3.999414	-0.562044	1.123760
H	-6.180727	-4.785167	1.620350
H	-4.555111	-2.913433	1.654883
H	-9.139285	-2.252234	-0.249549
H	-8.473048	-4.451322	0.670660
H	-8.565432	0.096950	-0.803034
H	-3.990046	3.895783	-0.612300
H	-6.286993	4.234292	-1.554556
H	-7.965832	2.419895	-1.441947
C	-9.999311	-1.210921	2.923987
C	-8.898733	-1.885353	3.443348
C	-7.662510	-1.215625	3.604130
C	-7.560372	0.160298	3.206849
C	-8.695580	0.825032	2.676193
C	-9.899032	0.140024	2.544026
C	-6.529159	-1.863012	4.137589
C	-6.333332	0.833212	3.350362
C	-5.199639	0.188879	3.911640
C	-5.298059	-1.183219	4.307013
C	-4.156190	-1.829785	4.848330
H	-4.228012	-2.878502	5.151657
C	-2.967950	-1.138209	4.991362
C	-2.876603	0.220400	4.607089
C	-3.972242	0.878798	4.077356
H	-6.606453	-2.911508	4.444029
H	-10.952348	-1.735732	2.814664

H	-8.982535	-2.935786	3.736776
H	-8.592987	1.881239	2.402711
H	-10.777169	0.657330	2.148217
H	-6.264786	1.872874	3.015120
H	-2.092087	-1.640544	5.410241
H	-1.930141	0.752033	4.736979
H	-3.920383	1.931106	3.780423
O	-7.440774	3.635797	2.037289
H	-6.634834	3.969959	2.470575
H	-7.176356	3.572400	1.106389
O	-4.743994	3.924696	2.868230
H	-4.368174	3.880688	1.974475
H	-4.337044	4.708416	3.266623

B

1 2

O	5.345995	1.950916	8.609692
C	3.706260	-0.030403	3.831012
C	2.730575	-0.066070	2.876519
C	2.968089	0.482947	1.573104
C	4.174615	1.048208	1.268474
C	4.990446	0.553545	3.551667
C	6.015001	0.588623	4.505969
C	5.226411	1.106772	2.246347
C	6.478691	1.669605	1.955800
C	7.275348	1.133959	4.207572
C	8.338444	1.144465	5.168537
C	7.511022	1.689513	2.905041
C	8.802737	2.242923	2.614192
C	9.798071	2.231090	3.555503
C	9.563076	1.672390	4.849302
H	5.240251	2.067129	9.563425
H	5.828509	1.105756	8.515721
H	3.531484	-0.458610	4.823462
H	1.761461	-0.522739	3.096672
H	2.179581	0.428872	0.816859
H	4.364498	1.452227	0.268887
H	5.845759	0.165329	5.502704
H	6.660668	2.081184	0.956412
H	8.145329	0.705277	6.152154
H	8.983363	2.659085	1.617961
H	10.783423	2.641382	3.317473
H	10.373811	1.663969	5.583727
O	6.861880	-0.351689	8.039674
C	6.619532	3.828125	6.360308
C	7.777383	4.445938	5.910294
C	7.847531	4.989251	4.609763
C	6.760042	4.909495	3.756040
C	5.489225	3.742635	5.509804
C	4.294949	3.129064	5.948741
C	5.558285	4.288476	4.184086
C	4.433770	4.187899	3.343788
C	3.150867	3.074140	5.117881
C	1.936736	2.505228	5.571884
C	3.221758	3.603876	3.788714
C	2.078796	3.540378	2.957586
C	0.898123	2.988778	3.433228
C	0.825584	2.472097	4.742362
H	6.550056	3.383723	7.358587
H	8.647307	4.513935	6.568988
H	8.768865	5.471943	4.274236
H	6.817725	5.323885	2.744914
H	4.276428	2.689503	6.954624
H	4.487438	4.590085	2.326187
H	1.885098	2.102905	6.587957
H	2.133493	3.938389	1.940133
H	0.016539	2.953151	2.787723
H	-0.112747	2.042718	5.103187
H	7.709928	-0.490262	8.486607
H	6.505961	-1.246350	7.934509

C

1 2

O	5.109593	6.207349	3.726013
C	4.000608	0.177990	2.461107
C	2.808499	0.638270	1.981888
C	2.694493	1.977981	1.479096
C	3.777014	2.811298	1.473909
C	5.167736	1.021014	2.467637

C	6.407749	0.569424	2.933750
C	5.051114	2.364089	1.968062
C	6.184673	3.190142	1.953844
C	7.544647	1.394342	2.911952
C	8.825998	0.935799	3.365624
C	7.429091	2.734586	2.408174
C	8.599279	3.567853	2.384827
C	9.805625	3.093864	2.823935
C	9.921323	1.756546	3.318915
H	5.188621	6.491446	2.805258
H	4.951483	7.047802	4.207747
H	4.093640	-0.847003	2.834666
H	1.931410	-0.015172	1.968718
H	1.733441	2.322288	1.085891
H	3.696072	3.830448	1.082207
H	6.499738	-0.458268	3.303332
H	6.098146	4.211408	1.567640
H	8.915287	-0.091229	3.734076
H	8.508941	4.586544	1.994119
H	10.693467	3.731497	2.787687
H	10.896662	1.389894	3.651461
O	4.695542	8.612805	5.023132
C	7.360550	1.575314	6.578282
C	8.379821	2.508272	6.442549
C	8.138877	3.752831	5.827615
C	6.878833	4.064489	5.335681
C	6.062103	1.865710	6.095578
C	4.998644	0.944928	6.220003
C	5.818641	3.132309	5.465888
C	4.529786	3.430154	4.977938
C	3.696007	1.248721	5.760321
C	2.621497	0.338729	5.910746
C	3.457003	2.515437	5.134736
C	2.153925	2.832358	4.690305
C	1.114585	1.927769	4.864113
C	1.350770	0.678586	5.470323
H	7.553129	0.610990	7.057860
H	9.380051	2.275584	6.817404
H	8.955406	4.472047	5.727419
H	6.671727	5.015747	4.833436
H	5.183311	-0.023777	6.697392
H	4.371967	4.397715	4.482398
H	2.801172	-0.630249	6.385877
H	1.976151	3.801108	4.215222
H	0.106969	2.183268	4.525826
H	0.524544	-0.025663	5.598177
H	5.375980	9.275811	5.202705
H	3.862710	9.099535	5.088036

D
1 2

C	-8.935868	-2.258714	0.693138
C	-7.562241	-2.330114	0.682436
C	-6.775981	-1.140602	0.684369
C	-7.438319	0.131552	0.694311
C	-8.865724	0.167958	0.703402
C	-9.594755	-0.996949	0.702932
C	-5.370089	-1.182239	0.662877
C	-6.667662	1.304638	0.683694
C	-5.259005	1.264002	0.619755
C	-4.597276	-0.006143	0.606984
C	-3.177546	-0.044195	0.530682
H	-2.671813	-1.014740	0.519382
C	-2.447840	1.125115	0.448600
C	-3.102932	2.380635	0.455998
C	-4.478600	2.450233	0.552069
H	-4.865582	-2.154484	0.644297
H	-9.531352	-3.175842	0.685547
H	-7.056448	-3.300590	0.665860
H	-9.369806	1.139570	0.706682
H	-10.687392	-0.960374	0.705379
H	-7.172960	2.276613	0.680657
H	-1.357801	1.084937	0.373006
H	-2.512680	3.298434	0.386002
H	-4.984943	3.420329	0.556767
C	-9.460188	-2.410441	4.174977
C	-8.083780	-2.395439	4.069271
C	-7.375783	-1.164058	4.008726
C	-8.114007	0.063539	4.039246

C	-9.534682	0.013793	4.128086
C	-10.191496	-1.196721	4.202613
C	-5.967893	-1.118390	3.931628
C	-7.416183	1.283589	3.991030
C	-6.010357	1.328107	3.952070
C	-5.271812	0.098774	3.925662
C	-3.843018	0.151165	3.906427
H	-3.280446	-0.787678	3.891913
C	-3.187799	1.356848	3.915934
C	-3.923301	2.577305	3.939246
C	-5.297666	2.564094	3.960171
H	-5.404307	-2.057777	3.926239
H	-9.992604	-3.363408	4.239601
H	-7.520270	-3.333536	4.051682
H	-10.097310	0.952245	4.154417
H	-11.281201	-1.224222	4.287748
H	-7.978704	2.223098	4.024244
H	-2.094941	1.387543	3.906260
H	-3.384855	3.529060	3.953537
H	-5.862266	3.501307	3.990522
O	-6.101268	0.027171	-2.154473
H	-5.467228	0.339127	-2.815461
H	-6.832215	-0.304646	-2.694780
O	-6.561336	0.128284	6.789900
H	-5.830068	0.472695	7.321669
H	-7.185369	-0.189084	7.457667

E
1 2

C	-8.733358	-2.692600	-3.839972
C	-7.492729	-2.659471	-3.203986
C	-6.904606	-1.433590	-2.880612
C	-7.565725	-0.233739	-3.202596
C	-8.806212	-0.273040	-3.844645
C	-9.390178	-1.499478	-4.160387
C	-5.574701	-1.332913	-2.167808
C	-6.888739	1.063236	-2.818424
C	-5.414959	0.965966	-3.166997
C	-4.748137	-0.240636	-2.823543
C	-3.381730	-0.384805	-3.107719
H	-2.873518	-1.320959	-2.857276
C	-2.681255	0.660804	-3.695018
C	-3.345469	1.854260	-4.041245
C	-4.705885	1.998294	-3.793511
H	-5.038753	-2.289438	-2.254455
H	-9.190085	-3.652801	-4.093944
H	-6.975217	-3.592107	-2.957915
H	-9.316390	0.660830	-4.101644
H	-10.359751	-1.527779	-4.664563
H	-7.340832	1.892888	-3.381656
H	-1.614104	0.553534	-3.906894
H	-2.788940	2.664394	-4.520241
H	-5.224386	2.919369	-4.077018
C	-9.147497	-1.617752	0.971548
C	-7.826207	-1.824143	0.572564
C	-7.158754	-0.839561	-0.165512
C	-7.812901	0.364361	-0.485848
C	-9.132744	0.569600	-0.071369
C	-9.800785	-0.421371	0.647729
C	-5.726676	-1.017134	-0.619121
C	-7.031357	1.401409	-1.268893
C	-5.655021	1.502039	-0.647226
C	-4.999514	0.266238	-0.300507
C	-3.742263	0.288769	0.334825
H	-3.302499	-0.657444	0.662297
C	-3.120378	1.500388	0.558019
C	-3.757793	2.721810	0.195231
C	-5.019979	2.721730	-0.376074
H	-5.263610	-1.832650	-0.049381
H	-9.673739	-2.390799	1.538495
H	-7.293933	-2.742106	0.842018
H	-9.641084	1.507817	-0.315597
H	-10.835451	-0.261717	0.962730
H	-7.531492	2.377459	-1.181752
H	-2.136083	1.534169	1.033158
H	-3.247560	3.669049	0.391566
H	-5.516073	3.662709	-0.629543
O	-4.464816	-2.497681	1.749737
H	-4.929626	-1.820064	2.281364

H	-4.187599	-3.169720	2.385767
O	-5.929970	-0.313439	2.709146
H	-5.904216	0.106045	3.581173
H	-6.874940	-0.434713	2.526024

F

1 2

C	-9.822325	-2.720407	-1.607628
C	-8.485138	-2.937119	-1.429935
C	-7.549154	-1.844831	-1.470741
C	-8.045684	-0.517109	-1.702956
C	-9.461447	-0.330543	-1.883199
C	-10.319273	-1.393361	-1.837051
C	-6.172504	-2.041927	-1.300574
C	-7.142900	0.554099	-1.749159
C	-5.765437	0.356900	-1.585268
C	-5.267688	-0.973345	-1.363271
C	-3.846416	-1.168380	-1.230637
H	-3.469974	-2.184615	-1.077251
C	-2.983681	-0.112469	-1.314279
C	-3.481238	1.216969	-1.531152
C	-4.823599	1.442406	-1.658152
H	-5.792693	-3.056483	-1.137605
H	-10.523960	-3.558977	-1.587628
H	-8.100954	-3.949113	-1.267199
H	-9.836927	0.679946	-2.075073
H	-11.391719	-1.241654	-1.988142
H	-7.520366	1.565569	-1.937254
H	-1.905869	-0.274100	-1.226230
H	-2.773886	2.047652	-1.609888
H	-5.203647	2.452973	-1.838327
C	-8.200222	-2.049723	2.423901
C	-7.220333	-1.675458	3.337402
C	-6.827122	-0.319073	3.432343
C	-7.447041	0.658134	2.585400
C	-8.443835	0.247907	1.674567
C	-8.812189	-1.091372	1.596340
C	-5.819660	0.085228	4.334174
C	-7.031536	2.005370	2.673595
C	-6.031787	2.417718	3.584936
C	-5.415735	1.439655	4.429449
C	-4.412271	1.843472	5.337334
H	-3.940318	1.094846	5.979905
C	-4.028410	3.176122	5.409674
C	-4.635209	4.138900	4.580016
C	-5.623964	3.768581	3.678998
H	-5.352457	-0.675903	4.971039
H	-8.499707	-3.098120	2.343880
H	-6.734385	-2.406867	3.991088
H	-8.917974	0.985677	1.020851
H	-9.573869	-1.400546	0.875916
H	-7.496074	2.749996	2.018358
H	-3.250655	3.482009	6.113993
H	-4.324395	5.184538	4.647994
H	-6.093891	4.518174	3.035666
O	-4.591115	0.541043	1.596430
H	-4.787910	-0.234210	1.049532
H	-4.038287	1.064678	0.997754
O	-5.192556	-2.722596	5.665750
H	-4.438105	-3.306063	5.499066
H	-5.533540	-3.030527	6.518165

G

1 2

C	-8.805763	-2.460187	-0.307289
C	-7.615931	-2.422229	0.422448
C	-7.088328	-1.197947	0.838864
C	-7.750938	-0.003000	0.510198
C	-8.933892	-0.044192	-0.231301
C	-9.465102	-1.270951	-0.634251
C	-5.800353	-1.098989	1.629370
C	-7.130303	1.298413	0.974449
C	-5.647225	1.235981	0.694896
C	-4.966715	0.010468	1.035998
C	-3.583791	-0.105731	0.808023
H	-3.075177	-1.040248	1.058298
C	-2.887195	0.961931	0.282163
C	-3.561304	2.171616	-0.058782

C	-4.924198	2.298253	0.131738
H	-5.245760	-2.044982	1.544800
H	-9.218657	-3.420836	-0.626597
H	-7.092021	-3.351352	0.668549
H	-9.443559	0.887780	-0.495628
H	-10.395070	-1.300705	-1.208406
H	-7.564203	2.133212	0.404735
H	-1.809768	0.886169	0.111839
H	-2.986874	3.000991	-0.481361
H	-5.441806	3.222154	-0.140093
C	-9.524050	-1.562938	4.489539
C	-8.170536	-1.712246	4.186090
C	-7.476912	-0.678956	3.550830
C	-8.145946	0.514705	3.224485
C	-9.500482	0.660794	3.533726
C	-10.189134	-0.376894	4.162655
C	-6.016582	-0.794549	3.177474
C	-7.348101	1.594851	2.525698
C	-5.994404	1.718052	3.205512
C	-5.320268	0.510898	3.528220
C	-4.069709	0.555393	4.163183
H	-3.576744	-0.385176	4.428727
C	-3.483762	1.784785	4.441166
C	-4.151948	2.983000	4.122308
C	-5.406930	2.948961	3.524236
H	-5.542741	-1.612904	3.736275
H	-10.063753	-2.371914	4.989279
H	-7.645119	-2.637667	4.443834
H	-10.019259	1.591799	3.283423
H	-11.248502	-0.259525	4.405624
H	-7.881455	2.553513	2.605687
H	-2.503991	1.825346	4.925063
H	-3.686534	3.943469	4.360501
H	-5.935240	3.879447	3.294129
O	-5.626788	-0.430780	-1.711938
H	-5.244569	-0.428594	-2.600788
H	-6.486497	-0.861943	-1.832016
O	-3.908025	-2.669670	4.814907
H	-3.316979	-3.426922	4.695827
H	-4.087531	-2.675648	5.766806

Ant2W3

A
1 2

O	5.363432	6.637620	0.957105
O	3.338317	6.578864	2.795796
C	4.907477	-0.264069	0.646768
C	3.584944	-0.138666	0.319868
C	3.009174	1.155608	0.106378
C	3.770421	2.283374	0.234645
C	5.740126	0.897210	0.789585
C	7.104772	0.799022	1.106665
C	5.161155	2.195531	0.583998
C	5.961233	3.338160	0.722306
C	7.917373	1.938198	1.215101
C	9.318842	1.848440	1.505042
C	7.332395	3.234151	1.021370
C	8.163838	4.392344	1.137451
C	9.504572	4.267318	1.407329
C	10.090321	2.978692	1.589610
H	5.603734	7.257161	0.253766
H	5.848399	6.944223	1.754537
H	5.355364	-1.252613	0.791019
H	2.961962	-1.029719	0.200338
H	1.953182	1.233149	-0.168029
H	3.336804	3.273729	0.062608
H	7.550665	-0.191855	1.250208
H	5.528063	4.333921	0.575001
H	9.766044	0.858190	1.638290
H	7.702001	5.373589	0.992967
H	10.135507	5.158269	1.475727
H	11.162133	2.898575	1.791565
H	2.608388	7.211375	2.742969
H	3.784839	6.625163	1.920347
O	5.916484	7.101975	3.579700
C	7.501044	1.295837	4.694007
C	8.563821	2.164700	4.869282
C	8.397485	3.554310	4.670740

C	7.173599	4.070997	4.285707
C	6.230614	1.791718	4.302330
C	5.121518	0.938164	4.121333
C	6.068088	3.201151	4.091580
C	4.810430	3.697646	3.693631
C	3.846485	1.438879	3.771533
C	2.719645	0.589579	3.643815
C	3.689022	2.845327	3.551622
C	2.417576	3.358415	3.201452
C	1.328821	2.503095	3.099711
C	1.479014	1.119686	3.324999
H	7.629975	0.221044	4.853494
H	9.539946	1.776068	5.171392
H	9.249196	4.223727	4.817055
H	7.028481	5.144408	4.127728
H	5.246012	-0.139263	4.276361
H	4.683564	4.769965	3.520173
H	2.837507	-0.485216	3.809774
H	2.321525	4.433816	3.021634
H	0.344544	2.903284	2.841958
H	0.611106	0.460229	3.241019
H	6.189342	7.860031	4.115123
H	4.935482	7.089887	3.620844

B
1 2

C	4.735877	-0.691787	2.898974
C	3.612649	-1.298742	2.344580
C	3.226010	-1.020549	1.020531
C	3.951789	-0.124753	0.241564
C	5.508549	0.198946	2.118439
C	6.661668	0.821799	2.651532
C	5.107415	0.493359	0.774337
C	5.861476	1.418162	0.013910
C	7.442437	1.711660	1.873964
C	8.610109	2.313106	2.396525
C	7.024707	2.028237	0.541489
C	7.780934	2.951053	-0.219500
C	8.920669	3.531011	0.318287
C	9.336997	3.209456	1.625718
H	5.034896	-0.871064	3.936805
H	3.021738	-1.996653	2.944418
H	2.338249	-1.504436	0.604232
H	3.639555	0.135701	-0.774424
H	6.919733	0.631093	3.700311
H	5.519258	1.668379	-0.997601
H	8.926367	2.071588	3.414520
H	7.457656	3.195336	-1.235713
H	9.503296	4.240535	-0.275499
H	10.236551	3.675317	2.036146
O	4.161218	1.957931	6.696140
O	6.151862	0.300730	5.664490
C	6.746443	3.842111	4.870431
C	7.850022	4.633340	5.027426
C	8.171554	5.639257	4.056259
C	7.394722	5.799488	2.944327
C	5.885756	4.001832	3.727829
C	4.734476	3.221276	3.553527
C	6.231197	4.979776	2.733408
C	5.426600	5.111429	1.593544
C	3.925038	3.361645	2.417590
C	2.735246	2.574586	2.233061
C	4.283697	4.319800	1.410042
C	3.435990	4.456460	0.254476
C	2.304924	3.697587	0.122269
C	1.951988	2.734596	1.125882
H	3.234709	1.771901	6.903266
H	4.276772	2.891743	6.923510
H	6.517829	3.047136	5.588115
H	8.497938	4.506354	5.899678
H	9.048291	6.274278	4.212301
H	7.639074	6.561340	2.197323
H	4.449378	2.506795	4.333499
H	5.689614	5.858177	0.835895
H	2.467198	1.845086	3.004643
H	3.698388	5.205023	-0.500618
H	1.640572	3.841312	-0.736932
H	1.042771	2.139688	1.001362
H	6.607678	-0.133413	6.398734

H	5.443646	0.818907	6.096617
O	3.865630	1.860637	-2.295092
H	3.370979	2.579680	-1.871550
H	3.613665	1.909638	-3.227640

C
1 2

C	3.462164	5.943799	18.252520
C	2.290612	5.961206	18.994491
C	1.662279	7.187047	19.304952
C	2.206997	8.388199	18.870687
C	4.038903	7.154197	17.791683
C	5.221301	7.166555	17.020760
C	3.401052	8.398587	18.110653
C	3.974562	9.607308	17.646921
C	5.785901	8.372461	16.542692
C	6.955781	8.382606	15.748176
C	5.152689	9.617003	16.869933
C	5.714483	10.825828	16.396103
C	6.866078	10.807110	15.618619
C	7.483877	9.585586	15.291431
H	3.952965	5.000960	18.022387
H	1.859081	5.030804	19.350064
H	0.746723	7.186361	19.888661
H	1.720854	9.331052	19.110025
H	5.705664	6.221970	16.777988
H	3.477019	10.550156	17.860144
H	7.439918	7.441139	15.500646
H	5.219431	11.764369	16.631205
H	7.288162	11.738277	15.252343
H	8.382162	9.584069	14.680583
C	8.481939	7.224461	18.830378
C	9.119640	8.347535	18.377525
C	8.599805	9.650978	18.677943
C	7.459069	9.788066	19.419379
C	7.280752	7.325845	19.614489
C	6.615664	6.191342	20.106097
C	6.758681	8.633019	19.916772
C	5.596742	8.743136	20.691631
C	5.461019	6.301780	20.895535
C	4.782174	5.148909	21.419383
C	4.937255	7.607990	21.193958
C	3.761304	7.710175	22.010054
C	3.146608	6.586823	22.500476
C	3.662934	5.287019	22.198814
H	8.883532	6.234897	18.621480
H	10.036304	8.261634	17.800017
H	9.129050	10.529094	18.318144
H	7.068092	10.774547	19.661403
H	7.021399	5.203119	19.891812
H	5.210150	9.732574	20.934395
H	5.187756	4.163022	21.201180
H	3.378345	8.700490	22.248260
H	2.268404	6.676066	23.133896
H	3.167879	4.409839	22.606344
O	2.654173	10.813834	15.244600
O	2.712395	8.192449	15.018985
H	3.393365	10.685380	14.579126
H	2.018321	11.489224	14.958749
H	1.993155	7.558382	14.877167
H	2.386489	9.099891	15.272079
O	4.394705	9.658498	13.715796
H	4.726794	9.625803	12.806723
H	3.927896	8.826099	14.001679

D
1 2

O	7.168685	-0.912119	0.928248
C	3.958633	0.930918	2.334135
C	2.870628	0.735652	1.494663
C	2.986166	0.964671	0.109459
C	4.193077	1.372729	-0.442819
C	5.200555	1.346500	1.795334
C	6.320259	1.546251	2.629649
C	5.323173	1.566601	0.384978
C	6.572094	1.963618	-0.142508
C	7.576849	1.927200	2.093551
C	8.707656	2.087674	2.922396
C	7.704981	2.140976	0.684149

C	8.962012	2.513212	0.152348
C	10.060684	2.654613	0.988270
C	9.935241	2.438703	2.373859
H	3.891490	0.779409	3.416617
H	1.912355	0.414329	1.910214
H	2.116380	0.817832	-0.536621
H	4.278702	1.544528	-1.520036
H	6.196124	1.399302	3.709911
H	6.667933	2.125252	-1.221668
H	8.604835	1.927620	3.999301
H	9.061850	2.679894	-0.924365
H	11.031256	2.933304	0.569424
H	10.809312	2.552181	3.020722
H	6.569350	-1.653132	0.760878
H	8.041848	-1.328629	0.902040
O	2.957641	2.606255	6.704112
O	4.921394	1.043312	5.413404
C	6.791048	4.749871	4.268438
C	7.987042	5.222871	3.809058
C	8.144129	5.588656	2.429573
C	7.098566	5.474119	1.559761
C	5.664161	4.617227	3.384583
C	4.420382	4.153024	3.835013
C	5.817364	4.991074	2.004697
C	4.720860	4.884696	1.140783
C	3.319864	4.058957	2.972926
C	2.038898	3.595570	3.431708
C	3.471509	4.431860	1.594272
C	2.331155	4.339277	0.726596
C	1.123716	3.904108	1.201110
C	0.975973	3.522587	2.573644
H	3.112055	3.323012	7.336970
H	2.115295	2.220469	6.984911
H	6.665088	4.470227	5.319559
H	8.833936	5.335727	4.492561
H	9.109275	5.968679	2.082496
H	7.212610	5.761474	0.509414
H	4.298822	3.861980	4.882865
H	4.834289	5.180383	0.091442
H	1.943660	3.314432	4.484999
H	2.442816	4.638587	-0.320626
H	0.258037	3.852574	0.534335
H	0.000082	3.182495	2.932427
H	5.019310	0.235722	5.936578
H	4.281270	1.577379	5.924377

E

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C	-0.432634	8.289833	13.459036
C	-1.816777	8.171497	13.518377
C	-2.636483	8.883669	12.622754
C	-2.078344	9.719865	11.663710
C	0.158747	9.136208	12.492711
C	1.563902	9.273221	12.411295
C	-0.673531	9.863668	11.578686
C	-0.066613	10.701668	10.614645
C	2.168000	10.113336	11.448257
C	3.574691	10.243271	11.377089
C	1.337961	10.840448	10.531127
C	1.947044	11.676065	9.566091
C	3.331530	11.786253	9.513205
C	4.142551	11.073358	10.415884
H	0.222298	7.740021	14.143177
H	-2.274702	7.518110	14.265360
H	-3.722526	8.775881	12.681850
H	-2.720013	10.269617	10.969148
H	2.187338	8.712304	13.109767
H	-0.700110	11.255294	9.913134
H	4.190177	9.685462	12.091679
H	1.320423	12.233239	8.863654
H	3.794455	12.433836	8.764013
H	5.229565	11.174840	10.360628
C	8.227554	7.963608	15.476061
C	8.962235	9.105701	15.335222
C	8.491188	10.346946	15.877667
C	7.301546	10.406054	16.544368
C	6.965288	7.982922	16.168075
C	6.183505	6.827353	16.322473
C	6.493384	9.228153	16.711573

C	5.264859	9.257617	17.385246
C	4.955370	6.860887	16.996523
C	4.147991	5.680971	17.169613
C	4.484613	8.104523	17.539179
C	3.223326	8.123824	18.232487
C	2.483739	6.984818	18.375921
C	2.955060	5.739429	17.836412
H	8.588825	7.013319	15.071274
H	9.922599	9.080003	14.813426
H	9.098305	11.248183	15.757444
H	6.944635	11.350432	16.966660
H	6.546672	5.877265	15.915382
H	4.915037	10.203344	17.814641
H	4.515090	4.730942	16.768980
H	2.872229	9.070737	18.655030
H	1.532631	7.009089	18.914872
H	2.359012	4.833213	17.977564
O	2.632765	9.984880	15.320780
O	2.326565	7.337316	14.934292
H	3.524870	9.783234	14.961658
H	2.791958	10.552645	16.086343
H	2.436432	6.678834	15.638478
H	2.281144	8.203262	15.401255
O	4.582994	8.626573	13.961812
H	5.455929	8.419718	14.329737
H	4.007361	7.888343	14.258830

F
1 2

C	2.160987	6.833217	13.153880
C	1.090686	6.294163	13.864590
C	1.178392	6.134354	15.254899
C	2.342201	6.503566	15.930242
C	3.333784	7.198212	13.823406
C	4.540933	7.743793	13.095581
C	3.428474	7.023589	15.217289
C	4.744622	7.373901	15.875590
C	5.151104	8.866811	13.908996
C	5.625674	10.052236	13.326135
C	5.248837	8.686131	15.312012
C	5.811758	9.694580	16.108501
C	6.305900	10.852127	15.514304
C	6.213097	11.029639	14.119254
H	2.084513	6.991964	12.074321
H	0.174281	6.011057	13.340013
H	0.332686	5.721391	15.811561
H	2.411788	6.376735	17.015423
H	4.217251	8.150631	12.128796
H	4.599197	7.474047	16.961412
H	5.511870	10.202980	12.249346
H	5.870584	9.562206	17.193458
H	6.752351	11.635669	16.132677
H	6.584203	11.952536	13.665738
C	8.039961	7.501813	12.783568
C	9.200817	7.845388	13.453831
C	9.302990	7.662968	14.858787
C	8.243560	7.137455	15.579311
C	6.940481	7.002830	13.502198
C	5.635164	6.618762	12.846504
C	7.045014	6.816241	14.923262
C	5.843072	6.245565	15.640575
C	5.252852	5.266648	13.408282
C	4.814692	4.213660	12.596738
C	5.352727	5.081427	14.806450
C	5.011504	3.846659	15.370299
C	4.557120	2.812577	14.557377
C	4.458960	2.996219	13.168974
H	7.965294	7.627777	11.699900
H	10.053426	8.250692	12.902377
H	10.232821	7.930595	15.367885
H	8.329445	6.981310	16.658259
H	5.791536	6.531480	11.761375
H	6.161346	5.875181	16.626139
H	4.746489	4.354644	11.513737
H	5.097773	3.700050	16.451300
H	4.282153	1.851592	14.999848
H	4.107782	2.177711	12.535204
O	2.609098	9.977101	12.306541
O	2.877205	11.323322	14.790612

H	1.870086	9.693571	12.904681
H	2.163048	10.506050	11.629175
H	3.663236	11.014376	15.261142
H	3.042378	11.068247	13.860604
O	0.827334	9.595232	14.302116
H	0.890954	8.786013	14.829324
H	1.387511	10.247174	14.778647

G
1 2

O	7.357486	0.761364	0.397771
C	4.113632	0.440464	1.644544
C	3.386000	0.109343	0.499135
C	3.363060	0.981707	-0.593522
C	4.065525	2.187210	-0.539650
C	4.806762	1.650913	1.706839
C	5.614767	2.058596	2.922348
C	4.779876	2.529271	0.610673
C	5.555766	3.826062	0.728219
C	6.935221	2.608469	2.449924
C	8.163208	2.302072	3.071966
C	6.909850	3.502457	1.309302
C	8.109086	4.028690	0.814657
C	9.298928	3.724463	1.450692
C	9.324667	2.860365	2.589793
H	8.054734	0.166028	0.088288
H	6.545357	0.376937	0.034336
H	4.141811	-0.246956	2.495950
H	2.837845	-0.835695	0.456537
H	2.797860	0.719895	-1.491935
H	4.054901	2.867795	-1.397026
H	5.803113	1.177124	3.552027
H	5.694693	4.261267	-0.272299
H	8.175438	1.627798	3.932025
H	8.094982	4.689854	-0.055561
H	10.239045	4.145971	1.083672
H	10.282941	2.640185	3.068051
O	3.527343	5.025785	6.285174
O	4.885530	2.671481	6.898003
C	6.577519	4.689917	5.027972
C	7.364601	5.838880	5.032919
C	7.341760	6.720451	3.938416
C	6.526491	6.456209	2.839984
C	5.781871	4.399790	3.908442
C	4.904877	3.158883	3.828612
C	5.752436	5.290210	2.809666
C	4.844377	4.922892	1.645177
C	3.551527	3.563023	3.291134
C	2.357904	3.083616	3.840569
C	3.516170	4.446824	2.197937
C	2.286942	4.842214	1.664145
C	1.097541	4.362563	2.215835
C	1.132048	3.484540	3.304163
H	2.859012	4.924423	5.590137
H	4.119013	5.710132	5.939082
H	6.541782	4.014962	5.890028
H	7.991513	6.066356	5.899729
H	7.951679	7.627907	3.958129
H	6.491516	7.156249	1.998963
H	4.799566	2.728459	4.832326
H	4.682382	5.812590	1.018700
H	2.397026	2.400276	4.695938
H	2.257668	5.532778	0.814990
H	0.137649	4.677911	1.798326
H	0.199122	3.112383	3.736330
H	4.782286	2.344340	7.800864
H	4.353357	3.494177	6.868362

H
1 2

O	3.550148	1.371479	1.356448
C	5.521447	-2.666268	0.200107
C	5.384652	-3.612837	-0.790191
C	5.835968	-3.344837	-2.109897
C	6.416903	-2.135129	-2.418985
C	6.117386	-1.403465	-0.085280
C	6.269366	-0.416936	0.912763
C	6.573051	-1.133685	-1.418108
C	7.163919	0.116935	-1.702951

C	6.854891	0.826725	0.622363
C	7.012704	1.825314	1.628914
C	7.313054	1.098423	-0.714097
C	7.912826	2.363579	-0.992537
C	8.054068	3.308741	0.002862
C	7.603361	3.040165	1.318807
H	3.952727	1.165118	0.500458
H	3.494497	2.339486	1.374467
H	5.178276	-2.871060	1.218316
H	4.928427	-4.580001	-0.563994
H	5.720741	-4.108703	-2.883155
H	6.766091	-1.930038	-3.435084
H	5.904806	-0.604089	1.929117
H	7.516581	0.320477	-2.719582
H	6.665429	1.603363	2.640996
H	8.263131	2.571430	-2.008089
H	8.519586	4.272080	-0.220511
H	7.728026	3.800058	2.091926
O	4.719200	5.551858	6.442630
C	7.708909	3.349941	4.828145
C	8.932508	3.980730	4.889195
C	9.063858	5.339891	4.490188
C	7.970560	6.041861	4.036825
C	6.557745	4.045076	4.350338
C	5.314487	3.402350	4.224483
C	6.688420	5.416433	3.946771
C	5.566416	6.093818	3.445244
C	4.192734	4.084581	3.716641
C	2.923583	3.440301	3.595459
C	4.319538	5.455017	3.317230
C	3.173572	6.131262	2.797869
C	1.967687	5.480588	2.683676
C	1.840438	4.120826	3.087326
H	7.603172	2.307312	5.144101
H	9.810229	3.439099	5.252055
H	10.040855	5.826520	4.550860
H	8.070120	7.089076	3.735258
H	5.210604	2.349501	4.507922
H	5.663690	7.141999	3.143742
H	2.836292	2.397074	3.912545
H	3.269501	7.178186	2.494575
H	1.096126	6.007608	2.286511
H	0.871951	3.620872	2.998693
H	5.214088	5.704119	7.259829
H	3.805000	5.729757	6.704579
O	4.704601	0.330906	3.652060
H	4.204724	0.630662	2.861779
H	4.127733	-0.320517	4.073939

Ant2W4

A
1 2

O	4.986330	7.035453	5.370134
O	4.825617	7.310977	2.688322
C	3.661182	0.497292	1.489222
C	2.324103	0.746025	1.250002
C	1.811460	2.063225	1.334279
C	2.642066	3.122085	1.647306
C	4.548388	1.564931	1.796922
C	5.925064	1.348117	2.023901
C	4.029465	2.899500	1.871683
C	4.905361	3.964184	2.165045
C	6.805725	2.412863	2.275259
C	8.206613	2.208856	2.463600
C	6.285748	3.748952	2.344025
C	7.178022	4.833400	2.588144
C	8.522888	4.596976	2.764743
C	9.041900	3.274267	2.701528
H	5.095166	7.727952	6.037197
H	4.065315	6.696976	5.493747
H	4.055857	-0.521428	1.427911
H	1.653567	-0.080303	0.998160
H	0.748530	2.239389	1.147567
H	2.260122	4.144775	1.729423
H	6.320556	0.327763	1.968358
H	4.518357	4.985654	2.227460
H	8.605471	1.191472	2.410274
H	6.762004	5.844142	2.633858

H	9.204869	5.431887	2.948094
H	10.113710	3.109262	2.841233
H	5.188242	8.132982	2.330768
H	4.989863	7.349227	3.663715
O	2.287538	6.365654	2.597496
O	2.539847	5.889061	5.246549
C	8.342493	1.843281	5.963556
C	9.123784	2.947739	6.227666
C	8.559115	4.248893	6.208536
C	7.220892	4.429414	5.924466
C	6.951571	1.989267	5.685456
C	6.121807	0.881319	5.430743
C	6.383645	3.306165	5.668989
C	5.006096	3.461980	5.407329
C	4.740613	1.032649	5.203818
C	3.881359	-0.087903	4.987482
C	4.172626	2.351275	5.200689
C	2.766404	2.506053	4.987206
C	1.971584	1.405959	4.783101
C	2.535464	0.096885	4.778205
H	1.636949	6.916162	2.139880
H	3.151110	6.833187	2.486145
H	8.776248	0.838856	5.982620
H	10.185456	2.823785	6.458707
H	9.193790	5.113743	6.421091
H	6.770631	5.427072	5.897095
H	6.555520	-0.125099	5.441934
H	4.568657	4.464464	5.405569
H	4.309229	-1.095553	4.998644
H	2.353512	3.519499	4.996971
H	0.896160	1.527449	4.624595
H	1.884655	-0.767455	4.617560
H	1.756761	6.077614	5.782246
H	2.272358	6.069260	4.311335

B

1 2

C	5.312950	11.794847	16.701055
C	6.128492	12.572397	15.895921
C	6.540375	12.100418	14.633728
C	6.131400	10.856466	14.177197
C	4.882705	10.519369	16.263603
C	4.031250	9.718602	17.050852
C	5.301519	10.041970	14.980136
C	4.847771	8.779866	14.532122
C	3.566594	8.459424	16.597838
C	2.673883	7.683656	17.367054
C	3.987482	7.980419	15.316683
C	3.506156	6.734312	14.852306
C	2.629976	5.990560	15.628559
C	2.209631	6.467408	16.884008
H	4.995168	12.156913	17.683213
H	6.462980	13.552971	16.243420
H	7.186207	12.723449	14.009238
H	6.444631	10.495763	13.193104
H	3.693425	10.093035	18.021141
H	5.148759	8.426593	13.541789
H	2.348423	8.054542	18.342864
H	3.824575	6.370048	13.871153
H	2.258041	5.030110	15.261978
H	1.514618	5.873569	17.483736
C	5.520721	7.505156	19.627022
C	5.094392	6.256848	19.272013
C	5.521510	5.664257	18.036297
C	6.360670	6.340583	17.199045
C	6.404239	8.251508	18.771327
C	6.871749	9.528068	19.117798
C	6.836067	7.657258	17.535799
C	7.712046	8.365711	16.705080
C	7.755168	10.233973	18.289404
C	8.251817	11.536694	18.639974
C	8.185951	9.640222	17.054711
C	9.102365	10.366298	16.221357
C	9.559903	11.600892	16.592926
C	9.124690	12.197181	17.819895
H	5.210162	7.952464	20.576923
H	4.434760	5.691846	19.937255
H	5.176320	4.659443	17.776375
H	6.698748	5.886772	16.261639

H	6.556293	9.974383	20.067806
H	8.052640	7.906381	15.769991
H	7.930119	11.982939	19.586541
H	9.440350	9.903786	15.288363
H	10.270702	12.137767	15.958158
H	9.508605	13.181031	18.104321
O	3.047748	12.102668	14.261553
O	2.815431	9.853147	12.787062
H	2.731334	12.977562	13.998057
H	2.503343	11.861870	15.050882
H	2.562217	10.033688	11.870994
H	2.928464	10.746803	13.201771
O	1.075496	8.936578	14.674193
O	1.575067	11.038387	16.295389
H	0.204876	8.734674	14.304881
H	1.636074	9.167365	13.893308
H	0.758731	11.446899	16.616073
H	1.275622	10.248296	15.775870

C
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O	7.012508	4.211757	-0.113585
O	4.529777	4.585356	1.096554
C	4.334501	-0.603320	4.326819
C	3.119222	-0.655461	3.659473
C	2.946378	0.021122	2.436009
C	3.984297	0.759216	1.880845
C	5.415324	0.134036	3.785123
C	6.667787	0.201064	4.429170
C	5.229546	0.833753	2.546496
C	6.292893	1.597639	2.014961
C	7.750531	0.926344	3.875365
C	9.020029	0.955381	4.495323
C	7.552404	1.651260	2.654305
C	8.618856	2.403009	2.105408
C	9.857972	2.403684	2.733599
C	10.060468	1.674573	3.920931
H	7.452797	4.772988	-0.766960
H	6.398051	3.650007	-0.634969
H	4.467321	-1.129230	5.277006
H	2.289582	-1.225815	4.084566
H	1.983078	-0.033053	1.922198
H	3.868110	1.291104	0.931535
H	6.812972	-0.333453	5.374281
H	6.130010	2.150039	1.086017
H	9.174917	0.404850	5.427565
H	8.434780	2.981248	1.193720
H	10.685089	2.975015	2.303899
H	11.043129	1.682917	4.400225
H	5.443973	4.855312	0.886584
H	4.090486	5.344168	1.532784
O	3.269587	6.392224	2.726454
O	4.783005	2.708718	-0.734416
C	6.903130	2.681560	7.229767
C	8.083464	3.296953	6.920868
C	8.209554	4.071752	5.719305
C	7.154802	4.194315	4.861430
C	5.764584	2.795180	6.357227
C	4.531905	2.194915	6.657324
C	5.895475	3.560058	5.148145
C	4.801251	3.669966	4.281017
C	3.427018	2.325993	5.804548
C	2.154164	1.728502	6.104867
C	3.565819	3.076676	4.587462
C	2.431767	3.200176	3.713283
C	1.234164	2.623537	4.040563
C	1.093904	1.874169	5.252890
H	3.326271	6.166412	3.666729
H	2.412369	6.831021	2.635622
H	6.799443	2.106411	8.155561
H	8.938056	3.216882	7.599080
H	9.159389	4.567631	5.499068
H	7.244372	4.785743	3.944159
H	4.426936	1.623768	7.586779
H	4.911692	4.204859	3.332206
H	2.046184	1.165067	7.037293
H	2.549621	3.782491	2.794932
H	0.371242	2.733500	3.376921
H	0.126591	1.426683	5.498454

H	4.371663	3.417969	-0.184015
H	4.265326	2.671259	-1.549691

D

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C	4.456320	7.693094	17.582123
C	4.536905	6.347985	17.361581
C	5.383385	5.829804	16.324246
C	6.118955	6.676480	15.542421
C	5.200407	8.619838	16.770510
C	5.114936	10.006859	16.953935
C	6.045293	8.101757	15.730608
C	6.764700	8.992841	14.926202
C	5.802425	10.899534	16.119558
C	5.677754	12.325711	16.260069
C	6.650567	10.380216	15.083887
C	7.349008	11.304372	14.231454
C	7.198172	12.653138	14.388295
C	6.346029	13.172923	15.419963
H	3.822195	8.088097	18.382339
H	3.966312	5.653045	17.983470
H	5.448585	4.748240	16.176207
H	6.779583	6.283474	14.762872
H	4.494077	10.404415	17.766068
H	7.433187	8.591972	14.155275
H	5.038658	12.720724	17.056022
H	8.010083	10.906391	13.454456
H	7.734746	13.347526	13.736098
H	6.246595	14.255485	15.538072
C	-0.259163	8.856775	13.802777
C	-0.872942	9.832464	14.575604
C	-0.609307	11.195316	14.345574
C	0.264347	11.583876	13.339292
C	0.631166	9.224709	12.769071
C	1.299482	8.253145	11.990415
C	0.893480	10.612080	12.530256
C	1.804645	10.977009	11.512662
C	2.202729	8.618364	10.965394
C	2.884860	7.644544	10.203010
C	2.455403	10.005847	10.718235
C	3.374724	10.372751	9.709876
C	4.022037	9.396013	8.966539
C	3.779257	8.032282	9.214938
H	-0.453736	7.796984	13.989860
H	-1.562272	9.541850	15.372429
H	-1.095425	11.952435	14.966181
H	0.476343	12.642709	13.166580
H	1.129478	7.193126	12.197736
H	2.025870	12.035412	11.349990
H	2.703156	6.584853	10.402705
H	3.572421	11.432459	9.525583
H	4.729227	9.685881	8.185172
H	4.300678	7.273921	8.625215
O	3.393967	7.610411	13.827903
O	2.531078	9.889045	15.049244
H	3.905152	7.009105	14.392315
H	4.071080	8.067883	13.268426
H	2.873374	9.893751	15.954239
H	2.806969	9.002322	14.703631
O	3.945989	11.464093	13.353721
O	4.969178	9.195751	12.269762
H	4.549891	12.050531	13.835595
H	3.434469	10.992274	14.060893
H	5.931966	9.183726	12.350191
H	4.707799	10.081051	12.632849

E

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C	6.409156	11.355831	13.768315
C	6.446559	12.032046	12.568051
C	6.023384	11.397678	11.357242
C	5.569282	10.095651	11.364038
C	5.973725	10.019742	13.796091
C	5.932083	9.193108	15.056672
C	5.544978	9.379657	12.571924
C	5.102119	7.942232	12.668317
C	4.638189	8.406099	15.081658
C	3.892753	8.238274	16.251961

C	4.225469	7.783772	13.893584
C	3.070055	6.996941	13.883517
C	2.346813	6.802613	15.061151
C	2.758873	7.425102	16.247632
H	6.702248	11.845599	14.699661
H	6.782777	13.071560	12.531262
H	6.046759	11.967657	10.424638
H	5.219460	9.616530	10.446819
H	5.961388	9.873257	15.919035
H	4.518915	7.695456	11.770554
H	4.211579	8.733168	17.174692
H	2.746963	6.519729	12.953118
H	1.458107	6.164986	15.057357
H	2.192165	7.274101	17.170870
C	6.948832	6.038511	16.333445
C	6.610794	4.684687	16.328975
C	6.203349	4.067869	15.142285
C	6.134265	4.804788	13.959401
C	6.879966	6.781604	15.152612
C	7.223710	8.255360	15.094597
C	6.469259	6.160780	13.958413
C	6.401574	7.015848	12.711099
C	8.068780	8.502362	13.854482
C	9.223815	9.294158	13.863513
C	7.652071	7.880638	12.652449
C	8.396775	8.065464	11.481289
C	9.524209	8.881248	11.493434
C	9.938950	9.496203	12.687049
H	7.274013	6.519910	17.261453
H	6.671721	4.104816	17.253711
H	5.945729	3.005418	15.138469
H	5.821278	4.321183	13.028403
H	7.803035	8.531671	15.987980
H	6.370306	6.366976	11.823336
H	9.557105	9.755889	14.798270
H	8.084852	7.569775	10.556588
H	10.099473	9.031187	10.575895
H	10.835846	10.121309	12.693791
O	3.394988	12.336096	12.593829
O	2.588091	9.824182	11.873214
H	2.683096	12.992577	12.591797
H	3.573144	12.180987	13.555402
H	1.892819	9.874503	11.201122
H	2.879628	10.762874	11.995182
O	1.659055	10.025313	14.461212
O	3.720956	11.532973	15.189664
H	1.579001	9.162780	14.894028
H	1.887581	9.805572	13.529386
H	3.404544	12.124479	15.888081
H	2.954917	10.911336	15.036053

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O	0.334996	2.606788	2.341351
C	6.056415	-1.743100	1.170212
C	7.017704	-2.742341	1.225223
C	8.352228	-2.468016	0.865438
C	8.724829	-1.196249	0.452910
C	6.408509	-0.438287	0.753238
C	5.444559	0.600290	0.701932
C	7.765647	-0.159317	0.389432
C	8.115364	1.156758	-0.009590
C	5.801438	1.904054	0.300347
C	4.840697	2.941700	0.298811
C	7.160387	2.191044	-0.063056
C	7.509215	3.511610	-0.431581
C	6.541806	4.511821	-0.438152
C	5.214068	4.231455	-0.070271
H	-0.478560	2.228323	2.705650
H	0.028547	3.116392	1.577050
H	5.018922	-1.949412	1.448521
H	6.740887	-3.749138	1.548079
H	9.099123	-3.264716	0.912080
H	9.762060	-0.987117	0.175153
H	4.402442	0.416947	0.999263
H	9.155619	1.374573	-0.274754
H	3.826840	2.703490	0.635659
H	8.544191	3.739998	-0.701649
H	6.820360	5.531173	-0.718784

H	4.473696	5.036094	-0.055067
O	3.573593	2.822699	6.219852
O	3.459907	0.621927	4.576273
C	7.605734	2.011970	3.392471
C	8.954965	2.107941	3.194442
C	9.557461	3.376150	2.900025
C	8.792975	4.507099	2.827312
C	6.765372	3.175248	3.303545
C	5.373569	3.088330	3.444994
C	7.369797	4.448858	3.028075
C	6.557883	5.589115	2.950607
C	4.559232	4.222923	3.317955
C	3.122320	4.131573	3.357734
C	5.165177	5.504846	3.087455
C	4.314110	6.660385	2.971230
C	2.955273	6.538458	3.038805
C	2.349226	5.249296	3.218046
H	2.988766	3.552076	5.963206
H	4.458800	3.204317	6.114300
H	7.137780	1.048628	3.623836
H	9.587620	1.218235	3.272212
H	10.639976	3.435226	2.754144
H	9.253935	5.478586	2.621917
H	4.915966	2.111400	3.633492
H	7.020279	6.564886	2.764203
H	2.660206	3.146452	3.446192
H	4.778931	7.639943	2.821432
H	2.319425	7.423351	2.946022
H	1.259625	5.153626	3.228199
H	3.214596	-0.148822	5.104958
H	3.435666	1.375918	5.210207
O	2.705369	1.066787	1.943835
H	1.816201	1.464850	1.971487
H	2.891668	0.862145	2.885436

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O	7.349905	-0.109254	0.663967
O	7.135313	-0.669594	3.388923
C	4.235535	0.434716	1.376056
C	3.474454	0.179881	0.232797
C	3.371024	1.148785	-0.771704
C	4.030196	2.371594	-0.635365
C	4.889505	1.663114	1.520259
C	5.726587	1.985441	2.736616
C	4.787057	2.635052	0.509777
C	5.527536	3.940272	0.718694
C	7.013326	2.636099	2.268996
C	8.273824	2.279931	2.788098
C	6.916791	3.626337	1.243401
C	8.077257	4.251269	0.772620
C	9.306766	3.930673	1.334581
C	9.404563	2.939831	2.341539
H	7.951876	-0.420224	-0.026593
H	6.479962	-0.077167	0.236434
H	4.345771	-0.323656	2.158027
H	2.960521	-0.779075	0.121814
H	2.777444	0.946882	-1.667409
H	3.956161	3.125805	-1.425664
H	5.973105	1.056843	3.267074
H	5.618100	4.466857	-0.243111
H	8.330719	1.463542	3.514029
H	8.009955	5.001112	-0.021339
H	10.213239	4.431771	0.983257
H	10.386254	2.683501	2.749258
H	7.284390	-1.582297	3.667062
H	7.306738	-0.667982	2.425542
O	3.600031	5.400986	5.680920
O	4.485442	2.944967	6.750777
C	6.716816	4.418348	5.010043
C	7.475312	5.571052	5.074003
C	7.367502	6.560206	4.062500
C	6.495461	6.392364	2.994746
C	5.866617	4.207715	3.904885
C	5.015874	2.963482	3.758050
C	5.752136	5.212196	2.889037
C	4.804933	4.921697	1.741066
C	3.630267	3.396036	3.333701
C	2.477834	2.880059	3.935165
C	3.519814	4.367256	2.322775

C	2.257178	4.805091	1.912968
C	1.108158	4.275003	2.502870
C	1.218624	3.315494	3.515949
H	2.833101	5.220278	5.114638
H	3.384724	6.234616	6.122827
H	6.729717	3.675725	5.811929
H	8.149423	5.739180	5.918336
H	7.966625	7.472134	4.138304
H	6.402784	7.166550	2.227532
H	4.955039	2.466309	4.734111
H	4.588463	5.860418	1.209536
H	2.579976	2.160020	4.752651
H	2.171215	5.566188	1.130526
H	0.121665	4.616363	2.177579
H	0.317439	2.908987	3.983495
H	4.207879	2.752259	7.655522
H	4.128704	3.836607	6.565083

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