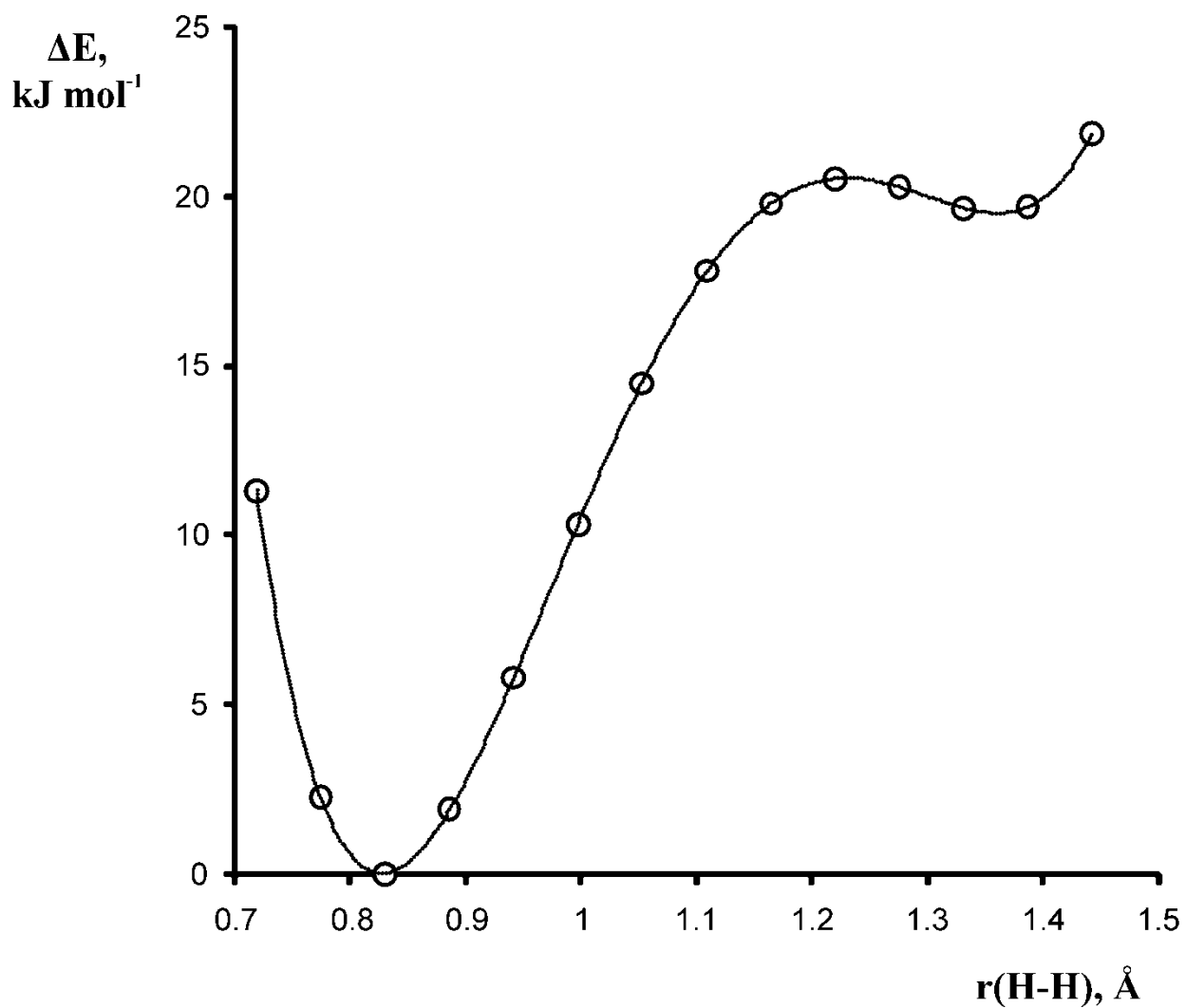


Supplementary information for the manuscript “Novel group 13 Lewis superacids and 13-15 donor-acceptor cryptands for hydrogen activation: a theoretical study” by Alexey Y. Timoshkin* and Keiji Morokuma.

Total energies E°_0 , standard enthalpies H°_{298} in Hartree, and standard entropies S°_{298} in cal $\text{mol}^{-1} \text{K}^{-1}$.

Compound	B3LYP/pVDZ			B3LYP/def2-TZVPP		
	E°_0	H°_{298}	S°_{298}	E°_0	H°_{298}	S°_{298}
H ₂	-1.1737901	-1.16053	31.227	-1.1800044	-1.166631	31.133
NH ₃	-56.5094755	-56.471622	46.015	-56.588622	-56.55057	45.967
PH ₃	-343.054335	-343.026707	50.248	-343.1774589	-343.149724	50.196
AsH ₃	-2237.43019	-2237.404478	53.27	-2237.711253	-2237.685676	53.256
[NH ₄] ⁺	-56.8557557	-56.803122	44.465	-56.9271387	-56.8739	44.406
[PH ₄] ⁺	-343.361699	-343.322808	48.65	-343.4854956	-343.446445	48.586
[AsH ₄] ⁺	-2237.72474	-2237.688749	51.68	-2238.006091	-2237.970007	51.633
N(C ₆ H ₅) ₃	-749.167189	-748.872813	124.411	-749.9762728	-749.682466	124.676
P(C ₆ H ₅) ₃	-1035.71527	-1035.424792	132.755	-1036.588097	-1036.297894	132.527
As(C ₆ H ₅) ₃	-2930.0866	-2929.797105	135.611	-2931.117891	-2930.828649	134.355
[HN(C ₆ H ₅) ₃] ⁺	-749.525111	-749.216817	124.046	-750.3365444	-750.028263	123.562
[HP(C ₆ H ₅) ₃] ⁺	-1036.0996	-1035.797986	132.024	-1036.976521	-1036.674789	131.895
[HAs(C ₆ H ₅) ₃] ⁺	-2930.44995	-2930.150471	136.52	-2931.48168	-2931.182302	137.236
N(2,6-Me ₂ C ₆ H ₃) ₃	-984.874579	-984.405537	154.69	-985.9400937	-985.470944	156.513
P(2,6-Me ₂ C ₆ H ₃) ₃	-1271.41229	-1270.947573	166.56	-1272.541875	-	-
As(2,6-Me ₂ C ₆ H ₃) ₃	-3165.78225	-3165.318675	170.542	-3167.071487	-3166.607632	172.853
[HN(2,6-Me ₂ C ₆ H ₃) ₃] ⁺	-985.229676	-984.746334	158.537	-986.2976872	-	-
[HP(2,6-Me ₂ C ₆ H ₃) ₃] ⁺	-1271.81151	-1271.33537	166.412	-1272.94524	-1272.46821	166.559
[HAs(2,6-Me ₂ C ₆ H ₃) ₃] ⁺	-3166.16575	-3165.691633	172.678	-3167.455251	-	-
B(C ₆ F ₅) ₃	-2206.60731	-2206.422813	189.105	-2209.206699	-2209.023184	188.322
Al(C ₆ F ₅) ₃	-2424.15991	-2423.979093	208.47	-2426.824697	-2426.644701	210.461
Ga(C ₆ F ₅) ₃	-4106.42556	-4106.245239	202.995	-4109.250885	-4109.071232	206.141
[HB(C ₆ F ₅) ₃] ⁻	-2207.30921	-2207.116224	198.905	-2209.919122	-2209.727294	197.895
[HAl(C ₆ F ₅) ₃] ⁻	-2424.86167	-2424.674964	204.499	-2427.533904	-2427.348135	206.033
[HGa(C ₆ F ₅) ₃] ⁻	-4107.12404	-4106.937472	207.819	-4109.957993	-4109.772443	207.889
B(C ₆ H ₂ F ₂) ₃ CF	-1450.22216	-1449.996293	144.316	-1451.878291	-1451.653659	144.56
Al(C ₆ H ₂ F ₂) ₃ CF	-1667.74681	-1667.52467	149.265	-1669.464772	-1669.243891	149.834
Ga(C ₆ H ₂ F ₂) ₃ CF	-3350.01266	-3349.790968	151.234	-3351.891657	-3351.671238	151.825
[HB(C ₆ H ₂ F ₂) ₃ CF] ⁻	-1450.95442	-1450.720024	142.3	-1452.618517	-1452.38558	142.777
[HAl(C ₆ H ₂ F ₂) ₃ CF] ⁻	-1668.47627	-1668.248016	148.504	-1670.199598	-1669.972805	149.054
[HGa(C ₆ H ₂ F ₂) ₃ CF] ⁻	-3350.74089	-3350.512872	150.705	-3352.626234	-3352.39968	151.258

Figure S1. Rigid PES scan for $\text{Al}(\text{C}_6\text{H}_2\text{F}_2)_3\text{CF}-\text{H}_2-\text{NH}_3$ system as a function of H-H distance. Energy values are given with respect to the structure shown in Figure 4,b. For all points Al-N distance is fixed at 4.3 Å.



Optimized geometries (xyz coordinates in angstroms B3LYP/def2-TZVPP level of theory).

B(C₆F₅)₃

B 0.0000816811 0.0009280218 0.3058384656
C 1.3058749086 0.7897752728 0.6656637867
C -0.0253780835 -1.5626859284 0.4122030047
C -1.2802517817 0.7756947209 -0.1603513947
C -0.0712884676 -4.3822766873 0.6040051254
C 1.0518374244 -2.3556892991 0.0062504845
C -1.1268289211 -2.258097718 0.9194046808
C -1.1625607502 -3.6378261897 1.0318568237
C 1.0425900115 -3.7383653974 0.0817103828
F 2.1466886876 -1.7863041784 -0.516452659
F -2.2014982771 -1.5880090193 1.3577928555
F -2.2269144345 -4.2555612352 1.5427190675
F 2.085237121 -4.4537417868 -0.3384672113
F -0.092843037 -5.7060526881 0.6940547341
C 3.6605498056 2.2122660473 1.3145196953
C 2.1092402163 0.4447849618 1.7563658141
C 1.7455033945 1.8856748522 -0.0825179767
C 2.902330691 2.5869961277 0.2132386436
C 3.2593309278 1.1371038818 2.0963051797
F 1.7616398026 -0.5767831964 2.5511549253
F 1.0580039878 2.2819252872 -1.162539939
F 3.293420024 3.612142847 -0.5427699023
F 3.9815393387 0.784515303 3.1590948528
F 4.7660514137 2.8801144373 1.6191525137
C -3.5890162946 2.1727947052 -1.001009424
C -2.0967775994 0.3124310171 -1.1960720977
C -1.6824844279 1.9764643165 0.4315998885
C -2.8166257581 2.6684038971 0.0410669656
C -3.2245750353 0.989255811 -1.6291472019
F -1.7842183708 -0.8180586596 -1.8444678873
F -0.9801257433 2.4927978969 1.4495434981
F -3.1726204791 3.7985962296 0.6504589858
F -3.9601714833 0.519616773 -2.636004999
F -4.6729633334 2.828722316 -1.395691851

Al(C₆F₅)₃

13 0.00208 0.00607 0.00125
6 1.94852 -0.21317 -0.00347
6 -1.1572 -1.57293 0.00371
6 -0.7873 1.79862 0.00233
6 -2.81812 -3.84018 0.00223
6 -1.03862 -2.5671 -0.95569

6	-2.14137	-1.76018	0.96245
6	-2.97195	-2.86928	0.98529
6	-1.84546	-3.69341	-0.9801
9	-0.10806	-2.43757	-1.92331
9	-2.29959	-0.83468	1.93053
9	-3.90367	-3.02013	1.92649
9	-1.70776	-4.6264	-1.922
9	-3.60337	-4.91205	0.00159
6	4.74034	-0.53938	-0.00892
6	2.59438	-1.0149	0.92574
6	2.75806	0.41887	-0.93538
6	4.13584	0.27343	-0.96092
6	3.96859	-1.19132	0.94599
9	1.86481	-1.64677	1.86742
9	2.19098	1.20245	-1.87463
9	4.88253	0.89079	-1.87635
9	4.55633	-1.96477	1.85868
9	6.06001	-0.69369	-0.01172
6	-1.92519	4.36916	0.00466
6	-1.7739	2.16431	-0.90161
6	-0.39415	2.77336	0.90749
6	-0.93994	4.04673	0.9308
6	-2.34962	3.4245	-0.92266
9	-2.19187	1.2672	-1.81709
9	0.55125	2.47823	1.82209
9	-0.5424	4.95657	1.82009
9	-3.29109	3.74327	-1.81079
9	-2.46306	5.58404	0.00589

Ga(C₆F₅)₃

31	0.00299	0.00072	-0.00199
6	1.96133	-0.26151	0.00076
6	-1.20371	-1.56425	-0.0005
6	-0.75266	1.82655	-0.00377
6	-2.92108	-3.78703	0.00154
6	-0.89912	-2.72234	-0.70143
6	-2.40077	-1.56097	0.70128
6	-3.26236	-2.6465	0.71812
6	-1.73204	-3.83007	-0.71617
9	0.23879	-2.78971	-1.41552
9	-2.75322	-0.47545	1.41317
9	-4.40202	-2.61381	1.40906
9	-1.41343	-4.92535	-1.40618
9	-3.73334	-4.8386	0.00258
6	4.7455	-0.63578	0.00406
6	2.55607	-1.31052	0.68758

6	2.81358	0.5931	-0.68419
6	4.18947	0.42669	-0.69789
6	3.92706	-1.51335	0.70457
9	1.7915	-2.16972	1.38476
9	2.30471	1.62372	-1.38246
9	4.98003	1.26175	-1.37232
9	4.46744	-2.52717	1.38084
9	6.06232	-0.81277	0.0056
6	-1.8292	4.42132	-0.0022
6	-1.9208	2.13267	-0.68769
6	-0.14417	2.86896	0.681
6	-0.65817	4.15602	0.69713
6	-2.46882	3.40565	-0.70219
9	-2.55701	1.17392	-1.38407
9	0.98365	2.64102	1.37732
9	-0.05267	5.13373	1.37139
9	-3.58898	3.66823	-1.37565
9	-2.33814	5.64867	-0.00166

[HB(C₆F₅)₃]⁻

B	-0.0034076261	-0.0039333652	0.7690969509
C	-1.4498090083	-0.65188522	0.3327394824
C	1.2830184896	-0.9286054936	0.3311191764
C	0.158846105	1.572885055	0.3325586962
C	3.5447550593	-2.5616641124	-0.2377569559
C	1.6201827853	-2.0463922008	1.0908049627
C	2.1380923857	-0.6880758999	-0.7387474108
C	3.2502804314	-1.4666183983	-1.0313507067
C	2.7184295709	-2.8551860826	0.8340321283
F	0.8599284303	-2.4066139102	2.1442363494
F	1.9103887141	0.340805319	-1.5819809313
F	4.0400132895	-1.1787772006	-2.0816529436
F	2.9928216992	-3.9199196004	1.6096931319
F	4.6136331556	-3.3303966501	-0.5051312155
C	-4.0042320888	-1.7786646635	-0.2246859717
C	-1.6714001423	-1.5380574176	-0.7156952045
C	-2.5885739574	-0.3530413466	1.0776834451
C	-3.8427933222	-0.8902274048	0.8253554676
C	-2.906976424	-2.1039252331	-1.0027990511
F	-0.6647094656	-1.8901330102	-1.5426226979
F	-2.5160023189	0.511083795	2.1098672033
F	-4.9039835982	-0.5633943379	1.5853886647
F	-3.0549041711	-2.9574671406	-2.0320328382
F	-5.2090205057	-2.3123781126	-0.4868472763
C	0.4654391297	4.3461037396	-0.2346355149
C	0.9833800834	2.4120584741	1.0785375989

C -0.4917859428 2.2042983699 -0.7217766464
C -0.3620423813 3.5559800261 -1.0134144926
C 1.1476948102 3.7658738374 0.821552957
F 1.6882330505 1.9221857446 2.1181304331
F -1.2941607369 1.5052994582 -1.5518714056
F -1.0206642796 4.1069981989 -2.0489301484
F 1.9577886682 4.5236545726 1.5831767229
F 0.6079446838 5.6551037198 -0.5016269002
H -0.0037549073 -0.0039269571 1.9732181501

[HAl(C₆F₅)₃]

Al -0.0163448307 -0.045416661 -0.7770628637
C 1.6737450807 0.9419759846 -0.1756332801
C -0.014372284 -1.9471793659 -0.0178788202
C -1.6756808768 0.9598888563 -0.1220587477
C 0.0660646135 -4.648363562 0.8383390522
C 0.8704144919 -2.8752740372 -0.5449823748
C -0.8518913066 -2.4425953991 0.9675405879
C -0.8348781352 -3.7612043505 1.4043270169
C 0.9321429514 -4.2028653622 -0.1480674343
F 1.7515035075 -2.4959170958 -1.4988868851
F -1.7504356419 -1.6344796542 1.5754155971
F -1.6716382465 -4.1924046809 2.3650067114
F 1.8118559144 -5.0613724886 -0.6937452821
F 0.1024910723 -5.9273181661 1.2436283986
C 4.0214269384 2.3997930988 0.4561375305
C 2.5825833181 0.5154695918 0.7783226539
C 2.0001357176 2.141348971 -0.7896520962
C 3.1413835853 2.8757895903 -0.5032941382
C 3.7409358617 1.208849273 1.1058060911
F 2.3718349255 -0.6318761205 1.4632518019
F 1.1717929085 2.66495376 -1.7223093605
F 3.4090137684 4.0351929828 -1.1300728515
F 4.5923500833 0.7497650461 2.0403338758
F 5.1338271506 3.0885965461 0.7551806702
C -4.068048434 2.3025962376 0.5918667107
C -2.9138109238 0.6137184284 -0.6409474992
C -1.7008581887 2.0100237819 0.7804429476
C -2.8578747871 2.6862389445 1.1462940702
C -4.1003602013 1.2525142625 -0.3124793986
F -3.0113875677 -0.4138116892 -1.5154896727
F -0.5609614427 2.4342918038 1.3725384301
F -2.8274478916 3.7017881323 2.02762303
F -5.2754100793 0.8746305054 -0.8464787875
F -5.1999544086 2.9397641978 0.9296789004
H -0.0421465924 -0.1171108945 -2.3661918212

[HGa(C₆F₅)₃]

Ga -0.0830850879 0.1202030404 -0.8994032973
C 1.6248342411 1.0259678167 -0.1803254843
C 0.0348235852 -1.8486114469 -0.2739471588
C -1.7605594647 1.0162981525 -0.091915543
C 0.2757141947 -4.5775368347 0.4377690941
C 0.8657583882 -2.7246778701 -0.9520443054
C -0.6641806498 -2.403656023 0.7844703159
C -0.5654241765 -3.7394677189 1.1520047416
C 1.0023290339 -4.0671959631 -0.62606069
F 1.6092311735 -2.2855730837 -1.9929624239
F -1.4949252269 -1.6463851723 1.5318374829
F -1.2661881468 -4.234754882 2.1875161957
F 1.8237020326 -4.8783508852 -1.3171144916
F 0.3887016868 -5.8719341092 0.7756267276
C 3.9929737848 2.2119115079 0.8106819619
C 2.029946134 0.8882526839 1.1362105227
C 2.4596303202 1.7898599606 -0.9778639095
C 3.6279094731 2.3823558862 -0.5148385085
C 3.1868632208 1.4574988391 1.6489514562
F 1.2783346434 0.1758646722 2.004617213
F 2.160697708 2.0055835882 -2.2769515449
F 4.409341431 3.1185232819 -1.3257940983
F 3.539299524 1.2967381509 2.9366931902
F 5.1173597006 2.7749694738 1.2805720018
C -4.1637923993 2.1769132937 0.8507044472
C -3.0041487873 0.4584369778 -0.33674273
C -1.7791767927 2.1892501282 0.6417738525
C -2.9446918393 2.7779730852 1.1172541516
C -4.1975015159 1.0031101582 0.1137102199
F -3.0995078171 -0.6855317499 -1.051652601
F -0.6297459067 2.8377588583 0.9349040095
F -2.9122682301 3.9193191527 1.828434364
F -5.3806429486 0.4199288244 -0.1484763586
F -5.3031215021 2.7278508346 1.2986870021
H -0.1784898373 0.1891075835 -2.4698287804

B(C₆H₂F₂)₃CF

C 0.8831514589 0. 1.503647736
B 1.2942900052 0. -0.0025858374
C 0.8831279915 1.3047302299 -0.7549467565
C 0.8831279915 -1.3047302299 -0.7549467565
C -0.5912822712 0. 3.8361768146
C 1.5280627568 0. 2.7279024209
C -0.5301154922 0. 1.4345120194

C -1.2600413753 0. 2.6107308153
C 0.7848132301 0. 3.9076194868
H 2.6079769075 0. 2.7825844066
C -1.1066126099 0. -0.002450605
F -2.5956217111 0. 2.6300947916
H 1.2588394448 0. 4.8790515006
F -1.3261404101 0. 4.9588791336
C -0.5910080453 -3.3276115174 -1.9162624451
C -0.5301938137 -1.2448996209 -0.7203855523
C 1.5281702274 -2.3662499104 -1.364738494
C 0.7851241675 -3.3894312573 -1.952001432
C -1.2599978831 -2.2650384096 -1.3060233048
H 2.6080925452 -2.4137578207 -1.3915393423
H 1.2593263989 -4.2319479318 -2.4354167777
F -2.595631189 -2.2821170755 -1.3152974841
F -1.3256880993 -4.301426754 -2.4751867961
C -0.5910080453 3.3276115174 -1.9162624451
C -0.5301938137 1.2448996209 -0.7203855523
C 1.5281702274 2.3662499104 -1.364738494
C 0.7851241675 3.3894312573 -1.952001432
C -1.2599978831 2.2650384096 -1.3060233048
H 2.6080925452 2.4137578207 -1.3915393423
H 1.2593263989 4.2319479318 -2.4354167777
F -2.595631189 2.2821170755 -1.3152974841
F -1.3256880993 4.301426754 -2.4751867961
F -2.4699645258 0. -0.0026616109

Al(C₆H₂F₂)₃CF

C -1.7836931471 0. -1.0784622937
Al -0.0038083814 0. -1.8206977785
C 0.8870922915 -1.5408442662 -1.0767938402
C 0.8870922915 1.5408442662 -1.0767938402
C -3.8792509913 0. 0.7187898471
C -3.0981899869 0. -1.5243098632
C -1.4944753188 0. 0.3116395882
C -2.5699169501 0. 1.2010964208
C -4.1617086735 0. -0.6285211936
H -3.3146607232 0. -2.5847045373
C -0.0035591289 0. 0.8020659696
F -2.4411301322 0. 2.5316653679
H -5.1928035078 0. -0.9537305384
F -4.8782963195 0. 1.6145226334
C 1.9431025413 3.3517506792 0.7198985692
C 0.7435025234 1.2906158375 0.3132852515
C 1.5469631888 2.677611741 -1.5229607135
C 2.0828758247 3.5966813328 -0.6274861239

C	1.2854307264	2.2196882471	1.2024465464
H	1.6542804287	2.8653536325	-2.5834018778
H	2.6006959333	4.4881863384	-0.9529947367
F	1.2227544704	2.1072336669	2.5330475807
F	2.4467226695	4.2146465817	1.6155957634
C	1.9431025413	-3.3517506792	0.7198985692
C	0.7435025234	-1.2906158375	0.3132852515
C	1.5469631888	-2.677611741	-1.5229607135
C	2.0828758247	-3.5966813328	-0.6274861239
C	1.2854307264	-2.2196882471	1.2024465464
H	1.6542804287	-2.8653536325	-2.5834018778
H	2.6006959333	-4.4881863384	-0.9529947367
F	1.2227544704	-2.1072336669	2.5330475807
F	2.4467226695	-4.2146465817	1.6155957634
F	-0.0054372931	0.	2.1693734929

Ga(C₆H₂F₂)₃CF

C	-1.7954598418	0.	1.0715934418
Ga	-0.003448283	0.	1.8643594816
C	0.8934664635	1.551260172	1.0698398368
C	0.8934664635	-1.551260172	1.0698398368
C	-3.8814688752	0.	-0.7206478971
C	-3.1039172675	0.	1.5255407431
C	-1.4952918598	0.	-0.3120649991
C	-2.5719821218	0.	-1.2017914377
C	-4.1653425207	0.	0.6265331292
H	-3.3169782141	0.	2.5860256231
C	-0.0035642707	0.	-0.7977481675
F	-2.4408266789	0.	-2.5316595064
H	-5.1967578119	0.	0.9506780767
F	-4.880028902	0.	-1.6173506414
C	1.9438896051	-3.3540026978	-0.7221607992
C	0.7439534195	-1.2914807797	-0.3137748848
C	1.5503032898	-2.682874202	1.5238878897
C	2.0847864208	-3.6001931606	0.6250453491
C	1.2861250468	-2.2217321365	-1.203352894
H	1.656210182	-2.8676732027	2.5843876308
H	2.6027672172	-4.4920331598	0.949330073
F	1.2218684597	-2.1072955278	-2.5332391029
F	2.4468769096	-4.216539181	-1.6189865483
C	1.9438896051	3.3540026978	-0.7221607992
C	0.7439534195	1.2914807797	-0.3137748848
C	1.5503032898	2.682874202	1.5238878897
C	2.0847864208	3.6001931606	0.6250453491
C	1.2861250468	2.2217321365	-1.203352894

H 1.656210182 2.8676732027 2.5843876308
H 2.6027672172 4.4920331598 0.949330073
F 1.2218684597 2.1072955278 -2.5332391029
F 2.4468769096 4.2165391809 -1.6189865483
F -0.0054274021 0. -2.1654210949

[HB(C₆H₂F₂)₃CF]⁻

C -0.7370803504 -1.2766606129 0.8018356994
C -0.7370803561 1.2766606096 0.8018356994
C 1.4741606895 0.0000000033 0.8018356994
C -1.9132073453 -3.3137723348 -0.6846809615
C -1.3578107681 -2.3517972397 1.428332454
C -0.7133062825 -1.2354827192 -0.6053353239
C -1.2995848101 -2.2509469217 -1.3431802972
C -1.9502359634 -3.3779077829 0.6913717797
H -1.3821682962 -2.3939857162 2.5104408022
C -0.0000000056 0. -1.1737090002
F -1.3125214921 -2.2733539123 -2.69219779
H -2.4370180848 -4.2210391539 1.1645865886
F -2.4812030428 -4.2975697464 -1.4291359662
C 3.8264146885 0.0000000085 -0.6846809615
C 1.4266125536 0.0000000032 -0.6053353239
C 2.7156215297 0.0000000061 1.428332454
C 3.9004719248 0.0000000087 0.6913717797
C 2.5991696133 0.0000000058 -1.3431802972
H 2.7643365862 0.0000000062 2.5104408022
H 4.8740361715 0.0000000109 1.1645865886
F 2.6250429774 0.0000000059 -2.69219779
F 4.9624060878 0.0000000111 -1.4291359662
C -1.9132073601 3.3137723263 -0.6846809615
C -0.713306288 1.2354827161 -0.6053353239
C -1.3578107786 2.3517972336 1.428332454
C -1.9502359784 3.3779077742 0.6913717797
C -1.2995848201 2.2509469159 -1.3431802972
H -1.3821683069 2.39398571 2.5104408022
H -2.4370181037 4.221039143 1.1645865886
F -1.3125215023 2.2733539064 -2.69219779
F -2.481203062 4.2975697353 -1.4291359662
F -0.0000000056 0. -2.5537410965
B -0.0000000056 0. 1.4939336839
H -0.0000000056 0. 2.707406661

[HAl(C₆H₂F₂)₃CF]⁻

C -0.8570734127 -1.4844946685 0.9420546944
C -0.8570733886 1.4844946824 0.9420546944
C 1.7141468007 -0.0000000139 0.9420546944

C -1.930704693 -3.3440785599 -0.8234990115
C -1.5153018442 -2.6245797336 1.3988753293
C -0.7364953013 -1.2756472573 -0.4495405071
C -1.2806412669 -2.2181356988 -1.3229879209
C -2.0590779607 -3.5664275777 0.528244551
H -1.6129103409 -2.7936426059 2.4656597644
C -0.0000000002 0. -0.943206836
F -1.2297816822 -2.1300443156 -2.667720284
H -2.5719789002 -4.4547980476 0.874154933
F -2.4446593731 -4.2342741619 -1.7088700736
C 3.8614093313 -0.0000000313 -0.8234990115
C 1.4729905814 -0.0000000119 -0.4495405071
C 3.0306036454 -0.0000000245 1.3988753293
C 4.1181558631 -0.0000000333 0.528244551
C 2.5612824973 -0.0000000207 -1.3229879209
H 3.225820636 -0.0000000261 2.4656597644
H 5.1439577278 -0.0000000416 0.874154933
F 2.4595633293 -0.0000000199 -2.667720284
F 4.8893186771 -0.0000000396 -1.7088700736
C -1.9307046389 3.3440785911 -0.8234990115
C -0.7364952807 1.2756472692 -0.4495405071
C -1.5153018017 2.6245797581 1.3988753293
C -2.059077903 3.566427611 0.528244551
C -1.280641231 2.2181357195 -1.3229879209
H -1.6129102957 2.793642632 2.4656597644
H -2.5719788281 4.4547980892 0.874154933
F -1.2297816477 2.1300443355 -2.667720284
F -2.4446593046 4.2342742015 -1.7088700736
F -0.0000000002 0. -2.326059867
Al -0.0000000002 0. 1.977918657
H -0.0000000002 0. 3.5822284532

[HGa(C₆H₂F₂)₃CF]⁺

Ga -0.0830850879 0.1202030404 -0.8994032973
C 1.6248342411 1.0259678167 -0.1803254843
C 0.0348235852 -1.8486114469 -0.2739471588
C -1.7605594647 1.0162981525 -0.091915543
C 0.2757141947 -4.5775368347 0.4377690941
C 0.8657583882 -2.7246778701 -0.9520443054
C -0.6641806498 -2.403656023 0.7844703159
C -0.5654241765 -3.7394677189 1.1520047416
C 1.0023290339 -4.0671959631 -0.62606069
F 1.6092311735 -2.2855730837 -1.9929624239
F -1.4949252269 -1.6463851723 1.5318374829
F -1.2661881468 -4.234754882 2.1875161957
F 1.8237020326 -4.8783508852 -1.3171144916

F 0.3887016868 -5.8719341092 0.7756267276
C 3.9929737848 2.2119115079 0.8106819619
C 2.029946134 0.8882526839 1.1362105227
C 2.4596303202 1.7898599606 -0.9778639095
C 3.6279094731 2.3823558862 -0.5148385085
C 3.1868632208 1.4574988391 1.6489514562
F 1.2783346434 0.1758646722 2.004617213
F 2.160697708 2.0055835882 -2.2769515449
F 4.409341431 3.1185232819 -1.3257940983
F 3.539299524 1.2967381509 2.9366931902
F 5.1173597006 2.7749694738 1.2805720018
C -4.1637923993 2.1769132937 0.8507044472
C -3.0041487873 0.4584369778 -0.33674273
C -1.7791767927 2.1892501282 0.6417738525
C -2.9446918393 2.7779730852 1.1172541516
C -4.1975015159 1.0031101582 0.1137102199
F -3.0995078171 -0.6855317499 -1.051652601
F -0.6297459067 2.8377588583 0.9349040095
F -2.9122682301 3.9193191527 1.828434364
F -5.3806429486 0.4199288244 -0.1484763586
F -5.3031215021 2.7278508346 1.2986870021
H -0.1784898373 0.1891075835 -2.4698287804

NH₃

N 0. 0. 0.9667538016
H 0.9404843854 0. 1.3431277774
H -0.4702421927 0.8144833696 1.3431277774
H -0.4702421927 -0.8144833696 1.3431277774

[NH₄]⁺

H -0.0000003661 -0.0000000177 -0.0239715736
N 0.0000000622 -0.0000000005 0.9999876585
H 0.9653982271 -0.0000139124 1.3413069988
H -0.4827108591 -0.836052248 1.3413076185
H -0.4826867531 0.8360661759 1.3413075905

N(C₆H₅)₃

6 -0.68235 1.24222 -0.00091
7 -0.00011 -0.00049 -0.00186
6 1.41725 -0.03 -0.001
6 -0.7347 -1.2128 -0.00078
6 -2.03266 3.70031 0.00182
6 -0.24047 2.29668 0.80487
6 -1.80976 1.43644 -0.8057
6 -2.47973 2.65206 -0.79551

6	-0.90709	3.51426	0.79742
1	0.62657	2.15714	1.43521
1	-2.15773	0.63112	-1.43731
1	-3.34956	2.7832	-1.42599
1	-0.55046	4.31759	1.42891
1	-2.55348	4.64814	0.00298
6	-2.18901	-3.61139	0.00094
6	-1.87528	-1.35396	0.79664
6	-0.33285	-2.29028	-0.7973
6	-1.05098	-3.47817	-0.78747
6	-2.59646	-2.54	0.78865
1	-2.19336	-0.53079	1.42094
1	0.54374	-2.19209	-1.42218
1	-0.72456	-4.2997	-1.41186
1	-3.4754	-2.62984	1.4137
1	-2.74978	-4.53613	0.00143
6	4.22125	-0.08842	0.00031
6	2.14835	0.84913	-0.80663
6	2.11039	-0.93849	0.80565
6	3.49808	-0.96926	0.79755
6	3.53618	0.82201	-0.79736
1	1.62421	1.55266	-1.43825
1	1.55689	-1.61943	1.43695
1	4.01619	-1.67883	1.42954
1	4.08389	1.50949	-1.42878
1	5.3025	-0.11103	0.00079

[HN(C₆H₅)₃]⁺

C	1.3372710922	0.573486924	0.2785192115
C	-0.1719812936	-1.444854196	0.2785192115
C	-1.1652897841	0.8713672708	0.2785192115
C	3.8360678542	1.5592389113	-0.3285425154
C	2.4011953855	0.2756499909	1.1171144574
C	1.4888057634	1.353259959	-0.8544834414
C	2.7561307975	1.8440225313	-1.1549233176
C	3.6586342123	0.7777984455	0.8083597686
H	2.2626152606	-0.3437856824	1.9949290314
H	0.6477616892	1.5912652586	-1.488427676
H	2.8912964065	2.4564428677	-2.0353097029
H	4.4949058809	0.5587755034	1.4571011317
H	4.8153782542	1.9503385197	-0.5663303163
C	-3.268374428	2.5425127519	-0.3285425154
C	-1.4393175806	1.941671203	1.1171144574
C	-1.9163603773	0.6127136281	-0.8544834414
C	-2.9750357491	1.4648680163	-1.1549233176
C	-2.502910312	2.7795709434	0.8083597686

H -0.833580489 2.131375131 1.9949290314
H -1.7019569758 -0.2346545557 -1.488427676
H -3.5729901227 1.2757146992 -2.0353097029
H -2.7313667146 3.6133149239 1.4571011317
H -4.0967318243 3.1950706323 -0.5663303163
C -0.5676934117 -4.1017516645 -0.3285425154
C 0.4275546284 -1.9659735884 -0.8544834414
C -0.9618777904 -2.2173211952 1.1171144574
C -1.1557238857 -3.5573693902 0.8083597686
C 0.2189049661 -3.3088905489 -1.1549233176
H 1.0541953011 -1.3566107041 -1.488427676
H -1.4290347571 -1.7875894499 1.9949290314
H -1.7635391518 -4.1720904287 1.4571011317
H 0.6816937308 -3.7321575682 -2.0353097029
H -0.7186464154 -5.1454091533 -0.5663303163
N 0.0000000048 -0.0000000004 0.6477995954
H 0.0000000048 -0.0000000004 1.668180166

N(2,6-Me₂C₆H₃)₃

C 0.4173324426 -1.3701134395 0.0026934694
C -1.3952192722 0.3236362077 0.0026934694
C 0.9778868073 1.0464772148 0.0026934694
C 1.2303899838 -4.0608345152 -0.004955363
C -0.1453941944 -2.2874748806 0.9204932807
C 1.3933175084 -1.817447676 -0.9184752393
C 1.7881329122 -3.1544238804 -0.8910171192
C 0.2660724869 -3.6191634541 0.8852330577
C -1.1538774291 -1.8985160297 1.9711567184
C 2.0163801057 -0.9307907934 -1.9661042778
H 2.5341298126 -3.4875669527 -1.6016743372
H -0.1698693899 -4.3139980946 1.5920234752
H 1.5424460029 -5.0966916828 -0.0084789849
C 2.9015908428 3.0959662381 -0.004955363
C 2.0537084382 1.0178223723 0.9204932807
C 0.8772970872 2.1153721937 -0.9184752393
C 1.8377447426 3.1257804654 -0.8910171192
C 3.0012512322 2.0400072578 0.8852330577
C 2.2211018098 -0.0500291537 1.9711567184
C -0.2021015962 2.2116317898 -1.9661042778
H 1.7532566561 3.9384042685 -1.6016743372
H 3.8209666208 2.0098878383 1.5920234752
H 3.6426414551 3.8841432617 -0.0084789849
C -4.1319808489 0.9648682601 -0.004955363
C -2.2706146179 -0.2979245347 -0.9184752393
C -1.9083142661 1.2696524912 0.9204932807
C -3.2673237413 1.5791561792 0.8852330577

C -3.625877677 0.028643398 -0.8910171192
C -1.8142785318 -1.2808410134 -1.9661042778
C -1.0672244029 1.9485451664 1.9711567184
H -3.6510972531 2.3041102394 1.5920234752
H -4.287386491 -0.4508373328 -1.6016743372
H -5.1850874802 1.212548404 -0.0084789849
N -0.0000000074 -0.0000000057 0.0049870688
H 2.930325683 0.2845215315 2.7272290701
H 2.5940524023 -0.9878616454 1.5568774747
H 1.2822186128 -0.281700637 2.471247483
H -0.8850692205 -0.9695835883 2.471247483
H -1.2187599735 -2.6799972635 2.7272290701
H -2.1525394878 -1.7525844714 1.5568774747
H -0.4415129368 2.7404460998 1.5568774747
H -0.3971494145 1.2512842083 2.471247483
H -1.7115657317 2.395475715 2.7272290701
H 0.0834776218 2.9412024455 -2.7228334255
H -1.1611426125 2.5222189239 -1.5490463592
H -0.3728016921 1.2595888355 -2.4660301852
H -0.9044350998 -0.9526501557 -2.4660301852
H -2.5888948624 -1.3983074837 -2.7228334255
H -1.6037343717 -2.2666884639 -1.5490463592
H 2.5054172184 -1.5428949788 -2.7228334255
H 2.764876962 -0.255530477 -1.5490463592
H 1.2772367697 -0.3069386967 -2.4660301852

[HN(2,6-Me₂C₆H₃)₃]⁺

6 0.86563 -1.22056 0.07033
6 0.62337 1.35958 0.07104
6 -1.49025 -0.13931 0.06973
6 2.39118 -3.51497 -0.19446
6 1.82675 -1.26718 -0.94966
6 0.66842 -2.28325 0.97053
6 1.44297 -3.42948 0.81023
6 2.57463 -2.44482 -1.0508
6 2.13772 -0.18826 -1.95858
6 -0.32371 -2.24837 2.10741
1 1.29927 -4.25604 1.49248
1 3.31752 -2.51046 -1.83378
1 2.98823 -4.40935 -0.30671
6 -4.24003 -0.30837 -0.1961
6 -2.01203 -0.94609 -0.95146
6 -2.311 0.56257 0.97102
6 -3.69097 0.4673 0.81034
6 -3.40593 -1.00233 -1.05339
6 -1.23292 -1.75515 -1.95987

6	-1.78371	1.40077	2.11007
1	-4.33446	1.00479	1.49322
1	-3.83484	-1.61069	-1.83776
1	-5.31319	-0.37622	-0.30882
6	1.85115	3.82569	-0.19543
6	1.63932	1.72101	0.97401
6	0.1876	2.21307	-0.95263
6	0.83554	3.4484	-1.05476
6	2.24633	2.96407	0.81326
6	2.10006	0.84647	2.11462
6	-0.89938	1.94107	-1.96419
1	0.52524	4.1227	-1.84106
1	3.03144	3.25387	1.49808
1	2.32887	4.78901	-0.30855
1	-1.90847	-2.08874	-2.74432
1	-0.78451	-2.64256	-1.51455
1	-0.43448	-1.19453	-2.43824
1	1.2534	0.21857	-2.44136
1	2.76887	-0.60587	-2.73976
1	2.67715	0.64676	-1.51297
1	-1.89362	1.99445	-1.52213
1	-0.80964	0.96972	-2.44277
1	-0.8495	2.69326	-2.74824
1	-2.61179	1.76068	2.71523
1	-1.22128	2.2692	1.76793
1	-1.13725	0.8346	2.78787
1	1.28647	0.57442	2.79429
1	2.82851	1.38271	2.71738
1	2.56749	-0.07741	1.77468
1	-0.21712	-3.14305	2.71549
1	-1.35662	-2.2037	1.76279
1	-0.1641	-1.40237	2.78308
7	-0.00063	-0.00058	0.34361
1	-0.00164	-0.00094	1.36561

PH₃

P 0. 0. 0.7746577796
H 1.1919108412 0. 1.5429335046
H -0.5959554206 1.0322250675 1.5429335046
H -0.5959554206 -1.0322250675 1.5429335046

[PH₄]⁺

H -0.0000005011 0.000000215 -0.3972940239
P 0.0000000611 0. 0.9999876541
H 1.317370048 -0.0000189925 1.4657476833

H -0.658701093 -1.140866227 1.4657484608
H -0.6586682094 1.140885198 1.465748496

PPh₃

C 0.056123985 1.6633835603 0.5626971875
P 0.0000000066 0.0000000007 1.3575583748
C 1.4124704362 -0.8802965703 0.5626971875
C -1.4685944016 -0.783086988 0.5626971875
C 0.2329527583 4.2614307172 -0.4807813092
C 0.8762405254 2.6248663594 1.1648065468
C -0.6842010159 2.032059823 -0.563104462
C -0.5983377646 3.3216372729 -1.0781893107
C 0.9730558887 3.908419667 0.6430828004
H 1.4404666136 2.3646063013 2.0521464335
H -1.334091602 1.3123728893 -1.0412844183
H -1.181789869 3.5897348101 -1.9496338717
H 1.6168071262 4.6358016774 1.120402895
H 0.298686753 5.2639727538 -0.8826643506
C -3.8069836263 -1.9289723567 -0.4807813092
C -2.7113212011 -0.5535866295 1.1648065468
C -1.4177149104 -1.6085653772 -0.563104462
C -2.5774533678 -2.1789943453 -1.0781893107
C -3.8713186541 -1.1115187192 0.6430828004
H -2.7680424232 0.0651775254 2.0521464335
H -0.4695024499 -1.8115436676 -1.0412844183
H -2.5179065935 -2.8183274582 -1.9496338717
H -4.8231255722 -0.917704799 1.120402895
H -4.7080774957 -2.3733160657 -0.8826643506
C 3.5740308877 -2.3324583585 -0.4807813092
C 2.1019159459 -0.4234944438 -0.563104462
C 1.8350806953 -2.0712797278 1.1648065468
C 2.8982627851 -2.7969009457 0.6430828004
C 3.1757911521 -1.1426429255 -1.0781893107
H 1.8035940716 0.4991707804 -1.0412844183
H 1.3275758293 -2.4297838246 2.0521464335
H 3.2063184657 -3.7180968763 1.120402895
H 3.6996964822 -0.7714073498 -1.9496338717
H 4.4093907624 -2.8906566861 -0.8826643506

[HP(C₆H₅)₃]⁺

C 0.9071741838 -1.4620438668 0.3394635432
C -1.7197542307 -0.0546139558 0.3394635432
C 0.8125800335 1.5166578296 0.3394635432
C 2.2646600659 -3.7632782665 -0.4092707753
C 0.689020089 -2.6575840825 1.0350951121
C 1.807225519 -1.4204629374 -0.7288502948

C	2.4816968981	-2.5766933519	-1.1004069976
C	1.3708341122	-3.8040761555	0.6576941053
H	-0.0029689374	-2.6959927113	1.8669571582
H	1.9888546587	-0.4961649688	-1.2597785135
H	3.1803441986	-2.547439036	-1.9248660354
H	1.2097846166	-4.7267857205	1.1974362175
H	2.7972203209	-4.6590302902	-0.6982205843
C	2.1267645427	3.8428922886	-0.4092707753
C	1.957025279	1.9255009493	1.0350951121
C	0.3265442247	2.2753346858	-0.7288502948
C	0.9906334468	3.4375592415	-1.1004069976
C	2.6090095278	3.0892152506	0.6576941053
H	2.3362826405	1.3454251877	1.8669571582
H	-0.5647358665	1.9704811506	-1.2597785135
H	0.6159748158	4.0279783941	-1.9248660354
H	3.4886241992	3.4110970787	1.1974362175
H	2.6362284233	4.7519790103	-0.6982205843
C	-4.391424622	-0.0796140152	-0.4092707753
C	-2.1337697571	-0.8548717415	-0.7288502948
C	-2.6460453813	0.7320831401	1.0350951121
C	-3.9798436533	0.7148609119	0.6576941053
C	-3.4723303582	-0.8608658827	-1.1004069976
H	-1.4241188055	-1.4743161748	-1.2597785135
H	-2.3333137164	1.3505675305	1.8669571582
H	-4.6984088292	1.3156886488	1.1974362175
H	-3.7963190278	-1.4805393511	-1.9248660354
H	-5.4334487575	-0.0929487131	-0.6982205843
P	-0.0000000044	0.0000000023	0.8365735758
H	-0.0000000044	0.0000000023	2.2376547329

P(2,6-Me₂C₆H₃)₃

6	-0.90344	-1.5019	0.11549
6	-0.85017	1.53571	0.11432
6	1.75649	-0.03318	0.11463
6	-2.33282	-3.88562	-0.32658
6	-2.04575	-1.81751	0.8973
6	-0.49836	-2.39985	-0.89942
6	-1.22043	-3.57986	-1.09119
6	-2.74381	-2.99855	0.65455
6	-2.55938	-0.91186	1.98947
6	0.66035	-2.15729	-1.83352
1	-0.90497	-4.26087	-1.87154
1	-3.61722	-3.22343	1.25329
1	-2.87848	-4.80419	-0.49829
6	4.53692	-0.07724	-0.32043
6	2.59748	-0.87782	0.88616

6	2.33581	0.77952	-0.88748
6	3.71928	0.74523	-1.07571
6	3.96983	-0.89054	0.64685
6	2.06548	-1.78994	1.96394
6	1.55032	1.67507	-1.81244
1	4.15396	1.37005	-1.84578
1	4.59853	-1.5444	1.2377
1	5.60578	-0.08953	-0.48887
6	-2.21228	3.96073	-0.3182
6	-1.84437	1.62786	-0.88782
6	-0.54392	2.68694	0.88652
6	-1.22392	3.87945	0.64872
6	-2.5112	2.84074	-1.07434
6	-2.22196	0.50021	-1.81514
6	0.5137	2.68604	1.96271
1	-0.97489	4.75107	1.24056
1	-3.26994	2.90298	-1.84416
1	-2.74018	4.89039	-0.48561
15	0.00198	0.00135	0.69378
1	2.88706	-2.28363	2.481
1	1.41381	-2.56663	1.55938
1	1.47421	-1.23894	2.69685
1	-1.77938	-0.68306	2.7171
1	-3.3928	-1.38213	2.50937
1	-2.91008	0.04503	1.59813
1	1.51281	2.51926	1.55559
1	0.34009	1.89378	2.69249
1	0.52383	3.64247	2.48341
1	2.17112	1.96699	-2.65866
1	1.21266	2.58764	-1.32084
1	0.66136	1.18451	-2.20309
1	-1.34878	-0.00525	-2.22253
1	-2.80352	0.88844	-2.65029
1	-2.82219	-0.26288	-1.31988
1	0.59376	-2.83082	-2.68708
1	1.62407	-2.32754	-1.35304
1	0.67665	-1.13771	-2.21223

[HP(2,6-Me₂C₆H₃)₃]⁺

C	0.4885741616	-1.7075927193	0.2461493602
C	-1.7251910428	0.4279220962	0.2081074138
C	1.2301499969	1.2774878563	0.290717676
C	1.2374962042	-4.3641665829	-0.1107153919
C	-0.0665525381	-2.7109556603	1.0807343056
C	1.411034509	-2.0370235766	-0.7725751355
C	1.7673905816	-3.3759263523	-0.9234856208

C 0.325523403 -4.0312573173 0.8776088291
C -1.0573101668 -2.4305955133 2.184335637
C 2.0392103637 -1.0436193639 -1.7169230051
H 2.4697801086 -3.6428800444 -1.7013760647
H -0.0957240559 -4.8046760241 1.5055067611
H 1.5296096792 -5.3958473084 -0.252610552
C 3.1716609672 3.2508057256 0.0040591533
C 2.3373779911 1.3059469236 1.1765343193
C 1.1013948757 2.2317157385 -0.7437525497
C 2.089115936 3.2082541058 -0.8586620442
C 3.2935597889 2.3036429671 1.0077180203
C 2.5388066319 0.3178788469 2.2996043829
C -0.0286590565 2.2704922084 -1.7411111758
H 2.0051239922 3.9428679073 -1.6479761641
H 4.1444213108 2.3312054546 1.6749186727
H 3.9251643328 4.018213063 -0.1106068611
C -4.3886519705 1.1202817998 -0.2069049922
C -2.4395004957 -0.170076999 -0.8546326616
C -2.3427829505 1.3807213568 1.0579242645
C -3.6756288976 1.7085288105 0.8250210163
C -3.7722360984 0.196115441 -1.0339178479
C -1.8636117672 -1.1772773566 -1.8175186076
C -1.6394983441 2.0593872961 2.2081162896
H -4.1545338483 2.4377482027 1.46437292
H -4.3300216604 -0.2510866942 -1.8454684508
H -5.4235391412 1.3881767024 -0.3714361542
P -0.0116607426 -0.0039357873 0.6213587416
H -0.0471039307 -0.0158986919 2.0123479413
H 3.5294934754 0.4417198897 2.7305854597
H 2.4537791576 -0.7188241229 1.9725948535
H 1.8199970374 0.4708745534 3.1091416204
H -0.5909958958 -1.9133234104 3.027203379
H -1.4576898022 -3.3648895495 2.5707712925
H -1.902651491 -1.8273485893 1.8520569202
H -0.6849970022 2.5009886395 1.9203083793
H -1.4501392514 1.3678095328 3.0335306034
H -2.2607170649 2.8594069314 2.6038404341
H 0.240173895 2.9137487877 -2.5761805681
H -0.9440460303 2.6687130703 -1.302462992
H -0.2677910662 1.2910778935 -2.1510905795
H -0.8779981829 -0.8985354627 -2.185470301
H -2.516319134 -1.2736696983 -2.6824305583
H -1.7714423453 -2.1650847693 -1.3651175587
H 2.4878185938 -1.5686344256 -2.557459092
H 2.8274010682 -0.465855193 -1.2333225789
H 1.3229367973 -0.332751034 -2.1245233306

AsH₃

As 0. 0. 0.7474250968
H 1.2669844535 0. 1.59568425
H -0.6334922268 1.097240723 1.59568425
H -0.6334922268 -1.097240723 1.59568425

[AsH₄]⁺

H -0.0000005394 0.0000000228 -0.4905581282
As 0.000000061 0. 0.999987654
H 1.4053003014 -0.00002026 1.496835682
H -0.702667298 -1.2170154162 1.4968365125
H -0.7026322199 1.2170356533 1.4968365498

AsPh₃

C -0.0000471358 1.7512119751 0.2731090265
As 0.0000000513 0.0000001154 1.1916758181
C 1.5166176028 -0.8755649493 0.2731090265
C -1.5165703131 -0.8756466797 0.2731090265
C 0.0687098707 4.3085622405 -0.864940931
C 0.7770366198 2.7633504975 0.8416302119
C -0.751396817 2.0396739918 -0.8657891855
C -0.7175243999 3.311566284 -1.4304099057
C 0.8181659263 4.0315329354 0.2734358422
H 1.354417385 2.5630731492 1.736409761
H -1.3683624889 1.2745618163 -1.316962491
H -1.3070692713 3.5214527824 -2.3137477631
H 1.4286438539 4.8036389172 0.7236821746
H 0.0935414367 5.2968970864 -1.3049214116
C -3.7656791126 -2.0947764981 -0.864940931
C -2.7816498635 -0.7087416677 0.8416302119
C -1.390710907 -1.6705655991 -0.8657891855
C -2.5091381514 -2.2771773715 -1.4304099057
C -3.9004927245 -1.3072138623 0.2734358422
H -2.8968949746 -0.1085765832 1.736409761
H -0.4196214903 -1.8223174565 -1.316962491
H -2.3961327553 -2.892681456 -2.3137477631
H -4.874395083 -1.1645774595 0.7236821746
H -4.6340179795 -2.5674391541 -1.3049214116
C 3.6969693957 -2.2137853963 -0.864940931
C 2.1421078779 -0.3691080465 -0.8657891855
C 2.0046133975 -2.0546084837 0.8416302119
C 3.0823269521 -2.7243187269 0.2734358422
C 3.2266627052 -1.0343885663 -1.4304099057
H 1.7879841331 0.5477559863 -1.316962491

H 1.5424777435 -2.4544962198 1.736409761
H 3.4457513829 -3.6390611116 0.7236821746
H 3.7032021805 -0.6287709802 -2.3137477631
H 4.5404766967 -2.7294575861 -1.3049214116

[HAsPh₃]⁺

C 0.1247755409 -1.8350047098 0.3541708872
C -1.6515484677 0.809443564 0.3541708872
C 1.5267729207 1.0255611438 0.3541708872
C 0.2732584614 -4.483156455 -0.4323234356
C -0.651284225 -2.7913553469 1.0111039611
C 0.9740943205 -2.1922775521 -0.6916824531
C 1.0424128213 -3.5248340566 -1.0824785532
C -0.5713154773 -4.1186135544 0.612308818
H -1.3087741534 -2.5160823115 1.825769996
H 1.5817011583 -1.4508819495 -1.1925267796
H 1.6998079966 -3.8117200381 -1.8914281781
H -1.1645917232 -4.8669132391 1.1191645012
H 0.3339418167 -5.5188046504 -0.7374241896
C 3.7458981449 2.4782269976 -0.4323234356
C 2.7430267503 0.8316489903 1.0111039611
C 1.4115208884 1.939729204 -0.6916824531
C 2.5313894229 2.6651730135 -1.0824785532
C 3.8524817015 1.5645330611 0.612308818
H 2.8333782729 0.1246094918 1.825769996
H 0.4656500434 2.0952343598 -1.1925267796
H 2.4511423832 3.3779369264 -1.8914281781
H 4.797166361 1.424890603 1.1191645012
H 4.6124541138 3.0486044226 -0.7374241896
C -4.0191566123 2.0049294554 -0.4323234356
C -2.385615215 0.2525483461 -0.6916824531
C -2.0917425314 1.9597063546 1.0111039611
C -3.2811662303 2.5540804913 0.612308818
C -3.5738022502 0.8596610411 -1.0824785532
H -2.0473512078 -0.6443524123 -1.1925267796
H -1.5246041256 2.3914728177 1.825769996
H -3.6325746439 3.4420226341 1.1191645012
H -4.1509503859 0.4337831097 -1.8914281781
H -4.9463959366 2.4702002258 -0.7374241896
As -0.000000002 -0.000000007 0.9063555478
H -0.000000002 -0.000000007 2.4096623835

As(2,6-Me₂C₆H₃)₃

C -1.7492009914 0.6481158434 -0.1883312107
C 1.4358852798 1.1907945727 -0.1883312107
C 0.3133157099 -1.838910416 -0.1883312107

C	-4.3360464466	1.6003727855	0.3462892626
C	-1.9562495496	1.5948254955	0.8359609541
C	-2.8549110545	0.1790407309	-0.9358730548
C	-4.1323124228	0.6598826354	-0.6498736628
C	-3.2534651725	2.0556729232	1.0787514763
C	-0.8658911557	2.1366101469	1.7256349027
C	-2.7230493797	-0.8489197519	-2.0350431582
H	-4.973482794	0.2884968179	-1.2216231099
H	-3.4087732499	2.7787674944	1.8696999029
H	-5.3316097695	1.9696405927	0.5554905395
C	0.7820597347	-4.5553127669	0.3462892626
C	-0.4030346198	-2.4915745533	0.8359609541
C	1.2724017051	-2.5619458636	-0.9358730548
C	1.4946810848	-3.9086288517	-0.6498736628
C	-0.1535323879	-3.8454199508	1.0787514763
C	-1.4174130882	-1.8181888106	1.7256349027
C	2.0967107599	-1.933770062	-2.0350431582
H	2.236895823	-4.4514108533	-1.2216231099
H	-0.7020966172	-4.3414679768	1.8696999029
H	0.9600460943	-5.6021297992	0.5554905395
C	3.5539867102	2.9549399816	0.3462892626
C	1.5825093476	2.3829051328	-0.9358730548
C	2.3592841676	0.8967490579	0.8359609541
C	3.4069975587	1.7897470277	1.0787514763
C	2.6376313363	3.2487462163	-0.6498736628
C	0.626338618	2.7826898141	-2.0350431582
C	2.2833042422	-0.3184213362	1.7256349027
H	4.1108698654	1.5627004825	1.8696999029
H	2.7365869694	4.1629140355	-1.2216231099
H	4.3715636735	3.6324892066	0.5554905395
As	-0.0000000006	0.	-0.9011315983
H	-1.6347125161	-2.4508311775	2.5854939453
H	-2.3583569009	-1.6279659745	1.2093849403
H	-1.0657720714	-0.8579414042	2.0971961563
H	-0.2101130162	1.3519563902	2.0971961563
H	-1.305125803	2.6411181551	2.5854939453
H	-0.2306814408	2.8563799741	1.2093849403
H	2.58903834	-1.2284139996	1.2093849403
H	1.2758850859	-0.4940149858	2.0971961563
H	2.9398383173	-0.1902869775	2.5854939453
H	2.7780101191	-2.6683259217	-2.4623100675
H	2.6982279506	-1.0980715035	-1.6722035449
H	1.4691429461	-1.5440976286	-2.8382755312
H	0.6026562984	2.044363928	-2.8382755312
H	0.9218329734	3.7399902965	-2.4623100675
H	-0.398156159	2.8857697027	-1.6722035449

H -3.6998430942 -1.0716643747 -2.4623100675
H -2.3000717934 -1.7876981991 -1.6722035449
H -2.0717992462 -0.5002662993 -2.8382755312

[HAs(2,6-Me₂C₆H₃)₃]⁺

6 -1.65154 -0.95915 -0.04182
6 1.65647 -0.95174 -0.0489
6 -0.00294 1.90414 -0.04753
6 -4.03325 -2.32216 0.33101
6 -1.95856 -2.04709 -0.88594
6 -2.51218 -0.55367 0.99499
6 -3.70499 -1.25855 1.15579
6 -3.16436 -2.71354 -0.67466
6 -1.06082 -2.52758 -1.99935
6 -2.23119 0.58485 1.94144
1 -4.38008 -0.96548 1.94849
1 -3.41582 -3.55299 -1.30881
1 -4.96364 -2.85343 0.47859
6 -0.01362 4.64737 0.33028
6 -0.79772 2.70934 -0.89051
6 0.77553 2.45083 0.9894
6 0.7508 3.83586 1.15274
6 -0.78257 4.08666 -0.67659
6 -1.65813 2.16771 -2.00543
6 1.62891 1.64346 1.93331
1 1.33914 4.27725 1.94587
1 -1.38881 4.72102 -1.30913
1 -0.01736 5.71839 0.48049
6 4.04307 -2.30466 0.32855
6 1.74509 -1.89762 0.98922
6 2.74929 -0.66351 -0.89344
6 3.93737 -1.36027 -0.67959
6 2.95958 -2.56408 1.15211
6 0.6216 -2.23466 1.9356
6 2.70451 0.35086 -2.00962
1 4.78847 -1.15024 -1.31327
1 3.05122 -3.29273 1.94627
1 4.97465 -2.83306 0.47886
33 -0.00011 -0.00435 -0.44478
1 -0.00374 -0.00521 -1.93895
1 -2.31863 2.94646 -2.37946
1 -2.28747 1.33532 -1.68758
1 -1.05708 1.82619 -2.85214
1 -1.05281 -1.83289 -2.84326
1 -1.41521 -3.48304 -2.37905
1 -0.02843 -2.67076 -1.67737

1	2.2956	1.31078	-1.69147
1	2.10718	-0.00188	-2.85438
1	3.70755	0.53697	-2.38633
1	1.91902	2.25382	2.78571
1	2.5439	1.29183	1.45555
1	1.11202	0.76797	2.32442
1	0.1295	-1.34962	2.33799
1	1.00606	-2.80082	2.78113
1	-0.14685	-2.84231	1.45675
1	-2.90853	0.53698	2.79127
1	-2.37195	1.55533	1.4647
1	-1.21619	0.56285	2.33659

Total energies E^0 , standard enthalpies H^0_{298} in Hartree,

Compound	B3LYP/def2-TZVPP E^0
Crypt_B_N	-3541.12212
Crypt_BH_HN	-3542.34569
Crypt_B_P	-3758.694674
Crypt_BH_HP	-3759.922162
Crypt_B_As	-5441.116359
Crypt_BH_HAs	-5442.344985
Crypt_Al_N	-3827.748228
Crypt_AlH_HN	-3828.968856
Crypt_Al_P	-4045.35607
Crypt_AlH_HP	-4046.533561
Crypt_Al_As	-5727.777317
Crypt_AlH_HAs	-5728.956968
Crypt_Ga_N	-5722.277292
Crypt_GaH_HN	-5723.477033
Crypt_Ga_P	-5939.883478
Crypt_GaH_HP	-5941.040729
Crypt_Ga_As	-7622.30669
Crypt_GaH_HAs	-7623.463069

Crypt_B_N

B	-2.840119453	-0.0000003126	0.0000000161
C	-3.2557414505	1.4523942127	-0.2917580509
C	-3.2557413438	-0.4735277193	1.4036896224
C	-3.2557412925	-0.9788675091	-1.111931533
C	-4.5377980064	-1.2448984342	3.6902837769
C	-2.5397304278	-0.8433339998	2.4999161977
C	-4.6703679841	-0.4685165903	1.3888347292
C	-5.2918258347	-0.8675620962	2.5717356476
C	-3.1439152818	-1.2488064193	3.7018685881
F	-6.6150812657	-0.921974302	2.7330309185
F	-5.1999909231	-1.6147537197	4.7866553534
C	-4.5377982871	3.818328085	-0.7670285776
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C	-4.4435765951	-1.2707945633	3.7670483684
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C	-4.3335597633	-0.4865550154	1.4423065696
C	-5.0701242017	-0.8693208537	2.5769492215
C	-3.0628301933	-1.3258253515	3.9301778404
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C	-5.0701241076	-1.797043742	-2.0413281651
F	-6.4023724566	-1.8527071619	-2.1045582256
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C	0.0082890175	6.6258784281	-1.3310112209
C	0.0082897384	-4.4656289793	-5.0726734898
C	1.1971710726	6.9012761477	-1.3863332891
C	4.7903341566	3.98984492	-0.8014828134
C	5.5829966752	5.1770321842	-1.0399658302
C	1.1971718234	-4.6512380524	-5.283513799
C	4.7903345907	-2.6890267574	-3.054565396
C	2.5411760801	6.9237083733	-1.3908394633
C	2.5411768334	-4.6663565099	-5.3006875007
C	3.7451923165	-4.5441872378	-5.1619109665
C	3.7451915829	6.742439854	-1.354426088
F	-0.7213766547	-0.96447129	2.8590069898
C	0.0082895048	-2.1602498529	6.4036848256
F	-0.7213768722	2.9582080292	-0.5942469637
F	-0.7213765503	-1.9937372798	-2.2647599283
C	5.1072069353	-4.3275288505	-4.9158007498
C	5.5829972385	-3.4891526717	-3.9634581653
C	5.3622655804	-0.9131466874	2.7068652989
C	4.79033445	-1.3008176721	3.8560484366
C	5.5829970559	-1.6878788738	5.0034242414
C	5.1072067089	-2.0934436969	6.2056505711
C	1.1971715801	-2.2500382771	6.6698472309
C	2.5411765893	-2.2573517936	6.6915271384
C	3.7451920788	-2.1982523212	6.5163372572
C	5.1072062367	6.4209730972	-1.2898495866
C	-1.1815721789	-1.9603829109	5.8112137886
C	-2.0992923719	-1.7052980102	5.0550587632
C	-1.1815719669	-4.0524676005	-4.6033480719
C	-1.1815726211	6.0128498848	-1.2078656297
C	-2.0992921875	-3.5251606818	-4.0043605163
C	-2.0992927566	5.2304578936	-1.0506981815
H	2.7950838331	2.0504006441	0.4890489042
H	6.3432771395	0.4711032869	-1.3965029457
H	4.9156562543	0.7961879067	-2.3601600687
H	2.7950839343	0.2251693568	2.0958555398
H	2.7950840431	-1.4487289862	1.53117465
H	2.7950840181	-0.6016715408	-2.0202233739
H	2.7950840917	-1.9276487078	-0.8529253304
H	4.9156564339	-2.4420523394	0.4905613444
H	6.3432772458	-1.4449583565	0.2902644159
H	6.3432770886	0.9738558506	1.1062387936
H	4.9156561682	1.6458649466	1.8695989545
H	6.4495231109	2.7664412526	-0.5557245695
H	6.4495234119	-1.8644918975	-2.1179457538
H	2.7950838684	1.7024794683	-1.242930029

H	3.711917277	-2.766353258	-3.1424033697
H	5.8183380093	-4.8684971107	-5.5303067172
H	6.6594642928	-3.4040418405	-3.8667776815
H	6.4495233144	-0.9019485544	2.6736705896
H	3.7119171322	-1.338224432	3.9669340665
H	6.6594641147	-1.6467064409	4.8813759283
H	5.8183377546	-2.3551372836	6.9813958576
H	3.7119168304	4.1045779788	-0.8245304948
H	6.6594637432	5.0507491215	-1.0145979756
H	5.8183372234	7.2236350771	-1.4510888889
F	-6.6356585636	0.3988103866	-1.1822057097
F	-6.6356584736	-1.223226182	0.2457224327
F	-6.6356586067	0.8244141484	0.9364832358
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Crypt_Ga_N

Ga	-2.0888979155	-0.0000002658	0.000000022
C	-2.9271181563	1.6977407931	-0.341043442
C	-2.9271180315	-0.5535185757	1.6408086754
C	-2.9271179715	-1.1442231715	-1.2997651872
C	-4.444430782	-1.2724659859	3.7720030099
C	-2.3440351641	-0.9450982296	2.8015786056
C	-4.3260384054	-0.4877871357	1.4459589776
C	-5.0662829681	-0.870587524	2.5807040459
C	-3.0639857104	-1.3291523956	3.9400402841
F	-6.3986055172	-0.8958399816	2.6555603104
F	-5.235186556	-1.6157392246	4.7895767046
C	-4.4444310689	3.9028828006	-0.7840139879
C	-4.3260385154	1.4961301635	-0.300543782
C	-2.3440353772	2.8987869181	-0.5823104409
C	-3.0639860102	4.0767506735	-0.8189406633
C	-5.0662831645	2.6702483494	-0.5364015041
C	-4.8652573788	-0.0000004389	0.0000000002
F	-6.3986057193	2.7477018893	-0.5519604541
F	-5.2351869204	4.9557640212	-0.9955175421
C	-4.4444306441	-2.6304180528	-2.9879890115
C	-4.3260383525	-1.0083442437	-1.1454151824
C	-2.3440350617	-1.9536895336	-2.2192681047
C	-3.0639855665	-2.7475992577	-3.1210995778
C	-5.0662828738	-1.7996621799	-2.0443025461
F	-6.3986054202	-1.8518635114	-2.1035998919
F	-5.235186381	-3.3400261826	-3.7940591707
C	-6.4152593428	-0.0000005356	-0.000000012
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C 5.6825774141 -1.8981785159 -2.1562115852
C 5.6825771075 2.8164236669 -0.565765088
C -0.1045152062 6.4769725447 -1.3010989015
C -0.1045145013 -4.3652712195 -4.9586733792
C 1.0998751395 6.6820686574 -1.3422987318
C 5.0039021652 3.9525346189 -0.7939878883
C 5.6579624579 5.213810566 -1.0473538958
C 1.0998758668 -4.503499271 -5.1156918286
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C 2.4442553977 6.7164319618 -1.3492016297
C 2.4442561286 -4.5266588916 -5.1419997857
C 3.6562341218 -4.4393616046 -5.042835634
C 3.6562334049 6.5869047654 -1.3231820885
F -0.9948007177 -0.9639944785 2.8575935111
C -0.10451473 -2.1117017513 6.2597723934
F -0.9948009351 2.9567454907 -0.5939531732
F -0.9948006133 -1.9927516048 -2.2636402461
C 5.0459632336 -4.3137752794 -4.9001775542
C 5.6579630254 -3.5139401093 -3.9916151402
C 5.6825773146 -0.9182444944 2.7219769225
C 5.0039024559 -1.2886532957 3.8199892972
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C 5.0459630076 -2.0867904041 6.1859280276
C 1.0998756308 -2.1785695871 6.4579907016
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C -1.3339008143 -1.93694688 5.7417417171
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C -1.3339012511 5.9409672767 -1.1934258022
C -2.334507107 -3.5453741873 -4.0273217726
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H	3.1848671945	-1.9107623968	-0.8372578759
H	5.3085558387	-2.4414285076	0.4904360368
H	6.7419154829	-1.4446623767	0.2902049676
H	6.7419153257	0.9736564109	1.1060122182
H	5.308555573	1.6454445445	1.8691213803
H	6.7705318808	2.8675393585	-0.5760332228
H	6.7705321929	-1.9326287328	-2.1953449336
H	3.1848669736	1.680467938	-1.2361397977
H	3.9203936118	-2.6661362443	-3.0285631576
H	5.6606403294	-4.9040212867	-5.5706599372
H	6.7424411882	-3.5098943591	-3.9870194908
H	6.7705320916	-0.9349097654	2.7713784313
H	3.9203934721	-1.2897444058	3.8232234945
H	6.7424410043	-1.6979126365	5.0331678089
H	5.6606400724	-2.3723221237	7.0323372963
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H	6.7424406214	5.2078078506	-1.0461480439
H	5.6606395375	7.2763440629	-1.4616771104
F	-6.9036039322	0.3989587611	-1.1826455923
F	-6.9036038422	-1.2236813425	0.24581386
F	-6.9036039754	0.8247208833	0.9368316847

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Ga	-1.5661630655	-0.0000002329	0.000000026
C	-2.6451249385	1.6417798273	-0.3298019573
C	-2.6451248177	-0.5352734755	1.5867243028
C	-2.6451247598	-1.1065072523	-1.2569222929
C	-4.1931091933	-1.2623222402	3.7419336893
C	-2.0905555355	-0.9327713574	2.765037786
C	-4.0459349878	-0.4802767482	1.4236957944
C	-4.8001910189	-0.8606866486	2.5513546747
C	-2.8148513943	-1.316662388	3.9030158773
F	-6.1362904162	-0.8860495651	2.6265383746
F	-4.9829506114	-1.6070679903	4.7638723885
C	-4.1931094781	3.8717701547	-0.7777640523
C	-4.0459350961	1.4730945123	-0.2959163582
C	-2.0905557459	2.8609782265	-0.5747153988
C	-2.8148516913	4.038441615	-0.8112451073
C	-4.800191213	2.6398806343	-0.5303012103
C	-4.5964387307	-0.0000004218	0.0000000022
F	-6.1362906161	2.7176729707	-0.5459282181
F	-4.9829509739	4.9291678358	-0.9901748764
C	-4.1931090568	-2.6094491045	-2.9641696208
C	-4.0459349358	-0.9928189267	-1.1277794165
C	-2.0905554346	-1.9282076658	-2.1903223216

C	-2.8148512519	-2.7217801592	-3.0917707215
C	-4.8001909258	-1.7791952893	-2.0210534625
F	-6.1362903204	-1.8316249591	-2.0806101859
F	-4.9829504376	-3.3221011832	-3.7736975145
C	-6.1469222014	-0.0000005185	-0.0000000099
N	2.7825842128	0.0000000383	0.000000006
C	3.2424805228	1.4162900575	-0.28450529
C	3.2424806768	-0.9545337921	-1.0842903705
C	3.2424806269	-0.4617560645	1.3687958514
C	4.7739766622	1.4510652852	-0.2914909316
C	5.2699837239	0.4642073375	-1.376061309
C	4.7739767689	-0.4730937816	1.4024048381
C	5.2699836737	0.959600741	1.0900459531
C	5.2699838286	-1.4238074982	0.2860155944
C	4.77397682	-0.9779710162	-1.1109136796
C	5.3773157668	-1.8886188424	-2.1453523784
C	5.3773154619	2.8022394507	-0.5629157592
C	0.000527631	6.6213218732	-1.3300958971
C	0.0005283514	-4.4625580088	-5.06918506
C	1.1903118958	6.8932333647	-1.3847176491
C	4.8002463385	3.9889552517	-0.801304096
C	5.5861182208	5.1803073943	-1.0406237567
C	1.1903126458	-4.6458174762	-5.277356365
C	4.8002467725	-2.6884271486	-3.0538842787
C	2.5343329684	6.9147388282	-1.3890376548
C	2.5343337207	-4.660311326	-5.2938205515
C	3.7388154739	-4.5398826261	-5.1570211979
C	3.738814741	6.7360528837	-1.353143069
F	-0.7333722565	-0.9666496111	2.8654642419
C	0.0005281179	-2.15876427	6.3992810718
F	-0.7333724745	2.9648893331	-0.5955891091
F	-0.7333721519	-1.9982402648	-2.2698750353
C	5.1024926724	-4.3278022629	-4.9161113288
C	5.5861187844	-3.4913600575	-3.965965617
C	5.377315668	-0.913620008	2.7082683786
C	4.8002466319	-1.3005276108	3.8551886021
C	5.5861186017	-1.6889466974	5.0065896196
C	5.102492446	-2.0935759604	6.2060426423
C	1.1903124028	-2.2474160714	6.6620741568
C	2.5343334769	-2.2544274337	6.6828583805
C	3.7388152363	-2.1961699638	6.5101644695
C	5.1024919737	6.4213787721	-1.289931079
C	-1.1919045174	-1.9605124795	5.81159787
C	-2.1125893389	-1.7064703203	5.0585338702
C	-1.1919043054	-4.0527354416	-4.6036523219
C	-1.1919049596	6.0132472924	-1.2079454615

C	-2.1125891543	-3.527584059	-4.0071133196
C	-2.1125897238	5.2340535784	-1.0514204856
H	2.8132758716	2.0506375349	0.4891922322
H	6.361241334	0.4711320758	-1.3965882818
H	4.9336948125	0.7962327584	-2.3602930204
H	2.8132759728	0.2252814983	2.0961086882
H	2.8132760816	-1.4489715553	1.5313081386
H	2.8132760566	-0.6016658589	-2.02050019
H	2.8132761302	-1.9279240097	-0.852954788
H	4.9336949921	-2.4421899031	0.4905889787
H	6.3612414403	-1.4450466527	0.2902821532
H	6.3612412831	0.9739153612	1.1063063928
H	4.9336947264	1.645957662	1.8697042723
H	6.4646382898	2.7713081449	-0.556702234
H	6.4646385913	-1.8677720246	-2.1216717729
H	2.8132759068	1.7026426321	-1.2431537194
H	3.7212631254	-2.7624673887	-3.1379892672
H	5.8089224187	-4.8714839424	-5.5336995695
H	6.6633200229	-3.4105057691	-3.8741202981
H	6.4646384936	-0.9035353167	2.6783742735
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H	6.6633198444	-1.6498333688	4.8906451632
H	5.8089221638	-2.3565821649	6.9856789551
H	3.7212626794	4.0988123201	-0.823372285
H	6.6633194723	5.0603399787	-1.0165245939
H	5.8089216322	7.2280667883	-1.4519791345
F	-6.6428547814	0.3988075924	-1.1821974281
F	-6.6428546915	-1.2232176134	0.2457207113
F	-6.6428548246	0.8244083727	0.9364766754
H	0.028976077	-0.0000001334	0.0000000385
H	1.7420654841	-0.0000000266	0.0000000519

Crypt_B_P

B	-2.6572245989	-0.0000003012	0.0000000175
C	-3.0753073523	1.4536743462	-0.2920152013
C	-3.0753072454	-0.4739450691	1.4049268181
C	-3.0753071941	-0.979730259	-1.112911574
C	-4.3662003211	-1.2446274294	3.6894804632
C	-2.3634271316	-0.8449351225	2.5046624817
C	-4.4904949196	-0.4683445653	1.3883248255
C	-5.1161227444	-0.8667079983	2.5692038567
C	-2.9726476193	-1.2497750216	3.7047398743
F	-6.4397861594	-0.9201443324	2.7276063256
F	-5.0316283043	-1.613884393	4.7840784178
C	-4.3662006018	3.8174969073	-0.7668616066
C	-4.4904950253	1.4364962242	-0.2885644767

C	-2.3634273222	2.5915684568	-0.5205961755
C	-2.9726479011	3.833285862	-0.7700332747
C	-5.1161229398	2.6583491262	-0.5340111806
C	-5.0980038924	-0.0000004535	-0.0000000016
F	-6.4397863669	2.8222477405	-0.5669352793
F	-5.0316286683	4.950074967	-0.9943747166
C	-4.3662001863	-2.5728707014	-2.9226188444
C	-4.4904948689	-0.9681529056	-1.0997603395
C	-2.3634270401	-1.746634183	-1.9840662467
C	-2.9726474839	-2.5835118031	-2.9347065544
C	-5.1161226505	-1.7916424917	-2.0351926815
F	-6.4397860597	-1.9021050195	-2.1606710829
F	-5.0316281295	-3.336191922	-3.7897037046
C	-6.638763051	-0.0000005495	-0.0000000138
P	2.5620634386	0.0000000243	0.0000000586
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C	3.468888032	-1.0694969592	-1.2148813123
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C	5.0026247386	-0.4794182444	1.4211526518
C	5.4778989076	0.9607575932	1.0913600522
C	5.4778990628	-1.4255239467	0.2863604002
C	5.0026247906	-0.9910448449	-1.1257647408
C	5.678758662	-1.8837032566	-2.1397686008
C	5.6787583579	2.7949459947	-0.5614506378
C	0.0633818032	6.2138250451	-1.2482376388
C	0.0633824795	-4.1879182588	-4.7572115799
C	1.2488214448	6.5055193451	-1.3068333757
C	5.0843289491	3.9742684648	-0.7983537973
C	5.7914913267	5.2063303882	-1.0458512696
C	1.2488221528	-4.3845107026	-4.9805283073
C	5.0843293816	-2.6785286976	-3.0426402785
C	2.587572128	6.6341342785	-1.3326696089
C	2.58757285	-4.4711928875	-5.0789939023
C	3.805306441	-4.4327309075	-5.0353035886
C	3.8053057252	6.5770664891	-1.3212057655
F	-1.022117719	-0.8227877987	2.4390108485
C	0.0633822601	-2.025907181	6.0054493354
F	-1.0221179046	2.5236389291	-0.5069504157
F	-1.0221176299	-1.7008517281	-1.9320603417
C	5.1977382157	-4.315631448	-4.9022860545
C	5.7914918933	-3.5088986963	-3.9858884205
C	5.6787585634	-0.9112420821	2.7012194877
C	5.0843292413	-1.2957392225	3.8409943109
C	5.7914917095	-1.6974310148	5.0317399419

C 5.1977379896 -2.0876883215 6.1885897769
C 1.2488219231 -2.1210088153 6.2873618278
C 2.5875726158 -2.1629413134 6.4116636874
C 3.8053062087 -2.1443352762 6.356509559
C 5.1977375188 6.4033203355 -1.2863034846
C -1.1448664765 -1.8364178754 5.4437409939
C -2.143208635 -1.6140556852 4.7845867406
C -1.1448662776 -3.7962093395 -4.3122548057
C -1.1448668906 5.6326265942 -1.1314860999
C -2.1432084602 -3.3365462064 -3.7901063313
C -2.143208999 4.9506010841 -0.9944803445
H 3.129081041 2.3074227469 0.4285723918
H 6.5713771169 0.4767196271 -1.413151566
H 5.130385634 0.7958044082 -2.3590232127
H 3.1290811616 0.1325975383 2.3431371924
H 3.1290812694 -1.5248658081 1.784000563
H 3.1290812545 -0.7825567599 -2.2125727658
H 3.1290813273 -2.0955149583 -1.0567357167
H 5.1303858135 -2.4408760259 0.4903250502
H 6.5713772244 -1.4621846357 0.2937248481
H 6.5713770653 0.9854658315 1.1194269881
H 5.1303855478 1.645072171 1.8686983987
H 6.7668957085 2.7582974889 -0.5540886374
H 6.7668960087 -1.85900323 -2.1117109924
H 3.129081076 1.9629175989 -1.2864012867
H 4.0039852582 -2.7218100736 -3.0918051317
H 5.8158923652 -4.9038149029 -5.570425508
H 6.8752339396 -3.4865372147 -3.960487252
H 6.7668959113 -0.8992933994 2.6657999046
H 4.0039851156 -1.31667664 3.9030594375
H 6.875233757 -1.6866136044 4.9996738178
H 5.8158921083 -2.3722222804 7.0320413584
H 4.0039848187 4.0384870562 -0.8112540962
H 6.8752333766 5.1731516989 -1.0391862885
H 5.8158915733 7.276037865 -1.461615598
F -7.1236896922 0.3994655677 -1.1841479748
F -7.1236896022 -1.2252358663 0.2461261294
F -7.1236897355 0.8257685593 0.9380217927

Crypt_BH_HP

5 1.928382 0.000111 -0.000186
6 2.617488 1.40559 -0.374768
6 2.619663 -1.026665 -1.029081
6 2.617819 -0.377117 1.404501
6 3.973719 -2.736374 -2.743462
6 1.952089 -1.870031 -1.874186

6	4.029187	-1.023086	-1.026013
6	4.69001	-1.89273	-1.897975
6	2.582278	-2.757647	-2.764233
9	6.020168	-1.998142	-2.003978
9	4.654939	-3.549185	-3.558282
6	3.967679	3.747614	-0.996932
6	4.027027	1.403359	-0.373022
6	1.948026	2.558191	-0.682054
6	2.576184	3.774049	-1.00502
6	4.685846	2.594601	-0.689539
6	4.635804	0.002118	0.001315
9	6.015736	2.741547	-0.7273
9	4.64714	4.860969	-1.292634
6	3.968602	-1.007537	3.743986
6	4.027367	-0.375458	1.40198
6	1.948613	-0.688163	2.556277
6	2.577114	-1.015409	3.770789
6	4.686521	-0.696383	2.591855
9	6.016455	-0.73549	2.738113
9	4.64829	-1.307377	4.856091
6	6.177025	0.003311	0.001905
15	-2.650015	0.00181	0.000993
6	-3.363902	1.605276	-0.435628
6	-3.364213	-0.424308	1.607212
6	-3.359985	-1.179026	-1.171005
6	-4.909234	1.458301	-0.397623
6	-5.365037	1.032657	1.025063
6	-4.905749	-1.072835	-1.067107
6	-5.361075	0.371581	-1.411653
6	-5.362189	-1.407463	0.379371
6	-4.90956	-0.387126	1.459808
6	-5.620044	-0.729698	2.746486
6	-5.61986	2.743579	-0.74558
6	-0.326566	6.27789	-1.673205
6	-0.325926	-1.690942	6.272175
6	-1.499043	6.609652	-1.763537
6	-5.101564	3.937661	-1.063501
6	-5.911319	5.094497	-1.373701
6	-1.498489	-1.779747	6.604072
6	-5.101514	-1.049951	3.93985
6	-2.839642	6.709704	-1.793467
6	-2.83911	-1.805039	6.705256
6	-4.052556	-1.774018	6.600366
6	-4.053089	6.603235	-1.76877
9	0.594529	-1.872311	-1.876105
6	-0.317515	-4.591484	-4.59947

9	0.590423	2.558736	-0.682739
9	0.591055	-0.689761	2.55698
6	-5.423583	-1.694363	6.317457
6	-5.911037	-1.36206	5.096367
6	-5.613738	-2.017784	-2.007365
6	-5.09376	-2.890501	-2.881152
6	-5.902636	-3.73858	-3.727819
6	-5.4149	-4.631696	-4.624198
6	-1.489843	-4.835875	-4.842039
6	-2.83042	-4.911687	-4.914171
6	-4.043852	-4.836605	-4.834562
6	-5.424068	6.318017	-1.697217
6	0.860839	-4.133857	-4.142178
6	1.7892	-3.578714	-3.586599
6	0.853113	-1.522593	5.648783
6	0.852279	5.653844	-1.505993
6	1.782499	-1.318019	4.891731
6	1.781468	4.89594	-1.303745
1	-3.007899	1.893538	-1.425805
1	-6.455879	1.060557	1.052745
1	-5.020591	1.76771	1.755407
1	-3.003349	-0.940485	-2.174062
1	-3.004536	-2.180459	-0.92387
1	-3.010581	0.289092	2.353088
1	-3.008454	-1.412831	1.901309
1	-5.016128	-2.406812	0.650991
1	-6.453011	-1.447242	0.388635
1	-6.451778	0.381139	-1.453149
1	-5.013341	0.636901	-2.412151
1	-6.703053	2.649067	-0.722456
1	-6.703253	-0.705575	2.652548
1	-3.009766	2.354701	0.273683
1	-4.02788	-1.088973	4.084132
1	-6.120799	-1.910938	7.11878
1	-6.987218	-1.32731	4.972172
1	-6.697111	-1.951147	-1.939146
1	-4.019988	-2.993992	-2.987743
1	-6.978861	-3.649431	-3.635141
1	-6.111964	-5.219363	-5.210621
1	-4.027943	4.082928	-1.099595
1	-6.987471	4.969001	-1.343208
1	-6.121363	7.119794	-1.911849
9	6.670365	0.885716	0.886152
9	6.67194	-1.202996	0.323835
9	6.67125	0.328234	-1.203993
1	0.724858	-0.000687	-0.000945

1 -1.239591 0.00308 0.002809

Crypt_Al_P

13 -0.933925 0.000731 -0.005849
6 -1.912793 -0.521963 1.612244
6 -1.954398 -1.115944 -1.255922
6 -1.935235 1.656182 -0.338698
6 -3.560167 -2.546125 -2.977786
6 -1.441594 -1.976111 -2.177026
6 -3.358005 -0.937822 -1.134875
6 -4.132109 -1.653637 -2.068022
6 -2.194244 -2.768479 -3.05684
9 -5.462007 -1.595985 -2.195066
9 -4.378349 -3.226611 -3.781849
6 -3.459564 -1.312829 3.749104
6 -3.321265 -0.520749 1.431685
6 -1.367101 -0.883277 2.804825
6 -2.089309 -1.251329 3.950301
6 -4.063515 -0.984354 2.533279
6 -3.890568 0.011418 0.037402
9 -5.387863 -1.163258 2.566088
9 -4.250627 -1.683269 4.757104
6 -3.507714 3.894997 -0.674153
6 -3.338998 1.491363 -0.21055
6 -1.408362 2.872187 -0.647015
6 -2.144113 4.045567 -0.871779
6 -4.09386 2.672413 -0.340398
9 -5.4162 2.779717 -0.176819
9 -4.310059 4.949239 -0.82888
6 -5.444994 0.016124 0.06866
15 1.576004 0.001594 0.020768
6 2.451302 0.390465 1.599827
6 2.399687 1.193342 -1.137093
6 2.401034 -1.583118 -0.460688
6 3.981353 0.351191 1.425492
6 4.435337 1.375957 0.357431
6 3.93525 -1.450842 -0.445419
6 4.428698 -1.057426 0.966626
6 4.376571 -0.361818 -1.457016
6 3.933415 1.066013 -1.077888
6 4.675446 2.022703 -1.989215
6 4.758448 0.653787 2.69114
6 0.526163 -1.217037 6.786943
6 0.422896 6.506209 -2.367435
6 1.645088 -0.86731 7.13203
6 4.400144 0.592823 3.981473

6	5.360713	0.842258	5.037601
6	1.534637	6.635685	-2.857728
6	4.300531	3.172611	-2.567609
6	2.896746	-0.377257	7.149212
6	2.782862	6.406962	-3.301845
6	3.86383	5.930807	-3.598626
6	3.983807	0.102978	6.882801
9	-0.085648	-2.116679	-2.239569
6	0.349614	-5.297594	-4.470867
9	-0.007815	-0.864854	2.919373
9	-0.053279	2.971543	-0.771262
6	5.052012	5.218609	-3.80767
6	5.247133	3.964889	-3.327639
6	4.673413	-2.714437	-0.839608
6	4.278251	-3.801864	-1.516664
6	5.218491	-4.855419	-1.843984
6	5.002909	-5.897775	-2.685217
6	1.461016	-5.789221	-4.342532
6	2.712651	-6.05681	-3.930349
6	3.802963	-6.067778	-3.387966
6	5.172898	0.632198	6.364559
6	-0.733822	-4.527454	-4.273842
6	-1.557824	-3.742067	-3.847136
6	-0.6652	5.958604	-1.800259
6	-0.575128	-1.420461	6.044559
6	-1.496102	5.205831	-1.330509
6	-1.423309	-1.443443	5.173766
1	2.117507	-0.336666	2.339973
1	5.527462	1.389967	0.342638
1	4.117795	2.379974	0.645994
1	2.052439	-2.363959	0.21946
1	2.029762	-1.843868	-1.450861
1	2.066999	2.191262	-0.85531
1	2.014086	1.008853	-2.143286
1	4.000328	-0.617606	-2.45013
1	5.466546	-0.379067	-1.525848
1	5.520641	-1.087021	0.970903
1	4.095812	-1.799441	1.69555
1	5.798221	0.898248	2.48216
1	5.714409	1.727873	-2.124321
1	2.10001	1.365481	1.947945
1	3.289473	3.551438	-2.469072
1	5.848472	5.6981	-4.364687
1	6.213854	3.508764	-3.511574
1	5.725186	-2.672551	-0.560867
1	3.256604	-3.917736	-1.861363

1	6.196022	-4.787992	-1.378462
1	5.795239	-6.620299	-2.841766
1	3.388909	0.33087	4.270378
1	6.328216	1.221448	4.727063
1	5.975536	0.866829	7.053882
9	-5.914037	0.736097	1.097803
9	-5.962911	0.545684	-1.049168
9	-5.939502	-1.225051	0.1942

Crypt_AIH_HP

Al	-1.82166745	-0.0000002488	0.000000024
C	-2.8575415989	1.6278479233	-0.3270033107
C	-2.8575414792	-0.5307312438	1.5732596056
C	-2.8575414218	-1.0971176197	-1.2462562473
C	-4.3681299988	-1.2649539492	3.7497348993
C	-2.2867943655	-0.9252781655	2.7428254833
C	-4.2600477788	-0.4813530371	1.4268862247
C	-4.9957174574	-0.865024744	2.5642141668
C	-2.9856556121	-1.3137348896	3.8943377845
F	-6.3315313239	-0.8944162338	2.6513398719
F	-5.1450340518	-1.6127642381	4.7807578935
C	-4.3681302841	3.87984204	-0.779385542
C	-4.2600478874	1.476395632	-0.2965794939
C	-2.2867945742	2.8379951951	-0.5700985549
C	-2.9856559084	4.0294624021	-0.80944136
C	-4.9957176525	2.6531863119	-0.5329740684
C	-4.8166457855	-0.0000004356	0.0000000005
F	-6.3315315256	2.7433350148	-0.551083232
F	-5.1450344156	4.9466392219	-0.9936845443
C	-4.368129862	-2.6148893136	-2.9703493453
C	-4.2600477268	-0.9950437974	-1.1303067163
C	-2.2867942655	-1.9127178631	-2.1727268675
C	-2.98565547	-2.7157284767	-3.0848963799
C	-4.9957173638	-1.7881629081	-2.0312401011
F	-6.3315312271	-1.8489203711	-2.100256674
F	-5.1450338773	-3.3338763519	-3.7870733554
C	-6.3638463717	-0.000000532	-0.0000000116
P	2.707886282	0.0000000336	0.0000000594
C	3.4257837431	1.6204266498	-0.325512392
C	3.4257839194	-1.0921152644	-1.2405742822
C	3.4257838623	-0.5283111502	1.5660868694
C	4.9695443469	1.4824926402	-0.2978040774
C	5.430083685	0.4662480927	-1.3821107424
C	4.969544456	-0.4833400949	1.4327782904
C	5.4300836345	0.9638193424	1.094838009
C	5.4300837901	-1.430066825	0.2872729757

C	4.9695445082	-0.9991520212	-1.1349739816
C	5.6326643262	-1.8962736017	-2.1540477196
C	5.6326640201	2.8135972423	-0.5651973153
C	-0.0191604542	6.4367856122	-1.2930261204
C	-0.0191597538	-4.3381865117	-4.9279068597
C	1.1796489292	6.6736005872	-1.3405976588
C	5.0340616112	3.9905934343	-0.8016331705
C	5.7337630679	5.2287634652	-1.0503576441
C	1.1796496553	-4.497792056	-5.109208796
C	5.0340620454	-2.6895312065	-3.0551384338
C	2.5248397264	6.7209646514	-1.3501121587
C	2.5248404576	-4.52971377	-5.1454699405
C	3.7392396126	-4.4562788419	-5.0620525568
C	3.7392388932	6.6120057358	-1.3282243885
F	-0.9258704062	-0.9501437964	2.816535586
C	-0.0191599808	-2.0985995097	6.2209330944
F	-0.9258706205	2.91426295	-0.5854192487
F	-0.9258703034	-1.9641197325	-2.2311162443
C	5.1291453404	-4.3264335238	-4.9145565289
C	5.7337636368	-3.5240178739	-4.0030628519
C	5.632664227	-0.9173229926	2.719245282
C	5.0340619047	-1.3010616917	3.8567718373
C	5.7337634524	-1.7047449243	5.0534207454
C	5.1291451141	-2.0929138314	6.2040798813
C	1.17964942	-2.1758087162	6.4498065972
C	2.5248402206	-2.1912508147	6.4955822732
C	3.7392393795	-2.1557266001	6.3902771479
C	5.129144642	6.4193479091	-1.2895231172
C	-1.2491576252	-1.9241736765	5.703877794
C	-2.2341699395	-1.6951862453	5.0250841678
C	-1.2491574171	-3.9776165265	-4.5183219549
C	-1.2491580592	5.9017895637	-1.1855557538
C	-2.2341697562	-3.5042578167	-3.9806161676
C	-2.2341703219	5.1994432383	-1.044467938
H	3.0717373685	2.3218502655	0.4312834939
H	6.5213103236	0.4785104129	-1.4184600489
H	5.085322947	0.7974538002	-2.3639125572
H	3.0717374898	0.1334577557	2.3577920028
H	3.0717375983	-1.5344274563	1.7951396115
H	3.0717375832	-0.7874226403	-2.2264229185
H	3.0717376564	-2.1086365107	-1.06331815
H	5.0853231269	-2.4459350217	0.4913413039
H	6.5213104315	-1.4676773133	0.2948282199
H	6.5213102718	0.9891677146	1.1236320969
H	5.0853228608	1.6484817672	1.8725714875
H	6.7193541571	2.7756330014	-0.5575710091

H 6.7193544591 -1.8706868121 -2.1249828042
H 3.0717374036 1.975178924 -1.294473666
H 3.9527676741 -2.7369014498 -3.1089479829
H 5.7513186799 -4.9134604907 -5.5813822849
H 6.8171619312 -3.5064088495 -3.9830601758
H 6.7193543613 -0.9049453381 2.6825540859
H 3.9527675309 -1.3239771004 3.9247003748
H 6.8171617478 -1.6962265169 5.028169616
H 5.7513184229 -2.3768883386 7.0458730663
H 3.9527672322 4.060878884 -0.8157521843
H 6.8171613652 5.2026362359 -1.0451091654
H 5.7513178867 7.2903494995 -1.4644905315
F -6.859577267 0.3989282916 -1.1825552616
F -6.859577177 -1.2235878747 0.2457950852
F -6.8595773101 0.8246578943 0.9367601299
H -0.2319311976 -0.0000001497 0.0000000364
H 1.2774612228 -0.0000000556 0.0000000482

Crypt_Ga_P

Ga 0. 0.0000000263 0.8419089108
C -1.4734117293 -0.8506746243 1.8886388885
C 0.0000000069 1.7013493394 1.8886388885
C 1.4734117225 -0.8506746362 1.8886388885
C 0.0000000159 3.943847494 3.4882839515
C 0.0000000119 2.9599897625 1.3660879315
C 0.0000000061 1.5008455686 3.2921553247
C 0.0000000108 2.6765417924 4.067540716
C 0.0000000167 4.1441150377 2.1175078534
F 0.000000011 2.7393907683 5.4021472352
F 0.0000000202 5.0023669026 4.300344337
C -3.4154721036 -1.9719236938 3.4882839515
C -1.2997703698 -0.7504227396 3.2921553247
C -2.5634263124 -1.4799948314 1.3660879315
C -3.5889088844 -2.0720574649 2.1175078534
C -2.3179531691 -1.3382708474 4.067540716
C 0. 0.0000000263 3.8347203035
F -2.372381979 -1.3696953351 5.4021472352
F -4.332176804 -2.5011833943 4.300344337
C 3.4154720877 -1.9719237213 3.4882839515
C 1.2997703638 -0.7504227501 3.2921553247
C 2.5634263005 -1.4799948521 1.3660879315
C 3.5889088677 -2.0720574938 2.1175078534
C 2.3179531583 -1.3382708661 4.067540716
F 2.372381968 -1.3696953543 5.4021472352
F 4.3321767838 -2.5011834293 4.300344337
C 0. 0.0000000263 5.3907710831

P 0. 0.0000000263 -1.7545267002
C -1.436833974 -0.8295564476 -2.5866164871
C 1.4368339673 -0.8295564592 -2.5866164871
C 0.0000000067 1.6591129858 -2.5866164871
C -1.3030657844 -0.7523253481 -4.1249827046
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C 2.418151806 -1.3961205828 -4.9166415375
C -2.4181518173 -1.3961205633 -4.9166415375
C -6.1075737597 -3.5262092951 -0.4446281784
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C -6.380542473 -3.6838078537 -2.9628596825
C 6.3805424433 -3.6838079052 -2.9628596825
C 6.0982552388 -3.5208293102 -4.135780307
C -6.0982552672 -3.520829261 -4.135780307
F 0.0000000125 3.0990060913 0.0123430185
C 0.0000000284 7.0524187185 -0.4446281784
F -2.683817985 -1.5495029954 0.0123430185
F 2.6838179725 -1.549503017 0.0123430185
C 5.591390867 -3.228191026 -5.4083244031
C 4.4285186523 -2.5568064335 -5.5947206856
C 0.0000000113 2.7922412251 -4.9166415375
C 0.0000000165 4.0870764168 -4.5701292481
C 0.0000000206 5.1136129102 -5.5947206856
C 0.000000026 6.4563820858 -5.4083244031
C 0.0000000298 7.3857982121 -1.6189820795
C 0.0000000297 7.3676158379 -2.9628596825
C 0.0000000284 7.0416586501 -4.135780307
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C 0.0000000254 6.2990256741 0.6688218185
C 0.0000000218 5.398594444 1.4836715538
C 5.4551162173 -3.1495128196 0.6688218185
C -5.4551162427 -3.1495127756 0.6688218185
C 4.6753198995 -2.6992972014 1.4836715538
C -4.6753199213 -2.6992971637 1.4836715538
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H -0.000000006 -1.4999917733 -5.6697633593
H -0.000000001 -2.4879167408 -4.2278783391

H	-0.8750006135	2.2097085785	-2.2402070937
H	0.8750006314	2.2097085715	-2.2402070937
H	1.4761634194	-1.8626270213	-2.2402070937
H	2.3511640479	-0.3470814901	-2.2402070937
H	2.1545991278	1.2439584012	-4.2278783391
H	1.299031007	0.7499959209	-5.6697633593
H	-1.2990310009	0.7499959314	-5.6697633593
H	-2.1545991178	1.2439584185	-4.2278783391
H	-2.2420414579	-1.2944432009	-5.9859494116
H	2.2420414474	-1.294443219	-5.9859494116
H	-1.4761634344	-1.8626270094	-2.2402070937
H	3.8119362585	-2.2008224191	-3.532989037
H	6.15425563	-3.5531611514	-6.2753390411
H	4.1220523075	-2.3798680052	-6.6200026278
H	0.0000000104	2.5888864988	-5.9859494116
H	0.0000000178	4.4016448865	-3.532989037
H	0.0000000192	4.7597360561	-6.6200026278
H	0.0000000287	7.1063223321	-6.2753390411
H	-3.8119362762	-2.2008223884	-3.532989037
H	-4.1220523267	-2.3798679719	-6.6200026278
H	-6.1542556586	-3.5531611018	-6.2753390411
F	-0.0000000005	-1.2469489595	5.8851857021
F	1.0798895015	0.6234745149	5.8851857021
F	-1.0798894964	0.6234745236	5.8851857021

Crypt_GaH_HP

Ga	-1.7961229307	-0.0000002472	0.0000000242
C	-2.8612320884	1.6360886714	-0.3286587182
C	-2.861231968	-0.5334179933	1.5812240067
C	-2.8612319104	-1.1026716189	-1.252565241
C	-4.3716230866	-1.2654720622	3.7512707547
C	-2.2858378904	-0.9272184361	2.7485770783
C	-4.2595491567	-0.4816505439	1.4277681318
C	-4.9971292279	-0.8655456323	2.5657582494
C	-2.9888396933	-1.3148106657	3.8975267351
F	-6.3330162369	-0.8942175277	2.6507508421
F	-5.1495796847	-1.6131908122	4.7820223974
C	-4.371623372	3.881431186	-0.7797047709
C	-4.2595492653	1.4773081393	-0.296762799
C	-2.2858380996	2.8439463579	-0.5712940287
C	-2.9888399899	4.0327620021	-0.8101041861
C	-4.9971294231	2.6547839707	-0.5332950073
C	-4.813004004	-0.0000004353	0.0000000005
F	-6.3330164386	2.7427255469	-0.5509608017
F	-5.1495800486	4.947947601	-0.9939473725
C	-4.3716229497	-2.6159603472	-2.9715659718

C	-4.2595491046	-0.9956587979	-1.1310053182
C	-2.2858377901	-1.9167287551	-2.1772829886
C	-2.9888395511	-2.7179523012	-3.0874225045
C	-4.9971291343	-1.7892396788	-2.0324632448
F	-6.3330161402	-1.8485096095	-2.0997900746
F	-5.1495795102	-3.3347581578	-3.7880750311
C	-6.3604896422	-0.0000005318	-0.0000000116
P	2.7157536655	0.0000000341	0.0000000595
C	3.4293072147	1.6210382398	-0.3256352486
C	3.4293073911	-1.092527456	-1.2410425062
C	3.4293073339	-0.528510548	1.56667795
C	4.9734113705	1.4827459528	-0.2978549629
C	5.4337139798	0.4662950007	-1.3822497921
C	4.9734114795	-0.4834226827	1.4330231082
C	5.4337139294	0.9639163094	1.0949481571
C	5.433714085	-1.4302106992	0.2873018773
C	4.9734115318	-0.9993227454	-1.1351679138
C	5.6354772053	-1.896810207	-2.1546572697
C	5.6354768991	2.8143934311	-0.5653572542
C	-0.022620329	6.4387638871	-1.2934235178
C	-0.0226196284	-4.3395198057	-4.9294213976
C	1.1765833064	6.673883756	-1.340654542
C	5.0355475534	3.9907768216	-0.8016700095
C	5.7332164949	5.2299994401	-1.0506059276
C	1.1765840325	-4.4979829029	-5.109425586
C	5.0355479876	-2.6896548035	-3.0552788323
C	2.5218187846	6.7197945738	-1.3498771128
C	2.5218195158	-4.5289251757	-5.1445741467
C	3.7362446278	-4.4553581826	-5.0610067456
C	3.7362439086	6.6106397068	-1.3279499797
F	-0.9273562219	-0.9526861159	2.82407185
C	-0.0226198554	-2.0992444913	6.2228450295
F	-0.9273564368	2.9220607058	-0.5869856675
F	-0.9273561188	-1.969375169	-2.2370860896
C	5.1263449214	-4.3265460045	-4.9146842998
C	5.733217064	-3.5248508813	-4.0040090959
C	5.6354771061	-0.9175825756	2.720014771
C	5.0355478469	-1.3011214818	3.8569490748
C	5.7332168796	-1.7051478919	5.0546152729
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C	1.1765837972	-2.1759010386	6.4500802703
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C	-2.2388810952	-1.6966153232	5.02932042

C -1.2535094204 -3.9803168835 -4.5213893904
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H 6.8166454603 -1.697242493 5.0311813007
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H 6.8166450774 5.2057524194 -1.0457351466
H 5.7472077347 7.2914445638 -1.4647105089
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F -6.8562426092 -1.2234820691 0.245773831
F -6.8562427424 0.824586585 0.9366791269
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Crypt_B_As

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C -3.0240897538 1.4541087507 -0.2921024638
C -3.0240896469 -0.4740866947 1.4053466525
C -3.0240895955 -0.9800230283 -1.1132441448
C -4.3169712016 -1.2446061323 3.6894173412
C -2.3134800238 -0.845379768 2.5059805658
C -4.4393702317 -0.4683072081 1.3882140964
C -5.0658799844 -0.8665101773 2.5686174606
C -2.9234338735 -1.2501038051 3.7057145052
F -6.3896289795 -0.9196062427 2.726011262
F -4.9832497289 -1.6136845053 4.7834858949

C	-4.3169714823	3.8174315978	-0.7668484861
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C	-2.3134802144	2.5929322782	-0.5208701399
C	-2.9234341554	3.8342943131	-0.7702358521
C	-5.0658801798	2.6577423862	-0.5338892972
C	-5.0465610256	-0.0000004502	-0.0000000012
F	-6.3896291869	2.8205973345	-0.5666037435
F	-4.9832500928	4.9494618875	-0.9942515598
C	-4.3169710668	-2.5728266797	-2.9225688416
C	-4.439370181	-0.9680756848	-1.0996726248
C	-2.3134799322	-1.7475533495	-1.9851103652
C	-2.9234337381	-2.5841914615	-2.9354786067
C	-5.0658798906	-1.7912335632	-2.0347281676
F	-6.3896288799	-1.9009926937	-2.1594075539
F	-4.9832495541	-3.335778721	-3.7892343373
C	-6.5874063415	-0.0000005463	-0.0000000134
As	2.3462222217	0.0000000108	0.0000000569
C	3.3799286924	1.6613801085	-0.3337391529
C	3.3799288732	-1.1197165823	-1.2719276402
C	3.3799288145	-0.5416633004	1.6056669881
C	4.9035138652	1.4803071999	-0.2973650655
C	5.3643923719	0.4653179646	-1.3793535518
C	4.903513974	-0.4826275769	1.4306661413
C	5.3643923215	0.9618966027	1.0926539025
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C	4.9035140263	-0.9976791121	-1.1333008449
C	5.6248660451	-1.8770598557	-2.1322221118
C	5.624865742	2.7850888376	-0.5594705261
C	0.1020109491	6.2304845252	-1.2515842064
C	0.1020116272	-4.199146208	-4.7699658265
C	1.2858051029	6.5287700223	-1.3115039878
C	5.0655455068	3.9806622035	-0.7996381765
C	5.8019995023	5.1959021587	-1.0437564391
C	1.2858058134	-4.4001809068	-4.998328676
C	5.06554594	-2.6828378736	-3.0475352303
C	2.6243503797	6.6598277583	-1.3378309329
C	2.6243511045	-4.4885094619	-5.0986644441
C	3.8419071455	-4.4468827489	-5.0513791927
C	3.8419064274	6.598064295	-1.3254238191
F	-0.9717193281	-0.8238060411	2.4420292609
C	0.1020114072	-2.0313387046	6.0215501505
F	-0.9717195139	2.5267620764	-0.5075777947
F	-0.9717192389	-1.7029566237	-1.9344513738
C	5.2317684281	-4.3162245933	-4.9029598324
C	5.8020000678	-3.5018704042	-3.9779047234
C	5.6248659468	-0.9080283361	2.6916928857

C	5.0655457995	-1.2978237887	3.8471736415
C	5.8019998843	-1.6940310755	5.0216614146
C	5.2317682019	-2.0879752547	6.1894403469
C	1.2858055829	-2.1285892815	6.3098328094
C	2.6243508694	-2.1713182119	6.4364955541
C	3.8419069125	-2.1511812338	6.3768032176
C	5.2317677311	6.4042004202	-1.2864802759
C	-1.1022638676	-1.83925409	5.4521484672
C	-2.0962617456	-1.6149097543	4.7871184889
C	-1.1022636684	-3.8020723134	-4.318914778
C	-1.1022642824	5.6413257907	-1.1332335999
C	-2.0962615707	-3.3383117255	-3.792111853
C	-2.0962621098	4.953220681	-0.9950065701
H	3.0576736892	2.3862169878	0.4151653744
H	6.4576095774	0.4794315118	-1.4211904988
H	5.0129700939	0.7959196894	-2.3593649663
H	3.0576738155	0.1093097664	2.4195960768
H	3.0576739235	-1.5526521181	1.858941889
H	3.0576739112	-0.8335647042	-2.2741070761
H	3.0576739842	-2.1500864158	-1.115132958
H	5.0129702734	-2.441229644	0.4903960829
H	6.4576096855	-1.4705025079	0.2953957459
H	6.4576095254	0.9910717977	1.1257950203
H	5.0129700077	1.645310486	1.8689691169
H	6.7112078704	2.715582995	-0.5455081202
H	6.7112081659	-1.830215042	-2.0790094178
H	3.0576737243	2.0407768149	-1.3044629315
H	3.9875283905	-2.744555344	-3.1176423274
H	5.8652257065	-4.8971590274	-5.5628648551
H	6.8847761041	-3.4646584953	-3.9356344033
H	6.7112080701	-0.8853671039	2.6245178115
H	3.9875282467	-1.3276796741	3.9356760163
H	6.8847759226	-1.6760297649	4.9682998673
H	5.8652254499	-2.3690024964	7.0224968779
H	3.9875279473	4.0722353576	-0.8180334796
H	6.8847755446	5.1406891418	-1.0326651864
H	5.8652249157	7.2661622147	-1.4596317692
F	-7.0723572416	0.399455491	-1.1841180944
F	-7.0723571515	-1.2252049464	0.2461199192
F	-7.0723572849	0.8257477256	0.9379981237

Crypt_BH_HAs

5	-1.9962	0.000195	-0.000186
6	-2.675851	-0.385101	1.403243
6	-2.677153	-1.022239	-1.035277
6	-2.675963	1.408379	-0.367699

6	-4.025044	-2.724669	-2.757447
6	-2.006912	-1.86016	-1.882686
6	-4.086725	-1.018902	-1.031978
6	-4.744295	-1.885457	-1.908837
6	-2.633468	-2.744949	-2.777491
9	-6.073829	-1.992065	-2.016925
9	-4.70487	-3.534192	-3.576114
6	-4.021965	-1.026342	3.739434
6	-4.085386	-0.383807	1.399859
6	-2.004747	-0.700726	2.551885
6	-2.630362	-1.03411	3.765799
6	-4.742052	-0.710023	2.589144
6	-4.693361	0.000982	0.000966
9	-6.071505	-0.749057	2.73657
9	-4.700956	-1.330829	4.850274
6	-4.022219	3.752248	-0.980287
6	-4.085479	1.405049	-0.366062
6	-2.00495	2.560814	-0.669403
6	-2.630622	3.778764	-0.98754
6	-4.742244	2.598154	-0.678235
9	-6.071699	2.745537	-0.717528
9	-4.701155	4.866502	-1.272111
6	-6.234571	0.002111	0.001937
33	2.356849	0.000491	0.000692
6	3.204201	-0.463696	1.684491
6	3.203705	1.690877	-0.44056
6	3.201864	-1.226864	-1.243741
6	4.733694	-0.404546	1.466107
6	5.1733	1.024238	1.037836
6	4.73166	-1.069044	-1.08437
6	5.171779	-1.413117	0.366536
6	5.171139	0.386935	-1.408574
6	4.73332	1.471982	-0.384589
6	5.489	2.740017	-0.715266
6	5.489712	-0.751866	2.729469
6	0.272625	-1.722554	6.267363
6	0.272535	6.288824	-1.643603
6	1.444241	-1.814627	6.601572
6	5.002843	-1.083354	3.933094
6	5.835165	-1.395364	5.073097
6	1.444099	6.624421	-1.731116
6	5.002166	3.947898	-1.030853
6	2.784909	-1.843387	6.706038
6	2.784726	6.729588	-1.758461
6	3.997922	6.621116	-1.730125
6	3.998088	-1.813547	6.597757

9	-0.648247	-1.857898	-1.880133
6	0.267701	-4.570856	-4.623603
9	-0.646039	-0.699352	2.547655
9	-0.646207	2.556386	-0.669298
6	5.366431	6.322786	-1.652085
6	5.834654	5.091208	-1.330114
6	5.48623	-1.989304	-2.018059
6	4.998456	-2.86731	-2.905102
6	5.830363	-3.697264	-3.746992
6	5.361661	-4.592356	-4.651827
6	1.439229	-4.814469	-4.870675
6	2.779896	-4.890003	-4.948504
6	3.993075	-4.810155	-4.869545
6	5.366669	-1.731682	6.30074
6	-0.908766	-4.112947	-4.160322
6	-1.838414	-3.561756	-3.603068
6	-0.904279	5.659207	-1.47923
6	-0.904209	-1.549781	5.640014
6	-1.834614	4.901674	-1.281264
6	-1.834434	-1.341928	4.884994
1	2.867513	-1.458151	1.973874
1	6.263897	1.058427	1.072814
1	4.822286	1.750377	1.774143
1	2.865233	-2.236082	-1.010607
1	2.864579	-0.980401	-2.249495
1	2.868209	2.439081	0.276152
1	2.866428	1.993914	-1.43081
1	4.818804	0.661558	-2.405086
1	6.261668	0.399641	-1.457237
1	6.262408	-1.461527	0.378123
1	4.820082	-2.413553	0.627267
1	6.569806	-0.716929	2.607408
1	6.569116	2.61716	-0.683619
1	2.868366	0.242452	2.442602
1	3.932577	4.115852	-1.074874
1	6.073881	7.117268	-1.859701
1	6.908557	4.949106	-1.293285
1	6.566458	-1.899304	-1.929824
1	3.928767	-2.990374	-3.026571
1	6.904323	-3.592869	-3.644332
1	6.068814	-5.168777	-5.237045
1	3.933272	-1.1304	4.100155
1	6.909098	-1.355999	4.931902
1	6.073928	-1.948294	7.092989
9	-6.726774	0.880375	0.890658
9	-6.728329	0.333137	-1.202309

9 -6.729224 -1.205646 0.318399
1 -0.786122 0 -0.000798
1 0.828665 0.00053 0.001001

Crypt_Al_As

Al -1.1583973639 -0.0000002078 0.0000000293
C -2.1499196101 1.6569800919 -0.3328553871
C -2.1499194883 -0.5402292107 1.6014148125
C -2.1499194298 -1.11675169 -1.2685593608
C -3.7333427552 -1.2614497348 3.7393473855
C -1.6212079578 -0.9417717227 2.7917178934
C -3.5578758318 -0.4802942511 1.4237477716
C -4.3240635921 -0.8572492816 2.5411652879
C -2.3604806087 -1.3226560052 3.9207829996
F -5.6585002309 -0.8795030793 2.6071325458
F -4.5382938496 -1.6014571061 4.7472399813
C -3.7333430397 3.8690941365 -0.7772264822
C -3.5578759401 1.4731483192 -0.2959271569
C -1.6212081702 2.8885841 -0.5802608767
C -2.360480907 4.0568252417 -0.8149380139
C -4.3240637855 2.6293377237 -0.528183333
C -4.1047007179 -0.0000003915 0.0000000062
F -5.6585004293 2.697593828 -0.5418946956
F -4.5382942107 4.9119583445 -0.986717812
C -3.7333426186 -2.6076455067 -2.9621208761
C -3.5578757798 -0.9928551403 -1.1278205833
C -1.6212078558 -1.9468130872 -2.2114569396
C -2.3604804655 -2.7341700847 -3.1058449261
C -4.3240634993 -1.7720896577 -2.0129819416
F -5.6585001357 -1.8180922139 -2.0652378684
F -4.5382936761 -3.310502494 -3.760522161
C -5.6590401297 -0.0000004884 -0.0000000061
As 1.5551826043 -0.0000000385 0.0000000506
C 2.5094012947 1.7045636033 -0.3424139022
C 2.5094014802 -1.1488209584 -1.3049883263
C 2.50940142 -0.5557425819 1.6474024029
C 4.0335491628 1.486038678 -0.2985164267
C 4.4734522819 0.4656529586 -1.3803467552
C 4.033549272 -0.4844962952 1.4362054642
C 4.4734522314 0.9625891556 1.0934406552
C 4.4734523869 -1.4282416838 0.2869063207
C 4.0335493245 -1.0015420346 -1.1376888271
C 4.8481108418 -1.8444547372 -2.0951846987
C 4.848110544 2.7367108598 -0.5497523389
C 0.2691747892 6.8453804289 -1.3751049351
C 0.2691755343 -4.6135662342 -5.2407209245

C	1.4463493954	7.1630809713	-1.4389248249
C	4.4918392123	4.0034518698	-0.8042161928
C	5.4927821219	5.0305418909	-1.0105387557
C	1.446350175	-4.8276860492	-5.4839476426
C	4.491839648	-2.6981974349	-3.0649826898
C	2.7905666193	7.1612897594	-1.4385649775
C	2.7905673987	-4.8264786897	-5.4825762429
C	3.972212425	-4.6325741225	-5.2623129234
C	3.9722116769	6.8735839642	-1.3807704061
F	-0.2631910292	-0.9812683452	2.9087990271
C	0.2691752925	-2.2318145508	6.6158259811
F	-0.2631912505	3.0097277652	-0.6045962757
F	-0.2631909229	-2.0284598758	-2.3042026423
C	5.2638844923	-4.2734716562	-4.8543951865
C	5.4927826694	-3.3904229395	-3.8513073928
C	4.8481107452	-0.8922556221	2.6449372672
C	4.4918395067	-1.305254001	3.8691991038
C	5.4927824918	-1.6401183303	4.8618463932
C	5.2638842684	-2.0672935034	6.1281328965
C	1.4463499221	-2.335395058	6.9228726169
C	2.7905671458	-2.3348109541	6.9211414015
C	3.9722121823	-2.241009505	6.6430835383
C	5.2638838022	6.3407657379	-1.2737374706
C	-0.862982386	-1.9998827458	5.9283042425
C	-1.7073516851	-1.7207160062	5.1007628061
C	-0.8629821694	-4.134120959	-4.6961011723
C	-0.862982837	6.1340031369	-1.2322029753
C	-1.7073514987	-3.557032507	-4.0405649301
C	-1.7073520731	5.2777477872	-1.060197801
H	2.1791184366	2.4199178773	0.4094263108
H	5.5642345945	0.4830417767	-1.4318926737
H	4.1170748051	0.7956465432	-2.3585554445
H	2.1791185653	0.0993446153	2.4522975572
H	2.1791186735	-1.564532476	1.8909972844
H	2.1791186622	-0.8553854001	-2.3004234285
H	2.1791187353	-2.1734242411	-1.1401137351
H	4.1170749845	-2.4403920822	0.4902278146
H	5.5642347034	-1.4815760731	0.2976201935
H	5.5642345422	0.9985349309	1.1342727266
H	4.1170747189	1.6447459027	1.8683278422
H	5.916842231	2.5347787395	-0.5091880473
H	5.9168425069	-1.7083588773	-1.9405884281
H	2.1791184717	2.074079627	-1.3121836555
H	3.4502462346	-2.8959567907	-3.2896248156
H	6.1086310695	-4.7218537735	-5.3637291268
H	6.5272981163	-3.1753852627	-3.6070381806

H 5.9168424174 -0.8264191617 2.4497767302
H 3.4502460829 -1.4009202011 4.1527847241
H 6.52729795 -1.5360937358 4.5534837643
H 6.1086308221 -2.2841985027 6.7711102264
H 3.450245767 4.2968772308 -0.8631597119
H 6.5272976036 4.7114798132 -0.9464453146
H 6.108630307 7.0060530126 -1.4073808404
F -6.1528836492 0.3986720419 -1.1817955184
F -6.1528835593 -1.2228017322 0.2456371786
F -6.1528836924 0.8241281326 0.93615831

Crypt_AIH_HAs

13 1.718656 0.001787 0.000435
6 2.702069 1.607859 -0.454816
6 2.69904 -1.196427 -1.164633
6 2.700963 -0.408949 1.619231
6 4.195967 -2.842164 -2.764123
6 2.119624 -2.077976 -2.020711
6 4.101381 -1.082682 -1.054291
6 4.830489 -1.945507 -1.893127
6 2.812611 -2.951158 -2.869184
9 6.165041 -2.013767 -1.959879
9 4.970616 -3.622633 -3.523008
6 4.202556 3.813687 -1.07984
6 4.104038 1.453189 -0.411653
6 2.124578 2.791181 -0.789368
6 2.819391 3.961471 -1.121225
6 4.835143 2.609859 -0.739182
6 4.657525 -0.000725 -0.001098
9 6.169885 2.699302 -0.764892
9 4.978804 4.859889 -1.376578
6 4.200811 -0.976188 3.840948
6 4.103056 -0.371491 1.463248
6 2.123105 -0.710362 2.811283
6 2.817651 -1.010779 3.990199
6 4.833691 -0.669544 2.628219
9 6.168364 -0.696378 2.718202
9 4.976814 -1.245843 4.894622
6 6.204327 -0.002191 -0.001798
33 -2.671041 0.001465 -0.002121
6 -3.566537 1.65989 -0.477035
6 -3.564443 -0.414987 1.672491
6 -3.566476 -1.240787 -1.198904
6 -5.093914 1.461504 -0.419996
6 -5.542974 1.050864 1.012943
6 -5.093822 -1.092443 -1.054426

6	-5.54393	0.353491	-1.416232
6	-5.542066	-1.402244	0.403549
6	-5.092289	-0.365971	1.474209
6	-5.796418	-0.690004	2.776041
6	-5.799049	2.751063	-0.789223
6	-0.169006	6.299092	-1.786324
6	-0.170372	-1.600461	6.348391
6	-1.368926	6.525525	-1.852278
6	-5.220972	3.916018	-1.118946
6	-5.927093	5.126484	-1.464053
6	-1.37017	-1.655368	6.578254
6	-5.21881	-0.98492	3.950472
6	-2.714553	6.579066	-1.869817
6	-2.71575	-1.665758	6.633507
6	-3.930814	-1.637372	6.533633
6	-3.929662	6.478766	-1.843783
9	0.75813	-2.122293	-2.062796
6	-0.176788	-4.697947	-4.55836
9	0.763198	2.852391	-0.805725
9	0.761725	-0.724057	2.872614
6	-5.322686	-1.587581	6.348966
6	-5.926426	-1.290146	5.170742
6	-5.799726	-2.05773	-1.984904
6	-5.223321	-2.928701	-2.826954
6	-5.931933	-3.832929	-3.70059
6	-5.328962	-4.704786	-4.54762
6	-1.376563	-4.869477	-4.721144
6	-2.722125	-4.912464	-4.75825
6	-3.937205	-4.840407	-4.683752
6	-5.321738	6.295117	-1.79438
6	1.056472	-4.308429	-4.183498
6	2.054092	-3.805902	-3.697881
6	1.062957	-1.471002	5.823722
6	1.064468	5.779737	-1.637737
6	2.06043	-1.301815	5.14546
6	2.062058	5.107532	-1.44639
1	-3.235222	1.946054	-1.474434
1	-6.634561	1.082793	1.044888
1	-5.193705	1.795661	1.731339
1	-3.235285	-1.025679	-2.214099
1	-3.23533	-2.247072	-0.945384
1	-3.232433	0.307425	2.417073
1	-3.232655	-1.401905	1.992827
1	-5.190999	-2.396309	0.689005
1	-6.63354	-1.44708	0.4176
1	-6.635679	0.364225	-1.459274

1	-5.195535	0.602953	-2.420753
1	-6.884919	2.691835	-0.774391
1	-6.882329	-0.674397	2.717035
1	-3.235192	2.429451	0.219055
1	-4.139242	-1.006965	4.031763
1	-5.941953	-1.803066	7.212647
1	-7.009845	-1.281409	5.143543
1	-6.885558	-2.013904	-1.940867
1	-4.143829	-2.989063	-2.88702
1	-7.015332	-3.813642	-3.678428
1	-5.948771	-5.345131	-5.165387
1	-4.141352	3.996889	-1.138886
1	-7.010555	5.099774	-1.45888
1	-5.939968	7.151707	-2.039141
9	6.699515	0.890993	0.86929
9	6.696829	-1.204363	0.336312
9	6.698168	0.305088	-1.211539
1	0.083298	0.003958	0.000176
1	-0.969312	0.002647	-0.003166

Crypt_Ga_As

Ga	-1.1098006598	-0.0000002047	0.0000000297
C	-2.1373140544	1.6676115495	-0.3349910417
C	-2.1373139317	-0.5436954071	1.6116897516
C	-2.1373138729	-1.1239169489	-1.276698645
C	-3.7223618417	-1.2619748651	3.7409040453
C	-1.604618558	-0.9445653938	2.7999992492
C	-3.5401903099	-0.4806209654	1.4247162627
C	-4.3095008284	-0.8576009659	2.5422077978
C	-2.3497142297	-1.3242307945	3.9254511908
F	-5.6439108482	-0.8788241378	2.6051199445
F	-4.5295852209	-1.6015611638	4.7475484438
C	-3.7223621263	3.8707048095	-0.7775500352
C	-3.5401904183	1.4741504157	-0.2961284584
C	-1.604618771	2.8971528016	-0.5819821633
C	-2.3497145283	4.0616554094	-0.8159083012
C	-4.3095010218	2.6304164072	-0.5284000194
C	-4.0830922054	-0.0000003902	0.0000000063
F	-5.6439110464	2.6955113946	-0.5414763746
F	-4.529585582	4.9122775105	-0.9867819261
C	-3.722361705	-2.6087310473	-2.9633539827
C	-3.5401902579	-0.9935305192	-1.1285877725
C	-1.6046184557	-1.9525881145	-2.2180170085
C	-2.3497140863	-2.7374254611	-3.1095428297
C	-4.3095007355	-1.7728166541	-2.0138077647
F	-5.6439107531	-1.8166887193	-2.0636435877

F	-4.5295850474	-3.3107176007	-3.7607665092
C	-5.6380014252	-0.0000004871	-0.0000000059
As	1.5425701482	-0.0000000393	0.0000000505
C	2.4923426435	1.7052735397	-0.3425565151
C	2.4923428291	-1.1492994345	-1.305531844
C	2.4923427689	-0.5559740455	1.6480885331
C	4.0169266722	1.4860113306	-0.2985109335
C	4.4563882424	0.4656835555	-1.3804374576
C	4.0169267814	-0.4844873805	1.4361790347
C	4.456388192	0.9626524061	1.0935125048
C	4.4563883474	-1.4283355343	0.2869251731
C	4.0169268339	-1.0015236051	-1.1376678913
C	4.8330129494	-1.8437632749	-2.0943992401
C	4.8330126516	2.7356849	-0.5495462437
C	0.2716454528	6.8570804515	-1.377455244
C	0.2716461991	-4.6214516726	-5.2496782866
C	1.4489632527	7.1742596184	-1.4411703995
C	4.4803889493	4.0034181784	-0.8042094251
C	5.4854152784	5.0268242845	-1.0097919604
C	1.4489640335	-4.8352200972	-5.4925058475
C	4.480389385	-2.6981747292	-3.0649568969
C	2.7931765188	7.1696193913	-1.4402382399
C	2.7931772991	-4.8320925932	-5.4889532843
C	3.9735065983	-4.6347244404	-5.2647555493
C	3.9735058499	6.8767744994	-1.381411323
F	-0.2496191599	-0.9850614694	2.9200430871
C	0.2716459569	-2.2356291346	6.6271336523
F	-0.2496193821	3.0213619701	-0.6069333629
F	-0.2496190532	-2.0363009539	-2.3131096148
C	5.2625945838	-4.271640854	-4.8523155104
C	5.4854158255	-3.3879173932	-3.8484612493
C	4.8330128528	-0.8919211274	2.643945713
C	4.4803892436	-1.3052430175	3.8691665428
C	5.485415648	-1.6389062715	4.8582534543
C	5.26259436	-2.0664078522	6.1255075371
C	1.4489637802	-2.3390396566	6.9336763965
C	2.7931770459	-2.3375266821	6.9291917054
C	3.9735063555	-2.2420497221	6.6461670813
C	5.262593894	6.3380492843	-1.2731917875
C	-0.8589701886	-2.0029537012	5.9374075566
C	-1.7008011124	-1.7230116683	5.1075678986
C	-0.8589699717	-4.1404691823	-4.7033123549
C	-0.8589706403	6.1434223162	-1.2340951067
C	-1.7008009257	-3.5617780583	-4.0459555783
C	-1.7008015009	5.2847890018	-1.0616122452
H	2.1617915065	2.4199124265	0.409669501

H	5.5471030885	0.4832135436	-1.43240185
H	4.0996618644	0.7956309614	-2.3585092583
H	2.1617916352	0.0995865333	2.4523229811
H	2.1617917434	-1.5647403613	1.8908709695
H	2.1617917321	-0.8551720673	-2.3005403042
H	2.1617918052	-2.1735672196	-1.1399169391
H	4.0996620439	-2.4403442944	0.4902182146
H	5.5471031975	-1.4821029177	0.2977260261
H	5.5471030362	0.9988900054	1.13467607
H	4.0996617783	1.6447136935	1.8682912556
H	5.9012866916	2.53148758	-0.5085269172
H	5.9012869671	-1.7061407434	-1.9380687665
H	2.1617915416	2.0739806843	-1.3124058758
H	3.4397706982	-2.8981933016	-3.2921653506
H	6.1105288181	-4.7173939502	-5.3586630481
H	6.5185527682	-3.1700027017	-3.6009239293
H	5.9012868777	-0.825346139	2.446595938
H	3.4397705464	-1.4020021145	4.1559918662
H	6.5185526022	-1.5334899201	4.5457652035
H	6.110528571	-2.2820410614	6.7647148669
H	3.4397702302	4.3001956531	-0.8638263192
H	6.5185522563	4.7034934348	-0.9448410053
H	6.1105280564	6.9994357483	-1.4060515595
F	-6.1318402409	0.3986168056	-1.1816317759
F	-6.1318401511	-1.222632307	0.2456031448
F	-6.1318402841	0.8240139477	0.9360286018

Crypt_GaH_HAs

31	1.62166	0.000688	0.00022
6	2.654234	-1.212055	-1.155702
6	2.655241	-0.395875	1.627261
6	2.656451	1.606716	-0.47152
6	4.155244	-0.937688	3.851563
6	2.073347	-0.684733	2.820674
6	4.052901	-0.358312	1.467035
6	4.785755	-0.643595	2.636212
6	2.771612	-0.971943	4.000735
9	6.120925	-0.667814	2.724829
9	4.931414	-1.195664	4.909058
6	4.152379	-2.869882	-2.736312
6	4.052087	-1.094005	-1.042749
6	2.071369	-2.100148	-2.002931
6	2.76862	-2.979615	-2.841321
6	4.78394	-1.96548	-1.873623
6	4.605408	-0.00191	-0.000424

9	6.119013	-2.032889	-1.937457
9	4.927686	-3.658252	-3.487757
6	4.15872	3.801804	-1.116746
6	4.053914	1.447474	-0.425236
6	2.075751	2.785597	-0.816994
6	2.775239	3.950097	-1.1595
6	4.787984	2.601445	-0.764294
9	6.123276	2.688335	-0.789895
9	4.935856	4.845415	-1.423688
6	6.152345	-0.003076	-0.000322
33	-2.766152	-0.00261	-0.000703
6	-3.632228	-1.256772	-1.192853
6	-3.626711	1.659292	-0.491397
6	-3.630475	-0.406494	1.682882
6	-5.16052	-1.100778	-1.048296
6	-5.605298	0.344807	-1.420266
6	-5.159213	-0.354406	1.478994
6	-5.608859	-1.397694	0.413475
6	-5.604006	1.061067	1.005676
6	-5.155866	1.461131	-0.431474
6	-5.857187	2.749518	-0.81087
6	-5.864949	-2.072877	-1.972923
6	-0.222234	-4.736199	-4.51431
6	-0.212446	6.280414	-1.845167
6	-1.422367	-4.907172	-4.676232
6	-5.285373	-2.949373	-2.807181
6	-5.987492	-3.863001	-3.676208
6	-1.412415	6.507045	-1.912228
6	-5.275927	3.909811	-1.151297
6	-2.76809	-4.94664	-4.712327
6	-2.758147	6.558799	-1.92791
6	-3.97353	6.461046	-1.899557
6	-3.983422	-4.873356	-4.640818
9	0.714344	-0.699221	2.887445
6	-0.218128	-1.539911	6.360243
9	0.712276	-2.14864	-2.049518
9	0.716862	2.85262	-0.83547
6	-5.36603	6.282424	-1.847676
6	-5.977401	5.119905	-1.506951
6	-5.862278	-0.668258	2.783973
6	-5.281835	-0.952348	3.959776
6	-5.983471	-1.248781	5.185612
6	-5.371912	-1.534932	6.362685
6	-1.418253	-1.593995	6.589537
6	-2.764003	-1.60526	6.641992
6	-3.979358	-1.580128	6.542916

6	-5.376009	-4.739932	-4.511944
6	1.017351	-1.415445	5.839676
6	2.013798	-1.251654	5.158301
6	1.022744	5.766417	-1.69361
6	1.013314	-4.348576	-4.14553
6	2.018645	5.093403	-1.495515
6	2.009979	-3.841354	-3.662455
1	-3.300235	-2.259977	-0.92934
1	-6.696602	0.357716	-1.464653
1	-5.255387	0.58655	-2.426152
1	-3.297993	-1.391826	2.006343
1	-3.294714	0.321804	2.419696
1	-3.292291	1.932551	-1.491227
1	-3.290566	2.431247	0.199354
1	-5.252898	1.8105	1.718307
1	-6.695183	1.096462	1.037327
1	-6.700233	-1.439146	0.426473
1	-5.261516	-2.390726	0.706628
1	-6.950639	-2.02909	-1.930272
1	-6.942978	2.692269	-0.79503
1	-3.297379	-1.046338	-2.207551
1	-4.196006	3.988125	-1.173849
1	-5.98113	7.139359	-2.099464
1	-7.060888	5.098021	-1.501298
1	-6.94802	-0.653895	2.725411
1	-4.201979	-0.971522	4.039484
1	-7.066957	-1.24267	5.163963
1	-5.98684	-1.745122	7.230877
1	-4.205575	-3.009171	-2.864173
1	-7.070965	-3.847241	-3.65995
1	-5.990888	-5.387118	-5.127703
9	6.647357	0.29185	-1.212809
9	6.647515	0.89893	0.861999
9	6.64553	-1.201402	0.350299
1	0.038507	0.000722	0.000655
1	-1.165224	-0.003455	-0.00009