

Exploring the Effectiveness of Different Lewis Pair Combinations in Caged Structures for the Catalysis of Ammonia Borane Dehydrogenation: A DFT Study

Supporting Information File

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I.

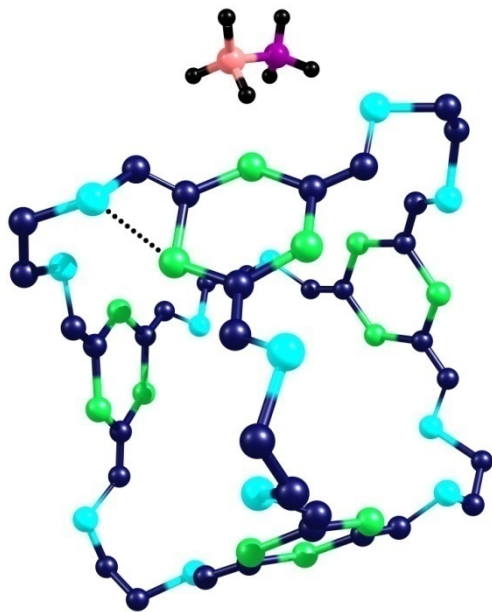


Fig. S1 The optimized structure of the reactant adduct species for the case of the P-Ge cage; the colour scheme is as follows: dark blue: carbon, violet: nitrogen, light blue: phosphorus, light green: germanium, light brown: boron; only the ammonia borane hydrogens are shown; the other hydrogens have been removed for the sake of clarity.

1	N-P cage case	B-P 86 functional (kcal/mol)	PBE Functional (kcal/mol)
	Ts-1	2.1	6.3
	Ts-2	31.0	32.2
2	C-P cage case		
	Ts-1	40.1	39.8
	Ts-2	31.0	31.4
3	N-Ge cage case		
	Ts-1	3.2	2.6
	Ts-2	31.5	31.6
4	P-Ge cage case		
	Ts-1	6.6	6.8
	Ts-2	22.8	22.8

Table.1 The comparison between the ΔE values for the barrier heights corresponding to the transition states obtained with the PBE and the B-P 86 functionals; all the values are ΔE values in kcal/mol.

1	N-P cage case	frequency (cm^{-1})
	N-P-cage-Ts-1	-997.4
	N-P-cage-(H2)-Ts-2	-958.8
	N-P-cage-Ts-1-C-N	-340.8
	N-P-cage-P-C-ring-Ts-1	-360.2
2	C-P cage case	
	C-P-cage-Ts-1	-1668.7
	C-P-cage-(H2)-Ts-2	-1087.1
	C-P-cage-Ts-1-C-C	-1162.7
	C-P-cage-P-C-ring-Ts-1	-306.3
3	N-Ge cage case	
	N-Ge-cage-Ts-1	-748.0
	N-Ge-cage-(H2)-Ts-2	-546.5
	N-Ge-cage- Ge -C-ring-Ts-1	-644.9
4	P-Ge cage case	
	P-Ge-cage-Ts-1	-283.7
	P-Ge-cage-(H2)-Ts-2	-985.1
	P- Ge -cage-H2-Ts-1-C-P	0949.6
	P-Ge-cage- Ge -C-ring-Ts-1	-225.3
5	N-C cage	
	N-C-cage-Ts-1	-1124.0
	N-C-cage-(H2)-Ts-2	-1479.7
	N-C-cage-Ts-1-C-N	-1030.3
6	P-C cage	
	P-C-cage-Ts-1	-903.4
	P-C-cage-(H2)-Ts-2	-1126.9
	P-C-cage-Ts-1-C-P	-467.9

Table.2 The frequency values (cm^{-1}) for all the transition states.

II. XYZ Coordinates of the optimized structures.

N-P-cage

C	11.488325	1.984960	-3.514911
C	12.224599	3.212886	-3.874505
N	12.641501	3.448350	-5.063219
C	13.366549	4.678446	-5.302227
C	14.770515	4.379953	-5.857435
N	15.607498	3.794719	-4.830872
C	16.106837	2.634141	-5.045896
C	16.956293	1.935375	-4.061884
P	17.667000	0.478327	-4.741461
C	18.662115	-0.228642	-3.450255
C	19.356084	-1.477548	-3.818722
N	19.356600	-1.952756	-5.009001
C	20.062929	-3.194591	-5.245337
C	19.109523	-4.260441	-5.811643
N	18.181321	-4.708818	-4.793928
C	16.927972	-4.558261	-5.013636
C	15.889847	-4.969813	-4.048534
P	16.512436	-5.508743	-2.474489
C	15.101743	-5.946879	-1.520578
P	13.349671	-5.919186	-1.820468
C	13.150790	-5.347138	-3.469790
C	11.729585	-5.307900	-3.868044
N	11.359231	-5.103079	-5.077455
C	9.940551	-5.072383	-5.365576
C	9.539294	-3.709701	-5.957642
N	9.591567	-2.681956	-4.939876
C	10.358242	-1.673659	-5.133483
C	10.499011	-0.580876	-4.151933
P	9.722786	-0.899294	-2.585833
C	10.003649	0.530924	-1.603225
C	9.390586	0.391798	-0.268142
N	9.360408	1.342782	0.590251
C	8.738950	1.079141	1.871894
C	9.743322	1.291284	3.017311
N	10.753384	0.252986	3.011805
C	11.981307	0.610602	2.928892
C	13.102152	-0.348421	2.899629
P	12.622873	-2.053580	2.843424
C	14.125022	-2.970345	2.806599
C	13.868586	-4.417435	2.808430
N	14.725659	-5.297888	3.195507
C	14.351742	-6.699298	3.074791
C	15.128394	-7.382768	1.933803
N	14.645083	-6.929297	0.648158
C	15.486655	-6.432635	-0.181758
P	10.865467	2.061876	-1.872154
P	11.435862	0.757621	-4.799639
P	17.024337	2.714501	-2.465389
C	18.108678	1.730532	-1.493449
C	18.281260	2.281157	-0.134718
N	19.165122	1.836447	0.679385
C	19.236991	2.420971	2.002113
C	18.964434	1.350533	3.073789
N	17.570948	0.960326	3.055600
C	17.288875	-0.275373	2.867939
C	15.901391	-0.774910	2.845606
P	15.841476	-2.527452	2.725862
P	19.001592	0.222525	-1.785348
P	14.656212	0.480592	2.930611
P	14.278155	-4.799827	-4.729806
N	16.891951	-4.940391	5.236203
B	17.104580	-3.423426	5.812103
H	19.895364	-1.989298	-2.993560
H	17.604006	3.115851	0.142905
H	20.264634	2.790879	2.156166

H	18.531716	3.264442	2.141063
H	19.175372	1.804600	4.056833
H	19.655659	0.497464	2.925785
H	10.991685	-5.481810	-3.057086
H	18.083313	-1.038205	2.736965
H	12.266194	1.682594	2.878527
H	10.172102	2.310820	2.945111
H	9.182021	1.214280	3.964397
H	8.315399	0.057257	1.943294
H	7.922119	1.808181	2.008897
H	8.939142	-0.598362	-0.046965
H	12.391709	3.936428	-3.049222
H	13.458972	5.309156	-4.395556
H	12.822092	5.249448	-6.073493
H	14.679612	3.740571	-6.758264
H	15.218739	5.343345	-6.154436
H	15.928894	2.096291	-6.000943
H	8.494600	-3.795095	-6.301790
H	10.181966	-3.487047	-6.832928
H	10.952466	-1.569260	-6.065341
H	9.733973	-5.839620	-6.130717
H	9.313455	-5.281673	-4.475886
H	12.862662	-4.733279	2.468908
H	13.269000	-6.829099	2.890306
H	14.607324	-7.213549	4.016173
H	16.217822	-7.221456	2.070314
H	14.929106	-8.465913	2.008197
H	16.566454	-6.356303	0.066794
H	16.556901	-4.114278	-5.961109
H	18.602447	-3.855588	-6.710128
H	19.723540	-5.125688	-6.114287
H	20.556362	-3.591962	-4.335827
H	20.835906	-3.005590	-6.009404
H	16.219470	-4.984891	4.434636
H	15.992450	-2.995444	6.071760
H	17.815713	-3.520103	6.799559
H	17.661484	-2.795275	4.920812
H	16.525388	-5.548934	5.974114
H	17.779640	-5.345129	4.924792

N-P-cage with NH₃BH₃

C	11.773473	2.370234	-5.214203
P	13.160666	3.454867	-5.445586
C	13.446281	4.218498	-3.885053
C	14.580170	5.161707	-3.951982
N	14.989255	5.843861	-2.946657
C	16.122569	6.725294	-3.144482
C	15.795588	8.156762	-2.693505
N	14.806451	8.758342	-3.564121
C	13.771584	9.287577	-3.024556
C	12.689702	9.918366	-3.806415
P	12.983114	9.993177	-5.559348
C	11.528840	10.689589	-6.260255
C	11.634741	10.802468	-7.728333
N	10.784642	11.454434	-8.430826
C	10.962966	11.479955	-9.867946
C	9.741691	10.865422	-10.573765
N	9.686556	9.434608	-10.356071
C	8.623780	8.951678	-9.825243
C	8.433578	7.515844	-9.549470
P	9.867104	6.503394	-9.815608
C	9.378192	4.857342	-9.446812
P	7.874705	4.125853	-8.848690
C	6.710635	5.434907	-8.724509
P	6.800727	7.187824	-8.988161
C	11.387074	1.622789	-6.427360
N	12.132336	1.579760	-7.468788

C	11.661061	0.838604	-8.620258
C	11.466118	1.779001	-9.823782
N	10.313363	2.629582	-9.618921
C	10.480431	3.900073	-9.655246
P	10.714547	2.010218	-3.858313
C	11.356175	2.938697	-2.482597
P	12.681271	4.078573	-2.285362
C	5.392077	4.950098	-8.273917
N	4.341580	5.684552	-8.287754
C	3.100031	5.112225	-7.810318
C	2.575166	5.898300	-6.594610
N	3.392153	5.632827	-5.429125
C	4.013783	6.614882	-4.888966
C	4.887804	6.452701	-3.711477
P	5.370519	8.004027	-3.045230
C	6.374537	7.637831	-1.626059
P	6.954015	6.147530	-0.897802
C	6.267325	4.824946	-1.861864
C	6.630292	3.471758	-1.401722
N	7.258602	3.248826	-0.306365
C	7.567781	1.875188	0.031940
C	9.085300	1.690662	0.210340
N	9.761623	1.795876	-1.066117
C	10.628581	2.727203	-1.215373
P	5.255985	4.765725	-3.297811
P	11.374154	10.451268	-2.765496
C	10.122431	11.097867	-3.848860
C	8.915537	11.588097	-3.153353
N	8.852664	11.687032	-1.877288
C	7.622534	12.171037	-1.285516
C	7.005368	11.102877	-0.366474
N	6.457946	10.013528	-1.147560
C	6.860185	8.822892	-0.894119
P	9.978007	11.252983	-5.595329
N	10.658692	6.831829	-4.293192
B	9.305487	6.482171	-5.155058
H	6.314418	2.638460	-2.063991
H	3.912445	7.649303	-5.278928
H	1.554314	5.537984	-6.382993
H	2.524630	6.975182	-6.852544
H	2.350205	5.207726	-8.613814
H	3.192050	4.041703	-7.537789
H	15.073862	5.245908	-4.943424
H	5.354600	3.894591	-7.932124
H	7.770017	9.607864	-9.552577
H	8.824289	11.389593	-10.238625
H	9.867614	11.041234	-11.655966
H	11.880179	10.952950	-10.198232
H	11.029609	12.535366	-10.181990
H	12.504169	10.294608	-8.195123
H	8.064095	11.879557	-3.802612
H	6.871975	12.476726	-2.040828
H	7.871030	13.044762	-0.659459
H	7.762161	10.771420	0.373071
H	6.173019	11.581495	0.177770
H	7.597643	8.623602	-0.087441
H	16.724942	8.746309	-2.779738
H	15.484508	8.150623	-1.629827
H	13.631528	9.285669	-1.922736
H	16.947436	6.361323	-2.507518
H	16.474698	6.741449	-4.195265
H	11.476875	4.345168	-9.860834
H	12.401061	2.347665	-10.002206
H	11.269281	1.144369	-10.704661
H	10.712943	0.298322	-8.427470
H	12.438200	0.105333	-8.892679
H	10.416825	1.086691	-6.382824
H	10.883548	3.418592	-0.385162
H	9.455957	2.421734	0.956369
H	9.252425	0.672297	0.600164

H	7.196149	1.149638	-0.719188
H	7.094752	1.647644	1.002603
H	9.632837	5.614065	-5.946517
H	8.982597	7.526148	-5.699416
H	11.019407	6.013717	-3.788043
H	11.416697	7.167266	-4.896999
H	8.482173	6.099485	-4.340739
H	10.489148	7.567362	-3.598477

N-P-cage-H₂

C	11.287696	2.176765	-2.089035
P	10.343571	0.683645	-1.902714
C	9.570116	0.790401	-0.326909
P	9.595365	1.995032	0.978462
C	10.652100	3.286914	0.425566
P	11.611334	3.553374	-1.047470
C	11.981879	2.288831	-3.387051
N	11.679861	1.545800	-4.385857
C	12.424086	1.704687	-5.617156
C	13.183821	0.408064	-5.959952
N	14.330790	0.234443	-5.093335
C	14.324890	-0.764172	-4.281510
C	15.412548	-1.021722	-3.339707
P	16.297929	0.389972	-2.827548
C	17.753605	-0.225985	-2.007372
P	18.352281	-1.949640	-2.292299
C	16.866672	-2.950657	-1.885688
C	17.080423	-4.163130	-1.095980
N	16.365299	-5.223233	-1.216092
C	16.661008	-6.349927	-0.356378
C	15.392689	-6.853862	0.351628
N	14.982098	-5.952927	1.408979
C	13.820705	-5.417006	1.328656
C	13.291116	-4.505928	2.362430
P	11.616941	-4.071375	2.046168
C	11.124343	-3.010942	3.384954
C	9.730417	-2.531945	3.312463
N	8.891262	-2.954002	2.440638
C	7.551476	-2.404072	2.465997
C	7.217097	-1.724734	1.126955
N	7.977394	-0.502363	0.968758
C	8.740779	-0.399269	-0.055441
P	15.305886	-2.641738	-2.531214
P	14.451758	-4.092704	3.643189
C	13.583004	-3.060518	4.770094
C	14.430590	-2.675454	5.914784
N	13.973882	-2.062402	6.943913
C	14.901433	-1.716198	8.000164
C	14.939480	-0.189662	8.199682
N	15.579607	0.445217	7.066262
C	14.887770	1.258015	6.357422
C	15.434922	1.922672	5.158346
P	16.943139	1.206571	4.556896
C	17.414040	2.168665	3.161463
P	16.696790	3.562877	2.325125
C	15.230130	3.954856	3.209189
P	14.408990	3.242798	4.616059
P	11.940734	-2.384464	4.809793
C	10.762948	4.364527	1.427455
N	11.360790	5.473216	1.190363
C	11.432214	6.456694	2.249530
C	12.900290	6.803538	2.558217
N	13.549848	5.691698	3.220502
C	14.530764	5.118329	2.628237
C	18.549992	0.747551	-1.428791
N	19.758004	0.551956	-0.855752
C	20.605442	1.607683	-0.325336
C	20.570325	1.744031	1.205230
N	19.313002	2.296239	1.653730

C	18.681210	1.684429	2.587817
H	17.926506	-4.126776	-0.374517
H	18.225825	1.793895	-1.450210
H	21.642589	1.416595	-0.643538
H	20.287129	2.558966	-0.774424
H	21.370210	2.456519	1.475677
H	20.815622	0.770746	1.682043
H	9.438793	-1.780630	4.076479
H	19.083919	0.751028	3.035729
H	14.909070	5.477615	1.648909
H	13.406031	7.102934	1.618912
H	12.902057	7.661536	3.250929
H	10.928062	6.130779	3.181420
H	10.945318	7.379709	1.891406
H	10.286171	4.163560	2.409987
H	12.769635	3.067541	-3.456785
H	13.142428	2.548149	-5.583246
H	11.699517	1.889449	-6.427715
H	12.472769	-0.441824	-5.914379
H	13.546367	0.505042	-6.997232
H	13.494352	-1.501262	-4.288813
H	6.146731	-1.457598	1.152338
H	7.380639	-2.444819	0.300413
H	8.807657	-1.213032	-0.808099
H	6.843985	-3.240496	2.596866
H	7.397775	-1.680018	3.290968
H	13.840102	1.511981	6.620538
H	13.909929	0.179781	8.376873
H	15.548182	0.013818	9.096445
H	15.929656	-2.085177	7.812100
H	14.533689	-2.162355	8.939512
H	15.501047	-2.961913	5.841714
H	13.142519	-5.630592	0.476306
H	14.600824	-7.017643	-0.405822
H	15.637264	-7.823245	0.819183
H	17.443767	-6.132141	0.398653
H	17.018680	-7.176322	-0.996181
H	19.034571	-2.166305	-1.025417
H	20.084207	-0.407207	-0.750782

N-P-cage-Ts-1

P	10.724772	2.063032	-2.080539
C	11.484726	1.962153	-3.662948
P	11.491223	0.739994	-4.952824
C	10.458004	-0.564955	-4.387791
P	9.549327	-0.859757	-2.889417
C	9.786247	0.566259	-1.890428
C	12.301574	3.157730	-3.948164
N	12.859749	3.363903	-5.083141
C	13.652754	4.564105	-5.246030
C	15.102821	4.208549	-5.618618
N	15.793311	3.627168	-4.486085
C	16.276171	2.446792	-4.613878
C	16.992394	1.750508	-3.527477
P	16.982660	2.602360	-1.968175
C	17.911115	1.600275	-0.861481
P	18.723771	0.026996	-1.005868
C	18.500540	-0.479756	-2.675026
P	17.664015	0.221778	-4.076695
C	18.002002	2.217484	0.476114
N	18.780047	1.778185	1.394853
C	18.764194	2.458955	2.673788
C	18.302665	1.511385	3.794550
N	16.902050	1.181993	3.640942
C	16.569144	-0.057615	3.656108
C	15.193525	-0.540128	3.470947
P	13.996251	0.657394	3.067360
C	12.421345	-0.154690	2.930751
P	11.964955	-1.845489	2.885074

C	13.401902	-2.788053	3.289649
P	15.070275	-2.306113	3.805448
C	13.124265	-4.188636	3.255202
N	13.989275	-5.174269	3.312541
C	13.494831	-6.548030	3.331035
C	14.095329	-7.416945	2.215084
N	13.715707	-6.934222	0.906299
C	14.656339	-6.678349	0.073354
C	14.435803	-6.174450	-1.292578
P	12.733684	-6.043826	-1.781709
C	12.754187	-5.428161	-3.427074
P	14.040748	-4.876360	-4.522068
C	15.556517	-5.176215	-3.683135
P	15.968573	-5.839273	-2.088021
C	16.722309	-4.780402	-4.497847
N	17.929382	-4.985343	-4.120130
C	19.004597	-4.555308	-4.989224
C	19.920019	-3.550766	-4.268510
N	19.259871	-2.271191	-4.117961
C	19.150438	-1.778088	-2.939830
C	11.394072	-5.330269	-3.991447
N	11.179951	-5.118576	-5.236929
C	9.807030	-5.023857	-5.688005
C	9.536246	-3.639378	-6.303494
N	9.532208	-2.620754	-5.274960
C	10.359994	-1.648476	-5.384262
C	11.321311	0.804456	2.755635
N	10.081011	0.477407	2.804204
C	9.096260	1.525586	2.635787
C	8.192908	1.248842	1.420699
N	8.919118	1.457345	0.185583
C	9.052476	0.465356	-0.613835
N	16.590879	-4.939408	3.178237
B	16.856462	-3.778170	2.184489
H	19.557395	-2.305856	-2.051582
H	17.357848	3.106277	0.642047
H	19.796400	2.771851	2.905869
H	18.113975	3.356285	2.672411
H	18.426625	2.055882	4.747613
H	18.957839	0.616949	3.816928
H	10.557760	-5.468347	-3.274632
H	17.338997	-0.845820	3.803640
H	11.627968	1.861588	2.604843
H	9.550317	2.531330	2.525301
H	8.448251	1.533880	3.529202
H	7.770762	0.227476	1.505837
H	7.363771	1.976197	1.451108
H	8.604078	-0.524844	-0.388144
H	12.401552	3.884697	-3.114890
H	13.655087	5.206932	-4.343288
H	13.228376	5.139731	-6.086351
H	15.099529	3.548335	-6.509013
H	15.615354	5.149610	-5.881764
H	16.185560	1.886974	-5.568667
H	8.530172	-3.672233	-6.755509
H	10.276326	-3.443214	-7.104977
H	11.045804	-1.569372	-6.254056
H	9.657207	-5.774840	-6.481962
H	9.073266	-5.211805	-4.879217
H	12.063028	-4.469888	3.156125
H	12.396229	-6.552590	3.242076
H	13.755975	-7.008714	4.299870
H	15.196927	-7.496065	2.338732
H	13.680007	-8.431701	2.345925
H	15.722177	-6.825660	0.354105
H	16.493299	-4.296145	-5.470338
H	18.642707	-4.105030	-5.934889
H	19.614601	-5.441967	-5.233027
H	20.253200	-3.983844	-3.304184
H	20.806759	-3.399223	-4.908028

H	15.267599	-5.053508	3.311957
H	15.880189	-2.857990	2.428213
H	17.852844	-3.120169	2.377296
H	16.561470	-4.063832	1.044076
H	17.034822	-4.795215	4.088812
H	16.951650	-5.821838	2.805467

N-P-cage-H₂-Ts-2

C	11.546638	2.023035	-5.570483
C	11.834219	3.020434	-4.521135
N	11.229395	3.036342	-3.391401
C	11.588181	4.068054	-2.440176
C	10.354520	4.901605	-2.052634
N	9.934460	5.738085	-3.157584
C	8.742700	5.592145	-3.605638
C	8.206346	6.383686	-4.729957
P	9.408367	7.391713	-5.564329
C	8.537356	8.229944	-6.840977
C	9.431954	9.111544	-7.615691
N	9.007434	9.912935	-8.521355
C	9.980086	10.718780	-9.229131
C	9.918634	10.434796	-10.740389
N	10.433390	9.112093	-11.029079
C	9.645181	8.265669	-11.580810
C	10.053699	6.883815	-11.900702
P	11.648024	6.420146	-11.265833
C	11.917054	4.765923	-11.796010
C	13.234795	4.259390	-11.364370
N	13.735515	3.170949	-11.818776
C	15.022888	2.744371	-11.310692
C	14.898564	1.371271	-10.625801
N	14.154084	1.491353	-9.389454
C	13.067395	0.822045	-9.270701
C	12.214258	0.889302	-8.068305
P	10.927879	-0.308216	-8.120697
C	10.016552	-0.113116	-6.607836
C	8.886833	-1.048551	-6.442635
N	8.641134	-2.000341	-7.264919
C	7.501972	-2.852140	-6.988912
C	6.486478	-2.813675	-8.140725
N	5.821894	-1.528472	-8.204490
C	5.721635	-0.955543	-9.347375
C	5.067006	0.347335	-9.551854
P	4.740273	0.659760	-11.277336
C	4.246489	2.392411	-11.343223
P	3.671702	3.528259	-10.127759
C	3.771065	2.685331	-8.585196
C	3.162152	3.392556	-7.447382
N	2.368612	4.389553	-7.596201
C	1.820192	5.009330	-6.407616
C	2.312970	6.461845	-6.269282
N	3.702822	6.489939	-5.864728
C	4.551961	7.062479	-6.634694
C	5.990941	7.132677	-6.312535
P	6.846507	8.226640	-7.389340
P	12.676889	2.154957	-6.910095
P	10.152292	0.974666	-5.232789
P	6.486724	6.096397	-4.956588
P	8.820171	6.046328	-12.831346
C	9.458760	4.416937	-13.137971
C	8.570512	3.546769	-13.931224
N	7.499517	3.970184	-14.494351
C	6.727186	3.037163	-15.286721
C	5.248886	3.045329	-14.876781
N	5.020232	2.375179	-13.605522
C	4.408135	3.000421	-12.635434
P	10.944216	3.585486	-12.698691
P	4.620446	1.213875	-8.090682
H	13.779518	4.885342	-10.627479
H	8.605210	8.538945	-11.856721

H	10.569503	11.170411	-11.242350
H	8.879060	10.580781	-11.096189
H	9.714927	11.779693	-9.082487
H	11.016765	10.561734	-8.869485
H	8.255329	-0.886145	-5.544305
H	10.511061	9.048231	-7.361237
H	4.239801	7.552170	-7.580822
H	2.126198	7.003650	-7.217976
H	1.719942	6.937165	-5.469635
H	2.068346	4.457598	-5.478638
H	0.722951	5.041105	-6.513786
H	3.404891	2.994147	-6.439944
H	4.072420	4.043670	-12.770153
H	4.888093	4.089870	-14.851612
H	4.681466	2.499111	-15.648765
H	7.123429	2.001356	-15.250713
H	6.769390	3.376907	-16.336211
H	8.897334	2.490175	-14.034561
H	5.722055	-3.580101	-7.920882
H	6.988034	-3.088943	-9.090555
H	6.130732	-1.436637	-10.262112
H	7.869458	-3.889311	-6.905424
H	6.986112	-2.584553	-6.044846
H	8.041350	4.859686	-3.153035
H	9.554067	4.223372	-1.694962
H	10.651577	5.563084	-1.221002
H	12.383843	4.743319	-2.813978
H	11.951419	3.572360	-1.523778
H	12.623520	3.762767	-4.764006
H	12.715907	0.143577	-10.076196
H	14.446727	0.649147	-11.335092
H	15.918681	1.031319	-10.379820
H	15.467826	3.467987	-10.598904
H	15.706709	2.626590	-12.168249
H	6.378183	1.091552	-12.252177
H	6.039931	1.556006	-12.953654

N-P-cage-H₂-C-N

C	2.575561	2.631690	-4.870754
P	1.633554	2.348064	-6.350605
C	0.888714	3.869147	-6.832992
P	0.940365	5.492612	-6.113245
C	1.924653	5.414482	-4.654344
C	1.979719	6.716003	-3.976944
C	2.637382	7.034224	-2.840958
C	2.626638	8.389188	-2.207504
C	2.180704	8.363829	-0.722063
C	0.756211	7.946965	-0.530996
C	0.369746	6.885600	0.210534
C	-0.993229	6.403661	0.467939
P	-0.985690	5.025289	1.565407
C	-2.667703	4.527032	1.841647
P	-4.189614	5.117355	1.182208
C	-3.833534	6.474858	0.093917
C	-4.977475	7.105170	-0.576980
C	-6.284655	6.780488	-0.472784
C	-7.389175	7.479717	-1.199748
C	-8.276531	6.518513	-2.032240
C	-7.539203	5.845860	-3.146486
C	-7.471357	4.507084	-3.315799
C	-6.780558	3.762630	-4.376171
P	-6.988735	2.024491	-4.181643
C	-6.119866	1.210520	-5.499837
P	-5.182192	1.839749	-6.852495
C	-5.167832	3.612411	-6.741275
C	-4.419991	4.341971	-7.772772
C	-3.689177	3.838004	-8.791502
C	-2.970506	4.676599	-9.801307
C	-1.463218	4.339743	-9.926712
C	-0.681793	4.617001	-8.681061

C	0.082659	3.700269	-8.048603
P	2.813002	4.077315	-3.894054
C	3.264509	1.472359	-4.291702
C	3.335986	0.218132	-4.791592
C	4.034351	-0.930006	-4.132706
C	3.196597	-2.224095	-4.021564
C	2.080513	-2.218458	-2.967188
C	0.898773	-1.282675	-3.285241
C	-0.238968	-1.358022	-2.273963
P	0.173301	-0.712458	-0.685703
C	-1.237822	-0.885142	0.363195
P	-2.860303	-1.520188	0.035853
C	-2.942026	-2.010303	-1.654411
C	-4.289603	-2.464232	-2.015721
C	-4.724578	-2.898270	-3.218871
C	-6.136765	-3.297884	-3.510568
C	-6.719073	-2.586692	-4.758433
C	-6.745863	-1.094672	-4.637479
C	-6.158529	-0.257096	-5.520725
P	-2.317134	7.242667	-0.367022
P	-5.907339	4.720748	-5.589878
P	-1.705028	-2.038088	-2.934840
C	-0.975785	-0.377379	1.714896
C	-1.857820	-0.197041	2.722041
C	-1.501613	0.344554	4.069680
C	-2.299643	1.624025	4.440695
C	-1.984504	2.788483	3.555872
C	-2.885885	3.399564	2.756614
H	-5.027310	-2.417032	-1.202373
H	0.068897	-0.095327	1.907021
H	-1.718456	-0.416690	4.841083
H	-0.419941	0.550126	4.121495
H	-2.056609	1.877526	5.487952
H	-4.467784	5.436512	-7.686865
H	-3.919079	3.026732	2.790277
H	1.162851	6.301195	0.697777
H	2.846989	7.698343	-0.149055
H	2.320925	9.381478	-0.313889
H	1.980006	9.072006	-2.782575
H	3.646068	8.815956	-2.239938
H	1.401895	7.514615	-4.462585
H	3.760710	1.660341	-3.329259
H	4.399988	-0.630570	-3.136086
H	4.932021	-1.173989	-4.732588
H	2.768553	-2.463198	-5.011361
H	3.886083	-3.050020	-3.782897
H	1.261126	-0.244428	-3.340642
H	-1.055048	4.947303	-10.755335
H	-1.340432	3.283978	-10.220280
H	0.110247	2.689937	-8.480835
H	-3.428735	4.521644	-10.795597
H	-3.096184	5.745158	-9.560340
H	-4.718654	7.938769	-1.244528
H	-6.974692	8.265906	-1.852309
H	-8.044097	7.988742	-0.468814
H	-8.729637	5.762658	-1.369503
H	-9.109362	7.112641	-2.451023
H	-7.991678	3.881396	-2.577312
H	-5.630742	-0.717436	-6.367923
H	-6.141984	-2.877449	-5.651582
H	-7.747374	-2.963186	-4.909860
H	-6.772504	-3.099697	-2.632336
H	-6.184820	-4.387145	-3.695482
H	-3.379769	1.405820	4.406729
H	1.691155	-3.244693	-2.858980
H	2.859399	-0.004375	-5.754428
H	-0.754909	5.635122	-8.279787
H	-3.599539	2.751808	-8.911662
H	-7.028369	6.508569	-3.855389
H	-6.586454	5.950021	0.176851

H	-0.944234	3.134921	3.563808
H	-2.916108	-0.437880	2.565027
H	-4.023593	-2.953107	-4.060170
H	-7.273555	-0.686691	-3.767476
H	0.001558	8.560537	-1.037303
H	3.221421	6.266540	-2.319715
H	2.502955	-1.947159	-1.984233
H	0.508550	-1.525204	-4.289635

N-P-cage-Ts-1-C-N

C	5.960481	-2.398154	1.524128
P	6.341902	-3.933987	2.290873
C	6.991972	-4.976888	1.008638
C	7.386141	-6.325348	1.460165
N	7.064636	-6.792755	2.608980
C	7.522352	-8.121686	2.957652
C	8.373929	-8.080568	4.237448
N	9.648551	-7.440115	3.984502
C	9.958628	-6.411262	4.683551
C	11.231187	-5.690995	4.503200
P	11.607527	-4.644289	5.868292
C	13.232364	-4.014138	5.573670
C	13.722508	-3.039561	6.563152
N	13.015130	-2.619973	7.545572
C	13.572700	-1.584933	8.389598
C	12.613100	-0.383354	8.456308
N	12.478739	0.241069	7.154846
C	11.307553	0.269704	6.634296
C	11.016583	0.850928	5.309374
P	9.281954	0.983341	5.047972
C	9.079751	1.719438	3.444846
P	10.202899	2.265708	2.207348
C	11.831414	1.961954	2.847690
P	12.446489	1.241986	4.329394
C	5.425751	-1.427972	2.499169
N	5.010076	-0.262338	2.166388
C	4.523702	0.613071	3.212494
C	5.349328	1.910911	3.258364
N	6.676748	1.657439	3.779579
C	7.679593	1.930189	3.029215
P	6.099203	-1.781581	-0.136982
C	6.750342	-3.106611	-1.090746
P	7.307272	-4.748948	-0.705207
C	12.919431	2.397984	1.949180
N	12.709217	3.165552	0.944561
C	13.837728	3.565717	0.130337
C	13.611912	3.200930	-1.346336
N	13.761616	1.776736	-1.553847
C	12.819087	1.135597	-2.139560
C	12.893758	-0.316225	-2.390610
P	11.420908	-0.945589	-3.115704
C	11.678829	-2.689983	-3.324024
C	10.588292	-3.385017	-4.033023
N	9.687250	-2.757635	-4.694567
C	8.649187	-3.532529	-5.342025
C	7.264993	-3.143983	-4.791933
N	7.116736	-3.608990	-3.428683
C	6.888354	-2.741219	-2.513851
P	14.434430	-1.053664	-1.906255
C	14.216501	-2.788478	-2.106049
C	15.370323	-3.511296	-1.548573
N	15.375428	-4.766332	-1.286755
C	16.578366	-5.314695	-0.694541
C	16.263031	-6.220035	0.504820
N	15.684914	-5.572279	1.688290
C	14.356758	-5.505461	1.816423
C	13.616162	-5.262364	3.048441
P	14.429444	-4.308296	4.315858
P	12.938776	-3.799500	-2.798968

P	12.007453	-5.977352	2.941687
B	14.815547	-2.594812	1.789114
N	16.267799	-2.976105	2.026333
H	13.938549	2.041491	2.206192
H	10.430001	-0.141463	7.176833
H	13.051573	0.354671	9.149510
H	11.641195	-0.720601	8.868942
H	13.669602	-1.983044	9.414645
H	14.571638	-1.245189	8.049464
H	10.598924	-4.493664	-3.978385
H	14.747141	-2.647157	6.386772
H	9.289407	-6.030661	5.483299
H	7.795950	-7.587664	5.044602
H	8.571090	-9.124532	4.535339
H	8.103645	-8.604707	2.146754
H	6.635157	-8.742270	3.170711
H	7.975122	-6.925848	0.735644
H	5.398773	-1.770414	3.555028
H	4.533357	0.138241	4.213857
H	3.485021	0.891710	2.965634
H	5.361374	2.369880	2.249564
H	4.839777	2.601540	3.951740
H	7.539229	2.356811	2.013448
H	6.508525	-3.654744	-5.411545
H	7.124687	-2.049224	-4.893864
H	6.770655	-1.663769	-2.753532
H	8.659176	-3.285782	-6.417235
H	8.791494	-4.625870	-5.228601
H	13.779561	-5.971783	1.005247
H	15.573499	-7.012821	0.180736
H	17.198438	-6.705686	0.825669
H	17.311010	-4.532666	-0.408243
H	17.067736	-5.963728	-1.444194
H	16.253555	-2.878150	-1.316048
H	11.892768	1.644897	-2.479263
H	12.627082	3.587759	-1.676362
H	14.398427	3.707734	-1.932359
H	14.796454	3.126355	0.470988
H	13.916586	4.665201	0.188930
H	16.200415	-4.671701	2.007714
H	14.133981	-3.605941	1.366452
H	14.225788	-2.490422	2.890637
H	14.651556	-1.691927	0.984809
H	16.595702	-2.883039	2.988966
H	16.952791	-2.546065	1.405433

C-P-cage

C	2.647699	2.732841	-4.927930
C	1.851993	2.514605	-6.141143
C	1.357758	3.442962	-6.989487
C	0.551006	3.120222	-8.206000
C	-0.891768	3.696366	-8.141929
C	-1.726616	3.042174	-7.088305
C	-2.203108	3.673090	-5.992724
C	-2.998584	3.089376	-4.907156
P	-2.974467	1.319993	-4.774795
C	-4.117412	0.839762	-3.522324
P	-5.019660	1.801304	-2.332831
C	-4.703303	3.506826	-2.648332
P	-3.788663	4.324769	-3.932822
P	2.892359	4.409237	-4.396271
C	3.849433	4.380957	-2.915536
P	4.595574	3.049927	-2.005264
C	4.197808	1.543706	-2.823675
C	4.812711	0.379726	-2.177082
C	4.990370	-0.845737	-2.718011
C	5.605143	-2.007388	-2.005972
C	4.585667	-3.155525	-1.747428
C	3.565393	-2.795655	-0.716128
C	2.243069	-2.667959	-0.963421

C	1.187500	-2.317906	-0.006223
P	-0.413720	-2.469237	-0.726891
C	-1.627421	-2.190941	0.536340
P	-1.479860	-1.626938	2.197120
C	0.247469	-1.391263	2.539154
C	0.596851	-0.826124	3.847793
C	-0.236816	-0.376534	4.811388
C	0.218942	0.208742	6.110474
C	-0.367027	1.618299	6.382311
C	0.053214	2.639149	5.371989
C	-0.810487	3.363851	4.627462
C	-0.508406	4.377470	3.609240
P	-1.986061	5.056060	2.931481
C	-1.535658	6.237044	1.684243
P	0.033681	6.788414	1.104874
C	1.294183	5.953475	2.036530
P	1.205199	4.709768	3.280696
P	3.144478	1.201853	-4.209205
C	4.033958	5.731474	-2.369236
C	4.840319	6.109092	-1.353163
C	4.941854	7.503644	-0.824496
C	4.574897	7.603494	0.681763
C	3.131553	7.321207	0.955529
C	2.685753	6.304411	1.725270
C	-2.631765	6.897659	0.964481
C	-3.960700	6.691970	1.096093
C	-5.005456	7.431022	0.321143
C	-5.963638	6.501502	-0.467118
C	-5.271933	5.705764	-1.527561
C	-5.355342	4.362723	-1.650051
C	-4.246815	-0.619355	-3.439489
C	-5.140875	-1.324541	-2.712070
C	-5.204816	-2.817106	-2.669917
C	-4.885215	-3.387517	-1.257902
C	-3.452023	-3.199521	-0.876686
C	-3.022042	-2.428017	0.145809
P	1.694403	-1.742280	1.594408
N	0.013244	-0.847797	-4.053456
B	0.168333	-2.077757	-5.118396
H	-5.966826	3.827980	-0.909881
H	-3.549621	-1.190437	-4.068809
H	-6.221044	-3.150926	-2.943508
H	-4.512083	-3.250924	-3.408672
H	-5.125349	-4.464980	-1.270626
H	3.442253	5.661702	2.196447
H	-3.780725	-1.948849	0.778516
H	1.900577	-2.877748	-1.987060
H	4.093222	-3.432898	-2.692992
H	5.156398	-4.037630	-1.407211
H	6.042939	-1.681433	-1.048432
H	6.426878	-2.420969	-2.615845
H	5.195254	0.550051	-1.161712
H	1.660746	1.460349	-6.387812
H	0.507651	2.029401	-8.354631
H	1.041618	3.548964	-9.097876
H	-0.845997	4.784136	-7.971039
H	-1.357539	3.542543	-9.131052
H	-2.003957	4.749464	-5.901636
H	5.979434	7.866328	-0.938973
H	4.299503	8.181330	-1.410093
H	3.439994	6.515575	-2.858649
H	4.819362	8.627058	1.017019
H	5.212130	6.916209	1.262111
H	1.675368	-0.749425	4.044132
H	1.320164	0.248946	6.139729
H	-0.095945	-0.449388	6.941160
H	-1.467308	1.561188	6.422563
H	-0.028829	1.931969	7.386500
H	-1.882061	3.182135	4.790072
H	-2.312523	7.649258	0.229107

H	-4.526260	8.143306	-0.370872
H	-5.620497	8.030652	1.016454
H	-6.491561	5.827680	0.227669
H	-6.735506	7.140084	-0.935106
H	-5.545336	-2.916824	-0.511138
H	-1.936725	1.975443	-7.231371
H	1.530965	4.507561	-6.791614
H	5.463609	5.359618	-0.850795
H	2.410004	7.995435	0.478808
H	1.133351	2.778636	5.244233
H	-1.321261	-0.419342	4.655044
H	-2.716436	-3.726062	-1.497030
H	-5.868474	-0.792914	-2.087061
H	-4.658807	6.277238	-2.234523
H	-4.326387	5.941681	1.807236
H	3.946359	-2.614214	0.296207
H	4.653893	-1.033923	-3.744782
H	-0.730014	-0.190764	-4.331451
H	0.478492	-1.569786	-6.185340
H	1.048399	-2.801291	-4.671580
H	0.888488	-0.309390	-3.975919
H	-0.918717	-2.634587	-5.157798
H	-0.221497	-1.198957	-3.113418

C-P-cage with NH₃BH₃

C	2.647699	2.732841	-4.927930
C	1.851993	2.514605	-6.141143
C	1.357758	3.442962	-6.989487
C	0.551007	3.120222	-8.206000
C	-0.891768	3.696366	-8.141929
C	-1.726616	3.042174	-7.088305
C	-2.203108	3.673090	-5.992724
C	-2.998584	3.089376	-4.907156
P	-2.974467	1.319993	-4.774795
C	-4.117412	0.839762	-3.522324
P	-5.019660	1.801304	-2.332831
C	-4.703303	3.506827	-2.648332
P	-3.788663	4.324769	-3.932822
P	2.892359	4.409237	-4.396271
C	3.849433	4.380957	-2.915536
P	4.595575	3.049927	-2.005264
C	4.197808	1.543706	-2.823675
C	4.812711	0.379726	-2.177082
C	4.990370	-0.845737	-2.718011
C	5.605143	-2.007388	-2.005972
C	4.585667	-3.155525	-1.747428
C	3.565394	-2.795655	-0.716128
C	2.243070	-2.667959	-0.963421
C	1.187500	-2.317906	-0.006223
P	-0.413720	-2.469237	-0.726891
C	-1.627421	-2.190941	0.536340
P	-1.479860	-1.626938	2.197120
C	0.247469	-1.391263	2.539154
C	0.596851	-0.826124	3.847793
C	-0.236816	-0.376534	4.811388
C	0.218942	0.208742	6.110474
C	-0.367027	1.618299	6.382311
C	0.053214	2.639149	5.371989
C	-0.810487	3.363851	4.627462
C	-0.508406	4.377470	3.609240
P	-1.986061	5.056060	2.931481
C	-1.535658	6.237044	1.684243
P	0.033681	6.788414	1.104874
C	1.294183	5.953475	2.036530
P	1.205199	4.709768	3.280696
P	3.144478	1.201853	-4.209205
C	4.033958	5.731474	-2.369236
C	4.840319	6.109092	-1.353164
C	4.941854	7.503644	-0.824496
C	4.574897	7.603494	0.681763

C	3.131553	7.321207	0.955529
C	2.685753	6.304411	1.725270
C	-2.631765	6.897659	0.964481
C	-3.960700	6.691970	1.096093
C	-5.005456	7.431022	0.321143
C	-5.963638	6.501502	-0.467118
C	-5.271933	5.705764	-1.527561
C	-5.355342	4.362723	-1.650051
C	-4.246815	-0.619355	-3.439489
C	-5.140875	-1.324541	-2.712070
C	-5.204816	-2.817106	-2.669917
C	-4.885215	-3.387517	-1.257902
C	-3.452023	-3.199521	-0.876686
C	-3.022042	-2.428017	0.145809
P	1.694403	-1.742280	1.594408
N	0.013244	-0.847797	-4.053456
B	0.168333	-2.077757	-5.118396
H	-5.966826	3.827980	-0.909881
H	-3.549621	-1.190437	-4.068809
H	-6.221044	-3.150926	-2.943508
H	-4.512083	-3.250924	-3.408672
H	-5.125349	-4.464980	-1.270626
H	3.442253	5.661702	2.196447
H	-3.780725	-1.948849	0.778516
H	1.900577	-2.877748	-1.987060
H	4.093222	-3.432898	-2.692992
H	5.156398	-4.037630	-1.407211
H	6.042939	-1.681433	-1.048432
H	6.426878	-2.420969	-2.615845
H	5.195254	0.550051	-1.161712
H	1.660746	1.460349	-6.387812
H	0.507651	2.029401	-8.354631
H	1.041618	3.548965	-9.097876
H	-0.845997	4.784136	-7.971039
H	-1.357539	3.542543	-9.131052
H	-2.003957	4.749464	-5.901636
H	5.979434	7.866328	-0.938973
H	4.299503	8.181330	-1.410093
H	3.439994	6.515575	-2.858649
H	4.819362	8.627058	1.017019
H	5.212130	6.916209	1.262111
H	1.675368	-0.749425	4.044132
H	1.320164	0.248946	6.139729
H	-0.095945	-0.449388	6.941160
H	-1.467308	1.561188	6.422563
H	-0.028829	1.931970	7.386500
H	-1.882061	3.182135	4.790072
H	-2.312523	7.649258	0.229107
H	-4.526260	8.143306	-0.370872
H	-5.620497	8.030652	1.016454
H	-6.491561	5.827680	0.227670
H	-6.735506	7.140084	-0.935106
H	-5.545336	-2.916824	-0.511138
H	-1.936725	1.975443	-7.231371
H	1.530965	4.507561	-6.791614
H	5.463609	5.359618	-0.850795
H	2.410004	7.995435	0.478808
H	1.133351	2.778636	5.244233
H	-1.321261	-0.419342	4.655044
H	-2.716436	-3.726062	-1.497030
H	-5.868474	-0.792914	-2.087061
H	-4.658807	6.277238	-2.234523
H	-4.326387	5.941682	1.807237
H	3.946360	-2.614214	0.296207
H	4.653893	-1.033923	-3.744782
H	-0.730014	-0.190764	-4.331451
H	0.478492	-1.569786	-6.185340
H	1.048399	-2.801291	-4.671580
H	0.888488	-0.309390	-3.975919
H	-0.918717	-2.634587	-5.157798

H -0.221497 -1.198957 -3.113418

C-P-cage-H₂

C 2.711914 2.802818 -4.920287
P 1.805030 2.561451 -6.411793
C 1.106576 4.117618 -6.899732
C 0.303732 4.126196 -8.129199
C -0.132874 3.062013 -8.837566
C -0.943359 3.150648 -10.091126
C -0.224797 2.530208 -11.321524
C 0.973107 3.313421 -11.754493
C 2.236896 2.836540 -11.759933
C 3.463961 3.537846 -12.157394
P 3.319677 5.271007 -12.511929
C 4.914408 5.883013 -12.943838
C 4.869943 7.324760 -13.215713
C 5.895163 8.159119 -13.494767
C 5.730422 9.623720 -13.753765
C 6.591992 10.517000 -12.824987
C 6.256796 10.361955 -11.374876
C 7.157332 10.030838 -10.424135
C 6.932869 9.832707 -8.987283
P 5.332180 10.253363 -8.348199
C 5.296324 9.812814 -6.642563
C 3.991719 10.091230 -6.027267
C 3.723195 10.203655 -4.708442
C 2.361076 10.424371 -4.132301
C 1.885492 9.229653 -3.256765
C 1.637504 7.989940 -4.055313
C 2.340720 6.843904 -3.927214
C 2.173504 5.603190 -4.694720
P 1.241883 5.729521 -6.201332
C 3.305379 1.542910 -4.459043
C 4.107030 1.324967 -3.392202
C 4.578576 -0.034504 -2.980983
C 6.103711 -0.199789 -2.826841
C 6.914955 -0.004109 -4.118622
C 7.381917 1.398794 -4.377215
C 8.209485 1.781332 -5.388660
P 8.847867 3.485292 -5.297293
C 9.767184 3.750933 -6.740598
C 10.616407 4.939385 -6.772408
C 11.343527 5.410105 -5.733590
C 12.186727 6.646047 -5.767989
C 11.498553 7.868056 -5.083735
C 10.422441 8.457550 -5.936611
C 9.100880 8.391303 -5.667588
C 8.006583 8.919078 -6.491592
P 6.505348 9.064314 -5.581041
P 2.995715 4.247133 -3.927904
P 8.974158 0.537070 -6.510816
C 9.088579 1.369086 -8.137110
C 8.877259 0.515891 -9.304184
C 9.616506 0.531466 -10.434673
C 9.337601 -0.282125 -11.658432
C 9.013534 0.593758 -12.902183
C 7.694085 1.290245 -12.802553
C 7.534916 2.631368 -12.787222
C 6.275995 3.379758 -12.679398
P 6.489005 5.076877 -13.099616
P 9.569093 2.997379 -8.396485
P 4.859031 2.462763 -12.128193
P 8.372424 9.177845 -8.206956
H 10.706882 5.450704 -7.740610
H 8.048125 -0.202201 -9.237282
H 10.223277 -0.894077 -11.904471
H 8.504894 -0.979685 -11.473223
H 9.010967 -0.069831 -13.785332
H 3.159351 10.234466 -6.729384
H 8.438177 3.248259 -12.886369

H 2.382674 1.794660 -11.441845
H 0.061868 1.490001 -11.095653
H -0.955728 2.488438 -12.148962
H -1.202612 4.200581 -10.304303
H -1.895115 2.606849 -9.951869
H 0.019082 5.124046 -8.490645
H 3.040723 0.664990 -5.065097
H 4.201651 -0.784475 -3.696986
H 4.120580 -0.281397 -2.004372
H 6.477645 0.490906 -2.051866
H 6.286182 -1.214621 -2.439987
H 7.086024 2.160209 -3.643758
H 0.953765 9.536476 -2.749042
H 2.631527 9.032262 -2.469974
H 3.116217 6.811039 -3.149589
H 2.367744 11.325212 -3.493469
H 1.630365 10.605062 -4.937134
H 3.865827 7.769027 -13.170907
H 4.668264 9.902826 -13.658289
H 6.023434 9.847382 -14.795947
H 7.660895 10.301487 -12.986973
H 6.430709 11.566870 -13.131125
H 8.191623 9.861100 -10.754932
H 8.796044 7.920482 -4.723076
H 11.093052 7.561594 -4.106352
H 12.275386 8.628058 -4.891875
H 12.431056 6.912863 -6.808897
H 13.141239 6.457831 -5.248728
H 9.820859 1.328102 -13.054990
H 7.808695 -0.656949 -4.083808
H 4.409018 2.164416 -2.754657
H 0.836818 8.049792 -4.802302
H 4.541206 10.103200 -3.984932
H 5.207073 10.517775 -11.099209
H 6.919428 7.769738 -13.534117
H 6.811941 0.642633 -12.731635
H 10.489288 1.193667 -10.477267
H 11.317768 4.858678 -4.786449
H 10.756445 8.949651 -6.858319
H 0.783367 4.346236 -12.070502
H 0.119188 2.049683 -8.499671
H 7.819382 -0.270359 -6.812614
H 6.335109 -0.376541 -4.986556

C-P-cage-Ts-1

P -1.834794 0.948769 -3.908555
C -2.514763 2.199342 -5.051998
P -2.163600 3.933589 -5.234967
C -1.072215 4.417118 -3.972085
P -0.126398 3.436003 -2.799631
C -0.458158 1.750848 -3.034135
C -3.434023 1.707069 -5.990360
C -3.656184 0.347266 -6.336342
C -4.866023 -0.018033 -7.182542
C -4.653100 -1.161471 -8.201781
C -3.758794 -0.771417 -9.334035
C -2.707316 -1.492146 -9.785266
C -1.761415 -1.123803 -10.848284
P -1.810595 0.556464 -11.414972
C -0.575713 0.771605 -12.654505
P 0.621261 -0.354055 -13.342267
C 0.438011 -1.884063 -12.502618
P -0.704041 -2.472176 -11.291384
C -0.589573 2.133932 -13.200419
C 0.372357 2.737159 -13.933430
C 0.248045 4.102890 -14.529602
C 1.411556 5.065026 -14.181423
C 1.401677 5.559941 -12.768804
C 2.450013 5.463876 -11.922331
C 2.560353 5.987907 -10.554401

P	1.058378	6.514690	-9.768185
C	1.468493	7.153692	-8.176460
P	3.009637	7.234890	-7.298475
C	4.280898	6.631860	-8.358745
P	4.227729	5.926586	-9.985712
C	5.595721	6.686424	-7.707886
C	6.809470	6.518612	-8.276613
C	8.100708	6.538537	-7.520564
C	8.837516	5.170110	-7.562593
C	8.041215	4.074909	-6.927954
C	7.618709	2.967641	-7.575758
C	6.774316	1.887155	-7.051927
P	6.199902	0.837537	-8.344018
C	5.141549	-0.393219	-7.625330
P	4.565094	-0.635238	-5.977941
C	5.336591	0.583410	-4.942618
P	6.483710	1.872895	-5.301416
C	4.987443	0.570539	-3.517720
C	4.172196	-0.279649	-2.854255
C	3.868649	-0.155420	-1.393188
C	2.355359	-0.120262	-1.076605
C	1.606159	0.924728	-1.848362
C	0.337592	0.774346	-2.294691
C	4.557258	-1.374684	-8.547667
C	4.896648	-1.613888	-9.833797
C	4.195767	-2.606707	-10.704581
C	3.521103	-1.936093	-11.932304
C	2.731382	-2.930984	-12.726056
C	1.400944	-2.930558	-12.937364
C	0.284401	7.653963	-7.466574
C	0.259467	8.419114	-6.352976
C	-0.981084	8.901637	-5.673579
C	-1.162382	8.316555	-4.240295
C	-1.562074	6.874682	-4.248693
C	-0.765796	5.850236	-3.874113
B	-0.224311	-0.231067	-6.129555
N	-1.068782	0.241102	-7.311894
H	0.964806	-3.792816	-13.454358
H	-1.489634	2.720776	-12.972624
H	0.226534	3.997109	-15.630183
H	-0.714048	4.557237	-14.241143
H	1.331089	5.934581	-14.859340
H	2.375797	4.580369	-14.407212
H	5.448839	1.375124	-2.927639
H	3.357579	4.974724	-12.303090
H	-0.680287	7.390801	-7.921207
H	-1.868263	8.662406	-6.281920
H	-0.938044	10.001691	-5.583285
H	-0.226618	8.449584	-3.673080
H	-1.936486	8.916885	-3.731817
H	0.215908	6.101382	-3.449370
H	-3.909689	2.457188	-6.641200
H	-5.209236	0.877404	-7.729810
H	-5.703876	-0.303802	-6.522944
H	-4.267219	-2.063560	-7.698738
H	-5.645907	-1.430643	-8.609107
H	-2.521427	-2.466186	-9.310342
H	2.245604	0.063855	0.008953
H	1.904207	-1.109567	-1.261496
H	-0.143779	-0.199979	-2.123016
H	4.309668	-1.008680	-0.845970
H	4.350289	0.753336	-0.996198
H	5.571430	6.905528	-6.631353
H	7.917955	6.823633	-6.471739
H	8.777389	7.299176	-7.948521
H	9.077011	4.908104	-8.606055
H	9.799734	5.291100	-7.033009
H	7.894310	2.869292	-8.635083
H	3.751872	-1.988670	-8.120660
H	3.432494	-3.144975	-10.120723

H	4.912533	-3.364159	-11.071682
H	2.878065	-1.113544	-11.588088
H	4.305483	-1.483946	-12.564087
H	-0.814000	1.160901	-7.678130
H	-1.064398	-0.419385	-8.094450
H	0.774462	0.392478	-5.866867
H	-0.265926	-1.423186	-5.933691
H	-0.985257	0.092886	-4.933986
H	-2.410468	0.283515	-6.961241
H	-3.415439	-0.387513	-5.549018
H	-3.992077	0.188448	-9.812837
H	1.307182	2.202370	-14.141980
H	0.485004	6.064095	-12.440341
H	1.206390	8.718702	-5.887468
H	-2.568074	6.653597	-4.626756
H	2.137141	1.860421	-2.057829
H	3.294646	-3.791107	-13.106783
H	5.708672	-1.041524	-10.297564
H	3.682671	-1.100844	-3.390263
H	7.757937	4.229250	-5.879881
H	6.880406	6.322991	-9.353158

C-P-cage-H₂-Ts-2

C	2.873333	2.949066	-4.747471
P	2.800900	4.633617	-4.239675
C	4.019093	4.877358	-2.970313
C	4.105372	6.220365	-2.383658
C	3.256169	7.257448	-2.550071
C	3.447716	8.606791	-1.934225
C	3.626342	9.732862	-2.990297
C	4.878530	9.582274	-3.794628
C	4.902165	9.404479	-5.133564
C	6.068191	9.217350	-6.005773
P	7.663125	9.171184	-5.227372
C	8.873218	8.887647	-6.475401
C	10.226318	8.818736	-5.909007
C	11.401702	8.849301	-6.573551
C	12.743934	8.745350	-5.922169
C	13.558411	7.514106	-6.406041
C	12.947529	6.210291	-6.000652
C	12.525267	5.264785	-6.868211
C	11.902853	3.971060	-6.559397
P	11.387982	3.713835	-4.879461
C	10.733150	2.083825	-4.749026
C	10.311764	1.787148	-3.374109
C	9.755669	0.650795	-2.899926
C	9.358702	0.437571	-1.473690
C	7.854858	0.096116	-1.302399
C	6.946972	1.226719	-1.668914
C	5.991517	1.157495	-2.621324
C	5.057960	2.207746	-3.046352
P	5.217798	3.795000	-2.267453
C	1.853374	2.642719	-5.759755
C	1.461666	1.420730	-6.181847
C	0.393274	1.162507	-7.196533
C	0.896311	0.352963	-8.419239
C	1.713557	1.150865	-9.404901
C	2.908235	0.655702	-9.952922
C	3.786338	1.450359	-10.722971
P	5.343931	0.655070	-11.091210
C	6.462896	1.880705	-11.629799
C	7.829449	1.453808	-11.974826
C	8.452330	0.304547	-11.640323
C	9.835451	-0.062753	-12.080740
C	10.761352	-0.501577	-10.920895
C	11.009818	0.575906	-9.912584
C	10.808137	0.431763	-8.584283
C	11.027064	1.420254	-7.521546
P	10.480870	0.811603	-5.961645
P	3.972312	1.626216	-4.306237

P	3.206635	3.121339	-11.043521
C	4.642320	4.107536	-11.479102
C	4.286488	5.518212	-11.680995
C	4.885678	6.385644	-12.525513
C	4.485643	7.813633	-12.718449
C	5.590888	8.827668	-12.306277
C	5.730024	8.976145	-10.825554
C	6.840477	8.671046	-10.119973
C	7.039724	8.807861	-8.671640
P	8.734880	8.631576	-8.227275
P	6.304828	3.660940	-11.763520
P	5.579546	9.035712	-7.688642
P	11.785131	2.955574	-7.992962
H	8.405190	2.181815	-12.562874
H	3.414972	5.879010	-11.118348
H	4.261355	7.981887	-13.786721
H	3.561176	8.031131	-12.158844
H	5.322681	9.806611	-12.742253
H	10.477163	2.601684	-2.655268
H	7.712240	8.305833	-10.680008
H	3.933443	9.391043	-5.652492
H	2.748759	9.756906	-3.657225
H	3.645064	10.696729	-2.450609
H	4.319227	8.593875	-1.259249
H	2.567367	8.862574	-1.318064
H	4.968324	6.380938	-1.722400
H	1.338049	3.515287	-6.183868
H	-0.058291	2.109882	-7.532690
H	-0.413097	0.576894	-6.719721
H	1.480026	-0.511873	-8.063534
H	0.014746	-0.053425	-8.945348
H	3.280336	-0.311508	-9.592564
H	7.692709	-0.173676	-0.242934
H	7.606857	-0.796931	-1.899441
H	5.882531	0.201713	-3.152132
H	9.940660	-0.402885	-1.053464
H	9.608605	1.328015	-0.873453
H	10.269160	8.749822	-4.813309
H	12.631619	8.707146	-4.826407
H	13.337433	9.648298	-6.152762
H	13.672146	7.554203	-7.501710
H	14.572605	7.595673	-5.975366
H	12.669871	5.465247	-7.938926
H	10.419187	-0.536700	-8.239672
H	10.340575	-1.390913	-10.423065
H	11.725236	-0.815236	-11.362746
H	10.291058	0.780937	-12.625456
H	9.779070	-0.902740	-12.798028
H	6.552617	8.529810	-12.754538
H	1.123282	1.824550	-10.045269
H	1.937078	0.528770	-5.755953
H	7.095284	2.162309	-1.115811
H	9.563735	-0.185070	-3.582716
H	12.837502	6.043419	-4.922456
H	11.401927	8.942559	-7.666133
H	4.849572	9.364866	-10.299759
H	5.721851	6.031135	-13.140676
H	7.933760	-0.426428	-11.007698
H	11.376698	1.531371	-10.305968
H	5.819402	9.598687	-3.231921
H	2.372675	7.137973	-3.188499
H	2.719801	3.181963	-9.281832
H	2.291974	2.461521	-8.863620

C-P-cage-H₂-C-C

C	2.575561	2.631690	-4.870754
P	1.633554	2.348064	-6.350605
C	0.888714	3.869147	-6.832992
P	0.940365	5.492612	-6.113245
C	1.924653	5.414482	-4.654344

C	1.979719	6.716003	-3.976944
C	2.637382	7.034224	-2.840958
C	2.626638	8.389188	-2.207504
C	2.180704	8.363829	-0.722063
C	0.756211	7.946965	-0.530996
C	0.369746	6.885600	0.210534
C	-0.993229	6.403661	0.467939
P	-0.985690	5.025289	1.565407
C	-2.667703	4.527032	1.841647
P	-4.189614	5.117355	1.182208
C	-3.833534	6.474858	0.093917
C	-4.977475	7.105170	-0.576980
C	-6.284655	6.780488	-0.472784
C	-7.389175	7.479717	-1.199748
C	-8.276531	6.518513	-2.032240
C	-7.539203	5.845860	-3.146486
C	-7.471357	4.507084	-3.315799
C	-6.780558	3.762630	-4.376171
P	-6.988735	2.024491	-4.181643
C	-6.119866	1.210520	-5.499837
P	-5.182192	1.839749	-6.852495
C	-5.167832	3.612411	-6.741275
C	-4.419991	4.341971	-7.772772
C	-3.689177	3.838004	-8.791502
C	-2.970506	4.676599	-9.801307
C	-1.463218	4.339743	-9.926712
C	-0.681793	4.617001	-8.681061
C	0.082659	3.700269	-8.048603
P	2.813002	4.077315	-3.894054
C	3.264509	1.472359	-4.291702
C	3.335986	0.218132	-4.791592
C	4.034351	-0.930006	-4.132706
C	3.196597	-2.224095	-4.021564
C	2.080513	-2.218458	-2.967188
C	0.898773	-1.282675	-3.285241
C	-0.238968	-1.358022	-2.273963
P	0.173301	-0.712458	-0.685703
C	-1.237822	-0.885142	0.363195
P	-2.860303	-1.520188	0.035853
C	-2.942026	-2.010303	-1.654411
C	-4.289603	-2.464232	-2.015721
C	-4.724578	-2.898270	-3.218871
C	-6.136765	-3.297884	-3.510568
C	-6.719073	-2.586692	-4.758433
C	-6.745863	-1.094672	-4.637479
C	-6.158529	-0.257096	-5.520725
P	-2.317134	7.242667	-0.367022
P	-5.907339	4.720748	-5.589878
P	-1.705028	-2.038088	-2.934840
C	-0.975785	-0.377379	1.714896
C	-1.857820	-0.197041	2.722041
C	-1.501613	0.344554	4.069680
C	-2.299643	1.624025	4.440695
C	-1.984504	2.788483	3.555872
C	-2.885885	3.399564	2.756614
H	-5.027310	-2.417032	-1.202373
H	0.068897	-0.095327	1.907021
H	-1.718456	-0.416690	4.841083
H	-0.419941	0.550126	4.121495
H	-2.056609	1.877526	5.487952
H	-4.467784	5.436512	-7.686865
H	-3.919079	3.026732	2.790277
H	1.162851	6.301195	0.697777
H	2.846989	7.698343	-0.149055
H	2.320925	9.381478	-0.313889
H	1.980006	9.072006	-2.782575
H	3.646068	8.815956	-2.239938
H	1.401895	7.514615	-4.462585
H	3.760710	1.660341	-3.329259
H	4.399988	-0.630570	-3.136086

H	4.932021	-1.173989	-4.732588
H	2.768553	-2.463198	-5.011361
H	3.886083	-3.050020	-3.782897
H	1.261126	-0.244428	-3.340642
H	-1.055048	4.947303	-10.755335
H	-1.340432	3.283978	-10.220280
H	0.110247	2.689937	-8.480835
H	-3.428735	4.521644	-10.795597
H	-3.096184	5.745158	-9.560340
H	-4.718654	7.938769	-1.244528
H	-6.974692	8.265906	-1.852309
H	-8.044097	7.988742	-0.468814
H	-8.729637	5.762658	-1.369503
H	-9.109362	7.112641	-2.451023
H	-7.991678	3.881396	-2.577312
H	-5.630742	-0.717436	-6.367923
H	-6.141984	-2.877449	-5.651582
H	-7.747374	-2.963186	-4.909860
H	-6.772504	-3.099697	-2.632336
H	-6.184820	-4.387145	-3.695482
H	-3.379769	1.405820	4.406729
H	1.691155	-3.244693	-2.858980
H	2.859399	-0.004375	-5.754428
H	-0.754909	5.635122	-8.279787
H	-3.599539	2.751808	-8.911662
H	-7.028369	6.508569	-3.855389
H	-6.586454	5.950021	0.176851
H	-0.944234	3.134921	3.563808
H	-2.916108	-0.437880	2.565027
H	-4.023593	-2.953107	-4.060170
H	-7.273555	-0.686691	-3.767476
H	0.001558	8.560537	-1.037303
H	3.221421	6.266540	-2.319715
H	2.502955	-1.947159	-1.984233
H	0.508550	-1.525204	-4.289635

C-P-cage-Ts-1-C-C

C	1.758378	3.015496	-2.819683
P	2.180977	2.064964	-1.395851
C	2.826197	0.511585	-1.958772
P	3.208456	-0.094578	-3.568477
C	2.760708	1.149744	-4.750333
C	3.029827	0.854833	-6.163381
C	3.496783	-0.294824	-6.697729
C	3.760598	-0.505061	-8.154642
C	5.258479	-0.786884	-8.463385
C	6.130357	0.399272	-8.203538
C	7.113821	0.439019	-7.278527
C	7.972659	1.578031	-6.930112
P	9.246871	1.109525	-5.807893
C	10.198828	2.556563	-5.415590
C	11.296295	2.396718	-4.453861
C	11.711013	1.269323	-3.835948
C	12.850930	1.213862	-2.868773
C	12.459413	0.629606	-1.486468
C	11.483355	1.478421	-0.734570
C	10.286477	1.039530	-0.287452
C	9.266163	1.781884	0.462740
P	9.578282	3.503533	0.769855
C	8.209436	4.159569	1.663309
C	8.379930	5.593387	1.931331
C	7.519125	6.428013	2.554148
C	7.766190	7.884680	2.785566
C	6.645124	8.793371	2.214478
C	6.572985	8.776586	0.720446
C	5.491998	8.384154	0.011238
C	5.345084	8.330296	-1.449010
P	3.654243	8.091729	-1.923669
C	3.571800	8.015750	-3.683239
P	4.824221	8.060799	-4.924605

C	6.365417	8.390260	-4.116342
P	6.817607	8.477274	-2.412110
C	1.092063	4.273962	-2.461584
C	0.252408	4.987444	-3.243466
C	-0.493186	6.208205	-2.812790
C	-0.292578	7.441263	-3.732900
C	1.022053	8.173586	-3.542459
C	2.195791	7.782460	-4.228403
P	2.059059	2.756533	-4.547944
C	7.526386	8.591191	-4.993756
C	7.511509	8.972718	-6.289253
C	8.736126	9.164592	-7.127242
C	8.894013	8.076654	-8.230938
C	9.256909	6.742002	-7.664333
C	8.448817	5.660008	-7.678939
C	8.715416	4.336990	-7.101721
P	10.058317	4.231035	-5.945619
P	7.542952	3.144026	-7.648831
C	3.165300	-0.468312	-0.918335
C	2.716362	-0.503863	0.354840
C	3.140278	-1.519765	1.368490
C	3.912311	-0.891061	2.564106
C	5.217601	-0.290711	2.149989
C	5.503467	1.027362	2.223296
C	6.725131	1.712633	1.784487
P	6.716464	3.406345	2.262032
P	7.895825	0.749501	0.860249
B	1.862167	9.785974	-6.154737
N	0.792512	10.277086	-5.169280
H	8.506391	8.460401	-4.515119
H	4.599633	8.085375	0.578931
H	6.843168	9.824066	2.560415
H	5.674743	8.493629	2.643298
H	7.824966	8.074974	3.873013
H	7.308105	-0.480818	-6.709829
H	9.322942	6.023688	1.566543
H	4.737209	1.682895	2.659867
H	3.281493	-0.128673	3.049554
H	4.085098	-1.689149	3.307611
H	3.767956	-2.290009	0.891415
H	2.252296	-2.033877	1.776632
H	3.842465	-1.272470	-1.236558
H	1.246919	4.618771	-1.430402
H	-0.229787	6.472913	-1.776094
H	-1.573543	5.968404	-2.815794
H	-0.395185	7.123750	-4.785851
H	-1.129264	8.134782	-3.539679
H	2.118834	6.940574	-4.927337
H	3.176392	-1.371070	-8.514078
H	3.423960	0.371289	-8.732425
H	2.812560	1.678746	-6.857232
H	5.331483	-1.076311	-9.526878
H	5.602081	-1.650259	-7.870381
H	10.028898	-0.007704	-0.499063
H	12.053263	-0.387339	-1.614356
H	13.387270	0.528582	-0.894291
H	13.284168	2.219299	-2.738938
H	13.651694	0.574866	-3.284130
H	11.839263	3.322943	-4.218684
H	7.481896	5.759372	-8.190947
H	7.961545	8.006121	-8.813784
H	9.685487	8.414224	-8.922742
H	9.636198	9.167615	-6.490929
H	8.689538	10.147200	-7.627495
H	8.739731	8.178108	2.359828
H	0.043225	4.632582	-4.260389
H	3.723901	-1.143450	-6.041520
H	5.914155	1.293219	-8.800673
H	11.197715	0.320748	-4.033485
H	11.785411	2.516268	-0.551075

H	6.561237	6.040862	2.921566
H	7.474745	9.106803	0.190817
H	6.550456	9.153459	-6.784980
H	10.239510	6.674619	-7.182451
H	5.956733	-0.983397	1.730491
H	2.009245	0.260757	0.698523
H	1.166581	8.622280	-2.550705
H	2.287795	8.707316	-5.515539
H	0.789612	9.374617	-4.279728
H	2.845433	10.494271	-6.186708
H	1.396513	9.357949	-7.188006
H	1.005212	11.145327	-4.675404
H	-0.162744	10.326536	-5.526551

N-Ge -cage

C	2.319010	3.839997	-4.469243
C	2.172850	2.506435	-5.028519
N	2.635166	1.450139	-4.459252
C	2.422301	0.174802	-5.113726
C	3.748108	-0.563001	-5.352973
N	4.550916	0.107414	-6.354763
C	5.761896	0.418554	-6.050898
C	6.666127	1.097165	-6.961558
Ge	6.070291	1.635640	-8.657457
C	7.218388	2.523033	-9.823114
C	6.738616	2.937803	-11.129819
N	7.479530	3.506768	-12.013707
C	6.864058	3.874543	-13.273233
C	7.009167	5.378122	-13.554445
N	6.211900	6.168866	-12.638481
C	6.810280	7.084773	-11.960537
C	6.142940	7.949760	-11.005227
Ge	4.312112	7.757416	-10.648705
C	3.470988	8.859416	-9.405684
C	2.046744	8.728869	-9.161025
N	1.377235	9.536066	-8.414539
C	-0.039444	9.289039	-8.245227
C	-0.411429	9.176879	-6.757417
N	0.164702	7.986630	-6.166368
C	0.948286	8.128996	-5.157212
C	1.619260	7.010346	-4.515235
Ge	2.601487	7.271018	-2.955550
C	3.518448	5.814304	-2.187177
C	4.267416	5.960268	-0.946107
N	4.392394	7.068550	-0.307154
C	5.180245	7.050699	0.910650
C	6.393135	7.991599	0.813360
N	7.344813	7.520761	-0.172584
C	7.663506	8.337239	-1.118455
C	8.585051	8.036774	-2.199888
Ge	8.745831	9.316170	-3.597697
C	10.106578	9.030292	-4.890281
Ge	11.075595	7.452230	-4.913971
C	10.811898	6.136297	-3.594556
C	11.538547	4.884843	-3.645076
N	12.358670	4.571643	-4.587797
C	12.999577	3.274630	-4.524020
C	12.864657	2.519320	-5.855439
N	11.486553	2.164108	-6.130505
C	10.968053	2.588469	-7.228076
C	9.595197	2.322594	-7.623679
Ge	8.986123	2.866886	-9.297985
Ge	1.480730	5.299295	-5.270553
Ge	3.310290	4.099992	-2.903420
Ge	8.429981	1.427285	-6.459642
Ge	7.112184	9.276526	-10.125130
C	6.279563	10.386513	-8.867870
C	7.039301	11.407071	-8.168798
N	8.260813	11.697948	-8.447437
C	8.906664	12.715994	-7.644702

C	10.129737	12.152897	-6.905461
N	9.742490	11.189143	-5.894905
C	10.368687	10.062117	-5.867570
Ge	4.473070	10.154154	-8.487769
Ge	9.654388	6.501744	-2.182226
N	6.285588	6.961558	-3.986727
B	6.026893	8.437069	-4.547167
H	8.611777	9.365903	-10.453919
H	1.534990	7.880453	-9.666654
H	3.435961	6.701935	-11.345106
H	7.902398	7.251508	-12.090885
H	6.639214	5.556545	-14.580122
H	8.084751	5.649799	-13.527692
H	7.386099	3.335512	-14.083691
H	5.789014	3.602229	-13.316525
H	4.743574	5.033990	-0.554770
H	5.666941	2.733184	-11.345943
H	9.988248	3.613500	-10.193435
H	11.575055	3.192100	-7.937656
H	13.311484	3.134748	-6.663636
H	13.452530	1.588287	-5.769981
H	12.602402	2.642820	-3.702097
H	14.079992	3.422357	-4.342948
H	11.344190	4.170404	-2.814311
H	9.574811	5.463499	-1.047449
H	8.226873	10.722515	-3.255578
H	11.165772	9.847552	-6.613423
H	10.842956	11.731697	-7.644366
H	10.627365	13.003981	-6.405189
H	8.218300	13.169701	-6.901552
H	9.263009	13.516979	-8.316362
H	6.505398	11.948016	-7.357761
H	6.879820	7.997876	1.804929
H	6.037127	9.021829	0.603123
H	7.201874	9.349167	-1.148388
H	4.544492	7.411200	1.738012
H	5.536249	6.031648	1.167156
H	8.844769	0.972391	-5.050225
H	6.169709	0.167965	-5.046893
H	4.279912	-0.678936	-4.385865
H	3.497996	-1.572340	-5.726622
H	1.885311	0.276274	-6.079157
H	1.809103	-0.456216	-4.446013
H	1.622430	2.432394	-5.991712
H	2.645774	8.682626	-2.354919
H	1.149665	9.137238	-4.736102
H	-0.100282	10.104824	-6.235470
H	-1.511261	9.099266	-6.695472
H	-0.380392	8.374838	-8.774125
H	-0.596321	10.149139	-8.658185
H	0.711240	5.021582	-6.571131
H	4.058011	2.967580	-2.179897
H	4.630045	1.403521	-9.143690
H	3.859618	11.064738	-7.412978
H	12.139988	7.302187	-6.014437
H	5.404456	9.073605	-3.726544
H	5.569829	8.398297	-5.668235
H	5.441579	6.554977	-3.549570
H	7.030699	7.009940	-3.251340
H	6.606997	6.312898	-4.712114
H	7.186915	8.960044	-4.679841

N-Ge-cage with NH₃BH₃

C	2.319010	3.839998	-4.469243
C	2.172850	2.506435	-5.028519
N	2.635166	1.450140	-4.459252
C	2.422301	0.174802	-5.113726
C	3.748108	-0.563001	-5.352973
N	4.550916	0.107414	-6.354763
C	5.761896	0.418554	-6.050898

C	6.666127	1.097165	-6.961558
Ge	6.070291	1.635640	-8.657457
C	7.218388	2.523033	-9.823114
C	6.738616	2.937803	-11.129819
N	7.479530	3.506768	-12.013707
C	6.864058	3.874543	-13.273233
C	7.009167	5.378122	-13.554445
N	6.211900	6.168866	-12.638481
C	6.810280	7.084773	-11.960537
C	6.142940	7.949760	-11.005227
Ge	4.312112	7.757416	-10.648705
C	3.470988	8.859416	-9.405684
C	2.046744	8.728869	-9.161025
N	1.377235	9.536066	-8.414539
C	-0.039444	9.289039	-8.245227
C	-0.411429	9.176879	-6.757417
N	0.164702	7.986630	-6.166368
C	0.948286	8.128996	-5.157212
C	1.619260	7.010346	-4.515235
Ge	2.601487	7.271018	-2.955550
C	3.518448	5.814304	-2.187177
C	4.267416	5.960268	-0.946107
N	4.392394	7.068550	-0.307154
C	5.180245	7.050699	0.910650
C	6.393135	7.991599	0.813360
N	7.344813	7.520761	-0.172584
C	7.663506	8.337239	-1.118455
C	8.585051	8.036774	-2.199888
Ge	8.745831	9.316170	-3.597697
C	10.106578	9.030292	-4.890281
Ge	11.075595	7.452230	-4.913972
C	10.811898	6.136297	-3.594556
C	11.538547	4.884843	-3.645076
N	12.358670	4.571643	-4.587797
C	12.999577	3.274630	-4.524020
C	12.864657	2.519320	-5.855439
N	11.486553	2.164108	-6.130505
C	10.968053	2.588469	-7.228076
C	9.595197	2.322594	-7.623679
Ge	8.986123	2.866886	-9.297985
Ge	1.480730	5.299295	-5.270553
Ge	3.310290	4.099992	-2.903420
Ge	8.429981	1.427285	-6.459642
Ge	7.112184	9.276526	-10.125130
C	6.279563	10.386513	-8.867870
C	7.039301	11.407071	-8.168798
N	8.260813	11.697948	-8.447437
C	8.906664	12.715994	-7.644702
C	10.129737	12.152897	-6.905461
N	9.742490	11.189143	-5.894905
C	10.368687	10.062117	-5.867570
Ge	4.473070	10.154154	-8.487769
Ge	9.654388	6.501744	-2.182226
N	6.285588	6.961558	-3.986727
B	6.026893	8.437069	-4.547167
H	8.611777	9.365903	-10.453919
H	1.534990	7.880453	-9.666654
H	3.435961	6.701935	-11.345106
H	7.902398	7.251508	-12.090885
H	6.639215	5.556545	-14.580122
H	8.084751	5.649799	-13.527692
H	7.386099	3.335512	-14.083691
H	5.789014	3.602229	-13.316525
H	4.743574	5.033990	-0.554770
H	5.666941	2.733184	-11.345943
H	9.988248	3.613500	-10.193435
H	11.575055	3.192100	-7.937656
H	13.311484	3.134748	-6.663636
H	13.452530	1.588287	-5.769981
H	12.602402	2.642820	-3.702097

H	14.079992	3.422357	-4.342948
H	11.344190	4.170404	-2.814311
H	9.574811	5.463499	-1.047449
H	8.226873	10.722515	-3.255578
H	11.165772	9.847552	-6.613423
H	10.842956	11.731697	-7.644366
H	10.627365	13.003981	-6.405189
H	8.218300	13.169701	-6.901552
H	9.263009	13.516979	-8.316362
H	6.505398	11.948016	-7.357761
H	6.879820	7.997876	1.804929
H	6.037127	9.021829	0.603123
H	7.201874	9.349167	-1.148388
H	4.544492	7.411200	1.738012
H	5.536249	6.031648	1.167156
H	8.844769	0.972391	-5.050225
H	6.169709	0.167965	-5.046893
H	4.279912	-0.678936	-4.385865
H	3.497996	-1.572340	-5.726622
H	1.885311	0.276274	-6.079157
H	1.809103	-0.456216	-4.446013
H	1.622430	2.432394	-5.991712
H	2.645774	8.682626	-2.354919
H	1.149665	9.137238	-4.736102
H	-0.100282	10.104824	-6.235470
H	-1.511261	9.099266	-6.695472
H	-0.380392	8.374838	-8.774125
H	-0.596321	10.149139	-8.658185
H	0.711240	5.021582	-6.571131
H	4.058011	2.967580	-2.179897
H	4.630045	1.403521	-9.143690
H	3.859618	11.064738	-7.412978
H	12.139988	7.302187	-6.014437
H	5.404456	9.073605	-3.726544
H	5.569829	8.398297	-5.668235
H	5.441579	6.554977	-3.549570
H	7.030699	7.009940	-3.251340
H	6.606997	6.312898	-4.712114
H	7.186915	8.960044	-4.679841

N-Ge-cage-Ts-1

C	2.599795	1.918159	-3.169653
C	1.739925	1.588581	-4.292536
N	1.498100	0.382857	-4.670835
C	0.629573	0.191424	-5.814496
C	1.329635	-0.612460	-6.922623
N	2.385036	0.157098	-7.548430
C	3.572254	-0.339235	-7.551332
C	4.719736	0.327528	-8.138677
Ge	6.376202	-0.521403	-8.172101
C	7.868881	0.328240	-8.924972
C	9.155060	-0.344358	-8.951106
N	9.330537	-1.556933	-8.556237
C	10.663793	-2.115977	-8.646090
C	11.124014	-2.697314	-7.300322
N	11.378391	-1.651735	-6.330302
C	10.733157	-1.686020	-5.218330
C	10.894707	-0.687626	-4.175249
Ge	12.019939	0.784224	-4.453548
C	12.212907	2.083762	-3.130182
Ge	11.276655	1.912015	-1.515261
C	10.187984	0.434435	-1.213315
C	9.508381	0.281543	0.060945
N	8.833515	-0.764984	0.382861
C	8.195670	-0.785639	1.683943
C	6.680386	-1.010620	1.561384
N	6.025809	0.131580	0.957832
C	5.310010	-0.070470	-0.092351
C	4.611741	0.984433	-0.803214
Ge	4.813857	2.775401	-0.284354

C	3.916920	4.128897	-1.194092
C	4.082958	5.512211	-0.783994
N	3.432578	6.490437	-1.307268
C	3.701525	7.825620	-0.813275
C	4.110602	8.774667	-1.950308
N	5.417483	8.445774	-2.481936
C	5.504415	8.201265	-3.743852
C	6.740386	7.876535	-4.426360
Ge	8.346019	7.719704	-3.496297
C	9.939091	7.326319	-4.391365
C	11.103730	7.143122	-3.609225
N	12.279958	6.707085	-4.006498
C	13.367204	6.655383	-3.034522
C	14.084307	5.296244	-2.998000
N	13.202392	4.228442	-2.585309
C	13.060211	3.228243	-3.384704
Ge	2.807291	3.692409	-2.641778
Ge	3.509866	0.564952	-2.244725
Ge	4.549116	2.041232	-8.881491
C	6.017430	2.889743	-9.648481
C	5.857572	4.207411	-10.238451
N	6.780487	4.810410	-10.900307
C	6.484692	6.135233	-11.407387
C	7.460807	7.183441	-10.847747
N	7.287471	7.358840	-9.421423
C	8.323784	7.198460	-8.671864
C	8.320990	7.316190	-7.228762
Ge	9.963334	7.138913	-6.303407
Ge	7.686646	2.035058	-9.652189
Ge	6.756635	7.639212	-6.287616
Ge	9.984243	-0.856307	-2.559808
N	12.821452	5.667215	-6.354320
B	11.582158	4.916621	-6.948040
H	3.219738	2.814180	-8.885389
H	10.011176	0.245568	-9.346068
H	8.955270	2.688872	-10.222588
H	4.866326	4.691318	-10.094490
H	6.605003	6.122715	-12.505330
H	5.446635	6.453076	-11.177883
H	7.235749	8.139653	-11.354772
H	8.497803	6.891499	-11.117308
H	9.603298	1.129249	0.774645
H	9.303939	6.949262	-9.137049
H	5.392454	7.796367	-6.983093
H	4.594059	8.244725	-4.382087
H	3.319039	8.762981	-2.728998
H	4.152563	9.794065	-1.526218
H	4.486873	7.838798	-0.028762
H	2.770957	8.224259	-0.371107
H	4.817288	5.699027	0.030143
H	5.729785	3.205495	0.873545
H	3.413480	-0.919968	-2.632579
H	1.279422	2.447412	-4.828624
H	0.265910	1.149735	-6.239411
H	-0.248883	-0.393312	-5.487957
H	1.693926	-1.570958	-6.498066
H	0.569390	-0.845355	-7.689195
H	3.763810	-1.334198	-7.091400
H	6.283953	-1.139288	2.584558
H	6.497885	-1.952053	1.002674
H	5.196836	-1.098127	-0.502803
H	8.609822	-1.632255	2.259749
H	8.377041	0.144473	2.261211
H	8.470930	7.864453	-1.967027
H	11.021619	7.389619	-2.534377
H	12.985522	6.884608	-2.024149
H	14.119933	7.425272	-3.284987
H	14.562721	5.094005	-3.982914
H	14.903463	5.388742	-2.262454
H	13.618695	3.208234	-4.349293

H	9.059950	-2.074248	-2.403685
H	10.010920	-2.505766	-5.011180
H	10.370329	-3.431463	-6.947988
H	12.070367	-3.237907	-7.480365
H	11.414396	-1.378590	-8.998773
H	10.640774	-2.950438	-9.370380
H	12.819945	1.000005	-5.747306
H	11.407356	2.937506	-0.376933
H	11.194436	7.787346	-6.994306
H	6.450793	-1.915521	-7.526189
H	2.055329	4.752887	-3.462534
H	12.565103	6.195878	-5.245623
H	10.484039	5.466273	-6.457882
H	11.471142	4.993966	-8.149671
H	11.444825	3.816645	-6.455243
H	13.179748	6.390240	-6.984128
H	13.587915	5.006744	-6.199156

N-Ge-cage-H₂

C	2.303679	3.622037	-4.527657
Ge	2.109107	1.909695	-5.270081
C	2.816118	0.421174	-4.404916
C	2.633100	-0.905333	-4.970212
N	2.980134	-1.985500	-4.365655
C	2.757348	-3.243409	-5.050226
C	4.071622	-4.010604	-5.270958
N	4.927541	-3.340815	-6.224473
C	6.137671	-3.072842	-5.861590
C	7.123091	-2.395489	-6.673181
Ge	6.686989	-1.727248	-8.328006
C	7.925325	-0.796111	-9.419902
C	7.543324	-0.345001	-10.741978
N	8.359550	0.179899	-11.590259
C	7.829326	0.585879	-12.875194
C	8.100403	2.072945	-13.156409
N	7.304606	2.927168	-12.298787
C	7.916786	3.777570	-11.553256
C	7.230238	4.676991	-10.641893
Ge	5.374791	4.537376	-10.403428
C	4.481989	5.697613	-9.252240
Ge	5.450637	7.006749	-8.324527
C	7.293923	7.154033	-8.548989
Ge	8.180163	5.981106	-9.714484
C	1.728802	4.784128	-5.180335
N	1.004419	4.722085	-6.241871
C	0.496972	5.964574	-6.786766
C	0.926631	6.153516	-8.250626
N	2.351925	6.390590	-8.354098
C	3.045128	5.583297	-9.076938
Ge	3.219439	3.824609	-2.919707
C	3.952157	2.336348	-2.045282
Ge	3.748263	0.641209	-2.793908
C	8.029195	8.174415	-7.825485
N	9.289990	8.387055	-7.972528
C	9.894876	9.435130	-7.176447
C	11.083641	8.902749	-6.360679
N	10.645084	7.993929	-5.320408
C	11.127069	6.801829	-5.321750
C	10.760190	5.789991	-4.345911
Ge	11.612492	4.137433	-4.353939
C	11.162311	2.828509	-3.086988
Ge	9.846668	3.193570	-1.816557
C	8.977812	4.852516	-1.801692
C	7.953766	5.126806	-0.807467
N	7.667735	4.317334	0.149606
C	6.608807	4.692878	1.064561
C	5.488716	3.640204	1.085258
N	4.758798	3.620395	-0.165438
C	4.656116	2.497547	-0.786659
Ge	9.430629	6.140219	-3.068669

Ge	8.918053	-2.273583	-5.962449
C	10.109598	-1.144319	-7.053515
C	11.385005	-0.836851	-6.626416
N	11.970511	-1.254778	-5.483024
C	13.314702	-0.901149	-5.054289
C	13.345664	-0.110101	-3.739050
N	12.765595	1.204083	-3.891323
C	11.825318	1.542615	-3.075842
Ge	9.611066	-0.471917	-8.740544
H	12.683977	3.903128	-5.432423
H	7.413272	6.092915	-0.908700
H	8.658452	7.468356	-3.020448
H	11.868496	6.496856	-6.092314
H	11.570588	9.769807	-5.880592
H	11.815294	8.436107	-7.052268
H	10.286685	10.210317	-7.859333
H	9.171621	9.920198	-6.488216
H	2.158719	-0.951433	-5.974725
H	7.438265	8.792201	-7.113821
H	9.701090	6.029484	-9.937667
H	9.025541	3.858114	-11.585155
H	9.188775	2.266372	-13.059121
H	7.809752	2.269333	-14.203864
H	6.739340	0.396487	-12.967732
H	8.342632	0.006037	-13.663525
H	6.473770	-0.485737	-11.013689
H	5.278168	-1.829214	-8.942642
H	9.610828	-3.670607	-5.814026
H	12.046328	-0.203123	-7.232549
H	13.771597	-0.296971	-5.850942
H	13.918598	-1.817321	-4.937151
H	12.859348	-0.706924	-2.935466
H	14.409823	-0.002390	-3.460534
H	11.485862	0.825664	-2.295063
H	3.798188	-5.004087	-5.673182
H	4.566739	-4.168755	-4.288832
H	6.476266	-3.375856	-4.843482
H	2.107962	-3.871010	-4.414312
H	2.254279	-3.107760	-6.030006
H	4.523229	3.467577	-11.105913
H	2.549175	4.744311	-9.612167
H	0.596636	5.273314	-8.840393
H	0.397467	7.042446	-8.637356
H	0.817419	6.850105	-6.199396
H	-0.606867	5.925493	-6.770488
H	1.940458	5.767725	-4.705551
H	4.400026	-0.529459	-0.396658
H	5.115143	1.578647	-0.359425
H	5.924048	2.652090	1.342542
H	4.789387	3.923297	1.892144
H	6.168837	5.682543	0.823132
H	7.033176	4.745095	2.082718
H	3.356576	5.257381	-2.377204
H	1.384462	1.664110	-6.603749
H	4.795848	7.985820	-7.335741
H	9.517150	2.061181	-0.830132
H	10.694783	0.381456	-9.434592
H	8.936311	-1.682216	-4.509147
H	11.420312	-1.836046	-4.851762

N-Ge-cage-H₂-Ts-2

C	2.102724	3.948887	-4.521056
C	1.952269	2.636170	-5.122397
N	2.483302	1.567792	-4.641019
C	2.261990	0.323529	-5.348914
C	3.589944	-0.360093	-5.709960
N	4.315228	0.389093	-6.715914
C	5.517232	0.756121	-6.441364
C	6.352536	1.517213	-7.353254

Ge	5.666878	2.123819	-8.989571
C	6.741313	3.093699	-10.161368
C	6.202012	3.555399	-11.427589
N	6.900022	4.170499	-12.316299
C	6.232877	4.587067	-13.532616
C	6.381390	6.099709	-13.761572
N	5.632616	6.857302	-12.779510
C	6.274582	7.703378	-12.053609
C	5.646149	8.514890	-11.026229
Ge	3.829061	8.288827	-10.619007
C	3.015116	9.341328	-9.316098
C	1.603676	9.169537	-9.020043
N	0.952232	9.925318	-8.208371
C	-0.449664	9.633481	-7.988036
C	-0.743039	9.398153	-6.497382
N	-0.128975	8.173338	-6.027082
C	0.690009	8.254064	-5.037864
C	1.388815	7.112416	-4.476458
Ge	2.484117	7.335003	-2.986130
C	3.397163	5.871960	-2.250545
C	4.250527	6.045787	-1.087914
N	4.382653	7.162309	-0.463361
C	5.273767	7.194435	0.678870
C	6.377018	8.249599	0.511348
N	7.308465	7.886310	-0.537074
C	7.602834	8.778730	-1.417227
C	8.536366	8.566287	-2.506108
Ge	9.064268	10.013384	-3.584153
C	10.318558	9.697218	-4.977623
Ge	11.094626	8.021595	-5.220643
C	10.619035	6.612173	-4.091563
C	11.246384	5.310733	-4.220571
N	12.191769	5.053678	-5.055792
C	12.738638	3.712399	-5.066596
C	12.552224	3.033638	-6.433361
N	11.164761	2.688464	-6.666888
C	10.598031	3.139733	-7.729653
C	9.214807	2.863950	-8.075921
Ge	8.521005	3.460842	-9.696783
Ge	1.202553	5.410753	-5.241475
Ge	3.202077	4.187752	-3.019909
Ge	8.120488	1.891383	-6.903504
Ge	6.638801	9.796788	-10.112416
C	5.833573	10.857628	-8.791419
C	6.599795	11.867776	-8.087548
N	7.828668	12.146251	-8.352053
C	8.463316	13.201784	-7.589492
C	9.816156	12.763381	-7.017337
N	9.681753	11.782794	-5.953503
C	10.427262	10.709332	-5.975943
Ge	4.027215	10.624735	-8.398821
Ge	9.298374	6.889476	-2.795578
H	8.127109	9.919373	-10.479280
H	1.089328	8.333879	-9.542966
H	2.946483	7.238053	-11.312078
H	7.367786	7.849407	-12.196621
H	5.969251	6.324774	-14.761253
H	7.460099	6.359326	-13.768056
H	6.714308	4.076681	-14.385802
H	5.154635	4.324293	-13.539842
H	4.801661	5.143333	-0.743850
H	5.124559	3.346363	-11.608439
H	9.465949	4.268773	-10.601680
H	11.169003	3.770892	-8.445564
H	12.969081	3.690569	-7.224904
H	13.141182	2.099501	-6.419490
H	12.293626	3.063371	-4.283736
H	13.824385	3.780073	-4.876424
H	10.875453	4.517298	-3.534897
H	8.924529	5.658521	-1.950903

H	8.974438	11.415848	-2.951656
H	11.130013	10.554107	-6.818845
H	10.450441	12.382442	-7.841603
H	10.306843	13.661321	-6.600794
H	7.820655	13.581695	-6.766694
H	8.661958	14.048387	-8.271255
H	6.062159	12.420167	-7.285352
H	6.928121	8.295685	1.468789
H	5.910874	9.242899	0.341576
H	7.137863	9.788545	-1.361817
H	4.682904	7.472391	1.569973
H	5.746784	6.209772	0.874881
H	8.609664	1.383982	-5.536700
H	5.974296	0.489578	-5.463129
H	4.181635	-0.512593	-4.783485
H	3.345770	-1.353758	-6.126379
H	1.661616	0.459304	-6.272450
H	1.710398	-0.362598	-4.681504
H	1.336189	2.587140	-6.047165
H	2.606497	8.761324	-2.424908
H	0.895726	9.238017	-4.561739
H	-0.416011	10.287971	-5.920282
H	-1.838073	9.303967	-6.388272
H	-0.797880	8.754326	-8.568715
H	-1.041640	10.510163	-8.306217
H	0.334749	5.148458	-6.483829
H	3.995951	3.035771	-2.381953
H	4.212256	1.878641	-9.424617
H	3.441160	11.513445	-7.289510
H	12.082453	7.885117	-6.392998
H	7.717982	10.753819	-4.936994
H	8.282084	11.255686	-5.346497

N-Ge-cage-H₂-C-N

C	2.360114	3.601417	-4.579795
Ge	2.146474	1.898530	-5.299649
C	2.856343	0.399930	-4.422413
C	2.690338	-0.922706	-4.998134
N	2.151142	-1.130409	-6.147615
C	2.039498	-2.497780	-6.611571
C	0.592736	-2.845108	-6.995324
N	-0.264152	-2.903381	-5.829115
C	-1.325888	-2.177026	-5.820102
C	-2.255730	-2.139046	-4.705447
Ge	-3.829936	-1.150528	-4.821748
C	-5.027866	-1.098969	-3.379601
Ge	-4.633645	-2.034599	-1.819164
C	-3.052305	-3.033635	-1.691365
C	-2.727832	-3.741808	-0.468868
N	-3.514904	-3.820248	0.546399
C	-3.033441	-4.531678	1.711242
C	-3.050488	-3.666719	2.973900
N	-2.261257	-2.445859	2.812230
C	-1.771612	-1.894296	4.080263
C	-0.915472	-0.664413	3.875238
Ge	-1.657543	1.035499	3.959286
C	-0.595323	2.563461	3.689994
C	-1.152517	3.891887	3.868915
N	-2.365924	4.114890	4.235607
C	-2.774197	5.493345	4.414864
C	-3.982513	5.853366	3.537893
N	-3.615720	5.942327	2.139220
C	-4.294594	5.257546	1.287659
C	-4.026192	5.273975	-0.139513
Ge	-5.159015	4.388009	-1.321640
C	-4.828580	4.437503	-3.167333
C	-5.722429	3.769216	-4.095634
N	-6.820681	3.198882	-3.743160
C	-7.609188	2.556098	-4.774761

C	-7.854306	1.074073	-4.447602
N	-6.624262	0.311375	-4.517489
C	-6.250250	-0.320139	-3.460962
Ge	3.298929	3.810791	-2.970574
C	4.011128	2.332724	-2.089203
Ge	3.780880	0.621944	-2.820601
C	1.805520	4.756926	-5.261609
N	1.968550	5.966174	-4.853793
C	1.353812	7.030429	-5.620525
C	0.404736	7.870820	-4.750931
N	-0.780327	7.121403	-4.386690
C	-1.047715	6.989399	-3.135078
C	-2.197051	6.258573	-2.632652
Ge	-3.348697	5.365671	-3.812495
C	4.745036	2.527932	-0.851809
N	5.340275	1.584254	-0.211344
C	6.039248	1.943196	1.007063
C	5.552931	1.122431	2.210007
N	4.188979	1.457209	2.566973
C	3.358006	0.488474	2.729496
C	1.963112	0.670720	3.081715
Ge	0.882084	-0.808503	3.428592
Ge	1.201691	2.374223	3.236520
Ge	-2.544631	6.212742	-0.803835
Ge	-1.871555	-3.079541	-3.130381
H	-5.639658	-1.925848	-0.662629
H	-1.574690	-1.535297	-6.693701
H	-4.070547	-0.378847	-6.129660
H	-6.874025	-0.289423	-2.540420
H	-8.553414	0.679447	-5.205977
H	-8.345239	1.000259	-3.455132
H	-8.595456	3.051411	-4.818658
H	-7.141581	2.631842	-5.778531
H	4.780615	3.571007	-0.466785
H	-5.412606	3.773594	-5.163947
H	-6.339315	3.614655	-0.710910
H	-5.138880	4.617319	1.625576
H	-4.797538	5.123130	3.721611
H	-4.336981	6.848138	3.862974
H	-1.953851	6.211485	4.206366
H	-3.081662	5.625110	5.467804
H	-0.459702	4.743550	3.688436
H	2.008487	3.663600	3.009438
H	-2.656995	-1.641004	4.691185
H	-4.091152	-3.388869	3.212885
H	-2.680431	-4.300705	3.810727
H	-2.003837	-4.929684	1.558401
H	-3.693663	-5.397498	1.896020
H	-1.728044	-4.232332	-0.437626
H	6.209110	1.377564	3.062333
H	5.682950	0.041381	1.993842
H	3.695891	-0.563679	2.598354
H	7.112400	1.719717	0.868514
H	5.943675	3.022694	1.247411
H	-1.546841	6.944065	0.109166
H	-0.385794	7.451434	-2.369825
H	0.961206	8.245030	-3.866828
H	0.092296	8.743373	-5.352037
H	0.796131	6.653873	-6.502901
H	2.152225	7.702724	-5.981711
H	1.216996	4.550598	-6.182526
H	4.317869	-0.649757	-2.142986
H	3.063264	-1.776536	-4.390637
H	2.402379	-3.233019	-5.863715
H	2.655391	-2.605453	-7.522320
H	0.234164	-2.117340	-7.752426
H	0.608435	-3.845180	-7.464330
H	1.343865	1.794046	-6.606825
H	3.509131	5.179575	-2.302249
H	-3.126767	5.344635	-5.334023

H	-0.579318	-3.889415	-2.934828
H	-3.143031	1.125962	4.349647
H	1.532102	-2.211746	3.360121
H	-1.468240	-2.608836	2.184389
H	-1.209326	-2.654181	4.672621

P-Ge-cagewith NH₃BH₃

C	2.324683	3.486812	-4.192953
Ge	1.948547	1.767160	-4.867549
C	2.691058	0.220228	-4.121976
C	2.337368	-1.067136	-4.651424
P	2.546104	-2.589895	-3.872994
C	2.001476	-3.784877	-5.227187
C	3.181351	-4.471586	-5.944196
P	4.083014	-3.326795	-7.144174
C	5.694986	-3.382612	-6.541889
C	6.846773	-2.732657	-7.102180
Ge	8.378185	-2.522265	-6.038467
C	9.920734	-1.627888	-6.639054
Ge	9.943316	-1.042225	-8.418115
C	8.450000	-1.232622	-9.552362
C	8.406072	-0.736863	-10.897725
P	9.404042	0.502910	-11.561234
C	8.800026	0.576794	-13.351542
C	8.538396	2.042591	-13.731983
P	7.350355	2.804721	-12.474835
C	8.178242	4.248993	-12.030689
C	7.715947	5.235595	-11.096438
Ge	8.981094	6.333944	-10.253035
C	8.509346	7.591878	-8.937891
C	9.485453	8.386697	-8.245245
P	11.128438	7.948887	-7.987475
C	11.826408	9.507667	-7.189399
C	12.699466	9.210884	-5.957729
P	11.768390	8.692749	-4.405983
C	11.859454	6.949261	-4.394828
C	11.188393	6.082360	-3.515328
Ge	11.817120	4.295281	-3.324369
C	11.127830	2.977359	-2.210387
C	11.676168	1.666448	-2.132506
P	13.320176	1.209050	-2.436928
C	13.208118	-0.676713	-2.336750
C	12.887087	-1.391791	-3.660743
P	11.048577	-1.369161	-4.078869
C	11.072010	-1.440796	-5.797272
C	1.842594	4.684233	-4.824582
P	1.393943	4.828988	-6.480614
C	0.815555	6.622837	-6.587568
C	1.497823	7.335991	-7.765022
P	3.365404	7.409036	-7.498048
C	3.976045	6.825696	-8.998781
C	5.364165	6.731358	-9.353678
Ge	6.687963	7.806207	-8.560047
Ge	3.388433	3.619064	-2.658111
C	4.245391	2.116197	-1.911316
C	5.172881	2.148654	-0.816706
P	5.684042	3.482357	0.147994
C	6.807924	2.564872	1.362507
C	7.855241	3.441853	2.055250
P	9.348484	4.099071	1.089196
Ge	9.516755	3.451310	-1.245239
C	9.137554	5.390673	-1.202932
Ge	9.668317	6.675334	-2.526197
Ge	5.905974	5.491202	-10.653172
Ge	3.914455	0.453552	-2.711468
Ge	6.939295	-2.111895	-8.874615
C	8.795963	5.552516	0.106905
B	9.686109	9.121991	-1.139602
N	9.602694	10.076666	-2.416464

H	12.847015	3.923373	-4.416365
H	8.468965	6.494935	0.565517
H	12.578126	6.503128	-5.100049
H	13.269636	10.115035	-5.689747
H	13.441878	8.428047	-6.183681
H	12.442632	10.009233	-7.956876
H	11.004801	10.196213	-6.936056
H	1.861945	-1.069268	-5.642902
H	9.126188	9.324883	-7.795789
H	10.422038	6.277788	-10.797183
H	9.195663	4.393260	-12.424874
H	9.476141	2.619465	-13.742447
H	8.096310	2.111417	-14.739313
H	7.883974	-0.025711	-13.452737
H	9.562068	0.133525	-14.013105
H	7.604911	-1.138071	-11.536503
H	5.820984	-2.425600	-9.888828
H	8.379933	-3.258792	-4.684253
H	12.033657	-1.284511	-6.308433
H	13.462948	-0.961285	-4.495598
H	13.172329	-2.456370	-3.585573
H	12.477884	-0.952585	-1.557376
H	14.193103	-1.015271	-1.977356
H	10.994800	0.873674	-1.784471
H	2.796812	-5.317795	-6.539250
H	3.896006	-4.888631	-5.217131
H	5.862555	-3.930779	-5.602201
H	1.378813	-4.552534	-4.738973
H	1.358463	-3.256355	-5.949060
H	4.788791	4.778503	-11.440783
H	3.254627	6.419735	-9.723589
H	1.281003	6.823762	-8.715775
H	1.118214	8.367078	-7.856431
H	1.028009	7.138232	-5.637598
H	-0.278364	6.626437	-6.724388
H	1.832736	5.595007	-4.208340
H	4.716012	-0.737765	-2.150998
H	5.616756	1.173406	-0.561916
H	7.291236	1.722207	0.844981
H	6.149685	2.131790	2.136130
H	7.388072	4.337322	2.500467
H	8.294921	2.879446	2.894556
H	3.644637	5.042751	-2.122408
H	0.900759	1.579842	-5.982432
H	6.294719	8.998002	-7.663684
H	8.294735	2.585812	-1.665841
H	11.286233	-0.523797	-8.969683
H	8.677278	10.072118	-2.856201
H	9.825464	11.044313	-2.165192
H	8.590455	8.857780	-0.709589
H	10.502988	9.531814	-0.350933
H	8.619598	7.455425	-3.368165
H	10.302299	9.768374	-3.166193
H	10.290528	8.045254	-1.544619

P-Ge-cage-Ts-1

C	2.550739	2.310117	-3.713762
C	1.877670	3.470628	-4.228160
P	1.299058	3.626057	-5.843058
C	0.450058	5.311880	-5.820640
C	0.851969	6.107473	-7.071255
P	2.720983	6.378380	-7.080578
C	3.149508	5.982701	-8.701994
C	4.469649	6.095014	-9.255759
Ge	4.978868	5.040266	-10.717251
C	6.744627	5.040269	-11.376288
Ge	7.964094	6.257714	-10.643426
C	7.492300	7.419732	-9.241645
Ge	5.748057	7.295337	-8.570613
Ge	3.769656	2.477570	-2.301453

C	4.862158	1.038982	-1.767170
Ge	4.630898	-0.593951	-2.660527
C	3.268584	-0.890249	-3.921955
C	2.992077	-2.183935	-4.481296
P	3.423809	-3.702250	-3.791037
C	2.887173	-4.901167	-5.144697
C	4.056752	-5.403511	-6.015126
P	4.662195	-4.114521	-7.252800
C	6.333544	-3.998882	-6.857120
C	7.320350	-3.195897	-7.524750
Ge	7.105313	-2.516993	-9.265783
C	8.390736	-1.423617	-10.081435
C	8.118196	-0.896400	-11.387568
P	8.864707	0.480436	-12.108576
C	8.051459	0.520055	-13.815245
C	7.613901	1.958639	-14.129738
P	6.506774	2.583841	-12.731572
C	7.209188	4.116229	-12.372148
Ge	2.268675	0.599572	-4.453280
C	5.904464	1.100219	-0.782672
P	6.323357	2.367472	0.307661
C	7.738223	1.512254	1.230230
C	8.797906	2.449802	1.815934
P	10.002695	3.379496	0.684643
C	9.072144	4.786613	-0.061520
C	9.132772	4.734374	-1.418971
Ge	9.794532	2.891763	-1.680241
C	11.265444	2.775117	-2.947946
C	12.079100	1.608878	-3.024615
P	13.690463	1.501909	-3.651359
C	13.984188	-0.364661	-3.594904
C	13.589017	-1.127012	-4.872446
P	11.730989	-1.429496	-5.003548
C	11.486370	-1.397485	-6.705932
C	10.263657	-1.719228	-7.391741
Ge	8.933976	-2.822156	-6.645249
Ge	9.053828	6.128366	-2.742506
C	10.419591	5.825858	-4.093547
C	10.663543	6.775351	-5.065088
P	9.806857	8.325109	-5.317790
C	11.030064	9.306330	-6.378018
C	10.409806	9.960882	-7.627703
P	10.015694	8.726433	-8.999278
C	8.370598	8.370847	-8.624556
Ge	11.413917	4.195302	-4.131624
Ge	9.980264	-1.079795	-9.129621
B	10.141523	8.627247	-1.473842
N	9.905260	9.688108	-2.564875
H	12.293159	4.078509	-5.397672
H	8.729795	5.648194	0.527056
H	11.416889	6.543349	-5.834188
H	11.483370	10.086357	-5.742960
H	11.847449	8.627786	-6.667669
H	11.129562	10.680957	-8.050445
H	9.502514	10.528785	-7.367789
H	2.423490	-2.197348	-5.422155
H	7.934780	8.932060	-7.785603
H	9.375099	6.261776	-11.264750
H	8.147670	4.378699	-12.882785
H	8.486541	2.623053	-14.228502
H	7.058613	1.998631	-15.080735
H	7.188281	-0.164226	-13.824718
H	8.768548	0.157551	-14.569604
H	7.300577	-1.378772	-11.943833
H	5.913189	-2.945992	-10.143920
H	9.185460	-3.574941	-5.323527
H	12.320920	-1.054270	-7.335609
H	13.944065	-0.602244	-5.773998
H	14.067429	-2.122251	-4.868927
H	13.467751	-0.783443	-2.715385

H	15.064024	-0.495453	-3.419235
H	11.655939	0.691652	-2.585130
H	3.718975	-6.274237	-6.603229
H	4.896773	-5.744784	-5.389503
H	6.681816	-4.553597	-5.972553
H	2.420044	-5.760235	-4.636244
H	2.108576	-4.430476	-5.766551
H	3.887002	4.191653	-11.398556
H	2.377038	5.541733	-9.349015
H	0.549196	5.578793	-7.989271
H	0.353013	7.090305	-7.078484
H	0.726294	5.853546	-4.902037
H	-0.641261	5.157756	-5.796064
H	1.801449	4.340915	-3.560639
H	5.632041	-1.710634	-2.301494
H	6.518704	0.188758	-0.711301
H	8.206961	0.769205	0.566851
H	7.276400	0.951927	2.062344
H	8.330681	3.237247	2.432869
H	9.445621	1.876396	2.498526
H	3.961049	3.891494	-1.716073
H	1.098771	0.361060	-5.427199
H	5.342721	8.358928	-7.531339
H	8.680604	1.848626	-1.975608
H	11.166989	-0.370125	-9.810766
H	9.856600	9.099795	-3.787187
H	9.392710	7.531820	-1.907945
H	9.057845	10.248035	-2.442409
H	10.698186	10.330221	-2.641420
H	9.535882	8.769437	-0.436900
H	11.266442	8.201570	-1.442651
H	7.657986	6.501956	-3.318876

P-Ge-cage-H₂

C	1.343752	3.789373	-4.461844
Ge	1.432133	1.996553	-5.034126
C	2.307946	0.671225	-4.042472
C	2.384508	-0.667784	-4.558625
P	3.502159	-1.879318	-4.065313
C	2.876269	-3.384845	-5.014848
C	4.005990	-4.368333	-5.368263
P	5.105236	-3.830576	-6.805804
C	6.385176	-3.001508	-5.995685
C	7.426087	-2.297305	-6.673531
Ge	7.125550	-1.391699	-8.259756
C	8.570627	-0.647331	-9.276681
C	8.244853	0.015945	-10.418800
P	9.391691	0.852591	-11.581278
C	8.526366	0.565806	-13.242168
C	7.924640	1.850485	-13.831596
P	6.517335	2.581466	-12.799399
C	7.292364	3.983997	-12.155955
C	6.736727	4.987987	-11.296971
Ge	4.896140	5.222035	-10.979329
C	4.253723	6.549825	-9.825688
Ge	5.504176	7.713887	-9.030678
C	7.351804	7.512157	-9.268543
Ge	7.925487	6.171757	-10.455639
C	0.743896	4.832525	-5.243553
P	0.493729	4.795982	-6.948645
C	-0.371247	6.445669	-7.266836
C	0.291828	7.127962	-8.473652
P	2.142204	7.303199	-8.136270
C	2.845516	6.633936	-9.559550
Ge	2.087940	4.211530	-2.793427
C	2.969750	2.928992	-1.737234
Ge	3.009154	1.164759	-2.366621
C	8.263149	8.377158	-8.573094
P	9.898582	7.994904	-8.191709
C	10.506891	9.589414	-7.382624

C	11.310685	9.242484	-6.121048
P	10.232593	8.225699	-4.948810
C	11.292730	6.940016	-4.505935
C	10.994762	5.890428	-3.575213
Ge	11.957947	4.284761	-3.662545
C	11.561707	2.811702	-2.558909
Ge	10.240212	3.040060	-1.250855
C	9.269331	4.644217	-1.065176
C	8.243730	4.858578	-0.082676
P	7.405016	3.664586	0.831296
C	6.290596	4.733111	1.919451
C	4.809115	4.340392	1.786162
P	4.121495	4.763182	0.078838
C	3.601544	3.220932	-0.480489
Ge	9.690895	6.051474	-2.227233
Ge	9.166259	-2.108894	-5.890854
C	10.616372	-1.486494	-6.841193
C	11.908301	-1.434239	-6.243177
P	12.497914	-2.527336	-5.033785
C	14.084114	-1.657080	-4.483804
C	13.896558	-0.605693	-3.374773
P	13.144102	0.998208	-4.021514
C	12.248572	1.551481	-2.661144
Ge	10.451153	-0.918647	-8.702780
H	13.167947	4.260797	-4.616476
H	7.931104	5.904503	0.058111
H	9.030868	7.412042	-1.927992
H	12.256766	6.868017	-5.031676
H	11.635768	10.160825	-5.605375
H	12.216337	8.670094	-6.376057
H	11.132155	10.142139	-8.102923
H	9.644063	10.228429	-7.137154
H	1.690216	-0.913580	-5.376336
H	7.849767	9.321556	-8.189152
H	9.397454	6.090033	-10.904515
H	8.356955	4.110564	-12.403889
H	8.705433	2.613071	-13.973927
H	7.507546	1.623915	-14.826470
H	7.762464	-0.217898	-13.131860
H	9.296710	0.167407	-13.921641
H	7.188575	0.172144	-10.687919
H	5.701381	-1.022549	-8.727805
H	9.207205	-2.301737	-4.361193
H	12.604997	-0.673180	-6.630032
H	14.568880	-1.207937	-5.366383
H	14.758736	-2.448641	-4.120423
H	13.279246	-1.002004	-2.553141
H	14.879770	-0.344187	-2.945233
H	12.144608	0.871178	-1.802683
H	3.565858	-5.332379	-5.669516
H	4.639100	-4.567648	-4.488252
H	6.459339	-3.085257	-4.901110
H	2.142049	-3.892878	-4.366003
H	2.336429	-3.057686	-5.917648
H	3.842959	4.399368	-11.747465
H	2.176541	6.151554	-10.287439
H	0.139726	6.539864	-9.392185
H	-0.141557	8.126809	-8.644908
H	-0.298584	7.077518	-6.367943
H	-1.441398	6.266648	-7.460085
H	0.495926	5.762472	-4.710005
H	3.542161	0.099219	-1.388987
H	3.831406	2.352273	0.154703
H	4.666549	3.266740	1.987224
H	4.211989	4.892190	2.531321
H	6.440991	5.795778	1.671233
H	6.614300	4.595049	2.964797
H	1.831344	5.636935	-2.265125
H	0.667169	1.531063	-6.288919
H	5.026789	8.958129	-8.256633

H	10.075852	1.893947	-0.233292
H	11.213585	0.423799	-8.896183
H	10.355549	-0.210693	-11.672071
H	11.082536	-1.957182	-9.677285

P-Ge-cage-H₂-Ts-2

C	0.780926	3.943613	-5.357735
C	-0.006007	4.695949	-6.294003
P	-0.740108	6.224315	-5.988559
C	-1.506147	6.639427	-7.664856
C	-2.941119	7.152244	-7.471906
P	-3.982227	5.828839	-6.614993
C	-4.815876	6.742511	-5.415440
C	-5.794751	6.225748	-4.501400
Ge	-6.088825	7.110490	-2.874940
C	-7.263960	6.438772	-1.568410
Ge	-8.233709	4.888158	-1.982546
C	-7.981861	3.944298	-3.589997
Ge	-6.799672	4.672851	-4.849723
Ge	0.919558	2.084001	-5.556600
C	1.844580	1.008415	-4.320877
Ge	2.737027	1.868977	-2.915177
C	2.634988	3.728573	-2.649588
C	3.232554	4.387663	-1.522930
P	3.592444	3.645423	-0.010728
C	4.401417	5.055604	0.950300
C	3.773703	5.152903	2.349638
P	1.921012	5.492168	2.203957
C	1.247317	4.302958	3.252120
C	-0.146932	4.156599	3.562666
Ge	-1.372575	5.579008	3.441790
C	-3.202501	5.360474	3.790089
C	-4.088699	6.478460	3.626484
P	-5.782673	6.383365	3.331018
C	-6.288291	8.203984	3.326408
C	-7.201142	8.487237	2.122812
P	-6.294511	8.053423	0.522954
C	-7.436710	7.042272	-0.277990
Ge	1.695542	4.739458	-3.918971
C	1.889929	-0.423875	-4.407685
P	0.727265	-1.420164	-5.196423
C	1.468425	-3.143178	-4.974706
C	0.388721	-4.125160	-4.496529
P	-0.316933	-3.569177	-2.833466
C	-2.011293	-3.745152	-3.084649
C	-3.025063	-3.551363	-2.086612
Ge	-2.735591	-3.863406	-0.269249
C	-4.089634	-3.586119	1.019530
C	-3.752692	-3.644382	2.381012
P	-4.847703	-3.249014	3.695161
C	-3.671095	-3.133487	5.166361
C	-3.505130	-1.715262	5.734393
P	-2.423733	-0.607671	4.651454
C	-3.131214	0.934497	4.945471
C	-2.618493	2.203746	4.510524
Ge	-0.797418	2.494696	4.138457
Ge	-4.744629	-2.974061	-2.614667
C	-6.108914	-2.598450	-1.397221
C	-7.391325	-2.111169	-1.805789
P	-7.704481	-1.199536	-3.238484
C	-9.593165	-1.119583	-3.251178
C	-10.034644	0.259913	-3.760142
P	-9.234008	1.595921	-2.691748
C	-8.644462	2.703338	-3.873490
Ge	-5.772459	-2.866631	0.458439
Ge	-3.782274	3.668287	4.370419
H	-2.361844	-3.948124	-4.107965
H	-5.027304	-3.019017	-4.130260
H	-8.228292	-2.284070	-1.111000
H	-9.991041	-1.919614	-3.896408

H	-9.970204	-1.302035	-2.231963
H	-11.130674	0.363936	-3.708956
H	-9.738159	0.405988	-4.810887
H	3.395477	5.471802	-1.616638
H	-8.698684	2.404444	-4.930979
H	-9.348248	4.483484	-0.997767
H	-8.345320	6.760757	0.275532
H	-8.131930	7.902281	2.187921
H	-7.483030	9.552541	2.097149
H	-5.385821	8.834314	3.292757
H	-6.813085	8.430533	4.269244
H	-3.621798	7.474798	3.615613
H	-0.878389	7.021565	3.215991
H	0.248861	1.412169	4.468946
H	-4.091560	0.957639	5.483042
H	-4.483895	-1.236513	5.897640
H	-3.012253	-1.780463	6.719465
H	-2.695614	-3.557664	4.878513
H	-4.093283	-3.787354	5.946550
H	-2.714866	-3.892070	2.648527
H	4.237557	5.973157	2.921955
H	3.934193	4.223917	2.918985
H	1.924421	3.540955	3.666234
H	5.483426	4.859646	1.028218
H	4.277399	5.999057	0.395590
H	-5.419130	8.487801	-2.700264
H	-4.523939	7.794455	-5.277993
H	-2.952251	8.075259	-6.870768
H	-3.398185	7.389465	-8.446704
H	-1.490814	5.744427	-8.306646
H	-0.887071	7.407446	-8.157142
H	-0.214559	4.210635	-7.259579
H	3.674781	1.001668	-2.052550
H	2.699039	-0.921992	-3.852734
H	2.302951	-3.094420	-4.257206
H	1.885202	-3.474671	-5.940005
H	-0.427123	-4.202415	-5.232976
H	0.816052	-5.134410	-4.376457
H	0.357428	1.479084	-6.858241
H	1.814048	6.272692	-3.814747
H	-6.775921	4.018935	-6.245178
H	-1.463498	-4.586681	0.219505
H	-5.210841	3.472155	4.915614
H	-5.493195	-1.404987	1.780865
H	-5.303722	-1.674112	2.579215
H	-7.037503	-3.234680	1.266753

P-Ge-cage-H₂-C-P

C	1.535025	3.717458	-4.301589
Ge	1.582053	1.926757	-4.858871
C	2.558603	0.613835	-3.932091
C	2.547933	-0.775464	-4.294063
P	1.300698	-1.578502	-5.169795
C	1.997585	-3.325742	-5.341930
C	0.915805	-4.356216	-4.984670
P	0.330415	-4.085706	-3.208931
C	-1.382885	-4.124720	-3.383394
C	-2.339661	-4.021587	-2.318047
Ge	-4.074807	-3.425619	-2.703933
C	-5.371671	-3.178159	-1.364088
Ge	-4.906503	-3.645565	0.391680
C	-3.176840	-4.218552	0.855924
C	-2.784055	-4.478989	2.213799
P	-3.513441	-3.788420	3.610685
C	-2.574275	-4.631458	5.014256
C	-2.143627	-3.605485	6.075244
P	-0.888355	-2.378718	5.374662
C	-1.687390	-0.870863	5.620828
C	-1.166611	0.429298	5.306978
Ge	-2.366905	1.850753	5.033871

C	-1.801634	3.556248	4.525068
C	-2.758723	4.707681	4.336763
P	-3.808382	4.975101	5.895053
C	-4.552478	6.694543	5.641288
C	-5.718561	6.745728	4.638023
P	-5.136453	6.976189	2.856099
C	-5.989160	5.731644	2.023852
C	-5.935025	5.421585	0.621023
Ge	-6.970612	3.993704	-0.014726
C	-7.005094	3.487137	-1.827331
C	-7.779664	2.389674	-2.335330
P	-8.378569	1.053320	-1.429706
C	-9.331225	0.086759	-2.743810
C	-8.974955	-1.405398	-2.665049
P	-7.121908	-1.644570	-2.948931
C	-6.681241	-2.649966	-1.620979
Ge	2.598691	4.206139	-2.827710
C	3.598705	2.950301	-1.858227
Ge	3.591835	1.170656	-2.468107
C	0.696109	4.646886	-5.003868
P	0.048196	6.107052	-4.357246
C	-0.849094	6.837675	-5.852024
C	-2.244457	7.332366	-5.444049
P	-3.278006	5.896984	-4.780869
C	-3.920795	6.552549	-3.323887
C	-4.831800	5.878789	-2.440594
Ge	-5.972062	4.496216	-3.019816
C	4.324373	3.366477	-0.691416
P	4.717500	2.353752	0.646417
C	5.726076	3.510677	1.749782
C	5.183877	3.436551	3.185723
P	3.335153	3.824392	3.148489
C	2.678546	2.610282	4.183954
C	1.290089	2.448313	4.500514
Ge	0.666284	0.788122	5.104034
Ge	0.020243	3.831504	4.307638
Ge	-4.877614	6.352452	-0.632136
Ge	-1.937189	-4.451718	-0.530304
H	-6.044029	-3.658040	1.431883
H	-1.791354	-4.155848	-4.404710
H	-4.443020	-3.279290	-4.193491
H	-7.445273	-2.845431	-0.853551
H	-9.527083	-1.970330	-3.433916
H	-9.254761	-1.825556	-1.686160
H	-10.410861	0.232149	-2.573597
H	-9.098300	0.494861	-3.740021
H	4.563435	4.437705	-0.615141
H	-7.938451	2.374867	-3.423897
H	-7.925775	3.348310	1.008569
H	-6.649442	5.088872	2.626018
H	-6.360675	5.854060	4.721563
H	-6.350289	7.618995	4.869709
H	-3.766872	7.415820	5.363910
H	-4.912988	6.987524	6.641474
H	-3.466728	4.516192	3.515118
H	0.477029	5.279342	4.034859
H	1.725175	-0.281630	5.438006
H	-2.720991	-0.903473	5.995600
H	-3.014580	-3.059355	6.470604
H	-1.671595	-4.123821	6.926303
H	-1.702637	-5.166993	4.605954
H	-3.238580	-5.386360	5.468042
H	-1.896325	-5.112984	2.355968
H	5.702783	4.159859	3.835237
H	5.339456	2.433969	3.614350
H	3.362349	1.837570	4.566648
H	6.785563	3.209089	1.715196
H	5.662605	4.537737	1.357211
H	-3.997530	7.547185	-0.216487
H	-3.549276	7.533445	-2.993489

H	-2.174908	8.120692	-4.677594
H	-2.766141	7.765585	-6.313420
H	-0.918253	6.078016	-6.647031
H	-0.249837	7.673365	-6.249572
H	0.384864	4.355207	-6.018219
H	4.565570	0.135411	-1.871452
H	3.376518	-1.387520	-3.906755
H	2.877619	-3.435642	-4.688826
H	2.338607	-3.471696	-6.380167
H	0.057034	-4.279842	-5.670443
H	1.316703	-5.379344	-5.073007
H	0.889052	1.598911	-6.196023
H	2.792470	5.690360	-2.459788
H	-6.151211	4.207828	-4.523146
H	-0.605878	-5.139395	-0.168529
H	-3.865947	1.508556	5.163077
H	-2.718658	5.407272	6.729006
H	-2.227951	5.637656	4.075271

P-Ge-cage-Ts-1-C-P

C	10.849799	5.260309	-11.989893
Ge	9.492007	5.074037	-10.696577
C	8.634260	6.544409	-9.914803
C	7.706561	6.315387	-8.845005
P	7.196678	7.476738	-7.681413
C	6.069409	6.466257	-6.552845
C	6.433771	6.799318	-5.097156
P	8.327127	6.696994	-4.889773
C	8.847851	8.231034	-3.988621
C	9.344297	7.930705	-2.760427
Ge	10.795531	8.737082	-1.729491
C	12.378301	7.609647	-2.172395
Ge	12.317883	5.686046	-2.537605
C	10.499123	4.993768	-2.251688
C	10.709701	4.115771	-1.186366
P	12.407694	4.009408	-0.776482
C	13.195335	2.353669	-1.235233
C	14.532304	2.384173	-1.991802
P	14.270010	2.451192	-3.866219
C	15.863868	2.807202	-4.411446
C	16.304537	2.878479	-5.775802
Ge	17.887816	3.803201	-6.166580
C	18.500400	4.059398	-7.927606
C	19.648714	4.864404	-8.236228
P	20.273273	6.110517	-7.223427
C	21.786493	6.716224	-8.176214
C	21.802663	8.252690	-8.129856
P	20.138710	8.893308	-8.756063
C	19.620795	9.905402	-7.459756
C	18.389054	10.640094	-7.432019
Ge	17.584969	11.017520	-5.783351
C	15.881281	11.809207	-5.669527
C	15.176808	12.067893	-4.445859
P	15.567319	11.537061	-2.851068
C	14.123502	12.271955	-1.877503
C	13.129469	11.215438	-1.367685
P	12.350467	10.220068	-2.790379
C	13.195707	8.555972	-2.702405
C	11.579142	4.150132	-12.537941
P	11.694934	2.571992	-11.857920
C	12.760200	1.668674	-13.129159
C	13.935327	0.943550	-12.450908
P	15.152947	2.168057	-11.683768
C	15.170913	1.670024	-10.035699
C	15.964391	2.250035	-8.987318
Ge	17.542474	3.226997	-9.308007
Ge	11.281912	6.995009	-12.548402
C	10.469292	8.519149	-11.798883
C	10.860988	9.862783	-12.112364
P	12.386558	10.349469	-12.751408

C	12.163174	12.219156	-12.920430
C	13.337451	12.951353	-12.252948
P	13.440383	12.476140	-10.427566
C	15.135200	12.264668	-10.206510
C	15.789424	11.949444	-8.967037
Ge	17.495967	11.177757	-9.001943
Ge	15.398606	2.062069	-7.211154
Ge	9.105436	8.255034	-10.542151
Ge	8.893109	5.991650	-2.654006
Ge	15.036752	12.288875	-7.275043
B	11.003294	4.767041	1.549441
N	12.468993	4.704011	2.017791
H	18.405412	10.676647	-4.524281
H	15.774821	12.297337	-11.101299
H	18.210594	11.096828	-10.366298
H	20.223506	9.914982	-6.539898
H	22.611098	8.656005	-8.760502
H	21.970467	8.613957	-7.103663
H	22.699432	6.300166	-7.721312
H	21.739346	6.354394	-9.214811
H	7.371471	5.276879	-8.708419
H	20.102297	4.723229	-9.228991
H	18.736771	4.253618	-4.960967
H	16.617848	3.059341	-3.649781
H	15.168391	3.221474	-1.663223
H	15.089822	1.459485	-1.773022
H	12.435244	1.790425	-1.800001
H	13.324249	1.835338	-0.270362
H	9.959516	3.412203	-0.803059
H	7.691371	5.619860	-1.736308
H	10.478815	8.937726	-0.222287
H	14.167394	8.374866	-3.181470
H	13.604457	10.530895	-0.650292
H	12.298453	11.713233	-0.841340
H	13.606908	13.012727	-2.506730
H	14.549557	12.812540	-1.016628
H	14.244363	12.642162	-4.554072
H	5.933201	6.126284	-4.385675
H	6.130111	7.825040	-4.841511
H	8.927507	9.204043	-4.491848
H	5.014956	6.711807	-6.759806
H	6.211618	5.394970	-6.762323
H	14.221265	1.101242	-6.952994
H	14.460044	0.885443	-9.735161
H	13.576341	0.247362	-11.675806
H	14.485529	0.346773	-13.197789
H	13.120021	2.380171	-13.889909
H	12.120471	0.934385	-13.647432
H	12.170350	4.359650	-13.442504
H	8.350560	9.516446	-10.080045
H	10.148443	10.655532	-11.837602
H	11.204813	12.517860	-12.465307
H	12.111728	12.475501	-13.991111
H	14.289582	12.705968	-12.749517
H	13.200791	14.043501	-12.325546
H	12.271531	7.125330	-13.722822
H	8.967457	3.683700	-10.287889
H	18.186891	3.249819	-10.708192
H	13.730929	13.096115	-7.134056
H	13.131031	5.316044	-3.813556
H	12.242138	4.382096	0.625408
H	10.889001	4.683587	0.156612
H	10.409002	3.735806	1.812888
H	10.436849	5.821963	1.758116
H	12.782502	3.914005	2.571411
H	12.979794	5.561466	2.206987

P-Ge-Cage-Ge-C-ring-Ts-1

C	0.539825	3.531988	-6.172027
C	0.750789	2.135904	-6.426219
P	1.764615	1.107809	-5.482160
C	1.541669	-0.573589	-6.313652
C	2.929938	-1.206950	-6.490028
P	4.033133	0.017570	-7.415002
C	5.496987	-0.037748	-6.504368
C	6.702141	0.671936	-6.824847
Ge	7.959763	1.016313	-5.481899
C	9.532118	2.002378	-5.813121
Ge	9.800808	2.644899	-7.553567
C	8.605758	2.298234	-8.968020
Ge	7.090110	1.274992	-8.569270
Ge	0.034897	4.666612	-7.574415
C	-0.120423	6.528681	-7.341544
Ge	0.283127	7.224390	-5.647089
C	0.781106	6.142392	-4.191438
C	1.124283	6.662055	-2.898487
P	1.747190	8.232157	-2.564470
C	1.888372	8.188145	-0.682081
C	3.321178	8.484044	-0.219887
P	4.524767	7.194556	-0.907151
C	6.030045	8.032796	-0.751710
C	7.330120	7.476860	-0.938725
Ge	7.746254	5.702465	-0.645528
C	9.533236	5.099321	-0.863500
Ge	11.185890	6.067073	-1.401819
C	10.702772	8.281350	-1.521611
Ge	8.732639	8.686352	-1.545701
P	9.460304	9.002304	-3.807676
C	9.385215	10.889387	-4.065644
C	8.226332	11.273044	-4.992780
P	8.447385	10.497635	-6.700298
C	6.825127	10.152422	-7.157929
C	6.403222	9.532221	-8.384694
Ge	7.569546	8.544875	-9.488365
C	7.007555	7.697074	-11.060382
Ge	5.200245	7.896996	-11.550902
C	3.984313	8.870009	-10.514052
Ge	4.606119	9.615628	-8.896516
Ge	0.806924	4.291754	-4.467677
C	-0.509437	7.458367	-8.364396
P	-0.880436	7.147650	-10.018440
C	-1.229867	8.896348	-10.638546
C	-0.075183	9.508672	-11.457940
P	1.400102	10.039402	-10.406361
C	2.627804	8.973915	-10.975547
C	7.970362	6.906977	-11.774225
P	7.712738	5.886785	-13.139793
C	9.449342	5.193502	-13.402469
C	9.671081	3.809810	-12.761094
P	9.943256	3.890442	-10.895658
C	8.808573	2.729831	-10.323412
C	10.552374	2.269299	-4.839147
P	10.581743	1.850761	-3.167793
C	12.326035	2.421862	-2.715715
C	12.567058	2.471394	-1.204823
P	11.804165	3.882169	-0.202424
C	10.009038	3.857816	-0.519034
C	10.973105	8.822642	-2.774121
B	12.234181	9.055553	0.607596
N	12.778313	7.637379	0.776279
H	9.018370	8.252978	-9.051210
H	2.356691	8.305718	-11.806513
H	4.634535	7.265482	-12.838972
H	8.996405	6.948282	-11.379620
H	9.585604	5.111734	-14.493073
H	10.195603	5.918913	-13.041305

H	10.581348	3.356245	-13.190132
H	8.834520	3.129820	-12.987053
H	1.056615	5.955643	-2.057671
H	8.133962	2.283522	-11.069549
H	11.161800	3.324413	-7.805045
H	11.430629	2.812033	-5.222337
H	12.521360	3.402937	-3.175315
H	13.027390	1.699373	-3.167270
H	12.231529	1.535425	-0.724310
H	13.647574	2.542780	-0.998379
H	9.374126	2.990121	-0.291998
H	6.760485	4.761219	0.084799
H	8.483513	10.081506	-0.894355
H	11.976740	9.053100	-3.152377
H	10.348317	11.164208	-4.527312
H	9.323161	11.418990	-3.103248
H	7.256403	10.976655	-4.564200
H	8.209538	12.368238	-5.120993
H	6.023254	10.446762	-6.464821
H	3.372489	8.475764	0.881456
H	3.639692	9.485009	-0.553083
H	5.987495	9.113471	-0.537440
H	1.195001	8.941768	-0.273632
H	1.553083	7.205394	-0.315000
H	7.669222	0.402859	-4.097827
H	5.494833	-0.602335	-5.560273
H	3.381705	-1.443510	-5.513713
H	2.866752	-2.146566	-7.062186
H	1.042297	-0.440000	-7.286190
H	0.892609	-1.211188	-5.692191
H	0.297459	1.722276	-7.339083
H	0.010672	8.728563	-5.449403
H	-0.559558	8.509776	-8.043997
H	-1.492279	9.543727	-9.786972
H	-2.125601	8.828631	-11.278066
H	0.260825	8.812431	-12.242609
H	-0.442482	10.417218	-11.964986
H	-0.268450	3.988741	-8.925251
H	1.000026	3.392914	-3.230859
H	6.224602	0.827679	-9.763645
H	3.633816	10.295179	-7.911808
H	11.439020	5.807769	-2.918446
H	11.347320	8.733493	-0.594045
H	12.313998	6.979756	-0.046855
H	12.516842	7.160224	1.644357
H	13.789058	7.539157	0.645564
H	12.969479	9.827156	0.056221
H	11.368735	9.372785	1.374489

P-Ge-Cage-Ge-C-ring-H₂

C	1.455581	3.726754	-4.377193
Ge	1.511988	1.943054	-4.952335
C	2.463113	0.616247	-4.016785
Ge	3.448260	1.150305	-2.513094
C	3.435118	2.921121	-1.878000
C	4.135983	3.322859	-0.691720
P	4.547698	2.290440	0.625217
C	5.554387	3.443073	1.732320
C	5.143307	3.253610	3.198791
P	3.313948	3.668918	3.416611
C	2.766292	2.387821	4.435408
C	1.438030	2.268800	4.947593
Ge	0.184917	3.727840	4.921795
C	-1.617305	3.472829	5.231559
C	-2.479694	4.599084	5.282611
P	-4.212030	4.566736	5.379932
C	-4.624272	6.411650	5.437881
C	-5.621407	6.786581	4.331275

P	-4.854504	6.499398	2.631319
C	-6.155504	5.786372	1.760113
C	-6.126582	5.446555	0.363856
Ge	-5.032789	6.347836	-0.871648
C	-4.909713	5.830780	-2.671844
Ge	-6.017063	4.425544	-3.250589
C	-7.143285	3.492879	-2.076969
C	-7.897564	2.376519	-2.571036
P	-8.515414	1.079832	-1.619354
C	-9.427487	0.039845	-2.905836
C	-9.029743	-1.436692	-2.757618
P	-7.168472	-1.634548	-3.013314
C	-6.709606	-2.573330	-1.644786
C	-5.385967	-3.062253	-1.374918
Ge	-4.115322	-3.357915	-2.731503
C	-2.359568	-3.901652	-2.360655
Ge	-1.922656	-4.251892	-0.565750
C	-3.138444	-3.985426	0.838108
C	-2.703632	-4.241271	2.180685
P	-3.438610	-3.677213	3.635574
C	-2.370054	-4.531719	4.940895
C	-2.016507	-3.577101	6.088132
P	-1.029255	-2.095301	5.452419
C	-1.459711	-0.862682	6.547315
C	-0.967509	0.531531	6.460641
Ge	-2.277737	1.628596	5.351049
Ge	2.471423	4.192894	-2.864035
C	0.647850	4.670136	-5.098514
P	-0.011564	6.126055	-4.457370
C	-0.860300	6.877538	-5.968854
C	-2.273797	7.349843	-5.597884
P	-3.304415	5.888882	-4.985722
C	-3.988577	6.515299	-3.533565
Ge	0.843844	0.693665	5.713659
Ge	-7.210532	4.062524	-0.283502
Ge	-4.879637	-3.423734	0.392353
C	2.464642	-0.767760	-4.396296
P	1.254208	-1.559500	-5.332929
C	1.940852	-3.314484	-5.467818
C	0.857913	-4.326329	-5.062218
P	0.292185	-3.975720	-3.294412
C	-1.422347	-4.046684	-3.438735
H	-5.991178	-3.375619	1.458916
H	-1.849319	-4.134015	-4.449098
H	-4.527376	-3.304949	-4.215958
H	-7.467099	-2.752532	-0.867377
H	-9.553964	-2.052820	-3.506608
H	-9.307295	-1.821661	-1.763662
H	-10.513075	0.160539	-2.756222
H	-9.191899	0.412032	-3.915331
H	4.361148	4.395414	-0.593845
H	-8.020617	2.313719	-3.662632
H	-8.269196	3.491281	0.679780
H	-7.053803	5.489649	2.322013
H	-6.548034	6.197598	4.419307
H	-5.900460	7.851073	4.410800
H	-3.699128	7.002855	5.348755
H	-5.060636	6.634672	6.425650
H	-2.001433	5.589974	5.231027
H	0.735250	5.167283	4.853978
H	1.837194	-0.471970	5.921534
H	-2.189348	-1.058776	7.344040
H	-2.923769	-3.213518	6.594287
H	-1.401539	-4.097898	6.840217
H	-1.458219	-4.926731	4.465369
H	-2.931391	-5.394277	5.335904
H	-1.771583	-4.818194	2.281774
H	5.732137	3.919617	3.850967
H	5.330190	2.219916	3.530031
H	3.468151	1.575097	4.673416

H	6.624811	3.213339	1.601498
H	5.402121	4.485789	1.411685
H	-4.307232	7.648011	-0.472882
H	-3.635857	7.498388	-3.187597
H	-2.236866	8.126899	-4.817669
H	-2.772252	7.791333	-6.476420
H	-0.894631	6.131798	-6.779067
H	-0.254074	7.725148	-6.329081
H	0.367907	4.390140	-6.124956
H	4.402201	0.104350	-1.903703
H	3.274442	-1.386589	-3.981134
H	2.830554	-3.411382	-4.825969
H	2.263339	-3.492253	-6.506779
H	-0.006987	-4.271974	-5.742222
H	1.252553	-5.354435	-5.113107
H	0.862732	1.633029	-6.315407
H	2.659023	5.671317	-2.470300
H	-6.139923	4.082413	-4.748467
H	-0.584932	-4.922698	-0.195067
H	-2.351662	0.907798	3.982286
H	-3.628478	1.528813	6.097836
H	-0.968792	1.028317	7.446248

C-P-cage-P-C-ring-Ts-1

C	2.920243	2.886795	-5.461851
P	3.809711	4.354190	-4.906754
C	2.552522	5.685583	-5.199668
P	1.999103	5.894529	-6.966094
C	1.431123	4.321177	-7.431678
C	0.755414	4.301139	-8.732301
C	0.301994	3.221860	-9.407957
C	-0.435841	3.282119	-10.708363
C	0.265383	2.508902	-11.858600
C	1.504664	3.184171	-12.350972
C	2.742943	2.646731	-12.306429
C	3.997137	3.250219	-12.772676
P	5.315657	2.082004	-12.781553
C	6.764498	2.890035	-13.414602
P	7.066501	4.556806	-13.896598
C	5.556592	5.470334	-13.699798
C	5.595480	6.903923	-14.014271
C	6.641974	7.635001	-14.455758
C	6.584903	9.105038	-14.725868
C	7.584718	9.920384	-13.860998
C	7.274125	9.865528	-12.398647
C	8.104482	9.347769	-11.467560
C	7.882697	9.224376	-10.021303
P	9.340480	8.673236	-9.199594
C	8.982018	8.521790	-7.468511
P	7.503460	8.806779	-6.551655
C	6.266403	9.412873	-7.670753
C	4.972519	9.768969	-7.072776
C	4.738276	10.090279	-5.782552
C	3.402879	10.453274	-5.215884
C	2.915894	9.450513	-4.130208
C	2.415369	8.159900	-4.704415
C	3.050053	6.980951	-4.619819
P	1.575870	2.736047	-6.574773
C	3.354613	1.594859	-4.928434
C	4.218282	1.368931	-3.909828
C	4.652325	0.007284	-3.458641
C	6.190082	-0.145736	-3.354858
C	6.906329	0.058305	-4.652990
C	7.909651	0.946588	-4.824810
C	8.683082	1.225012	-6.040797
P	8.382787	0.182290	-7.446275
C	9.394700	0.747694	-8.772228
P	10.540892	2.098658	-8.895384

C	10.644852	2.877743	-7.319255
C	11.604583	3.988901	-7.332797
C	11.987568	4.769038	-6.298649
C	12.974808	5.887285	-6.403273
C	12.384193	7.263967	-5.994080
C	11.342858	7.763059	-6.944590
C	10.064302	8.034924	-6.603926
P	3.956170	4.985395	-13.145778
P	6.255228	9.603114	-9.421242
P	9.777699	2.583071	-5.798391
C	9.199465	-0.061820	-9.981750
C	9.933558	-0.046103	-11.115653
C	9.649975	-0.889483	-12.317814
C	9.341471	-0.049666	-13.588738
C	8.062039	0.718118	-13.484243
C	7.973352	2.064737	-13.536972
H	12.062359	4.191970	-8.311096
H	8.358375	-0.767390	-9.936940
H	10.528606	-1.520951	-12.541111
H	8.808942	-1.571519	-12.112961
H	9.284935	-0.747697	-14.443312
H	4.124661	9.808187	-7.769492
H	8.903543	2.624237	-13.705435
H	2.838026	1.631512	-11.897288
H	0.495220	1.482787	-11.527871
H	-0.455045	2.423280	-12.692081
H	-0.591702	4.331407	-11.009427
H	-1.439735	2.839227	-10.574974
H	0.591983	5.286665	-9.190201
H	2.927537	0.714206	-5.427966
H	4.245627	-0.758653	-4.139104
H	4.233797	-0.208469	-2.457480
H	6.582259	0.556398	-2.600386
H	6.399267	-1.163465	-2.976449
H	8.187739	1.557751	-3.954681
H	2.104442	9.933421	-3.559530
H	3.737211	9.258187	-3.420818
H	4.007159	6.934767	-4.083393
H	3.469119	11.450396	-4.745429
H	2.651073	10.525927	-6.018434
H	4.645608	7.434359	-13.859395
H	5.561055	9.479718	-14.561854
H	6.829099	9.296303	-15.786459
H	8.609635	9.557235	-14.042656
H	7.549867	10.968554	-14.208327
H	9.076671	8.974152	-11.818003
H	9.782880	7.885270	-5.552290
H	11.969245	7.201155	-4.974810
H	13.220027	7.985877	-5.954667
H	13.374912	5.945711	-7.428696
H	13.832282	5.681614	-5.736991
H	10.180325	0.636281	-13.790092
H	6.574116	-0.559611	-5.495281
H	4.659405	2.221666	-3.378202
H	1.465163	8.212799	-5.251008
H	5.574933	10.093094	-5.073222
H	6.297733	10.261757	-12.095500
H	7.612595	7.151279	-14.617891
H	7.152395	0.122646	-13.341827
H	10.792068	0.631375	-11.194461
H	11.555957	4.600857	-5.304748
H	11.666657	7.898818	-7.983210
H	1.368595	4.188885	-12.769148
H	0.462134	2.220599	-8.990626
H	1.522742	5.386028	-4.612013
B	0.728321	4.963067	-3.347707
N	1.823909	4.157356	-2.664208
H	2.799695	4.169825	-3.355318
H	0.568317	6.077214	-2.931620
H	-0.121214	4.324128	-3.900823

H	1.627807	3.156164	-2.576994
H	2.132199	4.524614	-1.760440

C-P-cage-P-C-ring-H₂

C	2.848551	2.689376	-5.231425
P	3.266203	4.120246	-4.265958
C	2.485883	5.521700	-4.992944
P	1.451031	5.689367	-6.426968
C	1.233410	4.093076	-7.137498
C	0.374244	4.148145	-8.327281
C	-0.117849	3.114952	-9.045237
C	-0.985725	3.263802	-10.254385
C	-0.360191	2.649023	-11.536214
C	0.856492	3.382396	-12.002743
C	2.080636	2.825754	-12.130878
C	3.327281	3.474697	-12.555895
P	4.639676	2.309353	-12.703376
C	6.104462	3.188275	-13.187606
P	6.391876	4.888744	-13.541015
C	4.866516	5.769445	-13.317921
C	4.898850	7.218489	-13.551824
C	5.926720	7.960055	-14.019291
C	5.885509	9.443433	-14.203037
C	6.978707	10.183654	-13.385962
C	6.788540	10.068364	-11.906686
C	7.692637	9.527543	-11.060690
C	7.587577	9.374916	-9.603596
P	9.080842	8.747094	-8.911437
C	8.862062	8.612868	-7.153806
P	7.488015	8.972106	-6.111745
C	6.162461	9.578349	-7.125463
C	4.914187	9.941411	-6.442886
C	4.659676	9.940822	-5.116064
C	3.347249	10.325451	-4.510112
C	2.711615	9.194862	-3.657974
C	2.326057	7.996798	-4.466213
C	2.795830	6.748957	-4.248904
P	1.885971	2.502089	-6.694305
C	3.400820	1.402794	-4.790087
C	4.122231	1.142147	-3.677894
C	4.619372	-0.216545	-3.297209
C	6.146354	-0.271161	-3.040545
C	6.972768	-0.020111	-4.262066
C	7.942871	0.918600	-4.346573
C	8.804099	1.201042	-5.491475
P	8.688337	0.016532	-6.888822
C	9.179139	0.891759	-8.302129
P	9.612661	2.676964	-8.246773
C	10.874619	2.596835	-6.840041
C	11.819911	3.756890	-6.927758
C	11.923773	4.791368	-6.079989
C	12.913929	5.911920	-6.216778
C	12.325759	7.303463	-5.889577
C	11.224548	7.742462	-6.803024
C	10.001835	8.122344	-6.370300
P	3.271836	5.233979	-12.798555
P	6.035971	9.823271	-8.864202
P	9.885075	2.528592	-5.239165
C	9.071832	0.143645	-9.539435
C	9.463573	0.516311	-10.781443
C	9.329657	-0.352076	-11.994828
C	8.855274	0.408935	-13.254613
C	7.535960	1.093740	-13.080707
C	7.339222	2.407697	-13.325552
H	12.487573	3.732834	-7.800108
H	8.622489	-0.854357	-9.436954
H	10.312523	-0.802720	-12.230762
H	8.648797	-1.191780	-11.780124

H	8.787109	-0.322111	-14.081167
H	4.098593	10.255475	-7.109385
H	8.210810	2.986437	-13.662886
H	2.173457	1.756906	-11.892943
H	-0.119552	1.587779	-11.360362
H	-1.130880	2.675087	-12.327793
H	-1.213228	4.328095	-10.428903
H	-1.950703	2.755069	-10.077916
H	0.097569	5.161358	-8.650591
H	3.178094	0.554495	-5.452411
H	4.344956	-0.949950	-4.073259
H	4.115919	-0.537741	-2.366704
H	6.416977	0.445958	-2.248102
H	6.379852	-1.277924	-2.647241
H	8.112351	1.552486	-3.464925
H	1.813276	9.612799	-3.168103
H	3.405562	8.901253	-2.853295
H	3.495922	6.615756	-3.412267
H	3.490300	11.199818	-3.849466
H	2.642943	10.635222	-5.299383
H	3.965253	7.746476	-13.313323
H	4.890497	9.832374	-13.931117
H	6.044398	9.687842	-15.269072
H	7.973777	9.804152	-13.670640
H	6.947995	11.249150	-13.677297
H	8.632182	9.160890	-11.497126
H	9.823599	8.073450	-5.286795
H	11.966825	7.314238	-4.846957
H	13.152026	8.036329	-5.943847
H	13.346276	5.911775	-7.231108
H	13.755294	5.739333	-5.520674
H	9.618331	1.147251	-13.551546
H	6.763434	-0.658884	-5.128534
H	4.366824	1.956684	-2.985753
H	1.623369	8.176653	-5.288369
H	5.443776	9.635076	-4.413317
H	5.839294	10.450156	-11.512439
H	6.874896	7.471260	-14.273595
H	6.704072	0.472112	-12.729326
H	9.930447	1.494693	-10.937592
H	11.269404	4.833051	-5.200603
H	11.456836	7.761499	-7.874279
H	0.717654	4.444923	-12.236025
H	0.124355	2.087001	-8.750350
H	10.571480	2.672698	-9.322648
H	11.431760	1.649026	-6.950046

N-Ge-Cage-Ge-C-ring-Ts-1

C	2.811191	2.412093	-4.896370
C	2.316210	3.437911	-5.795647
N	2.334734	4.693898	-5.514536
C	1.786404	5.619738	-6.482785
C	0.633127	6.435937	-5.872356
N	-0.530949	5.604599	-5.646038
C	-0.934430	5.442251	-4.435288
C	-2.067582	4.604785	-4.082237
Ge	-2.592344	4.432154	-2.304659
C	-4.014896	3.300454	-1.842706
Ge	-4.933292	2.391043	-3.186380
C	-4.453916	2.606687	-4.983091
Ge	-2.997396	3.678137	-5.423487
Ge	2.768807	0.619636	-5.401944
C	3.373819	-0.709766	-4.227533
Ge	4.036122	-0.224708	-2.555464
C	4.112717	1.578287	-2.046127
C	4.672635	1.939830	-0.755669
N	5.236816	1.085480	0.022656
C	5.755269	1.541777	1.294066

C	5.096138	0.790045	2.466443
N	3.743745	1.239459	2.719976
C	2.759438	0.437354	2.446502
C	1.394896	0.806208	2.677585
Ge	1.181329	2.614407	3.284881
C	-0.558991	2.895745	4.064508
C	-1.457349	3.896632	3.560573
N	-2.658731	3.408525	3.315005
C	-3.815655	4.211056	2.953782
C	-4.648156	3.650589	1.804410
N	-4.027688	3.874884	0.508249
C	-4.447281	3.147379	-0.469576
Ge	3.485996	2.886481	-3.210058
C	3.331263	-2.112650	-4.597827
N	2.975793	-2.539296	-5.758326
C	2.976187	-3.972640	-5.972854
C	1.609394	-4.471217	-6.465260
N	0.591748	-4.332394	-5.442615
C	-0.483027	-3.698708	-5.755894
C	-1.587884	-3.472989	-4.841897
Ge	-1.464051	-3.959343	-3.033637
C	-2.891378	-3.660710	-1.875583
C	-2.794033	-4.042687	-0.476325
N	-3.756089	-3.897819	0.364127
C	-3.535524	-4.344546	1.725195
C	-3.675515	-3.211494	2.748205
N	-2.577741	-2.266822	2.651990
C	-2.766880	-1.073180	3.104177
C	-1.747501	-0.051277	3.151151
Ge	0.007221	-0.417179	2.581007
Ge	-3.155890	-2.697167	-5.477629
C	-4.610682	-2.415609	-4.329547
C	-5.832088	-1.809899	-4.824445
N	-6.030744	-1.504503	-6.059382
C	-7.264241	-0.820355	-6.384739
C	-6.976778	0.618765	-6.856525
N	-6.361394	1.379278	-5.788633
C	-5.210718	1.909898	-6.008585
Ge	-4.467337	-2.888392	-2.532559
Ge	-2.015806	1.551122	4.091622
H	-5.692066	-2.600635	-1.648025
H	-0.608805	-3.289431	-6.782679
H	-3.181264	-2.301052	-6.963722
H	-6.619594	-1.604677	-4.066328
H	-7.764144	-1.352267	-7.212155
H	-7.964781	-0.777372	-5.524965
H	-7.944795	1.082980	-7.114666
H	-6.351653	0.587083	-7.772439
H	4.602487	3.010428	-0.463987
H	-4.741818	1.843209	-7.014525
H	-6.044507	1.430160	-2.731624
H	-5.205138	2.352953	-0.291198
H	-4.874099	2.581129	1.991145
H	-5.614702	4.188787	1.832303
H	-3.487967	5.232422	2.694860
H	-4.465093	4.282763	3.845119
H	-1.225761	4.961796	3.415691
H	1.534889	3.805043	2.353439
H	-3.767679	-0.780568	3.499608
H	-4.665828	-2.725987	2.629025
H	-3.663333	-3.685809	3.749256
H	-2.538168	-4.813597	1.856636
H	-4.302990	-5.103538	1.960265
H	-1.828760	-4.488913	-0.152861
H	5.705176	0.985223	3.366811
H	5.149511	-0.297204	2.250681
H	2.963053	-0.577425	2.042723
H	6.836264	1.315916	1.322316
H	5.626390	2.633785	1.445183
H	-1.761031	5.180174	-1.248768

H	-0.414156	5.952431	-3.595314
H	0.995013	6.926007	-4.945097
H	0.362052	7.223837	-6.596327
H	1.424429	5.115257	-7.402808
H	2.578173	6.333046	-6.771939
H	1.906746	3.087018	-6.768434
H	4.473888	-1.372575	-1.631202
H	3.633260	-2.834558	-3.807311
H	3.260404	-4.537747	-5.060721
H	3.714105	-4.206253	-6.761236
H	1.344182	-3.939464	-7.402873
H	1.719346	-5.544510	-6.703447
H	2.182064	0.301240	-6.787485
H	3.556978	4.343792	-2.724989
H	-2.622250	3.767518	-6.911211
H	-0.190578	-4.577042	-2.433035
H	-2.947127	1.519848	5.331438
H	0.393910	-1.841781	2.137197
H	-0.398431	3.241594	5.543060
B	0.201816	3.427949	6.734029
N	1.680269	3.109271	6.357929
H	1.778759	2.930134	5.247462
H	2.340677	3.866031	6.551620
H	2.047164	2.253099	6.781995
H	0.035262	4.601683	6.972269
H	-0.284789	2.575236	7.439491

N-Ge-Cage-Ge-C-ring-H₂

C	2.397095	3.844702	-4.477858
Ge	2.315643	2.171088	-5.315389
C	3.099459	0.675484	-4.527743
C	2.973139	-0.611443	-5.183512
N	3.362619	-1.727306	-4.672864
C	3.084773	-2.932545	-5.428693
C	4.275785	-3.885986	-5.490771
N	5.352182	-3.389743	-6.347165
C	6.533164	-3.852975	-6.177747
C	7.654332	-3.398545	-7.030914
Ge	6.885569	-2.484110	-8.587773
C	7.887072	-1.242542	-9.501157
C	7.434759	-0.697238	-10.764223
N	8.165754	0.070572	-11.495979
C	7.635835	0.500106	-12.775204
C	7.913888	1.987207	-13.031380
N	7.134506	2.842172	-12.159154
C	7.765838	3.702509	-11.440386
C	7.106171	4.630147	-10.538468
Ge	5.249416	4.546051	-10.289729
C	4.393312	5.756704	-9.163348
Ge	5.402169	7.059315	-8.268785
C	7.246585	7.153034	-8.504336
Ge	8.096269	5.930005	-9.644407
C	1.764970	4.999205	-5.091291
N	1.007249	4.922927	-6.127836
C	0.466244	6.153833	-6.666083
C	0.861753	6.329438	-8.142294
N	2.288577	6.536348	-8.276688
C	2.955508	5.688028	-8.977659
Ge	3.284546	4.009263	-2.849441
C	4.062373	2.508513	-2.035321
Ge	3.971508	0.850277	-2.876747
C	8.006851	8.175942	-7.809388
N	9.269146	8.363459	-7.971829
C	9.895981	9.419321	-7.202423
C	11.062011	8.883100	-6.357080
N	10.593563	8.012787	-5.297260
C	11.059302	6.813702	-5.261678
C	10.677711	5.826466	-4.268238

Ge	11.485793	4.147145	-4.282159
C	11.007335	2.850331	-3.016639
Ge	9.715557	3.251119	-1.739467
C	8.899060	4.940069	-1.706763
C	7.893766	5.235391	-0.702084
N	7.595470	4.428056	0.254428
C	6.544948	4.813026	1.172616
C	5.424125	3.758663	1.194403
N	4.707347	3.735344	-0.063783
C	4.716883	2.644600	-0.745917
Ge	9.378949	6.217717	-2.973410
Ge	8.999622	-2.321817	-5.932624
C	10.131827	-1.295575	-7.139471
C	11.417878	-0.913166	-6.623940
N	11.806298	-1.222722	-5.428935
C	13.147182	-0.843750	-5.033957
C	13.166212	-0.106556	-3.687431
N	12.615889	1.229467	-3.796835
C	11.643189	1.544347	-3.017472
Ge	9.587122	-0.727140	-8.791854
H	12.518495	3.888691	-5.391811
H	7.374123	6.214356	-0.793452
H	8.652473	7.571866	-2.907379
H	11.802370	6.481781	-6.019786
H	11.561659	9.753997	-5.896988
H	11.792545	8.382880	-7.026418
H	10.314072	10.160747	-7.906706
H	9.178428	9.944629	-6.538232
H	2.485986	-0.599255	-6.183843
H	7.432303	8.819698	-7.107364
H	9.615922	5.933684	-9.879563
H	8.874336	3.772797	-11.495087
H	9.005002	2.167858	-12.939442
H	7.620654	2.202852	-14.074651
H	6.548223	0.303522	-12.874917
H	8.152859	-0.067834	-13.570967
H	6.413817	-0.987941	-11.096309
H	5.642003	-3.062508	-9.294244
H	9.747679	-3.411694	-5.130312
H	12.092581	-0.342857	-7.299785
H	13.656246	-0.217361	-5.796134
H	13.743513	-1.766276	-4.906519
H	12.637998	-0.724129	-2.931742
H	14.222469	-0.015747	-3.376489
H	11.247819	0.805361	-2.286370
H	3.911821	-4.836973	-5.919232
H	4.635328	-4.095471	-4.466556
H	6.763297	-4.589771	-5.381163
H	2.269640	-3.474978	-4.914105
H	2.737895	-2.716261	-6.461257
H	4.365142	3.485975	-10.966865
H	2.433530	4.845490	-9.481987
H	0.502025	5.451450	-8.718009
H	0.339160	7.225502	-8.520771
H	0.790307	7.048045	-6.094665
H	-0.636140	6.100302	-6.623397
H	1.965045	5.983267	-4.613552
H	4.651156	-0.335710	-2.172558
H	5.237303	1.742304	-0.356857
H	5.864708	2.773605	1.452588
H	4.717091	4.040070	1.994074
H	6.106313	5.803982	0.932598
H	6.969648	4.863663	2.190793
H	3.359193	5.417790	-2.238442
H	1.643961	1.954647	-6.681768
H	4.775682	8.076156	-7.300542
H	9.345384	2.131342	-0.753134
H	10.544167	0.128679	-9.638403
H	8.160199	-1.440099	-4.969938
H	8.261116	-4.250597	-7.385114

N-P-Cage-Ts-1-C-N

C	10.686425	1.081599	-2.249163
P	9.897332	-0.498639	-2.058745
C	9.284436	-0.539402	-0.411699
P	9.349551	0.590175	0.958682
C	10.193435	2.015570	0.370430
P	10.957712	2.446232	-1.174847
C	11.263055	1.322195	-3.586051
N	11.074512	0.531982	-4.577422
C	11.702802	0.860000	-5.840138
C	12.660706	-0.264102	-6.274644
N	13.828453	-0.291983	-5.419285
C	14.068238	-1.363004	-4.757716
C	15.216545	-1.495521	-3.840355
P	16.086891	0.021062	-3.526421
C	17.404401	-0.391395	-2.438063
P	17.930131	-1.896121	-1.652947
C	16.824315	-3.144873	-2.208091
C	17.162302	-4.462770	-1.635884
N	16.595410	-5.548418	-2.012806
C	16.992080	-6.784574	-1.371511
C	15.786411	-7.448847	-0.683539
N	15.384342	-6.688395	0.481324
C	14.182627	-6.245407	0.528838
C	13.668079	-5.445375	1.657098
P	11.934339	-5.186752	1.524878
C	11.472081	-4.230085	2.948857
C	10.035190	-3.903951	3.031131
N	9.162950	-4.385389	2.224813
C	7.783857	-3.975522	2.390780
C	7.266961	-3.293101	1.112094
N	7.897864	-2.001474	0.935582
C	8.582304	-1.806491	-0.130121
P	15.401838	-3.148833	-3.272851
P	14.906502	-4.937503	2.826251
C	14.057130	-4.029359	4.068266
C	14.974871	-3.563227	5.126404
N	14.559630	-3.020359	6.210107
C	15.541500	-2.593984	7.185418
C	15.419149	-1.085548	7.460902
N	15.924260	-0.310611	6.346988
C	15.134040	0.536010	5.793851
C	15.542647	1.395335	4.673796
P	17.247557	1.206514	4.152982
C	17.271802	1.878835	2.531947
P	16.064776	2.783526	1.566040
C	15.017908	3.509608	2.861500
P	14.250534	2.422657	4.120737
P	12.362895	-3.546884	4.302144
C	10.283909	3.063782	1.406036
N	10.674858	4.256110	1.145554
C	10.713915	5.222947	2.232287
C	12.118061	5.837802	2.352028
N	13.034652	4.898706	2.968779
C	14.023065	4.473863	2.286060
C	18.223650	0.791862	-2.113424
N	19.323927	0.721905	-1.459710
C	20.043520	1.951183	-1.203549
C	20.256567	2.157061	0.307123
N	19.005099	2.494404	0.962554
C	18.553911	1.669963	1.845311
H	17.953579	-4.463901	-0.856961
H	17.834983	1.763359	-2.485630
H	21.041587	1.861390	-1.666049
H	19.540125	2.843297	-1.628168

H	20.951529	3.005592	0.427477
H	20.732035	1.250084	0.729094
H	9.744217	-3.211261	3.848709
H	19.142422	0.779167	2.141823
H	14.214681	4.816703	1.247531
H	12.454173	6.178455	1.352684
H	12.042576	6.713224	3.017497
H	10.405622	4.800123	3.200140
H	10.020294	6.040610	1.962445
H	9.972296	2.765599	2.428994
H	11.870127	2.246000	-3.691434
H	12.256816	1.819533	-5.811161
H	10.911584	0.933927	-6.605408
H	12.111793	-1.226735	-6.289165
H	12.995198	-0.034156	-7.300586
H	13.418994	-2.258735	-4.853043
H	6.183631	-3.128515	1.240150
H	7.421907	-3.970751	0.248972
H	8.670316	-2.590820	-0.911138
H	7.175259	-4.882099	2.549520
H	7.635637	-3.295470	3.253219
H	14.089730	0.663936	6.151012
H	14.366542	-0.846057	7.713909
H	16.046809	-0.861520	8.340760
H	16.581818	-2.825997	6.881691
H	15.325526	-3.121348	8.130356
H	16.056871	-3.723978	4.936370
H	13.457694	-6.453896	-0.286049
H	14.968551	-7.577089	-1.420453
H	16.111115	-8.446751	-0.342857
H	17.803098	-6.645217	-0.629390
H	17.346837	-7.475239	-2.155454
H	15.837953	4.406797	3.638437
B	16.751124	5.397718	3.845096
N	17.770362	5.128440	2.671537
H	17.366438	4.412616	1.977749
H	17.996251	5.962944	2.122687
H	18.649688	4.701737	2.979966
H	16.112301	6.404452	3.663341
H	17.208479	5.146736	4.931053

N-P-Cage-H₂-C-N

C	11.290672	2.112068	-2.147741
P	10.373992	0.604264	-1.939726
C	9.618162	0.711365	-0.356391
P	9.663756	1.910000	0.953751
C	10.682399	3.221780	0.376841
P	11.589350	3.509773	-1.123960
C	11.976150	2.234140	-3.449302
N	11.767362	1.425557	-4.421491
C	12.505341	1.629388	-5.650709
C	13.350646	0.387478	-5.987311
N	14.453377	0.260153	-5.058511
C	14.536844	-0.811370	-4.360776
C	15.599596	-1.032730	-3.360945
P	16.632637	0.383189	-3.063239
C	17.808257	-0.120466	-1.858281
P	18.065847	-1.617866	-0.939123
C	16.850483	-2.753954	-1.506911
C	16.961046	-4.044544	-0.802088
N	16.270295	-5.079361	-1.108285
C	16.468207	-6.270729	-0.309114
C	15.161551	-6.704554	0.369246
N	14.733572	-5.725171	1.351579
C	13.471787	-5.495807	1.452789

C	12.904957	-4.554440	2.410619
P	11.178887	-4.545779	2.485521
C	10.814070	-3.225270	3.711841
C	9.484887	-2.632947	3.541848
N	8.720268	-2.962085	2.563724
C	7.410692	-2.349456	2.477011
C	7.183269	-1.727660	1.090195
N	7.974841	-0.527054	0.920982
C	8.778842	-0.469372	-0.074984
P	15.533330	-2.658727	-2.694692
P	14.005810	-3.383350	3.292697
C	13.263496	-3.627102	5.020160
C	14.233746	-3.201863	6.076700
N	14.005683	-2.224386	6.861089
C	15.003319	-1.889929	7.864732
C	15.156000	-0.370918	8.003027
N	15.774664	0.215466	6.830872
C	15.130289	1.141928	6.222674
C	15.651038	1.851020	5.038198
P	17.176350	1.211056	4.390444
C	17.605007	2.256367	3.043338
P	16.822998	3.648170	2.263864
C	15.352367	3.954336	3.176884
P	14.590506	3.177357	4.580306
P	11.668785	-2.628974	5.088911
C	10.798452	4.294522	1.383458
N	11.386509	5.409440	1.152366
C	11.451309	6.378869	2.226222
C	12.913972	6.721126	2.558276
N	13.568406	5.596852	3.195139
C	14.609604	5.106824	2.630845
C	18.751304	0.964479	-1.523995
N	19.793965	0.772996	-0.804387
C	20.639635	1.907864	-0.501194
C	20.746733	2.100284	1.022627
N	19.493487	2.583813	1.563631
C	18.891587	1.863175	2.436245
H	17.697832	-4.072888	0.028417
H	18.508626	1.965030	-1.939016
H	21.653516	1.688625	-0.877342
H	20.286143	2.849654	-0.966241
H	21.515917	2.869387	1.206507
H	21.079039	1.149712	1.485214
H	9.170032	-1.886040	4.300219
H	19.324088	0.904736	2.792280
H	15.014284	5.539959	1.692133
H	13.429803	7.054982	1.635954
H	12.901670	7.558936	3.276214
H	10.937776	6.037668	3.147350
H	10.966781	7.306748	1.877171
H	10.332020	4.082813	2.368618
H	12.683550	3.084433	-3.546422
H	13.164578	2.519807	-5.616560
H	11.776001	1.763182	-6.467502
H	12.696061	-0.506822	-6.007453
H	13.770008	0.538438	-6.996644
H	13.803270	-1.636555	-4.478318
H	6.119751	-1.438458	1.029829
H	7.384068	-2.490781	0.311798
H	8.867375	-1.308918	-0.796298
H	6.658656	-3.147698	2.603986
H	7.239691	-1.582748	3.258621
H	14.133787	1.477018	6.580109
H	14.164254	0.071062	8.228049
H	15.822116	-0.182517	8.862847
H	15.988114	-2.354135	7.660265
H	14.640108	-2.269242	8.835627
H	15.174218	-3.790827	6.129461
H	12.737794	-6.024193	0.809219
H	14.388160	-6.911013	-0.395607

H	15.373705	-7.650032	0.901668
H	17.250366	-6.137348	0.465610
H	16.780424	-7.087632	-0.982170
H	15.117929	-4.282503	3.431345
H	13.039832	-4.703127	5.133945

P-C-Cage with AB

C	11.865649	0.817948	-3.615354
C	11.821845	1.593783	-2.433218
C	10.849667	1.284855	-1.470032
C	9.938892	0.217398	-1.649233
C	10.013758	-0.529252	-2.834563
C	10.974496	-0.243575	-3.833257
C	12.741974	2.698100	-2.182607
P	14.085945	3.137265	-3.135643
C	14.738144	4.646284	-2.211346
C	16.203434	4.483558	-1.765533
P	16.380185	3.349411	-0.269681
C	17.400914	2.125411	-0.874740
C	17.887826	0.961677	-0.142297
C	17.657170	0.779510	1.241256
C	18.117299	-0.357763	1.920972
C	18.841518	-1.328030	1.190785
C	19.089874	-1.183716	-0.181571
C	18.609872	-0.023301	-0.831354
C	17.832623	-0.503037	3.344429
P	18.174140	-1.870626	4.303767
C	17.554251	-1.329804	5.999585
C	16.468906	-2.271709	6.554038
P	14.790264	-1.991206	5.744572
C	14.447307	-3.528341	5.091435
C	13.243649	-3.902568	4.356702
C	12.139359	-3.030144	4.216514
C	10.987548	-3.401981	3.507832
C	10.946926	-4.689219	2.921870
C	12.024995	-5.581351	3.036448
C	13.164915	-5.174011	3.768517
C	11.929833	-6.889242	2.392133
P	13.201210	-8.012242	2.192397
C	12.306090	-9.486049	1.432666
C	13.095034	-10.148129	0.285103
P	12.868375	-9.254215	-1.358640
C	14.298172	-8.327096	-1.440652
C	14.628033	-7.370939	-2.495071
C	15.946492	-6.906256	-2.616328
C	16.322218	-5.999083	-3.633636
C	15.334674	-5.548237	-4.523188
C	13.989210	-5.968681	-4.416222
C	13.655918	-6.884524	-3.403201
C	12.939878	-5.477452	-5.303954
P	13.110339	-4.247796	-6.471668
C	11.393196	-4.191046	-7.243490
C	10.779125	-2.778018	-7.211506
P	10.085821	-2.331042	-5.516302
C	11.065734	-1.007585	-5.073612
C	17.692084	-5.520967	-3.791137
P	18.995617	-5.826968	-2.736277
C	20.419733	-4.952053	-3.607020
C	21.106739	-3.903334	-2.712133
P	20.101839	-2.315549	-2.564134
C	19.824335	-2.229521	-0.884156
C	9.882238	-2.455117	3.400913
P	8.389802	-2.729091	2.623753
C	7.511490	-1.082633	2.888374
C	7.246677	-0.338054	1.565535
P	8.775922	0.544374	0.905215
C	8.930627	-0.130175	-0.652858

N	12.080628	-5.294568	-0.712588
B	10.554003	-5.784663	-1.058128
H	17.104870	1.543328	1.794797
H	20.200054	-3.033989	-0.239899
H	19.216146	-2.214849	1.708519
H	17.330645	0.358471	3.801440
H	18.429067	-1.351363	6.671012
H	17.197514	-0.288764	5.961632
H	16.331321	-2.070535	7.629901
H	16.768133	-3.326861	6.455667
H	11.959942	-5.947109	-5.156987
H	15.188069	-4.330742	5.195986
H	12.179882	-2.042280	4.682437
H	10.067734	-1.483626	3.875636
H	8.079184	-0.455139	3.592985
H	6.546549	-1.321423	3.366109
H	6.839539	-1.016437	0.799969
H	6.492261	0.447622	1.740190
H	8.235116	-0.919102	-0.964242
H	9.314166	-1.354825	-2.987683
H	12.606101	1.057297	-4.382750
H	12.530377	3.267533	-1.269024
H	14.084765	4.877507	-1.356008
H	14.668101	5.494176	-2.913614
H	16.834137	4.122532	-2.592916
H	16.598566	5.466323	-1.458015
H	17.720985	2.170235	-1.922925
H	9.928068	-2.740215	-7.911854
H	11.506465	-2.019171	-7.539214
H	11.855528	-0.673345	-5.757975
H	11.519433	-4.506753	-8.293180
H	10.731999	-4.925765	-6.758766
H	10.066457	-4.993727	2.350486
H	10.938151	-7.127600	1.987460
H	11.294536	-9.193632	1.112546
H	12.189778	-10.213124	2.255171
H	14.165662	-10.226952	0.531176
H	12.717607	-11.171799	0.132235
H	15.070594	-8.450960	-0.671526
H	15.611852	-4.846736	-5.314395
H	17.857775	-4.894662	-4.676262
H	20.071478	-4.504860	-4.551023
H	21.149064	-5.737623	-3.867330
H	21.323274	-4.311692	-1.712749
H	22.071559	-3.619244	-3.164716
H	16.706689	-7.276034	-1.923520
H	12.619225	-7.222921	-3.310306
H	14.001504	-5.867844	3.884249
H	18.804794	0.109308	-1.898795
H	10.795346	1.883887	-0.557616
H	9.861498	-5.431273	-0.116548
H	10.245890	-5.230683	-2.099921
H	12.432566	-5.747284	0.141465
H	12.732701	-5.530386	-1.471145
H	10.609899	-7.000191	-1.167942
H	12.126466	-4.281216	-0.569036

P-C-Cage-Ts-1-C-P

C	14.333215	-7.682015	-1.957566
C	12.971525	-7.948425	-1.753647
C	12.042170	-7.452176	-2.696933
C	12.450748	-6.698689	-3.806951
C	13.832538	-6.452172	-3.978238
C	14.784734	-6.927969	-3.065315
C	12.566956	-8.719324	-0.583510
P	10.968604	-9.046621	-0.087988
C	11.247976	-10.072361	1.469338

C	10.684883	-9.393261	2.732173
P	11.769903	-7.974703	3.338258
C	10.687789	-6.658031	3.287338
C	10.977035	-5.281791	3.674067
C	12.203496	-4.897581	4.261846
C	12.465763	-3.566222	4.618044
C	11.456622	-2.600878	4.395660
C	10.221761	-2.945728	3.824975
C	10.000647	-4.296013	3.470338
C	13.747186	-3.239432	5.232254
P	14.406976	-1.686354	5.474931
C	15.953024	-2.104808	6.469303
C	17.221946	-1.366781	6.021582
P	17.964747	-1.981102	4.388007
C	17.619631	-0.590962	3.297868
C	17.583965	-0.743528	1.813929
C	18.092136	-1.893539	1.186265
C	18.156051	-2.001772	-0.215116
C	17.688596	-0.917655	-0.986356
C	17.157580	0.237213	-0.390931
C	17.113624	0.306230	1.022071
C	16.714547	1.331651	-1.246468
P	15.879162	2.736181	-0.760305
C	15.762146	3.690975	-2.383291
C	14.313100	3.986604	-2.811279
P	13.461558	2.483399	-3.565502
C	12.125660	2.281453	-2.526245
C	11.091149	1.259456	-2.629941
C	11.011052	0.362020	-3.719439
C	10.019023	-0.627009	-3.787367
C	9.076302	-0.705046	-2.736254
C	9.120783	0.169393	-1.641085
C	10.135932	1.152497	-1.609670
C	8.131603	0.036289	-0.577709
P	8.077549	0.946519	0.862943
C	6.564085	0.231900	1.728622
C	6.916023	-0.410291	3.084071
P	7.683370	-2.122489	2.901097
C	9.204810	-1.915767	3.643092
C	9.995934	-1.532811	-4.930048
P	8.970614	-2.879660	-5.134269
C	9.500317	-3.518801	-6.827281
C	9.988581	-4.978634	-6.781916
P	11.716819	-5.139732	-6.045921
C	11.445165	-6.199141	-4.737976
C	18.716046	-3.210792	-0.806874
P	18.811594	-3.583575	-2.468408
C	19.719156	-5.237019	-2.439980
C	18.968199	-6.341314	-3.205760
P	17.488965	-7.009731	-2.246461
C	16.194798	-6.631645	-3.290221
H	12.968389	-5.656720	4.444861
H	9.482312	-0.925664	4.024953
H	11.634929	-1.565441	4.697099
H	14.335972	-4.111226	5.542674
H	15.718019	-1.816524	7.509740
H	16.113835	-3.193379	6.460410
H	17.999767	-1.517607	6.790239
H	17.046109	-0.279235	5.967766
H	10.738808	-1.308255	-5.704931
H	16.949229	0.183522	3.686301
H	18.440520	-2.726907	1.802638
H	19.099020	-3.936717	-0.079222
H	19.922214	-5.539676	-1.400888
H	20.694954	-5.062363	-2.924850
H	18.648278	-5.989509	-4.198745
H	19.647223	-7.195855	-3.364691
H	16.404520	-6.094151	-4.222965
H	14.167584	-5.876042	-4.844573
H	10.977927	-7.658203	-2.556059

H	13.398950	-9.090892	0.026708
H	12.318535	-10.302258	1.585070
H	10.723264	-11.029503	1.310321
H	9.654460	-9.040826	2.569233
H	10.651260	-10.130347	3.552283
H	9.669573	-6.821395	2.913766
H	10.051305	-5.370119	-7.811381
H	9.280879	-5.618460	-6.232269
H	10.422938	-6.538964	-4.532114
H	8.609410	-3.456982	-7.474629
H	10.265333	-2.856271	-7.261426
H	17.744431	-0.974721	-2.076603
H	16.951391	1.199782	-2.309210
H	16.310434	3.157590	-3.175339
H	16.287903	4.645568	-2.211700
H	13.719963	4.377980	-1.970206
H	14.320169	4.763371	-3.594708
H	12.015257	2.954657	-1.667818
H	8.291920	-1.465590	-2.779447
H	7.379359	-0.743544	-0.746285
H	6.047809	-0.483774	1.069887
H	5.875443	1.076617	1.897484
H	7.577281	0.242402	3.675119
H	5.990495	-0.550717	3.667670
H	10.180781	1.845008	-0.764773
H	11.742479	0.439432	-4.528492
H	16.737270	1.214594	1.499841
H	9.038690	-4.582643	3.037324
H	15.063931	-8.067527	-1.241786
H	18.815481	-0.093833	3.553224
B	20.106724	0.464227	3.814848
N	20.428368	-0.722469	4.758668
H	19.279561	-1.521982	4.726733
H	20.546732	0.387817	2.698068
H	19.802285	1.495504	4.354067
H	20.564200	-0.498923	5.744224
H	21.133755	-1.386650	4.440866

P-C-Cage-Ts-1

C	-1.736902	0.726795	-3.976068
C	-2.736804	1.707175	-4.061398
C	-2.467685	2.987205	-3.524778
C	-1.244567	3.287211	-2.908691
C	-0.258538	2.276330	-2.851181
C	-0.488257	0.992430	-3.367271
C	-4.010340	1.379779	-4.693588
P	-5.370224	2.403123	-4.799807
C	-6.603435	1.329987	-5.738549
C	-7.912926	1.128492	-4.953907
P	-7.703850	-0.081546	-3.523328
C	-8.232892	0.841488	-2.190425
C	-8.298753	0.388841	-0.804968
C	-8.661219	1.297250	0.200976
C	-8.729813	0.911814	1.560239
C	-8.431033	-0.419124	1.889602
C	-8.057804	-1.362498	0.904747
C	-8.008620	-0.943637	-0.432446
C	-7.729637	-2.747456	1.223487
P	-7.500057	-3.406785	2.778877
C	-7.166479	-5.220623	2.381243
C	-5.811881	-5.711761	2.921765
P	-4.351653	-5.142903	1.871571
C	-3.348863	-4.411581	3.039965
C	-2.031766	-3.826506	2.815387
C	-1.421722	-3.116063	3.858190
C	-0.138088	-2.528344	3.721390
C	0.527200	-2.693426	2.490997
C	-0.065909	-3.385831	1.411031

C	-1.335818	-3.956050	1.591077
C	0.476550	-1.764936	4.792764
P	-0.376492	-1.162186	6.169270
C	0.980428	-0.263238	7.138540
C	0.360330	1.107992	7.458170
P	-0.590410	1.505068	5.894586
C	-1.991429	2.502298	6.216181
C	-2.624847	3.281299	5.239690
C	-3.966806	3.686540	5.375350
C	-4.594310	4.542462	4.461313
C	-3.776952	5.183481	3.469311
C	-2.460575	4.853994	3.247040
C	-1.880394	3.687419	3.998117
C	-1.602869	5.546857	2.320919
P	-2.074020	6.590468	1.039655
C	-0.396744	7.211301	0.431574
C	-0.155115	6.929496	-1.062887
P	0.278673	5.126811	-1.396305
C	-1.038366	4.618656	-2.351488
C	-6.004822	4.846391	4.501824
P	-7.203660	4.013552	5.404154
C	-8.770056	4.938016	4.898937
C	-9.804440	4.005289	4.238434
P	-9.341320	3.520136	2.475337
C	-9.102311	1.838265	2.624251
C	0.586977	-3.519508	0.113453
P	1.965742	-2.668304	-0.417599
C	2.213966	-3.369978	-2.150776
C	2.177263	-2.284798	-3.242621
P	0.429590	-1.674162	-3.606799
C	0.563805	-0.011247	-3.255034
B	-0.985808	1.799949	2.156248
N	0.149235	1.276716	2.984726
H	-1.945159	-3.024213	4.813468
H	0.090662	-4.209799	-0.579476
H	-1.793580	-4.511840	0.769110
H	-3.708837	-4.336570	4.073308
H	-5.793303	-6.814833	2.898081
H	-5.666344	-5.407703	3.970134
H	-7.975936	-5.793958	2.863932
H	-7.249251	-5.392924	1.296702
H	-1.846535	5.330205	-2.558246
H	-7.596542	-3.396124	0.348873
H	-8.492651	-0.734819	2.934145
H	-9.202873	1.376161	3.613741
H	-9.964745	3.100910	4.845831
H	-10.773278	4.528580	4.169148
H	-8.516592	5.781657	4.238172
H	-9.208282	5.363380	5.817387
H	-6.323410	5.646722	3.822182
H	-4.214535	6.012477	2.905045
H	-0.811954	3.843815	4.221656
H	-2.494003	2.370640	7.180449
H	-0.372539	1.032914	8.276765
H	1.093924	1.880464	7.727167
H	1.883134	-0.157486	6.518099
H	1.254509	-0.824880	8.043143
H	1.529398	-1.492113	4.645572
H	-0.388892	8.302148	0.596149
H	0.410576	6.788315	1.050547
H	-0.529853	5.349925	2.447134
H	0.704586	7.526017	-1.412566
H	-1.025736	7.225159	-1.668782
H	-8.901748	2.327800	-0.072928
H	-8.539583	1.882810	-2.348206
H	-8.309846	2.087822	-4.587589
H	-8.673182	0.694235	-5.625001
H	-6.144987	0.364191	-6.002783
H	-6.823293	1.857190	-6.682334
H	-4.069204	0.366643	-5.109127

H	0.707689	2.500120	-2.391297
H	1.518075	0.372384	-2.873933
H	2.828323	-1.435780	-2.981471
H	2.559943	-2.710109	-4.185673
H	1.470528	-4.157865	-2.347706
H	3.206718	-3.850820	-2.153515
H	-1.924959	-0.264745	-4.396163
H	-3.235226	3.763120	-3.587464
H	-7.734553	-1.665921	-1.205694
H	1.535004	-2.285291	2.369540
H	-4.535604	3.323831	6.236216
H	0.168685	0.252267	3.070116
H	1.077283	1.612443	2.716597
H	-1.956353	1.102286	2.072269
H	-0.764832	2.734142	1.441493
H	-1.869361	2.789221	3.251463
H	0.009725	1.558784	4.242109

P-C-Cage-H₂

C	11.912246	1.138183	-3.560977
C	11.800777	1.854908	-2.360200
C	10.963212	1.337025	-1.345319
C	10.238762	0.148541	-1.522867
C	10.377216	-0.544411	-2.747614
C	11.198657	-0.063103	-3.777641
C	12.541483	3.102396	-2.206172
P	12.386829	4.220239	-0.928217
C	13.653932	5.532621	-1.406384
C	13.032819	6.935277	-1.536677
P	12.014296	7.135372	-3.111740
C	10.499296	7.611239	-2.490325
C	9.306143	7.933341	-3.265035
C	9.319588	8.038956	-4.675601
C	8.156855	8.334764	-5.401928
C	6.954438	8.540007	-4.687749
C	6.899731	8.440196	-3.290491
C	8.093267	8.144318	-2.592662
C	8.220201	8.415573	-6.856882
P	6.896742	8.653816	-7.905339
C	7.724193	8.643431	-9.597932
C	7.212017	7.497324	-10.490916
P	7.955960	5.826650	-10.034759
C	6.569659	4.903265	-9.669179
C	6.548737	3.492442	-9.295919
C	7.714370	2.692429	-9.305875
C	7.678554	1.330458	-8.972602
C	6.431439	0.757274	-8.635503
C	5.253114	1.518999	-8.604837
C	5.331054	2.890479	-8.941824
C	3.997017	0.858388	-8.269330
P	2.499448	1.596286	-7.915158
C	1.386978	0.075310	-7.817723
C	0.376821	0.063217	-6.664046
P	1.059497	-0.155069	-4.922015
C	1.392062	1.550864	-4.402591
C	2.169442	1.875901	-3.317771
C	3.009198	0.812452	-2.639594
C	3.650368	1.213725	-1.327531
C	3.549385	2.505851	-0.895224
C	2.867924	3.545472	-1.638755
C	2.199717	3.206135	-2.805351
C	2.866681	4.885714	-1.084427
P	2.435104	6.335934	-1.883664
C	2.595496	7.595808	-0.486130
C	3.452880	8.811941	-0.879072
P	5.290784	8.397012	-0.963674
C	5.619920	8.633871	-2.619625
C	4.363218	0.185337	-0.606367

P	5.615852	0.441667	0.534686
C	5.977916	-1.318108	1.114249
C	7.491199	-1.590103	1.178352
P	8.267012	-1.621141	-0.540238
C	9.365744	-0.319244	-0.452651
C	8.916192	0.558138	-9.000307
P	9.114848	-1.054343	-8.483261
C	10.938042	-1.361330	-8.854731
C	11.738295	-1.772245	-7.604996
P	12.076973	-0.318168	-6.452716
C	11.278232	-0.809375	-5.028287
H	10.259617	7.887752	-5.212514
H	4.799506	8.930249	-3.284182
H	6.040638	8.776864	-5.239018
H	9.223006	8.285795	-7.281458
H	7.475590	9.607766	-10.072204
H	8.818977	8.605930	-9.488071
H	7.514489	7.690699	-11.534141
H	6.112531	7.440806	-10.476277
H	4.112146	-0.846490	-0.886299
H	5.584361	5.384227	-9.699494
H	8.667404	3.144279	-9.592327
H	9.788775	1.107979	-9.374075
H	11.380029	-0.476144	-9.337304
H	10.970365	-2.183917	-9.589485
H	11.230792	-2.580320	-7.055725
H	12.722362	-2.158422	-7.919436
H	10.735774	-1.762365	-5.025116
H	9.826909	-1.477179	-2.896715
H	10.874616	1.878139	-0.399777
H	13.232912	3.326172	-3.027416
H	14.172041	5.239158	-2.332476
H	14.407794	5.546683	-0.600929
H	12.420341	7.182892	-0.655850
H	13.841968	7.683334	-1.592495
H	10.364460	7.664376	-1.403279
H	7.668596	-2.579172	1.632694
H	8.000998	-0.843101	1.806199
H	9.417253	0.271480	0.469919
H	5.542895	-1.430401	2.122201
H	5.471063	-2.043495	0.458662
H	6.382093	-0.308602	-8.398381
H	4.058988	-0.236633	-8.243845
H	2.004869	-0.835769	-7.801918
H	0.827908	0.062812	-8.770599
H	-0.225543	0.986084	-6.648445
H	-0.334144	-0.763080	-6.818175
H	0.791726	2.335608	-4.873743
H	3.992408	2.776400	0.067719
H	3.229215	4.951664	-0.050794
H	2.989275	7.106901	0.418625
H	1.572777	7.937049	-0.250970
H	3.119054	9.239056	-1.837477
H	3.341238	9.597735	-0.113248
H	1.609479	3.967613	-3.323111
H	2.394202	-0.097970	-2.485563
H	4.416724	3.489098	-8.951212
H	8.069347	8.072036	-1.502153
H	12.563201	1.520839	-4.351414
H	2.396391	-0.584765	-5.254794
H	3.808072	0.488437	-3.335307

P-C-Cage-H₂-C-P

C	11.885181	0.823919	-3.685501
C	11.885025	1.621259	-2.517573
C	10.916736	1.362319	-1.535641
C	9.963729	0.328373	-1.686683
C	9.991743	-0.435936	-2.862517

C	10.955040	-0.209360	-3.872610
C	12.848436	2.695000	-2.299851
P	14.174113	3.089269	-3.297479
C	14.926268	4.554436	-2.378479
C	16.345869	4.264489	-1.853512
P	16.326082	3.122384	-0.352352
C	17.309616	1.832563	-0.878921
C	17.629187	0.623626	-0.130588
C	18.381166	-0.384178	-0.751650
C	18.676581	-1.596656	-0.094822
C	18.196537	-1.775870	1.216646
C	17.447252	-0.781005	1.870180
C	17.183113	0.409782	1.196439
C	16.913767	-1.003765	3.262520
P	18.281635	-1.477215	4.486146
C	17.453793	-1.156880	6.154421
C	16.495332	-2.272604	6.610415
P	14.744619	-2.048488	5.951422
C	14.417422	-3.560176	5.233058
C	13.183034	-3.932543	4.548840
C	13.050183	-5.223967	4.017413
C	11.879152	-5.627649	3.333945
C	10.835939	-4.700300	3.195095
C	10.936992	-3.385987	3.706613
C	12.108952	-3.026720	4.386711
C	11.716637	-6.963188	2.769872
P	12.906800	-8.180196	2.673360
C	11.950854	-9.592155	1.866173
C	12.593987	-10.073001	0.551651
P	12.294997	-8.883738	-0.881305
C	13.886549	-8.434793	-1.297459
C	14.282174	-7.519972	-2.362319
C	13.360828	-6.990880	-3.295091
C	13.761880	-6.099992	-4.301903
C	15.128296	-5.743150	-4.376959
C	16.072286	-6.247313	-3.470360
C	15.629091	-7.144720	-2.471790
C	17.466711	-5.834859	-3.588377
P	18.724485	-6.209838	-2.500596
C	20.211667	-5.387532	-3.314407
C	20.901054	-4.361288	-2.393823
P	19.997602	-2.707051	-2.334936
C	19.444031	-2.665485	-0.721700
C	12.763219	-5.580124	-5.229331
P	13.007312	-4.381152	-6.416557
C	11.302226	-4.274560	-7.215707
C	10.711737	-2.853109	-7.161915
P	10.087890	-2.394724	-5.442788
C	11.017542	-1.009522	-5.090781
C	9.879332	-2.394609	3.544416
P	8.474382	-2.559122	2.592807
C	7.605049	-0.913566	2.896120
C	7.336401	-0.137753	1.593672
P	8.889738	0.680744	0.904426
C	8.961132	0.029421	-0.669764
H	13.868389	-5.938206	4.141483
H	10.053578	-1.451380	4.076699
H	12.198751	-2.015208	4.790907
H	15.182861	-4.345851	5.261548
H	16.402597	-2.236056	7.709011
H	16.884876	-3.269570	6.351230
H	18.291401	-1.083685	6.867230
H	16.947622	-0.178086	6.157505
H	11.766062	-0.672990	-5.818516
H	16.197995	-1.840825	3.261752
H	18.410350	-2.713772	1.736104
H	19.655204	-3.519566	-0.066878
H	21.026768	-4.760923	-1.375442
H	21.908938	-4.146535	-2.786386
H	19.918273	-4.931884	-4.272940

H	20.922487	-6.199668	-3.542972
H	17.685697	-5.205352	-4.459275
H	15.457598	-5.057279	-5.161814
H	12.309802	-7.284543	-3.231394
H	14.720984	-8.835032	-0.709035
H	13.673289	-10.249784	0.678148
H	12.137794	-11.033774	0.259401
H	10.901042	-9.298287	1.711280
H	11.953247	-10.422805	2.592305
H	10.721755	-7.161255	2.352634
H	11.433616	-4.570422	-8.270330
H	10.620828	-5.006263	-6.754384
H	11.761553	-6.009647	-5.107100
H	9.839296	-2.799953	-7.834808
H	11.440160	-2.105654	-7.512024
H	18.739834	-0.227649	-1.772552
H	17.734463	1.868251	-1.889415
H	16.984621	3.842279	-2.644855
H	16.808858	5.211355	-1.528567
H	14.258470	4.868585	-1.561649
H	14.972370	5.386143	-3.101623
H	12.686970	3.270984	-1.380595
H	9.253654	-1.230377	-2.999087
H	8.213268	-0.713696	-0.971824
H	6.878966	-0.786269	0.830510
H	6.621558	0.676324	1.801047
H	8.182498	-0.305816	3.609895
H	6.642068	-1.155003	3.377254
H	10.896312	1.977230	-0.632276
H	12.629367	1.017322	-4.462376
H	16.601150	1.190600	1.693495
H	9.923583	-5.000679	2.673458
H	16.355305	-7.557352	-1.766487
H	16.371543	-0.114056	3.613642
H	18.973870	-0.216269	4.430346

P-C-Cage

C	11.812043	0.751729	-3.648790
C	11.791820	1.545557	-2.478709
C	10.805756	1.285333	-1.515262
C	9.855311	0.251992	-1.685605
C	9.907339	-0.513187	-2.860174
C	10.886812	-0.282542	-3.853682
C	12.751456	2.618610	-2.241642
P	14.103520	3.000416	-3.207509
C	14.824239	4.486657	-2.298503
C	16.280732	4.258911	-1.851336
P	16.404337	3.151370	-0.330531
C	17.349482	1.856250	-0.910442
C	17.781033	0.691549	-0.146086
C	18.469097	-0.340087	-0.800829
C	18.905792	-1.495129	-0.111804
C	18.642732	-1.589095	1.262336
C	17.950758	-0.571006	1.957766
C	17.535755	0.559929	1.240319
C	17.660456	-0.655554	3.384709
P	17.951756	-1.996984	4.395952
C	17.364739	-1.360704	6.070784
C	16.257421	-2.240070	6.681202
P	14.580931	-1.954970	5.868082
C	14.195807	-3.513694	5.294472
C	12.982648	-3.893879	4.579345
C	12.872674	-5.190167	4.055436
C	11.726128	-5.606937	3.339819
C	10.676937	-4.691087	3.172135
C	10.750717	-3.375151	3.684916
C	11.903614	-2.999908	4.389439

C	11.599381	-6.945090	2.772162
P	12.811090	-8.144152	2.726498
C	11.918956	-9.569666	1.873075
C	12.623242	-10.016528	0.578143
P	12.335051	-8.822249	-0.852252
C	13.928708	-8.395436	-1.282387
C	14.322005	-7.495916	-2.361431
C	13.395060	-6.976704	-3.294286
C	13.789563	-6.099333	-4.315192
C	15.156469	-5.749081	-4.407204
C	16.106543	-6.245818	-3.502864
C	15.669153	-7.126579	-2.486884
C	17.501197	-5.842236	-3.643492
P	18.779448	-6.231888	-2.584625
C	20.247069	-5.392879	-3.418989
C	20.910970	-4.331449	-2.521211
P	19.926902	-2.725046	-2.443701
C	19.620169	-2.581325	-0.772790
C	12.784310	-5.588644	-5.240436
P	13.016644	-4.394666	-6.435003
C	11.308586	-4.305489	-7.229876
C	10.697954	-2.892759	-7.170864
P	10.043986	-2.455059	-5.457578
C	10.968990	-1.074857	-5.075656
C	9.680476	-2.399952	3.507280
P	8.273517	-2.598007	2.564671
C	7.387654	-0.956241	2.839445
C	7.141966	-0.189059	1.527137
P	8.703301	0.636997	0.867099
C	8.828984	-0.042569	-0.691479
H	13.694419	-5.895478	4.203352
H	9.842596	-1.447007	4.025888
H	11.970095	-1.989580	4.800895
H	14.917073	-4.327530	5.437578
H	16.135311	-1.978892	7.745932
H	16.525392	-3.307127	6.635672
H	18.246114	-1.377849	6.733877
H	17.039983	-0.311833	5.987236
H	11.729490	-0.732574	-5.788303
H	17.191522	0.240190	3.809564
H	18.982834	-2.471979	1.810022
H	19.964260	-3.375498	-0.098964
H	21.084356	-4.720094	-1.505656
H	21.896243	-4.069216	-2.942422
H	19.940410	-4.962697	-4.385024
H	20.977956	-6.190400	-3.633800
H	17.707371	-5.210626	-4.516071
H	15.481715	-5.076941	-5.205531
H	12.343969	-7.267163	-3.218225
H	14.763827	-8.796699	-0.695680
H	13.702555	-10.161412	0.740801
H	12.207858	-10.987475	0.259494
H	10.868396	-9.300493	1.682545
H	11.916390	-10.408855	2.589160
H	10.624438	-7.156254	2.315947
H	11.443258	-4.595080	-8.285845
H	10.637837	-5.048679	-6.771400
H	11.784881	-6.021092	-5.110794
H	9.833727	-2.845324	-7.854708
H	11.420372	-2.132155	-7.504838
H	18.675850	-0.246774	-1.870250
H	17.665633	1.856018	-1.960493
H	16.890904	3.849723	-2.671630
H	16.725397	5.226961	-1.565292
H	14.183268	4.756906	-1.445086
H	14.794562	5.329808	-3.009420
H	12.565578	3.202379	-1.331764
H	9.172869	-1.308301	-3.010695
H	8.097387	-0.797875	-1.003007
H	6.705872	-0.844821	0.757804

H	6.417304	0.621222	1.714666
H	7.945460	-0.340853	3.562141
H	6.415713	-1.200824	3.300363
H	10.769964	1.898107	-0.610999
H	12.566802	0.949509	-4.414140
H	17.008999	1.360534	1.766367
H	9.780275	-5.002696	2.630296
H	16.399631	-7.529835	-1.780674

P-C-Cage-(H2)-Ts-2

C	5.685993	-0.707605	-0.410366
C	5.451998	-2.064324	-0.142110
C	4.681412	-2.807778	-1.065710
C	4.139221	-2.217032	-2.216290
C	4.398118	-0.847310	-2.452313
C	5.161084	-0.077520	-1.562280
C	6.001367	-2.653855	1.073680
P	5.717562	-4.233306	1.649638
C	6.750781	-4.264077	3.225745
C	5.907676	-4.583212	4.474531
P	4.855865	-3.118993	5.028147
C	3.286506	-3.785257	5.011303
C	2.051277	-3.101081	5.377495
C	0.824583	-3.753636	5.184269
C	-0.404699	-3.136625	5.513206
C	-0.375311	-1.845542	6.060151
C	0.840452	-1.154691	6.269602
C	2.038756	-1.798639	5.928622
C	0.889940	0.193207	6.825333
P	-0.447622	1.185580	7.190566
C	0.387420	2.733097	7.869973
C	0.082075	3.987511	7.029152
P	1.093755	4.064860	5.439990
C	-0.122640	4.077177	4.245324
C	0.080570	4.161603	2.803175
C	-1.024509	4.039735	1.947861
C	-0.889671	4.123289	0.542744
C	0.387422	4.350788	0.008665
C	1.526334	4.475769	0.837477
C	1.351970	4.382629	2.226374
C	-2.031515	4.004037	-0.357931
P	-3.596118	3.477671	0.068246
C	-4.543839	3.757074	-1.538406
C	-5.605487	2.676134	-1.804885
P	-4.895152	1.106886	-2.578574
C	-5.346636	-0.125022	-1.427889
C	-4.642588	-1.347696	-1.399764
C	-4.751990	-2.237592	-0.304841
C	-3.896341	-3.333639	-0.154945
C	-2.914364	-3.576917	-1.157758
C	-2.762528	-2.761592	-2.273236
C	-3.602929	-1.587791	-2.387765
C	-1.819493	-3.036013	-3.342890
P	-0.548538	-4.178905	-3.322051
C	0.127801	-4.026976	-5.077499
C	1.665068	-4.052279	-5.109711
P	2.417631	-2.457821	-4.442673
C	3.329364	-3.027314	-3.118664
C	-3.984747	-4.253728	0.971142
P	-4.791488	-3.976841	2.449382
C	-4.549478	-5.625148	3.334615
C	-3.824222	-5.481631	4.685215
P	-1.961886	-5.263047	4.491819
C	-1.691942	-3.792347	5.310301
C	2.865181	4.706665	0.306982
P	3.318520	4.746218	-1.335883
C	5.162940	5.120850	-1.217218
C	6.034724	4.043289	-1.890290

P	6.167784	2.470590	-0.858078
C	5.377892	1.334550	-1.854512
H	-2.017737	3.891536	2.379562
H	3.637976	4.847259	1.072447
H	2.221042	4.496080	2.879730
H	-1.172218	3.998400	4.553948
H	0.354200	4.885246	7.609549
H	-0.992549	4.061824	6.800044
H	-0.010090	2.877137	8.888760
H	1.472322	2.569911	7.963717
H	3.299786	-4.095613	-2.872005
H	1.902187	0.580750	6.993461
H	-1.317255	-1.361089	6.330267
H	-2.551502	-3.244583	5.715539
H	-4.244564	-4.654945	5.278920
H	-3.964048	-6.406458	5.270183
H	-4.027567	-6.335846	2.675024
H	-5.560989	-6.029317	3.510035
H	-3.432998	-5.192982	0.839283
H	-2.285099	-4.465684	-1.061074
H	-3.821448	-1.259876	-3.413412
H	-6.033801	0.099178	-0.606589
H	-6.152693	2.424583	-0.883206
H	-6.337686	3.061046	-2.533266
H	-3.847251	3.860236	-2.385058
H	-5.049974	4.730314	-1.419902
H	-1.822119	4.270266	-1.401479
H	-0.262074	-4.889374	-5.645037
H	-0.265835	-3.117186	-5.557246
H	-1.942087	-2.405458	-4.233242
H	2.006449	-4.150568	-6.153801
H	2.059306	-4.917306	-4.554117
H	0.819283	-4.765833	4.771996
H	3.152433	-4.821034	4.676407
H	5.271753	-5.467045	4.310290
H	6.582377	-4.817571	5.315161
H	7.292355	-3.312742	3.343292
H	7.506555	-5.055868	3.088952
H	6.633593	-1.978114	1.662684
H	3.993899	-0.376205	-3.352054
H	4.957196	1.670358	-2.810091
H	5.662608	3.803819	-2.898557
H	7.061038	4.430244	-2.003993
H	5.452514	5.266757	-0.164906
H	5.317915	6.082982	-1.734502
H	6.286614	-0.122369	0.290822
H	4.497476	-3.868339	-0.875035
H	2.987245	-1.282031	6.096856
H	0.504905	4.434225	-1.074946
H	-5.533937	-2.059643	0.438104
H	-3.155072	0.601647	-2.270333
H	-2.873957	-0.304990	-2.222505

N-C-Cage With AB

C	10.415058	1.540793	-2.959865
C	11.169284	1.766666	-4.128769
C	11.019230	0.900828	-5.217421
C	10.129636	-0.192098	-5.148261
C	9.389707	-0.399648	-3.980664
C	9.528078	0.464698	-2.877148
C	12.118273	2.890860	-4.220480
N	12.328090	3.690066	-3.243769
C	13.282466	4.765040	-3.442283
C	12.648108	6.124244	-3.111528
N	11.635867	6.468547	-4.089285
C	10.456669	6.729137	-3.674003
C	9.353161	7.078433	-4.585567
C	9.535601	7.086743	-5.984909

C	8.481824	7.434833	-6.837497
C	7.230323	7.771522	-6.284599
C	7.034106	7.766151	-4.900927
C	8.105113	7.414921	-4.055282
C	8.700300	7.447343	-8.295626
N	7.785339	7.794096	-9.119784
C	8.102960	7.764743	-10.535289
C	7.080992	6.913391	-11.303246
N	7.221767	5.512072	-10.962972
C	6.193223	4.886784	-10.535175
C	6.230007	3.463914	-10.154523
C	7.432652	2.726453	-10.191319
C	7.447462	1.371440	-9.841659
C	6.247223	0.748988	-9.443380
C	5.049163	1.466914	-9.400053
C	5.049637	2.830089	-9.756837
C	3.811381	0.783670	-8.988164
N	2.672417	1.363133	-8.966618
C	1.522095	0.587068	-8.545518
C	0.777981	1.284785	-7.398002
N	1.568901	1.268136	-6.182909
C	1.810223	2.383928	-5.608750
C	2.606181	2.494270	-4.375091
C	2.796214	3.748925	-3.790893
C	3.554895	3.886907	-2.611789
C	4.121021	2.750817	-2.027083
C	3.939763	1.478161	-2.603733
C	3.184352	1.359191	-3.772989
C	4.534328	0.274024	-2.000521
N	5.209327	0.301489	-0.915652
C	5.751989	-0.948115	-0.419594
C	7.268882	-0.841046	-0.205646
N	7.966422	-0.733392	-1.472721
C	8.762476	0.252282	-1.637317
C	3.765037	5.201625	-1.984754
N	3.257947	6.281733	-2.445252
C	3.537715	7.517296	-1.740452
C	4.136443	8.567850	-2.686513
N	5.473131	8.190975	-3.103299
C	5.716047	8.132918	-4.357131
C	8.713896	0.618481	-9.901750
N	8.779823	-0.630635	-9.636348
C	10.078599	-1.272902	-9.723338
C	10.420592	-1.988651	-8.408155
N	10.660421	-1.028165	-7.350310
C	9.971692	-1.123023	-6.278280
H	10.519946	6.830089	-6.386442
H	4.937382	8.365150	-5.112792
H	6.419507	8.042978	-6.965157
H	9.706314	7.129942	-8.632925
H	8.028711	8.796636	-10.920073
H	9.123950	7.387162	-10.739407
H	7.300342	7.024034	-12.379141
H	6.059514	7.301457	-11.112863
H	4.356643	-0.672369	-2.552316
H	5.206679	5.384467	-10.430812
H	8.348164	3.231430	-10.512905
H	9.608119	1.207234	-10.186491
H	10.891388	-0.565770	-9.979397
H	10.022777	-2.042311	-10.512831
H	9.615592	-2.709572	-8.160298
H	11.355196	-2.552187	-8.571828
H	9.213924	-1.921824	-6.137522
H	8.695631	-1.239792	-3.900538
H	10.546911	2.225244	-2.118129
H	12.635760	3.002971	-5.193444
H	13.692930	4.790840	-4.470668
H	14.117261	4.610704	-2.736922
H	12.255472	6.106372	-2.074573
H	13.446578	6.884087	-3.169024

H	10.197987	6.710726	-2.594866
H	7.599813	-1.773092	0.284560
H	7.485317	0.006210	0.476169
H	8.926725	1.008306	-0.841597
H	5.293794	-1.150634	0.564039
H	5.534929	-1.805857	-1.087904
H	6.276558	-0.310092	-9.175759
H	3.929293	-0.281402	-8.699111
H	1.789794	-0.443712	-8.236699
H	0.826369	0.522460	-9.399929
H	0.496194	2.310027	-7.712960
H	-0.147785	0.713788	-7.208953
H	1.425297	3.342649	-6.014122
H	4.714839	2.828092	-1.113420
H	4.397025	5.198701	-1.072842
H	4.216165	7.373364	-0.875128
H	2.579977	7.918680	-1.366411
H	3.449242	8.726945	-3.542099
H	4.212230	9.514138	-2.123326
H	2.360921	4.646241	-4.237348
H	3.028033	0.384788	-4.241927
H	4.104964	3.377992	-9.720930
H	7.938002	7.418134	-2.975391
H	11.599086	1.047260	-6.133561
N	9.551299	3.625344	-7.290545
B	10.911853	3.827965	-8.188719
H	8.726280	3.484173	-7.885411
H	9.628690	2.808357	-6.673468
H	9.366166	4.442519	-6.696643
H	10.719865	4.817996	-8.874169
H	11.822397	3.977824	-7.391339
H	11.030457	2.812271	-8.853082

N-C-Cage-Ts-1-C-N

C	-2.133529	4.643623	3.045231
C	-1.101246	3.990475	3.723791
C	0.234845	4.348272	3.455086
C	0.532752	5.345557	2.522487
C	-0.520043	5.994833	1.848309
C	-1.850483	5.652017	2.102887
C	-1.431855	2.940796	4.701481
N	-0.549421	2.333549	5.398933
C	-1.002482	1.316282	6.328160
C	-0.287847	-0.019026	6.076748
N	-0.710495	-0.608660	4.821346
C	0.193067	-0.910916	3.968860
C	-0.106861	-1.513233	2.660075
C	0.945945	-1.861490	1.809603
C	0.693331	-2.440107	0.550423
C	-0.627987	-2.663350	0.154669
C	-1.701217	-2.316925	0.998798
C	-1.433146	-1.744255	2.244873
C	-3.097530	-2.542643	0.591892
N	-3.418810	-3.099023	-0.513319
C	-4.828924	-3.260890	-0.808687
C	-5.184018	-2.618878	-2.158018
N	-5.106420	-1.172925	-2.082165
C	-4.347262	-0.568776	-2.914481
C	-4.186802	0.894327	-2.935379
C	-3.386797	1.483690	-3.917660
C	-3.219525	2.881784	-3.967263
C	-3.862639	3.681133	-3.018121
C	-4.674611	3.103242	-2.022448
C	-4.828391	1.714783	-1.987103
C	-2.397299	3.516260	-5.010308
N	-1.846588	2.856592	-5.956656
C	-1.093902	3.587308	-6.956300
C	0.301691	2.984869	-7.159935

N	1.199067	3.283616	-6.042898
C	1.778385	2.237463	-5.448664
C	2.473862	2.413274	-4.146621
C	3.056802	1.310249	-3.517230
C	3.735397	1.456102	-2.294284
C	3.837513	2.724373	-1.711909
C	3.252516	3.843448	-2.327692
C	2.562892	3.675908	-3.536606
C	3.354404	5.186217	-1.734242
N	4.044249	5.435729	-0.687251
C	4.089237	6.803342	-0.208379
C	3.695732	6.885938	1.272798
N	2.280555	6.626505	1.451806
C	1.937687	5.697524	2.260449
C	4.357742	0.304607	-1.620161
N	4.320109	-0.883115	-2.090705
C	4.982899	-1.931865	-1.340264
C	4.016749	-3.083179	-1.025950
N	3.024581	-2.678607	-0.048453
C	1.791186	-2.813746	-0.356053
C	-5.367944	3.929024	-1.020838
N	-5.332708	5.206926	-1.023595
C	-6.057084	5.906239	0.019943
C	-5.129507	6.859112	0.789049
N	-4.166078	6.117530	1.578806
C	-2.924932	6.347496	1.376589
H	-2.880051	0.871891	-4.667836
H	-5.937863	3.365512	-0.253365
H	-5.451535	1.239990	-1.225451
H	-3.765616	-1.123244	-3.679586
H	-6.228506	-2.890144	-2.388741
H	-4.531442	-3.043053	-2.947805
H	-5.036394	-4.341627	-0.892523
H	-5.484504	-2.840953	-0.018857
H	2.691183	5.102696	2.817148
H	-3.866227	-2.197262	1.313753
H	-0.853353	-3.109272	-0.817073
H	1.478519	-3.230276	-1.335934
H	3.565117	-3.450513	-1.969542
H	4.611168	-3.901894	-0.584711
H	5.434233	-1.564738	-0.396278
H	5.789210	-2.340996	-1.973189
H	4.876582	0.535670	-0.666589
H	4.370056	2.865731	-0.768566
H	2.069761	4.528704	-4.009604
H	1.390949	1.227916	-5.646909
H	0.196449	1.897284	-7.319600
H	0.722331	3.411482	-8.088885
H	-1.004087	4.668245	-6.722374
H	-1.635983	3.490524	-7.914041
H	-2.297994	4.619090	-4.934579
H	5.132587	7.154796	-0.292089
H	3.444692	7.486946	-0.797841
H	2.799039	5.987077	-2.266823
H	3.895246	7.917570	1.610489
H	4.336741	6.197873	1.860415
H	1.984065	-1.691595	2.105353
H	1.269256	-0.735451	4.175864
H	0.808682	0.136748	6.129540
H	-0.578942	-0.707122	6.889272
H	-2.099440	1.158361	6.289574
H	-0.736091	1.645826	7.347214
H	-2.512103	2.706728	4.800461
H	-0.271334	6.771341	1.121040
H	-2.587252	7.096746	0.630893
H	-4.650344	7.558825	0.074252
H	-5.757780	7.446166	1.480551
H	-6.549829	5.216953	0.735392
H	-6.837115	6.521058	-0.461211
H	-3.178188	4.383743	3.232265

H	1.031430	3.827262	3.991606
H	-2.246072	-1.464725	2.919344
H	-3.752047	4.768077	-3.033560
H	3.010363	0.317198	-3.970441
H	2.225464	3.918968	-6.513366
H	3.090866	1.924639	-6.318693
B	3.968719	2.586712	-7.055644
N	3.389854	4.024604	-7.076601
H	3.904479	2.045116	-8.140027
H	4.991203	2.483463	-6.413044
H	3.252017	4.410151	-8.011807
H	3.927888	4.700997	-6.531735

N-C-Cage-Ts-1

C	11.041937	1.964724	-1.985622
C	11.744410	2.079551	-3.200841
C	11.597692	1.087810	-4.174624
C	10.755365	-0.017748	-3.956512
C	10.072432	-0.123052	-2.742287
C	10.212858	0.864613	-1.747177
C	12.629007	3.214374	-3.491073
N	12.796037	4.219967	-2.717613
C	13.711295	5.250685	-3.163997
C	13.032495	6.626042	-3.241706
N	11.949906	6.666712	-4.220153
C	10.779397	7.137641	-3.866156
C	9.635003	7.259648	-4.702905
C	8.396755	7.527579	-4.096859
C	7.220925	7.647785	-4.842460
C	7.306335	7.513239	-6.248408
C	8.502096	7.273357	-6.906919
C	9.717106	7.051507	-6.145509
C	8.565548	7.175902	-8.364945
N	7.550047	7.332729	-9.132978
C	7.745231	7.139256	-10.554538
C	6.770112	6.082630	-11.098588
N	7.071996	4.767489	-10.566755
C	6.141926	4.151293	-9.943109
C	6.314446	2.815111	-9.349162
C	5.204344	2.163995	-8.803663
C	5.327242	0.877888	-8.242187
C	6.578181	0.255784	-8.230640
C	7.709200	0.900595	-8.767815
C	7.570642	2.176717	-9.321255
C	4.169771	0.171982	-7.670744
N	2.985216	0.653403	-7.670114
C	1.930269	-0.145942	-7.077312
C	1.210391	0.627012	-5.961964
N	2.067273	0.788353	-4.802972
C	2.294886	1.976903	-4.390226
C	3.148949	2.275368	-3.229313
C	3.806169	1.253301	-2.516240
C	4.614473	1.557300	-1.417237
C	4.773619	2.902226	-1.029061
C	4.130902	3.927604	-1.726762
C	3.316279	3.603910	-2.829306
C	4.324970	5.323918	-1.303286
N	3.717755	6.305588	-1.851106
C	3.998953	7.640020	-1.359824
C	4.468165	8.558366	-2.497390
N	5.791249	8.195274	-2.964174
C	5.939729	7.977177	-4.219626
C	5.290324	0.470392	-0.691205
N	5.993373	0.667879	0.358405
C	6.620554	-0.479062	0.984370
C	8.131940	-0.257754	1.142866
N	8.794088	-0.261183	-0.147301

C	9.501308	0.755723	-0.462839
C	9.028728	0.247762	-8.762232
N	9.205640	-0.950488	-8.351496
C	10.543817	-1.504863	-8.413454
C	10.968450	-2.086484	-7.057329
N	11.221745	-1.031553	-6.095879
C	10.580299	-1.051656	-4.990557
H	4.220636	2.639775	-8.806509
H	9.867709	0.861557	-9.149378
H	8.432260	2.702084	-9.740195
H	5.132243	4.596346	-9.821694
H	6.899000	6.044441	-12.194243
H	5.730611	6.401550	-10.880738
H	7.519950	8.088439	-11.072364
H	8.783893	6.843359	-10.809207
H	9.621517	1.617769	0.225337
H	9.561813	6.923105	-8.783327
H	6.411716	7.647551	-6.863396
H	5.080790	8.050647	-4.919563
H	3.709790	8.548291	-3.307619
H	4.517721	9.583721	-2.089902
H	4.754544	7.646866	-0.547613
H	3.058478	8.058765	-0.961885
H	5.039753	5.474404	-0.467837
H	5.413177	3.124301	-0.171575
H	3.669903	0.219496	-2.842853
H	1.850399	2.861096	-4.892024
H	0.846524	1.593939	-6.364444
H	0.335669	0.027623	-5.655518
H	2.298411	-1.110954	-6.673539
H	1.185843	-0.360495	-7.863111
H	4.390186	-0.825729	-7.236791
H	6.195209	-0.589258	1.997074
H	6.444022	-1.422629	0.428970
H	5.150105	-0.545917	-1.114268
H	8.530727	-1.102474	1.730683
H	8.307359	0.677219	1.712462
H	8.338176	7.663751	-3.013621
H	10.652769	7.443041	-2.816775
H	12.646503	6.900811	-2.246253
H	13.801741	7.367810	-3.520126
H	14.182017	5.006573	-4.140907
H	14.526139	5.338350	-2.424696
H	13.167199	3.140130	-4.459697
H	9.414625	-0.971763	-2.540260
H	9.851691	-1.853213	-4.751143
H	10.200352	-2.808030	-6.712671
H	11.914226	-2.633869	-7.213145
H	11.300877	-0.768021	-8.750263
H	10.528460	-2.338828	-9.137050
H	12.121607	1.159410	-5.130398
H	11.159699	2.748381	-1.233381
H	10.646739	7.391152	-6.616898
H	6.702432	-0.742177	-7.803324
H	2.822762	4.417073	-3.366862
H	12.199022	6.197036	-5.377942
N	12.378339	5.551060	-6.544890
B	11.035661	4.800148	-6.808267
H	10.085859	5.653659	-6.343427
H	10.711437	4.703752	-7.973779
H	10.904326	3.831947	-6.092706
H	12.658599	6.166896	-7.312440
H	13.149950	4.892034	-6.411463

N-C-Cage-H2-C-N

C	3.125770	1.296400	-3.801219
C	2.485297	2.410387	-4.344231

C	2.670647	3.661620	-3.731750
C	3.480504	3.800140	-2.595023
C	4.103212	2.662963	-2.052833
C	3.929745	1.410495	-2.648859
C	1.573895	2.260354	-5.543035
N	1.657878	3.405323	-6.453723
C	0.758106	3.328106	-7.606521
C	-0.617718	3.957674	-7.349712
N	-1.415173	3.198074	-6.405249
C	-2.005587	3.834829	-5.465294
C	-2.858569	3.172927	-4.465497
C	-3.044407	1.775901	-4.471162
C	-3.861971	1.159948	-3.519852
C	-4.502860	1.951711	-2.547069
C	-4.329975	3.338280	-2.526833
C	-3.501740	3.943376	-3.492314
C	-4.040598	-0.300932	-3.555284
N	-4.816185	-0.924894	-2.753378
C	-4.915532	-2.365622	-2.883529
C	-4.606065	-3.062797	-1.550573
N	-3.198991	-2.951812	-1.219129
C	-2.886364	-2.449276	-0.085842
C	-1.493160	-2.284881	0.359751
C	-0.413048	-2.642994	-0.470591
C	0.905754	-2.479013	-0.038871
C	1.148909	-1.946697	1.242330
C	0.089137	-1.587339	2.079530
C	-1.234506	-1.760175	1.628865
C	0.379588	-1.031478	3.410767
N	-0.531741	-0.727671	4.254350
C	-0.117397	-0.185312	5.533639
C	-0.808711	1.156113	5.815756
N	-0.320629	2.192769	4.926845
C	-1.179614	2.846380	4.242084
C	-0.811447	3.922013	3.307167
C	0.536170	4.255818	3.066782
C	0.870193	5.278710	2.175202
C	-0.158144	5.978130	1.513363
C	-1.499544	5.659011	1.739646
C	-1.818974	4.624476	2.641102
C	-2.548476	6.404911	1.026189
N	-3.796899	6.194347	1.203801
C	-4.734822	6.985226	0.431396
C	-5.675386	6.081670	-0.380667
N	-4.957134	5.410314	-1.446460
C	-5.017238	4.134421	-1.497027
C	2.287002	5.602092	1.939981
N	2.662774	6.551752	1.171148
C	4.086094	6.773828	1.007157
C	4.485706	6.705747	-0.474274
N	4.396703	5.348341	-0.975040
C	3.654396	5.131341	-1.993891
C	2.010314	-2.859819	-0.934134
N	3.240884	-2.779626	-0.597226
C	4.237214	-3.168961	-1.576525
C	5.204619	-2.010817	-1.865552
N	4.527293	-0.934906	-2.562536
C	4.589042	0.237348	-2.054989
H	-2.538682	1.185955	-5.239471
H	-5.603618	3.550460	-0.757756
H	-5.139454	1.456125	-1.810184
H	-3.457761	-0.834273	-4.334356
H	-5.958861	-2.609030	-3.148701
H	-4.251764	-2.772618	-3.673027
H	-4.840553	-4.133941	-1.676367
H	-5.267756	-2.652342	-0.760870
H	3.018263	4.964565	2.478717
H	-3.660332	-2.108392	0.632530
H	-0.631240	-3.049998	-1.460933
H	1.705227	-3.227842	-1.935624

H	3.787899	-3.514086	-2.529773
H	4.828419	-3.997861	-1.150789
H	5.674764	-1.678871	-0.917599
H	5.997811	-2.401828	-2.526325
H	5.152054	0.433761	-1.118591
H	4.725942	2.779883	-1.162890
H	2.179388	4.536911	-4.164452
H	0.528660	2.185263	-5.200749
H	0.609292	2.285995	-7.959465
H	1.218765	3.889437	-8.434133
H	-0.486392	5.014118	-7.037826
H	-1.158131	3.950578	-8.314171
H	-1.905711	4.934641	-5.355964
H	5.539346	7.026637	-0.547128
H	3.863761	7.419406	-1.052424
H	3.096340	5.953787	-2.488862
H	4.313131	7.792806	1.364847
H	4.702645	6.056013	1.585387
H	2.185132	-1.820302	1.565539
H	1.455981	-0.892231	3.642898
H	0.981129	-0.053864	5.607685
H	-0.434920	-0.891901	6.320093
H	-1.907944	1.022442	5.755943
H	-0.551616	1.447892	6.848694
H	-2.266524	2.636268	4.320883
H	0.118407	6.773609	0.817424
H	-2.184904	7.173924	0.313548
H	-4.233075	7.698993	-0.253079
H	-5.357357	7.561296	1.137269
H	-6.186443	5.374595	0.303882
H	-6.439777	6.730237	-0.842507
H	-2.871900	4.384105	2.806213
H	1.313086	3.695512	3.592206
H	-2.052556	-1.472382	2.293676
H	-3.375620	5.028393	-3.463180
H	3.013070	0.309357	-4.255906
H	2.622678	3.500938	-6.775413
H	1.796347	1.294969	-6.047199

N-C-Cage-H₂

C	3.253280	1.397004	-3.874926
C	2.683658	2.539970	-4.485485
C	2.890838	3.917570	-3.878391
C	3.683558	3.908994	-2.583931
C	4.187811	2.747637	-2.081161
C	3.999273	1.465346	-2.711748
C	1.947735	2.396808	-5.643114
N	1.385242	3.424128	-6.333571
C	0.609079	3.273655	-7.550670
C	-0.815073	3.838084	-7.438048
N	-1.611946	3.081061	-6.498524
C	-2.164757	3.716141	-5.534843
C	-2.999202	3.070512	-4.512529
C	-3.198124	1.675725	-4.497693
C	-4.000222	1.081980	-3.520046
C	-4.609147	1.893692	-2.542618
C	-4.419493	3.278108	-2.541268
C	-3.608869	3.861022	-3.534103
C	-4.190185	-0.378149	-3.526649
N	-4.953276	-0.980495	-2.697398
C	-5.056955	-2.423713	-2.791730
C	-4.700680	-3.089240	-1.454537
N	-3.286474	-2.955592	-1.164356
C	-2.953108	-2.445948	-0.039765
C	-1.554818	-2.263083	0.379399
C	-0.482477	-2.604358	-0.468339
C	0.840168	-2.428682	-0.053564

C	1.094265	-1.898984	1.226742
C	0.042629	-1.556195	2.080994
C	-1.284803	-1.741951	1.647689
C	0.343890	-1.010154	3.414031
N	-0.561226	-0.725401	4.271205
C	-0.139497	-0.194386	5.552598
C	-0.823713	1.148930	5.845268
N	-0.327744	2.187657	4.963723
C	-1.178326	2.835665	4.263727
C	-0.797825	3.908274	3.330241
C	0.553091	4.242615	3.110662
C	0.902592	5.263979	2.223329
C	-0.115225	5.959713	1.541454
C	-1.460421	5.637868	1.744400
C	-1.794608	4.607018	2.644790
C	-2.498393	6.379360	1.011127
N	-3.749784	6.164623	1.163708
C	-4.676121	6.963923	0.386220
C	-5.652627	6.074986	-0.397744
N	-4.974204	5.372558	-1.469632
C	-5.065948	4.098157	-1.503238
C	2.324668	5.588909	2.021593
N	2.721606	6.546657	1.274046
C	4.151002	6.766896	1.158947
C	4.608958	6.717238	-0.306488
N	4.536297	5.373263	-0.837549
C	3.863917	5.193644	-1.919062
C	1.939624	-2.804009	-0.958700
N	3.169773	-2.743313	-0.618646
C	4.165793	-3.133049	-1.597532
C	5.146503	-1.984050	-1.880496
N	4.503192	-0.905694	-2.600517
C	4.586321	0.276729	-2.103117
H	-2.712019	1.069093	-5.265330
H	-5.647204	3.535365	-0.744144
H	-5.231706	1.413034	-1.784162
H	-3.625274	-0.930224	-4.305841
H	-6.108475	-2.673014	-3.015385
H	-4.419494	-2.847993	-3.593650
H	-4.926498	-4.165229	-1.552803
H	-5.344754	-2.671536	-0.653984
H	3.041859	4.944874	2.571306
H	-3.716143	-2.113864	0.694597
H	-0.708591	-3.011675	-1.456824
H	1.630344	-3.154836	-1.965199
H	3.715291	-3.469948	-2.553333
H	4.746427	-3.970006	-1.172147
H	5.602495	-1.651989	-0.924606
H	5.951313	-2.396397	-2.515421
H	5.135184	0.455192	-1.153641
H	4.756215	2.801310	-1.147755
H	3.400575	4.579319	-4.612469
H	1.785136	1.405769	-6.072558
H	0.554195	2.200772	-7.781779
H	1.117954	3.773048	-8.394229
H	-0.770575	4.921530	-7.190760
H	-1.275817	3.748478	-8.437650
H	-2.048066	4.815206	-5.424911
H	5.664932	7.042190	-0.325992
H	4.015230	7.446789	-0.896936
H	3.366299	6.057611	-2.413918
H	4.366667	7.780246	1.540352
H	4.743172	6.039264	1.749969
H	2.133880	-1.764078	1.535230
H	1.421364	-0.862959	3.635453
H	0.959775	-0.068328	5.624259
H	-0.458217	-0.904467	6.335369
H	-1.923606	1.021693	5.782541
H	-0.566215	1.431400	6.880542
H	-2.265716	2.621907	4.326536

H	0.172202	6.755244	0.849680
H	-2.124180	7.151539	0.307028
H	-4.164406	7.654771	-0.314491
H	-5.275401	7.567838	1.089238
H	-6.168715	5.389524	0.304556
H	-6.408955	6.737013	-0.853892
H	-2.849981	4.366460	2.794086
H	1.321621	3.684593	3.650796
H	-2.097087	-1.469804	2.326065
H	-3.469088	4.944631	-3.520025
H	3.103019	0.415196	-4.333617
H	1.905351	4.399033	-3.700329
H	1.532153	4.368441	-5.986323

N-C-Cage

C	10.426076	1.527844	-2.947934
C	11.184325	1.752432	-4.113630
C	11.037735	0.887167	-5.201086
C	10.144018	-0.199938	-5.140289
C	9.399837	-0.407900	-3.976115
C	9.534142	0.455187	-2.871289
C	12.122885	2.881757	-4.210058
N	12.333547	3.696266	-3.247500
C	13.280463	4.772827	-3.464231
C	12.641103	6.137703	-3.172038
N	11.643343	6.471775	-4.170196
C	10.467793	6.766897	-3.763469
C	9.368669	7.127567	-4.673205
C	8.128870	7.486868	-4.137821
C	7.055237	7.838810	-4.978787
C	7.240178	7.825811	-6.363713
C	8.483449	7.466595	-6.920464
C	9.538100	7.119028	-6.071716
C	8.691389	7.448600	-8.377458
N	7.791835	7.803646	-9.213392
C	8.114326	7.741991	-10.625630
C	7.087069	6.893541	-11.388870
N	7.212767	5.491619	-11.041576
C	6.172128	4.881423	-10.618635
C	6.180921	3.460984	-10.232360
C	4.991476	2.850769	-9.825543
C	4.971823	1.494017	-9.445841
C	6.158985	0.757093	-9.478753
C	7.366537	1.356912	-9.887725
C	7.368325	2.703619	-10.260389
C	3.726313	0.840301	-9.012183
N	2.595210	1.435979	-9.001570
C	1.438010	0.688686	-8.548859
C	0.724537	1.420060	-7.402788
N	1.527469	1.398780	-6.195889
C	1.800071	2.514990	-5.635817
C	2.607474	2.618100	-4.409497
C	3.175934	1.477022	-3.810384
C	3.941204	1.586884	-2.646344
C	4.143029	2.857629	-2.072608
C	3.586153	3.999973	-2.654111
C	2.816893	3.870951	-3.827343
C	3.815632	5.313555	-2.031099
N	3.299461	6.394757	-2.476935
C	3.601482	7.629908	-1.780233
C	4.185886	8.674857	-2.741494
N	5.517759	8.295827	-3.170554
C	5.744722	8.217494	-4.426157
C	4.518352	0.373229	-2.046476
N	5.190807	0.384064	-0.959375
C	5.702501	-0.880231	-0.466256
C	7.217950	-0.809984	-0.230479
N	7.937452	-0.720597	-1.486360

C	8.750500	0.253646	-1.642163
C	8.626320	0.597066	-9.929759
N	8.703062	-0.646757	-9.644979
C	10.004693	-1.281046	-9.732052
C	10.370773	-1.979418	-8.414997
N	10.634186	-1.012673	-7.366306
C	9.971742	-1.117233	-6.277883
H	4.055394	3.413229	-9.793051
H	9.521009	1.178895	-10.234295
H	8.290581	3.194486	-10.579888
H	5.194151	5.396698	-10.521057
H	7.307671	6.996927	-12.465439
H	6.069527	7.293235	-11.202257
H	8.063020	8.767744	-11.030074
H	9.131244	7.343066	-10.816493
H	8.910899	1.009675	-0.845825
H	9.692944	7.106788	-8.711680
H	6.425657	8.093777	-7.040819
H	4.956265	8.436897	-5.175536
H	3.487298	8.824367	-3.589529
H	4.266385	9.626009	-2.187180
H	4.299816	7.483711	-0.931404
H	2.654757	8.036533	-1.384610
H	4.470948	5.308295	-1.135480
H	4.744242	2.928874	-1.162998
H	3.003520	0.504448	-4.277283
H	1.434131	3.478018	-6.048466
H	0.465090	2.447744	-7.728481
H	-0.213022	0.875221	-7.195624
H	1.692448	-0.340189	-8.222762
H	0.727978	0.619764	-9.391063
H	3.829376	-0.217529	-8.692705
H	5.225786	-1.080336	0.509184
H	5.475837	-1.727788	-1.144158
H	4.326468	-0.568354	-2.601722
H	7.518695	-1.748979	0.265958
H	7.443740	0.032833	0.453688
H	7.968800	7.501646	-3.057177
H	10.211032	6.771735	-2.683916
H	12.232665	6.138154	-2.141203
H	13.441796	6.895764	-3.227203
H	13.697626	4.776206	-4.491593
H	14.113636	4.639408	-2.752592
H	12.646408	2.984390	-5.183172
H	8.697864	-1.242109	-3.902428
H	9.219816	-1.920132	-6.130790
H	9.568891	-2.695952	-8.145372
H	11.299741	-2.549280	-8.590768
H	10.810114	-0.569942	-10.005779
H	9.949503	-2.058940	-10.513487
H	11.611812	1.038601	-6.118434
H	10.550253	2.214129	-2.106691
H	10.512374	6.835344	-6.476869
H	6.172248	-0.296097	-9.188368
H	2.388719	4.773340	-4.270276

N-C-Cage-(H₂)-Ts-2

C	11.219547	0.892340	-5.430474
C	11.477906	1.716481	-4.331910
C	10.629667	1.653457	-3.209030
C	9.539770	0.779165	-3.185312
C	9.294842	-0.045461	-4.300434
C	10.127065	0.003501	-5.421873
C	12.627652	2.633982	-4.374658
N	12.964689	3.377085	-3.390441
C	14.116703	4.242093	-3.557916
C	13.760555	5.702493	-3.245830

N	12.873777	6.250669	-4.254027
C	11.768294	6.760784	-3.863636
C	10.783809	7.347137	-4.787182
C	9.627915	7.937938	-4.269825
C	8.665642	8.510044	-5.124964
C	8.875396	8.478707	-6.505895
C	10.035257	7.886933	-7.044500
C	10.980751	7.325908	-6.181848
C	10.270020	7.845905	-8.496552
N	9.471447	8.369348	-9.346762
C	9.808093	8.260187	-10.752592
C	8.662877	7.607831	-11.541298
N	8.534410	6.203417	-11.203433
C	7.406464	5.794279	-10.762733
C	7.155636	4.394560	-10.382131
C	5.878672	4.017443	-9.958931
C	5.607794	2.685279	-9.589803
C	6.631825	1.736371	-9.650679
C	7.923837	2.099033	-10.078105
C	8.176870	3.425621	-10.436711
C	4.267224	2.268342	-9.152734
N	3.257636	3.053725	-9.153763
C	1.974347	2.513336	-8.747754
C	1.256262	3.432068	-7.757184
N	1.845120	3.392450	-6.421977
C	2.023975	4.512829	-5.755684
C	2.765297	4.455157	-4.544084
C	3.334569	5.607929	-3.981806
C	4.277859	5.517890	-2.954445
C	4.665226	4.236985	-2.495691
C	4.120846	3.066495	-3.009103
C	3.168780	3.140247	-4.085235
C	4.455804	1.753323	-2.452949
N	5.192613	1.587806	-1.417373
C	5.419126	0.233839	-0.953150
C	6.904815	-0.019681	-0.664828
N	7.682509	-0.065712	-1.887956
C	8.671920	0.736312	-1.997194
C	4.855868	6.713488	-2.332908
N	4.565465	7.907720	-2.695897
C	5.183632	9.003681	-1.976231
C	5.995885	9.906255	-2.917002
N	7.221615	9.254863	-3.336587
C	7.448842	9.143246	-4.589313
C	9.010898	1.109101	-10.149873
N	8.832366	-0.135345	-9.918971
C	9.982027	-1.014635	-10.003913
C	10.170096	-1.793719	-8.693342
N	10.570901	-0.905817	-7.619417
C	9.838907	-0.867921	-6.571707
H	5.068559	4.748654	-9.906717
H	10.007401	1.513757	-10.422474
H	9.170735	3.736146	-10.768040
H	6.543288	6.481724	-10.646327
H	8.916684	7.676528	-12.613031
H	7.728282	8.178495	-11.366942
H	9.942953	9.281064	-11.149925
H	10.744201	7.692116	-10.927976
H	8.935889	1.448107	-1.188150
H	11.198198	7.327042	-8.814401
H	8.145430	8.912980	-7.193120
H	6.737141	9.529637	-5.347798
H	5.358657	10.215754	-3.770246
H	6.276045	10.809943	-2.348233
H	5.841290	8.660927	-1.151093
H	4.378262	9.620334	-1.540908
H	5.566367	6.520325	-1.502205
H	5.383972	4.147008	-1.676350
H	2.416015	2.347438	-4.146967
H	1.760083	5.485740	-6.197052

H	1.245928	4.460452	-8.163794
H	0.212325	3.085800	-7.670981
H	2.048968	1.489125	-8.326684
H	1.338396	2.456781	-9.648573
H	4.179946	1.210413	-8.829607
H	4.878515	0.108404	0.002283
H	5.043644	-0.532793	-1.661692
H	4.014125	0.884376	-2.986216
H	6.984399	-1.007733	-0.179118
H	7.272110	0.747953	0.046405
H	9.449018	7.968996	-3.192326
H	11.490071	6.792183	-2.789874
H	13.337191	5.765519	-2.222780
H	14.698886	6.283000	-3.268304
H	14.554739	4.180374	-4.574913
H	14.885500	3.927491	-2.830953
H	13.195881	2.639346	-5.327887
H	8.438046	-0.722701	-4.267028
H	8.932649	-1.500571	-6.473465
H	9.239707	-2.352010	-8.463566
H	10.981519	-2.523651	-8.855170
H	10.918835	-0.473358	-10.246941
H	9.789407	-1.751210	-10.802678
H	11.859304	0.922069	-6.315717
H	10.842922	2.305448	-2.358577
H	11.888419	6.859983	-6.573003
H	6.449893	0.696159	-9.370066
H	3.053897	6.597457	-4.351918
H	3.688732	2.544521	-5.488555
H	2.963193	2.678416	-6.135506