

Electronic Supplementary Information

Theoretical study of fructose adsorption and conversion to trioses on metal–organic frameworks

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Table S1 Adsorption energy of fructose and the overall barrier of the reaction without thermal correction on NU-1000 with 4- and 8-connected linkers, and UIO-66 with 4- and 11-connected linkers.

MOFs	Zr-NU-1000		Hf-UIO-66	
	4-connected	8-connected	4-connected	11-connected
Fructose adsorption (kcal/mol)	-58.1	-57.9	-60.4	-59.5
Overall barrier (kcal/mol)	37.1	37.2	36.3	36.4

Table S1. Optimized key distances of the species involved in the ring-opening of fructose over Zr-NU-1000.

Distance (Å)	Isolated cluster	Ads	TS1	Int1	TS2	Int2
Zr-O2	-	2.33	2.29	2.14	2.15	2.26
Zr-O	2.03	2.13	2.17	2.25	2.14	2.17
O2-H1	0.97	1.03	1.14	1.69	2.56	2.89
O-H1	-	1.53	1.28	1.00	1.50	1.72
C1-O2	1.39	1.42	1.40	1.36	1.26	1.23
C1-O1	1.44	1.41	1.42	1.44	1.81	2.33
O1-H1	2.66	2.37	2.41	2.45	1.04	0.99

Table S2. Optimized key distances of the species involved in the retro-aldol fragmentation pathway over Zr-NU-1000.

Distance (Å)	Int2	Int2_Ro_1	TS3_1	Int3_1	TS4_1	Prod_1
Zr-O2	2.26	2.32	2.10	2.07	2.22	2.29
Zr-O	2.17	2.08	2.26	2.36	2.16	2.08
C1-O2	1.23	1.22	1.29	1.33	1.26	1.22
C2-C3	1.53	1.55	2.46	3.00	3.26	3.13
O4-H2	0.97	0.96	1.22	1.71	3.20	2.76
O-H2	-	3.64	1.20	1.00	1.36	5.18
C2-H2	2.70	3.20	3.59	3.59	1.31	1.10

Table S3. Optimized key distances of the species involved in an intramolecular hydrogen shift pathway over Zr-NU-1000.

Distance (Å)	Int2	Int2_Ro_2	TS3_2	Prod_2
Zr-O4	5.57	2.45	2.32	2.33
Zr-O	2.17	2.01	2.12	2.10
C2-C3	1.55	1.53	2.00	3.67
O4-H3	0.96	0.98	1.33	3.87
C2-H3	3.20	2.34	1.42	1.10
C3-O4	1.42	1.44	1.36	1.22

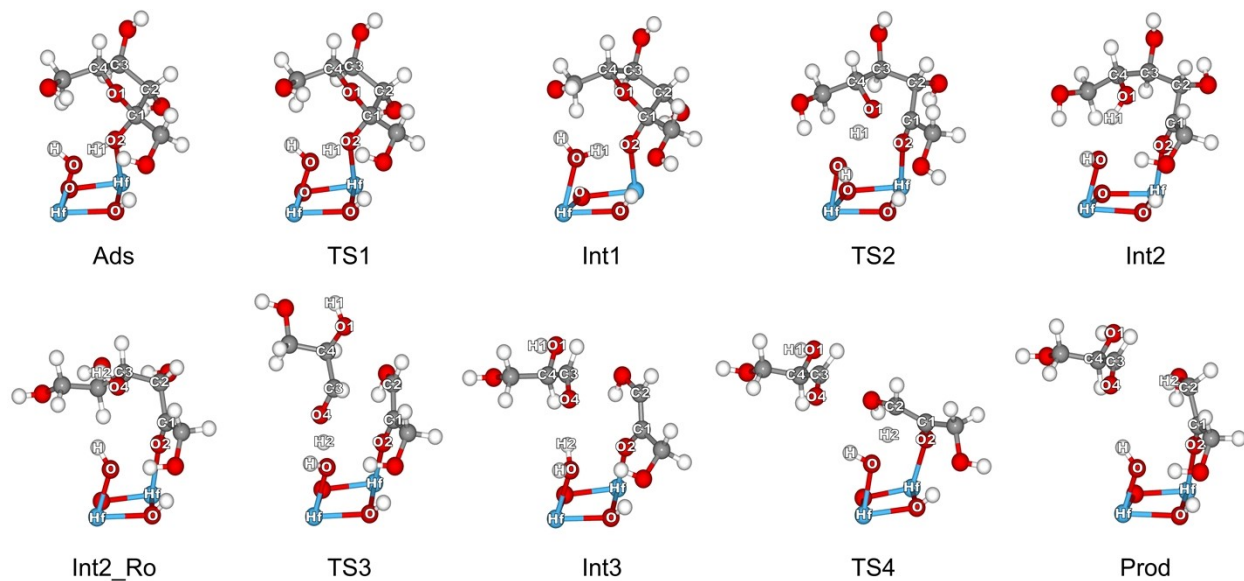


Figure S1. Optimized structures of the fructose conversion into GLA and DHA over Hf-NU-1000.

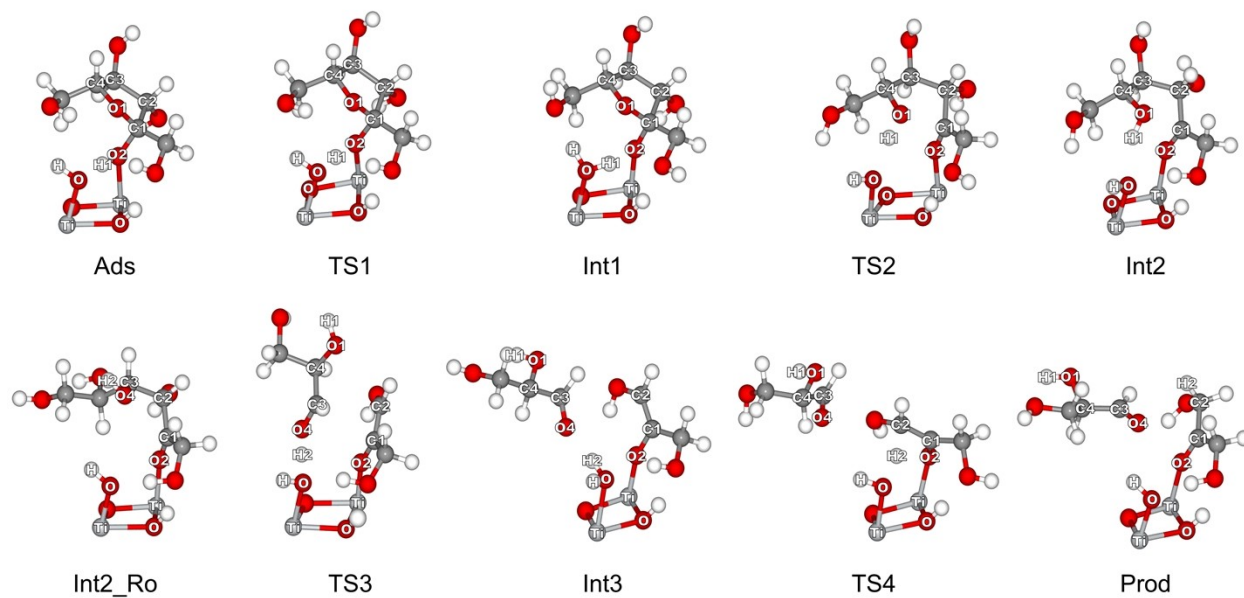


Figure S2. Optimized structures of the fructose conversion into GLA and DHA over Ti-NU-1000.

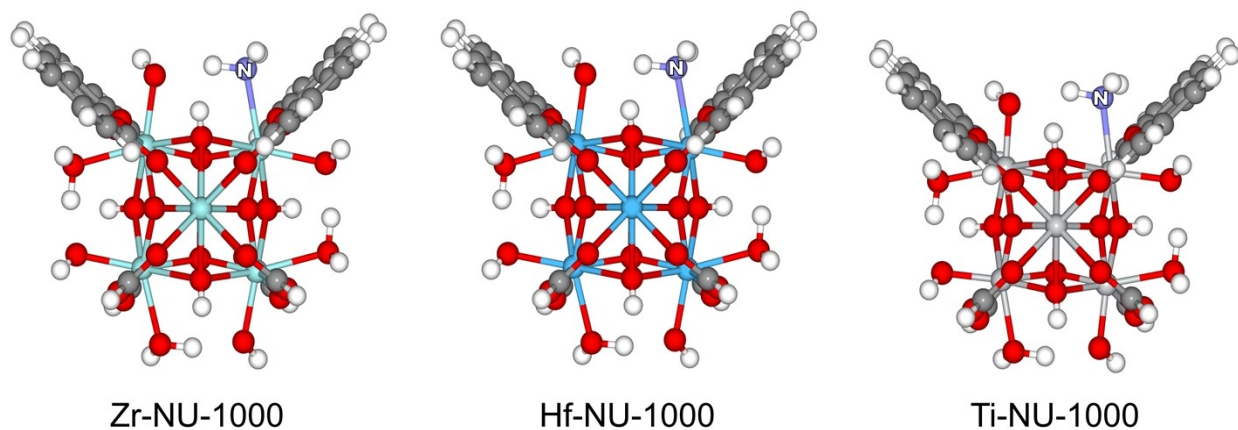


Figure S3. Optimized structures of the ammonia adsorption on NU-1000 MOFs and their binding free energies.

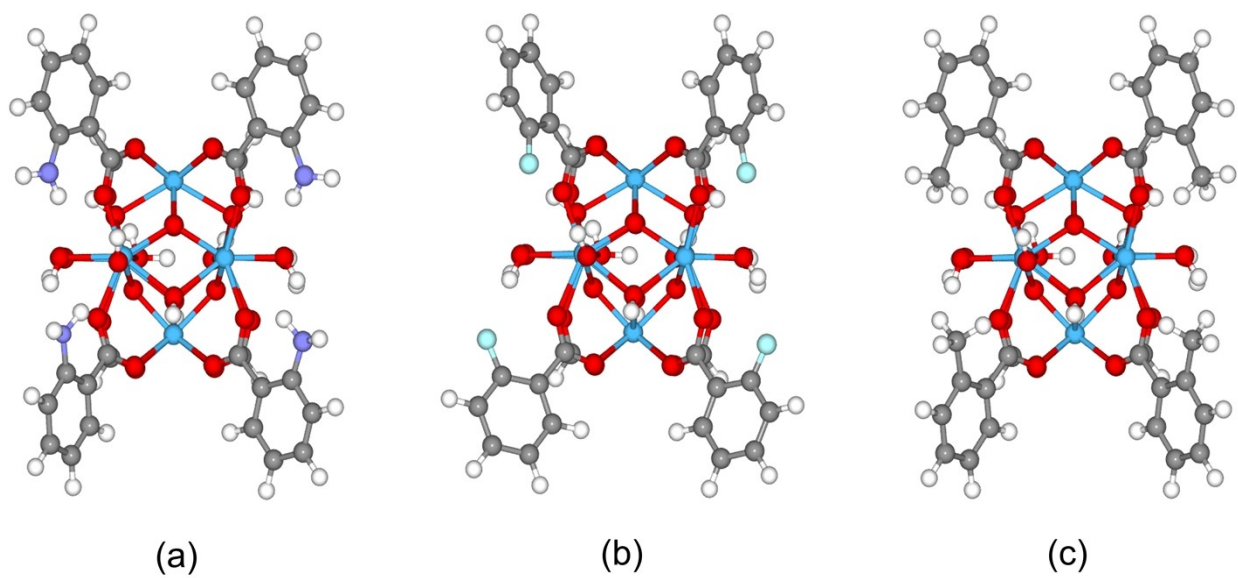


Figure S4. Cluster models of the functionalized Hf-NU-1000; (a) -NH₂, (b) -F, and (c) -CH₃. Hf, O, C, H, N and F are represented in blue, red, grey, white, dark blue, and green, respectively.

Turnover frequencies (TOF).

The turnover frequencies (TOF) for the catalytic pathways are calculated by using the energy span model of Kozuch and Shaik⁴² through equation (1):

$$TOF = \frac{k_B T}{h} \frac{e^{-\Delta G_r/RT} - 1}{\sum_{i=1, j=0}^N e^{(T_i - I_j - \delta G_{ij}/RT)}} \quad (1)$$

k_B is Boltzmann's constant, h is Planck's constant, T is the absolute temperature, R is the universal gas constant, N is the number of steps in the catalytic cycle, ΔG_r is the reaction's Gibbs free energy, T_i represents the energies of transition states, I_j denotes the energies of intermediates, and δG_{ij} is defined as ΔG_r if $i > j$ and 0 if $i \leq j$. In this study, the reaction is exergonic ($\Delta G_r < 0$), and Equation 1 can be simplified to:

$$TOF \approx \frac{k_B T}{h} e^{-\delta G/RT} \quad (2)$$

with δG being defined to be $T_{TDTS} - I_{TDI}$, as the TDI precedes the TDTS for all catalytic cycles in this work. In Equation 2, the TOF is contributed by two states forming the energy span so-called the TOF-determining intermediate (TDI) and TOF-determining transition state (TDTS). In our work, the TDI is Int1, whereas the TDTS is TS4.

Coordinates of all optimized structures.

1. Zr-NU-1000 case

Zr-NU-1000

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086956000	2.683362000	3.474348000
H	4.063785000	-3.157376000	3.120923000
H	-4.031448000	2.543433000	3.686468000
H	-4.029729000	-2.994711000	3.375702000
C	5.678221000	-2.765225000	-1.968617000
C	-5.649623000	-2.654502000	-2.168031000
C	4.334716000	-3.004251000	-2.287446000
C	-4.294245000	-2.873606000	-2.447464000
C	4.015928000	-3.929002000	-3.290650000
C	-3.932161000	-3.748086000	-3.480157000
C	5.027546000	-4.604846000	-3.966247000
C	-4.914367000	-4.393807000	-4.225056000
C	6.363864000	-4.363671000	-3.643253000
C	-6.263287000	-4.170067000	-3.944400000
C	6.687689000	-3.444053000	-2.644448000
C	-6.629590000	-3.300494000	-2.915801000
C	5.642417000	3.002280000	-1.555784000
C	-5.694195000	2.738366000	-1.818856000
C	4.305595000	3.214983000	-1.916359000
C	-4.352012000	3.027893000	-2.096938000
C	3.987027000	4.232951000	-2.824620000
C	-4.037169000	4.070745000	-2.977899000
C	4.993353000	5.029369000	-3.363372000
C	-5.052460000	4.813154000	-3.573678000
C	6.322985000	4.817967000	-2.994966000
C	-6.388096000	4.518312000	-3.295445000
C	6.646069000	3.804827000	-2.090923000
C	-6.707524000	3.480992000	-2.417917000

H	5.91000000	-2.041419000	-1.185130000
H	-5.913874000	-1.971177000	-1.358783000
H	2.965771000	-4.102970000	-3.532551000
H	-2.871781000	-3.910644000	-3.681015000
H	4.775296000	-5.322943000	-4.749665000
H	-4.629197000	-5.075792000	-5.029303000
H	7.733789000	-3.255763000	-2.393033000
H	-7.685593000	-3.126421000	-2.697288000
H	5.874001000	2.203213000	-0.848922000
H	-5.922504000	1.924687000	-1.128001000
H	2.942199000	4.376227000	-3.107933000
H	-2.986603000	4.288503000	-3.179680000
H	4.742265000	5.817767000	-4.076547000
H	-4.803286000	5.626903000	-4.258490000
H	7.687086000	3.640229000	-1.803699000
H	-7.753105000	3.251630000	-2.200222000
H	-7.033735000	-4.676908000	-4.530556000
H	7.157537000	-4.894971000	-4.173957000
H	-7.184619000	5.101103000	-3.764486000
H	7.112208000	5.445066000	-3.416753000
H	-1.925409000	-2.954614000	0.622181000
H	-0.871017000	1.410804000	5.075646000
H	-0.010757000	0.106277000	4.800275000
H	0.021232000	4.010961000	0.564979000
H	0.652989000	4.302714000	2.640349000
H	0.868467000	4.306687000	-0.740435000
H	1.962876000	-0.169559000	3.582645000
H	-1.937445000	2.793681000	0.826078000
H	-0.605581000	-1.982688000	5.137817000
H	0.894888000	-4.438700000	2.213880000
H	0.691959000	-4.440747000	-1.138847000
H	0.036124000	-4.156529000	0.910138000
O	-1.063919000	-0.101326000	2.190762000
O	-3.619477000	1.286652000	2.167780000
O	-3.610371000	1.334904000	-0.630233000
O	-3.608551000	-1.508232000	2.086284000
O	-2.049388000	-2.646119000	3.248123000
O	0.044268000	-4.080035000	1.924787000
O	2.076556000	-2.825573000	3.005400000
O	2.047127000	-2.549146000	-1.862241000
O	3.630235000	-1.526407000	2.023340000
O	3.601356000	-1.433256000	-0.689278000
O	3.649088000	1.283984000	2.096557000
O	3.585104000	1.355086000	-0.652664000
O	2.030867000	2.689980000	-1.555499000
O	2.098445000	2.450776000	3.238011000

O	1.071278000	1.381143000	0.725378000
O	1.410840000	-0.120622000	2.792358000
O	0.036194000	-1.507218000	4.598789000
O	-0.022937000	1.118272000	4.713751000
O	1.071491000	-1.551540000	0.711826000
O	-1.386655000	-2.157503000	0.702945000
O	-2.026573000	-2.362188000	-1.968573000
O	0.006853000	-3.935474000	-0.687607000
O	-3.622137000	-1.444752000	-0.688212000
O	-0.005233000	3.781635000	2.167725000
O	0.018324000	3.949761000	-0.448571000
O	-1.393729000	1.998128000	0.770033000
O	-2.046890000	2.256393000	3.451979000
O	-2.074446000	2.502800000	-1.771691000
O	1.331427000	-0.052916000	-1.415530000
O	-1.079007000	-0.057158000	-0.749515000
Hf	2.535838000	-0.053703000	0.697589000
Hf	-0.021675000	-1.860507000	2.537706000
Hf	0.036224000	1.712038000	2.490636000
Hf	-0.047621000	1.740609000	-1.114049000
Hf	-2.539398000	-0.065881000	0.715114000
Hf	0.020779000	-1.855474000	-0.994698000
H	1.862959000	0.025816000	-2.217973000
O	0.063981000	1.618933000	-3.135157000
H	-0.697872000	1.841724000	-3.677665000

Zr-NU-1000 adsorption O2 mode

C	-3.248217000	-2.182786000	-1.650097000
C	-3.229703000	-2.386601000	2.899998000
C	-3.232304000	2.034304000	3.104001000
C	3.276892000	2.141996000	2.939207000
C	3.226874000	2.366332000	-1.338705000
C	3.259377000	-2.277981000	-1.561482000
C	-3.265317000	2.236121000	-1.457290000
C	3.257197000	-2.506585000	2.716367000
H	4.089823000	2.704071000	3.450200000
H	4.063883000	-3.140757000	3.147131000
H	-4.030453000	2.565567000	3.668987000
H	-4.031490000	-2.988154000	3.383001000
C	5.677622000	-2.581911000	-2.126090000
C	-5.560712000	-2.078875000	-2.591632000
C	4.350679000	-3.007017000	-2.271970000
C	-4.320946000	-2.728847000	-2.527648000
C	4.070058000	-4.108749000	-3.091190000
C	-4.086720000	-3.853042000	-3.329646000
C	5.097143000	-4.771442000	-3.757194000

C	-5.073738000	-4.312298000	-4.197111000
C	6.414704000	-4.333823000	-3.616120000
C	-6.299411000	-3.649365000	-4.271129000
C	6.702702000	-3.239041000	-2.800181000
C	-6.542528000	-2.534392000	-3.466544000
C	5.637004000	2.970531000	-1.664399000
C	-5.689826000	2.688222000	-1.888473000
C	4.291044000	3.182076000	-1.989342000
C	-4.346542000	2.968392000	-2.171996000
C	3.953312000	4.161716000	-2.931887000
C	-4.030412000	3.935714000	-3.134324000
C	4.949024000	4.920537000	-3.540386000
C	-5.044387000	4.611970000	-3.805649000
C	6.288080000	4.709652000	-3.208031000
C	-6.380605000	4.328033000	-3.520022000
C	6.630468000	3.734877000	-2.269500000
C	-6.702112000	3.366682000	-2.560495000
H	5.883592000	-1.726491000	-1.480380000
H	-5.727367000	-1.204670000	-1.958554000
H	3.040898000	-4.464031000	-3.184972000
H	-3.122969000	-4.363572000	-3.267909000
H	4.870979000	-5.636132000	-4.384949000
H	-4.879569000	-5.184725000	-4.824490000
H	7.734004000	-2.897326000	-2.688253000
H	-7.502351000	-2.016288000	-3.525618000
H	5.883262000	2.201497000	-0.929747000
H	-5.919734000	1.934395000	-1.132993000
H	2.901187000	4.308527000	-3.184748000
H	-2.980308000	4.147160000	-3.343681000
H	4.682081000	5.679659000	-4.279143000
H	-4.793695000	5.363955000	-4.557061000
H	7.678813000	3.570623000	-2.010031000
H	-7.748311000	3.146626000	-2.336161000
H	-7.070650000	-4.003949000	-4.959267000
H	7.220720000	-4.851480000	-4.141474000
H	-7.176106000	4.859288000	-4.048221000
H	7.069176000	5.307287000	-3.684249000
H	-1.933875000	-2.915234000	0.605547000
H	-0.885087000	1.318093000	5.124498000
H	-0.010913000	0.028379000	4.809497000
H	0.033592000	4.027903000	0.646319000
H	0.683867000	4.267697000	2.698370000
H	0.922784000	4.305899000	-0.635808000
H	1.974245000	-0.215291000	3.564936000
H	-1.943682000	2.795149000	0.830054000
H	-0.633094000	-2.031787000	5.069146000

H	0.897060000	-4.460540000	2.160691000
H	-0.401726000	-4.527514000	-1.306217000
H	0.023574000	-4.186935000	0.863625000
O	-1.055421000	-0.098935000	2.190131000
O	-3.619670000	1.293262000	2.166642000
O	-3.613156000	1.362810000	-0.609403000
O	-3.614305000	-1.504671000	2.091834000
O	-2.050988000	-2.658816000	3.235743000
O	0.038330000	-4.111366000	1.884687000
O	2.076417000	-2.844877000	2.977591000
O	2.065705000	-2.530279000	-1.902927000
O	3.633041000	-1.527609000	2.024944000
O	3.602025000	-1.438004000	-0.689257000
O	3.642003000	1.280713000	2.104081000
O	3.596353000	1.402273000	-0.607982000
O	2.021301000	2.686801000	-1.559461000
O	2.101277000	2.441467000	3.269779000
O	1.064387000	1.412737000	0.777108000
O	1.409097000	-0.141578000	2.785848000
O	0.038328000	-1.551832000	4.570140000
O	-0.030124000	1.047732000	4.762014000
O	1.057634000	-1.569617000	0.660830000
O	-1.402515000	-2.114904000	0.688622000
O	-2.055440000	-2.519753000	-1.898166000
O	0.023335000	-3.942315000	-0.669832000
O	-3.603054000	-1.388967000	-0.729255000
O	-0.009609000	3.784129000	2.233938000
O	0.052996000	3.976370000	-0.369951000
O	-1.387474000	2.006917000	0.799484000
O	-2.050714000	2.232463000	3.481651000
O	-2.064252000	2.518465000	-1.747559000
O	1.382695000	0.015379000	-1.317453000
O	-1.083320000	-0.040579000	-0.783600000
H	1.910121000	0.043229000	-2.141270000
O	-0.019262000	1.550693000	-3.157033000
H	-0.833175000	1.936529000	-3.509487000
Zr	2.512614000	-0.071597000	0.695373000
Zr	-0.014953000	-1.889511000	2.490082000
Zr	0.032491000	1.705656000	2.557246000
Zr	-0.025685000	1.753499000	-1.015868000
Zr	-2.526640000	-0.068981000	0.721139000
Zr	-0.001172000	-1.874898000	-1.113373000
C	-1.379309000	-2.784908000	-5.093353000
C	0.094809000	-2.857804000	-4.684621000
C	0.452903000	-1.381778000	-4.527115000
C	-1.534651000	-1.389347000	-5.711911000

C	1.926714000	-0.991120000	-4.654830000
C	-2.597861000	-0.517954000	-5.064569000
H	2.554938000	-1.803130000	-4.259635000
H	0.698912000	-3.287427000	-5.511650000
H	-1.954889000	-2.831536000	-4.159043000
H	-1.547755000	0.998435000	-5.551966000
H	2.153409000	-0.898961000	-5.731530000
H	1.584619000	0.859011000	-4.051600000
H	-2.505993000	-0.596579000	-3.961252000
H	-3.599386000	-0.896836000	-5.325807000
H	1.156888000	-3.548689000	-3.187247000
H	-0.124174000	0.017681000	-3.237028000
H	-1.360935000	-3.837038000	-6.718747000
H	-1.716442000	-1.451500000	-6.798798000
O	-1.841782000	-3.845793000	-5.882476000
O	2.270411000	0.168233000	-3.942538000
O	-2.495641000	0.810889000	-5.502535000
O	-0.083804000	-1.004170000	-3.275346000
O	0.234618000	-3.595168000	-3.500682000
O	-0.254024000	-0.740125000	-5.557294000

Zr-NU-1000 adsorption O3 mode

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087259000	2.689888000	3.469103000
H	4.061728000	-3.151149000	3.136149000
H	-4.030391000	2.553642000	3.680041000
H	-4.031760000	-2.992335000	3.377220000
C	5.671846000	-2.582553000	-2.177708000
C	-5.591307000	-2.155701000	-2.542524000
C	4.328764000	-2.932864000	-2.366706000
C	-4.292773000	-2.678093000	-2.593511000
C	3.995972000	-3.888066000	-3.335575000
C	-3.969975000	-3.632102000	-3.568531000
C	4.987943000	-4.480136000	-4.110708000
C	-4.931175000	-4.053262000	-4.483357000
C	6.324383000	-4.124778000	-3.919764000
C	-6.220956000	-3.521004000	-4.433514000
C	6.664176000	-3.177987000	-2.951755000
C	-6.549530000	-2.573998000	-3.462423000

C	5.627411000	3.053842000	-1.544743000
C	-5.688918000	2.757441000	-1.820092000
C	4.289751000	3.234335000	-1.919934000
C	-4.345947000	3.007735000	-2.131535000
C	3.958947000	4.236731000	-2.841040000
C	-4.027002000	3.985298000	-3.082873000
C	4.953520000	5.048571000	-3.378719000
C	-5.038740000	4.701608000	-3.715469000
C	6.283777000	4.868327000	-2.996513000
C	-6.374872000	4.447825000	-3.401761000
C	6.619189000	3.871237000	-2.079192000
C	-6.698607000	3.476249000	-2.453270000
H	5.918063000	-1.836422000	-1.419883000
H	-5.826806000	-1.414276000	-1.776364000
H	2.950457000	-4.162142000	-3.477212000
H	-2.959350000	-4.046695000	-3.583145000
H	4.712632000	-5.220911000	-4.865258000
H	-4.677193000	-4.801974000	-5.237249000
H	7.710262000	-2.901194000	-2.802471000
H	-7.559175000	-2.159051000	-3.423894000
H	5.868439000	2.267277000	-0.827066000
H	-5.920489000	1.994951000	-1.073915000
H	2.914382000	4.358250000	-3.134887000
H	-2.976457000	4.171742000	-3.313127000
H	4.692668000	5.824902000	-4.101526000
H	-4.786324000	5.462596000	-4.457276000
H	7.660605000	3.731108000	-1.780803000
H	-7.744588000	3.280237000	-2.206677000
H	-6.974266000	-3.848461000	-5.153949000
H	7.105571000	-4.588021000	-4.527428000
H	-7.168429000	5.011304000	-3.898569000
H	7.063678000	5.507487000	-3.417493000
H	-1.933558000	-2.948863000	0.626478000
H	-0.883321000	1.361435000	5.101331000
H	-0.013506000	0.066308000	4.807905000
H	0.033514000	4.013442000	0.596313000
H	0.684174000	4.275361000	2.653460000
H	0.914522000	4.287197000	-0.691269000
H	1.963372000	-0.181835000	3.588179000
H	-1.936758000	2.796651000	0.827070000
H	-0.634205000	-2.005256000	5.090152000
H	0.894140000	-4.463818000	2.176143000
H	0.811049000	-4.394524000	-1.081310000
H	0.029558000	-4.168157000	0.879706000
O	-1.063447000	-0.100929000	2.196478000
O	-3.622244000	1.291520000	2.167773000

O	-3.614200000	1.348716000	-0.622549000
O	-3.613217000	-1.509035000	2.087724000
O	-2.052433000	-2.650334000	3.247423000
O	0.040152000	-4.106997000	1.895328000
O	2.076300000	-2.837820000	2.986032000
O	2.060204000	-2.610368000	-1.799343000
O	3.638407000	-1.526828000	2.029897000
O	3.615867000	-1.422048000	-0.702215000
O	3.648497000	1.283429000	2.102698000
O	3.597360000	1.388060000	-0.626637000
O	2.020655000	2.660546000	-1.589121000
O	2.099788000	2.454080000	3.247306000
O	1.066110000	1.391656000	0.744686000
O	1.412623000	-0.124961000	2.797501000
O	0.037889000	-1.530850000	4.586677000
O	-0.028593000	1.082044000	4.745039000
O	1.069624000	-1.543229000	0.698794000
O	-1.383690000	-2.159301000	0.699269000
O	-2.049138000	-2.498627000	-1.891659000
O	0.027211000	-3.962390000	-0.721181000
O	-3.623464000	-1.434143000	-0.699904000
O	-0.004509000	3.784735000	2.189427000
O	0.047394000	3.955924000	-0.419085000
O	-1.389968000	2.002518000	0.782356000
O	-2.048805000	2.246134000	3.465550000
O	-2.066969000	2.501972000	-1.766269000
O	1.381150000	-0.030998000	-1.355398000
O	-1.077434000	-0.057910000	-0.738989000
H	1.921370000	0.006310000	-2.155249000
O	-0.039597000	1.351623000	-3.139290000
H	-0.840293000	1.656565000	-3.587792000
Zr	2.532427000	-0.073312000	0.699929000
Zr	-0.013261000	-1.877193000	2.511824000
Zr	0.036334000	1.708846000	2.524298000
Zr	-0.037997000	1.730655000	-1.061494000
Zr	-2.532836000	-0.075287000	0.726420000
Zr	0.015959000	-1.874909000	-1.067377000
C	-1.044517000	-0.717353000	-5.452890000
C	-0.636462000	-1.734421000	-4.401589000
C	0.264344000	-2.667388000	-5.197652000
C	-1.206402000	-1.603083000	-6.689740000
C	0.431398000	-4.055316000	-4.614197000
C	-0.732550000	-0.987498000	-7.984816000
H	0.817796000	-3.962709000	-3.587330000
H	-1.535404000	-2.308220000	-4.106912000
H	-0.211684000	-0.008312000	-5.600270000

H	-0.390162000	-2.681989000	-8.781369000
H	-0.547395000	-4.562709000	-4.562923000
H	1.006368000	-4.950541000	-6.222350000
H	0.310130000	-0.636812000	-7.841689000
H	-1.344062000	-0.100948000	-8.213615000
H	-0.022283000	-0.154666000	-3.288854000
H	2.132554000	-2.770966000	-5.576286000
H	-2.904753000	-0.506053000	-4.929900000
H	-2.267968000	-1.902158000	-6.796048000
O	-2.157026000	0.073930000	-5.128565000
O	1.385060000	-4.790155000	-5.348630000
O	-0.850924000	-1.879327000	-9.056452000
O	1.500219000	-2.061126000	-5.383149000
O	-0.034645000	-1.193785000	-3.260720000
O	-0.446224000	-2.799192000	-6.433959000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087277000	2.690437000	3.468677000
H	4.061475000	-3.150197000	3.138067000
H	-4.030349000	2.553857000	3.679975000
H	-4.031391000	-2.990822000	3.379680000
C	5.679759000	-2.695577000	-2.061628000
C	-5.639033000	-2.341013000	-2.386634000
C	4.332114000	-2.974195000	-2.326207000
C	-4.303799000	-2.733887000	-2.546333000
C	4.000811000	-3.907448000	-3.318049000
C	-3.963574000	-3.620693000	-3.576143000
C	5.004429000	-4.551552000	-4.035411000
C	-4.943586000	-4.102490000	-4.438925000
C	6.345042000	-4.271497000	-3.766962000
C	-6.271473000	-3.704735000	-4.277082000
C	6.680977000	-3.343455000	-2.779370000
C	-6.617910000	-2.825588000	-3.249517000
C	5.629801000	3.044062000	-1.555908000
C	-5.690093000	2.736949000	-1.837829000
C	4.290730000	3.233202000	-1.921642000
C	-4.346779000	3.013259000	-2.124173000
C	3.959481000	4.242971000	-2.834531000

C	-4.028719000	4.023699000	-3.040801000
C	4.954669000	5.053405000	-3.373314000
C	-5.041584000	4.747119000	-3.663452000
C	6.286435000	4.863998000	-3.000877000
C	-6.378187000	4.466307000	-3.375803000
C	6.622414000	3.859504000	-2.091905000
C	-6.701020000	3.461393000	-2.462512000
H	5.922019000	-1.966379000	-1.286174000
H	-5.887513000	-1.648084000	-1.580497000
H	2.953490000	-4.126706000	-3.531680000
H	-2.922194000	-3.931405000	-3.682755000
H	4.733263000	-5.276510000	-4.806512000
H	-4.671074000	-4.791876000	-5.241382000
H	7.730416000	-3.124815000	-2.569169000
H	-7.657621000	-2.515158000	-3.123598000
H	5.871299000	2.252119000	-0.844370000
H	-5.920926000	1.948925000	-1.118623000
H	2.913559000	4.372341000	-3.120204000
H	-2.977922000	4.231378000	-3.250894000
H	4.693052000	5.836277000	-4.088812000
H	-4.789712000	5.534956000	-4.376944000
H	7.664934000	3.712192000	-1.800916000
H	-7.747328000	3.243418000	-2.236766000
H	-7.041006000	-4.082439000	-4.954775000
H	7.132986000	-4.778664000	-4.329285000
H	-7.172733000	5.034755000	-3.865352000
H	7.066897000	5.502029000	-3.422547000
H	-1.934843000	-2.947204000	0.620753000
H	-0.884402000	1.356418000	5.100616000
H	-0.014102000	0.061896000	4.805105000
H	0.033176000	4.014790000	0.600279000
H	0.684028000	4.274582000	2.656132000
H	0.918471000	4.287966000	-0.684272000
H	1.962500000	-0.183875000	3.585555000
H	-1.938144000	2.798989000	0.828402000
H	-0.634488000	-2.008895000	5.083786000
H	0.893911000	-4.464928000	2.168993000
H	0.808831000	-4.391480000	-1.096631000
H	0.033054000	-4.165317000	0.871074000
O	-1.063270000	-0.101191000	2.193310000
O	-3.622058000	1.292276000	2.167241000
O	-3.612809000	1.347414000	-0.624745000
O	-3.613545000	-1.508078000	2.089060000
O	-2.051673000	-2.652881000	3.243310000
O	0.041032000	-4.106370000	1.887100000
O	2.076006000	-2.838630000	2.983279000

O	2.059202000	-2.586915000	-1.826161000
O	3.638708000	-1.526488000	2.030215000
O	3.613407000	-1.420007000	-0.702555000
O	3.648655000	1.284048000	2.102229000
O	3.597648000	1.389413000	-0.626240000
O	2.021117000	2.662275000	-1.590817000
O	2.099820000	2.453118000	3.248481000
O	1.065680000	1.397262000	0.745719000
O	1.411944000	-0.125478000	2.794860000
O	0.037729000	-1.533318000	4.581590000
O	-0.029267000	1.078100000	4.744492000
O	1.069865000	-1.542259000	0.693698000
O	-1.384637000	-2.157708000	0.692322000
O	-2.044802000	-2.466119000	-1.913857000
O	0.033176000	-3.952999000	-0.726201000
O	-3.619636000	-1.432352000	-0.697803000
O	-0.005453000	3.785654000	2.191507000
O	0.049192000	3.959471000	-0.415789000
O	-1.390870000	2.005292000	0.782290000
O	-2.048815000	2.245407000	3.466523000
O	-2.067029000	2.504791000	-1.766536000
O	1.381495000	-0.018542000	-1.349363000
O	-1.074333000	-0.051689000	-0.739471000
H	1.925676000	0.016954000	-2.145431000
O	-0.045997000	1.349581000	-3.146450000
H	-0.833755000	1.672831000	-3.603309000
Zr	2.530180000	-0.072527000	0.700784000
Zr	-0.013944000	-1.878348000	2.505784000
Zr	0.034696000	1.708381000	2.524770000
Zr	-0.039878000	1.734547000	-1.060381000
Zr	-2.534490000	-0.076437000	0.723107000
Zr	0.015598000	-1.867840000	-1.077028000
C	-0.521874000	-1.798578000	-4.410916000
C	-0.822154000	-0.846825000	-5.559495000
C	-0.864615000	-1.835254000	-6.722321000
C	0.440827000	-2.797526000	-5.035433000
C	-0.661595000	-1.270378000	-8.111844000
C	0.266097000	-4.213127000	-4.547227000
H	-1.391806000	-0.466007000	-8.279903000
H	0.030011000	-0.158492000	-5.696882000
H	-1.465069000	-2.303272000	-4.134951000
H	1.155303000	-4.973323000	-6.062208000
H	0.349293000	-0.836872000	-8.198364000
H	-0.204613000	-2.922152000	-8.986635000
H	-0.775801000	-4.530594000	-4.756630000
H	0.393243000	-4.238872000	-3.451783000

H	-2.723139000	-0.669487000	-5.495248000
H	-2.266424000	-2.852444000	-7.533550000
H	-0.038528000	-0.145167000	-3.299095000
H	1.481016000	-2.469372000	-4.852908000
O	0.023192000	-1.184710000	-3.268216000
O	-0.909998000	-2.268392000	-9.075188000
O	1.207314000	-5.091194000	-5.105389000
O	-2.110062000	-2.476453000	-6.652178000
O	-1.968029000	-0.066002000	-5.418060000
O	0.198205000	-2.738925000	-6.457081000

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C	-3.248184000	-2.182850000	-1.650098000
C	-3.229715000	-2.386601000	2.899990000
C	-3.232292000	2.034305000	3.104012000
C	3.276888000	2.142018000	2.939210000
C	3.226910000	2.366317000	-1.338692000
C	3.259301000	-2.277949000	-1.561551000
C	-3.265283000	2.236128000	-1.457275000
C	3.257175000	-2.506569000	2.716404000
H	4.086653000	2.698129000	3.461475000
H	4.061821000	-3.142643000	3.148200000
H	-4.030091000	2.551522000	3.682057000
H	-4.030490000	-2.987428000	3.384939000
C	5.644212000	-2.460319000	-2.300798000
C	-5.664712000	-2.606118000	-2.168127000
C	4.316271000	-2.893479000	-2.410289000
C	-4.314218000	-2.857675000	-2.441899000
C	3.987133000	-3.878454000	-3.351082000
C	-3.970043000	-3.748326000	-3.466745000
C	4.970271000	-4.419786000	-4.172615000
C	-4.964630000	-4.379148000	-4.208156000
C	6.289416000	-3.977658000	-4.064520000
C	-6.308964000	-4.123637000	-3.932394000
C	6.625173000	-2.999377000	-3.127776000
C	-6.657550000	-3.237044000	-2.912362000
C	5.611868000	3.114486000	-1.449359000
C	-5.690068000	2.713077000	-1.869162000
C	4.293984000	3.233505000	-1.911567000
C	-4.345879000	3.016694000	-2.121954000
C	3.990942000	4.159346000	-2.919710000
C	-4.025339000	4.059066000	-3.001602000
C	4.999815000	4.955180000	-3.456951000
C	-5.037051000	4.787537000	-3.620338000
C	6.308780000	4.840442000	-2.986635000
C	-6.374445000	4.478661000	-3.367170000

C	6.613579000	3.920360000	-1.981730000
C	-6.699516000	3.441327000	-2.491675000
H	5.886073000	-1.693064000	-1.562640000
H	-5.915777000	-1.910106000	-1.365464000
H	2.949249000	-4.209222000	-3.428402000
H	-2.912555000	-3.934737000	-3.663486000
H	4.709138000	-5.186753000	-4.905190000
H	-4.693130000	-5.074855000	-5.005467000
H	7.658267000	-2.654981000	-3.043857000
H	-7.709897000	-3.038072000	-2.697226000
H	5.829270000	2.384793000	-0.666728000
H	-5.922816000	1.899440000	-1.179690000
H	2.967309000	4.223988000	-3.295606000
H	-2.974050000	4.289629000	-3.184694000
H	4.763761000	5.669820000	-4.248856000
H	-4.783453000	5.601529000	-4.303162000
H	7.638468000	3.830816000	-1.614608000
H	-7.746498000	3.200776000	-2.293951000
H	-7.089329000	-4.618954000	-4.515335000
H	7.060259000	-4.397760000	-4.714858000
H	-7.168017000	5.050508000	-3.854270000
H	7.097080000	5.469709000	-3.407082000
H	-1.943811000	-2.939668000	0.599870000
H	-0.882750000	1.355478000	5.098321000
H	-0.015248000	0.058763000	4.798621000
H	0.058681000	4.017149000	0.594200000
H	0.688415000	4.272845000	2.652973000
H	0.905372000	4.324776000	-0.718091000
H	1.961311000	-0.187482000	3.577259000
H	-1.933296000	2.801730000	0.820362000
H	-0.629773000	-2.011213000	5.079096000
H	0.894435000	-4.458651000	2.141124000
H	0.737702000	-4.397428000	-1.133559000
H	0.015421000	-4.159072000	0.853734000
O	-1.061397000	-0.100344000	2.178694000
O	-3.620882000	1.292013000	2.166860000
O	-3.614421000	1.349715000	-0.623561000
O	-3.613722000	-1.507076000	2.090140000
O	-2.050089000	-2.656952000	3.235486000
O	0.036732000	-4.103043000	1.870377000
O	2.075263000	-2.841239000	2.976910000
O	2.059924000	-2.635031000	-1.763679000
O	3.637653000	-1.530428000	2.023600000
O	3.619813000	-1.413655000	-0.712075000
O	3.648060000	1.274618000	2.112051000
O	3.587887000	1.417417000	-0.589699000

O	2.023633000	2.616282000	-1.664161000
O	2.099048000	2.453211000	3.247763000
O	1.073829000	1.404355000	0.743916000
O	1.409004000	-0.129176000	2.787699000
O	0.036324000	-1.531894000	4.572365000
O	-0.029680000	1.075599000	4.738493000
O	1.056124000	-1.542090000	0.685364000
O	-1.395163000	-2.149011000	0.673790000
O	-2.045861000	-2.405224000	-1.961879000
O	-0.014986000	-3.942409000	-0.737268000
O	-3.618891000	-1.417617000	-0.704861000
O	0.001515000	3.786165000	2.182030000
O	0.063400000	3.953780000	-0.422091000
O	-1.388050000	2.006395000	0.776840000
O	-2.047727000	2.247474000	3.463700000
O	-2.068398000	2.502952000	-1.767340000
O	1.384655000	-0.031185000	-1.353325000
O	-1.079461000	-0.047052000	-0.770090000
H	1.923071000	0.000223000	-2.159581000
O	-0.051220000	1.515847000	-3.158485000
H	-0.946068000	1.678478000	-3.485023000
Zr	2.523586000	-0.078736000	0.701588000
Zr	-0.019853000	-1.880615000	2.496761000
Zr	0.034822000	1.709584000	2.522253000
Zr	-0.036381000	1.732292000	-1.055285000
Zr	-2.538702000	-0.076463000	0.712780000
Zr	0.010147000	-1.861673000	-1.095657000
C	2.094175000	-1.332193000	-6.619171000
C	3.104699000	-0.308930000	-6.058483000
C	2.212703000	0.711200000	-5.296553000
C	0.898840000	-1.158679000	-5.687633000
C	2.246485000	2.151204000	-5.779576000
C	1.027271000	-1.860568000	-4.351878000
H	3.294655000	2.489431000	-5.844677000
H	3.587220000	0.193015000	-6.920967000
H	2.535212000	-2.340054000	-6.603872000
H	0.124901000	-0.301241000	-3.488249000
H	1.830179000	2.178710000	-6.805841000
H	0.838291000	2.511504000	-4.454600000
H	2.067987000	-1.799888000	-3.998198000
H	0.780185000	-2.928244000	-4.450148000
H	4.138549000	-0.403964000	-4.437358000
H	2.261132000	1.521514000	-3.544441000
H	1.224507000	-0.227493000	-7.934883000
H	-0.047996000	-1.419877000	-6.184367000
O	1.734953000	-1.047639000	-7.947132000

O	1.573111000	2.996873000	-4.894806000
O	0.133925000	-1.296965000	-3.398319000
O	2.579353000	0.682330000	-3.933832000
O	4.055467000	-0.929155000	-5.246819000
O	0.877591000	0.256898000	-5.497520000

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C	-3.248206000	-2.182808000	-1.650101000
C	-3.229697000	-2.386599000	2.899994000
C	-3.232298000	2.034296000	3.104003000
C	3.276894000	2.141996000	2.939183000
C	3.226890000	2.366296000	-1.338701000
C	3.259332000	-2.277910000	-1.561464000
C	-3.265308000	2.236126000	-1.457290000
C	3.257192000	-2.506596000	2.716376000
H	4.089215000	2.684282000	3.471035000
H	4.062722000	-3.141268000	3.148611000
H	-4.029781000	2.553423000	3.680450000
H	-4.031045000	-2.986155000	3.385355000
C	5.674809000	-2.611794000	-2.143082000
C	-5.666159000	-2.574266000	-2.186369000
C	4.334048000	-2.982804000	-2.318419000
C	-4.316859000	-2.840705000	-2.452058000
C	4.015616000	-4.018038000	-3.210363000
C	-3.976050000	-3.729808000	-3.479417000
C	5.022485000	-4.667925000	-3.918538000
C	-4.972838000	-4.344083000	-4.231619000
C	6.353867000	-4.288592000	-3.742830000
C	-6.315903000	-4.073991000	-3.963751000
C	6.678354000	-3.261848000	-2.855316000
C	-6.661140000	-3.189151000	-2.941051000
C	5.641614000	2.904782000	-1.696471000
C	-5.687329000	2.718660000	-1.868800000
C	4.296543000	3.263505000	-1.854320000
C	-4.342557000	3.024470000	-2.116560000
C	3.974248000	4.466588000	-2.494873000
C	-4.020724000	4.075940000	-2.984861000
C	4.983005000	5.299314000	-2.967209000
C	-5.031265000	4.810703000	-3.597903000
C	6.321683000	4.931908000	-2.815722000
C	-6.369019000	4.498773000	-3.350662000
C	6.650069000	3.733084000	-2.181597000
C	-6.695586000	3.452704000	-2.486183000
H	5.906948000	-1.806019000	-1.443963000
H	-5.914762000	-1.879836000	-1.381580000
H	2.969406000	-4.307257000	-3.334107000

H	-2.919592000	-3.927702000	-3.670220000
H	4.769599000	-5.470581000	-4.614383000
H	-4.703990000	-5.037864000	-5.031450000
H	7.720370000	-2.963421000	-2.723272000
H	-7.712531000	-2.978848000	-2.732171000
H	5.878300000	1.966902000	-1.189962000
H	-5.921419000	1.898285000	-1.187834000
H	2.924527000	4.725045000	-2.637367000
H	-2.969567000	4.310690000	-3.162947000
H	4.726384000	6.236040000	-3.466945000
H	-4.776487000	5.631978000	-4.271417000
H	7.697086000	3.445649000	-2.061908000
H	-7.742857000	3.209849000	-2.293089000
H	-7.097979000	-4.556315000	-4.555208000
H	7.142585000	-4.792904000	-4.305386000
H	-7.161700000	5.075227000	-3.833667000
H	7.112673000	5.583955000	-3.194347000
H	-1.935035000	-2.944690000	0.602102000
H	-0.882228000	1.351024000	5.104295000
H	-0.015085000	0.054292000	4.800994000
H	0.029941000	4.013536000	0.593922000
H	0.684617000	4.272637000	2.650052000
H	0.909913000	4.285737000	-0.694636000
H	1.964910000	-0.186708000	3.574448000
H	-1.930380000	2.794051000	0.811513000
H	-0.632706000	-2.013879000	5.075193000
H	0.894646000	-4.463217000	2.159455000
H	0.740156000	-4.418215000	-1.143709000
H	0.031667000	-4.164306000	0.861153000
O	-1.058742000	-0.103063000	2.177382000
O	-3.619839000	1.292150000	2.166243000
O	-3.613997000	1.356581000	-0.618561000
O	-3.612659000	-1.508191000	2.087873000
O	-2.050018000	-2.656107000	3.236030000
O	0.041537000	-4.105116000	1.877760000
O	2.075829000	-2.840732000	2.980589000
O	2.060334000	-2.596090000	-1.820418000
O	3.635714000	-1.532355000	2.019012000
O	3.618154000	-1.416335000	-0.714862000
O	3.643169000	1.292745000	2.089600000
O	3.593156000	1.354735000	-0.669553000
O	2.016984000	2.669969000	-1.567517000
O	2.099780000	2.448440000	3.254638000
O	1.067941000	1.399461000	0.742799000
O	1.411530000	-0.127884000	2.785706000
O	0.036396000	-1.535098000	4.571785000

O	-0.030605000	1.071194000	4.741051000
O	1.068099000	-1.543404000	0.680627000
O	-1.387810000	-2.153086000	0.677112000
O	-2.046936000	-2.423434000	-1.947681000
O	0.011102000	-3.944666000	-0.726884000
O	-3.616515000	-1.410767000	-0.708053000
O	-0.003628000	3.780442000	2.186855000
O	0.042527000	3.954588000	-0.421432000
O	-1.384784000	1.998618000	0.773108000
O	-2.047513000	2.244458000	3.465307000
O	-2.064486000	2.489856000	-1.778627000
O	1.372623000	-0.016602000	-1.367760000
O	-1.078433000	-0.050376000	-0.773344000
H	1.910927000	0.019786000	-2.180519000
O	-0.081149000	1.457320000	-3.208105000
H	-0.914879000	1.871902000	-3.475273000
Zr	2.528681000	-0.070180000	0.685834000
Zr	-0.013788000	-1.880816000	2.496845000
Zr	0.033872000	1.706804000	2.527328000
Zr	-0.022495000	1.725419000	-1.055183000
Zr	-2.536946000	-0.078475000	0.712649000
Zr	0.015694000	-1.865170000	-1.088305000
C	4.024219000	-0.464501000	-5.724693000
C	2.630218000	-0.993495000	-6.167202000
C	1.675902000	-0.567969000	-5.014992000
C	3.675966000	0.550086000	-4.646331000
C	0.860632000	-1.709471000	-4.443330000
C	3.340345000	1.915703000	-5.237445000
H	0.225709000	-2.107840000	-5.251923000
H	2.706913000	-2.096574000	-6.207290000
H	4.508130000	0.005543000	-6.593792000
H	1.832738000	2.218960000	-4.043708000
H	1.517852000	-2.512638000	-4.083843000
H	-0.167526000	-0.327598000	-3.399150000
H	2.864567000	1.772626000	-6.228109000
H	4.292794000	2.438444000	-5.429668000
H	1.535160000	0.151448000	-7.231701000
H	0.457518000	0.920963000	-4.734079000
H	4.547574000	-1.830001000	-4.450573000
H	4.446039000	0.626154000	-3.862079000
O	4.885341000	-1.478035000	-5.285348000
O	0.045617000	-1.298822000	-3.353247000
O	2.580648000	2.725586000	-4.399901000
O	0.834536000	0.431925000	-5.508195000
O	2.208591000	-0.524319000	-7.408086000
O	2.527417000	-0.050566000	-3.995850000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087891000	2.710815000	3.446078000
H	4.060507000	-3.138434000	3.157008000
H	-4.030501000	2.572073000	3.662682000
H	-4.033486000	-2.971029000	3.399688000
C	5.663307000	-2.722645000	-2.113094000
C	-5.636272000	-2.262570000	-2.386709000
C	4.310194000	-3.030516000	-2.301031000
C	-4.346416000	-2.808788000	-2.440728000
C	3.948505000	-4.052754000	-3.189952000
C	-4.105469000	-3.924686000	-3.252778000
C	4.930295000	-4.756018000	-3.882225000
C	-5.134639000	-4.480078000	-4.007146000
C	6.277295000	-4.442066000	-3.693702000
C	-6.412581000	-3.922946000	-3.958825000
C	6.642200000	-3.425357000	-2.809716000
C	-6.662119000	-2.814308000	-3.147949000
C	5.636564000	2.935768000	-1.722455000
C	-5.685391000	2.730914000	-1.864062000
C	4.286250000	3.171226000	-2.011480000
C	-4.341369000	2.954863000	-2.191715000
C	3.941236000	4.162864000	-2.938970000
C	-4.019137000	3.849389000	-3.220328000
C	4.933449000	4.909864000	-3.567499000
C	-5.029221000	4.510723000	-3.912191000
C	6.276865000	4.673999000	-3.271606000
C	-6.366053000	4.287100000	-3.579429000
C	6.626740000	3.686978000	-2.348795000
C	-6.693084000	3.397714000	-2.554440000
H	5.926659000	-1.925315000	-1.415660000
H	-5.811449000	-1.396832000	-1.745041000
H	2.888604000	-4.286415000	-3.323813000
H	-3.104951000	-4.361500000	-3.288520000
H	4.645948000	-5.554692000	-4.571102000
H	-4.934859000	-5.346362000	-4.640941000
H	7.696729000	-3.180866000	-2.663708000
H	-7.662913000	-2.378300000	-3.110369000

H	5.888883000	2.157412000	-0.999920000
H	-5.919509000	2.031178000	-1.059518000
H	2.885795000	4.330226000	-3.163434000
H	-2.969106000	4.007998000	-3.470919000
H	4.660252000	5.679280000	-4.293193000
H	-4.774409000	5.203414000	-4.717300000
H	7.678468000	3.502520000	-2.118462000
H	-7.739690000	3.224370000	-2.293896000
H	-7.218890000	-4.354958000	-4.556383000
H	7.047289000	-4.994033000	-4.238134000
H	-7.158022000	4.808325000	-4.122815000
H	7.055407000	5.261649000	-3.764091000
H	-1.913487000	-2.935425000	0.577630000
H	-0.888743000	1.303334000	5.130928000
H	-0.016697000	0.012482000	4.809105000
H	0.037824000	4.031599000	0.673832000
H	0.688703000	4.258562000	2.719449000
H	0.920500000	4.331040000	-0.609862000
H	1.967151000	-0.212776000	3.583403000
H	-1.935618000	2.805575000	0.848890000
H	-0.636687000	-2.049174000	5.053131000
H	0.903226000	-4.467611000	2.108981000
H	0.663785000	-4.390295000	-1.264173000
H	0.048956000	-4.150344000	0.806419000
O	-1.056387000	-0.106142000	2.189906000
O	-3.619213000	1.291621000	2.167489000
O	-3.615710000	1.373472000	-0.598700000
O	-3.610371000	-1.509208000	2.084168000
O	-2.049534000	-2.670784000	3.220398000
O	0.052014000	-4.105143000	1.827699000
O	2.075082000	-2.848608000	2.965443000
O	2.053377000	-2.543115000	-1.841440000
O	3.640372000	-1.529331000	2.026939000
O	3.632371000	-1.424558000	-0.707286000
O	3.646710000	1.279885000	2.107799000
O	3.601221000	1.417574000	-0.595618000
O	2.018418000	2.686625000	-1.559510000
O	2.101354000	2.436943000	3.272972000
O	1.071458000	1.412623000	0.783381000
O	1.413442000	-0.141696000	2.795968000
O	0.036064000	-1.564671000	4.560286000
O	-0.034447000	1.032701000	4.767120000
O	1.071503000	-1.534851000	0.671511000
O	-1.380438000	-2.134718000	0.656234000
O	-2.054378000	-2.473054000	-1.949432000
O	-0.003822000	-3.910512000	-0.758294000

O	-3.588441000	-1.379796000	-0.733451000
O	-0.005613000	3.779223000	2.251872000
O	0.057424000	3.984795000	-0.344590000
O	-1.383100000	2.014919000	0.813848000
O	-2.051676000	2.226043000	3.487470000
O	-2.060474000	2.513808000	-1.742840000
O	1.403074000	0.027477000	-1.320271000
O	-1.070568000	-0.017756000	-0.760283000
H	1.909305000	0.011640000	-2.158090000
O	-0.035617000	1.429095000	-3.140563000
H	-0.861270000	1.763836000	-3.529592000
Zr	2.535954000	-0.073324000	0.695872000
Zr	-0.008530000	-1.892782000	2.476970000
Zr	0.035471000	1.696722000	2.565461000
Zr	-0.015134000	1.765401000	-0.992105000
Zr	-2.524172000	-0.066292000	0.723000000
Zr	0.032267000	-1.825459000	-1.127621000
C	-1.716372000	-2.380573000	-5.225257000
C	-0.281567000	-2.755528000	-4.818658000
C	0.341055000	-1.389209000	-4.523159000
C	-1.607726000	-0.926351000	-5.700055000
C	1.852206000	-1.255890000	-4.648031000
C	-2.485485000	0.062374000	-4.949384000
H	2.330660000	-2.125582000	-4.181046000
H	0.240132000	-3.197808000	-5.689189000
H	-2.336599000	-2.411417000	-4.317318000
H	-1.169401000	1.347338000	-5.477450000
H	2.121267000	-1.253313000	-5.718542000
H	1.810619000	0.659032000	-4.237620000
H	-2.412372000	-0.134733000	-3.860146000
H	-3.541833000	-0.079157000	-5.230217000
H	-0.965147000	-3.552087000	-3.184021000
H	-0.090449000	0.147428000	-3.216659000
H	-1.795023000	-3.307810000	-6.921324000
H	-1.808851000	-0.851538000	-6.782831000
O	-2.332430000	-3.264383000	-6.121361000
O	2.344848000	-0.111246000	-3.983161000
O	-2.110121000	1.388457000	-5.248576000
O	-0.100136000	-0.996749000	-3.257763000
O	-0.182036000	-3.658066000	-3.754664000
O	-0.232137000	-0.547690000	-5.516054000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000

C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.088579000	2.715207000	3.440269000
H	4.060121000	-3.127618000	3.172667000
H	-4.029260000	2.580579000	3.656220000
H	-4.031973000	-2.967990000	3.405660000
C	5.656735000	-2.550605000	-2.249221000
C	-5.655209000	-2.319171000	-2.321601000
C	4.329984000	-2.996106000	-2.313235000
C	-4.352992000	-2.829957000	-2.414632000
C	4.015678000	-4.121326000	-3.088160000
C	-4.104981000	-3.936503000	-3.237455000
C	5.015307000	-4.788878000	-3.790861000
C	-5.140275000	-4.516907000	-3.964058000
C	6.333417000	-4.333571000	-3.731459000
C	-6.431366000	-3.996432000	-3.875566000
C	6.652540000	-3.213791000	-2.961504000
C	-6.687694000	-2.897550000	-3.053481000
C	5.634132000	2.927802000	-1.750885000
C	-5.681498000	2.684125000	-1.931407000
C	4.281987000	3.151641000	-2.042083000
C	-4.333626000	2.931000000	-2.224705000
C	3.931555000	4.110582000	-3.001291000
C	-4.000345000	3.821872000	-3.253018000
C	4.920445000	4.836056000	-3.659821000
C	-5.003524000	4.457980000	-3.977915000
C	6.265496000	4.612659000	-3.361540000
C	-6.344440000	4.211422000	-3.679445000
C	6.620839000	3.658691000	-2.406442000
C	-6.682350000	3.324852000	-2.655535000
H	5.887013000	-1.680227000	-1.631258000
H	-5.835236000	-1.460479000	-1.671949000
H	2.978887000	-4.465980000	-3.124593000
H	-3.093631000	-4.342565000	-3.306418000
H	4.766737000	-5.669641000	-4.387225000
H	-4.934290000	-5.373717000	-4.608668000
H	7.685094000	-2.860584000	-2.912597000
H	-7.698879000	-2.490079000	-2.984505000
H	5.890517000	2.176885000	-1.000946000
H	-5.923706000	1.986100000	-1.127764000
H	2.874966000	4.267294000	-3.227158000
H	-2.946913000	3.998976000	-3.475536000
H	4.643112000	5.579210000	-4.410848000

H	-4.740174000	5.148910000	-4.781817000
H	7.673752000	3.485593000	-2.172465000
H	-7.732185000	3.132879000	-2.422660000
H	-7.242704000	-4.448824000	-4.450976000
H	7.116849000	-4.856587000	-4.285179000
H	-7.131096000	4.712303000	-4.249034000
H	7.041026000	5.184601000	-3.876733000
H	-1.924589000	-2.919023000	0.567711000
H	-0.889045000	1.276780000	5.147032000
H	-0.019171000	-0.014166000	4.805668000
H	0.037581000	4.036729000	0.703336000
H	0.694756000	4.246750000	2.741051000
H	0.919423000	4.337570000	-0.582332000
H	1.963356000	-0.221716000	3.584546000
H	-1.933146000	2.814043000	0.859371000
H	-0.637106000	-2.065259000	5.030314000
H	0.903597000	-4.468622000	2.052263000
H	0.662814000	-4.376227000	-1.274408000
H	0.032315000	-4.135094000	0.761825000
O	-1.057199000	-0.104535000	2.187138000
O	-3.619662000	1.291258000	2.168950000
O	-3.620657000	1.387612000	-0.588736000
O	-3.613804000	-1.505569000	2.089124000
O	-2.048120000	-2.677045000	3.208066000
O	0.051020000	-4.099286000	1.785146000
O	2.074941000	-2.853203000	2.954189000
O	2.066413000	-2.605727000	-1.791205000
O	3.642448000	-1.534997000	2.017936000
O	3.629499000	-1.384887000	-0.741587000
O	3.644165000	1.281665000	2.105155000
O	3.604644000	1.420540000	-0.596343000
O	2.016650000	2.700068000	-1.539320000
O	2.102016000	2.430948000	3.282421000
O	1.067615000	1.416202000	0.790740000
O	1.413945000	-0.145075000	2.794643000
O	0.036422000	-1.575794000	4.543473000
O	-0.037099000	1.009599000	4.775508000
O	1.071864000	-1.521287000	0.658894000
O	-1.388761000	-2.120179000	0.645034000
O	-2.060151000	-2.468884000	-1.956532000
O	-0.029851000	-3.899559000	-0.800478000
O	-3.586634000	-1.365333000	-0.740378000
O	-0.004277000	3.774197000	2.273448000
O	0.055829000	3.992593000	-0.316672000
O	-1.382911000	2.021544000	0.829584000
O	-2.052575000	2.218666000	3.495768000

O	-2.055661000	2.517126000	-1.731247000
O	1.397991000	0.046422000	-1.339571000
O	-1.074910000	0.004564000	-0.764781000
H	1.888206000	-0.013853000	-2.182488000
O	-0.030717000	1.457495000	-3.181536000
H	-0.843310000	1.696234000	-3.677566000
Zr	2.533763000	-0.081976000	0.692096000
Zr	-0.007695000	-1.895721000	2.453711000
Zr	0.031573000	1.689002000	2.584441000
Zr	-0.015348000	1.771552000	-0.953922000
Zr	-2.530214000	-0.068416000	0.722004000
Zr	0.020533000	-1.810002000	-1.172883000
C	-1.730872000	-2.429952000	-5.227696000
C	-0.321968000	-2.916702000	-4.869066000
C	0.393249000	-1.608784000	-4.486642000
C	-1.514364000	-0.978468000	-5.670538000
C	1.903763000	-1.644783000	-4.652527000
C	-2.345217000	0.038165000	-4.907865000
H	2.267421000	-2.598790000	-4.234730000
H	0.158871000	-3.328258000	-5.777579000
H	-2.330058000	-2.436314000	-4.305959000
H	-1.028577000	1.262581000	-5.599285000
H	2.146880000	-1.618257000	-5.728261000
H	3.422733000	-0.532968000	-4.143883000
H	-2.269341000	-0.169168000	-3.822206000
H	-3.409315000	-0.045238000	-5.183683000
H	-0.893237000	-3.682330000	-3.183800000
H	0.068109000	0.471620000	-3.323694000
H	-1.894145000	-3.344029000	-6.923843000
H	-1.710283000	-0.874526000	-6.753604000
O	-2.435232000	-3.237756000	-6.132474000
O	2.474539000	-0.539778000	-3.971471000
O	-1.897432000	1.359252000	-5.179410000
O	0.022634000	-1.220169000	-3.234471000
O	-0.264758000	-3.911335000	-3.891349000
O	-0.126315000	-0.688772000	-5.471266000

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C	-3.248200000	-2.182800000	-1.650100000
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C	-3.265300000	2.236100000	-1.457300000
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H	4.089503000	2.688958000	3.467115000
H	4.063576000	-3.146366000	3.140293000
H	-4.029087000	2.560465000	3.675553000
H	-4.030579000	-2.992512000	3.378708000
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C	-5.667081000	-2.290682000	-2.289437000
C	4.331047000	-2.875290000	-2.416978000
C	-4.349728000	-2.722040000	-2.500145000
C	4.030960000	-3.917722000	-3.305111000
C	-4.082887000	-3.635677000	-3.527693000
C	5.026068000	-4.456973000	-4.116448000
C	-5.113939000	-4.107881000	-4.334079000
C	6.327264000	-3.955718000	-4.051450000
C	-6.421903000	-3.674071000	-4.118803000
C	6.633100000	-2.918198000	-3.169229000
C	-6.697106000	-2.765059000	-3.095647000
C	5.648497000	2.922415000	-1.682741000
C	-5.686891000	2.701870000	-1.877052000
C	4.303187000	3.188284000	-1.970374000
C	-4.343550000	3.028805000	-2.105432000
C	3.980968000	4.226075000	-2.854761000
C	-4.025658000	4.103608000	-2.945133000
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C	-5.039360000	4.843988000	-3.544561000
C	6.326084000	4.715211000	-3.152290000
C	-6.375774000	4.511862000	-3.317090000
C	6.654396000	3.684188000	-2.270582000
C	-6.698854000	3.439595000	-2.483993000
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H	3.007818000	-4.299920000	-3.343759000
H	-3.057440000	-3.967256000	-3.699258000
H	4.787576000	-5.273457000	-4.801803000
H	-4.892528000	-4.810864000	-5.139719000
H	7.652470000	-2.529254000	-3.115691000
H	-7.721014000	-2.422807000	-2.928827000
H	5.884075000	2.113888000	-0.988005000
H	-5.917417000	1.862184000	-1.218674000
H	2.930445000	4.428344000	-3.074651000
H	-2.976490000	4.345688000	-3.118153000
H	4.730701000	5.791721000	-4.134108000
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H	-7.744997000	3.179891000	-2.306735000
H	-7.231053000	-4.042821000	-4.753928000
H	7.107383000	-4.378387000	-4.689050000

H	-7.170550000	5.092246000	-3.792327000
H	7.116459000	5.312448000	-3.613252000
H	-1.940969000	-2.931602000	0.604250000
H	-0.882909000	1.355302000	5.106676000
H	-0.013853000	0.059942000	4.806122000
H	0.023238000	4.010223000	0.609695000
H	0.683585000	4.272856000	2.663135000
H	0.898721000	4.290534000	-0.677587000
H	1.964843000	-0.177946000	3.580374000
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H	-0.637602000	-2.004895000	5.082224000
H	0.898026000	-4.457510000	2.150096000
H	0.743543000	-4.404030000	-1.130542000
H	0.021526000	-4.160449000	0.859220000
O	-1.058285000	-0.099570000	2.180064000
O	-3.622917000	1.290422000	2.169591000
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O	-3.613645000	-1.504958000	2.092669000
O	-2.050738000	-2.653994000	3.240602000
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O	2.077169000	-2.837450000	2.989071000
O	2.077875000	-2.665008000	-1.758120000
O	3.635981000	-1.531247000	2.020953000
O	3.619789000	-1.404101000	-0.720891000
O	3.645010000	1.283783000	2.100566000
O	3.593359000	1.396316000	-0.620058000
O	2.027634000	2.689310000	-1.578106000
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O	1.062792000	1.413009000	0.746398000
O	1.409696000	-0.122050000	2.792778000
O	0.034541000	-1.529003000	4.580252000
O	-0.029004000	1.077215000	4.747456000
O	1.067757000	-1.543536000	0.699641000
O	-1.388407000	-2.144548000	0.684923000
O	-2.060540000	-2.484932000	-1.942663000
O	-0.006742000	-3.951663000	-0.727126000
O	-3.591691000	-1.421171000	-0.692989000
O	-0.011759000	3.786909000	2.204170000
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O	-1.397467000	2.000013000	0.785822000
O	-2.048750000	2.240283000	3.470588000
O	-2.064878000	2.489801000	-1.765950000
O	1.376177000	-0.018236000	-1.334907000
O	-1.098491000	-0.043303000	-0.795781000
H	1.849706000	-0.062139000	-2.185806000
O	0.112778000	1.815052000	-3.190311000

H	0.980299000	2.168225000	-3.428458000
Zr	2.518230000	-0.073768000	0.696902000
Zr	-0.016517000	-1.879536000	2.504042000
Zr	0.029920000	1.710844000	2.530813000
Zr	-0.039781000	1.721152000	-1.052425000
Zr	-2.538005000	-0.073043000	0.716266000
Zr	0.015234000	-1.864290000	-1.082363000
C	-1.811399000	-1.594926000	-5.318712000
C	-0.449540000	-2.296566000	-5.328780000
C	0.439457000	-1.454999000	-4.418848000
C	-1.555226000	-0.091033000	-5.430049000
C	1.902113000	-1.326982000	-4.756207000
C	-2.490915000	0.730376000	-4.564848000
H	2.324322000	-2.339413000	-4.604762000
H	-0.044850000	-2.334279000	-6.356000000
H	-2.249604000	-1.804788000	-4.327409000
H	-1.611125000	2.361075000	-4.064558000
H	2.022580000	-1.062448000	-5.820109000
H	3.471628000	-0.499194000	-3.947358000
H	-2.376444000	0.390988000	-3.512822000
H	-3.522121000	0.471964000	-4.863615000
H	-0.826275000	-3.563107000	-3.938175000
H	-0.082656000	0.803316000	-4.276937000
H	-2.375784000	-1.948214000	-7.132488000
H	-1.649454000	0.229901000	-6.483806000
O	-2.733597000	-2.083909000	-6.246660000
O	2.514624000	-0.379592000	-3.910268000
O	-2.301039000	2.103138000	-4.701827000
O	0.099481000	-1.512269000	-3.203308000
O	-0.500329000	-3.612182000	-4.853027000
O	-0.174822000	0.117691000	-5.060363000

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C	-3.248200000	-2.182800000	-1.650100000
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C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
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H	4.062342000	-3.150402000	3.135928000
H	-4.029918000	2.547625000	3.685478000
H	-4.031429000	-2.990836000	3.378986000
C	5.670551000	-2.548390000	-2.196440000

C	-5.641870000	-2.329137000	-2.374992000
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C	-4.317183000	-2.766191000	-2.507795000
C	3.999661000	-3.843557000	-3.376979000
C	-3.998350000	-3.724737000	-3.477956000
C	4.997734000	-4.415609000	-4.160890000
C	-4.990553000	-4.233989000	-4.310266000
C	6.332118000	-4.056378000	-3.963050000
C	-6.306616000	-3.789777000	-4.179122000
C	6.666771000	-3.123154000	-2.980804000
C	-6.631584000	-2.838269000	-3.210382000
C	5.647570000	2.939610000	-1.636531000
C	-5.683579000	2.800903000	-1.755686000
C	4.305837000	3.199981000	-1.943454000
C	-4.340727000	3.089667000	-2.029299000
C	3.991052000	4.245822000	-2.820445000
C	-4.020553000	4.191563000	-2.832153000
C	5.002067000	5.020405000	-3.381926000
C	-5.029582000	4.993841000	-3.353933000
C	6.336556000	4.757148000	-3.069671000
C	-6.366584000	4.698404000	-3.082455000
C	6.657387000	3.716724000	-2.196537000
C	-6.692212000	3.601376000	-2.283829000
H	5.910776000	-1.814554000	-1.424963000
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H	4.735508000	-5.146233000	-4.929450000
H	-4.735314000	-4.974832000	-5.071095000
H	7.711097000	-2.841979000	-2.827531000
H	-7.662265000	-2.490674000	-3.109762000
H	5.877689000	2.120966000	-0.952251000
H	-5.917501000	1.941436000	-1.124751000
H	2.943224000	4.439247000	-3.059199000
H	-2.970611000	4.407306000	-3.039310000
H	4.750585000	5.832752000	-4.067546000
H	-4.775095000	5.852810000	-3.978708000
H	7.701997000	3.510936000	-1.952339000
H	-7.738600000	3.370843000	-2.071449000
H	-7.084307000	-4.186391000	-4.836423000
H	7.115203000	-4.506161000	-4.578240000
H	-7.158960000	5.327302000	-3.495601000
H	7.130264000	5.365594000	-3.509817000
H	-1.936067000	-2.941841000	0.601349000
H	-0.878291000	1.370185000	5.094235000
H	-0.012734000	0.071653000	4.797209000

H	0.008552000	3.996663000	0.560769000
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H	0.928262000	4.230304000	-0.699216000
H	1.964861000	-0.174089000	3.570726000
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H	-0.636358000	-1.994167000	5.084426000
H	0.896590000	-4.456812000	2.183882000
H	0.692025000	-4.451001000	-1.148013000
H	0.030858000	-4.172723000	0.883712000
O	-1.058848000	-0.100080000	2.170369000
O	-3.620545000	1.292972000	2.165013000
O	-3.611817000	1.327860000	-0.646679000
O	-3.612122000	-1.506967000	2.088866000
O	-2.051179000	-2.651643000	3.242689000
O	0.040422000	-4.106101000	1.901962000
O	2.076244000	-2.835612000	2.990242000
O	2.068923000	-2.633295000	-1.787341000
O	3.635695000	-1.528396000	2.026305000
O	3.613887000	-1.423487000	-0.699440000
O	3.646379000	1.281311000	2.104153000
O	3.584219000	1.389901000	-0.620980000
O	2.026490000	2.684686000	-1.582514000
O	2.097901000	2.462286000	3.236668000
O	1.059699000	1.403334000	0.731567000
O	1.407835000	-0.120626000	2.784206000
O	0.033599000	-1.519275000	4.578576000
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O	1.061528000	-1.550703000	0.695711000
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O	-0.000753000	-3.959260000	-0.691440000
O	-3.615161000	-1.426742000	-0.696935000
O	-0.018334000	3.784648000	2.158476000
O	0.040100000	3.933426000	-0.454064000
O	-1.396572000	1.987897000	0.757156000
O	-2.047035000	2.249555000	3.459574000
O	-2.066166000	2.471681000	-1.798438000
O	1.370100000	-0.043110000	-1.345425000
O	-1.090909000	-0.062099000	-0.811499000
H	1.909160000	-0.066882000	-2.162008000
O	0.119712000	1.720501000	-3.239878000
H	0.357124000	2.599660000	-3.561399000
Zr	2.523384000	-0.077395000	0.692306000
Zr	-0.015357000	-1.880561000	2.505506000
Zr	0.031073000	1.713333000	2.512783000
Zr	-0.027974000	1.694000000	-1.078550000

Zr	-2.534955000	-0.081841000	0.709257000
Zr	0.023745000	-1.888232000	-1.081316000
C	-1.685052000	-1.823686000	-5.376521000
C	-0.218863000	-2.237794000	-5.552112000
C	0.576451000	-1.535063000	-4.471157000
C	-1.833957000	-0.299459000	-5.470756000
C	1.897511000	-0.895940000	-4.788864000
C	-2.740889000	0.242215000	-4.378947000
H	2.649715000	-1.706712000	-4.731326000
H	0.146996000	-1.912906000	-6.549016000
H	-1.973131000	-2.165526000	-4.367442000
H	-2.272495000	2.020890000	-3.789368000
H	1.887448000	-0.556311000	-5.838681000
H	1.528149000	0.762424000	-3.821506000
H	-2.337529000	-0.079229000	-3.396029000
H	-3.735748000	-0.229310000	-4.480844000
H	-0.919297000	-4.004057000	-5.717754000
H	-0.482059000	0.891947000	-4.618865000
H	-2.396616000	-2.192301000	-7.144493000
H	-2.269148000	-0.042177000	-6.458190000
O	-2.503305000	-2.559000000	-6.256680000
O	2.270028000	0.110476000	-3.900297000
O	-2.864093000	1.633650000	-4.453496000
O	0.154793000	-1.604976000	-3.317313000
O	-0.090610000	-3.624557000	-5.386371000
O	-0.546319000	0.285238000	-5.400430000

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C	-3.248176000	-2.182749000	-1.650145000
C	-3.229671000	-2.386628000	2.900039000
C	-3.232271000	2.034303000	3.103989000
C	3.276917000	2.141961000	2.939201000
C	3.226788000	2.366226000	-1.338730000
C	3.259299000	-2.277814000	-1.561550000
C	-3.265239000	2.236079000	-1.457301000
C	3.257152000	-2.506579000	2.716496000
H	4.087163000	2.695084000	3.464290000
H	4.060406000	-3.142401000	3.152081000
H	-4.030004000	2.554448000	3.680470000
H	-4.031273000	-2.974434000	3.399735000
C	5.682419000	-2.678181000	-2.065735000
C	-5.657169000	-2.583982000	-2.231027000
C	4.336849000	-2.945069000	-2.348005000
C	-4.313708000	-2.963279000	-2.344056000
C	4.011049000	-3.831540000	-3.383190000
C	-3.968979000	-4.076514000	-3.122646000

C	5.017908000	-4.442900000	-4.125034000
C	-4.957800000	-4.799509000	-3.782566000
C	6.357178000	-4.175136000	-3.836714000
C	-6.294502000	-4.408657000	-3.679527000
C	6.687603000	-3.293027000	-2.806887000
C	-6.642963000	-3.300854000	-2.905113000
C	5.640278000	2.937311000	-1.711626000
C	-5.691128000	2.794730000	-1.802658000
C	4.291564000	3.163741000	-2.012686000
C	-4.346622000	3.026341000	-2.125330000
C	3.948372000	4.137231000	-2.959362000
C	-4.025110000	3.978887000	-3.100494000
C	4.941975000	4.877498000	-3.593763000
C	-5.035307000	4.678557000	-3.756951000
C	6.284319000	4.653633000	-3.283635000
C	-6.372907000	4.435145000	-3.440922000
C	6.631876000	3.683532000	-2.342219000
C	-6.699409000	3.495481000	-2.460450000
H	5.919144000	-1.982268000	-1.258789000
H	-5.904917000	-1.715739000	-1.617040000
H	2.957978000	-4.029781000	-3.595970000
H	-2.915319000	-4.355545000	-3.198440000
H	4.759339000	-5.132987000	-4.931511000
H	-4.687299000	-5.669463000	-4.385107000
H	7.735874000	-3.083131000	-2.582610000
H	-7.689291000	-2.997281000	-2.825193000
H	5.890374000	2.170191000	-0.976308000
H	-5.922440000	2.050782000	-1.037137000
H	2.893166000	4.291637000	-3.195262000
H	-2.971905000	4.156600000	-3.329748000
H	4.671035000	5.631987000	-4.335985000
H	-4.780375000	5.420916000	-4.516839000
H	7.682820000	3.507787000	-2.101258000
H	-7.745977000	3.310622000	-2.207758000
H	-7.069317000	-4.972024000	-4.205176000
H	7.147351000	-4.656212000	-4.418319000
H	-7.164685000	4.983410000	-3.956879000
H	7.063914000	5.236637000	-3.780183000
H	-1.932222000	-2.935627000	0.570539000
H	-0.888348000	1.338031000	5.092578000
H	-0.016218000	0.045527000	4.791744000
H	0.018532000	4.027136000	0.604364000
H	0.689916000	4.267964000	2.659625000
H	0.874817000	4.313790000	-0.697002000
H	1.962115000	-0.197761000	3.570209000
H	-1.943413000	2.799639000	0.832176000

H	-0.634471000	-2.026838000	5.058311000
H	0.903661000	-4.447212000	2.104513000
H	0.695938000	-4.385943000	-1.213958000
H	0.029360000	-4.144801000	0.814532000
O	-1.062827000	-0.103918000	2.172380000
O	-3.623079000	1.293268000	2.166297000
O	-3.628908000	1.382160000	-0.600600000
O	-3.612716000	-1.511335000	2.083993000
O	-2.048713000	-2.666793000	3.222875000
O	0.042298000	-4.100242000	1.833562000
O	2.073815000	-2.849875000	2.965070000
O	2.062609000	-2.580580000	-1.839987000
O	3.637701000	-1.524395000	2.034135000
O	3.612508000	-1.441666000	-0.683366000
O	3.647711000	1.283214000	2.103747000
O	3.598987000	1.391412000	-0.621630000
O	2.028021000	2.710981000	-1.526570000
O	2.099471000	2.449313000	3.254263000
O	1.067099000	1.409402000	0.753531000
O	1.408234000	-0.133434000	2.782363000
O	0.035742000	-1.544902000	4.559625000
O	-0.031880000	1.062479000	4.737852000
O	1.057721000	-1.542749000	0.673978000
O	-1.397003000	-2.136130000	0.647907000
O	-2.053445000	-2.383106000	-1.996109000
O	-0.012709000	-3.910678000	-0.764322000
O	-3.622548000	-1.380019000	-0.739772000
O	-0.009065000	3.786432000	2.201488000
O	0.013013000	3.979421000	-0.410719000
O	-1.395064000	2.007784000	0.773641000
O	-2.048884000	2.242896000	3.466716000
O	-2.077597000	2.474021000	-1.806468000
O	1.381955000	-0.005692000	-1.337728000
O	-1.090867000	-0.026659000	-0.797501000
H	1.901379000	0.000844000	-2.167734000
O	0.145571000	1.767840000	-3.140987000
H	-0.616025000	1.817939000	-3.728442000
Zr	2.526240000	-0.066083000	0.690179000
Zr	-0.016588000	-1.884386000	2.480826000
Zr	0.036906000	1.707800000	2.521554000
Zr	-0.026729000	1.755465000	-1.065906000
Zr	-2.530637000	-0.068200000	0.704568000
Zr	0.023709000	-1.825922000	-1.110943000
C	-1.564461000	-0.396429000	-5.858298000
C	-0.472429000	-1.479519000	-5.693084000
C	0.432515000	-1.096279000	-4.529426000

C	-2.613317000	-0.448608000	-4.749066000
C	1.696172000	-0.360050000	-4.875041000
C	-3.533475000	0.755567000	-4.722301000
H	2.409695000	-1.162156000	-5.155072000
H	0.145770000	-1.445345000	-6.610096000
H	-2.087899000	-0.615121000	-6.809289000
H	-5.109831000	1.186852000	-3.649000000
H	1.510487000	0.200321000	-5.811832000
H	1.544691000	1.114443000	-3.678025000
H	-3.940180000	0.950289000	-5.738430000
H	-2.970552000	1.653735000	-4.400845000
H	-1.865263000	-2.706955000	-5.139651000
H	-4.101135000	-1.635501000	-4.366739000
H	-1.462731000	1.479350000	-6.393705000
H	-2.120704000	-0.507108000	-3.755010000
O	-0.911993000	0.858536000	-5.905147000
O	2.245521000	0.423961000	-3.879995000
O	-4.548918000	0.419342000	-3.814093000
O	0.123422000	-1.426144000	-3.393557000
O	-0.985676000	-2.760711000	-5.557120000
O	-3.364599000	-1.620803000	-4.997375000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.089589000	2.712016000	3.442352000
H	4.061170000	-3.145046000	3.146287000
H	-4.029875000	2.578686000	3.657470000
H	-4.032617000	-2.988355000	3.380567000
C	5.678716000	-2.605799000	-2.141443000
C	-5.465109000	-1.783270000	-2.719298000
C	4.333982000	-2.923704000	-2.369222000
C	-4.337546000	-2.603195000	-2.575613000
C	4.002730000	-3.848340000	-3.368559000
C	-4.220499000	-3.760636000	-3.353173000
C	5.003279000	-4.447302000	-4.128450000
C	-5.218199000	-4.091753000	-4.266266000
C	6.342037000	-4.128758000	-3.894354000
C	-6.325077000	-3.257798000	-4.425417000
C	6.678010000	-3.207991000	-2.900868000

C	-6.446637000	-2.101957000	-3.652211000
C	5.633365000	2.983885000	-1.646345000
C	-5.650196000	2.347632000	-2.222237000
C	4.287002000	3.208409000	-1.961567000
C	-4.325005000	2.781126000	-2.356663000
C	3.950100000	4.227276000	-2.861821000
C	-3.993328000	3.672183000	-3.384694000
C	4.945222000	5.011804000	-3.437511000
C	-4.970497000	4.117700000	-4.270882000
C	6.284463000	4.785527000	-3.116453000
C	-6.287375000	3.672949000	-4.138763000
C	6.626793000	3.771363000	-2.220782000
C	-6.626206000	2.789500000	-3.111950000
H	5.920280000	-1.881298000	-1.361574000
H	-5.538087000	-0.884704000	-2.102317000
H	2.949583000	-4.082259000	-3.540877000
H	-3.342211000	-4.398649000	-3.236872000
H	4.740385000	-5.166401000	-4.907673000
H	-5.125219000	-4.999117000	-4.866932000
H	7.725844000	-2.958337000	-2.719139000
H	-7.309255000	-1.443482000	-3.783437000
H	5.879948000	2.184449000	-0.945190000
H	-5.894306000	1.657839000	-1.412114000
H	2.898436000	4.387571000	-3.107363000
H	-2.958171000	4.008369000	-3.474783000
H	4.677999000	5.802744000	-4.141987000
H	-4.706899000	4.815845000	-5.068890000
H	7.675227000	3.594043000	-1.970830000
H	-7.658641000	2.449162000	-3.001216000
H	-7.095512000	-3.507589000	-5.158759000
H	7.127399000	-4.599907000	-4.490437000
H	-7.054525000	4.024693000	-4.833326000
H	7.065507000	5.401931000	-3.568075000
H	-1.927081000	-2.926909000	0.600488000
H	-0.891911000	1.306518000	5.145855000
H	-0.018206000	0.014427000	4.823933000
H	0.056902000	4.021554000	0.673953000
H	0.694796000	4.252283000	2.722162000
H	0.991849000	4.250136000	-0.583914000
H	1.968504000	-0.202522000	3.598978000
H	-1.917944000	2.803595000	0.838711000
H	-0.643060000	-2.036010000	5.066796000
H	0.886356000	-4.474154000	2.167813000
H	0.750551000	-4.405825000	-1.124544000
H	0.040885000	-4.156840000	0.854474000
O	-1.056160000	-0.102208000	2.195905000

O	-3.620654000	1.289567000	2.170548000
O	-3.622893000	1.388038000	-0.589436000
O	-3.614023000	-1.502988000	2.093099000
O	-2.051797000	-2.657694000	3.235388000
O	0.040324000	-4.104713000	1.880770000
O	2.076936000	-2.840173000	2.979407000
O	2.073269000	-2.634677000	-1.772168000
O	3.642545000	-1.530524000	2.025803000
O	3.618956000	-1.403819000	-0.713532000
O	3.643646000	1.278880000	2.107822000
O	3.594492000	1.415399000	-0.599245000
O	2.013519000	2.662014000	-1.590749000
O	2.102496000	2.438642000	3.277436000
O	1.078466000	1.409954000	0.786383000
O	1.414764000	-0.135878000	2.811253000
O	0.034019000	-1.554003000	4.577328000
O	-0.037560000	1.036749000	4.781589000
O	1.070782000	-1.523249000	0.691960000
O	-1.380355000	-2.136080000	0.684155000
O	-2.074712000	-2.562205000	-1.902948000
O	0.024824000	-3.942887000	-0.689804000
O	-3.579053000	-1.406479000	-0.701230000
O	-0.001547000	3.774783000	2.255512000
O	0.098494000	3.966496000	-0.343246000
O	-1.373342000	2.006893000	0.833201000
O	-2.052662000	2.223478000	3.492801000
O	-2.069329000	2.598293000	-1.665018000
O	1.364888000	0.001639000	-1.352861000
O	-1.095850000	-0.018440000	-0.770811000
H	1.829826000	-0.019825000	-2.212907000
O	-0.138998000	1.625385000	-3.210012000
H	-0.401129000	2.488540000	-3.555735000
Zr	2.539894000	-0.091628000	0.694477000
Zr	-0.005605000	-1.889469000	2.492347000
Zr	0.036110000	1.692819000	2.582464000
Zr	-0.017678000	1.727633000	-0.952006000
Zr	-2.532254000	-0.076734000	0.734037000
Zr	0.016557000	-1.867492000	-1.115129000
C	-1.926200000	-0.049887000	-5.042587000
C	-0.700823000	-2.164024000	-5.279372000
C	0.226633000	-1.537220000	-4.470589000
C	-3.113528000	-0.639323000	-5.723651000
C	1.448103000	-0.828896000	-5.003714000
C	-4.296336000	0.313483000	-5.584671000
H	2.250223000	-1.576624000	-5.130710000
H	-0.631996000	-2.186383000	-6.368134000

H	-1.203734000	0.487924000	-5.688305000
H	-6.066777000	0.375954000	-6.375879000
H	1.244607000	-0.437876000	-6.020794000
H	1.257647000	0.808111000	-3.960080000
H	-4.013627000	1.315648000	-5.964813000
H	-4.557403000	0.419882000	-4.515261000
H	-1.629248000	-2.885448000	-3.784561000
H	-3.652471000	-1.030433000	-7.506683000
H	-1.072024000	0.912470000	-3.457739000
H	-3.385738000	-1.584848000	-5.206176000
O	-2.007762000	0.214037000	-3.808649000
O	1.963327000	0.154176000	-4.145196000
O	-5.337305000	-0.251114000	-6.346415000
O	0.056297000	-1.583917000	-3.194953000
O	-1.617918000	-3.001240000	-4.761186000
O	-2.805709000	-0.854792000	-7.074779000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.085480000	2.699234000	3.462379000
H	4.059313000	-3.129318000	3.171385000
H	-4.027611000	2.556527000	3.681161000
H	-4.029913000	-2.973820000	3.402210000
C	5.692313000	-2.590610000	-2.095539000
C	-5.669394000	-2.467693000	-2.242830000
C	4.359807000	-2.972484000	-2.293840000
C	-4.338038000	-2.875164000	-2.396848000
C	4.066053000	-4.012419000	-3.186209000
C	-4.029065000	-3.916418000	-3.281042000
C	5.090517000	-4.661943000	-3.868439000
C	-5.039441000	-4.545182000	-4.001854000
C	6.416790000	-4.276173000	-3.666251000
C	-6.363006000	-4.126962000	-3.856726000
C	6.715709000	-3.240074000	-2.780520000
C	-6.676907000	-3.086769000	-2.978872000
C	5.641554000	2.949623000	-1.643045000
C	-5.659728000	2.963201000	-1.594891000
C	4.298107000	3.209264000	-1.943366000
C	-4.326564000	3.144081000	-1.987203000

C	3.978505000	4.261722000	-2.810638000
C	-4.003041000	4.176386000	-2.875618000
C	4.985770000	5.043006000	-3.369494000
C	-5.001090000	5.003463000	-3.384236000
C	6.321927000	4.778740000	-3.065487000
C	-6.329778000	4.808858000	-3.003455000
C	6.647792000	3.731852000	-2.202022000
C	-6.657467000	3.791384000	-2.104301000
H	5.905336000	-1.779009000	-1.397648000
H	-5.890304000	-1.648944000	-1.556040000
H	3.022052000	-4.296653000	-3.338305000
H	-2.986473000	-4.220577000	-3.394817000
H	4.855840000	-5.472174000	-4.562500000
H	-4.793806000	-5.356613000	-4.690080000
H	7.753684000	-2.937794000	-2.623799000
H	-7.713393000	-2.759839000	-2.867107000
H	5.875625000	2.126125000	-0.966031000
H	-5.891095000	2.158335000	-0.893877000
H	2.929428000	4.456943000	-3.042188000
H	-2.958644000	4.310912000	-3.164462000
H	4.730369000	5.861453000	-4.046380000
H	-4.744156000	5.804914000	-4.080463000
H	7.693683000	3.524877000	-1.964710000
H	-7.695866000	3.648117000	-1.796112000
H	-7.155100000	-4.613150000	-4.431529000
H	7.221086000	-4.785482000	-4.202690000
H	-7.113002000	5.457156000	-3.403450000
H	7.112914000	5.391551000	-3.504380000
H	-1.939295000	-2.926874000	0.577935000
H	-0.878499000	1.303205000	5.120826000
H	-0.017026000	0.005618000	4.776456000
H	0.022183000	4.006673000	0.594549000
H	0.681358000	4.262294000	2.634833000
H	0.940888000	4.242105000	-0.670983000
H	1.959282000	-0.203236000	3.558564000
H	-1.930109000	2.808285000	0.812829000
H	-0.637167000	-2.036842000	5.017629000
H	0.894913000	-4.468265000	2.080272000
H	0.652876000	-4.432132000	-1.227524000
H	0.030604000	-4.143047000	0.777357000
O	-1.058410000	-0.097033000	2.160447000
O	-3.621811000	1.299391000	2.162145000
O	-3.626739000	1.348577000	-0.636959000
O	-3.618006000	-1.501826000	2.094495000
O	-2.047493000	-2.671631000	3.207076000
O	0.044169000	-4.100106000	1.805998000

O	2.073873000	-2.848346000	2.956876000
O	2.081751000	-2.638772000	-1.792732000
O	3.641892000	-1.535641000	2.016793000
O	3.606482000	-1.376518000	-0.736383000
O	3.643402000	1.279132000	2.108098000
O	3.582292000	1.421529000	-0.591297000
O	2.016612000	2.659213000	-1.621565000
O	2.096234000	2.450736000	3.253026000
O	1.059645000	1.422508000	0.751540000
O	1.408056000	-0.133002000	2.769281000
O	0.035070000	-1.549645000	4.526832000
O	-0.031869000	1.031006000	4.741447000
O	1.062719000	-1.527502000	0.647275000
O	-1.399909000	-2.128975000	0.638980000
O	-2.066094000	-2.411718000	-2.001603000
O	-0.023922000	-3.929219000	-0.760242000
O	-3.605069000	-1.397527000	-0.715540000
O	-0.015535000	3.776243000	2.177677000
O	0.051561000	3.949506000	-0.424971000
O	-1.397359000	2.004396000	0.773232000
O	-2.047333000	2.237425000	3.471656000
O	-2.067564000	2.440804000	-1.828409000
O	1.370572000	0.014548000	-1.367447000
O	-1.092758000	-0.025020000	-0.806182000
H	1.902955000	0.021021000	-2.196111000
O	0.110456000	1.724100000	-3.356358000
H	0.205395000	2.615810000	-3.715264000
Zr	2.523115000	-0.097250000	0.682081000
Zr	-0.008384000	-1.894803000	2.438063000
Zr	0.026342000	1.699102000	2.546996000
Zr	-0.017052000	1.694597000	-0.994968000
Zr	-2.537996000	-0.089431000	0.705972000
Zr	0.017283000	-1.856091000	-1.211482000
C	-2.374811000	0.071954000	-5.611691000
C	-0.060544000	-1.844040000	-5.532068000
C	0.687464000	-1.515937000	-4.454088000
C	-3.487662000	-0.275241000	-4.666164000
C	2.125430000	-1.134886000	-4.582716000
C	-4.356266000	0.959070000	-4.477795000
H	2.788983000	-1.910069000	-4.172608000
H	0.282601000	-1.796939000	-6.565055000
H	-2.516362000	-0.288464000	-6.656231000
H	-5.972892000	1.348590000	-3.475452000
H	2.381936000	-1.036085000	-5.652639000
H	1.774613000	0.717206000	-4.062900000
H	-4.734005000	1.293543000	-5.465394000

H	-3.732444000	1.773641000	-4.067270000
H	-1.514282000	-2.275398000	-4.421801000
H	-5.001012000	-1.446471000	-4.633429000
H	-0.609923000	1.311838000	-3.908597000
H	-3.030406000	-0.519529000	-3.679161000
O	-1.445109000	0.803517000	-5.316911000
O	2.457592000	0.055574000	-3.868995000
O	-5.402775000	0.584682000	-3.622424000
O	0.106722000	-1.564587000	-3.259008000
O	-1.361329000	-2.209814000	-5.386699000
O	-4.223031000	-1.334391000	-5.198358000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086797000	2.684442000	3.475514000
H	4.063150000	-3.142348000	3.146970000
H	-4.030922000	2.539219000	3.691836000
H	-4.031856000	-2.990546000	3.379214000
C	5.588607000	-2.270620000	-2.510403000
C	-5.649589000	-2.328257000	-2.341175000
C	4.282672000	-2.778598000	-2.531366000
C	-4.327031000	-2.761681000	-2.499764000
C	3.924105000	-3.722039000	-3.503738000
C	-4.019569000	-3.706174000	-3.486893000
C	4.859476000	-4.151606000	-4.442074000
C	-5.025798000	-4.219951000	-4.299178000
C	6.159089000	-3.641935000	-4.416358000
C	-6.342213000	-3.783204000	-4.140868000
C	6.522173000	-2.701994000	-3.450223000
C	-6.652958000	-2.833706000	-3.164469000
C	5.627512000	3.061115000	-1.535851000
C	-5.685490000	2.844574000	-1.625903000
C	4.292404000	3.229066000	-1.925139000
C	-4.358146000	3.090174000	-1.999775000
C	3.965244000	4.210459000	-2.869576000
C	-4.064858000	4.154415000	-2.862323000
C	4.961498000	5.014658000	-3.416198000
C	-5.090117000	4.958278000	-3.350773000
C	6.289307000	4.848002000	-3.019373000

C	-6.413050000	4.708692000	-2.977270000
C	6.620878000	3.871406000	-2.078744000
C	-6.709080000	3.653840000	-2.112191000
H	5.850500000	-1.534300000	-1.747399000
H	-5.870264000	-1.576403000	-1.580651000
H	2.899423000	-4.101889000	-3.509707000
H	-2.982024000	-4.025667000	-3.604882000
H	4.576536000	-4.888256000	-5.197682000
H	-4.783973000	-4.958150000	-5.066834000
H	7.539530000	-2.304712000	-3.429800000
H	-7.679571000	-2.478169000	-3.050360000
H	5.864715000	2.290395000	-0.799611000
H	-5.895569000	2.010120000	-0.954406000
H	2.922011000	4.320527000	-3.173021000
H	-3.026926000	4.330566000	-3.147057000
H	4.703681000	5.775272000	-4.156722000
H	-4.859661000	5.784976000	-4.026398000
H	7.660225000	3.742825000	-1.767799000
H	-7.743141000	3.464024000	-1.812630000
H	-7.130050000	-4.181248000	-4.785211000
H	6.892363000	-3.979404000	-5.152712000
H	-7.215853000	5.345211000	-3.358286000
H	7.070129000	5.482162000	-3.446326000
H	-1.938195000	-2.948098000	0.622143000
H	-0.880780000	1.372480000	5.081295000
H	-0.014284000	0.072869000	4.793096000
H	0.035320000	4.002288000	0.561146000
H	0.680805000	4.273959000	2.623840000
H	0.916997000	4.250091000	-0.730736000
H	1.965325000	-0.174087000	3.575106000
H	-1.926963000	2.786098000	0.786485000
H	-0.643271000	-1.991969000	5.076290000
H	0.904834000	-4.453196000	2.174756000
H	0.641394000	-4.475547000	-1.124462000
H	0.007585000	-4.179840000	0.891030000
O	-1.059037000	-0.099334000	2.177029000
O	-3.618496000	1.301867000	2.156806000
O	-3.603974000	1.296512000	-0.674124000
O	-3.611073000	-1.504407000	2.091815000
O	-2.050956000	-2.654890000	3.240726000
O	0.042636000	-4.105430000	1.908724000
O	2.077241000	-2.831776000	2.995019000
O	2.110152000	-2.773304000	-1.617114000
O	3.636754000	-1.541466000	2.006918000
O	3.630326000	-1.368548000	-0.759667000
O	3.646967000	1.281091000	2.103806000

O	3.597242000	1.387228000	-0.628469000
O	2.024003000	2.658563000	-1.594120000
O	2.098625000	2.461399000	3.238022000
O	1.069322000	1.391847000	0.723594000
O	1.413756000	-0.122354000	2.784774000
O	0.032510000	-1.518987000	4.576387000
O	-0.025717000	1.089404000	4.728565000
O	1.063836000	-1.538893000	0.691891000
O	-1.387364000	-2.157894000	0.682138000
O	-2.050181000	-2.403982000	-1.987575000
O	-0.061960000	-3.984482000	-0.683067000
O	-3.608290000	-1.464871000	-0.671348000
O	-0.007511000	3.780873000	2.161876000
O	0.045046000	3.936275000	-0.451967000
O	-1.386138000	1.987155000	0.752076000
O	-2.046919000	2.250147000	3.459413000
O	-2.074939000	2.514401000	-1.768363000
O	1.351183000	-0.051472000	-1.414530000
O	-1.074994000	-0.075559000	-0.791685000
H	1.942406000	-0.043926000	-2.191921000
O	-0.087001000	1.730916000	-3.239884000
H	-0.882693000	2.210924000	-3.521950000
Zr	2.527001000	-0.079477000	0.682602000
Zr	-0.013185000	-1.877480000	2.501972000
Zr	0.038493000	1.708736000	2.506792000
Zr	-0.034950000	1.703030000	-1.083316000
Zr	-2.524905000	-0.084670000	0.705202000
Zr	0.031122000	-1.916259000	-1.087015000
C	-0.559820000	-0.355898000	-4.795891000
C	0.505577000	-1.121145000	-4.289180000
C	1.903429000	-0.910967000	-4.808224000
H	2.285233000	-1.897955000	-5.126114000
H	-0.505199000	0.038023000	-5.818766000
H	1.882082000	-0.257151000	-5.697470000
H	3.625669000	-0.669589000	-3.889057000
H	-1.779928000	-1.365278000	-3.701390000
H	-0.168536000	0.665100000	-4.075036000
O	2.717756000	-0.355431000	-3.793599000
O	0.303319000	-1.863237000	-3.284658000
O	-1.832548000	-0.686273000	-4.403065000
C	-3.432204000	1.088606000	-5.361292000
C	-4.593815000	0.448866000	-4.641761000
C	-5.818969000	1.342206000	-4.696147000
H	-3.142023000	0.552903000	-6.303932000
H	-7.596765000	1.261884000	-3.925856000
H	-6.136916000	1.449858000	-5.752680000

H	-5.562061000	2.347633000	-4.317448000
H	-5.595510000	-1.183915000	-4.768745000
H	-4.299140000	0.352284000	-3.572592000
O	-2.881220000	2.098603000	-4.996360000
O	-6.810436000	0.707166000	-3.920896000
O	-4.840833000	-0.795680000	-5.232170000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086614000	2.691347000	3.468847000
H	4.061235000	-3.149605000	3.139871000
H	-4.030156000	2.549125000	3.684797000
H	-4.031462000	-2.985331000	3.386063000
C	5.673102000	-2.555100000	-2.181099000
C	-5.652425000	-2.451481000	-2.303038000
C	4.337772000	-2.940539000	-2.352661000
C	-4.324519000	-2.887909000	-2.402963000
C	4.024006000	-3.941959000	-3.281211000
C	-4.015921000	-3.979038000	-3.225163000
C	5.029986000	-4.548132000	-4.028310000
C	-5.020295000	-4.624897000	-3.940272000
C	6.358392000	-4.155276000	-3.855694000
C	-6.338209000	-4.177397000	-3.849444000
C	6.677753000	-3.159093000	-2.932110000
C	-6.652851000	-3.089425000	-3.031310000
C	5.634060000	3.001487000	-1.637609000
C	-5.675821000	2.900728000	-1.698026000
C	4.290548000	3.183771000	-1.988602000
C	-4.342920000	3.039385000	-2.111519000
C	3.951652000	4.134865000	-2.959398000
C	-4.031708000	3.912097000	-3.161866000
C	4.944903000	4.896111000	-3.569009000
C	-5.042837000	4.624019000	-3.802463000
C	6.281463000	4.717060000	-3.208818000
C	-6.368955000	4.477480000	-3.392127000
C	6.624589000	3.769880000	-2.242665000
C	-6.683943000	3.619134000	-2.336572000
H	5.902194000	-1.774051000	-1.453922000
H	-5.874988000	-1.595878000	-1.663895000

H	2.980001000	-4.241229000	-3.399577000
H	-2.982241000	-4.323090000	-3.290466000
H	4.780894000	-5.332800000	-4.746526000
H	-4.772389000	-5.475692000	-4.578128000
H	7.717327000	-2.852112000	-2.797633000
H	-7.685516000	-2.739903000	-2.959979000
H	5.880983000	2.252148000	-0.882983000
H	-5.899776000	2.216369000	-0.876574000
H	2.901498000	4.253859000	-3.234526000
H	-2.987915000	4.013027000	-3.467035000
H	4.678014000	5.631825000	-4.331164000
H	-4.797154000	5.298138000	-4.626056000
H	7.671072000	3.629974000	-1.962056000
H	-7.721042000	3.509775000	-2.011610000
H	-7.125462000	-4.677798000	-4.418500000
H	7.148361000	-4.629598000	-4.442900000
H	-7.161147000	5.036434000	-3.895757000
H	7.060319000	5.317250000	-3.685631000
H	-1.932182000	-2.936554000	0.591916000
H	-0.884306000	1.362260000	5.093579000
H	-0.014454000	0.068000000	4.800857000
H	0.024427000	4.023318000	0.590024000
H	0.686782000	4.277902000	2.649577000
H	0.870550000	4.321981000	-0.716443000
H	1.963517000	-0.183994000	3.579832000
H	-1.936356000	2.803216000	0.826506000
H	-0.634430000	-2.009910000	5.081784000
H	0.905869000	-4.445102000	2.121839000
H	0.727302000	-4.375876000	-1.179559000
H	0.026793000	-4.146312000	0.836116000
O	-1.061130000	-0.099959000	2.180164000
O	-3.624088000	1.295083000	2.165056000
O	-3.629071000	1.370466000	-0.609804000
O	-3.611211000	-1.506699000	2.089155000
O	-2.049769000	-2.659995000	3.234123000
O	0.044435000	-4.097183000	1.852306000
O	2.074889000	-2.842381000	2.980277000
O	2.062723000	-2.592056000	-1.833288000
O	3.636952000	-1.525233000	2.032603000
O	3.612795000	-1.438298000	-0.689222000
O	3.649966000	1.281019000	2.106706000
O	3.601032000	1.396584000	-0.614694000
O	2.025812000	2.690004000	-1.551155000
O	2.099653000	2.455618000	3.245960000
O	1.068129000	1.404768000	0.748629000
O	1.409483000	-0.125418000	2.791629000

O	0.034293000	-1.531337000	4.577854000
O	-0.029061000	1.082975000	4.738690000
O	1.067998000	-1.547326000	0.696187000
O	-1.392201000	-2.140452000	0.670238000
O	-2.047894000	-2.401106000	-1.991753000
O	-0.011646000	-3.917862000	-0.762288000
O	-3.605445000	-1.409319000	-0.713255000
O	-0.007637000	3.790862000	2.190356000
O	0.018272000	3.969869000	-0.424254000
O	-1.392678000	2.007792000	0.770634000
O	-2.048754000	2.246839000	3.462419000
O	-2.075916000	2.473365000	-1.801083000
O	1.386447000	-0.016696000	-1.331852000
O	-1.091469000	-0.031383000	-0.781817000
H	1.884565000	-0.020306000	-2.173798000
O	0.109539000	1.685031000	-3.158671000
H	-0.702161000	1.659460000	-3.678337000
Zr	2.530750000	-0.060546000	0.694996000
Zr	-0.015928000	-1.877301000	2.503780000
Zr	0.038306000	1.714510000	2.516130000
Zr	-0.024450000	1.748920000	-1.082564000
Zr	-2.531486000	-0.063963000	0.714025000
Zr	0.022391000	-1.822626000	-1.067643000
C	0.136354000	-2.704651000	-5.327300000
C	0.626600000	-1.597266000	-4.442182000
C	1.734420000	-0.696635000	-4.894951000
H	2.590413000	-1.350818000	-5.150513000
H	0.929178000	-3.485638000	-5.282143000
H	1.405600000	-0.262452000	-5.861180000
H	1.363081000	0.880647000	-3.803341000
H	-1.255488000	-2.975487000	-4.005064000
H	0.111567000	-2.372581000	-6.378271000
O	2.131565000	0.249828000	-3.975341000
O	0.113876000	-1.499547000	-3.334088000
O	-1.107512000	-3.185781000	-4.948310000
C	-2.208954000	-0.715240000	-5.930050000
C	-3.338839000	-0.796565000	-4.948265000
C	-3.830491000	0.568945000	-4.500332000
H	-2.343710000	-1.361338000	-6.836387000
H	-5.285309000	1.154933000	-3.345664000
H	-4.151187000	1.160523000	-5.381056000
H	-2.998927000	1.115143000	-4.012957000
H	-5.076841000	-1.588708000	-4.864937000
H	-2.895995000	-1.291302000	-4.054619000
O	-1.222942000	-0.030272000	-5.770325000
O	-4.898211000	0.316268000	-3.625890000

O -4.358533000 -1.564926000 -5.513068000

Zr-NU-1000 Int2_Ro'

C -3.248200000 -2.182800000 -1.650100000

C -3.229700000 -2.386600000 2.900000000

C -3.232300000 2.034300000 3.104000000

C 3.276900000 2.142000000 2.939200000

C 3.226900000 2.366300000 -1.338700000

C 3.259300000 -2.277900000 -1.561500000

C -3.265300000 2.236100000 -1.457300000

C 3.257200000 -2.506600000 2.716400000

H 4.092210000 2.689062000 3.462497000

H 4.065314000 -3.141724000 3.144028000

H -4.029495000 2.568141000 3.668345000

H -4.030860000 -2.991075000 3.380381000

C 5.663862000 -2.438264000 -2.247854000

C -5.602664000 -2.218541000 -2.503637000

C 4.339875000 -2.866833000 -2.408717000

C -4.302026000 -2.736856000 -2.548383000

C 4.039374000 -3.817164000 -3.393854000

C -3.986375000 -3.736626000 -3.478097000

C 5.046776000 -4.329244000 -4.206987000

C -4.958708000 -4.208108000 -4.355512000

C 6.363757000 -3.895926000 -4.042588000

C -6.250064000 -3.678368000 -4.316298000

C 6.670480000 -2.951218000 -3.062261000

C -6.570744000 -2.684111000 -3.390397000

C 5.654432000 2.848370000 -1.761276000

C -5.690642000 2.660029000 -1.961438000

C 4.308241000 3.128456000 -2.029557000

C -4.340930000 2.900517000 -2.247689000

C 3.981496000 4.118079000 -2.965738000

C -3.995549000 3.758548000 -3.299928000

C 4.988405000 4.818444000 -3.624187000

C -4.991976000 4.369435000 -4.056139000

C 6.327912000 4.539973000 -3.347897000

C -6.336196000 4.132262000 -3.763438000

C 6.659586000 3.555624000 -2.415294000

C -6.684478000 3.278481000 -2.715292000

H 5.882550000 -1.697797000 -1.475783000

H -5.831592000 -1.441962000 -1.770849000

H 3.006553000 -4.154495000 -3.510972000

H -2.968451000 -4.132711000 -3.497071000

H 4.807248000 -5.073169000 -4.970214000

H -4.710573000 -4.990643000 -5.076066000

H 7.701201000 -2.614068000 -2.931877000

H	-7.581612000	-2.271211000	-3.359567000
H	5.892030000	2.073648000	-1.029424000
H	-5.941022000	1.987677000	-1.138331000
H	2.928478000	4.319759000	-3.173660000
H	-2.936611000	3.923744000	-3.510601000
H	4.729257000	5.585519000	-4.357447000
H	-4.721110000	5.035132000	-4.878963000
H	7.708338000	3.340519000	-2.197543000
H	-7.736974000	3.095789000	-2.485989000
H	-7.010937000	-4.044224000	-5.009996000
H	7.154353000	-4.298641000	-4.680113000
H	-7.117288000	4.615560000	-4.355672000
H	7.117630000	5.092888000	-3.862424000
H	-1.950118000	-2.923151000	0.597515000
H	-0.883840000	1.357770000	5.101013000
H	-0.012811000	0.064407000	4.810033000
H	0.028524000	4.040805000	0.647935000
H	0.689097000	4.265665000	2.715104000
H	0.872003000	4.352817000	-0.655440000
H	1.965778000	-0.184276000	3.577246000
H	-1.953417000	2.792145000	0.836743000
H	-0.634885000	-2.011655000	5.087424000
H	0.894542000	-4.444591000	2.154468000
H	0.738081000	-4.385728000	-1.113051000
H	0.014340000	-4.151441000	0.865044000
O	-1.062135000	-0.103848000	2.182286000
O	-3.624461000	1.290663000	2.169532000
O	-3.626406000	1.343948000	-0.621976000
O	-3.611010000	-1.506982000	2.090115000
O	-2.050551000	-2.655852000	3.242646000
O	0.033592000	-4.097027000	1.883355000
O	2.076680000	-2.843603000	2.982728000
O	2.070179000	-2.660107000	-1.781495000
O	3.630697000	-1.528967000	2.021279000
O	3.598623000	-1.421392000	-0.707216000
O	3.643396000	1.286483000	2.094866000
O	3.582531000	1.356156000	-0.655096000
O	2.041971000	2.750498000	-1.496344000
O	2.103143000	2.448110000	3.259101000
O	1.063157000	1.404922000	0.744534000
O	1.407689000	-0.127402000	2.791797000
O	0.035784000	-1.535459000	4.583731000
O	-0.027442000	1.078895000	4.747987000
O	1.052483000	-1.537769000	0.684504000
O	-1.396354000	-2.137436000	0.683317000
O	-2.044358000	-2.448466000	-1.928466000

O	-0.014734000	-3.933437000	-0.715289000
O	-3.625747000	-1.438405000	-0.697865000
O	-0.008479000	3.789282000	2.249769000
O	0.023341000	3.994100000	-0.363067000
O	-1.397367000	2.003944000	0.807816000
O	-2.051025000	2.230747000	3.479568000
O	-2.082374000	2.579780000	-1.679653000
O	1.333717000	-0.025412000	-1.418399000
O	-1.107549000	-0.030184000	-0.815823000
H	1.930864000	-0.011217000	-2.184310000
O	0.035928000	2.028851000	-3.080360000
H	0.820011000	2.163791000	-3.630465000
Zr	2.505095000	-0.053228000	0.698385000
Zr	-0.023447000	-1.876058000	2.510535000
Zr	0.030382000	1.711934000	2.526922000
Zr	-0.042167000	1.794049000	-1.085278000
Zr	-2.534194000	-0.055159000	0.709802000
Zr	-0.010021000	-1.843675000	-1.064934000
C	0.350959000	-0.747619000	-4.381945000
C	1.741169000	-0.592752000	-4.993616000
C	1.887600000	0.681940000	-5.823394000
C	-0.750753000	-0.905332000	-5.411829000
C	2.099893000	0.539750000	-7.298795000
C	-2.105288000	-1.012971000	-4.746613000
H	3.045666000	-0.039979000	-7.412334000
H	1.961953000	-1.475254000	-5.633010000
H	0.143681000	0.167634000	-3.796824000
H	-3.937049000	-0.867646000	-5.377082000
H	1.306589000	-0.116139000	-7.702272000
H	2.122234000	2.427484000	-7.245214000
H	-2.205610000	-0.206878000	-3.990343000
H	-2.178329000	-1.977101000	-4.221475000
H	3.547970000	-0.464408000	-4.194822000
H	-1.589421000	0.350153000	-6.593041000
H	1.248015000	-2.231096000	-3.397811000
H	-0.575418000	-1.829799000	-6.007982000
O	0.340980000	-1.878984000	-3.491969000
O	2.152127000	1.755535000	-7.945975000
O	-3.060658000	-0.883733000	-5.776919000
O	1.950607000	1.774186000	-5.295286000
O	2.636158000	-0.555705000	-3.891065000
O	-0.694652000	0.230823000	-6.239920000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000

C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.092172000	2.702096000	3.448505000
H	4.063260000	-3.138032000	3.152164000
H	-4.030772000	2.573540000	3.660684000
H	-4.032732000	-2.974595000	3.396382000
C	5.691472000	-2.694455000	-1.998855000
C	-5.649293000	-2.395040000	-2.333366000
C	4.352385000	-2.987117000	-2.285518000
C	-4.315293000	-2.791038000	-2.490475000
C	4.048800000	-3.940002000	-3.266700000
C	-3.983851000	-3.744862000	-3.461813000
C	5.070829000	-4.590982000	-3.951977000
C	-4.977663000	-4.300238000	-4.261953000
C	6.403740000	-4.295147000	-3.661304000
C	-6.306002000	-3.901783000	-4.101936000
C	6.712142000	-3.347450000	-2.684286000
C	-6.640130000	-2.948452000	-3.139099000
C	5.638117000	2.698501000	-1.944340000
C	-5.669934000	2.524486000	-2.107074000
C	4.295231000	3.061356000	-2.115908000
C	-4.327712000	2.887136000	-2.272019000
C	3.962552000	4.053945000	-3.047719000
C	-3.977744000	3.837293000	-3.241027000
C	4.958076000	4.675069000	-3.796438000
C	-4.962479000	4.417820000	-4.035167000
C	6.293768000	4.314136000	-3.615048000
C	-6.299629000	4.052671000	-3.867261000
C	6.632507000	3.326822000	-2.688037000
C	-6.651891000	3.106977000	-2.903212000
H	5.911131000	-1.949085000	-1.232180000
H	-5.887700000	-1.645149000	-1.576696000
H	3.000268000	-4.162176000	-3.478550000
H	-2.937284000	-4.038015000	-3.571593000
H	4.830087000	-5.335524000	-4.714372000
H	-4.718311000	-5.046804000	-5.016083000
H	7.755406000	-3.117339000	-2.456688000
H	-7.679286000	-2.634126000	-3.019074000
H	5.880425000	1.919237000	-1.219253000
H	-5.922425000	1.776913000	-1.352756000
H	2.913851000	4.327847000	-3.183940000
H	-2.924307000	4.103859000	-3.355981000

H	4.691921000	5.442217000	-4.526623000
H	-4.689075000	5.159021000	-4.789716000
H	7.678415000	3.044877000	-2.547621000
H	-7.698209000	2.820418000	-2.775933000
H	-7.085225000	-4.335461000	-4.733438000
H	7.205918000	-4.807194000	-4.198149000
H	-7.071651000	4.507050000	-4.493034000
H	7.075105000	4.803283000	-4.201637000
H	-1.944861000	-2.913167000	0.569859000
H	-0.886086000	1.321260000	5.124291000
H	-0.017811000	0.027123000	4.809412000
H	0.022936000	4.057784000	0.710910000
H	0.691778000	4.254043000	2.757091000
H	0.859240000	4.391179000	-0.595526000
H	1.964847000	-0.201201000	3.574476000
H	-1.958537000	2.800992000	0.850171000
H	-0.639660000	-2.037514000	5.058087000
H	0.890479000	-4.461301000	2.143259000
H	0.758483000	-4.389086000	-1.169396000
H	0.041178000	-4.155834000	0.835575000
O	-1.058239000	-0.104643000	2.171330000
O	-3.617750000	1.290228000	2.167647000
O	-3.627057000	1.374557000	-0.598280000
O	-3.607529000	-1.510335000	2.083002000
O	-2.048849000	-2.666511000	3.226790000
O	0.039763000	-4.102349000	1.855510000
O	2.075138000	-2.848504000	2.967691000
O	2.067084000	-2.576644000	-1.858362000
O	3.633447000	-1.525948000	2.026411000
O	3.594766000	-1.404987000	-0.710339000
O	3.640930000	1.285864000	2.096085000
O	3.579644000	1.373999000	-0.638209000
O	2.043942000	2.782708000	-1.462960000
O	2.103458000	2.436149000	3.275711000
O	1.061128000	1.422592000	0.765058000
O	1.406260000	-0.135638000	2.789935000
O	0.032188000	-1.554749000	4.562125000
O	-0.033250000	1.045404000	4.760603000
O	1.057012000	-1.527439000	0.663715000
O	-1.385476000	-2.131338000	0.657338000
O	-2.050041000	-2.466420000	-1.916990000
O	0.033252000	-3.928118000	-0.731887000
O	-3.612647000	-1.392634000	-0.722827000
O	-0.008647000	3.785089000	2.288242000
O	0.016012000	4.019049000	-0.304508000
O	-1.392302000	2.020045000	0.815734000

O	-2.051859000	2.224128000	3.489588000
O	-2.071029000	2.548949000	-1.703397000
O	1.335709000	0.024372000	-1.412312000
O	-1.088790000	-0.000683000	-0.829667000
H	1.993600000	-0.005639000	-2.126283000
O	0.102749000	2.289082000	-3.078164000
H	0.972846000	2.625889000	-3.328072000
Zr	2.507825000	-0.063792000	0.701265000
Zr	-0.019517000	-1.886646000	2.483657000
Zr	0.028398000	1.702666000	2.555435000
Zr	-0.041804000	1.823266000	-1.018941000
Zr	-2.529379000	-0.061406000	0.700244000
Zr	0.006663000	-1.854736000	-1.117777000
C	0.089084000	-0.479833000	-4.058561000
C	1.909313000	-0.499208000	-4.879255000
C	1.783346000	0.630625000	-5.874058000
C	-1.025096000	-0.062098000	-4.976511000
C	1.185842000	0.345293000	-7.225348000
C	-2.347116000	-0.240710000	-4.208902000
H	2.041211000	0.076824000	-7.874157000
H	2.187688000	-1.456079000	-5.373780000
H	0.416882000	0.369624000	-3.444906000
H	-3.176389000	1.246770000	-5.084753000
H	0.583105000	-0.587250000	-7.158961000
H	-0.135482000	1.682809000	-7.124872000
H	-2.240460000	0.185161000	-3.187962000
H	-2.544346000	-1.313021000	-4.088501000
H	2.996393000	0.781074000	-4.044655000
H	-0.590644000	1.800921000	-4.545462000
H	1.016106000	-1.397288000	-4.234746000
H	-1.089946000	-0.673574000	-5.892175000
O	-0.004730000	-1.688633000	-3.436207000
O	0.521594000	1.410085000	-7.790100000
O	-3.403913000	0.321883000	-4.918663000
O	2.235071000	1.706743000	-5.530406000
O	2.778571000	-0.162730000	-3.871317000
O	-0.850637000	1.280303000	-5.363982000

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C	-3.248236000	-2.182785000	-1.650095000
C	-3.229693000	-2.386607000	2.899996000
C	-3.232298000	2.034294000	3.103998000
C	3.276901000	2.142002000	2.939200000
C	3.226899000	2.366298000	-1.338699000
C	3.259313000	-2.277896000	-1.561490000
C	-3.265292000	2.236093000	-1.457311000

C	3.257207000	-2.506598000	2.716400000
H	4.090575000	2.694111000	3.459741000
H	4.062286000	-3.147624000	3.140363000
H	-4.028998000	2.572142000	3.664725000
H	-4.032579000	-2.980694000	3.389619000
C	5.686984000	-2.619129000	-2.074781000
C	-5.657862000	-2.426034000	-2.299288000
C	4.349037000	-2.942521000	-2.332007000
C	-4.318336000	-2.786280000	-2.492138000
C	4.043807000	-3.862618000	-3.342342000
C	-3.985937000	-3.706826000	-3.494570000
C	5.063095000	-4.448628000	-4.088891000
C	-4.982101000	-4.261159000	-4.292522000
C	6.394526000	-4.119409000	-3.830559000
C	-6.315633000	-3.897509000	-4.097165000
C	6.704684000	-3.205091000	-2.821945000
C	-6.651916000	-2.979946000	-3.100999000
C	5.646267000	2.723763000	-1.901946000
C	-5.679067000	2.665389000	-1.979559000
C	4.306223000	3.106319000	-2.060918000
C	-4.328128000	2.941066000	-2.223663000
C	3.987444000	4.159897000	-2.927694000
C	-3.976208000	3.865895000	-3.215757000
C	4.993699000	4.823638000	-3.621773000
C	-4.965981000	4.507857000	-3.953759000
C	6.326105000	4.438770000	-3.459509000
C	-6.311594000	4.230967000	-3.705340000
C	6.651524000	3.387706000	-2.601020000
C	-6.666707000	3.310704000	-2.718089000
H	5.907165000	-1.898269000	-1.284763000
H	-5.899310000	-1.705864000	-1.515380000
H	2.996238000	-4.104202000	-3.534965000
H	-2.936302000	-3.976188000	-3.630105000
H	4.820359000	-5.167183000	-4.875265000
H	-4.720480000	-4.980144000	-5.072268000
H	7.747220000	-2.950082000	-2.617986000
H	-7.695451000	-2.694121000	-2.951055000
H	5.880936000	1.904413000	-1.218307000
H	-5.934358000	1.937734000	-1.206927000
H	2.939296000	4.431227000	-3.064465000
H	-2.916945000	4.066690000	-3.391841000
H	4.739145000	5.641075000	-4.299808000
H	-4.690119000	5.228563000	-4.727019000
H	7.694282000	3.089098000	-2.471796000
H	-7.720060000	3.093830000	-2.526873000
H	-7.097044000	-4.330902000	-4.726147000

H	7.194325000	-4.579359000	-4.416062000
H	-7.088198000	4.734577000	-4.286137000
H	7.114884000	4.960525000	-4.006798000
H	-1.935564000	-2.930861000	0.576015000
H	-0.886437000	1.335265000	5.113534000
H	-0.016332000	0.041649000	4.808752000
H	0.012599000	4.028109000	0.649195000
H	0.690100000	4.259785000	2.700831000
H	0.860388000	4.342364000	-0.650182000
H	1.963506000	-0.195534000	3.577170000
H	-1.955565000	2.790026000	0.837593000
H	-0.635490000	-2.027324000	5.074989000
H	0.892539000	-4.460628000	2.155990000
H	0.779007000	-4.386005000	-1.153115000
H	0.041676000	-4.159557000	0.851098000
O	-1.061420000	-0.108392000	2.178167000
O	-3.621945000	1.285621000	2.173216000
O	-3.628455000	1.374583000	-0.599475000
O	-3.609523000	-1.510816000	2.084246000
O	-2.050455000	-2.661208000	3.235424000
O	0.039274000	-4.106735000	1.869147000
O	2.075293000	-2.848282000	2.968763000
O	2.063308000	-2.565454000	-1.868587000
O	3.636089000	-1.517208000	2.042111000
O	3.598943000	-1.453503000	-0.667149000
O	3.643801000	1.290207000	2.092450000
O	3.590457000	1.367793000	-0.648027000
O	2.038680000	2.751329000	-1.494211000
O	2.101883000	2.440827000	3.265601000
O	1.062412000	1.406952000	0.755313000
O	1.406518000	-0.133260000	2.791252000
O	0.035133000	-1.548697000	4.573482000
O	-0.032547000	1.058394000	4.753158000
O	1.057493000	-1.539334000	0.679153000
O	-1.384263000	-2.144072000	0.670055000
O	-2.051615000	-2.477181000	-1.909603000
O	0.042044000	-3.931101000	-0.728967000
O	-3.612240000	-1.392849000	-0.720924000
O	-0.008417000	3.780999000	2.239228000
O	0.011084000	3.979091000	-0.365404000
O	-1.397482000	2.003316000	0.805268000
O	-2.050049000	2.231273000	3.480105000
O	-2.064714000	2.512618000	-1.732411000
O	1.378257000	-0.005058000	-1.381707000
O	-1.081756000	-0.028555000	-0.796153000
H	2.017432000	-0.004764000	-2.115475000

O	0.136934000	1.882203000	-3.130069000
H	1.051057000	2.085503000	-3.387218000
Zr	2.514946000	-0.071399000	0.703513000
Zr	-0.021946000	-1.885952000	2.497035000
Zr	0.027504000	1.702679000	2.540373000
Zr	-0.039804000	1.762479000	-1.041463000
Zr	-2.537868000	-0.067563000	0.707307000
Zr	0.018070000	-1.853706000	-1.093288000
C	0.075655000	-0.448819000	-4.176572000
C	3.679552000	-0.052087000	-4.749470000
C	2.866088000	1.061712000	-5.386778000
C	-0.967060000	0.094076000	-5.109092000
C	2.452766000	0.894558000	-6.831062000
C	-2.358383000	0.060071000	-4.478340000
H	3.372581000	0.899647000	-7.445453000
H	4.717839000	-0.010580000	-5.136810000
H	1.115316000	-0.082795000	-4.321136000
H	-2.979882000	1.473002000	-5.601606000
H	2.066060000	-0.146393000	-6.935450000
H	0.778849000	1.809841000	-6.759488000
H	-2.305334000	0.586451000	-3.502716000
H	-2.639848000	-0.980205000	-4.262629000
H	4.088230000	0.775673000	-3.038445000
H	-0.441571000	1.876948000	-4.712496000
H	3.292124000	-1.034281000	-5.066950000
H	-0.966016000	-0.568225000	-5.998680000
O	-0.166260000	-1.310930000	-3.347995000
O	1.592761000	1.858832000	-7.298849000
O	-3.312363000	0.605095000	-5.336138000
O	2.528050000	2.019734000	-4.721802000
O	3.625987000	-0.014672000	-3.354644000
O	-0.629074000	1.383457000	-5.557024000

2. Hf-NU-1000 case

Hf-NU-1000

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000

H	4.086956000	2.683362000	3.474348000
H	4.063785000	-3.157376000	3.120923000
H	-4.031448000	2.543433000	3.686468000
H	-4.029729000	-2.994711000	3.375702000
C	5.678221000	-2.765225000	-1.968617000
C	-5.649623000	-2.654502000	-2.168031000
C	4.334716000	-3.004251000	-2.287446000
C	-4.294245000	-2.873606000	-2.447464000
C	4.015928000	-3.929002000	-3.290650000
C	-3.932161000	-3.748086000	-3.480157000
C	5.027546000	-4.604846000	-3.966247000
C	-4.914367000	-4.393807000	-4.225056000
C	6.363864000	-4.363671000	-3.643253000
C	-6.263287000	-4.170067000	-3.944400000
C	6.687689000	-3.444053000	-2.644448000
C	-6.629590000	-3.300494000	-2.915801000
C	5.642417000	3.002280000	-1.555784000
C	-5.694195000	2.738366000	-1.818856000
C	4.305595000	3.214983000	-1.916359000
C	-4.352012000	3.027893000	-2.096938000
C	3.987027000	4.232951000	-2.824620000
C	-4.037169000	4.070745000	-2.977899000
C	4.993353000	5.029369000	-3.363372000
C	-5.052460000	4.813154000	-3.573678000
C	6.322985000	4.817967000	-2.994966000
C	-6.388096000	4.518312000	-3.295445000
C	6.646069000	3.804827000	-2.090923000
C	-6.707524000	3.480992000	-2.417917000
H	5.910000000	-2.041419000	-1.185130000
H	-5.913874000	-1.971177000	-1.358783000
H	2.965771000	-4.102970000	-3.532551000
H	-2.871781000	-3.910644000	-3.681015000
H	4.775296000	-5.322943000	-4.749665000
H	-4.629197000	-5.075792000	-5.029303000
H	7.733789000	-3.255763000	-2.393033000
H	-7.685593000	-3.126421000	-2.697288000
H	5.874001000	2.203213000	-0.848922000
H	-5.922504000	1.924687000	-1.128001000
H	2.942199000	4.376227000	-3.107933000
H	-2.986603000	4.288503000	-3.179680000
H	4.742265000	5.817767000	-4.076547000
H	-4.803286000	5.626903000	-4.258490000
H	7.687086000	3.640229000	-1.803699000
H	-7.753105000	3.251630000	-2.200222000
H	-7.033735000	-4.676908000	-4.530556000
H	7.157537000	-4.894971000	-4.173957000

H	-7.184619000	5.101103000	-3.764486000
H	7.112208000	5.445066000	-3.416753000
H	-1.925409000	-2.954614000	0.622181000
H	-0.871017000	1.410804000	5.075646000
H	-0.010757000	0.106277000	4.800275000
H	0.021232000	4.010961000	0.564979000
H	0.652989000	4.302714000	2.640349000
H	0.868467000	4.306687000	-0.740435000
H	1.962876000	-0.169559000	3.582645000
H	-1.937445000	2.793681000	0.826078000
H	-0.605581000	-1.982688000	5.137817000
H	0.894888000	-4.438700000	2.213880000
H	0.691959000	-4.440747000	-1.138847000
H	0.036124000	-4.156529000	0.910138000
O	-1.063919000	-0.101326000	2.190762000
O	-3.619477000	1.286652000	2.167780000
O	-3.610371000	1.334904000	-0.630233000
O	-3.608551000	-1.508232000	2.086284000
O	-2.049388000	-2.646119000	3.248123000
O	0.044268000	-4.080035000	1.924787000
O	2.076556000	-2.825573000	3.005400000
O	2.047127000	-2.549146000	-1.862241000
O	3.630235000	-1.526407000	2.023340000
O	3.601356000	-1.433256000	-0.689278000
O	3.649088000	1.283984000	2.096557000
O	3.585104000	1.355086000	-0.652664000
O	2.030867000	2.689980000	-1.555499000
O	2.098445000	2.450776000	3.238011000
O	1.071278000	1.381143000	0.725378000
O	1.410840000	-0.120622000	2.792358000
O	0.036194000	-1.507218000	4.598789000
O	-0.022937000	1.118272000	4.713751000
O	1.071491000	-1.551540000	0.711826000
O	-1.386655000	-2.157503000	0.702945000
O	-2.026573000	-2.362188000	-1.968573000
O	0.006853000	-3.935474000	-0.687607000
O	-3.622137000	-1.444752000	-0.688212000
O	-0.005233000	3.781635000	2.167725000
O	0.018324000	3.949761000	-0.448571000
O	-1.393729000	1.998128000	0.770033000
O	-2.046890000	2.256393000	3.451979000
O	-2.074446000	2.502800000	-1.771691000
O	1.331427000	-0.052916000	-1.415530000
O	-1.079007000	-0.057158000	-0.749515000
Hf	2.535838000	-0.053703000	0.697589000
Hf	-0.021675000	-1.860507000	2.537706000

Hf	0.036224000	1.712038000	2.490636000
Hf	-0.047621000	1.740609000	-1.114049000
Hf	-2.539398000	-0.065881000	0.715114000
Hf	0.020779000	-1.855474000	-0.994698000
H	1.862959000	0.025816000	-2.217973000
O	0.063981000	1.618933000	-3.135157000
H	-0.697872000	1.841724000	-3.677665000

Hf-NU-1000 Ads

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087096000	2.710822000	3.445922000
H	4.062296000	-3.141093000	3.148664000
H	-4.032939000	2.564839000	3.664986000
H	-4.033794000	-2.968444000	3.400828000
C	5.661243000	-2.729608000	-2.109575000
C	-5.635300000	-2.255093000	-2.386454000
C	4.307001000	-3.027043000	-2.306214000
C	-4.345799000	-2.801715000	-2.445195000
C	3.941866000	-4.034849000	-3.210160000
C	-4.106021000	-3.912130000	-3.265061000
C	4.921769000	-4.734295000	-3.908932000
C	-5.135878000	-4.461413000	-4.022974000
C	6.270020000	-4.431214000	-3.711307000
C	-6.413406000	-3.903751000	-3.970004000
C	6.638193000	-3.428955000	-2.812285000
C	-6.661875000	-2.800746000	-3.151091000
C	5.637684000	2.931028000	-1.724045000
C	-5.687454000	2.717826000	-1.866685000
C	4.287595000	3.164201000	-2.015521000
C	-4.344020000	2.951692000	-2.189526000
C	3.942477000	4.147223000	-2.952027000
C	-4.024360000	3.854788000	-3.211432000
C	4.934824000	4.888826000	-3.586693000
C	-5.036482000	4.514470000	-3.901843000
C	6.278142000	4.656357000	-3.287524000
C	-6.372835000	4.280635000	-3.574142000
C	6.627974000	3.677489000	-2.356019000
C	-6.697325000	3.382908000	-2.555626000
H	5.926523000	-1.942748000	-1.401048000

H	-5.809157000	-1.394062000	-1.738144000
H	2.880784000	-4.259371000	-3.350288000
H	-3.105633000	-4.349124000	-3.304033000
H	4.635086000	-5.521540000	-4.609899000
H	-4.936941000	-5.323211000	-4.663120000
H	7.693684000	-3.192964000	-2.659505000
H	-7.662394000	-2.364450000	-3.109874000
H	5.889603000	2.158410000	-0.995193000
H	-5.919011000	2.011704000	-1.067002000
H	2.886824000	4.309653000	-3.179321000
H	-2.974444000	4.021370000	-3.457616000
H	4.661899000	5.651011000	-4.320107000
H	-4.783676000	5.213684000	-4.701927000
H	7.679695000	3.495540000	-2.123512000
H	-7.743598000	3.201829000	-2.298951000
H	-7.220314000	-4.330988000	-4.570166000
H	7.038523000	-4.980337000	-4.260679000
H	-7.166460000	4.800522000	-4.116408000
H	7.056786000	5.239978000	-3.784656000
H	-1.912020000	-2.934013000	0.581472000
H	-0.879890000	1.326188000	5.118810000
H	-0.015006000	0.028161000	4.799772000
H	0.031788000	4.022236000	0.661353000
H	0.658103000	4.282461000	2.714702000
H	0.900447000	4.331778000	-0.631963000
H	1.967486000	-0.207951000	3.581457000
H	-1.935770000	2.797445000	0.846368000
H	-0.610361000	-2.040670000	5.082119000
H	0.895620000	-4.461287000	2.132008000
H	0.652054000	-4.408980000	-1.248399000
H	0.046425000	-4.144684000	0.824632000
O	-1.055798000	-0.106185000	2.191536000
O	-3.614066000	1.286582000	2.166845000
O	-3.612135000	1.366923000	-0.600332000
O	-3.605928000	-1.508771000	2.080439000
O	-2.047805000	-2.669665000	3.217909000
O	0.050761000	-4.087985000	1.845841000
O	2.074702000	-2.841940000	2.975770000
O	2.049403000	-2.535890000	-1.843250000
O	3.634526000	-1.528559000	2.022675000
O	3.629601000	-1.427919000	-0.702389000
O	3.645690000	1.279189000	2.105004000
O	3.599575000	1.408007000	-0.601011000
O	2.020990000	2.692836000	-1.545981000
O	2.099556000	2.431440000	3.270651000
O	1.074539000	1.409701000	0.778558000

O	1.413493000	-0.140051000	2.794052000
O	0.037667000	-1.552867000	4.561926000
O	-0.031954000	1.048536000	4.745643000
O	1.073545000	-1.539077000	0.679998000
O	-1.377352000	-2.134619000	0.661805000
O	-2.051757000	-2.473381000	-1.946102000
O	-0.003944000	-3.911638000	-0.745950000
O	-3.585584000	-1.383441000	-0.728101000
O	-0.008555000	3.774384000	2.239377000
O	0.046657000	3.969820000	-0.357987000
O	-1.382174000	2.007805000	0.807607000
O	-2.050400000	2.233788000	3.479280000
O	-2.062419000	2.518358000	-1.738269000
O	1.397499000	0.021033000	-1.324433000
O	-1.071247000	-0.023636000	-0.768415000
H	1.914163000	0.013873000	-2.155662000
O	-0.006985000	1.536775000	-3.126993000
H	-0.824039000	1.904841000	-3.497358000
Hf	2.535936000	-0.065992000	0.695946000
Hf	-0.008885000	-1.883275000	2.484825000
Hf	0.037244000	1.695856000	2.549816000
Hf	-0.015160000	1.764676000	-1.008129000
Hf	-2.520880000	-0.064304000	0.720811000
Hf	0.036399000	-1.827698000	-1.094258000
C	-1.731339000	-2.361383000	-5.237182000
C	-0.292075000	-2.738506000	-4.842468000
C	0.326562000	-1.371079000	-4.551720000
C	-1.630954000	-0.905564000	-5.707068000
C	1.833796000	-1.204681000	-4.654719000
C	-2.510768000	0.083956000	-4.960864000
H	2.326410000	-2.066903000	-4.187239000
H	0.225803000	-3.175380000	-5.717378000
H	-2.341425000	-2.397583000	-4.322202000
H	-1.193418000	1.393149000	-5.409618000
H	2.109191000	-1.193720000	-5.723677000
H	1.693964000	0.698267000	-4.171067000
H	-2.428498000	-0.103590000	-3.869838000
H	-3.567360000	-0.070261000	-5.232154000
H	-0.965232000	-3.534761000	-3.203885000
H	-0.117929000	0.019864000	-3.206344000
H	-1.838267000	-3.263534000	-6.945367000
H	-1.822526000	-0.826961000	-6.790990000
O	-2.353933000	-3.242317000	-6.130283000
O	2.289375000	-0.050751000	-3.984015000
O	-2.153934000	1.406007000	-5.282818000
O	-0.129098000	-1.010189000	-3.260289000

O	-0.186579000	-3.642419000	-3.781499000
O	-0.255057000	-0.520310000	-5.511585000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086842000	2.714386000	3.442434000
H	4.061768000	-3.137449000	3.154833000
H	-4.032254000	2.568267000	3.662723000
H	-4.033253000	-2.965759000	3.404837000
C	5.661623000	-2.730321000	-2.109748000
C	-5.640189000	-2.278143000	-2.369037000
C	4.307743000	-3.034450000	-2.298076000
C	-4.346407000	-2.813756000	-2.435092000
C	3.943212000	-4.057236000	-3.185248000
C	-4.103324000	-3.925858000	-3.251772000
C	4.923217000	-4.764701000	-3.875765000
C	-5.134224000	-4.487707000	-3.998976000
C	6.271081000	-4.454445000	-3.686991000
C	-6.416181000	-3.941100000	-3.938553000
C	6.638708000	-3.437262000	-2.804655000
C	-6.667910000	-2.836413000	-3.122923000
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O	-2.047851000	2.243650000	3.466469000
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O	1.375402000	-0.013880000	-1.334775000
O	-1.098088000	-0.041680000	-0.796417000

H	1.849851000	-0.057833000	-2.184765000
O	0.106457000	1.817951000	-3.181831000
H	0.964756000	2.184822000	-3.431009000
Hf	2.518134000	-0.073548000	0.696150000
Hf	-0.016281000	-1.874099000	2.497326000
Hf	0.029551000	1.705238000	2.525124000
Hf	-0.038543000	1.721976000	-1.046208000
Hf	-2.537028000	-0.072267000	0.715387000
Hf	0.013082000	-1.857927000	-1.077409000
C	-1.819345000	-1.588252000	-5.310613000
C	-0.463095000	-2.301216000	-5.316798000
C	0.435198000	-1.468115000	-4.408779000
C	-1.552844000	-0.086772000	-5.428458000
C	1.896434000	-1.341719000	-4.751608000
C	-2.485688000	0.746225000	-4.571027000
H	2.320119000	-2.352851000	-4.595466000
H	-0.058759000	-2.344857000	-6.343872000
H	-2.261320000	-1.791706000	-4.319668000
H	-1.569835000	2.358515000	-4.079919000
H	2.013128000	-1.084337000	-5.817703000
H	3.467636000	-0.506893000	-3.953682000
H	-2.382949000	0.405197000	-3.518066000
H	-3.517975000	0.502026000	-4.877005000
H	-0.857445000	-3.562016000	-3.925355000
H	-0.081880000	0.799416000	-4.270517000
H	-2.383508000	-1.941268000	-7.124471000
H	-1.640850000	0.228710000	-6.484521000
O	-2.742774000	-2.074800000	-6.238873000
O	2.510640000	-0.388624000	-3.913868000
O	-2.276634000	2.116236000	-4.706263000
O	0.099029000	-1.520180000	-3.193099000
O	-0.526010000	-3.615464000	-4.838230000
O	-0.173664000	0.115963000	-5.053935000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086176000	2.689243000	3.470003000
H	4.063608000	-3.148748000	3.134658000
H	-4.031709000	2.545132000	3.684140000

H	-4.031601000	-2.983438000	3.386497000
C	5.671182000	-2.566354000	-2.182954000
C	-5.641984000	-2.336955000	-2.371545000
C	4.329698000	-2.917527000	-2.378274000
C	-4.316969000	-2.773730000	-2.501343000
C	3.998070000	-3.863139000	-3.358836000
C	-3.997799000	-3.742023000	-3.461574000
C	4.996203000	-4.447791000	-4.133291000
C	-4.990237000	-4.261783000	-4.287110000
C	6.331712000	-4.093980000	-3.933036000
C	-6.306707000	-3.817711000	-4.159303000
C	6.667473000	-3.153702000	-2.957897000
C	-6.631885000	-2.856169000	-3.200537000
C	5.647107000	2.937466000	-1.637948000
C	-5.684247000	2.784338000	-1.772663000
C	4.305439000	3.196565000	-1.946287000
C	-4.341647000	3.079012000	-2.040841000
C	3.990575000	4.238751000	-2.827653000
C	-4.023255000	4.177265000	-2.849246000
C	5.001629000	5.011096000	-3.392130000
C	-5.033853000	4.970499000	-3.381598000
C	6.336070000	4.749285000	-3.078332000
C	-6.370691000	4.669431000	-3.115263000
C	6.656929000	3.712429000	-2.200946000
C	-6.694539000	3.575767000	-2.311353000
H	5.911650000	-1.826636000	-1.417166000
H	-5.872326000	-1.580432000	-1.618717000
H	2.947691000	-4.128487000	-3.504651000
H	-2.961193000	-4.077448000	-3.545291000
H	4.733233000	-5.183968000	-4.896294000
H	-4.735066000	-5.010618000	-5.040123000
H	7.712705000	-2.876892000	-2.802815000
H	-7.662934000	-2.508873000	-3.102601000
H	5.876834000	2.121370000	-0.950483000
H	-5.916403000	1.927439000	-1.137588000
H	2.942611000	4.429831000	-3.067728000
H	-2.973315000	4.396936000	-3.052182000
H	4.750298000	5.820470000	-4.081331000
H	-4.780808000	5.826620000	-4.010882000
H	7.701541000	3.507747000	-1.955804000
H	-7.740765000	3.340773000	-2.103026000
H	-7.084656000	-4.222447000	-4.811324000
H	7.114878000	-4.553611000	-4.540799000
H	-7.164299000	5.291265000	-3.536676000
H	7.129810000	5.356026000	-3.520769000
H	-1.932701000	-2.938498000	0.596723000

H	-0.871570000	1.374089000	5.090279000
H	-0.012594000	0.069203000	4.786214000
H	0.008862000	3.987243000	0.568600000
H	0.639456000	4.301850000	2.623545000
H	0.924926000	4.229153000	-0.695666000
H	1.962919000	-0.177467000	3.568253000
H	-1.942580000	2.777845000	0.796459000
H	-0.609047000	-1.997758000	5.100180000
H	0.888475000	-4.453831000	2.187806000
H	0.657686000	-4.467966000	-1.157507000
H	0.031208000	-4.160592000	0.880236000
O	-1.059574000	-0.100864000	2.172915000
O	-3.615465000	1.288798000	2.164163000
O	-3.610117000	1.328374000	-0.642938000
O	-3.609300000	-1.506358000	2.085619000
O	-2.048666000	-2.655352000	3.232304000
O	0.040255000	-4.088660000	1.900841000
O	2.075817000	-2.831660000	2.993548000
O	2.066199000	-2.621870000	-1.792226000
O	3.631533000	-1.528870000	2.020573000
O	3.612825000	-1.419701000	-0.700542000
O	3.643748000	1.279350000	2.102575000
O	3.581682000	1.391712000	-0.615376000
O	2.025234000	2.681260000	-1.584300000
O	2.096056000	2.452612000	3.240854000
O	1.060938000	1.402770000	0.733830000
O	1.407530000	-0.123082000	2.780716000
O	0.036058000	-1.516776000	4.570128000
O	-0.026955000	1.087779000	4.716207000
O	1.062582000	-1.551384000	0.694808000
O	-1.387670000	-2.146062000	0.678550000
O	-2.049137000	-2.446110000	-1.936907000
O	-0.006149000	-3.950405000	-0.688611000
O	-3.613436000	-1.420081000	-0.699885000
O	-0.021413000	3.776720000	2.158857000
O	0.041599000	3.920200000	-0.448483000
O	-1.394448000	1.984286000	0.759704000
O	-2.046419000	2.252196000	3.456712000
O	-2.063543000	2.477740000	-1.785843000
O	1.369598000	-0.037735000	-1.342671000
O	-1.091077000	-0.060223000	-0.811710000
H	1.910060000	-0.061879000	-2.157742000
O	0.107280000	1.717383000	-3.229683000
H	0.338007000	2.593380000	-3.563461000
Hf	2.522935000	-0.077510000	0.693027000
Hf	-0.015260000	-1.875478000	2.499191000

Hf	0.030577000	1.707205000	2.508935000
Hf	-0.025564000	1.695223000	-1.070237000
Hf	-2.533706000	-0.081603000	0.708227000
Hf	0.022542000	-1.881254000	-1.076840000
C	-1.692883000	-1.836096000	-5.359583000
C	-0.227489000	-2.256398000	-5.528218000
C	0.567566000	-1.545446000	-4.453417000
C	-1.836456000	-0.311868000	-5.459085000
C	1.889338000	-0.910621000	-4.775524000
C	-2.744430000	0.236349000	-4.371178000
H	2.640076000	-1.721926000	-4.705625000
H	0.141416000	-1.942653000	-6.527650000
H	-1.985024000	-2.173588000	-4.350317000
H	-2.245192000	2.009540000	-3.790305000
H	1.882715000	-0.584702000	-5.829656000
H	1.517804000	0.755932000	-3.820797000
H	-2.348867000	-0.091018000	-3.387055000
H	-3.743252000	-0.224616000	-4.479365000
H	-0.928479000	-4.022743000	-5.687077000
H	-0.484242000	0.878902000	-4.604334000
H	-2.398734000	-2.208742000	-7.128989000
H	-2.265242000	-0.054897000	-6.449248000
O	-2.510048000	-2.571907000	-6.240297000
O	2.261328000	0.106267000	-3.899093000
O	-2.854659000	1.628923000	-4.442488000
O	0.146516000	-1.608719000	-3.298262000
O	-0.103920000	-3.641674000	-5.347536000
O	-0.546337000	0.268096000	-5.383578000

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C	-3.248200000	-2.182800000	-1.650100000
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C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086486000	2.699664000	3.459201000
H	4.061838000	-3.140990000	3.150129000
H	-4.031754000	2.551634000	3.679518000
H	-4.031174000	-2.968585000	3.405253000
C	5.681530000	-2.691644000	-2.054886000
C	-5.657325000	-2.578074000	-2.231054000
C	4.335714000	-2.956923000	-2.337468000
C	-4.314706000	-2.960207000	-2.343938000

C	4.009125000	-3.855070000	-3.362300000
C	-3.972238000	-4.074847000	-3.121454000
C	5.015505000	-4.479282000	-4.094016000
C	-4.962384000	-4.795706000	-3.781705000
C	6.355041000	-4.212581000	-3.805819000
C	-6.298238000	-4.401632000	-3.679432000
C	6.686242000	-3.318984000	-2.786185000
C	-6.644516000	-3.292805000	-2.905461000
C	5.640303000	2.939719000	-1.703992000
C	-5.691364000	2.778638000	-1.818845000
C	4.292088000	3.165637000	-2.007774000
C	-4.346424000	3.015847000	-2.135174000
C	3.950160000	4.141334000	-2.952654000
C	-4.024131000	3.964551000	-3.113751000
C	4.944500000	4.884512000	-3.582498000
C	-5.034211000	4.654357000	-3.780782000
C	6.286312000	4.661072000	-3.269716000
C	-6.372325000	4.405257000	-3.471251000
C	6.632651000	3.688576000	-2.330308000
C	-6.699540000	3.469864000	-2.486832000
H	5.918387000	-1.986823000	-1.255734000
H	-5.902732000	-1.709012000	-1.617278000
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H	-2.918931000	-4.355438000	-3.196986000
H	4.756432000	-5.178466000	-4.892470000
H	-4.693682000	-5.666503000	-4.383854000
H	7.734740000	-3.110027000	-2.562048000
H	-7.690203000	-2.986874000	-2.826045000
H	5.889043000	2.170739000	-0.970145000
H	-5.922538000	2.037337000	-1.050766000
H	2.895237000	4.294190000	-3.190784000
H	-2.970342000	4.146048000	-3.337429000
H	4.674620000	5.640766000	-4.323327000
H	-4.778884000	5.393317000	-4.543851000
H	7.683224000	3.513096000	-2.087500000
H	-7.746598000	3.280772000	-2.239305000
H	-7.074127000	-4.963330000	-4.205286000
H	7.144859000	-4.703564000	-4.379568000
H	-7.164051000	4.945806000	-3.995365000
H	7.066517000	5.246248000	-3.762745000
H	-1.929931000	-2.930991000	0.568452000
H	-0.880894000	1.344129000	5.089049000
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H	0.018446000	4.014945000	0.608534000
H	0.660959000	4.285537000	2.666502000
H	0.865782000	4.314334000	-0.699301000

H	1.960541000	-0.198966000	3.567072000
H	-1.940684000	2.795782000	0.832546000
H	-0.607625000	-2.028740000	5.074858000
H	0.893170000	-4.445374000	2.115682000
H	0.680507000	-4.397905000	-1.207472000
H	0.030920000	-4.132414000	0.815831000
O	-1.063328000	-0.103709000	2.174225000
O	-3.618265000	1.289120000	2.165527000
O	-3.627073000	1.379890000	-0.599699000
O	-3.610116000	-1.510048000	2.081266000
O	-2.046534000	-2.668964000	3.213649000
O	0.040826000	-4.082599000	1.837581000
O	2.073355000	-2.845388000	2.969573000
O	2.060549000	-2.571967000	-1.842623000
O	3.633258000	-1.525132000	2.027784000
O	3.611622000	-1.437066000	-0.685455000
O	3.645198000	1.281383000	2.102181000
O	3.596737000	1.392005000	-0.617515000
O	2.026801000	2.704630000	-1.532254000
O	2.097492000	2.440682000	3.256924000
O	1.068383000	1.410408000	0.753570000
O	1.407698000	-0.134578000	2.778584000
O	0.037760000	-1.540582000	4.551866000
O	-0.031406000	1.064100000	4.721506000
O	1.059058000	-1.542481000	0.673670000
O	-1.395760000	-2.130881000	0.646012000
O	-2.052396000	-2.387140000	-1.990542000
O	-0.012407000	-3.903611000	-0.755623000
O	-3.619794000	-1.376778000	-0.739382000
O	-0.012590000	3.778728000	2.199664000
O	0.012802000	3.962375000	-0.408680000
O	-1.393413000	2.003107000	0.775584000
O	-2.048246000	2.245824000	3.463561000
O	-2.075196000	2.480432000	-1.794469000
O	1.381456000	-0.003498000	-1.334865000
O	-1.090516000	-0.025640000	-0.798812000
H	1.901912000	0.005106000	-2.163979000
O	0.137227000	1.756925000	-3.135047000
H	-0.617716000	1.815053000	-3.728651000
Hf	2.525442000	-0.065813000	0.689543000
Hf	-0.015791000	-1.878334000	2.475445000
Hf	0.035966000	1.702390000	2.517052000
Hf	-0.023664000	1.751738000	-1.060703000
Hf	-2.529702000	-0.068182000	0.704216000
Hf	0.023210000	-1.821688000	-1.106282000
C	-1.565633000	-0.425591000	-5.852891000

C	-0.478456000	-1.510650000	-5.668498000
C	0.424669000	-1.115012000	-4.508312000
C	-2.623025000	-0.465637000	-4.751399000
C	1.687298000	-0.381059000	-4.860585000
C	-3.536826000	0.743313000	-4.736423000
H	2.401720000	-1.187897000	-5.125785000
H	0.143874000	-1.490083000	-6.583382000
H	-2.083069000	-0.652694000	-6.805241000
H	-5.120515000	1.185278000	-3.678464000
H	1.503525000	0.162345000	-5.807819000
H	1.524201000	1.105405000	-3.676623000
H	-3.933839000	0.936986000	-5.756629000
H	-2.972352000	1.639882000	-4.413323000
H	-1.886703000	-2.725023000	-5.122535000
H	-4.122973000	-1.641191000	-4.380343000
H	-1.456025000	1.443821000	-6.406478000
H	-2.138360000	-0.522756000	-3.753382000
O	-0.909816000	0.826973000	-5.907917000
O	2.232733000	0.419506000	-3.878119000
O	-4.561509000	0.414866000	-3.835850000
O	0.115713000	-1.435979000	-3.369218000
O	-0.996458000	-2.787733000	-5.515526000
O	-3.379318000	-1.634299000	-5.002654000

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C	-3.248563000	-2.182400000	-1.650041000
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C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.258923000	-2.278209000	-1.561151000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.088455000	2.715250000	3.439208000
H	4.062442000	-3.144395000	3.143533000
H	-4.031701000	2.573228000	3.659047000
H	-4.032717000	-2.982762000	3.386034000
C	5.677003000	-2.611137000	-2.141090000
C	-5.473195000	-1.805716000	-2.712810000
C	4.331887000	-2.930877000	-2.363739000
C	-4.336268000	-2.613062000	-2.571597000
C	3.998520000	-3.864396000	-3.354129000
C	-4.208839000	-3.769913000	-3.348534000
C	4.997562000	-4.470093000	-4.110669000
C	-5.204519000	-4.112301000	-4.259602000
C	6.336755000	-4.149158000	-3.882219000

C	-6.320687000	-3.290542000	-4.416639000
C	6.674756000	-3.219713000	-2.897509000
C	-6.453394000	-2.136048000	-3.643227000
C	5.633448000	2.979416000	-1.647317000
C	-5.656712000	2.380843000	-2.192830000
C	4.287495000	3.203782000	-1.964503000
C	-4.326652000	2.792740000	-2.345251000
C	3.952105000	4.218538000	-2.869968000
C	-3.994024000	3.678517000	-3.377583000
C	4.948310000	4.999245000	-3.448941000
C	-4.975400000	4.139749000	-4.250894000
C	6.287121000	4.773224000	-3.125828000
C	-6.297573000	3.717203000	-4.100345000
C	6.627974000	3.763098000	-2.225028000
C	-6.637172000	2.839611000	-3.068853000
H	5.919590000	-1.879754000	-1.367970000
H	-5.555002000	-0.908027000	-2.095667000
H	2.944833000	-4.100054000	-3.521103000
H	-3.324085000	-4.398890000	-3.232531000
H	4.733181000	-5.196325000	-4.882750000
H	-5.102874000	-5.018965000	-4.859921000
H	7.722954000	-2.968272000	-2.720322000
H	-7.324279000	-1.487991000	-3.771744000
H	5.878505000	2.183033000	-0.942152000
H	-5.900698000	1.694870000	-1.379417000
H	2.900657000	4.377801000	-3.117162000
H	-2.954732000	3.997780000	-3.480705000
H	4.682376000	5.786844000	-4.157641000
H	-4.711092000	4.833001000	-5.052917000
H	7.676092000	3.585958000	-1.973620000
H	-7.673491000	2.516361000	-2.944510000
H	-7.089999000	-3.549072000	-5.148135000
H	7.120936000	-4.625368000	-4.475825000
H	-7.068096000	4.081131000	-4.784745000
H	7.069049000	5.386621000	-3.579998000
H	-1.926006000	-2.924659000	0.598790000
H	-0.881571000	1.314297000	5.141537000
H	-0.016866000	0.014213000	4.811220000
H	0.053011000	4.008861000	0.675325000
H	0.667434000	4.269842000	2.722579000
H	0.979056000	4.252374000	-0.590404000
H	1.967251000	-0.205239000	3.594991000
H	-1.917951000	2.797837000	0.840535000
H	-0.616951000	-2.036113000	5.083009000
H	0.877236000	-4.470557000	2.174972000
H	0.716162000	-4.426464000	-1.130113000

H	0.039508000	-4.146105000	0.853888000
O	-1.056939000	-0.102975000	2.197811000
O	-3.615748000	1.286168000	2.169125000
O	-3.620108000	1.384623000	-0.589391000
O	-3.611441000	-1.502029000	2.090311000
O	-2.049697000	-2.659912000	3.227158000
O	0.039182000	-4.087318000	1.883204000
O	2.076456000	-2.835696000	2.983475000
O	2.070212000	-2.624840000	-1.774869000
O	3.638321000	-1.530315000	2.021001000
O	3.618321000	-1.402340000	-0.712458000
O	3.642020000	1.277588000	2.105941000
O	3.591550000	1.416420000	-0.594627000
O	2.012483000	2.660227000	-1.591300000
O	2.100439000	2.430684000	3.278275000
O	1.079824000	1.407367000	0.786974000
O	1.414837000	-0.137554000	2.806519000
O	0.036865000	-1.548741000	4.569553000
O	-0.035474000	1.039144000	4.762688000
O	1.070372000	-1.526522000	0.691851000
O	-1.381764000	-2.132247000	0.682946000
O	-2.072885000	-2.557260000	-1.899982000
O	0.017448000	-3.936783000	-0.682566000
O	-3.579396000	-1.401135000	-0.703452000
O	-0.004051000	3.766886000	2.248248000
O	0.093715000	3.949025000	-0.344906000
O	-1.372348000	2.001961000	0.830115000
O	-2.051297000	2.228343000	3.487006000
O	-2.067176000	2.591453000	-1.667428000
O	1.367407000	0.005665000	-1.348813000
O	-1.093179000	-0.020678000	-0.770164000
H	1.834540000	-0.018768000	-2.207481000
O	-0.132426000	1.627371000	-3.197594000
H	-0.383418000	2.489115000	-3.554776000
Hf	2.540104000	-0.091354000	0.695065000
Hf	-0.005601000	-1.884248000	2.486820000
Hf	0.036097000	1.686597000	2.575163000
Hf	-0.013084000	1.724274000	-0.949073000
Hf	-2.530888000	-0.077874000	0.732563000
Hf	0.015787000	-1.862346000	-1.107251000
C	-1.909111000	-0.057257000	-5.048831000
C	-0.662305000	-2.209875000	-5.266540000
C	0.244506000	-1.562633000	-4.454245000
C	-3.082394000	-0.672064000	-5.730596000
C	1.479358000	-0.871502000	-4.977891000
C	-4.285258000	0.258309000	-5.608241000

H	2.286278000	-1.621182000	-5.054715000
H	-0.578660000	-2.246671000	-6.353771000
H	-1.177109000	0.465430000	-5.696647000
H	-6.050013000	0.275124000	-6.416646000
H	1.304958000	-0.514380000	-6.012484000
H	1.255619000	0.785890000	-3.967040000
H	-4.021564000	1.263500000	-5.994131000
H	-4.556944000	0.367043000	-4.541708000
H	-1.613859000	-2.908291000	-3.775304000
H	-3.603194000	-1.092584000	-7.512016000
H	-1.052591000	0.921632000	-3.456385000
H	-3.340246000	-1.617702000	-5.205223000
O	-1.993670000	0.213870000	-3.819779000
O	1.971620000	0.140919000	-4.138063000
O	-5.307241000	-0.335128000	-6.373843000
O	0.051527000	-1.581536000	-3.179218000
O	-1.593183000	-3.033861000	-4.750594000
O	-2.762558000	-0.895370000	-7.077463000

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C	-3.248200000	-2.182800000	-1.650100000
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C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
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H	4.061046000	-3.128639000	3.167920000
H	-4.029154000	2.552680000	3.681390000
H	-4.029896000	-2.969308000	3.406200000
C	5.689881000	-2.595365000	-2.098762000
C	-5.666770000	-2.467377000	-2.249168000
C	4.356444000	-2.976027000	-2.292843000
C	-4.334490000	-2.871865000	-2.402904000
C	4.058854000	-4.018565000	-3.180927000
C	-4.021861000	-3.907279000	-3.292630000
C	5.080808000	-4.671997000	-3.863174000
C	-5.029626000	-4.533414000	-4.019325000
C	6.408117000	-4.287437000	-3.665319000
C	-6.354211000	-4.118428000	-3.874130000
C	6.710716000	-3.248640000	-2.783978000
C	-6.671743000	-3.083910000	-2.990793000
C	5.641778000	2.940959000	-1.648943000
C	-5.660797000	2.954888000	-1.599700000

C	4.298614000	3.202853000	-1.948697000
C	-4.327656000	3.139203000	-1.990088000
C	3.980582000	4.251750000	-2.820922000
C	-4.005277000	4.171507000	-2.878927000
C	4.989184000	5.027396000	-3.385177000
C	-5.004682000	4.995160000	-3.390338000
C	6.325027000	4.761039000	-3.081518000
C	-6.333468000	4.797236000	-3.011418000
C	6.649324000	3.717590000	-2.213308000
C	-6.659876000	3.779980000	-2.111500000
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H	-5.889919000	-1.652807000	-1.558126000
H	3.013849000	-4.300924000	-3.329680000
H	-2.978213000	-4.207534000	-3.406898000
H	4.843317000	-5.484262000	-4.553903000
H	-4.781130000	-5.339743000	-4.712488000
H	7.749504000	-2.947203000	-2.630983000
H	-7.709020000	-2.759375000	-2.879303000
H	5.874252000	2.119864000	-0.968475000
H	-5.890734000	2.149863000	-0.898458000
H	2.931678000	4.447894000	-3.052532000
H	-2.960655000	4.307811000	-3.166247000
H	4.735118000	5.842931000	-4.066066000
H	-4.748892000	5.796342000	-4.087298000
H	7.694985000	3.508874000	-1.976526000
H	-7.698397000	3.634466000	-1.804686000
H	-7.144334000	-4.602508000	-4.453423000
H	7.210410000	-4.799775000	-4.201870000
H	-7.117813000	5.442978000	-3.413376000
H	7.117058000	5.369447000	-3.524615000
H	-1.936756000	-2.925670000	0.574923000
H	-0.866663000	1.310116000	5.120695000
H	-0.015420000	0.004092000	4.766496000
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H	0.650907000	4.280438000	2.642627000
H	0.933884000	4.243642000	-0.667459000
H	1.957687000	-0.206761000	3.556720000
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H	-0.608882000	-2.038925000	5.037576000
H	0.884959000	-4.465839000	2.090646000
H	0.621438000	-4.449188000	-1.224842000
H	0.028130000	-4.132575000	0.780590000
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O	-3.616936000	1.295946000	2.160684000
O	-3.623409000	1.347748000	-0.634072000
O	-3.615297000	-1.500793000	2.091864000

O	-2.045798000	-2.673012000	3.200564000
O	0.042100000	-4.083507000	1.812059000
O	2.073501000	-2.843956000	2.961505000
O	2.078685000	-2.631306000	-1.791240000
O	3.637274000	-1.535235000	2.011931000
O	3.606574000	-1.375416000	-0.735087000
O	3.641444000	1.277737000	2.106003000
O	3.579203000	1.422699000	-0.586670000
O	2.015385000	2.658420000	-1.620862000
O	2.094466000	2.442027000	3.255441000
O	1.061811000	1.417802000	0.753765000
O	1.408229000	-0.135402000	2.766364000
O	0.038296000	-1.545372000	4.521777000
O	-0.029729000	1.032277000	4.724715000
O	1.061023000	-1.530852000	0.648223000
O	-1.400571000	-2.126059000	0.640555000
O	-2.062980000	-2.413146000	-1.992475000
O	-0.030269000	-3.922312000	-0.750055000
O	-3.605950000	-1.395528000	-0.715846000
O	-0.018511000	3.767622000	2.175797000
O	0.051503000	3.933114000	-0.419146000
O	-1.394749000	1.999987000	0.772906000
O	-2.046176000	2.240654000	3.467024000
O	-2.065785000	2.443383000	-1.822500000
O	1.371617000	0.017184000	-1.363506000
O	-1.092554000	-0.027240000	-0.804613000
H	1.901670000	0.016638000	-2.193048000
O	0.103567000	1.723579000	-3.329120000
H	0.225554000	2.605572000	-3.703508000
Hf	2.524066000	-0.096937000	0.682824000
Hf	-0.009284000	-1.889623000	2.434976000
Hf	0.026384000	1.691474000	2.541798000
Hf	-0.013962000	1.695506000	-0.989769000
Hf	-2.536648000	-0.091109000	0.704944000
Hf	0.016226000	-1.851152000	-1.199902000
C	-2.379031000	0.074061000	-5.591634000
C	-0.073327000	-1.849145000	-5.520187000
C	0.678300000	-1.522030000	-4.444707000
C	-3.503952000	-0.275385000	-4.661273000
C	2.117057000	-1.145944000	-4.580444000
C	-4.376123000	0.957346000	-4.480567000
H	2.781415000	-1.919599000	-4.169006000
H	0.267286000	-1.810497000	-6.554278000
H	-2.508403000	-0.280952000	-6.639374000
H	-6.000818000	1.344639000	-3.490831000
H	2.370576000	-1.051878000	-5.651494000

H	1.763329000	0.704250000	-4.062407000
H	-4.752113000	1.285601000	-5.470889000
H	-3.756621000	1.776214000	-4.072224000
H	-1.523585000	-2.270009000	-4.402069000
H	-5.014136000	-1.450815000	-4.645521000
H	-0.617970000	1.314010000	-3.883996000
H	-3.059945000	-0.520291000	-3.668493000
O	-1.453623000	0.806309000	-5.283282000
O	2.451861000	0.047909000	-3.872557000
O	-5.423705000	0.583940000	-3.625915000
O	0.101869000	-1.558275000	-3.247971000
O	-1.377656000	-2.204220000	-5.368206000
O	-4.232633000	-1.333636000	-5.204417000

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C	-3.248200000	-2.182800000	-1.650100000
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C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086202000	2.688023000	3.471498000
H	4.064272000	-3.142347000	3.143543000
H	-4.032421000	2.536944000	3.690738000
H	-4.031687000	-2.985019000	3.384997000
C	5.601585000	-2.293364000	-2.475348000
C	-5.648742000	-2.317131000	-2.344808000
C	4.291964000	-2.790685000	-2.513662000
C	-4.327230000	-2.753596000	-2.503590000
C	3.941164000	-3.737781000	-3.485409000
C	-4.020768000	-3.693735000	-3.495122000
C	4.887504000	-4.180946000	-4.406207000
C	-5.026993000	-4.200440000	-4.311805000
C	6.190637000	-3.681537000	-4.363326000
C	-6.342554000	-3.761315000	-4.152771000
C	6.546135000	-2.738215000	-3.397724000
C	-6.652258000	-2.816027000	-3.171944000
C	5.628138000	3.057350000	-1.534647000
C	-5.684641000	2.843487000	-1.635212000
C	4.293562000	3.225625000	-1.925656000
C	-4.355909000	3.088667000	-2.004248000
C	3.968157000	4.204591000	-2.873233000
C	-4.058763000	4.154716000	-2.863237000
C	4.965628000	5.006423000	-3.421092000

C	-5.081482000	4.961396000	-3.352355000
C	6.292878000	4.839676000	-3.022387000
C	-6.405834000	4.712419000	-2.983373000
C	6.622737000	3.865279000	-2.078855000
C	-6.705806000	3.655277000	-2.122413000
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H	-5.868100000	-1.568488000	-1.580731000
H	2.913904000	-4.110160000	-3.504749000
H	-2.983385000	-4.013703000	-3.613337000
H	4.610483000	-4.920387000	-5.161279000
H	-4.785935000	-4.934803000	-5.083383000
H	7.566158000	-2.348741000	-3.363981000
H	-7.678136000	-2.458448000	-3.057598000
H	5.863628000	2.288347000	-0.796054000
H	-5.897361000	2.008024000	-0.965785000
H	2.925259000	4.313548000	-3.178298000
H	-3.019525000	4.330371000	-3.143514000
H	4.709269000	5.765190000	-4.164028000
H	-4.847939000	5.789829000	-4.024797000
H	7.661696000	3.736593000	-1.766639000
H	-7.740939000	3.465831000	-1.826346000
H	-7.130520000	-4.153924000	-4.800289000
H	6.932559000	-4.029673000	-5.085925000
H	-7.206680000	5.351243000	-3.364675000
H	7.074693000	5.471978000	-3.450274000
H	-1.935659000	-2.944779000	0.620438000
H	-0.873054000	1.379539000	5.075578000
H	-0.012515000	0.073939000	4.781039000
H	0.031362000	3.991153000	0.560660000
H	0.650151000	4.294143000	2.625519000
H	0.899801000	4.253513000	-0.741043000
H	1.963992000	-0.175222000	3.570479000
H	-1.928172000	2.780827000	0.787635000
H	-0.614115000	-1.992085000	5.093857000
H	0.893604000	-4.450140000	2.188251000
H	0.625448000	-4.488516000	-1.117695000
H	0.008635000	-4.167926000	0.893581000
O	-1.059647000	-0.099320000	2.178364000
O	-3.614151000	1.295700000	2.157874000
O	-3.604108000	1.299607000	-0.667818000
O	-3.608714000	-1.504374000	2.088143000
O	-2.048617000	-2.655950000	3.232691000
O	0.040284000	-4.087520000	1.914146000
O	2.076824000	-2.827554000	2.998403000
O	2.103924000	-2.756396000	-1.635410000
O	3.632787000	-1.540290000	2.003644000

O	3.625972000	-1.370054000	-0.753709000
O	3.644800000	1.279713000	2.101661000
O	3.593851000	1.386454000	-0.624884000
O	2.023683000	2.656763000	-1.594563000
O	2.096567000	2.453204000	3.239574000
O	1.068566000	1.391445000	0.722736000
O	1.413562000	-0.123062000	2.779438000
O	0.036839000	-1.513678000	4.568595000
O	-0.024800000	1.092380000	4.710187000
O	1.065339000	-1.541529000	0.691580000
O	-1.386636000	-2.153427000	0.681168000
O	-2.049436000	-2.412786000	-1.978879000
O	-0.059345000	-3.977402000	-0.671958000
O	-3.605818000	-1.458063000	-0.673538000
O	-0.010697000	3.773939000	2.155362000
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O	-2.046090000	2.254695000	3.454666000
O	-2.072866000	2.510900000	-1.764211000
O	1.350351000	-0.048481000	-1.411565000
O	-1.076777000	-0.075330000	-0.794436000
H	1.941772000	-0.044301000	-2.188413000
O	-0.078096000	1.740238000	-3.230924000
H	-0.863314000	2.230902000	-3.521470000
Hf	2.526819000	-0.079191000	0.683804000
Hf	-0.012884000	-1.871325000	2.496828000
Hf	0.037244000	1.704350000	2.499917000
Hf	-0.032023000	1.699272000	-1.079583000
Hf	-2.524491000	-0.084610000	0.704775000
Hf	0.028496000	-1.911418000	-1.080209000
C	-0.560727000	-0.345094000	-4.789026000
C	0.494082000	-1.121460000	-4.277251000
C	1.894982000	-0.934601000	-4.796536000
H	2.267526000	-1.931123000	-5.095275000
H	-0.500333000	0.039898000	-5.814887000
H	1.880976000	-0.297592000	-5.698080000
H	3.620440000	-0.681645000	-3.887570000
H	-1.789905000	-1.340455000	-3.694745000
H	-0.163218000	0.672996000	-4.072358000
O	2.712545000	-0.367737000	-3.791115000
O	0.278964000	-1.852663000	-3.267442000
O	-1.837574000	-0.660213000	-4.395280000
C	-3.430241000	1.107248000	-5.376128000
C	-4.590428000	0.468866000	-4.652881000
C	-5.817028000	1.359753000	-4.712615000
H	-3.140069000	0.567430000	-6.316495000

H	-7.598360000	1.275873000	-3.950841000
H	-6.131857000	1.465498000	-5.770321000
H	-5.562951000	2.366028000	-4.334273000
H	-5.592152000	-1.164265000	-4.775298000
H	-4.295504000	0.377908000	-3.583361000
O	-2.880820000	2.120200000	-5.017191000
O	-6.810216000	0.723807000	-3.940284000
O	-4.835271000	-0.778900000	-5.237575000

Hf-NU-1000 Prod

C	-3.248130000	-2.182803000	-1.650070000
C	-3.229697000	-2.386603000	2.899987000
C	-3.232303000	2.034299000	3.103990000
C	3.276900000	2.142000000	2.939202000
C	3.226892000	2.366304000	-1.338693000
C	3.259228000	-2.277902000	-1.561510000
C	-3.265286000	2.236104000	-1.457304000
C	3.257196000	-2.506599000	2.716396000
H	4.085863000	2.695839000	3.464101000
H	4.062209000	-3.146258000	3.141723000
H	-4.031889000	2.546510000	3.683663000
H	-4.030956000	-2.977000000	3.395680000
C	5.679084000	-2.613691000	-2.122849000
C	-5.672506000	-2.596350000	-2.107565000
C	4.336294000	-2.937387000	-2.354380000
C	-4.332096000	-2.920921000	-2.356482000
C	4.013958000	-3.877125000	-3.342458000
C	-4.023052000	-3.933996000	-3.271815000
C	5.020239000	-4.484710000	-4.088069000
C	-5.041634000	-4.615691000	-3.930769000
C	6.356666000	-4.158161000	-3.851632000
C	-6.374751000	-4.284072000	-3.687085000
C	6.684108000	-3.222615000	-2.869184000
C	-6.689856000	-3.271874000	-2.776626000
C	5.633030000	3.018548000	-1.599395000
C	-5.680537000	2.854901000	-1.695307000
C	4.292211000	3.202773000	-1.959720000
C	-4.348905000	3.042636000	-2.086150000
C	3.958865000	4.175728000	-2.910660000
C	-4.041476000	3.979575000	-3.081081000
C	4.954317000	4.956426000	-3.491371000
C	-5.058333000	4.706426000	-3.693418000
C	6.288108000	4.774138000	-3.122604000
C	-6.386325000	4.511169000	-3.307224000
C	6.625957000	3.805237000	-2.176378000
C	-6.695174000	3.591434000	-2.302461000

H	5.913388000	-1.877847000	-1.351487000
H	-5.897104000	-1.797785000	-1.398045000
H	2.962849000	-4.120738000	-3.513449000
H	-2.975681000	-4.178351000	-3.458102000
H	4.764431000	-5.218177000	-4.856289000
H	-4.796022000	-5.404813000	-4.644466000
H	7.730015000	-2.966706000	-2.685480000
H	-7.733300000	-3.007904000	-2.588542000
H	5.875450000	2.252595000	-0.860200000
H	-5.898504000	2.119504000	-0.918360000
H	2.910772000	4.297851000	-3.192426000
H	-2.997342000	4.109644000	-3.372040000
H	4.691434000	5.710160000	-4.237163000
H	-4.817805000	5.429576000	-4.475871000
H	7.670276000	3.662738000	-1.889140000
H	-7.733525000	3.454715000	-1.987363000
H	-7.173646000	-4.815733000	-4.209905000
H	7.146725000	-4.635461000	-4.436404000
H	-7.183366000	5.086076000	-3.785403000
H	7.068852000	5.389134000	-3.576903000
H	-1.928408000	-2.937854000	0.592600000
H	-0.876115000	1.365215000	5.084983000
H	-0.013086000	0.064535000	4.785687000
H	0.030628000	4.008274000	0.593427000
H	0.653127000	4.294497000	2.659019000
H	0.884689000	4.304351000	-0.710849000
H	1.963547000	-0.186098000	3.571921000
H	-1.934138000	2.798562000	0.823960000
H	-0.607547000	-2.014194000	5.092361000
H	0.899370000	-4.442432000	2.129227000
H	0.665397000	-4.410662000	-1.193369000
H	0.023070000	-4.138953000	0.838673000
O	-1.061113000	-0.101832000	2.181635000
O	-3.618866000	1.293213000	2.161910000
O	-3.618581000	1.336398000	-0.634815000
O	-3.609310000	-1.505264000	2.087303000
O	-2.046801000	-2.665412000	3.219882000
O	0.044037000	-4.082138000	1.857080000
O	2.074196000	-2.838727000	2.981930000
O	2.062687000	-2.601321000	-1.813318000
O	3.633246000	-1.527106000	2.024979000
O	3.612071000	-1.425723000	-0.696161000
O	3.647314000	1.279133000	2.104860000
O	3.597041000	1.398172000	-0.610086000
O	2.024137000	2.669927000	-1.578226000
O	2.097374000	2.446625000	3.248135000

O	1.069675000	1.405722000	0.743290000
O	1.410042000	-0.128086000	2.783409000
O	0.037313000	-1.529856000	4.565177000
O	-0.027012000	1.081620000	4.719048000
O	1.069171000	-1.546214000	0.690442000
O	-1.390430000	-2.139495000	0.660259000
O	-2.053479000	-2.356173000	-2.032039000
O	-0.030533000	-3.914088000	-0.748848000
O	-3.598122000	-1.418758000	-0.700834000
O	-0.012289000	3.781049000	2.187880000
O	0.032822000	3.948852000	-0.422629000
O	-1.392739000	2.001246000	0.772623000
O	-2.048073000	2.247181000	3.460873000
O	-2.073249000	2.500219000	-1.770722000
O	1.382070000	-0.016041000	-1.345582000
O	-1.079891000	-0.037504000	-0.775432000
H	1.900256000	-0.006395000	-2.174104000
O	0.050352000	1.663127000	-3.162936000
H	-0.768986000	1.833936000	-3.644370000
Hf	2.529571000	-0.062958000	0.691691000
Hf	-0.014431000	-1.872853000	2.493084000
Hf	0.038086000	1.706898000	2.508430000
Hf	-0.031086000	1.739930000	-1.078419000
Hf	-2.528929000	-0.066584000	0.712079000
Hf	0.030374000	-1.829713000	-1.073267000
C	-0.733222000	-1.314764000	-5.475949000
C	0.336297000	-1.111749000	-4.463887000
C	1.630404000	-0.467151000	-4.892217000
H	2.333559000	-1.301863000	-5.077366000
H	-0.293534000	-1.840350000	-6.347821000
H	1.475573000	0.015591000	-5.877536000
H	1.464236000	1.062718000	-3.752562000
H	-1.792416000	-2.057187000	-4.030025000
H	-0.960639000	-0.291212000	-5.849225000
O	2.180371000	0.389231000	-3.954403000
O	0.124742000	-1.481783000	-3.316115000
O	-1.856972000	-1.959046000	-5.003155000
C	-3.456630000	0.262967000	-5.396693000
C	-4.625633000	-0.186387000	-4.562310000
C	-5.692576000	0.893951000	-4.509160000
H	-3.385093000	-0.251420000	-6.390603000
H	-7.295793000	1.157493000	-3.457383000
H	-6.098448000	1.045521000	-5.529798000
H	-5.239606000	1.844673000	-4.181172000
H	-5.869703000	-1.648121000	-4.563244000
H	-4.251175000	-0.321121000	-3.521658000

O	-2.679061000	1.125809000	-5.059394000
O	-6.682732000	0.433098000	-3.621120000
O	-5.121926000	-1.372035000	-5.110709000

3. Ti-NU-1000 case

Ti-NU-1000

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.124342000	2.647321000	3.449736000
H	4.125467000	-3.090437000	3.099295000
H	-4.064694000	2.518931000	3.663572000
H	-4.026581000	-2.975129000	3.403880000
C	5.694690000	-2.756388000	-1.824880000
C	-5.705514000	-2.626430000	-1.873240000
C	4.372682000	-3.004104000	-2.217598000
C	-4.393095000	-2.867519000	-2.299453000
C	4.109473000	-3.937418000	-3.228606000
C	-4.154572000	-3.764364000	-3.348529000
C	5.159379000	-4.615734000	-3.840374000
C	-5.219632000	-4.412791000	-3.965945000
C	6.474865000	-4.367985000	-3.444900000
C	-6.526588000	-4.169872000	-3.539415000
C	6.740995000	-3.438985000	-2.437573000
C	-6.767977000	-3.277524000	-2.493675000
C	5.697135000	2.787539000	-1.388609000
C	-5.704050000	2.682251000	-1.770521000
C	4.410820000	3.109300000	-1.840925000
C	-4.374483000	3.007146000	-2.069222000
C	4.237069000	4.146222000	-2.766604000
C	-4.094467000	4.065462000	-2.943203000
C	5.339638000	4.853798000	-3.235683000
C	-5.135982000	4.789843000	-3.514981000
C	6.619480000	4.533032000	-2.779804000
C	-6.459725000	4.460883000	-3.218396000
C	6.796611000	3.501339000	-1.856442000
C	-6.742201000	3.408036000	-2.346564000
H	5.877483000	-2.024938000	-1.035508000
H	-5.870041000	-1.925599000	-1.052713000
H	3.074640000	-4.115616000	-3.527112000

H	-3.123721000	-3.938739000	-3.662974000
H	4.953114000	-5.341269000	-4.630337000
H	-5.032722000	-5.112143000	-4.784041000
H	7.771135000	-3.246567000	-2.129761000
H	-7.791321000	-3.089450000	-2.161006000
H	5.811681000	1.976558000	-0.666867000
H	-5.900081000	1.856947000	-1.083708000
H	3.227994000	4.378323000	-3.113524000
H	-3.052538000	4.310621000	-3.158023000
H	5.203147000	5.658870000	-3.961170000
H	-4.916697000	5.616218000	-4.194678000
H	7.798947000	3.252714000	-1.500598000
H	-7.778691000	3.153216000	-2.114920000
H	-7.362205000	-4.679873000	-4.025002000
H	7.298003000	-4.902074000	-3.925608000
H	-7.276545000	5.029925000	-3.668883000
H	7.484486000	5.090295000	-3.147500000
H	-1.861184000	-2.844172000	0.574286000
H	-0.894355000	1.546321000	4.635835000
H	-0.073152000	0.195201000	4.539575000
H	0.071260000	3.740867000	0.459813000
H	0.742535000	3.825627000	2.671685000
H	0.891397000	3.877822000	-0.884500000
H	1.861538000	-0.172375000	3.446132000
H	-1.877528000	2.653055000	0.835653000
H	-0.698475000	-2.052113000	4.701988000
H	0.926178000	-4.000163000	2.306964000
H	0.742938000	-4.011692000	-1.261373000
H	0.085903000	-3.914628000	0.971649000
O	-1.083925000	-0.110917000	2.079259000
O	-3.574769000	1.267888000	2.149811000
O	-3.566756000	1.320761000	-0.607778000
O	-3.595584000	-1.524310000	2.053692000
O	-2.034983000	-2.627582000	3.225285000
O	0.036319000	-3.798262000	1.957959000
O	2.105294000	-2.862836000	3.032179000
O	2.051883000	-2.544830000	-1.882650000
O	3.554544000	-1.504761000	1.985102000
O	3.540636000	-1.393302000	-0.684688000
O	3.592506000	1.258914000	2.072276000
O	3.466454000	1.326588000	-0.595689000
O	2.069916000	2.729363000	-1.625532000
O	2.108019000	2.460365000	3.239236000
O	1.064960000	1.267989000	0.686766000
O	1.336785000	-0.115310000	2.635458000
O	-0.010706000	-1.523908000	4.269366000

O	-0.018922000	1.179373000	4.405919000
O	1.063781000	-1.468772000	0.695229000
O	-1.351010000	-2.028260000	0.672099000
O	-2.072652000	-2.374970000	-2.029695000
O	0.029537000	-3.615992000	-0.738671000
O	-3.533460000	-1.370820000	-0.664627000
O	0.023321000	3.435721000	2.151216000
O	0.011016000	3.654054000	-0.529496000
O	-1.347746000	1.849483000	0.739693000
O	-2.056652000	2.281228000	3.454031000
O	-2.072253000	2.490611000	-1.777326000
O	1.204461000	-0.071683000	-1.375094000
O	-1.104504000	-0.068280000	-0.693542000
Ti	2.491048000	-0.015177000	0.693935000
Ti	-0.126886000	-1.697029000	2.404898000
Ti	0.059842000	1.563474000	2.302677000
Ti	-0.140056000	1.569387000	-1.031562000
Ti	-2.508582000	-0.092592000	0.630623000
Ti	0.105321000	-1.735175000	-0.825202000
H	1.708387000	-0.021867000	-2.199119000
O	-0.014743000	1.613834000	-2.849502000
H	-0.793803000	2.005571000	-3.270106000

Ti-NU-1000 Ads

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.110390000	2.677052000	3.443399000
H	4.122314000	-3.068300000	3.136354000
H	-4.084376000	2.523915000	3.627847000
H	-4.038310000	-2.953032000	3.410555000
C	5.675091000	-2.673159000	-2.056178000
C	-5.691146000	-2.210073000	-2.189176000
C	4.333304000	-3.009115000	-2.275720000
C	-4.410640000	-2.744502000	-2.387523000
C	4.008589000	-4.035607000	-3.173529000
C	-4.229598000	-3.790792000	-3.302095000
C	5.019093000	-4.717424000	-3.845550000
C	-5.314413000	-4.289591000	-4.016794000
C	6.354970000	-4.377289000	-3.626560000
C	-6.586183000	-3.750793000	-3.819623000

C	6.681335000	-3.355729000	-2.732837000
C	-6.773315000	-2.712275000	-2.905399000
C	5.678890000	2.779638000	-1.638564000
C	-5.716272000	2.582121000	-1.799418000
C	4.355835000	3.108017000	-1.960664000
C	-4.396759000	2.893719000	-2.153301000
C	4.098257000	4.139127000	-2.873069000
C	-4.147088000	3.816700000	-3.176819000
C	5.153304000	4.834372000	-3.456930000
C	-5.210302000	4.422537000	-3.839128000
C	6.470154000	4.505554000	-3.131372000
C	-6.523818000	4.113370000	-3.482069000
C	6.731145000	3.478802000	-2.222447000
C	-6.775838000	3.194136000	-2.462078000
H	5.904063000	-1.871680000	-1.351434000
H	-5.812023000	-1.397025000	-1.470819000
H	2.957471000	-4.292163000	-3.330573000
H	-3.231104000	-4.206734000	-3.455178000
H	4.765447000	-5.519781000	-4.541897000
H	-5.164106000	-5.098213000	-4.735010000
H	7.727552000	-3.091781000	-2.563393000
H	-7.769673000	-2.291419000	-2.752680000
H	5.858098000	1.972629000	-0.925766000
H	-5.887536000	1.860154000	-0.998672000
H	3.061644000	4.379665000	-3.118213000
H	-3.113497000	4.038458000	-3.446321000
H	4.950127000	5.636462000	-4.170132000
H	-5.015474000	5.139070000	-4.640110000
H	7.762323000	3.223025000	-1.968617000
H	-7.804502000	2.954393000	-2.183652000
H	-7.437054000	-4.141342000	-4.383117000
H	7.147150000	-4.913076000	-4.154995000
H	-7.357036000	4.591474000	-4.002997000
H	7.297854000	5.052613000	-3.589260000
H	-1.861666000	-2.788750000	0.543720000
H	-0.903793000	1.472807000	4.666170000
H	-0.060490000	0.136399000	4.535449000
H	0.081783000	3.788411000	0.552411000
H	0.741960000	3.846145000	2.748527000
H	0.923815000	3.935562000	-0.779722000
H	1.895417000	-0.209123000	3.431071000
H	-1.855078000	2.676887000	0.825067000
H	-0.692404000	-2.089308000	4.636646000
H	0.916878000	-4.023379000	2.232144000
H	0.771925000	-3.982571000	-1.288180000
H	0.078310000	-3.888760000	0.897425000

O	-1.059532000	-0.094585000	2.078673000
O	-3.546715000	1.266894000	2.136628000
O	-3.543271000	1.325500000	-0.589190000
O	-3.583068000	-1.515757000	2.050691000
O	-2.038126000	-2.652015000	3.206819000
O	0.032877000	-3.794634000	1.888181000
O	2.101566000	-2.879905000	2.995100000
O	2.045408000	-2.534127000	-1.841257000
O	3.559237000	-1.508422000	1.980760000
O	3.582611000	-1.402736000	-0.690671000
O	3.601529000	1.263852000	2.082486000
O	3.524994000	1.372747000	-0.578480000
O	2.041349000	2.713935000	-1.575637000
O	2.099851000	2.440643000	3.256620000
O	1.082433000	1.328068000	0.746384000
O	1.357054000	-0.129614000	2.631336000
O	0.007550000	-1.557947000	4.227309000
O	-0.020141000	1.127714000	4.436265000
O	1.069194000	-1.449627000	0.667054000
O	-1.331011000	-1.985700000	0.638471000
O	-2.076342000	-2.508031000	-1.951151000
O	0.036328000	-3.589409000	-0.793407000
O	-3.510967000	-1.332222000	-0.710982000
O	0.020821000	3.457266000	2.229840000
O	0.040735000	3.701099000	-0.440127000
O	-1.318680000	1.873390000	0.774375000
O	-2.070310000	2.268544000	3.496883000
O	-2.075944000	2.553776000	-1.730203000
O	1.355948000	0.007413000	-1.215681000
O	-1.048702000	-0.016868000	-0.704902000
H	1.869300000	-0.005689000	-2.054909000
O	-0.024052000	1.553001000	-2.806920000
H	-0.850694000	1.971872000	-3.114481000
Ti	2.483109000	-0.060149000	0.680911000
Ti	-0.091841000	-1.702803000	2.354241000
Ti	0.091923000	1.581710000	2.355401000
Ti	-0.047416000	1.610883000	-0.915717000
Ti	-2.466298000	-0.058665000	0.660626000
Ti	0.110073000	-1.704942000	-0.939897000
C	-1.804138000	-2.161361000	-5.168060000
C	-0.384598000	-2.652300000	-4.820595000
C	0.308373000	-1.352676000	-4.407567000
C	-1.622907000	-0.682920000	-5.520507000
C	1.817153000	-1.255548000	-4.529364000
C	-2.463858000	0.291071000	-4.717812000
H	2.280652000	-2.150330000	-4.101308000

H	0.105305000	-3.010552000	-5.746607000
H	-2.408425000	-2.237741000	-4.253475000
H	-1.108724000	1.589390000	-5.086414000
H	2.074730000	-1.211939000	-5.601176000
H	1.888375000	0.662974000	-4.137288000
H	-2.375800000	0.039971000	-3.638763000
H	-3.527847000	0.186100000	-4.982595000
H	-0.930129000	-3.455364000	-3.154880000
H	-0.132933000	-0.072791000	-2.988948000
H	-1.949215000	-2.951028000	-6.928285000
H	-1.781675000	-0.510076000	-6.598886000
O	-2.481073000	-2.928290000	-6.123852000
O	2.331224000	-0.142215000	-3.826324000
O	-2.069821000	1.617820000	-4.972338000
O	-0.114106000	-1.072286000	-3.068224000
O	-0.320936000	-3.677274000	-3.887436000
O	-0.232526000	-0.379219000	-5.262520000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.103739000	2.690437000	3.440647000
H	4.125994000	-3.050555000	3.150905000
H	-4.082705000	2.530164000	3.624058000
H	-4.042867000	-2.944964000	3.412049000
C	5.680228000	-2.663584000	-2.041397000
C	-5.676081000	-2.184244000	-2.247827000
C	4.340869000	-3.004167000	-2.268436000
C	-4.402802000	-2.751838000	-2.392804000
C	4.023996000	-4.032021000	-3.167632000
C	-4.220154000	-3.835544000	-3.262434000
C	5.040476000	-4.710871000	-3.833482000
C	-5.296729000	-4.339390000	-3.985906000
C	6.374026000	-4.366230000	-3.607238000
C	-6.560993000	-3.766484000	-3.843755000
C	6.692324000	-3.343167000	-2.712341000
C	-6.749515000	-2.690223000	-2.974579000
C	5.663729000	2.869559000	-1.598802000
C	-5.713663000	2.621623000	-1.773530000
C	4.335451000	3.152659000	-1.941966000

C	-4.393278000	2.904587000	-2.147629000
C	4.057238000	4.178298000	-2.854451000
C	-4.139513000	3.810008000	-3.185605000
C	5.097067000	4.912658000	-3.417632000
C	-5.199620000	4.427989000	-3.841535000
C	6.418967000	4.628504000	-3.071404000
C	-6.513986000	4.148227000	-3.463810000
C	6.700499000	3.607471000	-2.162131000
C	-6.770053000	3.245865000	-2.429886000
H	5.902975000	-1.861050000	-1.335916000
H	-5.797767000	-1.341899000	-1.563953000
H	2.974357000	-4.291317000	-3.330587000
H	-3.226734000	-4.276860000	-3.371732000
H	4.793305000	-5.514180000	-4.531034000
H	-5.145808000	-5.178366000	-4.668233000
H	7.736737000	-3.075643000	-2.537486000
H	-7.740009000	-2.242813000	-2.865444000
H	5.858595000	2.066277000	-0.885850000
H	-5.888204000	1.911830000	-0.962601000
H	3.017290000	4.384227000	-3.116327000
H	-3.105086000	4.007005000	-3.470755000
H	4.877863000	5.710432000	-4.130926000
H	-5.002035000	5.130755000	-4.653976000
H	7.735606000	3.386585000	-1.892037000
H	-7.799385000	3.028806000	-2.135701000
H	-7.405050000	-4.160178000	-4.415217000
H	7.170816000	-4.899647000	-4.131147000
H	-7.344756000	4.635919000	-3.979734000
H	7.234502000	5.206125000	-3.513274000
H	-1.874708000	-2.777608000	0.546830000
H	-0.908002000	1.441226000	4.682347000
H	-0.061372000	0.107362000	4.527922000
H	0.095323000	3.791127000	0.562703000
H	0.756816000	3.838622000	2.753606000
H	0.940872000	3.919686000	-0.772443000
H	1.893154000	-0.216913000	3.425598000
H	-1.840162000	2.696254000	0.816856000
H	-0.681874000	-2.109573000	4.608937000
H	0.906783000	-4.032424000	2.203319000
H	0.779717000	-3.966319000	-1.294191000
H	0.076096000	-3.872673000	0.864934000
O	-1.063444000	-0.089930000	2.078460000
O	-3.548260000	1.264155000	2.139344000
O	-3.546668000	1.335055000	-0.579717000
O	-3.581801000	-1.508408000	2.053805000
O	-2.040476000	-2.662543000	3.196463000

O	0.027336000	-3.790979000	1.858353000
O	2.104294000	-2.892012000	2.980494000
O	2.051240000	-2.537016000	-1.844424000
O	3.554907000	-1.508617000	1.975502000
O	3.578733000	-1.401133000	-0.685553000
O	3.605139000	1.262517000	2.090315000
O	3.538324000	1.389744000	-0.574363000
O	2.026542000	2.676056000	-1.603895000
O	2.095487000	2.434847000	3.259572000
O	1.074426000	1.333233000	0.751726000
O	1.356746000	-0.133550000	2.624884000
O	0.014866000	-1.571130000	4.203546000
O	-0.025162000	1.102109000	4.442953000
O	1.062267000	-1.442384000	0.652847000
O	-1.340568000	-1.975309000	0.626757000
O	-2.073588000	-2.509912000	-1.941925000
O	0.035536000	-3.576553000	-0.808878000
O	-3.516938000	-1.324345000	-0.720860000
O	0.025009000	3.459960000	2.241286000
O	0.056881000	3.691323000	-0.429539000
O	-1.316918000	1.882895000	0.787857000
O	-2.069600000	2.263815000	3.499190000
O	-2.071064000	2.535228000	-1.742126000
O	1.372502000	0.010819000	-1.195933000
O	-1.044219000	-0.002452000	-0.684958000
H	1.875201000	0.006094000	-2.043471000
O	-0.067029000	1.362237000	-2.836139000
H	-0.911879000	1.740172000	-3.152667000
Ti	2.477544000	-0.106979000	0.680405000
Ti	-0.086621000	-1.703816000	2.324773000
Ti	0.087806000	1.583753000	2.373970000
Ti	-0.024589000	1.592240000	-0.859842000
Ti	-2.476939000	-0.059353000	0.676630000
Ti	0.082681000	-1.696048000	-1.017440000
C	-1.753210000	-2.270329000	-5.127927000
C	-0.327362000	-2.700291000	-4.739391000
C	0.320379000	-1.375922000	-4.316143000
C	-1.618669000	-0.787344000	-5.478964000
C	1.828002000	-1.260060000	-4.487579000
C	-2.501397000	0.148151000	-4.675748000
H	2.316158000	-2.153772000	-4.086752000
H	0.195599000	-3.047769000	-5.651878000
H	-2.382949000	-2.368856000	-4.234030000
H	-1.197843000	1.471977000	-5.142931000
H	2.051518000	-1.203749000	-5.566251000
H	1.935835000	0.658113000	-4.122158000

H	-2.417549000	-0.115873000	-3.600604000
H	-3.558852000	0.016052000	-4.956283000
H	-0.877550000	-3.515025000	-3.083448000
H	-0.117048000	0.169547000	-2.958445000
H	-1.804143000	-3.081513000	-6.883579000
H	-1.785036000	-0.621384000	-6.557865000
O	-2.369709000	-3.066906000	-6.102334000
O	2.361787000	-0.148129000	-3.793983000
O	-2.134287000	1.492872000	-4.897222000
O	-0.084079000	-1.053430000	-3.009500000
O	-0.249870000	-3.722374000	-3.802276000
O	-0.245927000	-0.434776000	-5.220120000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.099617000	2.689593000	3.449861000
H	4.128719000	-3.034964000	3.165223000
H	-4.078224000	2.534205000	3.627727000
H	-4.041711000	-2.944907000	3.414558000
C	5.705900000	-2.553817000	-2.018875000
C	-5.671485000	-2.168328000	-2.279817000
C	4.384546000	-2.948605000	-2.265004000
C	-4.403668000	-2.753285000	-2.396274000
C	4.123249000	-3.975041000	-3.183692000
C	-4.224261000	-3.858487000	-3.238956000
C	5.175343000	-4.597101000	-3.850412000
C	-5.297995000	-4.365012000	-3.965388000
C	6.490272000	-4.197542000	-3.605554000
C	-6.556227000	-3.772062000	-3.854492000
C	6.754086000	-3.176727000	-2.690543000
C	-6.741914000	-2.675124000	-3.011001000
C	5.671912000	2.863808000	-1.564324000
C	-5.697109000	2.564465000	-1.940494000
C	4.349912000	3.147799000	-1.930886000
C	-4.365209000	2.922531000	-2.179590000
C	4.090268000	4.166039000	-2.857006000
C	-4.069311000	3.926088000	-3.110504000
C	5.141857000	4.890399000	-3.412122000
C	-5.098111000	4.564082000	-3.796397000

C	6.457293000	4.604894000	-3.043003000
C	-6.426069000	4.202213000	-3.558709000
C	6.720545000	3.592426000	-2.118584000
C	-6.723972000	3.203322000	-2.631036000
H	5.886131000	-1.757405000	-1.294044000
H	-5.791410000	-1.313109000	-1.611706000
H	3.087652000	-4.278915000	-3.359337000
H	-3.234838000	-4.315025000	-3.319501000
H	4.970692000	-5.399890000	-4.562295000
H	-5.150979000	-5.223563000	-4.623933000
H	7.784175000	-2.868477000	-2.498012000
H	-7.728347000	-2.213918000	-2.923449000
H	5.851218000	2.069067000	-0.837343000
H	-5.904888000	1.784344000	-1.205717000
H	3.054506000	4.373974000	-3.133956000
H	-3.022764000	4.188963000	-3.277885000
H	4.936804000	5.682765000	-4.135749000
H	-4.867940000	5.350942000	-4.518752000
H	7.750407000	3.372545000	-1.827926000
H	-7.763229000	2.923898000	-2.443487000
H	-7.397825000	-4.167798000	-4.428222000
H	7.314983000	-4.687198000	-4.129064000
H	-7.233069000	4.704621000	-4.097727000
H	7.281794000	5.175668000	-3.477181000
H	-1.915336000	-2.746898000	0.560179000
H	-0.908408000	1.421706000	4.687691000
H	-0.058938000	0.092152000	4.509802000
H	0.105578000	3.799503000	0.557040000
H	0.765994000	3.833846000	2.753581000
H	0.933512000	3.900517000	-0.790235000
H	1.891684000	-0.205733000	3.403035000
H	-1.854035000	2.712511000	0.802706000
H	-0.671090000	-2.116589000	4.579077000
H	0.898340000	-4.019540000	2.155575000
H	0.806849000	-3.957044000	-1.252054000
H	0.057802000	-3.840956000	0.819056000
O	-1.075486000	-0.080039000	2.068383000
O	-3.557180000	1.265990000	2.140772000
O	-3.579569000	1.330793000	-0.599602000
O	-3.589402000	-1.502743000	2.060519000
O	-2.040878000	-2.666414000	3.184978000
O	0.017282000	-3.773377000	1.818941000
O	2.107045000	-2.906677000	2.966975000
O	2.076729000	-2.591913000	-1.845819000
O	3.549839000	-1.508954000	1.972027000
O	3.549038000	-1.371163000	-0.700578000

O	3.604932000	1.268789000	2.088831000
O	3.527235000	1.375312000	-0.595022000
O	2.035184000	2.695060000	-1.611512000
O	2.092320000	2.438149000	3.257016000
O	1.036977000	1.346137000	0.734166000
O	1.348908000	-0.123119000	2.606661000
O	0.021172000	-1.571981000	4.174869000
O	-0.026379000	1.089589000	4.438774000
O	1.052551000	-1.431359000	0.636244000
O	-1.368890000	-1.951434000	0.617860000
O	-2.081196000	-2.525362000	-1.939692000
O	0.021306000	-3.580845000	-0.827049000
O	-3.525706000	-1.321062000	-0.727794000
O	0.020671000	3.469985000	2.249249000
O	0.048059000	3.700071000	-0.432096000
O	-1.338792000	1.893629000	0.795437000
O	-2.067831000	2.259206000	3.496108000
O	-2.063976000	2.544639000	-1.697348000
O	1.309910000	0.033484000	-1.229077000
O	-1.092814000	0.027259000	-0.720325000
H	1.801392000	0.023682000	-2.075383000
O	-0.031846000	1.709903000	-2.929405000
H	-0.887662000	1.690817000	-3.426898000
Ti	2.434379000	-0.138823000	0.670633000
Ti	-0.087676000	-1.698551000	2.291294000
Ti	0.076272000	1.595584000	2.373915000
Ti	-0.067927000	1.589009000	-0.854066000
Ti	-2.491969000	-0.060632000	0.688079000
Ti	0.022505000	-1.694692000	-1.117930000
C	-1.764521000	-2.251184000	-5.148724000
C	-0.328465000	-2.715632000	-4.856040000
C	0.315488000	-1.443323000	-4.267162000
C	-1.654671000	-0.725656000	-5.269819000
C	1.806219000	-1.296938000	-4.505131000
C	-2.576925000	0.011693000	-4.320967000
H	2.328819000	-2.193490000	-4.141040000
H	0.172439000	-2.956959000	-5.813033000
H	-2.371262000	-2.495481000	-4.266773000
H	-2.543605000	1.752973000	-5.225347000
H	1.977202000	-1.193146000	-5.588972000
H	3.174026000	0.029320000	-3.994956000
H	-2.360119000	-0.306090000	-3.288628000
H	-3.631539000	-0.241695000	-4.537990000
H	-0.688183000	-3.636645000	-3.209985000
H	0.614149000	1.186219000	-3.436580000
H	-1.837788000	-2.803168000	-7.001209000

H	-1.863533000	-0.413509000	-6.311085000
O	-2.399550000	-2.891297000	-6.222161000
O	2.237829000	-0.124629000	-3.819246000
O	-2.359770000	1.410131000	-4.342753000
O	-0.018952000	-1.360829000	-2.943087000
O	-0.222959000	-3.837476000	-4.043330000
O	-0.294399000	-0.384254000	-5.000400000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.114404000	2.668477000	3.446106000
H	4.122365000	-3.076239000	3.125973000
H	-4.076454000	2.537273000	3.628097000
H	-4.044400000	-2.954690000	3.398880000
C	5.649698000	-2.314542000	-2.304397000
C	-5.725955000	-2.240628000	-2.013714000
C	4.364477000	-2.869734000	-2.366059000
C	-4.443370000	-2.652381000	-2.403674000
C	4.123340000	-3.969301000	-3.201393000
C	-4.295274000	-3.483310000	-3.522081000
C	5.155400000	-4.504653000	-3.967927000
C	-5.413355000	-3.887826000	-4.245438000
C	6.431189000	-3.941360000	-3.910525000
C	-6.686859000	-3.478791000	-3.850599000
C	6.676559000	-2.846661000	-3.079734000
C	-6.841867000	-2.657027000	-2.732468000
C	5.695385000	2.630838000	-1.709101000
C	-5.714614000	2.416116000	-1.920450000
C	4.384341000	3.020731000	-2.012524000
C	-4.419060000	2.919046000	-2.098403000
C	4.163660000	4.030667000	-2.957298000
C	-4.219272000	4.060217000	-2.885771000
C	5.240613000	4.641678000	-3.593346000
C	-5.303130000	4.689201000	-3.490397000
C	6.544952000	4.251234000	-3.286315000
C	-6.590716000	4.179707000	-3.317318000
C	6.770614000	3.246867000	-2.343424000
C	-6.795098000	3.043444000	-2.532852000
H	5.819542000	-1.466350000	-1.637571000

H	-5.823695000	-1.593877000	-1.140085000
H	3.120015000	-4.401673000	-3.231717000
H	-3.299441000	-3.796355000	-3.841933000
H	4.965922000	-5.366518000	-4.611588000
H	-5.285993000	-4.520269000	-5.126472000
H	7.676626000	-2.409986000	-3.032720000
H	-7.839472000	-2.337097000	-2.422898000
H	5.847664000	1.845666000	-0.965899000
H	-5.849880000	1.530264000	-1.297409000
H	3.136521000	4.321664000	-3.186308000
H	-3.207760000	4.452597000	-3.010431000
H	5.064210000	5.426570000	-4.332379000
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H	7.792235000	2.945423000	-2.100643000
H	-7.803563000	2.646341000	-2.397642000
H	-7.563780000	-3.798617000	-4.418866000
H	7.239745000	-4.360678000	-4.513869000
H	-7.440460000	4.672310000	-3.796069000
H	7.390124000	4.733229000	-3.783709000
H	-1.863913000	-2.799461000	0.554216000
H	-0.897956000	1.482428000	4.677398000
H	-0.059426000	0.144189000	4.543810000
H	0.007869000	3.748489000	0.522173000
H	0.737288000	3.840707000	2.707125000
H	0.909056000	3.878289000	-0.754815000
H	1.891643000	-0.192715000	3.443779000
H	-1.889235000	2.633154000	0.817315000
H	-0.695285000	-2.080026000	4.653562000
H	0.914811000	-4.026747000	2.271780000
H	0.764580000	-4.029611000	-1.192729000
H	0.063381000	-3.901775000	0.941024000
O	-1.065031000	-0.108295000	2.085677000
O	-3.558772000	1.261654000	2.145258000
O	-3.531374000	1.318926000	-0.598386000
O	-3.579234000	-1.513854000	2.048540000
O	-2.043281000	-2.648271000	3.220187000
O	0.028149000	-3.799687000	1.934069000
O	2.102348000	-2.870059000	3.012670000
O	2.074351000	-2.657729000	-1.772880000
O	3.558398000	-1.513048000	1.975500000
O	3.563505000	-1.377909000	-0.710085000
O	3.597333000	1.260161000	2.082953000
O	3.499361000	1.356371000	-0.586781000
O	2.067130000	2.790142000	-1.532621000
O	2.101737000	2.451982000	3.249418000
O	1.064437000	1.316668000	0.745542000

O	1.353880000	-0.123871000	2.642738000
O	0.008378000	-1.553341000	4.244748000
O	-0.017898000	1.134692000	4.439846000
O	1.068742000	-1.456769000	0.691711000
O	-1.332709000	-1.997684000	0.657088000
O	-2.097512000	-2.554533000	-1.954537000
O	0.018511000	-3.623626000	-0.727457000
O	-3.483088000	-1.340087000	-0.687653000
O	-0.000687000	3.448046000	2.215455000
O	0.001792000	3.660840000	-0.469217000
O	-1.340262000	1.838648000	0.769024000
O	-2.066330000	2.260590000	3.490345000
O	-2.084926000	2.549488000	-1.771849000
O	1.339731000	-0.016853000	-1.207214000
O	-1.061749000	-0.046945000	-0.728757000
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H	0.043878000	2.551375000	-3.132846000
Ti	2.469222000	-0.057398000	0.690680000
Ti	-0.083917000	-1.708903000	2.371738000
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Ti	-0.064142000	1.539403000	-0.944882000
Ti	-2.473515000	-0.084883000	0.675729000
Ti	0.102916000	-1.738296000	-0.914669000
C	-1.848709000	-1.566838000	-5.122017000
C	-0.547973000	-2.380157000	-4.989581000
C	0.423459000	-1.619735000	-4.109258000
C	-1.557875000	-0.071947000	-5.326481000
C	1.855937000	-1.462549000	-4.516373000
C	-2.451571000	0.761394000	-4.432490000
H	2.309946000	-2.462618000	-4.358398000
H	-0.107257000	-2.555433000	-5.987154000
H	-2.354850000	-1.691302000	-4.151003000
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H	-1.738817000	0.192563000	-6.385927000
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C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
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H	-4.048717000	-2.941457000	3.406218000
C	5.699286000	-2.531987000	-2.046473000
C	-5.676930000	-2.090412000	-2.264443000
C	4.377431000	-2.917828000	-2.301364000
C	-4.408043000	-2.654873000	-2.450038000
C	4.111909000	-3.901445000	-3.264372000
C	-4.217815000	-3.631048000	-3.435660000
C	5.160282000	-4.491917000	-3.964373000
C	-5.283686000	-4.033762000	-4.234239000
C	6.476416000	-4.104723000	-3.706663000
C	-6.545026000	-3.466010000	-4.050179000
C	6.744143000	-3.125588000	-2.748546000
C	-6.740764000	-2.496356000	-3.064583000
C	5.698584000	2.748701000	-1.507966000
C	-5.710805000	2.675697000	-1.719214000
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C	-4.134284000	4.128893000	-2.847758000
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C	6.588496000	4.472413000	-2.947077000
C	-6.506296000	4.513176000	-3.068454000
C	6.788513000	3.438178000	-2.031253000
C	-6.764968000	3.416337000	-2.245022000
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H	-5.802910000	-1.328426000	-1.492712000
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H	4.951801000	-5.259063000	-4.713441000
H	-5.128517000	-4.787685000	-5.009129000

H	7.774737000	-2.823885000	-2.549031000
H	-7.729005000	-2.052841000	-2.923482000
H	5.830433000	1.936584000	-0.790578000
H	-5.888316000	1.818653000	-1.067032000
H	3.183344000	4.389963000	-3.112068000
H	-3.099835000	4.396392000	-3.073163000
H	5.138841000	5.627319000	-4.057590000
H	-4.988733000	5.729479000	-4.010221000
H	7.801729000	3.168917000	-1.724350000
H	-7.795262000	3.139664000	-2.010551000
H	-7.381240000	-3.779458000	-4.679964000
H	7.298554000	-4.569331000	-4.256304000
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H	7.445758000	5.011387000	-3.357770000
H	-1.865960000	-2.831560000	0.548242000
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H	-0.053571000	0.137737000	4.509366000
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H	0.738521000	3.835474000	2.636665000
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H	-0.687946000	-2.080330000	4.632569000
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H	0.745945000	-4.061251000	-1.259762000
H	0.084534000	-3.926398000	0.933172000
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O	0.032217000	-3.817938000	1.923935000
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O	2.070668000	-2.613445000	-1.829445000
O	3.557132000	-1.514975000	1.974626000
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O	3.604511000	1.258367000	2.090183000
O	3.481838000	1.358587000	-0.577002000
O	2.062473000	2.731390000	-1.621040000
O	2.095048000	2.461184000	3.223776000
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O	1.052922000	-1.480251000	0.664170000
O	-1.339112000	-2.026008000	0.644285000

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O	-0.000789000	3.440940000	2.147697000
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O	-1.352720000	1.816416000	0.730197000
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O	-2.077634000	2.464398000	-1.830671000
O	1.318132000	-0.047601000	-1.228605000
O	-1.080482000	-0.082068000	-0.757512000
H	1.849086000	-0.052038000	-2.058789000
O	0.071489000	1.584087000	-2.903173000
H	-0.156846000	2.488313000	-3.164324000
Ti	2.459261000	-0.075096000	0.662404000
Ti	-0.082926000	-1.723287000	2.345372000
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Ti	-0.085960000	1.492743000	-0.984414000
Ti	-2.486893000	-0.112093000	0.668157000
Ti	0.090304000	-1.775330000	-0.948408000
C	-1.686397000	-1.883414000	-5.173622000
C	-0.224400000	-2.340451000	-5.238903000
C	0.542288000	-1.579482000	-4.175256000
C	-1.789018000	-0.364254000	-5.360550000
C	1.885804000	-0.999125000	-4.514956000
C	-2.738978000	0.268688000	-4.360350000
H	2.616436000	-1.819249000	-4.383817000
H	0.198642000	-2.095592000	-6.237135000
H	-2.037081000	-2.163358000	-4.166359000
H	-2.454050000	2.061186000	-3.689353000
H	1.898168000	-0.737098000	-5.585575000
H	1.593346000	0.765727000	-3.718947000
H	-2.406522000	-0.019245000	-3.341808000
H	-3.749841000	-0.162040000	-4.500718000
H	-0.964501000	-4.099157000	-5.281836000
H	-0.489574000	0.796065000	-4.444138000
H	-2.284658000	-2.353344000	-6.960797000
H	-2.141795000	-0.147111000	-6.388555000
O	-2.472293000	-2.646454000	-6.059136000
O	2.283624000	0.066794000	-3.704632000
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H	-4.072539000	2.521734000	3.649825000
H	-4.035874000	-2.950017000	3.418074000
C	5.698118000	-2.643214000	-1.971208000
C	-5.733371000	-2.418587000	-1.867085000
C	4.368612000	-2.958223000	-2.278894000
C	-4.449251000	-2.879598000	-2.184437000
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C	-5.417230000	-4.643708000	-3.525152000
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C	-6.696078000	-4.176991000	-3.213998000
C	6.737316000	-3.275668000	-2.647224000
C	-6.852825000	-3.063697000	-2.387325000
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C	6.474471000	4.495439000	-3.137040000
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H	-5.295014000	-5.514307000	-4.173227000
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H	7.274112000	-4.719494000	-4.161549000
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H	7.303103000	5.039625000	-3.596789000
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O	2.062016000	-2.565989000	-1.856436000
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O	3.601320000	1.259300000	2.086156000
O	3.524965000	1.376023000	-0.574793000
O	2.043859000	2.714485000	-1.577452000
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O	1.074483000	1.326906000	0.735787000
O	1.352985000	-0.124681000	2.624492000
O	0.007150000	-1.551183000	4.224952000
O	-0.018741000	1.137524000	4.419202000
O	1.068515000	-1.459850000	0.675606000
O	-1.338326000	-1.994209000	0.626691000
O	-2.102965000	-2.441554000	-2.062081000
O	0.011167000	-3.580267000	-0.792586000
O	-3.478533000	-1.314703000	-0.705850000
O	0.011449000	3.455381000	2.184456000
O	-0.000543000	3.677541000	-0.495901000

O	-1.334152000	1.850639000	0.735020000
O	-2.062118000	2.270023000	3.476953000
O	-2.083397000	2.466920000	-1.828992000
O	1.366417000	0.000064000	-1.198158000
O	-1.045703000	-0.041818000	-0.731075000
H	1.875444000	0.000786000	-2.039449000
O	0.059004000	1.627530000	-2.830595000
H	-0.774539000	1.931835000	-3.216744000
Ti	2.479713000	-0.055269000	0.685705000
Ti	-0.094368000	-1.705303000	2.352478000
Ti	0.080648000	1.581289000	2.330790000
Ti	-0.050628000	1.579310000	-0.965466000
Ti	-2.462903000	-0.083100000	0.636585000
Ti	0.119928000	-1.697667000	-0.932343000
C	-1.605882000	-0.684945000	-5.653952000
C	-0.581511000	-1.773599000	-5.237420000
C	0.366003000	-1.199684000	-4.202086000
C	-2.689483000	-0.447186000	-4.601985000
C	1.617534000	-0.511205000	-4.659636000
C	-3.435437000	0.861606000	-4.812668000
H	2.324893000	-1.337844000	-4.868573000
H	0.010803000	-2.010773000	-6.139687000
H	-2.124786000	-1.064143000	-6.555066000
H	-5.067867000	1.597483000	-4.028562000
H	1.414192000	-0.039711000	-5.637253000
H	1.535116000	1.067843000	-3.572674000
H	-3.730502000	0.962175000	-5.880015000
H	-2.792867000	1.725883000	-4.553467000
H	-1.586001000	-2.778216000	-3.915521000
H	-4.381063000	-1.268381000	-4.216091000
H	-1.392035000	1.059676000	-6.505456000
H	-2.235992000	-0.403158000	-3.584295000
O	-0.865126000	0.489547000	-5.935904000
O	2.200039000	0.357259000	-3.746186000
O	-4.561426000	0.779514000	-3.977139000
O	0.082483000	-1.372682000	-3.027463000
O	-1.166149000	-2.941425000	-4.787023000
O	-3.588361000	-1.518599000	-4.713336000

Ti-NU-1000 TS3

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000

C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.100694000	2.701021000	3.434525000
H	4.114268000	-3.091247000	3.120463000
H	-4.093629000	2.539065000	3.597323000
H	-4.061031000	-2.947109000	3.380068000
C	5.701093000	-2.582296000	-2.016575000
C	-5.414633000	-1.459919000	-2.662993000
C	4.373526000	-2.924881000	-2.301500000
C	-4.407632000	-2.428049000	-2.560367000
C	4.097985000	-3.876334000	-3.292761000
C	-4.467262000	-3.580143000	-3.353552000
C	5.140623000	-4.479172000	-3.990358000
C	-5.527233000	-3.765159000	-4.237955000
C	6.462546000	-4.135633000	-3.702112000
C	-6.525263000	-2.793249000	-4.346194000
C	6.740926000	-3.187763000	-2.716113000
C	-6.464984000	-1.637284000	-3.561291000
C	5.661954000	2.896646000	-1.566225000
C	-5.705448000	2.346089000	-2.027246000
C	4.335580000	3.166347000	-1.926597000
C	-4.391074000	2.758797000	-2.280896000
C	4.060335000	4.193058000	-2.838254000
C	-4.132048000	3.624044000	-3.350823000
C	5.099772000	4.941185000	-3.383797000
C	-5.172412000	4.058420000	-4.167998000
C	6.419684000	4.669915000	-3.020330000
C	-6.478849000	3.634766000	-3.918838000
C	6.698878000	3.648036000	-2.111379000
C	-6.744413000	2.783379000	-2.844684000
H	5.893476000	-1.837431000	-1.242315000
H	-5.340409000	-0.567594000	-2.035993000
H	3.056883000	-4.131740000	-3.504919000
H	-3.677219000	-4.329320000	-3.269875000
H	4.923970000	-5.221086000	-4.762267000
H	-5.577433000	-4.670675000	-4.846598000
H	7.775955000	-2.919688000	-2.492796000
H	-7.241719000	-0.872724000	-3.649931000
H	5.854962000	2.092520000	-0.853669000
H	-5.889571000	1.682834000	-1.179440000
H	3.022243000	4.389005000	-3.114210000
H	-3.103298000	3.945969000	-3.527164000
H	4.882092000	5.739370000	-4.097207000
H	-4.966505000	4.731436000	-5.003602000
H	7.732352000	3.436930000	-1.827322000
H	-7.769116000	2.462157000	-2.642674000

H	-7.358549000	-2.941313000	-5.038710000
H	7.280566000	-4.609569000	-4.249975000
H	-7.294641000	3.974463000	-4.561378000
H	7.235146000	5.258026000	-3.448344000
H	-1.840854000	-2.785814000	0.574102000
H	-0.913035000	1.452878000	4.697517000
H	-0.062315000	0.121340000	4.558818000
H	0.092925000	3.778442000	0.570618000
H	0.751239000	3.845779000	2.772462000
H	0.981206000	3.867045000	-0.735007000
H	1.903410000	-0.199287000	3.479485000
H	-1.822353000	2.679715000	0.812521000
H	-0.706875000	-2.087125000	4.634232000
H	0.891980000	-4.059127000	2.316451000
H	0.808858000	-4.044986000	-1.175075000
H	0.098731000	-3.894345000	0.952836000
O	-1.041544000	-0.094832000	2.109970000
O	-3.533573000	1.250672000	2.143172000
O	-3.547216000	1.334058000	-0.585112000
O	-3.560915000	-1.502244000	2.047248000
O	-2.053116000	-2.658506000	3.232232000
O	0.028129000	-3.798164000	1.950563000
O	2.099178000	-2.852381000	3.014301000
O	2.071497000	-2.597103000	-1.828198000
O	3.574477000	-1.513441000	1.980819000
O	3.560993000	-1.396438000	-0.679236000
O	3.611132000	1.260220000	2.096796000
O	3.539698000	1.389410000	-0.578732000
O	2.027236000	2.672342000	-1.608944000
O	2.095651000	2.431595000	3.264477000
O	1.094576000	1.324266000	0.777429000
O	1.373068000	-0.127277000	2.673947000
O	0.014411000	-1.566943000	4.247839000
O	-0.025792000	1.115470000	4.472232000
O	1.107463000	-1.446512000	0.712174000
O	-1.304883000	-1.986215000	0.670582000
O	-2.151508000	-2.737692000	-1.854963000
O	0.095367000	-3.632159000	-0.668643000
O	-3.463710000	-1.332617000	-0.705084000
O	0.023016000	3.456412000	2.263816000
O	0.079457000	3.669325000	-0.419295000
O	-1.300821000	1.864939000	0.815280000
O	-2.079289000	2.264676000	3.519500000
O	-2.089655000	2.624611000	-1.678941000
O	1.351708000	-0.013081000	-1.187168000
O	-1.046685000	-0.010132000	-0.673851000

H	1.818582000	0.006162000	-2.054377000
O	-0.095437000	1.539522000	-2.844609000
H	-0.346491000	2.443707000	-3.085290000
Ti	2.492356000	-0.124361000	0.699078000
Ti	-0.046130000	-1.710159000	2.368185000
Ti	0.107577000	1.581055000	2.397331000
Ti	-0.013147000	1.540926000	-0.825969000
Ti	-2.452155000	-0.073506000	0.723303000
Ti	0.109594000	-1.753434000	-0.963716000
C	-1.812159000	-0.076712000	-4.806903000
C	-0.539133000	-2.377232000	-4.914502000
C	0.266228000	-1.618411000	-4.091463000
C	-2.900895000	-0.741412000	-5.551469000
C	1.538037000	-0.975815000	-4.589306000
C	-4.145165000	0.162218000	-5.630035000
H	2.346716000	-1.724855000	-4.537923000
H	-0.366119000	-2.440266000	-5.991189000
H	-1.014927000	0.435446000	-5.373584000
H	-5.528167000	-1.163383000	-5.858885000
H	1.427116000	-0.726939000	-5.663253000
H	1.254561000	0.770877000	-3.718928000
H	-3.886642000	1.100387000	-6.145509000
H	-4.495997000	0.419390000	-4.614290000
H	-1.630990000	-3.048891000	-3.483069000
H	-3.271035000	-1.236179000	-7.346786000
H	-1.171728000	0.788582000	-3.172613000
H	-3.194323000	-1.644919000	-4.968847000
O	-2.001809000	0.183838000	-3.581120000
O	1.981221000	0.120616000	-3.835171000
O	-5.120521000	-0.476371000	-6.407931000
O	-0.048792000	-1.532921000	-2.833094000
O	-1.511887000	-3.162928000	-4.465558000
O	-2.463818000	-1.070326000	-6.837897000

Ti-NU-1000 Int3

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.090088000	2.718433000	3.433761000
H	4.129249000	-3.040576000	3.156348000
H	-4.076042000	2.532367000	3.633283000

H	-4.037022000	-2.947712000	3.419605000
C	5.715182000	-2.529997000	-1.983395000
C	-5.716161000	-2.435961000	-2.016494000
C	4.398953000	-2.905175000	-2.279796000
C	-4.411592000	-2.884495000	-2.261137000
C	4.156304000	-3.872701000	-3.264118000
C	-4.200752000	-3.976311000	-3.110652000
C	5.219907000	-4.459943000	-3.942850000
C	-5.282628000	-4.612287000	-3.712370000
C	6.530487000	-4.084258000	-3.642983000
C	-6.579106000	-4.149917000	-3.483617000
C	6.776235000	-3.119744000	-2.664477000
C	-6.795034000	-3.059122000	-2.637131000
C	5.640206000	2.961857000	-1.590832000
C	-5.733343000	2.404771000	-1.852110000
C	4.303953000	3.203614000	-1.934147000
C	-4.438653000	2.862765000	-2.124731000
C	3.995739000	4.232523000	-2.832591000
C	-4.247771000	3.905430000	-3.040181000
C	5.011534000	5.010100000	-3.381803000
C	-5.341025000	4.476536000	-3.685226000
C	6.341159000	4.765997000	-3.035364000
C	-6.631434000	4.012931000	-3.415127000
C	6.653524000	3.742000000	-2.139668000
C	-6.825732000	2.980183000	-2.496345000
H	5.882354000	-1.772838000	-1.215266000
H	-5.860903000	-1.584155000	-1.348274000
H	3.123469000	-4.151700000	-3.486364000
H	-3.179912000	-4.315187000	-3.297403000
H	5.028505000	-5.214418000	-4.709235000
H	-5.114133000	-5.465742000	-4.372563000
H	7.802434000	-2.826319000	-2.432326000
H	-7.810160000	-2.697599000	-2.457220000
H	5.858759000	2.155271000	-0.888475000
H	-5.860223000	1.590120000	-1.136322000
H	2.950966000	4.409213000	-3.096032000
H	-3.231120000	4.254046000	-3.233025000
H	4.767578000	5.810323000	-4.084361000
H	-5.191327000	5.290610000	-4.398251000
H	7.694596000	3.551852000	-1.868932000
H	-7.834306000	2.618672000	-2.281581000
H	-7.427533000	-4.643751000	-3.964132000
H	7.365247000	-4.545860000	-4.175984000
H	-7.489276000	4.468621000	-3.916780000
H	7.138107000	5.376968000	-3.466171000
H	-1.913393000	-2.730364000	0.564744000

H	-0.926013000	1.404915000	4.703049000
H	-0.072999000	0.073883000	4.530815000
H	0.094045000	3.795509000	0.575128000
H	0.779088000	3.820917000	2.753402000
H	0.996018000	3.898986000	-0.720271000
H	1.876722000	-0.224166000	3.451817000
H	-1.805005000	2.705979000	0.787248000
H	-0.690837000	-2.128149000	4.583365000
H	0.893725000	-4.030974000	2.163355000
H	0.648770000	-4.041093000	-1.325899000
H	0.063596000	-3.841664000	0.819273000
O	-1.058727000	-0.078712000	2.070273000
O	-3.552579000	1.285823000	2.127306000
O	-3.518642000	1.299199000	-0.607369000
O	-3.590378000	-1.501620000	2.066560000
O	-2.037805000	-2.670277000	3.178971000
O	0.019093000	-3.771982000	1.823453000
O	2.108164000	-2.895425000	2.976085000
O	2.085729000	-2.619091000	-1.830549000
O	3.556577000	-1.509906000	1.970635000
O	3.542261000	-1.382504000	-0.677531000
O	3.617265000	1.258700000	2.108059000
O	3.557271000	1.407746000	-0.583562000
O	2.008309000	2.647261000	-1.617273000
O	2.088386000	2.424125000	3.264660000
O	1.090123000	1.333424000	0.772262000
O	1.352388000	-0.139667000	2.643500000
O	0.008250000	-1.583326000	4.190893000
O	-0.040310000	1.073123000	4.464157000
O	1.073679000	-1.438513000	0.658807000
O	-1.360016000	-1.938686000	0.607326000
O	-2.088799000	-2.420105000	-2.048348000
O	-0.015432000	-3.587661000	-0.789331000
O	-3.513681000	-1.339326000	-0.707436000
O	0.027259000	3.457399000	2.258082000
O	0.092463000	3.691536000	-0.417815000
O	-1.296034000	1.883278000	0.796355000
O	-2.066596000	2.246996000	3.507916000
O	-2.100512000	2.623265000	-1.715794000
O	1.357495000	0.018601000	-1.225643000
O	-1.039779000	0.038067000	-0.739500000
H	1.860212000	0.081863000	-2.073798000
O	-0.049863000	1.648929000	-2.988790000
H	-0.242220000	2.582829000	-3.162756000
Ti	2.470383000	-0.193796000	0.692272000
Ti	-0.087176000	-1.703973000	2.303999000

Ti	0.082352000	1.579757000	2.410169000
Ti	0.052561000	1.554478000	-0.786125000
Ti	-2.460601000	-0.053629000	0.653409000
Ti	0.058471000	-1.708951000	-1.123926000
C	-3.062960000	0.023473000	-4.739260000
C	-0.391371000	-1.920536000	-5.135892000
C	0.481766000	-1.455781000	-4.205345000
C	-4.493291000	-0.332083000	-4.450358000
C	1.868265000	-0.988487000	-4.518408000
C	-5.426227000	0.786276000	-4.896766000
H	2.610670000	-1.754964000	-4.246025000
H	-0.170490000	-1.907619000	-6.205586000
H	-2.676110000	-0.301239000	-5.735089000
H	-7.341859000	1.053869000	-4.776904000
H	1.964382000	-0.835311000	-5.608770000
H	1.563094000	0.845800000	-3.889901000
H	-5.338409000	0.911246000	-5.994646000
H	-5.134609000	1.738939000	-4.419939000
H	-1.684723000	-2.460522000	-3.842171000
H	-5.718776000	-1.728023000	-4.906940000
H	-0.873859000	1.195107000	-3.299635000
H	-4.592473000	-0.411849000	-3.346149000
O	-2.389464000	0.663425000	-3.961160000
O	2.255688000	0.170775000	-3.795626000
O	-6.716155000	0.368737000	-4.521557000
O	0.079630000	-1.473514000	-2.939569000
O	-1.589239000	-2.435284000	-4.825006000
O	-4.795541000	-1.525546000	-5.111031000

Ti-NU-1000 TS4

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.093815000	2.676904000	3.471202000
H	4.127680000	-3.047160000	3.152902000
H	-4.080821000	2.516303000	3.640870000
H	-4.040377000	-2.958056000	3.401946000
C	5.624523000	-2.043337000	-2.368959000
C	-5.691966000	-2.287064000	-2.176900000
C	4.388066000	-2.700631000	-2.440739000
C	-4.389699000	-2.742033000	-2.420539000

C	4.202274000	-3.730146000	-3.373526000
C	-4.157729000	-3.683546000	-3.429686000
C	5.241787000	-4.099463000	-4.223162000
C	-5.219346000	-4.166647000	-4.188322000
C	6.470230000	-3.440172000	-4.150222000
C	-6.514812000	-3.703610000	-3.951380000
C	6.659664000	-2.412459000	-3.224699000
C	-6.750964000	-2.762831000	-2.945870000
C	5.674900000	2.897996000	-1.403575000
C	-5.707150000	2.741939000	-1.609877000
C	4.378574000	3.140587000	-1.875763000
C	-4.393662000	3.031390000	-2.005824000
C	4.166764000	4.119298000	-2.854736000
C	-4.148270000	4.091073000	-2.886451000
C	5.241964000	4.845374000	-3.359390000
C	-5.210492000	4.847869000	-3.373338000
C	6.531927000	4.603242000	-2.884230000
C	-6.518838000	4.551091000	-2.986399000
C	6.746591000	3.631221000	-1.905438000
C	-6.767173000	3.498943000	-2.102386000
H	5.750105000	-1.245892000	-1.632837000
H	-5.847982000	-1.549196000	-1.386383000
H	3.232815000	-4.232424000	-3.414963000
H	-3.134471000	-4.018836000	-3.610899000
H	5.096080000	-4.905691000	-4.945646000
H	-5.037476000	-4.900026000	-4.976886000
H	7.621838000	-1.898692000	-3.168044000
H	-7.763904000	-2.394177000	-2.768803000
H	5.816708000	2.135091000	-0.635165000
H	-5.869237000	1.925804000	-0.900546000
H	3.149918000	4.291379000	-3.213847000
H	-3.120468000	4.301202000	-3.184100000
H	5.075447000	5.604905000	-4.126735000
H	-5.019139000	5.673098000	-4.062746000
H	7.756224000	3.446802000	-1.531064000
H	-7.791278000	3.272357000	-1.796465000
H	-7.346266000	-4.075994000	-4.554706000
H	7.284855000	-3.729796000	-4.818161000
H	-7.350139000	5.145440000	-3.372881000
H	7.374738000	5.176490000	-3.278164000
H	-1.919095000	-2.803352000	0.598762000
H	-0.893056000	1.479574000	4.631698000
H	-0.049618000	0.143175000	4.505797000
H	0.076590000	3.747771000	0.463250000
H	0.741273000	3.844989000	2.672323000
H	0.907181000	3.848261000	-0.878949000

H	1.906264000	-0.198267000	3.387770000
H	-1.863557000	2.654706000	0.780268000
H	-0.677605000	-2.078048000	4.630495000
H	0.912022000	-4.021413000	2.261062000
H	0.683850000	-4.071130000	-1.208195000
H	0.045279000	-3.914939000	0.936542000
O	-1.070647000	-0.100929000	2.066849000
O	-3.555850000	1.269679000	2.135393000
O	-3.557715000	1.291229000	-0.634895000
O	-3.586360000	-1.508154000	2.057922000
O	-2.041185000	-2.650026000	3.209963000
O	0.021331000	-3.801311000	1.929035000
O	2.105149000	-2.881770000	3.004180000
O	2.135391000	-2.800601000	-1.689531000
O	3.549583000	-1.528223000	1.950258000
O	3.509503000	-1.332641000	-0.723968000
O	3.616171000	1.264067000	2.093924000
O	3.500775000	1.351349000	-0.597749000
O	2.052406000	2.702521000	-1.627491000
O	2.088616000	2.450570000	3.221440000
O	1.051799000	1.301348000	0.690516000
O	1.356256000	-0.132644000	2.594773000
O	0.018330000	-1.548215000	4.212907000
O	-0.010233000	1.133691000	4.400479000
O	1.027811000	-1.466485000	0.645924000
O	-1.369325000	-2.009636000	0.650630000
O	-2.069581000	-2.428250000	-2.001767000
O	-0.045133000	-3.660456000	-0.719592000
O	-3.540386000	-1.394579000	-0.670695000
O	0.016555000	3.449476000	2.163004000
O	0.020446000	3.642143000	-0.524333000
O	-1.338571000	1.843265000	0.737226000
O	-2.067265000	2.274338000	3.480541000
O	-2.078054000	2.523603000	-1.759319000
O	1.273691000	-0.040220000	-1.288333000
O	-1.095589000	-0.063308000	-0.729142000
H	1.857816000	0.009522000	-2.075976000
O	-0.066444000	1.634127000	-2.912818000
H	-0.844961000	2.163900000	-3.166062000
Ti	2.444792000	-0.110681000	0.643773000
Ti	-0.092954000	-1.709294000	2.340515000
Ti	0.097111000	1.580505000	2.314061000
Ti	-0.092040000	1.534428000	-0.964759000
Ti	-2.476928000	-0.084123000	0.675623000
Ti	0.032377000	-1.793442000	-0.974166000
C	-0.556660000	-0.348486000	-4.595553000

C	0.479115000	-1.103989000	-4.021291000
C	1.892126000	-0.988066000	-4.529322000
H	2.278254000	-2.016301000	-4.645776000
H	-0.457486000	0.051147000	-5.611907000
H	1.895469000	-0.508675000	-5.523247000
H	3.586514000	-0.566947000	-3.616338000
H	-1.830497000	-1.287395000	-3.510215000
H	-0.116484000	0.641810000	-3.822122000
O	2.674466000	-0.245758000	-3.613992000
O	0.213699000	-1.768494000	-2.974759000
O	-1.838292000	-0.607738000	-4.219596000
C	-3.454804000	1.084472000	-5.338989000
C	-4.594165000	0.452705000	-4.583832000
C	-5.870317000	1.279582000	-4.721076000
H	-3.177584000	0.526121000	-6.274060000
H	-6.751382000	0.848439000	-3.064966000
H	-6.181059000	1.290560000	-5.777552000
H	-5.686377000	2.324289000	-4.415027000
H	-5.621518000	-1.159450000	-4.690353000
H	-4.305217000	0.450985000	-3.506251000
O	-2.908954000	2.110867000	-5.014395000
O	-6.919715000	0.677776000	-4.001046000
O	-4.791071000	-0.841995000	-5.074235000

Ti-NU-1000 Prod

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.104092000	2.668816000	3.462364000
H	4.119434000	-3.077350000	3.130481000
H	-4.089549000	2.504910000	3.637597000
H	-4.037143000	-2.963782000	3.400746000
C	5.687548000	-2.479098000	-2.131355000
C	-5.715189000	-2.384704000	-2.003527000
C	4.367956000	-2.903718000	-2.328764000
C	-4.417945000	-2.808360000	-2.321622000
C	4.093901000	-3.911246000	-3.263264000
C	-4.229205000	-3.789841000	-3.302498000
C	5.129939000	-4.487279000	-3.992790000
C	-5.326589000	-4.339118000	-3.958770000
C	6.443771000	-4.058813000	-3.794782000

C	-6.615786000	-3.909719000	-3.644444000
C	6.720612000	-3.055617000	-2.864784000
C	-6.809000000	-2.933073000	-2.665603000
C	5.669900000	2.880041000	-1.531517000
C	-5.710950000	2.754255000	-1.608332000
C	4.351940000	3.137760000	-1.929330000
C	-4.394971000	3.052657000	-1.979234000
C	4.095036000	4.127624000	-2.886139000
C	-4.140238000	4.122711000	-2.846706000
C	5.146768000	4.852314000	-3.439345000
C	-5.197211000	4.878567000	-3.349464000
C	6.458532000	4.595683000	-3.037296000
C	-6.511094000	4.575043000	-2.978506000
C	6.718427000	3.610309000	-2.083307000
C	-6.764948000	3.515870000	-2.105744000
H	5.878732000	-1.692702000	-1.398906000
H	-5.841036000	-1.618976000	-1.235032000
H	3.059839000	-4.237297000	-3.400683000
H	-3.217133000	-4.118250000	-3.550293000
H	4.915249000	-5.276219000	-4.717262000
H	-5.175332000	-5.104823000	-4.722711000
H	7.749229000	-2.721828000	-2.711433000
H	-7.819782000	-2.601217000	-2.416334000
H	5.847899000	2.103738000	-0.784870000
H	-5.884930000	1.916583000	-0.930088000
H	3.062568000	4.309407000	-3.191698000
H	-3.104823000	4.345404000	-3.114679000
H	4.945115000	5.620579000	-4.189338000
H	-4.998719000	5.715627000	-4.023105000
H	7.745638000	3.411179000	-1.769406000
H	-7.791526000	3.280940000	-1.816673000
H	-7.475814000	-4.340268000	-4.163280000
H	7.256620000	-4.510957000	-4.368124000
H	-7.338997000	5.171515000	-3.369407000
H	7.283310000	5.166504000	-3.470919000
H	-1.873721000	-2.790494000	0.566039000
H	-0.896687000	1.511325000	4.630542000
H	-0.056470000	0.173074000	4.524519000
H	0.071287000	3.762206000	0.477839000
H	0.732496000	3.864410000	2.685378000
H	0.879985000	3.913619000	-0.873125000
H	1.902263000	-0.188995000	3.427581000
H	-1.861839000	2.654973000	0.804919000
H	-0.695797000	-2.058586000	4.650149000
H	0.916071000	-4.015316000	2.256274000
H	0.674212000	-4.022080000	-1.275099000

H	0.065779000	-3.890953000	0.925711000
O	-1.054194000	-0.090274000	2.074397000
O	-3.543172000	1.266312000	2.134167000
O	-3.552079000	1.316602000	-0.606325000
O	-3.584599000	-1.516003000	2.051890000
O	-2.038764000	-2.640296000	3.219167000
O	0.028848000	-3.789795000	1.918400000
O	2.100202000	-2.867093000	3.010147000
O	2.069730000	-2.623055000	-1.805049000
O	3.562738000	-1.515853000	1.974667000
O	3.558837000	-1.388863000	-0.691234000
O	3.610205000	1.259648000	2.091048000
O	3.529488000	1.374544000	-0.577408000
O	2.040072000	2.690897000	-1.596006000
O	2.096026000	2.456560000	3.228283000
O	1.086541000	1.319814000	0.722688000
O	1.363433000	-0.122452000	2.627117000
O	0.010186000	-1.535863000	4.239861000
O	-0.011844000	1.161061000	4.412197000
O	1.064794000	-1.461643000	0.685351000
O	-1.343501000	-1.986252000	0.652855000
O	-2.079702000	-2.429442000	-2.026823000
O	-0.017400000	-3.600700000	-0.743525000
O	-3.508696000	-1.355163000	-0.690548000
O	0.017340000	3.460854000	2.170029000
O	0.007609000	3.669406000	-0.512161000
O	-1.325705000	1.853455000	0.729676000
O	-2.072184000	2.288892000	3.484381000
O	-2.090385000	2.474041000	-1.834388000
O	1.359096000	-0.022058000	-1.210439000
O	-1.055527000	-0.043495000	-0.727536000
H	1.837659000	-0.031465000	-2.066338000
O	0.050808000	1.612686000	-2.842282000
H	-0.820002000	1.659015000	-3.266384000
Ti	2.486876000	-0.066002000	0.672709000
Ti	-0.085043000	-1.699621000	2.370476000
Ti	0.106589000	1.588123000	2.317171000
Ti	-0.043870000	1.576228000	-0.987478000
Ti	-2.452287000	-0.065585000	0.663196000
Ti	0.090028000	-1.715713000	-0.904946000
C	-0.024340000	-2.854373000	-4.904965000
C	0.525738000	-1.691918000	-4.134420000
C	1.543102000	-0.780460000	-4.759125000
H	2.392543000	-1.419744000	-5.061839000
H	0.812515000	-3.375175000	-5.404243000
H	1.117000000	-0.392530000	-5.706478000

H	1.275107000	0.835023000	-3.695399000
H	-1.181026000	-3.276730000	-3.395916000
H	-0.615568000	-2.411620000	-5.739523000
O	2.014944000	0.210034000	-3.917064000
O	0.150195000	-1.516105000	-2.986555000
O	-0.735800000	-3.749011000	-4.133572000
C	-2.623518000	-0.676157000	-4.609530000
C	-3.975588000	-0.081754000	-4.347541000
C	-4.111431000	1.333026000	-4.876677000
H	-2.630652000	-1.796324000	-4.692631000
H	-5.513967000	2.659998000	-4.605815000
H	-3.840743000	1.351560000	-5.951132000
H	-3.399348000	1.991539000	-4.348035000
H	-5.789994000	-0.534302000	-4.742777000
H	-4.068240000	-0.040943000	-3.231683000
O	-1.605677000	-0.031598000	-4.724991000
O	-5.451781000	1.699674000	-4.673280000
O	-4.928887000	-0.940712000	-4.905827000

4. functionalized Hf-NU-1000 case

4.1 -NH₂

Hf-NU-1000 (-NH₂)

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.085552000	2.702322000	3.456423000
H	4.063154000	-3.148474000	3.135327000
H	-4.032628000	2.554401000	3.674720000
H	-4.031616000	-2.979607000	3.390692000
C	5.658853000	-2.792746000	-1.811985000
C	-5.605863000	-2.523568000	-2.295249000
C	4.329524000	-3.079471000	-2.179089000
C	-4.266170000	-2.942148000	-2.390027000
C	4.080518000	-4.127165000	-3.113725000
C	-3.946897000	-4.100803000	-3.157117000
C	5.190851000	-4.826885000	-3.634739000
C	-5.010539000	-4.775150000	-3.798350000
C	6.484778000	-4.517338000	-3.255085000
C	-6.316369000	-4.328347000	-3.700005000
C	6.732882000	-3.492099000	-2.333631000

C	-6.629936000	-3.189940000	-2.946167000
C	5.579557000	3.009092000	-1.763314000
C	-5.668059000	2.649972000	-1.871279000
C	4.225399000	3.100780000	-2.128184000
C	-4.329814000	3.001444000	-2.129786000
C	3.848042000	3.874060000	-3.267544000
C	-4.054676000	4.086867000	-3.014855000
C	4.882516000	4.543485000	-3.963260000
C	-5.155952000	4.763205000	-3.588153000
C	6.204744000	4.455339000	-3.565179000
C	-6.459231000	4.389410000	-3.314984000
C	6.572027000	3.682658000	-2.455469000
C	-6.731030000	3.321006000	-2.450366000
H	5.814610000	-1.986560000	-1.093547000
H	-5.810126000	-1.640225000	-1.687205000
H	5.007758000	-5.631065000	-4.352541000
H	-4.779987000	-5.668090000	-4.385855000
H	7.752872000	-3.246447000	-2.034534000
H	-7.659821000	-2.838068000	-2.869581000
H	5.821460000	2.387391000	-0.898626000
H	-5.839822000	1.817607000	-1.186799000
H	4.615349000	5.140657000	-4.839666000
H	-4.956173000	5.598021000	-4.265539000
H	7.615957000	3.609801000	-2.146613000
H	-7.759069000	3.025816000	-2.234785000
H	-7.107092000	-4.877525000	-4.217618000
H	7.315885000	-5.082477000	-3.684452000
H	-7.280114000	4.939722000	-3.782036000
H	6.967639000	4.993524000	-4.133813000
H	-1.939211000	-2.925987000	0.600207000
H	-0.875504000	1.379058000	5.101250000
H	-0.015447000	0.076582000	4.808583000
H	0.003524000	4.049320000	0.613994000
H	0.664630000	4.290389000	2.675558000
H	0.846869000	4.353848000	-0.694124000
H	1.959743000	-0.191781000	3.591030000
H	-1.943072000	2.800258000	0.850329000
H	-0.608632000	-2.013900000	5.120321000
H	0.904233000	-4.438227000	2.124164000
H	0.784075000	-4.368446000	-1.149890000
H	0.023896000	-4.139724000	0.842228000
O	-1.062567000	-0.104073000	2.186028000
O	-3.615968000	1.286183000	2.167756000
O	-3.604838000	1.341703000	-0.619214000
O	-3.603895000	-1.509210000	2.082902000
O	-2.046823000	-2.661798000	3.231763000

O	0.048865000	-4.076747000	1.852433000
O	2.073882000	-2.836442000	2.985128000
O	2.034807000	-2.494681000	-1.908574000
O	3.631001000	-1.525352000	2.025070000
O	3.574664000	-1.406375000	-0.703631000
O	3.652630000	1.273053000	2.111259000
O	3.606109000	1.384203000	-0.615469000
O	2.016848000	2.720261000	-1.431596000
O	2.098313000	2.441099000	3.247585000
O	1.065411000	1.377362000	0.755809000
O	1.409559000	-0.131816000	2.800142000
O	0.031831000	-1.530130000	4.587071000
O	-0.029095000	1.090317000	4.732450000
O	1.076834000	-1.543912000	0.695652000
O	-1.385385000	-2.139988000	0.683537000
O	-2.007866000	-2.349408000	-1.950843000
O	0.004901000	-3.918773000	-0.801816000
O	-3.617546000	-1.399689000	-0.721288000
O	-0.003858000	3.779982000	2.205367000
O	-0.007365000	4.003022000	-0.402150000
O	-1.389670000	2.011488000	0.795274000
O	-2.048604000	2.244776000	3.467061000
O	-2.055114000	2.501045000	-1.737118000
O	1.316467000	0.000211000	-1.443096000
O	-1.071019000	-0.018055000	-0.767531000
H	1.912778000	0.055216000	-2.199618000
O	0.170054000	2.018034000	-3.101028000
H	-0.634517000	2.058133000	-3.628838000
Hf	2.547801000	-0.039081000	0.705641000
Hf	-0.023175000	-1.863132000	2.521975000
Hf	0.031444000	1.706472000	2.520026000
Hf	-0.030553000	1.793648000	-1.063916000
Hf	-2.541364000	-0.053920000	0.703661000
Hf	0.024123000	-1.810674000	-1.007745000
N	-2.675186000	-4.580657000	-3.297633000
H	-1.954818000	-4.204487000	-2.690335000
H	-2.581415000	-5.545794000	-3.580737000
N	2.820432000	-4.508164000	-3.490080000
H	2.745702000	-5.073641000	-4.324309000
H	2.076621000	-3.844012000	-3.312184000
N	2.562844000	3.998705000	-3.713413000
H	1.837216000	3.353100000	-3.396807000
H	2.458394000	4.338217000	-4.659764000
N	-2.791296000	4.480538000	-3.350051000
H	-2.687450000	5.387174000	-3.782451000
H	-2.020525000	4.129164000	-2.793291000

Hf-NU-1000 (-NH₂) Ads

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086269000	2.727511000	3.427920000
H	4.061394000	-3.127496000	3.169062000
H	-4.034177000	2.574090000	3.654332000
H	-4.031683000	-2.953262000	3.421508000
C	5.658498000	-2.701317000	-1.954654000
C	-5.512152000	-2.578761000	-2.600661000
C	4.321993000	-3.034206000	-2.247315000
C	-4.196603000	-3.024089000	-2.411022000
C	4.056762000	-4.082447000	-3.178774000
C	-3.781694000	-4.263891000	-2.966289000
C	5.164814000	-4.733774000	-3.768407000
C	-4.716736000	-4.986035000	-3.727754000
C	6.465629000	-4.378688000	-3.460641000
C	-6.005570000	-4.511758000	-3.929206000
C	6.727882000	-3.352032000	-2.544577000
C	-6.418155000	-3.302492000	-3.362750000
C	5.595174000	2.960675000	-1.731649000
C	-5.635205000	2.400174000	-2.130279000
C	4.248918000	3.091700000	-2.114619000
C	-4.325689000	2.906804000	-2.226747000
C	3.920018000	3.878496000	-3.257018000
C	-4.077012000	4.038554000	-3.058890000
C	4.981452000	4.503208000	-3.949507000
C	-5.174227000	4.599009000	-3.752137000
C	6.295721000	4.369457000	-3.536889000
C	-6.447411000	4.070649000	-3.642241000
C	6.618751000	3.594852000	-2.415858000
C	-6.693295000	2.957495000	-2.827303000
H	5.822868000	-1.896324000	-1.236799000
H	-5.793991000	-1.630804000	-2.136388000
H	4.971938000	-5.539532000	-4.482320000
H	-4.411245000	-5.939224000	-4.167597000
H	7.753164000	-3.069076000	-2.301698000
H	-7.434192000	-2.934864000	-3.515061000
H	5.806010000	2.334684000	-0.862429000
H	-5.787476000	1.538185000	-1.478032000

H	4.743317000	5.105736000	-4.830500000
H	-4.994787000	5.467519000	-4.391633000
H	7.655174000	3.487138000	-2.092180000
H	-7.698375000	2.541812000	-2.739617000
H	-6.701215000	-5.100102000	-4.532337000
H	7.291022000	-4.909143000	-3.942515000
H	-7.265768000	4.533399000	-4.199978000
H	7.084572000	4.874404000	-4.100433000
H	-1.951379000	-2.908324000	0.583181000
H	-0.882907000	1.289462000	5.136985000
H	-0.017304000	-0.004961000	4.798464000
H	0.021057000	4.046210000	0.693306000
H	0.664467000	4.269686000	2.737250000
H	0.922932000	4.337018000	-0.579302000
H	1.961366000	-0.233862000	3.573031000
H	-1.943669000	2.803099000	0.869230000
H	-0.602109000	-2.075149000	5.057712000
H	0.900276000	-4.440939000	2.063581000
H	0.651053000	-4.388876000	-1.230867000
H	0.009961000	-4.130076000	0.782858000
O	-1.066647000	-0.108231000	2.185535000
O	-3.612130000	1.287591000	2.165220000
O	-3.599606000	1.342412000	-0.619152000
O	-3.610262000	-1.512570000	2.078192000
O	-2.045797000	-2.683977000	3.196648000
O	0.039502000	-4.085557000	1.801416000
O	2.072237000	-2.858351000	2.946738000
O	2.038831000	-2.515359000	-1.871594000
O	3.632822000	-1.525652000	2.026622000
O	3.595185000	-1.415132000	-0.698236000
O	3.644016000	1.267883000	2.117943000
O	3.598056000	1.434982000	-0.564445000
O	2.005049000	2.698090000	-1.499354000
O	2.099166000	2.424196000	3.281020000
O	1.068971000	1.414928000	0.803266000
O	1.405963000	-0.153528000	2.787745000
O	0.038633000	-1.575132000	4.540267000
O	-0.036431000	1.017568000	4.756603000
O	1.052546000	-1.536816000	0.646713000
O	-1.400909000	-2.118271000	0.633653000
O	-2.024126000	-2.333103000	-1.946227000
O	-0.080800000	-3.924364000	-0.806150000
O	-3.668202000	-1.386028000	-0.761315000
O	-0.012231000	3.772458000	2.264205000
O	0.046957000	4.009525000	-0.328959000
O	-1.386330000	2.016329000	0.833997000

O	-2.053319000	2.222886000	3.494182000
O	-2.049432000	2.564854000	-1.669508000
O	1.391152000	0.054871000	-1.327880000
O	-1.069722000	0.003629000	-0.768885000
H	1.922282000	0.081456000	-2.147622000
O	0.017207000	1.717935000	-3.114122000
H	-0.837308000	2.023864000	-3.456886000
Hf	2.530623000	-0.064226000	0.695317000
Hf	-0.016353000	-1.882265000	2.456084000
Hf	0.029985000	1.689710000	2.571423000
Hf	-0.014882000	1.791743000	-0.964174000
Hf	-2.534979000	-0.062369000	0.706945000
Hf	0.019244000	-1.803710000	-1.147801000
C	-1.710158000	-2.329427000	-5.182507000
C	-0.239137000	-2.608557000	-4.824303000
C	0.313657000	-1.211705000	-4.570082000
C	-1.716546000	-0.858197000	-5.621446000
C	1.812914000	-0.978983000	-4.713696000
C	-2.596816000	0.067009000	-4.795981000
H	2.351754000	-1.835708000	-4.285565000
H	0.270612000	-3.029485000	-5.717234000
H	-2.307643000	-2.445160000	-4.266257000
H	-1.389157000	1.451858000	-5.327079000
H	2.056104000	-0.933590000	-5.789927000
H	1.601158000	0.891373000	-4.138576000
H	-2.439316000	-0.134799000	-3.717109000
H	-3.658044000	-0.141301000	-5.007176000
H	-0.897794000	-3.887142000	-3.502204000
H	-0.089481000	0.155127000	-3.202907000
H	-1.787473000	-3.138237000	-6.939908000
H	-1.987054000	-0.767018000	-6.687079000
O	-2.261510000	-3.231004000	-6.104590000
O	2.247199000	0.168598000	-4.024123000
O	-2.332256000	1.412368000	-5.111589000
O	-0.117907000	-0.861854000	-3.273769000
O	-0.048607000	-3.436104000	-3.709901000
O	-0.347623000	-0.408495000	-5.519732000
N	-2.496160000	-4.784828000	-2.805229000
H	-1.985224000	-4.501328000	-1.966293000
H	-2.461553000	-5.789579000	-2.942406000
N	2.800725000	-4.506291000	-3.501740000
H	2.708677000	-5.148381000	-4.275503000
H	1.988453000	-3.951378000	-3.253124000
N	2.639790000	4.061983000	-3.705740000
H	1.905788000	3.468691000	-3.332542000
H	2.533702000	4.380621000	-4.658523000

N	-2.841932000	4.591046000	-3.219564000
H	-2.783029000	5.509108000	-3.634192000
H	-2.094052000	4.283321000	-2.610457000

Hf-NU-1000 (-NH₂) TS1

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086205000	2.728766000	3.426732000
H	4.060818000	-3.125031000	3.173419000
H	-4.033283000	2.576168000	3.653649000
H	-4.030874000	-2.953050000	3.423139000
C	5.658538000	-2.652766000	-2.005954000
C	-5.513566000	-2.595595000	-2.592502000
C	4.323597000	-3.018460000	-2.263465000
C	-4.199394000	-3.039249000	-2.390961000
C	4.060534000	-4.082686000	-3.177130000
C	-3.787320000	-4.293985000	-2.913824000
C	5.168970000	-4.715734000	-3.785467000
C	-4.723452000	-5.032181000	-3.658657000
C	6.468374000	-4.328059000	-3.512740000
C	-6.010604000	-4.559295000	-3.873778000
C	6.728509000	-3.285410000	-2.614518000
C	-6.420718000	-3.335422000	-3.337773000
C	5.606205000	2.962466000	-1.640044000
C	-5.635767000	2.401641000	-2.125095000
C	4.270223000	3.135084000	-2.044771000
C	-4.324720000	2.902769000	-2.231544000
C	3.981187000	4.010970000	-3.131181000
C	-4.075886000	4.025058000	-3.076149000
C	5.064616000	4.670424000	-3.752549000
C	-5.173793000	4.582942000	-3.770322000
C	6.367341000	4.487871000	-3.322480000
C	-6.448444000	4.060491000	-3.649703000
C	6.653037000	3.629713000	-2.253554000
C	-6.694678000	2.956119000	-2.823019000
H	5.821315000	-1.836396000	-1.300718000
H	-5.793779000	-1.635863000	-2.151971000
H	4.977743000	-5.533982000	-4.485502000
H	-4.420493000	-5.997362000	-4.073432000
H	7.752492000	-2.976425000	-2.399269000

H	-7.435585000	-2.968958000	-3.500376000
H	5.789358000	2.274811000	-0.812437000
H	-5.788615000	1.546584000	-1.463998000
H	4.853319000	5.340793000	-4.590251000
H	-4.993785000	5.444573000	-4.418905000
H	7.679859000	3.484213000	-1.914476000
H	-7.700775000	2.544791000	-2.727125000
H	-6.707049000	-5.160445000	-4.463218000
H	7.294042000	-4.845250000	-4.008387000
H	-7.267582000	4.520806000	-4.208290000
H	7.175538000	5.021104000	-3.829629000
H	-1.954083000	-2.908990000	0.583903000
H	-0.880209000	1.277301000	5.144788000
H	-0.016982000	-0.017913000	4.793824000
H	0.030153000	4.036257000	0.697665000
H	0.667533000	4.265449000	2.735801000
H	0.940543000	4.328955000	-0.569058000
H	1.959532000	-0.237865000	3.569609000
H	-1.940487000	2.804883000	0.867525000
H	-0.600032000	-2.079790000	5.047185000
H	0.894483000	-4.444423000	2.061401000
H	0.632597000	-4.394700000	-1.224698000
H	0.006425000	-4.126032000	0.776924000
O	-1.067996000	-0.107263000	2.185793000
O	-3.612914000	1.287259000	2.166371000
O	-3.599425000	1.348770000	-0.614294000
O	-3.613373000	-1.511983000	2.079593000
O	-2.045860000	-2.684109000	3.193277000
O	0.035062000	-4.086131000	1.799337000
O	2.072360000	-2.859416000	2.942243000
O	2.041312000	-2.530356000	-1.856658000
O	3.634555000	-1.526373000	2.025995000
O	3.598240000	-1.412755000	-0.700232000
O	3.642181000	1.269038000	2.116442000
O	3.585429000	1.436645000	-0.561863000
O	2.000450000	2.671597000	-1.552058000
O	2.098824000	2.422714000	3.283968000
O	1.069354000	1.419288000	0.803997000
O	1.405375000	-0.154818000	2.783713000
O	0.040804000	-1.577894000	4.531679000
O	-0.036283000	1.007199000	4.757866000
O	1.047714000	-1.535889000	0.640203000
O	-1.407789000	-2.115778000	0.628914000
O	-2.027701000	-2.332383000	-1.953342000
O	-0.090125000	-3.923415000	-0.792003000
O	-3.667028000	-1.377379000	-0.767891000

O	-0.010535000	3.770129000	2.262560000
O	0.064377000	3.997352000	-0.326363000
O	-1.385058000	2.016543000	0.837490000
O	-2.053047000	2.222149000	3.494979000
O	-2.045135000	2.560980000	-1.671716000
O	1.397733000	0.050905000	-1.316211000
O	-1.069923000	0.002125000	-0.759955000
H	1.915263000	0.062613000	-2.145223000
O	-0.042002000	1.541833000	-3.130508000
H	-0.900733000	1.821628000	-3.494775000
Hf	2.527052000	-0.076916000	0.694565000
Hf	-0.016377000	-1.885733000	2.443487000
Hf	0.028329000	1.686045000	2.578205000
Hf	-0.013607000	1.774138000	-0.946427000
Hf	-2.538092000	-0.067406000	0.710044000
Hf	0.014637000	-1.804216000	-1.181193000
C	-1.673983000	-2.396455000	-5.157667000
C	-0.212443000	-2.672864000	-4.765695000
C	0.351208000	-1.276408000	-4.516915000
C	-1.666953000	-0.926242000	-5.601527000
C	1.856516000	-1.085249000	-4.692305000
C	-2.542652000	0.000501000	-4.771399000
H	2.382542000	-1.946325000	-4.259059000
H	0.309052000	-3.119149000	-5.639714000
H	-2.297493000	-2.510232000	-4.259392000
H	-1.346163000	1.354566000	-5.411090000
H	2.092490000	-1.056533000	-5.770516000
H	1.760435000	0.812923000	-4.230108000
H	-2.395043000	-0.211844000	-3.694488000
H	-3.605386000	-0.189878000	-4.994673000
H	-0.896407000	-3.932485000	-3.435982000
H	-0.059115000	0.304211000	-3.214695000
H	-1.690917000	-3.222610000	-6.908693000
H	-1.948894000	-0.839583000	-6.665044000
O	-2.201251000	-3.300517000	-6.093514000
O	2.333293000	0.058298000	-4.018203000
O	-2.248784000	1.351520000	-5.060211000
O	-0.059477000	-0.875851000	-3.256565000
O	-0.045578000	-3.480648000	-3.630842000
O	-0.298319000	-0.489807000	-5.514420000
N	-2.504877000	-4.814797000	-2.735639000
H	-1.989862000	-4.511562000	-1.905895000
H	-2.471078000	-5.822309000	-2.849696000
N	2.807049000	-4.540217000	-3.464595000
H	2.713862000	-5.189151000	-4.232697000
H	1.989130000	-3.993801000	-3.214582000

N	2.711778000	4.252178000	-3.585869000
H	1.974506000	3.633493000	-3.268197000
H	2.624917000	4.641946000	-4.513844000
N	-2.839292000	4.570837000	-3.246403000
H	-2.777487000	5.485896000	-3.667067000
H	-2.091346000	4.260543000	-2.638670000

Hf-NU-1000 (-NH₂) Int1

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.085805000	2.732638000	3.422927000
H	4.059107000	-3.120953000	3.181539000
H	-4.032265000	2.581777000	3.649713000
H	-4.029988000	-2.950594000	3.427105000
C	5.658684000	-2.646266000	-2.017526000
C	-5.534961000	-2.591674000	-2.537957000
C	4.324491000	-3.027520000	-2.253194000
C	-4.212894000	-3.031667000	-2.380352000
C	4.059619000	-4.120187000	-3.132253000
C	-3.812037000	-4.280508000	-2.928736000
C	5.167473000	-4.766018000	-3.728011000
C	-4.771235000	-5.014404000	-3.651142000
C	6.466917000	-4.363211000	-3.477542000
C	-6.065402000	-4.544812000	-3.820618000
C	6.727897000	-3.291367000	-2.614834000
C	-6.462973000	-3.326584000	-3.261069000
C	5.609615000	2.937007000	-1.655870000
C	-5.627732000	2.375166000	-2.160249000
C	4.273863000	3.118656000	-2.058158000
C	-4.321143000	2.886774000	-2.255567000
C	3.991483000	3.985247000	-3.153516000
C	-4.072276000	4.001220000	-3.108363000
C	5.079487000	4.625790000	-3.786285000
C	-5.166702000	4.549375000	-3.813461000
C	6.381677000	4.434371000	-3.358487000
C	-6.440660000	4.019529000	-3.701206000
C	6.661412000	3.585771000	-2.280504000
C	-6.684635000	2.916979000	-2.873376000
H	5.821996000	-1.808210000	-1.338276000
H	-5.804278000	-1.637919000	-2.077908000

H	4.975471000	-5.606470000	-4.400950000
H	-4.477952000	-5.974197000	-4.084901000
H	7.751744000	-2.969940000	-2.417498000
H	-7.483870000	-2.962549000	-3.387840000
H	5.788787000	2.256805000	-0.821356000
H	-5.780629000	1.523169000	-1.495155000
H	4.872242000	5.288675000	-4.630929000
H	-4.987055000	5.410430000	-4.463391000
H	7.687665000	3.432815000	-1.943055000
H	-7.688119000	2.497675000	-2.784605000
H	-6.777993000	-5.143360000	-4.393357000
H	7.291731000	-4.891193000	-3.963247000
H	-7.258634000	4.472979000	-4.267071000
H	7.193876000	4.952778000	-3.874505000
H	-1.957177000	-2.899214000	0.573684000
H	-0.877022000	1.257743000	5.160786000
H	-0.018224000	-0.038149000	4.791765000
H	0.033820000	4.037800000	0.722033000
H	0.672683000	4.256055000	2.751280000
H	0.949929000	4.328696000	-0.542996000
H	1.957508000	-0.241842000	3.572762000
H	-1.936606000	2.812546000	0.878316000
H	-0.603391000	-2.091866000	5.031106000
H	0.904315000	-4.446568000	1.992455000
H	0.646914000	-4.371639000	-1.277716000
H	0.004765000	-4.112916000	0.722068000
O	-1.067045000	-0.107690000	2.183825000
O	-3.613880000	1.289060000	2.165693000
O	-3.606297000	1.357715000	-0.610537000
O	-3.615233000	-1.507347000	2.085189000
O	-2.045133000	-2.691234000	3.183013000
O	0.044047000	-4.081728000	1.742745000
O	2.071636000	-2.863381000	2.932106000
O	2.045705000	-2.542807000	-1.839175000
O	3.637233000	-1.526606000	2.026447000
O	3.600289000	-1.394376000	-0.714056000
O	3.641957000	1.268750000	2.117490000
O	3.581695000	1.447778000	-0.551038000
O	1.998509000	2.677740000	-1.553636000
O	2.098958000	2.419821000	3.288480000
O	1.066541000	1.421651000	0.809532000
O	1.405927000	-0.156057000	2.785364000
O	0.039489000	-1.587322000	4.520723000
O	-0.036980000	0.989647000	4.764556000
O	1.053777000	-1.522774000	0.637612000
O	-1.410022000	-2.107029000	0.625008000

O	-2.032024000	-2.342725000	-1.952639000
O	-0.091633000	-3.905685000	-0.866425000
O	-3.659964000	-1.364952000	-0.770881000
O	-0.009702000	3.766619000	2.277937000
O	0.070727000	4.002223000	-0.304124000
O	-1.384372000	2.021944000	0.850227000
O	-2.053937000	2.215419000	3.501282000
O	-2.044656000	2.571994000	-1.655676000
O	1.393113000	0.073809000	-1.328392000
O	-1.079566000	0.022614000	-0.764659000
H	1.894257000	0.055749000	-2.167775000
O	-0.040008000	1.545007000	-3.171158000
H	-0.868740000	1.748826000	-3.665700000
Hf	2.532738000	-0.081961000	0.691844000
Hf	-0.013292000	-1.889755000	2.428024000
Hf	0.026901000	1.679032000	2.591909000
Hf	-0.013493000	1.779879000	-0.919140000
Hf	-2.541876000	-0.069925000	0.711420000
Hf	0.013940000	-1.783124000	-1.202022000
C	-1.714122000	-2.322290000	-5.209075000
C	-0.250043000	-2.704258000	-4.964658000
C	0.362529000	-1.376340000	-4.506593000
C	-1.654508000	-0.807320000	-5.488265000
C	1.863933000	-1.214753000	-4.719163000
C	-2.538768000	-0.016158000	-4.532381000
H	2.383268000	-2.075317000	-4.277770000
H	0.206785000	-2.982230000	-5.938974000
H	-2.270486000	-2.499745000	-4.276061000
H	-2.582509000	1.703949000	-5.487441000
H	2.091804000	-1.201140000	-5.799408000
H	1.911831000	0.708801000	-4.434431000
H	-2.296854000	-0.289256000	-3.493945000
H	-3.597629000	-0.288423000	-4.703516000
H	-0.916164000	-4.030001000	-3.698221000
H	0.025459000	0.542360000	-3.260813000
H	-1.878741000	-3.015903000	-7.006804000
H	-1.966182000	-0.605309000	-6.530527000
O	-2.375156000	-3.088401000	-6.182668000
O	2.365607000	-0.063236000	-4.067835000
O	-2.345878000	1.384060000	-4.609269000
O	0.009437000	-1.100446000	-3.223322000
O	-0.047799000	-3.737500000	-4.042212000
O	-0.282197000	-0.433160000	-5.388912000
N	-2.529154000	-4.800328000	-2.797446000
H	-1.958985000	-4.469949000	-2.015571000
H	-2.490534000	-5.807396000	-2.908866000

N	2.805938000	-4.598291000	-3.392708000
H	2.714071000	-5.240189000	-4.167888000
H	1.995210000	-4.016927000	-3.207213000
N	2.723174000	4.234569000	-3.607046000
H	1.981310000	3.629824000	-3.274891000
H	2.635798000	4.612574000	-4.539741000
N	-2.828569000	4.542036000	-3.290584000
H	-2.789863000	5.491034000	-3.635431000
H	-2.106279000	4.252862000	-2.640228000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.088477000	2.690309000	3.465635000
H	4.064236000	-3.144179000	3.140635000
H	-4.032236000	2.549088000	3.680322000
H	-4.030385000	-2.984621000	3.387824000
C	5.617225000	-2.380562000	-2.315574000
C	-5.527603000	-2.258740000	-2.626045000
C	4.300837000	-2.863450000	-2.437279000
C	-4.238173000	-2.809799000	-2.553522000
C	4.020245000	-3.874071000	-3.406651000
C	-3.912172000	-3.937533000	-3.355520000
C	5.089294000	-4.328786000	-4.211926000
C	-4.910539000	-4.455181000	-4.200444000
C	6.371275000	-3.827282000	-4.069634000
C	-6.171207000	-3.882613000	-4.266563000
C	6.650874000	-2.842804000	-3.113723000
C	-6.492011000	-2.772534000	-3.478680000
C	5.622871000	2.916846000	-1.618814000
C	-5.650099000	2.620963000	-1.961389000
C	4.282482000	3.237474000	-1.902337000
C	-4.315846000	3.047141000	-2.090457000
C	4.001001000	4.381807000	-2.704165000
C	-4.033244000	4.244640000	-2.811125000
C	5.091984000	5.138754000	-3.183532000
C	-5.124063000	4.950387000	-3.366130000
C	6.399696000	4.793756000	-2.888587000
C	-6.424164000	4.497458000	-3.231892000
C	6.679632000	3.672928000	-2.098072000

C	-6.703153000	3.319819000	-2.526090000
H	5.795670000	-1.615035000	-1.557979000
H	-5.739087000	-1.398675000	-1.986886000
H	4.883708000	-5.101869000	-4.957472000
H	-4.669274000	-5.319655000	-4.824767000
H	7.661745000	-2.448803000	-2.997720000
H	-7.484118000	-2.321095000	-3.531055000
H	5.801315000	2.039029000	-0.995452000
H	-5.827027000	1.705652000	-1.393684000
H	4.883603000	6.018606000	-3.798535000
H	-4.919108000	5.870961000	-3.919383000
H	7.709476000	3.400555000	-1.861868000
H	-7.728859000	2.963334000	-2.419301000
H	-6.915882000	-4.308746000	-4.943294000
H	7.167495000	-4.209505000	-4.713538000
H	-7.237299000	5.071894000	-3.683267000
H	7.214589000	5.407502000	-3.280692000
H	-1.952737000	-2.921719000	0.616939000
H	-0.876324000	1.367591000	5.097029000
H	-0.013551000	0.065204000	4.790540000
H	0.006420000	4.004274000	0.582693000
H	0.655267000	4.296780000	2.628059000
H	0.914798000	4.286275000	-0.675628000
H	1.959917000	-0.178720000	3.573524000
H	-1.949695000	2.784320000	0.814666000
H	-0.606936000	-2.000014000	5.098413000
H	0.890956000	-4.441283000	2.132238000
H	0.747122000	-4.423103000	-1.076845000
H	-0.004788000	-4.146445000	0.852647000
O	-1.065401000	-0.093936000	2.178627000
O	-3.616716000	1.285717000	2.168343000
O	-3.611018000	1.325713000	-0.642590000
O	-3.613874000	-1.510498000	2.083234000
O	-2.048937000	-2.652438000	3.234508000
O	0.032382000	-4.081475000	1.869741000
O	2.075287000	-2.836737000	2.985856000
O	2.059550000	-2.653945000	-1.723245000
O	3.631742000	-1.528787000	2.020240000
O	3.614913000	-1.403609000	-0.714442000
O	3.640511000	1.279423000	2.101361000
O	3.581482000	1.388906000	-0.620625000
O	2.009342000	2.638159000	-1.607312000
O	2.097357000	2.452334000	3.247404000
O	1.063777000	1.408603000	0.742836000
O	1.406422000	-0.121585000	2.784909000
O	0.037972000	-1.517029000	4.570011000

O	-0.029786000	1.084958000	4.724569000
O	1.059685000	-1.546522000	0.697699000
O	-1.399939000	-2.134820000	0.688966000
O	-2.033615000	-2.465093000	-1.859301000
O	-0.043349000	-3.974232000	-0.755517000
O	-3.646823000	-1.396852000	-0.736675000
O	-0.016017000	3.781724000	2.166721000
O	0.039607000	3.949405000	-0.437650000
O	-1.396674000	1.994357000	0.780820000
O	-2.047562000	2.253195000	3.460438000
O	-2.043505000	2.479393000	-1.743738000
O	1.364523000	-0.029162000	-1.337104000
O	-1.103325000	-0.051023000	-0.794015000
H	1.838542000	-0.069485000	-2.188018000
O	0.076066000	1.785420000	-3.194818000
H	0.994029000	1.943197000	-3.451770000
Hf	2.521665000	-0.082404000	0.691003000
Hf	-0.019405000	-1.866425000	2.494693000
Hf	0.029493000	1.708169000	2.519366000
Hf	-0.036402000	1.700466000	-1.040683000
Hf	-2.547087000	-0.076636000	0.708706000
N	-2.654413000	-4.537182000	-3.366340000
H	-2.076670000	-4.347752000	-2.548415000
H	-2.684445000	-5.520520000	-3.614303000
N	2.784533000	-4.435989000	-3.571497000
H	2.616337000	-4.967416000	-4.414409000
H	1.989385000	-3.957645000	-3.163489000
N	2.727184000	4.805195000	-2.992166000
H	1.984812000	4.124484000	-2.886583000
H	2.632541000	5.466025000	-3.751208000
N	-2.771570000	4.730769000	-2.990802000
H	-2.676124000	5.686931000	-3.299119000
H	-2.012265000	4.317937000	-2.463218000
Hf	0.009465000	-1.864758000	-1.088801000
C	-1.866133000	-1.701196000	-5.238489000
C	-0.457856000	-2.273230000	-5.380932000
C	0.380452000	-1.411518000	-4.430953000
C	-1.715225000	-0.183601000	-5.310334000
C	1.829285000	-1.188709000	-4.801980000
C	-2.671823000	0.568205000	-4.410701000
H	2.311554000	-2.179656000	-4.717209000
H	-0.104432000	-2.125303000	-6.422306000
H	-2.214533000	-1.980198000	-4.228981000
H	-1.945064000	2.304853000	-3.964822000
H	1.903128000	-0.864349000	-5.853530000
H	3.384160000	-0.353617000	-3.964565000

H	-2.483192000	0.260364000	-3.359799000
H	-3.692363000	0.226545000	-4.658692000
H	-1.142898000	-3.871615000	-4.523385000
H	-0.232185000	0.818700000	-4.182573000
H	-2.527264000	-2.030291000	-7.024383000
H	-1.855810000	0.155905000	-6.353654000
O	-2.812933000	-2.225260000	-6.123183000
O	2.424964000	-0.250000000	-3.928891000
O	-2.599172000	1.949976000	-4.587647000
O	0.098469000	-1.565261000	-3.202354000
O	-0.358456000	-3.625843000	-5.058978000
O	-0.338828000	0.091533000	-4.969133000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.088573000	2.683601000	3.472061000
H	4.064926000	-3.148078000	3.133464000
H	-4.032371000	2.543522000	3.684902000
H	-4.030031000	-2.990760000	3.380673000
C	5.594718000	-2.309652000	-2.388418000
C	-5.525756000	-2.211081000	-2.624488000
C	4.289222000	-2.828918000	-2.473245000
C	-4.244263000	-2.783166000	-2.564100000
C	4.004987000	-3.832381000	-3.449290000
C	-3.939497000	-3.902642000	-3.384003000
C	5.057262000	-4.241581000	-4.299974000
C	-4.949567000	-4.397500000	-4.227909000
C	6.328214000	-3.704115000	-4.193235000
C	-6.202045000	-3.806478000	-4.280110000
C	6.612563000	-2.727912000	-3.230273000
C	-6.501231000	-2.699788000	-3.478831000
C	5.618773000	2.957399000	-1.574423000
C	-5.657161000	2.651068000	-1.902598000
C	4.278136000	3.255491000	-1.879492000
C	-4.320539000	3.057409000	-2.066696000
C	3.988557000	4.398246000	-2.681026000
C	-4.039574000	4.248791000	-2.799607000
C	5.073837000	5.177510000	-3.137427000

C	-5.135121000	4.969398000	-3.327308000
C	6.382301000	4.855200000	-2.820889000
C	-6.437316000	4.536210000	-3.156476000
C	6.669501000	3.735638000	-2.031030000
C	-6.714761000	3.364220000	-2.440179000
H	5.776950000	-1.550353000	-1.625322000
H	-5.721591000	-1.355348000	-1.974691000
H	4.848467000	-5.008347000	-5.051134000
H	-4.722495000	-5.256210000	-4.865287000
H	7.614867000	-2.305835000	-3.142769000
H	-7.486040000	-2.231708000	-3.521802000
H	5.802178000	2.079612000	-0.952356000
H	-5.832781000	1.739405000	-1.328758000
H	4.860245000	6.056200000	-3.752305000
H	-4.931491000	5.884990000	-3.889300000
H	7.700043000	3.481542000	-1.778027000
H	-7.742404000	3.023197000	-2.305034000
H	-6.956788000	-4.213694000	-4.957350000
H	7.111974000	-4.051304000	-4.871287000
H	-7.253768000	5.121447000	-3.587672000
H	7.192378000	5.486043000	-3.195510000
H	-1.952659000	-2.925408000	0.625202000
H	-0.873357000	1.394574000	5.084060000
H	-0.011347000	0.090638000	4.792892000
H	0.010946000	4.005620000	0.565023000
H	0.653818000	4.303272000	2.619188000
H	0.907389000	4.292092000	-0.701662000
H	1.962205000	-0.165931000	3.573455000
H	-1.949116000	2.781576000	0.802870000
H	-0.607427000	-1.981405000	5.116418000
H	0.891977000	-4.434331000	2.159651000
H	0.753655000	-4.427387000	-1.037872000
H	-0.011563000	-4.152138000	0.884917000
O	-1.064752000	-0.092364000	2.178331000
O	-3.616781000	1.285347000	2.168217000
O	-3.607466000	1.311660000	-0.652031000
O	-3.611834000	-1.511370000	2.082372000
O	-2.049450000	-2.645692000	3.244549000
O	0.030742000	-4.079545000	1.898518000
O	2.075883000	-2.831733000	2.995911000
O	2.060851000	-2.676111000	-1.698658000
O	3.629752000	-1.529760000	2.017926000
O	3.615468000	-1.405994000	-0.715492000
O	3.641689000	1.279601000	2.100176000
O	3.584608000	1.378222000	-0.631522000
O	2.012157000	2.630932000	-1.608915000

O	2.097684000	2.457436000	3.239107000
O	1.064936000	1.400802000	0.727974000
O	1.407279000	-0.115873000	2.785377000
O	0.037011000	-1.503126000	4.583147000
O	-0.026107000	1.107254000	4.716500000
O	1.060747000	-1.548283000	0.708230000
O	-1.396702000	-2.140883000	0.700166000
O	-2.029817000	-2.465154000	-1.862872000
O	-0.045367000	-3.980458000	-0.736149000
O	-3.641568000	-1.412012000	-0.723682000
O	-0.013341000	3.784910000	2.155758000
O	0.038982000	3.946025000	-0.452817000
O	-1.395992000	1.991376000	0.771361000
O	-2.046919000	2.258588000	3.454126000
O	-2.047614000	2.483757000	-1.740602000
O	1.353286000	-0.049323000	-1.364283000
O	-1.099791000	-0.063490000	-0.796585000
H	1.841563000	-0.097789000	-2.205648000
O	0.040019000	1.855499000	-3.181762000
H	0.952140000	1.930066000	-3.488959000
Hf	2.523624000	-0.074211000	0.689318000
Hf	-0.021976000	-1.858426000	2.513788000
Hf	0.031256000	1.714156000	2.502984000
Hf	-0.041137000	1.704976000	-1.073166000
Hf	-2.547072000	-0.071603000	0.705642000
N	-2.688509000	-4.517290000	-3.412837000
H	-2.099779000	-4.329453000	-2.602528000
H	-2.735854000	-5.503235000	-3.648206000
N	2.779867000	-4.421640000	-3.582128000
H	2.596234000	-4.977905000	-4.404954000
H	1.992665000	-3.994065000	-3.109072000
N	2.712350000	4.798234000	-2.990448000
H	1.979922000	4.103621000	-2.902760000
H	2.620033000	5.459979000	-3.749068000
N	-2.778964000	4.715833000	-3.009068000
H	-2.665170000	5.649146000	-3.373446000
H	-2.001253000	4.265549000	-2.542929000
Hf	0.009739000	-1.871814000	-1.049852000
C	-1.865704000	-1.689229000	-5.236880000
C	-0.472829000	-2.303248000	-5.428910000
C	0.461538000	-1.618831000	-4.448865000
C	-1.790785000	-0.167188000	-5.393593000
C	1.853495000	-1.258150000	-4.876360000
C	-2.709722000	0.546879000	-4.417848000
H	2.384898000	-2.227842000	-4.952216000
H	-0.120718000	-2.124813000	-6.464249000

H	-2.153648000	-1.934707000	-4.199283000
H	-1.935459000	2.271736000	-4.037941000
H	1.823991000	-0.822258000	-5.888436000
H	3.423024000	-0.534486000	-3.972921000
H	-2.434360000	0.232724000	-3.386611000
H	-3.741102000	0.191400000	-4.586937000
H	-1.267206000	-3.908387000	-4.662254000
H	-0.358714000	0.861258000	-4.446175000
H	-2.660443000	-2.062514000	-6.959076000
H	-2.091116000	0.095938000	-6.428132000
O	-2.841105000	-2.293156000	-6.039137000
O	2.467167000	-0.400363000	-3.946064000
O	-2.674267000	1.933085000	-4.569508000
O	0.154677000	-1.646142000	-3.253745000
O	-0.459229000	-3.681233000	-5.174737000
O	-0.440161000	0.238754000	-5.225857000
Hf-NU-1000 (-NH ₂) Int2_Ro			
C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087220000	2.713723000	3.442232000
H	4.060763000	-3.135989000	3.159250000
H	-4.032503000	2.565468000	3.665240000
H	-4.030845000	-2.959864000	3.415418000
C	5.646494000	-2.745035000	-2.008143000
C	-5.591205000	-2.559037000	-2.375729000
C	4.306382000	-2.894196000	-2.405086000
C	-4.262833000	-3.019317000	-2.325019000
C	4.012544000	-3.606621000	-3.604538000
C	-3.923658000	-4.280029000	-2.903218000
C	5.093920000	-4.147445000	-4.331588000
C	-4.964898000	-5.005172000	-3.529862000
C	6.403235000	-3.996428000	-3.905212000
C	-6.256581000	-4.513297000	-3.591219000
C	6.694113000	-3.288606000	-2.733917000
C	-6.587240000	-3.277416000	-3.016900000
C	5.594099000	2.996805000	-1.679379000
C	-5.666171000	2.613455000	-1.902641000
C	4.248443000	3.151754000	-2.053931000
C	-4.330034000	2.912971000	-2.220819000
C	3.916018000	4.033585000	-3.123885000

C	-4.056845000	3.812634000	-3.291267000
C	4.975511000	4.725212000	-3.753238000
C	-5.154963000	4.366488000	-3.984951000
C	6.290103000	4.563638000	-3.350919000
C	-6.459499000	4.053967000	-3.643836000
C	6.615785000	3.694056000	-2.302909000
C	-6.729603000	3.170312000	-2.592014000
H	5.833372000	-2.180839000	-1.092664000
H	-5.800897000	-1.596508000	-1.902458000
H	4.878815000	-4.694073000	-5.254111000
H	-4.727059000	-5.973584000	-3.978109000
H	7.725015000	-3.164984000	-2.398636000
H	-7.609054000	-2.897258000	-3.061734000
H	5.805425000	2.299488000	-0.866419000
H	-5.836392000	1.909386000	-1.086581000
H	4.735572000	5.403413000	-4.577098000
H	-4.954325000	5.055472000	-4.810312000
H	7.652243000	3.563911000	-1.987508000
H	-7.757650000	2.922421000	-2.322783000
H	-7.025629000	-5.104706000	-4.094617000
H	7.210578000	-4.436080000	-4.496404000
H	-7.280698000	4.506665000	-4.205768000
H	7.076737000	5.122171000	-3.864979000
H	-1.959410000	-2.906324000	0.570650000
H	-0.886663000	1.323759000	5.109261000
H	-0.018665000	0.028229000	4.794229000
H	0.024194000	4.035815000	0.649029000
H	0.671382000	4.278735000	2.702889000
H	0.888684000	4.341853000	-0.646679000
H	1.958102000	-0.214328000	3.575218000
H	-1.942503000	2.797423000	0.843256000
H	-0.600770000	-2.053486000	5.076310000
H	0.912500000	-4.426045000	2.015829000
H	0.695121000	-4.352101000	-1.219009000
H	-0.017257000	-4.124491000	0.769214000
O	-1.066219000	-0.105883000	2.176560000
O	-3.616167000	1.282936000	2.171045000
O	-3.606778000	1.382632000	-0.581264000
O	-3.608778000	-1.509908000	2.082262000
O	-2.044985000	-2.681835000	3.201530000
O	0.039465000	-4.082154000	1.779169000
O	2.071604000	-2.858795000	2.947986000
O	2.042805000	-2.585288000	-1.794787000
O	3.634250000	-1.518489000	2.039057000
O	3.608567000	-1.455000000	-0.668032000
O	3.644407000	1.273924000	2.110305000

O	3.601366000	1.406850000	-0.595520000
O	2.007246000	2.681297000	-1.504281000
O	2.098878000	2.431985000	3.269521000
O	1.067501000	1.407054000	0.777239000
O	1.404612000	-0.143588000	2.787676000
O	0.036929000	-1.557596000	4.551213000
O	-0.036837000	1.047007000	4.739777000
O	1.053258000	-1.542608000	0.673490000
O	-1.404206000	-2.120312000	0.635677000
O	-2.035864000	-2.334629000	-1.996595000
O	-0.092627000	-3.910650000	-0.880806000
O	-3.632422000	-1.374656000	-0.750836000
O	-0.005515000	3.778274000	2.233856000
O	0.030832000	3.989641000	-0.369758000
O	-1.383520000	2.011649000	0.807533000
O	-2.050078000	2.236630000	3.476441000
O	-2.051089000	2.513730000	-1.722680000
O	1.381372000	0.008797000	-1.328277000
O	-1.087496000	-0.002918000	-0.798516000
H	1.914423000	0.045052000	-2.148274000
O	0.136589000	1.905749000	-3.124730000
H	-0.667172000	1.889503000	-3.657296000
Hf	2.532040000	-0.061600000	0.696403000
Hf	-0.023944000	-1.875640000	2.472935000
Hf	0.033532000	1.700011000	2.541809000
Hf	-0.020412000	1.777348000	-1.021272000
Hf	-2.540018000	-0.053174000	0.701031000
N	-2.661603000	-4.792554000	-2.896033000
H	-1.924794000	-4.356229000	-2.344969000
H	-2.554929000	-5.770892000	-3.121689000
N	2.741275000	-3.726802000	-4.117356000
H	2.602644000	-4.437231000	-4.823775000
H	1.976529000	-3.594020000	-3.464822000
N	2.635075000	4.253721000	-3.556765000
H	1.908861000	3.600691000	-3.275768000
H	2.541571000	4.658032000	-4.478194000
N	-2.786871000	4.116838000	-3.709308000
H	-2.688064000	4.942106000	-4.284198000
H	-2.033636000	3.915377000	-3.060167000
Hf	0.018724000	-1.788274000	-1.101749000
C	-1.389485000	-0.724353000	-5.964342000
C	-0.214969000	-1.713023000	-5.699361000
C	0.575297000	-1.188930000	-4.515349000
C	-2.454663000	-0.758770000	-4.877612000
C	1.786383000	-0.359381000	-4.825380000
C	-3.495068000	0.345358000	-4.997114000

H	2.573977000	-1.113625000	-5.031594000
H	0.450068000	-1.666807000	-6.585921000
H	-1.880345000	-1.054920000	-6.901486000
H	-5.072287000	-0.606127000	-4.395047000
H	1.609958000	0.138614000	-5.800243000
H	1.450283000	1.145529000	-3.668630000
H	-3.867914000	0.406421000	-6.038385000
H	-3.046446000	1.320581000	-4.757158000
H	-1.534053000	-3.021198000	-5.183009000
H	-3.546262000	-2.232524000	-4.190883000
H	-0.491113000	0.724237000	-6.916205000
H	-1.990695000	-0.674570000	-3.875822000
O	-0.920018000	0.603319000	-6.062568000
O	2.213085000	0.509739000	-3.846474000
O	-4.535141000	0.130042000	-4.076843000
O	0.206057000	-1.463835000	-3.380508000
O	-0.616888000	-3.029377000	-5.521420000
O	-3.076804000	-2.031381000	-5.015872000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087523000	2.724834000	3.429417000
H	4.061388000	-3.139635000	3.151934000
H	-4.031759000	2.579271000	3.653121000
H	-4.033143000	-2.976987000	3.391980000
C	5.652264000	-2.588217000	-2.111458000
C	-5.394529000	-1.824621000	-2.811084000
C	4.310813000	-2.920563000	-2.373278000
C	-4.303031000	-2.670750000	-2.560886000
C	4.016214000	-3.841981000	-3.422277000
C	-4.194698000	-3.907974000	-3.251263000
C	5.100031000	-4.375351000	-4.155158000
C	-5.183381000	-4.210061000	-4.211313000
C	6.408960000	-4.029414000	-3.868693000
C	-6.230172000	-3.338832000	-4.468605000
C	6.700682000	-3.129026000	-2.836657000
C	-6.353119000	-2.136116000	-3.763347000
C	5.596779000	3.045303000	-1.484001000
C	-5.572751000	2.190495000	-2.359694000

C	4.280949000	3.191924000	-1.960148000
C	-4.262505000	2.686666000	-2.458109000
C	4.027160000	4.100602000	-3.026707000
C	-3.918247000	3.519691000	-3.558678000
C	5.120256000	4.817192000	-3.559388000
C	-4.916068000	3.804646000	-4.512250000
C	6.402072000	4.658179000	-3.061734000
C	-6.200077000	3.294125000	-4.393363000
C	6.653801000	3.768435000	-2.010561000
C	-6.542220000	2.477790000	-3.309747000
H	5.838975000	-1.875803000	-1.306217000
H	-5.439715000	-0.887903000	-2.249626000
H	4.883905000	-5.081189000	-4.961978000
H	-5.110458000	-5.154738000	-4.756741000
H	7.732339000	-2.854631000	-2.611073000
H	-7.175095000	-1.448348000	-3.972098000
H	5.756115000	2.332181000	-0.673237000
H	-5.800425000	1.556523000	-1.500702000
H	4.934457000	5.512736000	-4.382420000
H	-4.659308000	4.444883000	-5.361116000
H	7.663773000	3.641180000	-1.617817000
H	-7.554757000	2.083326000	-3.205033000
H	-6.965717000	-3.602435000	-5.232835000
H	7.217262000	-4.467412000	-4.460014000
H	-6.947300000	3.547134000	-5.150629000
H	7.220063000	5.234838000	-3.500991000
H	-1.942158000	-2.909375000	0.595807000
H	-0.883459000	1.299347000	5.151949000
H	-0.017514000	0.001502000	4.814990000
H	0.060563000	4.020911000	0.689128000
H	0.675628000	4.263963000	2.730536000
H	0.996601000	4.271849000	-0.569311000
H	1.966961000	-0.214656000	3.595320000
H	-1.914522000	2.797212000	0.851625000
H	-0.612100000	-2.051428000	5.080015000
H	0.877808000	-4.469497000	2.122072000
H	0.773599000	-4.386857000	-1.100390000
H	0.014850000	-4.139018000	0.821775000
O	-1.059479000	-0.105118000	2.199443000
O	-3.616308000	1.285145000	2.170471000
O	-3.628076000	1.396141000	-0.583870000
O	-3.610933000	-1.502998000	2.088682000
O	-2.049114000	-2.665592000	3.220922000
O	0.034502000	-4.084849000	1.847160000
O	2.074491000	-2.844186000	2.967860000
O	2.052869000	-2.611005000	-1.753634000

O	3.638479000	-1.526976000	2.026689000
O	3.609335000	-1.402173000	-0.705927000
O	3.642198000	1.270874000	2.114143000
O	3.574284000	1.428285000	-0.570011000
O	1.998496000	2.635052000	-1.605210000
O	2.100251000	2.427249000	3.282882000
O	1.080560000	1.406665000	0.796500000
O	1.412808000	-0.143757000	2.808333000
O	0.037539000	-1.559386000	4.565745000
O	-0.037713000	1.026830000	4.770521000
O	1.060387000	-1.519570000	0.684133000
O	-1.388148000	-2.123777000	0.677088000
O	-2.052676000	-2.538741000	-1.879822000
O	-0.004388000	-3.942786000	-0.743524000
O	-3.582258000	-1.376578000	-0.726882000
O	0.000613000	3.766158000	2.255486000
O	0.107769000	3.969684000	-0.333760000
O	-1.366646000	2.003112000	0.852081000
O	-2.052662000	2.223309000	3.493596000
O	-2.065170000	2.651140000	-1.575901000
O	1.350610000	0.015741000	-1.362289000
O	-1.100536000	-0.003384000	-0.772642000
H	1.823972000	0.014567000	-2.217152000
O	-0.220730000	1.690985000	-3.182012000
H	-0.654223000	2.494847000	-3.509129000
Hf	2.543642000	-0.092354000	0.695116000
Hf	-0.008443000	-1.885147000	2.481279000
Hf	0.037009000	1.682889000	2.586642000
Hf	-0.012121000	1.738831000	-0.928502000
Hf	-2.536621000	-0.071816000	0.732682000
N	-3.220999000	-4.826967000	-2.960881000
H	-2.394739000	-4.502751000	-2.469610000
H	-3.049991000	-5.540429000	-3.655795000
N	2.746968000	-4.247102000	-3.729643000
H	2.602483000	-4.713712000	-4.613484000
H	1.974686000	-3.727491000	-3.328814000
N	2.773957000	4.324100000	-3.540709000
H	2.066619000	3.637741000	-3.304221000
H	2.741344000	4.698889000	-4.479181000
N	-2.641082000	4.018070000	-3.756637000
H	-2.604986000	4.826969000	-4.366112000
H	-2.103742000	4.118797000	-2.899731000
Hf	0.006942000	-1.842739000	-1.113697000
C	-1.937385000	-0.028235000	-4.991687000
C	-0.687948000	-2.133975000	-5.304638000
C	0.234514000	-1.517638000	-4.484864000

C	-3.116063000	-0.600795000	-5.699697000
C	1.436172000	-0.770087000	-5.009015000
C	-4.284822000	0.365057000	-5.539737000
H	2.274149000	-1.483693000	-5.100536000
H	-0.631914000	-2.127924000	-6.394115000
H	-1.220408000	0.546648000	-5.612239000
H	-6.076635000	0.452956000	-6.267228000
H	1.236566000	-0.410388000	-6.037947000
H	1.156984000	0.872851000	-3.984628000
H	-3.974637000	1.378108000	-5.868905000
H	-4.559520000	0.427784000	-4.470417000
H	-1.628141000	-2.852023000	-3.822449000
H	-3.644069000	-0.913413000	-7.501603000
H	-1.092645000	0.897208000	-3.391693000
H	-3.399303000	-1.557758000	-5.211131000
O	-2.011169000	0.170525000	-3.748043000
O	1.893685000	0.253181000	-4.162497000
O	-5.322919000	-0.141051000	-6.342026000
O	0.077064000	-1.608132000	-3.207545000
O	-1.603719000	-2.983064000	-4.795686000
O	-2.797796000	-0.777586000	-7.054301000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087687000	2.731821000	3.420766000
H	4.060583000	-3.134535000	3.160363000
H	-4.031012000	2.588539000	3.644845000
H	-4.032762000	-2.970605000	3.400192000
C	5.658357000	-2.638439000	-2.050814000
C	-5.461656000	-1.971063000	-2.731745000
C	4.317527000	-2.953793000	-2.336663000
C	-4.307934000	-2.737547000	-2.523752000
C	4.030851000	-3.893232000	-3.372054000
C	-4.152910000	-3.981360000	-3.200396000
C	5.122258000	-4.459954000	-4.067847000
C	-5.167353000	-4.364369000	-4.106200000
C	6.430040000	-4.129619000	-3.759021000
C	-6.288801000	-3.575470000	-4.312289000
C	6.713570000	-3.212020000	-2.739849000

C	-6.454098000	-2.366652000	-3.621462000
C	5.599172000	3.028056000	-1.495527000
C	-5.533827000	2.202881000	-2.454980000
C	4.281875000	3.185711000	-1.965157000
C	-4.208022000	2.659611000	-2.517819000
C	4.030736000	4.098978000	-3.028504000
C	-3.784368000	3.407087000	-3.649933000
C	5.127104000	4.807450000	-3.565366000
C	-4.714720000	3.635724000	-4.679367000
C	6.409941000	4.636728000	-3.074687000
C	-6.018375000	3.166217000	-4.595527000
C	6.659370000	3.742999000	-2.026227000
C	-6.442692000	2.449341000	-3.473526000
H	5.838932000	-1.912459000	-1.256385000
H	-5.540929000	-1.030257000	-2.181310000
H	4.912435000	-5.179555000	-4.864054000
H	-5.061010000	-5.313126000	-4.638428000
H	7.744363000	-2.949897000	-2.496378000
H	-7.341225000	-1.748494000	-3.776885000
H	5.757017000	2.312692000	-0.686549000
H	-5.820569000	1.630871000	-1.570305000
H	4.942816000	5.506226000	-4.385957000
H	-4.395509000	4.202570000	-5.558749000
H	7.670150000	3.606486000	-1.638786000
H	-7.469017000	2.084766000	-3.402282000
H	-7.054073000	-3.913961000	-5.016867000
H	7.243921000	-4.593509000	-4.322285000
H	-6.712145000	3.365658000	-5.415771000
H	7.230532000	5.207213000	-3.517092000
H	-1.944181000	-2.900352000	0.583464000
H	-0.878412000	1.273636000	5.176562000
H	-0.018527000	-0.024888000	4.815176000
H	0.064816000	4.026415000	0.723133000
H	0.679178000	4.254085000	2.757972000
H	1.001394000	4.292625000	-0.533758000
H	1.963842000	-0.226202000	3.595164000
H	-1.912693000	2.804137000	0.862983000
H	-0.612312000	-2.069844000	5.062772000
H	0.874475000	-4.472579000	2.084837000
H	0.762775000	-4.372797000	-1.140659000
H	0.016167000	-4.126670000	0.782707000
O	-1.061483000	-0.106009000	2.195952000
O	-3.616435000	1.284821000	2.171182000
O	-3.653220000	1.415093000	-0.579001000
O	-3.612724000	-1.503058000	2.088311000
O	-2.048336000	-2.671921000	3.210761000

O	0.034236000	-4.080739000	1.811089000
O	2.073774000	-2.849055000	2.956570000
O	2.052619000	-2.587562000	-1.780071000
O	3.639792000	-1.526306000	2.027480000
O	3.606893000	-1.396905000	-0.708225000
O	3.640610000	1.270725000	2.114121000
O	3.570022000	1.435207000	-0.562799000
O	1.994654000	2.636454000	-1.608318000
O	2.101174000	2.420057000	3.293312000
O	1.078662000	1.414180000	0.811651000
O	1.410698000	-0.148862000	2.808029000
O	0.036820000	-1.572750000	4.552724000
O	-0.038591000	1.003487000	4.781151000
O	1.060421000	-1.512771000	0.673063000
O	-1.395473000	-2.111100000	0.664235000
O	-2.055391000	-2.525532000	-1.882933000
O	-0.008969000	-3.926700000	-0.772833000
O	-3.593308000	-1.359093000	-0.745514000
O	0.000618000	3.762400000	2.281411000
O	0.115490000	3.980249000	-0.301574000
O	-1.367049000	2.008459000	0.871144000
O	-2.054518000	2.213969000	3.503831000
O	-2.059411000	2.651184000	-1.544370000
O	1.346902000	0.042326000	-1.357968000
O	-1.108622000	0.020198000	-0.777418000
H	1.817386000	0.060857000	-2.217219000
O	-0.287871000	1.696970000	-3.233258000
H	-0.842844000	2.451129000	-3.524558000
Hf	2.543386000	-0.095668000	0.695742000
Hf	-0.008911000	-1.889489000	2.463283000
Hf	0.032477000	1.676322000	2.607118000
Hf	-0.005249000	1.751777000	-0.895571000
Hf	-2.541327000	-0.068131000	0.730065000
N	-3.113884000	-4.828778000	-2.947203000
H	-2.294922000	-4.459192000	-2.475167000
H	-2.938620000	-5.561041000	-3.620674000
N	2.762522000	-4.288125000	-3.700037000
H	2.635127000	-4.748909000	-4.590168000
H	1.990633000	-3.732906000	-3.348705000
N	2.777213000	4.335124000	-3.535223000
H	2.065358000	3.654845000	-3.295594000
H	2.741958000	4.714341000	-4.471790000
N	-2.478108000	3.877729000	-3.807140000
H	-2.414151000	4.621479000	-4.494853000
H	-2.042253000	4.128667000	-2.922968000
Hf	0.004551000	-1.821389000	-1.144163000

C	-2.212440000	-0.099438000	-5.023197000
C	-0.375199000	-2.333458000	-5.316294000
C	0.388255000	-1.593945000	-4.464512000
C	-3.257639000	-0.898552000	-5.719194000
C	1.673232000	-0.920780000	-4.860442000
C	-4.603315000	-0.164682000	-5.677374000
H	2.520100000	-1.602025000	-4.664897000
H	-0.206753000	-2.413156000	-6.390690000
H	-1.474604000	0.421394000	-5.682862000
H	-5.818105000	-1.648948000	-5.825394000
H	1.681707000	-0.725584000	-5.949677000
H	1.190884000	0.827058000	-4.107479000
H	-4.508148000	0.808540000	-6.185023000
H	-4.896854000	0.029473000	-4.629764000
H	-1.478271000	-2.897685000	-3.894701000
H	-3.684182000	-1.395915000	-7.501567000
H	-0.960220000	0.945118000	-3.349493000
H	-3.373647000	-1.845998000	-5.146819000
O	-2.227979000	0.071445000	-3.809904000
O	1.968786000	0.244643000	-4.112586000
O	-5.560084000	-0.903551000	-6.389762000
O	0.043384000	-1.563554000	-3.194130000
O	-1.384256000	-3.110097000	-4.846289000
O	-2.873267000	-1.130280000	-7.044594000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.084488000	2.698647000	3.462716000
H	4.063847000	-3.144169000	3.141373000
H	-4.033346000	2.538505000	3.687713000
H	-4.031641000	-2.989019000	3.379900000
C	5.631513000	-2.370034000	-2.285569000
C	-5.624315000	-2.244645000	-2.323157000
C	4.306975000	-2.810255000	-2.468071000
C	-4.305356000	-2.679620000	-2.548779000
C	4.027581000	-3.749693000	-3.505464000
C	-4.034251000	-3.526603000	-3.664104000
C	5.108133000	-4.209616000	-4.291191000
C	-5.123090000	-3.907602000	-4.482552000

C	6.400627000	-3.761672000	-4.078427000
C	-6.406834000	-3.458340000	-4.235549000
C	6.676313000	-2.827516000	-3.072664000
C	-6.673370000	-2.610153000	-3.150234000
C	5.573024000	3.114798000	-1.573386000
C	-5.682036000	2.687837000	-1.700603000
C	4.247591000	3.165233000	-2.038336000
C	-4.358678000	3.079035000	-1.980811000
C	3.935222000	3.947150000	-3.189540000
C	-4.132820000	4.280692000	-2.715361000
C	4.994616000	4.652814000	-3.804710000
C	-5.266447000	4.989911000	-3.181837000
C	6.286833000	4.598722000	-3.311924000
C	-6.553289000	4.564559000	-2.909261000
C	6.592523000	3.826666000	-2.183903000
C	-6.777759000	3.406543000	-2.150404000
H	5.809348000	-1.650000000	-1.484666000
H	-5.790312000	-1.591330000	-1.463998000
H	4.902852000	-4.933180000	-5.085059000
H	-4.926178000	-4.558518000	-5.338508000
H	7.693992000	-2.471629000	-2.905621000
H	-7.685429000	-2.248498000	-2.961351000
H	5.770035000	2.489622000	-0.699861000
H	-5.813567000	1.782360000	-1.102949000
H	4.772204000	5.254351000	-4.690522000
H	-5.103167000	5.904279000	-3.758562000
H	7.611912000	3.783045000	-1.797166000
H	-7.793910000	3.081007000	-1.919709000
H	-7.217460000	-3.768474000	-4.900045000
H	7.207527000	-4.144361000	-4.708489000
H	-7.398834000	5.145377000	-3.286115000
H	7.073019000	5.165567000	-3.817408000
H	-1.945791000	-2.928853000	0.623316000
H	-0.871930000	1.380337000	5.092901000
H	-0.013458000	0.074301000	4.792183000
H	0.012609000	4.008456000	0.560140000
H	0.649660000	4.297512000	2.617908000
H	0.888314000	4.272883000	-0.735433000
H	1.963875000	-0.174759000	3.580850000
H	-1.933346000	2.781498000	0.794241000
H	-0.616325000	-1.991912000	5.102176000
H	0.891709000	-4.449392000	2.177199000
H	0.727906000	-4.454079000	-1.030999000
H	-0.008329000	-4.162366000	0.896574000
O	-1.059478000	-0.096511000	2.182185000
O	-3.612019000	1.295608000	2.157292000

O	-3.585221000	1.278058000	-0.683951000
O	-3.608021000	-1.500940000	2.092269000
O	-2.048728000	-2.655175000	3.234862000
O	0.035507000	-4.085911000	1.912984000
O	2.076190000	-2.828704000	2.996708000
O	2.088878000	-2.744817000	-1.635083000
O	3.633099000	-1.538213000	2.007518000
O	3.602776000	-1.365223000	-0.748078000
O	3.647586000	1.265230000	2.119880000
O	3.599952000	1.423221000	-0.576861000
O	2.001522000	2.632632000	-1.561926000
O	2.095626000	2.456648000	3.234467000
O	1.062337000	1.387008000	0.738604000
O	1.412324000	-0.122156000	2.790596000
O	0.034071000	-1.512722000	4.576889000
O	-0.026265000	1.092981000	4.721728000
O	1.066627000	-1.536166000	0.697863000
O	-1.379503000	-2.150611000	0.691254000
O	-2.031366000	-2.426387000	-1.942483000
O	-0.045424000	-3.985497000	-0.698661000
O	-3.594841000	-1.472664000	-0.655865000
O	-0.014576000	3.775971000	2.153759000
O	0.024025000	3.937819000	-0.456330000
O	-1.387952000	1.985649000	0.761061000
O	-2.046796000	2.253525000	3.458979000
O	-2.059598000	2.507931000	-1.756069000
O	1.343808000	-0.040791000	-1.416110000
O	-1.073923000	-0.070758000	-0.796092000
H	1.946943000	-0.033169000	-2.185094000
O	-0.015499000	1.866880000	-3.228210000
H	-0.861407000	2.246059000	-3.519123000
Hf	2.534408000	-0.071712000	0.693468000
Hf	-0.012802000	-1.866475000	2.504947000
Hf	0.032796000	1.707821000	2.514193000
Hf	-0.026322000	1.705257000	-1.050884000
Hf	-2.526278000	-0.087225000	0.705809000
N	-2.784117000	-3.957204000	-3.982861000
H	-2.025460000	-3.790155000	-3.331944000
H	-2.685204000	-4.667057000	-4.692428000
N	2.763364000	-4.174899000	-3.797711000
H	2.650376000	-4.969674000	-4.409193000
H	2.016429000	-3.925660000	-3.158308000
N	2.676977000	4.050185000	-3.715737000
H	1.961370000	3.395423000	-3.412135000
H	2.611495000	4.384140000	-4.667054000
N	-2.894326000	4.794038000	-2.931717000

H	-2.795684000	5.510778000	-3.635636000
H	-2.101232000	4.189365000	-2.756266000
Hf	0.029172000	-1.897550000	-1.067735000
C	-0.499917000	-0.251115000	-4.719918000
C	0.516978000	-1.097609000	-4.249593000
C	1.922994000	-0.930360000	-4.766525000
H	2.302103000	-1.931933000	-5.028791000
H	-0.428297000	0.155032000	-5.737653000
H	1.913690000	-0.314576000	-5.682531000
H	3.619935000	-0.710880000	-3.785818000
H	-1.781705000	-1.235339000	-3.676518000
H	-0.062679000	0.765396000	-4.010627000
O	2.735129000	-0.321971000	-3.773886000
O	0.269889000	-1.880749000	-3.281006000
O	-1.787449000	-0.498381000	-4.316436000
C	-3.286951000	1.283355000	-5.348403000
C	-4.476035000	0.658893000	-4.675109000
C	-5.725264000	1.512588000	-4.902183000
H	-2.998412000	0.776328000	-6.308200000
H	-6.797738000	1.082115000	-3.366576000
H	-5.927958000	1.569725000	-5.983669000
H	-5.560176000	2.541436000	-4.535228000
H	-5.523244000	-0.931836000	-4.858532000
H	-4.260403000	0.644534000	-3.582334000
O	-2.715765000	2.271610000	-4.947944000
O	-6.844394000	0.898200000	-4.314374000
O	-4.665348000	-0.626487000	-5.190564000

Hf-NU-1000 (-NH₂) Prod

C	-3.248231000	-2.182834000	-1.650024000
C	-3.229707000	-2.386619000	2.899993000
C	-3.232311000	2.034297000	3.104036000
C	3.276909000	2.141996000	2.939211000
C	3.226880000	2.366317000	-1.338676000
C	3.259265000	-2.277860000	-1.561520000
C	-3.265214000	2.236112000	-1.457405000
C	3.257208000	-2.506609000	2.716385000
H	4.084977000	2.707011000	3.452864000
H	4.061663000	-3.139099000	3.153079000
H	-4.032056000	2.552901000	3.677108000
H	-4.030565000	-2.970116000	3.403901000
C	5.660021000	-2.602798000	-2.068588000
C	-5.580621000	-2.527041000	-2.394996000
C	4.321983000	-2.885787000	-2.395637000
C	-4.249076000	-2.971750000	-2.385279000
C	4.048008000	-3.726847000	-3.511184000

C	-3.889066000	-4.144851000	-3.106411000
C	5.139321000	-4.249026000	-4.234628000
C	-4.901790000	-4.791004000	-3.847268000
C	6.447241000	-3.958182000	-3.881683000
C	-6.198441000	-4.306037000	-3.876447000
C	6.720385000	-3.126607000	-2.790489000
C	-6.555706000	-3.165858000	-3.144513000
C	5.589733000	3.023448000	-1.655059000
C	-5.649410000	2.887549000	-1.600987000
C	4.250778000	3.134559000	-2.068477000
C	-4.336773000	3.034070000	-2.089433000
C	3.929129000	3.950427000	-3.193465000
C	-4.092997000	3.929080000	-3.173738000
C	4.992716000	4.625111000	-3.834895000
C	-5.203738000	4.601935000	-3.733339000
C	6.299103000	4.510185000	-3.392803000
C	-6.484700000	4.421659000	-3.240329000
C	6.613915000	3.705545000	-2.290711000
C	-6.721920000	3.562876000	-2.158250000
H	5.835288000	-1.947691000	-1.213623000
H	-5.816404000	-1.638953000	-1.804843000
H	4.934552000	-4.894280000	-5.093737000
H	-4.641418000	-5.687984000	-4.415628000
H	7.749144000	-2.892998000	-2.512098000
H	-7.580599000	-2.791013000	-3.160299000
H	5.793608000	2.374724000	-0.800874000
H	-5.795538000	2.209959000	-0.756897000
H	4.762173000	5.251108000	-4.701495000
H	-5.031357000	5.276409000	-4.576666000
H	7.644288000	3.613058000	-1.943580000
H	-7.729495000	3.430170000	-1.761258000
H	-6.948936000	-4.829145000	-4.474557000
H	7.265740000	-4.385125000	-4.466723000
H	-7.314516000	4.961073000	-3.704059000
H	7.088635000	5.053589000	-3.918448000
H	-1.962246000	-2.908560000	0.587055000
H	-0.879688000	1.353666000	5.096366000
H	-0.015692000	0.055653000	4.790451000
H	0.013171000	4.022485000	0.601424000
H	0.665839000	4.289197000	2.656209000
H	0.853051000	4.341295000	-0.708750000
H	1.957950000	-0.196405000	3.574084000
H	-1.941427000	2.799169000	0.830376000
H	-0.597475000	-2.029072000	5.092391000
H	0.907466000	-4.423540000	2.046860000
H	0.724936000	-4.364704000	-1.145653000

H	-0.023938000	-4.128439000	0.800393000
O	-1.067004000	-0.099790000	2.177573000
O	-3.617970000	1.288602000	2.165096000
O	-3.615018000	1.352883000	-0.614798000
O	-3.609588000	-1.509618000	2.082394000
O	-2.045937000	-2.670294000	3.214318000
O	0.034776000	-4.080019000	1.809897000
O	2.072099000	-2.851171000	2.962084000
O	2.047483000	-2.610220000	-1.784739000
O	3.633130000	-1.523043000	2.031947000
O	3.601590000	-1.439520000	-0.680735000
O	3.646587000	1.268258000	2.117431000
O	3.598536000	1.419035000	-0.578519000
O	2.006084000	2.668519000	-1.525354000
O	2.096416000	2.444952000	3.249175000
O	1.061837000	1.397910000	0.757299000
O	1.405075000	-0.133851000	2.785381000
O	0.039045000	-1.538058000	4.561279000
O	-0.031800000	1.072722000	4.725941000
O	1.055779000	-1.549717000	0.685612000
O	-1.405280000	-2.124095000	0.656384000
O	-2.025062000	-2.352067000	-1.959211000
O	-0.083654000	-3.932012000	-0.849537000
O	-3.636390000	-1.375441000	-0.748097000
O	-0.010547000	3.782493000	2.193141000
O	0.009374000	3.967395000	-0.416324000
O	-1.392552000	2.006954000	0.779791000
O	-2.048730000	2.246916000	3.463398000
O	-2.058668000	2.464551000	-1.778971000
O	1.383774000	-0.016374000	-1.336282000
O	-1.086548000	-0.018111000	-0.793951000
H	1.897601000	-0.015415000	-2.168822000
O	0.144330000	1.821265000	-3.151270000
H	-0.622429000	1.599396000	-3.700725000
Hf	2.531109000	-0.062079000	0.696275000
Hf	-0.022773000	-1.867963000	2.487202000
Hf	0.032757000	1.707894000	2.519321000
Hf	-0.015416000	1.755435000	-1.058709000
Hf	-2.537584000	-0.061592000	0.701411000
N	-2.615830000	-4.662908000	-3.121288000
H	-1.964595000	-4.383133000	-2.390575000
H	-2.542553000	-5.626144000	-3.421314000
N	2.766788000	-4.006823000	-3.945320000
H	2.675434000	-4.842748000	-4.508584000
H	2.043029000	-3.865043000	-3.247492000
N	2.657442000	4.121875000	-3.671217000

H	1.935246000	3.473471000	-3.370808000
H	2.583049000	4.454635000	-4.622295000
N	-2.857018000	4.104882000	-3.720504000
H	-2.731122000	4.863312000	-4.374430000
H	-2.053740000	3.769210000	-3.200540000
Hf	0.012180000	-1.804529000	-1.081803000
C	-0.036875000	-2.369684000	-5.550723000
C	0.565517000	-1.465246000	-4.512420000
C	1.687093000	-0.555705000	-4.920557000
H	2.508418000	-1.228542000	-5.239031000
H	0.687837000	-3.210371000	-5.645576000
H	1.357743000	-0.040625000	-5.846285000
H	1.402399000	0.970712000	-3.754919000
H	-1.433453000	-2.957160000	-4.307781000
H	-0.042774000	-1.870917000	-6.533033000
O	2.145066000	0.314528000	-3.952820000
O	0.157939000	-1.565851000	-3.357661000
O	-1.325417000	-2.785638000	-5.262628000
C	-2.256717000	-0.282937000	-5.695435000
C	-3.416144000	-0.470621000	-4.766084000
C	-4.254314000	0.814812000	-4.729590000
H	-2.377332000	-0.773299000	-6.694883000
H	-5.347843000	0.968038000	-3.136390000
H	-4.528023000	1.093079000	-5.763053000
H	-3.652294000	1.641729000	-4.317284000
H	-5.034254000	-1.498769000	-4.751564000
H	-2.989432000	-0.635992000	-3.748987000
O	-1.282292000	0.394791000	-5.433465000
O	-5.440679000	0.586241000	-4.017011000
O	-4.183648000	-1.543727000	-5.215847000

4.2 -F

Hf-NU-1000 (-F)

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.088842000	2.677629000	3.477165000
H	4.064409000	-3.151431000	3.128934000
H	-4.030895000	2.539887000	3.690744000
H	-4.029640000	-2.992335000	3.378983000

C	5.648405000	-2.553618000	-2.222722000
C	-5.653063000	-2.651120000	-2.101289000
C	4.331078000	-3.037395000	-2.259535000
C	-4.306440000	-2.867836000	-2.438077000
C	4.100235000	-4.231980000	-2.959108000
C	-4.041234000	-3.732043000	-3.513307000
C	5.126903000	-4.907856000	-3.610108000
C	-5.067818000	-4.351763000	-4.220442000
C	6.418517000	-4.391493000	-3.573072000
C	-6.390851000	-4.116240000	-3.861926000
C	6.683178000	-3.211313000	-2.875700000
C	-6.687324000	-3.262307000	-2.797805000
C	5.610804000	2.793864000	-1.966021000
C	-5.640924000	3.001622000	-1.552680000
C	4.296094000	3.268712000	-1.850270000
C	-4.359307000	2.995038000	-2.124409000
C	4.054520000	4.597448000	-2.227242000
C	-4.176222000	3.718125000	-3.312813000
C	5.064814000	5.416482000	-2.718199000
C	-5.216074000	4.430737000	-3.901385000
C	6.354643000	4.908582000	-2.844654000
C	-6.470885000	4.435009000	-3.299709000
C	6.631417000	3.594076000	-2.465521000
C	-6.686975000	3.717804000	-2.121656000
H	5.829035000	-1.634464000	-1.662472000
H	-5.856268000	-1.978594000	-1.266383000
H	4.892317000	-5.835635000	-4.133800000
H	-4.804022000	-5.013019000	-5.047074000
H	7.696760000	-2.808322000	-2.840151000
H	-7.724342000	-3.074383000	-2.514174000
H	5.801616000	1.766233000	-1.651513000
H	-5.784217000	2.426400000	-0.635949000
H	4.821008000	6.444652000	-2.989226000
H	-5.020641000	4.968746000	-4.830111000
H	7.643934000	3.196907000	-2.556641000
H	-7.671560000	3.716053000	-1.650654000
H	-7.194002000	-4.603727000	-4.419222000
H	7.223440000	-4.920155000	-4.088399000
H	-7.285474000	4.998901000	-3.759744000
H	7.148377000	5.549090000	-3.235339000
H	-1.916823000	-2.957047000	0.619171000
H	-0.871856000	1.409405000	5.063038000
H	-0.010529000	0.105693000	4.789049000
H	0.056210000	4.022334000	0.537226000
H	0.662584000	4.303129000	2.636873000
H	0.849152000	4.346427000	-0.806159000

H	1.965207000	-0.170467000	3.574339000
H	-1.918691000	2.805901000	0.826747000
H	-0.607487000	-1.982774000	5.125128000
H	0.898336000	-4.443158000	2.200887000
H	0.653352000	-4.445359000	-1.201029000
H	0.050910000	-4.156666000	0.890060000
O	-1.061044000	-0.099841000	2.186020000
O	-3.621500000	1.288613000	2.166768000
O	-3.620575000	1.353382000	-0.614013000
O	-3.608866000	-1.506666000	2.087595000
O	-2.048371000	-2.649393000	3.242136000
O	0.052484000	-4.078688000	1.905728000
O	2.076520000	-2.825214000	3.004504000
O	2.049414000	-2.531324000	-1.859471000
O	3.629363000	-1.532049000	2.013864000
O	3.621005000	-1.416288000	-0.713304000
O	3.646484000	1.290410000	2.087781000
O	3.607118000	1.337752000	-0.690683000
O	2.032132000	2.663065000	-1.567332000
O	2.099586000	2.449438000	3.241862000
O	1.082660000	1.383171000	0.716242000
O	1.414401000	-0.121164000	2.783245000
O	0.036718000	-1.508109000	4.588327000
O	-0.022008000	1.117823000	4.704549000
O	1.076160000	-1.547193000	0.699652000
O	-1.383413000	-2.156131000	0.698195000
O	-2.030042000	-2.351606000	-1.966791000
O	0.011941000	-3.927313000	-0.700528000
O	-3.627291000	-1.447288000	-0.686378000
O	0.008790000	3.782974000	2.157182000
O	0.031106000	3.950447000	-0.472141000
O	-1.385516000	2.003309000	0.769618000
O	-2.046519000	2.258785000	3.448067000
O	-2.077678000	2.508817000	-1.756496000
O	1.320680000	-0.049831000	-1.433039000
O	-1.084055000	-0.052535000	-0.749211000
H	1.852903000	0.029081000	-2.234887000
O	0.030983000	1.625120000	-3.141057000
H	-0.698604000	1.959952000	-3.672455000
Hf	2.539575000	-0.053515000	0.686324000
Hf	-0.017402000	-1.861195000	2.526836000
Hf	0.043389000	1.714778000	2.481536000
Hf	-0.048585000	1.743706000	-1.123997000
Hf	-2.537671000	-0.063029000	0.715654000
Hf	0.016474000	-1.852826000	-1.006965000
F	-2.999575000	3.718258000	-3.939333000

F	2.838279000	5.138332000	-2.088491000
F	-2.795450000	-3.992333000	-3.898615000
F	2.884718000	-4.781035000	-2.996553000

Hf-NU-1000 (-F) Ads

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.089776000	2.705154000	3.447964000
H	4.063114000	-3.136729000	3.153907000
H	-4.033242000	2.563451000	3.666255000
H	-4.033858000	-2.966086000	3.403903000
C	5.686875000	-2.665334000	-1.991127000
C	-5.538831000	-2.052297000	-2.633413000
C	4.352644000	-2.996816000	-2.279877000
C	-4.326471000	-2.748001000	-2.511245000
C	4.136237000	-3.997963000	-3.240247000
C	-4.173081000	-3.917444000	-3.266906000
C	5.190413000	-4.639122000	-3.883639000
C	-5.161295000	-4.375399000	-4.128339000
C	6.499937000	-4.284858000	-3.575729000
C	-6.345744000	-3.652999000	-4.244112000
C	6.750884000	-3.293544000	-2.625433000
C	-6.538246000	-2.490875000	-3.494185000
C	5.547144000	2.672798000	-2.215334000
C	-5.678067000	2.691598000	-1.903186000
C	4.283008000	3.219032000	-1.952487000
C	-4.334027000	2.893567000	-2.255999000
C	4.074693000	4.562014000	-2.291473000
C	-4.072559000	3.692558000	-3.381370000
C	5.068652000	5.333832000	-2.881236000
C	-5.102129000	4.264688000	-4.122508000
C	6.306731000	4.757472000	-3.152684000
C	-6.423157000	4.053287000	-3.742136000
C	6.548937000	3.423939000	-2.819235000
C	-6.715515000	3.264931000	-2.627126000
H	5.856304000	-1.890916000	-1.241349000
H	-5.659133000	-1.143036000	-2.039908000
H	4.960277000	-5.411487000	-4.618984000
H	-4.979361000	-5.287049000	-4.698430000
H	7.776626000	-3.013604000	-2.379211000

H	-7.467935000	-1.926335000	-3.584462000
H	5.711857000	1.630046000	-1.936829000
H	-5.876722000	2.065452000	-1.031258000
H	4.855389000	6.378162000	-3.113631000
H	-4.842945000	4.868372000	-4.993267000
H	7.520743000	2.972928000	-3.027640000
H	-7.751442000	3.098498000	-2.326148000
H	-7.124039000	-4.004088000	-4.925198000
H	7.327024000	-4.788546000	-4.081072000
H	-7.228976000	4.506750000	-4.323819000
H	7.087955000	5.359396000	-3.622103000
H	-1.911492000	-2.940338000	0.585160000
H	-0.883210000	1.316742000	5.109056000
H	-0.014235000	0.020950000	4.788435000
H	0.063845000	4.030030000	0.637523000
H	0.669056000	4.279081000	2.712564000
H	0.887270000	4.357718000	-0.690799000
H	1.968987000	-0.212488000	3.567645000
H	-1.923772000	2.801535000	0.840555000
H	-0.609518000	-2.042478000	5.065636000
H	0.880717000	-4.466497000	2.178604000
H	0.633246000	-4.434141000	-1.229391000
H	0.059173000	-4.155114000	0.846213000
O	-1.057244000	-0.105223000	2.186941000
O	-3.614171000	1.286277000	2.167069000
O	-3.630480000	1.378351000	-0.595558000
O	-3.607603000	-1.511519000	2.077088000
O	-2.048246000	-2.667763000	3.217108000
O	0.042941000	-4.092547000	1.873750000
O	2.075351000	-2.843231000	2.973230000
O	2.062377000	-2.538739000	-1.861665000
O	3.633575000	-1.530261000	2.018800000
O	3.620191000	-1.429551000	-0.696202000
O	3.639781000	1.288595000	2.092056000
O	3.616901000	1.381129000	-0.646365000
O	2.022854000	2.671361000	-1.554684000
O	2.100756000	2.427498000	3.279255000
O	1.079874000	1.415293000	0.772238000
O	1.413587000	-0.141795000	2.781508000
O	0.041577000	-1.554502000	4.549458000
O	-0.032834000	1.042747000	4.738862000
O	1.064211000	-1.538975000	0.660048000
O	-1.380766000	-2.137323000	0.655281000
O	-2.056880000	-2.482723000	-1.921731000
O	0.020160000	-3.926429000	-0.683875000
O	-3.611459000	-1.392015000	-0.731493000

O	0.002658000	3.774210000	2.233466000
O	0.059077000	3.966046000	-0.377453000
O	-1.377853000	2.006246000	0.809674000
O	-2.050333000	2.236119000	3.478005000
O	-2.062828000	2.531972000	-1.701063000
O	1.383020000	0.015256000	-1.336319000
O	-1.081600000	-0.030265000	-0.776468000
H	1.898680000	0.034204000	-2.167512000
O	-0.031041000	1.586242000	-3.140888000
H	-0.809616000	2.043070000	-3.491115000
Hf	2.525080000	-0.071430000	0.686429000
Hf	-0.007322000	-1.885584000	2.469368000
Hf	0.040224000	1.698165000	2.546518000
Hf	-0.018468000	1.758818000	-1.007881000
Hf	-2.518811000	-0.066916000	0.719909000
Hf	0.023843000	-1.859062000	-1.131680000
F	-2.827289000	3.924650000	-3.789735000
F	2.908120000	5.160972000	-2.014997000
F	-3.049535000	-4.645225000	-3.166242000
F	2.900873000	-4.376270000	-3.574051000
C	-1.677763000	-2.576917000	-5.143963000
C	-0.230648000	-2.800734000	-4.675270000
C	0.291145000	-1.372232000	-4.518263000
C	-1.696529000	-1.142410000	-5.685026000
C	1.790894000	-1.133910000	-4.658164000
C	-2.665046000	-0.218031000	-4.964837000
H	2.325499000	-1.978898000	-4.207145000
H	0.343120000	-3.309609000	-5.475601000
H	-2.317035000	-2.619860000	-4.252240000
H	-1.522598000	1.249423000	-5.401901000
H	2.034940000	-1.114520000	-5.734749000
H	1.596902000	0.763675000	-4.147024000
H	-2.546157000	-0.350633000	-3.868299000
H	-3.699962000	-0.509737000	-5.208471000
H	-0.985882000	-3.782260000	-3.166058000
H	-0.175798000	0.074634000	-3.229336000
H	-1.646991000	-3.554008000	-6.814374000
H	-1.908242000	-1.127825000	-6.767546000
O	-2.181735000	-3.555493000	-6.011356000
O	2.226702000	0.032001000	-3.999222000
O	-2.479961000	1.116536000	-5.349969000
O	-0.172637000	-0.953013000	-3.254375000
O	-0.102272000	-3.517709000	-3.474163000
O	-0.357386000	-0.638291000	-5.529083000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.089348000	2.710000000	3.443404000
H	4.062620000	-3.132223000	3.161078000
H	-4.032753000	2.567154000	3.663421000
H	-4.033290000	-2.962452000	3.409008000
C	5.682544000	-2.609191000	-2.060462000
C	-5.570398000	-2.150090000	-2.570656000
C	4.351073000	-2.999002000	-2.279888000
C	-4.325871000	-2.792062000	-2.481685000
C	4.133726000	-4.056884000	-3.176787000
C	-4.148063000	-3.962128000	-3.231210000
C	5.184593000	-4.696677000	-3.826978000
C	-5.145132000	-4.473177000	-4.051644000
C	6.491342000	-4.281706000	-3.591499000
C	-6.362987000	-3.803933000	-4.133783000
C	6.743033000	-3.233308000	-2.704789000
C	-6.578931000	-2.641247000	-3.391249000
C	5.543098000	2.679168000	-2.222340000
C	-5.677318000	2.648012000	-1.940167000
C	4.279041000	3.222786000	-1.953957000
C	-4.331728000	2.893675000	-2.258661000
C	4.067256000	4.566321000	-2.287868000
C	-4.067852000	3.732835000	-3.354347000
C	5.057726000	5.341785000	-2.878532000
C	-5.097564000	4.300306000	-4.099635000
C	6.295706000	4.767997000	-3.156187000
C	-6.420066000	4.042856000	-3.754806000
C	6.541345000	3.433820000	-2.827783000
C	-6.714452000	3.214473000	-2.669698000
H	5.852697000	-1.791600000	-1.358225000
H	-5.710635000	-1.241748000	-1.980385000
H	4.954210000	-5.516104000	-4.509397000
H	-4.944959000	-5.384535000	-4.616066000
H	7.766883000	-2.906132000	-2.515317000
H	-7.534876000	-2.118430000	-3.454701000
H	5.710435000	1.635842000	-1.947234000
H	-5.877130000	1.991881000	-1.090900000
H	4.842304000	6.386636000	-3.106522000
H	-4.836434000	4.938034000	-4.945218000

H	7.513168000	2.985167000	-3.041045000
H	-7.751561000	3.011922000	-2.396260000
H	-7.148812000	-4.197306000	-4.782303000
H	7.315987000	-4.783393000	-4.102809000
H	-7.225423000	4.492349000	-4.340229000
H	7.074362000	5.372591000	-3.626405000
H	-1.912971000	-2.937765000	0.577708000
H	-0.882981000	1.299677000	5.117353000
H	-0.015313000	0.003789000	4.784934000
H	0.069367000	4.028454000	0.651864000
H	0.672559000	4.272075000	2.722015000
H	0.893610000	4.360828000	-0.676893000
H	1.966717000	-0.220585000	3.565936000
H	-1.921198000	2.806156000	0.845499000
H	-0.607834000	-2.053854000	5.052290000
H	0.879436000	-4.468959000	2.156205000
H	0.620207000	-4.427075000	-1.244785000
H	0.057573000	-4.147579000	0.823285000
O	-1.058478000	-0.105863000	2.186112000
O	-3.614146000	1.286377000	2.167357000
O	-3.631219000	1.381978000	-0.593310000
O	-3.609597000	-1.510402000	2.078657000
O	-2.047725000	-2.672302000	3.209287000
O	0.042133000	-4.092122000	1.853933000
O	2.075049000	-2.846815000	2.965113000
O	2.063375000	-2.539416000	-1.858513000
O	3.634964000	-1.530798000	2.018327000
O	3.623509000	-1.424860000	-0.700857000
O	3.639122000	1.287551000	2.093559000
O	3.618583000	1.392928000	-0.635145000
O	2.019440000	2.660368000	-1.570734000
O	2.100619000	2.423893000	3.283870000
O	1.079518000	1.418093000	0.778356000
O	1.413115000	-0.145663000	2.778901000
O	0.042651000	-1.562379000	4.538687000
O	-0.034129000	1.027849000	4.742315000
O	1.061890000	-1.536595000	0.650885000
O	-1.385856000	-2.132200000	0.644942000
O	-2.056101000	-2.458184000	-1.936713000
O	0.012144000	-3.916646000	-0.695942000
O	-3.616266000	-1.387649000	-0.736062000
O	0.003872000	3.771079000	2.241907000
O	0.067226000	3.964878000	-0.364505000
O	-1.377377000	2.009348000	0.815776000
O	-2.050593000	2.232499000	3.481742000
O	-2.059241000	2.524948000	-1.703057000

O	1.394571000	0.024084000	-1.325639000
O	-1.077586000	-0.022747000	-0.769085000
H	1.903671000	0.027333000	-2.160480000
O	-0.062967000	1.480559000	-3.144587000
H	-0.887780000	1.849895000	-3.500392000
Hf	2.524867000	-0.078409000	0.687196000
Hf	-0.007180000	-1.889874000	2.454536000
Hf	0.038346000	1.693211000	2.556253000
Hf	-0.014546000	1.757026000	-0.986733000
Hf	-2.520987000	-0.069266000	0.720316000
Hf	0.020423000	-1.849557000	-1.162345000
F	-2.822614000	4.012854000	-3.726447000
F	2.900179000	5.161661000	-2.004485000
F	-2.993219000	-4.643967000	-3.160484000
F	2.900739000	-4.495700000	-3.436490000
C	-1.671693000	-2.522291000	-5.132705000
C	-0.232453000	-2.797900000	-4.667862000
C	0.338181000	-1.390677000	-4.488837000
C	-1.634064000	-1.084432000	-5.668065000
C	1.847089000	-1.220825000	-4.642201000
C	-2.553045000	-0.119869000	-4.933510000
H	2.348357000	-2.078449000	-4.178387000
H	0.318350000	-3.315567000	-5.479800000
H	-2.318025000	-2.550773000	-4.245651000
H	-1.311279000	1.240465000	-5.447088000
H	2.095588000	-1.222557000	-5.717636000
H	1.779556000	0.698095000	-4.238713000
H	-2.457949000	-0.287915000	-3.840701000
H	-3.602336000	-0.330649000	-5.198690000
H	-0.996075000	-3.824353000	-3.190645000
H	-0.114585000	0.207390000	-3.233061000
H	-1.649250000	-3.503112000	-6.801279000
H	-1.858910000	-1.059871000	-6.748021000
O	-2.203377000	-3.477285000	-6.011931000
O	2.331160000	-0.063550000	-3.994597000
O	-2.264152000	1.212842000	-5.274409000
O	-0.103099000	-0.939915000	-3.249052000
O	-0.114928000	-3.529339000	-3.474469000
O	-0.275795000	-0.639491000	-5.527246000

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C	-3.248200000	-2.182800000	-1.650100000
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C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000

C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.089620000	2.707805000	3.445496000
H	4.062580000	-3.129056000	3.165224000
H	-4.031644000	2.568593000	3.663476000
H	-4.032672000	-2.966193000	3.405606000
C	5.603622000	-2.365838000	-2.421656000
C	-5.558489000	-2.041176000	-2.585905000
C	4.335212000	-2.961064000	-2.338353000
C	-4.348562000	-2.745469000	-2.485162000
C	4.145152000	-4.173358000	-3.018478000
C	-4.226369000	-3.928048000	-3.226150000
C	5.162989000	-4.763155000	-3.762195000
C	-5.244383000	-4.390929000	-4.050359000
C	6.403551000	-4.137616000	-3.842687000
C	-6.425054000	-3.660864000	-4.145230000
C	6.627515000	-2.934722000	-3.170022000
C	-6.585589000	-2.483911000	-3.410733000
C	5.576146000	2.738004000	-2.104967000
C	-5.674864000	2.691321000	-1.907361000
C	4.273249000	3.234172000	-1.950371000
C	-4.329433000	2.917773000	-2.241233000
C	4.025980000	4.543918000	-2.384334000
C	-4.066354000	3.767907000	-3.328762000
C	5.018163000	5.323524000	-2.968101000
C	-5.096642000	4.361238000	-4.053251000
C	6.294875000	4.793728000	-3.132096000
C	-6.418596000	4.119795000	-3.695156000
C	6.577823000	3.497661000	-2.697584000
C	-6.712052000	3.283099000	-2.616235000
H	5.755063000	-1.434544000	-1.871784000
H	-5.656968000	-1.124011000	-2.001232000
H	4.961962000	-5.710972000	-4.263675000
H	-5.085745000	-5.313391000	-4.609773000
H	7.602695000	-2.447326000	-3.224213000
H	-7.512564000	-1.912311000	-3.483599000
H	5.772918000	1.727447000	-1.741456000
H	-5.874605000	2.030581000	-1.061835000
H	4.771576000	6.339451000	-3.279852000
H	-4.836058000	5.007288000	-4.892704000
H	7.581190000	3.084669000	-2.816021000
H	-7.748541000	3.094051000	-2.331154000
H	-7.225599000	-4.016396000	-4.797682000
H	7.201423000	-4.598816000	-4.429018000
H	-7.224092000	4.589340000	-4.264399000

H	7.074185000	5.403197000	-3.594824000
H	-1.914641000	-2.930082000	0.578480000
H	-0.880675000	1.295719000	5.126568000
H	-0.016832000	-0.002935000	4.785367000
H	0.068305000	4.026218000	0.656781000
H	0.678106000	4.267124000	2.718820000
H	0.879324000	4.362746000	-0.682267000
H	1.964692000	-0.217556000	3.573793000
H	-1.915815000	2.811445000	0.846940000
H	-0.611391000	-2.052538000	5.047322000
H	0.885805000	-4.473827000	2.107329000
H	0.610283000	-4.421145000	-1.277975000
H	0.048817000	-4.137961000	0.787240000
O	-1.056314000	-0.103231000	2.186198000
O	-3.614954000	1.286683000	2.168116000
O	-3.633906000	1.387517000	-0.590349000
O	-3.611328000	-1.505186000	2.085028000
O	-2.047331000	-2.673095000	3.207139000
O	0.049644000	-4.085189000	1.817870000
O	2.075379000	-2.844444000	2.966415000
O	2.067916000	-2.594666000	-1.788585000
O	3.637139000	-1.535758000	2.010744000
O	3.639171000	-1.393891000	-0.734557000
O	3.638799000	1.290273000	2.090504000
O	3.624522000	1.394856000	-0.637843000
O	2.015282000	2.655270000	-1.565675000
O	2.100766000	2.424216000	3.284104000
O	1.077487000	1.412208000	0.776357000
O	1.416366000	-0.142610000	2.783081000
O	0.040954000	-1.560825000	4.536234000
O	-0.034532000	1.023328000	4.746014000
O	1.071276000	-1.526350000	0.658141000
O	-1.387696000	-2.125013000	0.652177000
O	-2.062856000	-2.487695000	-1.931522000
O	-0.009185000	-3.909450000	-0.741881000
O	-3.598453000	-1.378985000	-0.732844000
O	0.008282000	3.767523000	2.238744000
O	0.059568000	3.960424000	-0.361201000
O	-1.376296000	2.011537000	0.819220000
O	-2.049945000	2.231850000	3.481887000
O	-2.054579000	2.506488000	-1.714405000
O	1.393344000	0.027476000	-1.343448000
O	-1.080780000	-0.014749000	-0.767770000
H	1.876924000	-0.028302000	-2.189680000
O	-0.072794000	1.434757000	-3.179532000
H	-0.896141000	1.686761000	-3.647717000

Hf	2.533412000	-0.086160000	0.683982000
Hf	-0.004337000	-1.890339000	2.449747000
Hf	0.037619000	1.688488000	2.563820000
Hf	-0.014589000	1.748886000	-0.965934000
Hf	-2.525747000	-0.072917000	0.723711000
Hf	0.018067000	-1.838126000	-1.166975000
F	-2.822134000	4.036032000	-3.711533000
F	2.823445000	5.105717000	-2.212733000
F	-3.111999000	-4.663223000	-3.142239000
F	2.979557000	-4.817022000	-2.952691000
C	-1.742607000	-2.561504000	-5.159094000
C	-0.326967000	-3.001044000	-4.773258000
C	0.367953000	-1.664510000	-4.459404000
C	-1.559715000	-1.117170000	-5.642885000
C	1.877810000	-1.696700000	-4.640032000
C	-2.398754000	-0.102981000	-4.883633000
H	2.246018000	-2.637872000	-4.197060000
H	0.161085000	-3.444627000	-5.664875000
H	-2.350297000	-2.554548000	-4.244211000
H	-1.095885000	1.137016000	-5.561188000
H	2.110652000	-1.700314000	-5.718083000
H	3.379664000	-0.520861000	-4.235572000
H	-2.309855000	-0.301165000	-3.796757000
H	-3.463428000	-0.211370000	-5.150506000
H	-1.028672000	-3.842730000	-3.171051000
H	0.019447000	0.444903000	-3.327203000
H	-1.863187000	-3.539783000	-6.823313000
H	-1.779413000	-1.042272000	-6.723255000
O	-2.420625000	-3.411322000	-6.046793000
O	2.447877000	-0.568176000	-3.996277000
O	-1.981883000	1.219896000	-5.174862000
O	0.010442000	-1.222032000	-3.222410000
O	-0.239541000	-3.925456000	-3.732799000
O	-0.174565000	-0.797114000	-5.478594000

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C	-3.248200000	-2.182800000	-1.650100000
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C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.090227000	2.686104000	3.467642000
H	4.064996000	-3.144464000	3.139203000

H	-4.031287000	2.550432000	3.680636000
H	-4.031110000	-2.986380000	3.384255000
C	5.598993000	-2.263269000	-2.447975000
C	-5.605327000	-2.058030000	-2.464207000
C	4.332995000	-2.870691000	-2.417964000
C	-4.340089000	-2.662786000	-2.547913000
C	4.141674000	-3.998179000	-3.232226000
C	-4.169852000	-3.657098000	-3.521767000
C	5.154720000	-4.493725000	-4.048202000
C	-5.195839000	-4.031314000	-4.381526000
C	6.393019000	-3.859324000	-4.067029000
C	-6.433401000	-3.405471000	-4.280006000
C	6.618576000	-2.739422000	-3.264167000
C	-6.641579000	-2.415921000	-3.316875000
C	5.610037000	2.784537000	-1.974106000
C	-5.675707000	2.628571000	-1.956906000
C	4.291468000	3.256372000	-1.889618000
C	-4.336358000	3.005459000	-2.143379000
C	4.046671000	4.564471000	-2.330523000
C	-4.082668000	4.090209000	-2.998441000
C	5.056004000	5.365767000	-2.852450000
C	-5.113828000	4.763048000	-3.645944000
C	6.349306000	4.859892000	-2.946201000
C	-6.430285000	4.359339000	-3.448160000
C	6.629963000	3.565745000	-2.504293000
C	-6.715805000	3.288981000	-2.598574000
H	5.751322000	-1.398426000	-1.798456000
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H	4.950484000	-5.377102000	-4.655036000
H	-4.996745000	-4.804203000	-5.124675000
H	7.591525000	-2.244668000	-3.270348000
H	-7.612198000	-1.923478000	-3.234497000
H	5.804262000	1.775886000	-1.603806000
H	-5.869831000	1.791371000	-1.284580000
H	4.809064000	6.379241000	-3.171830000
H	-4.859659000	5.597854000	-4.300442000
H	7.645863000	3.171600000	-2.566965000
H	-7.748015000	2.972597000	-2.437853000
H	-7.239417000	-3.693468000	-4.958613000
H	7.186818000	-4.247696000	-4.708915000
H	-7.237550000	4.888080000	-3.960219000
H	7.142762000	5.486370000	-3.359455000
H	-1.933533000	-2.934763000	0.606877000
H	-0.877096000	1.367608000	5.086412000
H	-0.013340000	0.065505000	4.783982000
H	0.055958000	4.002925000	0.572664000

H	0.664228000	4.293164000	2.649240000
H	0.851436000	4.332333000	-0.771235000
H	1.964440000	-0.176748000	3.569411000
H	-1.928041000	2.794064000	0.803980000
H	-0.612733000	-1.997739000	5.092089000
H	0.889460000	-4.456402000	2.173900000
H	0.689569000	-4.447679000	-1.163067000
H	0.036961000	-4.155189000	0.863103000
O	-1.057761000	-0.097347000	2.176094000
O	-3.617722000	1.284693000	2.169649000
O	-3.634310000	1.351320000	-0.621796000
O	-3.610804000	-1.504351000	2.088743000
O	-2.048675000	-2.655016000	3.232500000
O	0.044541000	-4.085254000	1.885805000
O	2.077202000	-2.830799000	2.995818000
O	2.077427000	-2.646899000	-1.754745000
O	3.631866000	-1.533903000	2.011756000
O	3.631997000	-1.402925000	-0.724034000
O	3.640035000	1.288303000	2.090546000
O	3.612496000	1.380803000	-0.648621000
O	2.027370000	2.643999000	-1.609146000
O	2.099480000	2.447040000	3.254708000
O	1.072935000	1.411042000	0.734876000
O	1.411361000	-0.121801000	2.780379000
O	0.037684000	-1.518621000	4.566853000
O	-0.028520000	1.084953000	4.718483000
O	1.068991000	-1.545362000	0.694608000
O	-1.386850000	-2.143369000	0.684597000
O	-2.062588000	-2.494570000	-1.916535000
O	0.002404000	-3.951124000	-0.703304000
O	-3.606346000	-1.425119000	-0.692886000
O	-0.000013000	3.780299000	2.175866000
O	0.040495000	3.922045000	-0.440094000
O	-1.389915000	1.993243000	0.777868000
O	-2.046929000	2.252366000	3.458615000
O	-2.062081000	2.474076000	-1.747869000
O	1.370874000	-0.030715000	-1.339793000
O	-1.104942000	-0.052797000	-0.802377000
H	1.843853000	-0.063746000	-2.191338000
O	0.079427000	1.778652000	-3.195272000
H	0.908853000	2.192771000	-3.467011000
Hf	2.519519000	-0.079256000	0.687970000
Hf	-0.013700000	-1.873862000	2.493287000
Hf	0.034999000	1.709635000	2.512915000
Hf	-0.035330000	1.706741000	-1.058108000
Hf	-2.535298000	-0.074476000	0.714744000

Hf	0.012198000	-1.876115000	-1.085993000
F	-2.844888000	4.529684000	-3.204658000
F	2.824842000	5.102509000	-2.229935000
F	-3.002740000	-4.297416000	-3.650159000
F	2.977319000	-4.647744000	-3.242320000
C	-1.819610000	-1.677409000	-5.264561000
C	-0.433288000	-2.313433000	-5.361144000
C	0.426084000	-1.477782000	-4.415539000
C	-1.612607000	-0.163669000	-5.350560000
C	1.889292000	-1.332788000	-4.747183000
C	-2.547287000	0.608382000	-4.441163000
H	2.316063000	-2.341712000	-4.587012000
H	-0.052032000	-2.232782000	-6.396026000
H	-2.199809000	-1.925765000	-4.259105000
H	-1.756064000	2.311314000	-4.005802000
H	2.010091000	-1.074548000	-5.812516000
H	3.450394000	-0.456100000	-3.974714000
H	-2.358919000	0.284798000	-3.393965000
H	-3.573666000	0.283219000	-4.689416000
H	-0.878313000	-3.763517000	-4.175751000
H	-0.117512000	0.778540000	-4.244222000
H	-2.442706000	-2.044359000	-7.058001000
H	-1.753791000	0.173686000	-6.393855000
O	-2.771171000	-2.173532000	-6.159910000
O	2.491803000	-0.371060000	-3.908718000
O	-2.460942000	1.989944000	-4.596111000
O	0.086067000	-1.566949000	-3.199274000
O	-0.392159000	-3.661662000	-5.009404000
O	-0.223799000	0.075101000	-5.025270000

Hf-NU-1000 (-F) Int2

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.090373000	2.682130000	3.471271000
H	4.065425000	-3.146096000	3.135884000
H	-4.031499000	2.547303000	3.683063000
H	-4.030809000	-2.989169000	3.381198000
C	5.602610000	-2.272612000	-2.437487000
C	-5.595786000	-2.060939000	-2.489351000
C	4.329790000	-2.866378000	-2.424805000

C	-4.329547000	-2.665304000	-2.557925000
C	4.130762000	-3.975908000	-3.261691000
C	-4.148043000	-3.658317000	-3.529961000
C	5.142601000	-4.467359000	-4.081746000
C	-5.161581000	-4.033645000	-4.402557000
C	6.388348000	-3.847426000	-4.081400000
C	-6.400288000	-3.407654000	-4.316593000
C	6.621577000	-2.745318000	-3.256414000
C	-6.620717000	-2.418693000	-3.355650000
C	5.613378000	2.787474000	-1.961418000
C	-5.678314000	2.630728000	-1.944064000
C	4.294839000	3.259500000	-1.877783000
C	-4.339882000	3.009074000	-2.133146000
C	4.052421000	4.571448000	-2.308570000
C	-4.089445000	4.100192000	-2.981096000
C	5.064229000	5.376274000	-2.820266000
C	-5.123405000	4.777440000	-3.619533000
C	6.357518000	4.870333000	-2.913542000
C	-6.439052000	4.372167000	-3.419593000
C	6.635771000	3.572392000	-2.481326000
C	-6.721153000	3.295670000	-2.576697000
H	5.760498000	-1.420733000	-1.772496000
H	-5.740286000	-1.289578000	-1.730929000
H	4.931580000	-5.336442000	-4.706682000
H	-4.952465000	-4.805360000	-5.144083000
H	7.599984000	-2.261522000	-3.247799000
H	-7.592170000	-1.926005000	-3.285907000
H	5.805501000	1.775496000	-1.599177000
H	-5.869892000	1.788585000	-1.277227000
H	4.819034000	6.392462000	-3.132264000
H	-4.871830000	5.616600000	-4.269449000
H	7.651670000	3.178142000	-2.543580000
H	-7.752715000	2.978032000	-2.414108000
H	-7.197466000	-3.695051000	-5.005743000
H	7.181407000	-4.232824000	-4.725961000
H	-7.248365000	4.904487000	-3.924718000
H	7.152842000	5.499670000	-3.318791000
H	-1.932427000	-2.937769000	0.609825000
H	-0.874961000	1.383695000	5.077649000
H	-0.011908000	0.080585000	4.784596000
H	0.057717000	4.004857000	0.563666000
H	0.662884000	4.296327000	2.645159000
H	0.843094000	4.337898000	-0.785532000
H	1.965456000	-0.169397000	3.567815000
H	-1.929505000	2.791495000	0.798719000
H	-0.612886000	-1.987520000	5.102201000

H	0.890862000	-4.450949000	2.189301000
H	0.678101000	-4.452447000	-1.153649000
H	0.034167000	-4.158120000	0.880698000
O	-1.058205000	-0.097112000	2.174475000
O	-3.617787000	1.284556000	2.169323000
O	-3.632602000	1.340610000	-0.629553000
O	-3.609794000	-1.505083000	2.088119000
O	-2.048775000	-2.651804000	3.237384000
O	0.044126000	-4.083526000	1.901470000
O	2.077471000	-2.827761000	3.001501000
O	2.076490000	-2.654465000	-1.744261000
O	3.630309000	-1.535043000	2.009371000
O	3.631591000	-1.402113000	-0.726312000
O	3.640594000	1.288069000	2.089961000
O	3.610651000	1.373217000	-0.655335000
O	2.030196000	2.646203000	-1.608291000
O	2.099588000	2.450092000	3.249581000
O	1.073644000	1.406899000	0.724949000
O	1.411267000	-0.118944000	2.779263000
O	0.036752000	-1.510883000	4.573743000
O	-0.026098000	1.097992000	4.712539000
O	1.068189000	-1.545944000	0.698746000
O	-1.386188000	-2.146161000	0.689678000
O	-2.056685000	-2.478059000	-1.918916000
O	-0.004241000	-3.952302000	-0.690683000
O	-3.613307000	-1.437863000	-0.687119000
O	0.000879000	3.782215000	2.170109000
O	0.037949000	3.922035000	-0.447546000
O	-1.390947000	1.990902000	0.772899000
O	-2.046662000	2.255146000	3.455232000
O	-2.065186000	2.482297000	-1.741849000
O	1.360948000	-0.042179000	-1.359549000
O	-1.104550000	-0.059488000	-0.806352000
H	1.840929000	-0.079653000	-2.205919000
O	0.058651000	1.829804000	-3.182582000
H	0.899921000	2.199071000	-3.478465000
Hf	2.520039000	-0.074010000	0.685763000
Hf	-0.015799000	-1.869193000	2.503975000
Hf	0.035746000	1.712810000	2.501623000
Hf	-0.039247000	1.712517000	-1.080433000
Hf	-2.536368000	-0.071954000	0.711310000
Hf	0.012104000	-1.878392000	-1.063382000
F	-2.853087000	4.541295000	-3.188742000
F	2.830929000	5.109495000	-2.207558000
F	-2.977723000	-4.303149000	-3.641170000
F	2.957872000	-4.610618000	-3.294887000

C	-1.825446000	-1.646269000	-5.267214000
C	-0.452951000	-2.310412000	-5.419629000
C	0.478399000	-1.634768000	-4.431655000
C	-1.672220000	-0.126770000	-5.412491000
C	1.904477000	-1.375771000	-4.813788000
C	-2.576115000	0.616170000	-4.443130000
H	2.388678000	-2.373710000	-4.772061000
H	-0.073222000	-2.173432000	-6.448321000
H	-2.151939000	-1.878548000	-4.237622000
H	-1.767959000	2.315027000	-4.031426000
H	1.947403000	-1.029162000	-5.859298000
H	3.460556000	-0.503856000	-4.035078000
H	-2.320811000	0.283981000	-3.412006000
H	-3.613160000	0.283573000	-4.629871000
H	-1.083980000	-3.842461000	-4.420837000
H	-0.199796000	0.826399000	-4.436006000
H	-2.569891000	-2.018279000	-7.012881000
H	-1.942385000	0.158186000	-6.448851000
O	-2.808700000	-2.199588000	-6.095441000
O	2.503114000	-0.464051000	-3.927077000
O	-2.510650000	2.001103000	-4.578746000
O	0.127419000	-1.622662000	-3.245864000
O	-0.479512000	-3.687147000	-5.163760000
O	-0.301445000	0.207429000	-5.223241000

Hf-NU-1000 (-F) Int2_Ro

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.088403000	2.691874000	3.464329000
H	4.062948000	-3.136437000	3.154630000
H	-4.031048000	2.548708000	3.683329000
H	-4.030624000	-2.968692000	3.406248000
C	5.634105000	-2.442370000	-2.317001000
C	-5.678731000	-2.586921000	-2.067257000
C	4.340491000	-2.985728000	-2.305936000
C	-4.344356000	-2.938718000	-2.326287000
C	4.134959000	-4.178388000	-3.015338000
C	-4.119985000	-3.989888000	-3.229032000
C	5.162882000	-4.799050000	-3.717989000
C	-5.169537000	-4.663216000	-3.845014000

C	6.431047000	-4.225494000	-3.724996000
C	-6.481238000	-4.287560000	-3.570920000
C	6.670013000	-3.043385000	-3.021989000
C	-6.739151000	-3.244119000	-2.680334000
C	5.565981000	2.684179000	-2.162496000
C	-5.676718000	2.846599000	-1.695400000
C	4.288351000	3.219293000	-1.946179000
C	-4.350016000	3.023677000	-2.119064000
C	4.072849000	4.549968000	-2.327806000
C	-4.128213000	3.915058000	-3.180596000
C	5.072932000	5.318176000	-2.912817000
C	-5.176700000	4.589086000	-3.802307000
C	6.325268000	4.752181000	-3.135486000
C	-6.481257000	4.390328000	-3.359919000
C	6.574898000	3.431585000	-2.758993000
C	-6.733837000	3.517650000	-2.299097000
H	5.793724000	-1.522422000	-1.751529000
H	-5.850874000	-1.767534000	-1.367197000
H	4.948820000	-5.730178000	-4.244781000
H	-4.934089000	-5.471677000	-4.538473000
H	7.665082000	-2.594915000	-3.021470000
H	-7.766515000	-2.945582000	-2.463885000
H	5.735762000	1.652136000	-1.850031000
H	-5.846026000	2.147403000	-0.874451000
H	4.852297000	6.352730000	-3.179740000
H	-4.945176000	5.264923000	-4.627017000
H	7.557888000	2.988154000	-2.927804000
H	-7.754688000	3.360982000	-1.945897000
H	-7.304753000	-4.814387000	-4.058343000
H	7.237508000	-4.710946000	-4.279199000
H	-7.301994000	4.922200000	-3.846358000
H	7.111249000	5.351908000	-3.599870000
H	-1.921962000	-2.940238000	0.573437000
H	-0.881420000	1.345322000	5.077460000
H	-0.015409000	0.046894000	4.771646000
H	0.045630000	4.021172000	0.575731000
H	0.667395000	4.287397000	2.655778000
H	0.845579000	4.345139000	-0.765189000
H	1.963020000	-0.197640000	3.559952000
H	-1.926078000	2.806246000	0.830839000
H	-0.609343000	-2.026482000	5.066805000
H	0.900762000	-4.449547000	2.108868000
H	0.633003000	-4.414402000	-1.270640000
H	0.045871000	-4.137776000	0.804197000
O	-1.060401000	-0.103425000	2.171537000
O	-3.619852000	1.289871000	2.165539000

O	-3.633398000	1.377600000	-0.602836000
O	-3.610956000	-1.507548000	2.084647000
O	-2.045931000	-2.671509000	3.209583000
O	0.051529000	-4.083628000	1.825973000
O	2.074019000	-2.843958000	2.972644000
O	2.064029000	-2.559051000	-1.843153000
O	3.631934000	-1.530512000	2.018222000
O	3.625844000	-1.417366000	-0.710058000
O	3.642369000	1.289469000	2.091382000
O	3.616210000	1.371744000	-0.656387000
O	2.028064000	2.678258000	-1.547311000
O	2.098450000	2.439728000	3.259593000
O	1.075680000	1.410539000	0.743603000
O	1.410913000	-0.133921000	2.770930000
O	0.038319000	-1.540063000	4.545040000
O	-0.030394000	1.065843000	4.713044000
O	1.066318000	-1.543080000	0.666537000
O	-1.391551000	-2.137137000	0.646001000
O	-2.058759000	-2.367905000	-2.007660000
O	-0.008303000	-3.900773000	-0.765089000
O	-3.613301000	-1.392499000	-0.720784000
O	-0.000937000	3.778926000	2.183350000
O	0.021018000	3.956953000	-0.437629000
O	-1.389640000	2.006131000	0.773359000
O	-2.047457000	2.248708000	3.459153000
O	-2.074676000	2.471734000	-1.785439000
O	1.371618000	-0.004064000	-1.349040000
O	-1.089948000	-0.030846000	-0.785562000
H	1.893917000	0.007660000	-2.175754000
O	0.087144000	1.696010000	-3.147864000
H	-0.613480000	2.067413000	-3.693941000
Hf	2.526415000	-0.065858000	0.680249000
Hf	-0.012097000	-1.879240000	2.468916000
Hf	0.040476000	1.704975000	2.508013000
Hf	-0.030485000	1.744388000	-1.069102000
Hf	-2.530377000	-0.067849000	0.706275000
Hf	0.018247000	-1.825844000	-1.110268000
F	-2.902246000	4.133689000	-3.658191000
F	2.893116000	5.143319000	-2.101749000
F	-2.883513000	-4.379051000	-3.534430000
F	2.941984000	-4.778410000	-3.016193000
C	-1.566862000	-0.489963000	-5.885135000
C	-0.485966000	-1.583559000	-5.646251000
C	0.417607000	-1.154426000	-4.506293000
C	-2.578367000	-0.388984000	-4.750661000
C	1.671549000	-0.407573000	-4.867452000

C	-3.500357000	0.809259000	-4.888149000
H	2.397561000	-1.210608000	-5.112419000
H	0.135459000	-1.617023000	-6.562227000
H	-2.136464000	-0.808728000	-6.779997000
H	-5.172130000	1.296730000	-3.988050000
H	1.488414000	0.112118000	-5.828757000
H	1.479912000	1.095329000	-3.705415000
H	-3.881860000	0.878603000	-5.926420000
H	-2.953938000	1.741834000	-4.664031000
H	-1.715130000	-2.817773000	-4.794217000
H	-4.136426000	-1.408647000	-4.278430000
H	-0.594179000	0.828535000	-6.942751000
H	-2.062032000	-0.301779000	-3.769067000
O	-0.984056000	0.783910000	-6.063512000
O	2.203215000	0.422108000	-3.904006000
O	-4.543491000	0.567592000	-3.968211000
O	0.119003000	-1.466676000	-3.363033000
O	-1.007134000	-2.852180000	-5.461106000
O	-3.338991000	-1.577042000	-4.803481000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.090573000	2.709030000	3.442684000
H	4.062541000	-3.144829000	3.142937000
H	-4.031953000	2.568895000	3.663083000
H	-4.032516000	-2.987220000	3.380761000
C	5.683100000	-2.695186000	-2.008810000
C	-5.308940000	-1.530367000	-2.871246000
C	4.342399000	-2.934343000	-2.350035000
C	-4.323723000	-2.500093000	-2.631203000
C	4.098924000	-3.790172000	-3.436033000
C	-4.343718000	-3.658875000	-3.414334000
C	5.136705000	-4.385020000	-4.147248000
C	-5.288653000	-3.848742000	-4.416890000
C	6.454412000	-4.133280000	-3.778592000
C	-6.235786000	-2.856627000	-4.655502000
C	6.730835000	-3.285453000	-2.704612000
C	-6.251559000	-1.696634000	-3.878725000
C	5.572378000	2.767313000	-2.097536000

C	-5.675863000	2.633641000	-1.991891000
C	4.271534000	3.257474000	-1.913838000
C	-4.328566000	2.761246000	-2.363178000
C	4.022162000	4.585004000	-2.284822000
C	-4.059851000	3.314210000	-3.623087000
C	5.010709000	5.394186000	-2.831468000
C	-5.076686000	3.747457000	-4.468093000
C	6.286979000	4.872079000	-3.025029000
C	-6.402716000	3.624064000	-4.063389000
C	6.570863000	3.556063000	-2.656771000
C	-6.705582000	3.060746000	-2.822048000
H	5.871375000	-2.026689000	-1.167027000
H	-5.286442000	-0.625279000	-2.258366000
H	4.887489000	-5.038391000	-4.984678000
H	-5.258421000	-4.770655000	-4.999161000
H	7.763316000	-3.085462000	-2.412407000
H	-6.987346000	-0.913074000	-4.073437000
H	5.768963000	1.737585000	-1.793061000
H	-5.886103000	2.179276000	-1.021540000
H	4.763731000	6.424404000	-3.091720000
H	-4.806559000	4.169682000	-5.437667000
H	7.572264000	3.147798000	-2.803667000
H	-7.744178000	2.957703000	-2.502652000
H	-6.964802000	-2.991340000	-5.457534000
H	7.268150000	-4.602739000	-4.335951000
H	-7.202116000	3.969640000	-4.723027000
H	7.064872000	5.503128000	-3.460399000
H	-1.920307000	-2.926867000	0.598568000
H	-0.883676000	1.321174000	5.132150000
H	-0.017024000	0.021419000	4.807171000
H	0.082982000	4.017672000	0.647021000
H	0.680374000	4.270502000	2.712881000
H	0.938066000	4.315636000	-0.669433000
H	1.968578000	-0.200727000	3.593024000
H	-1.901553000	2.806733000	0.835055000
H	-0.618736000	-2.028101000	5.082624000
H	0.876920000	-4.472767000	2.189358000
H	0.673184000	-4.451015000	-1.157751000
H	0.048111000	-4.150654000	0.861376000
O	-1.054965000	-0.099775000	2.195445000
O	-3.616462000	1.286246000	2.169251000
O	-3.633796000	1.396144000	-0.582497000
O	-3.611353000	-1.498651000	2.094014000
O	-2.049822000	-2.657334000	3.229498000
O	0.042700000	-4.086243000	1.891540000
O	2.077188000	-2.831615000	2.988809000

O	2.072817000	-2.618369000	-1.768331000
O	3.639076000	-1.533457000	2.016029000
O	3.629355000	-1.401749000	-0.716636000
O	3.639091000	1.283850000	2.097293000
O	3.616820000	1.399688000	-0.629278000
O	2.013904000	2.629659000	-1.602206000
O	2.101750000	2.430486000	3.281484000
O	1.088780000	1.407541000	0.779915000
O	1.417247000	-0.134765000	2.803670000
O	0.036804000	-1.542668000	4.569497000
O	-0.035807000	1.046131000	4.757149000
O	1.073132000	-1.524277000	0.692247000
O	-1.378663000	-2.132951000	0.688164000
O	-2.080400000	-2.574596000	-1.889270000
O	0.024559000	-3.934916000	-0.666521000
O	-3.583666000	-1.421323000	-0.688238000
O	0.010650000	3.768981000	2.234559000
O	0.094774000	3.945924000	-0.370022000
O	-1.365886000	2.003994000	0.828392000
O	-2.050693000	2.233488000	3.482199000
O	-2.072163000	2.596108000	-1.652922000
O	1.359817000	-0.003142000	-1.355204000
O	-1.101517000	-0.022221000	-0.772312000
H	1.818894000	-0.024089000	-2.218713000
O	-0.164663000	1.641216000	-3.196014000
H	-0.466026000	2.498545000	-3.529429000
Hf	2.542317000	-0.092867000	0.688689000
Hf	-0.003703000	-1.882594000	2.487675000
Hf	0.041496000	1.691343000	2.568701000
Hf	-0.011725000	1.722025000	-0.952890000
Hf	-2.530493000	-0.079134000	0.735643000
Hf	0.012176000	-1.869901000	-1.105718000
F	-2.806979000	3.399642000	-4.089164000
F	2.815107000	5.134564000	-2.081891000
F	-3.452168000	-4.624469000	-3.191884000
F	2.855137000	-4.058272000	-3.837827000
C	-1.878683000	-0.027018000	-5.061618000
C	-0.722674000	-2.181354000	-5.267565000
C	0.209740000	-1.573945000	-4.451886000
C	-3.042062000	-0.570420000	-5.821924000
C	1.449655000	-0.894785000	-4.974651000
C	-4.184200000	0.437674000	-5.756678000
H	2.251571000	-1.650321000	-5.031462000
H	-0.645530000	-2.197514000	-6.355699000
H	-1.113756000	0.507286000	-5.661900000
H	-5.880056000	0.609859000	-6.685439000

H	1.285345000	-0.549026000	-6.014215000
H	1.232195000	0.785848000	-3.992900000
H	-3.823685000	1.427174000	-6.104545000
H	-4.513365000	0.547460000	-4.705767000
H	-1.646575000	-2.941172000	-3.784364000
H	-3.481967000	-0.930709000	-7.639856000
H	-1.063306000	0.934969000	-3.439973000
H	-3.386923000	-1.503749000	-5.326111000
O	-2.016289000	0.217185000	-3.831418000
O	1.940305000	0.127619000	-4.142441000
O	-5.199990000	-0.064790000	-6.592530000
O	0.031234000	-1.611675000	-3.175743000
O	-1.672450000	-2.989757000	-4.765542000
O	-2.658816000	-0.793982000	-7.152248000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.090694000	2.714900000	3.435833000
H	4.061880000	-3.140497000	3.150118000
H	-4.031773000	2.575310000	3.656997000
H	-4.032128000	-2.980680000	3.389472000
C	5.686793000	-2.618653000	-2.052821000
C	-5.423435000	-1.757442000	-2.795732000
C	4.349826000	-2.947184000	-2.329089000
C	-4.341287000	-2.618822000	-2.570533000
C	4.117844000	-3.899603000	-3.334798000
C	-4.309290000	-3.827101000	-3.278936000
C	5.162870000	-4.498588000	-4.031912000
C	-5.301537000	-4.167317000	-4.192718000
C	6.476411000	-4.152357000	-3.731805000
C	-6.358218000	-3.285773000	-4.410650000
C	6.741593000	-3.208683000	-2.737844000
C	-6.423248000	-2.077135000	-3.710554000
C	5.562179000	2.730352000	-2.141310000
C	-5.663099000	2.658879000	-2.019882000
C	4.272366000	3.240821000	-1.935842000
C	-4.310877000	2.756510000	-2.381563000
C	4.034934000	4.569885000	-2.308768000
C	-4.020736000	3.281989000	-3.648828000

C	5.024727000	5.362191000	-2.877235000
C	-5.021564000	3.710065000	-4.513604000
C	6.289457000	4.820492000	-3.091809000
C	-6.352905000	3.617105000	-4.118615000
C	6.561149000	3.502055000	-2.722932000
C	-6.676952000	3.088655000	-2.867720000
H	5.866608000	-1.878224000	-1.271604000
H	-5.445986000	-0.817974000	-2.237068000
H	4.922032000	-5.230945000	-4.803854000
H	-5.231215000	-5.123736000	-4.712296000
H	7.770800000	-2.934878000	-2.498847000
H	-7.251125000	-1.384491000	-3.879970000
H	5.749094000	1.698653000	-1.836961000
H	-5.889262000	2.227992000	-1.042391000
H	4.788038000	6.394712000	-3.137884000
H	-4.737900000	4.101774000	-5.491706000
H	7.553477000	3.078596000	-2.887160000
H	-7.720307000	3.010628000	-2.556928000
H	-7.143362000	-3.553934000	-5.122622000
H	7.295721000	-4.624040000	-4.279051000
H	-7.139651000	3.954170000	-4.796921000
H	7.068163000	5.438099000	-3.544607000
H	-1.919397000	-2.921135000	0.588774000
H	-0.881169000	1.300998000	5.151018000
H	-0.018582000	0.000534000	4.806911000
H	0.084245000	4.025544000	0.672626000
H	0.683986000	4.264365000	2.733548000
H	0.942626000	4.328996000	-0.641545000
H	1.965637000	-0.210704000	3.594030000
H	-1.898806000	2.816132000	0.845736000
H	-0.617643000	-2.043303000	5.067076000
H	0.873384000	-4.473103000	2.158280000
H	0.639828000	-4.446396000	-1.196349000
H	0.047388000	-4.139840000	0.827796000
O	-1.055876000	-0.098651000	2.192255000
O	-3.615872000	1.285215000	2.170329000
O	-3.640820000	1.412154000	-0.572412000
O	-3.613116000	-1.501119000	2.090675000
O	-2.048913000	-2.661287000	3.221177000
O	0.041444000	-4.081171000	1.861395000
O	2.076207000	-2.835867000	2.978221000
O	2.073723000	-2.606315000	-1.782448000
O	3.640388000	-1.532356000	2.017444000
O	3.625695000	-1.394266000	-0.719975000
O	3.637924000	1.284186000	2.096989000
O	3.614239000	1.405446000	-0.623125000

O	2.011213000	2.637352000	-1.595556000
O	2.102448000	2.424378000	3.290310000
O	1.089109000	1.412937000	0.792955000
O	1.416100000	-0.138505000	2.803931000
O	0.036467000	-1.552336000	4.557376000
O	-0.037476000	1.027940000	4.765679000
O	1.072920000	-1.515972000	0.682152000
O	-1.387203000	-2.120511000	0.674283000
O	-2.079802000	-2.549978000	-1.901014000
O	0.013259000	-3.919813000	-0.687780000
O	-3.594798000	-1.393431000	-0.715290000
O	0.012166000	3.766766000	2.253912000
O	0.098873000	3.957348000	-0.345964000
O	-1.364831000	2.012147000	0.842229000
O	-2.051797000	2.227755000	3.489340000
O	-2.065052000	2.588294000	-1.647392000
O	1.356958000	0.020241000	-1.361315000
O	-1.103465000	-0.001280000	-0.774094000
H	1.810415000	0.006216000	-2.230290000
O	-0.180856000	1.689323000	-3.234668000
H	-0.527038000	2.546530000	-3.527728000
Hf	2.544105000	-0.096679000	0.689304000
Hf	-0.003736000	-1.884800000	2.471246000
Hf	0.038743000	1.687179000	2.585985000
Hf	-0.003385000	1.732505000	-0.921600000
Hf	-2.532898000	-0.074267000	0.732888000
Hf	0.010076000	-1.851937000	-1.133877000
F	-2.758403000	3.353113000	-4.098782000
F	2.839398000	5.136642000	-2.086160000
F	-3.330158000	-4.700381000	-3.062693000
F	2.879013000	-4.266164000	-3.665227000
C	-2.106017000	-0.015051000	-5.061052000
C	-0.550368000	-2.351116000	-5.267891000
C	0.284247000	-1.649451000	-4.447575000
C	-3.163687000	-0.767632000	-5.790802000
C	1.583868000	-1.039931000	-4.894067000
C	-4.482437000	0.011057000	-5.780215000
H	2.390073000	-1.777591000	-4.745022000
H	-0.416870000	-2.426577000	-6.347664000
H	-1.318284000	0.459357000	-5.693658000
H	-5.710109000	-1.455432000	-6.011586000
H	1.558268000	-0.821210000	-5.978509000
H	1.251461000	0.733088000	-4.116145000
H	-4.341619000	0.986771000	-6.272344000
H	-4.802334000	0.201167000	-4.738837000
H	-1.576991000	-3.000517000	-3.803997000

H	-3.557209000	-1.237688000	-7.591872000
H	-0.977230000	1.066939000	-3.403649000
H	-3.326433000	-1.716948000	-5.230919000
O	-2.191899000	0.206992000	-3.852759000
O	1.979018000	0.088953000	-4.135580000
O	-5.446073000	-0.682347000	-6.531682000
O	0.010328000	-1.597044000	-3.167075000
O	-1.563147000	-3.101778000	-4.779421000
O	-2.752519000	-1.004527000	-7.107864000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087728000	2.684333000	3.472948000
H	4.062994000	-3.138738000	3.151339000
H	-4.032955000	2.534143000	3.692659000
H	-4.031241000	-2.981283000	3.390431000
C	5.674373000	-2.653659000	-2.104058000
C	-5.669938000	-2.523612000	-2.147030000
C	4.325927000	-2.851693000	-2.435321000
C	-4.331094000	-2.799946000	-2.467144000
C	4.049511000	-3.572851000	-3.606260000
C	-4.090288000	-3.633747000	-3.571187000
C	5.064480000	-4.080942000	-4.411426000
C	-5.131585000	-4.191638000	-4.306547000
C	6.393531000	-3.881304000	-4.047356000
C	-6.447622000	-3.906144000	-3.959532000
C	6.701636000	-3.165884000	-2.889408000
C	-6.721234000	-3.061898000	-2.879752000
C	5.597582000	2.780233000	-2.017064000
C	-5.669858000	2.870701000	-1.630001000
C	4.287606000	3.262779000	-1.882021000
C	-4.345322000	3.072882000	-2.047954000
C	4.043412000	4.586016000	-2.273505000
C	-4.107061000	4.092395000	-2.986065000
C	5.046166000	5.394169000	-2.797111000
C	-5.147107000	4.863207000	-3.498325000
C	6.331185000	4.878836000	-2.943150000
C	-6.450185000	4.641115000	-3.061567000
C	6.610600000	3.568723000	-2.550662000

C	-6.715054000	3.645129000	-2.119431000
H	5.888019000	-2.082645000	-1.198436000
H	-5.856300000	-1.858100000	-1.302360000
H	4.791564000	-4.629858000	-5.314191000
H	-4.885349000	-4.830731000	-5.155333000
H	7.742384000	-3.007161000	-2.600951000
H	-7.752079000	-2.822930000	-2.612205000
H	5.790587000	1.757085000	-1.687645000
H	-5.848830000	2.077804000	-0.901834000
H	4.801375000	6.419914000	-3.076499000
H	-4.909468000	5.635858000	-4.230755000
H	7.619982000	3.166668000	-2.655287000
H	-7.734578000	3.474254000	-1.766830000
H	-7.263882000	-4.339784000	-4.541964000
H	7.190252000	-4.286712000	-4.675092000
H	-7.261008000	5.257042000	-3.458069000
H	7.119395000	5.510652000	-3.358484000
H	-1.928481000	-2.942231000	0.609910000
H	-0.875281000	1.375076000	5.066905000
H	-0.013458000	0.070321000	4.771211000
H	0.059954000	4.005887000	0.543791000
H	0.662924000	4.292840000	2.624973000
H	0.865226000	4.315633000	-0.799374000
H	1.963375000	-0.177707000	3.563855000
H	-1.911754000	2.795451000	0.789808000
H	-0.613593000	-1.995190000	5.079582000
H	0.894996000	-4.449585000	2.168917000
H	0.574279000	-4.493006000	-1.175926000
H	0.015990000	-4.162422000	0.870103000
O	-1.058785000	-0.095907000	2.172653000
O	-3.614132000	1.295266000	2.158099000
O	-3.623694000	1.315831000	-0.657547000
O	-3.609650000	-1.504913000	2.087066000
O	-2.047610000	-2.658600000	3.226246000
O	0.044171000	-4.083366000	1.892282000
O	2.075931000	-2.827963000	2.992290000
O	2.097347000	-2.727024000	-1.652986000
O	3.635270000	-1.542982000	2.000316000
O	3.631153000	-1.366618000	-0.756824000
O	3.642560000	1.285414000	2.094350000
O	3.613552000	1.374279000	-0.654413000
O	2.026960000	2.639103000	-1.603307000
O	2.097498000	2.451194000	3.244612000
O	1.078316000	1.396659000	0.717631000
O	1.415548000	-0.123377000	2.771170000
O	0.037616000	-1.515039000	4.556268000

O	-0.025546000	1.089410000	4.703818000
O	1.066261000	-1.534254000	0.678881000
O	-1.387129000	-2.145594000	0.671135000
O	-2.050487000	-2.389724000	-1.978673000
O	-0.063853000	-3.961904000	-0.685884000
O	-3.616530000	-1.452550000	-0.680085000
O	0.002756000	3.776583000	2.149511000
O	0.043594000	3.924689000	-0.468397000
O	-1.380564000	1.990074000	0.755839000
O	-2.046143000	2.258245000	3.452467000
O	-2.069346000	2.500074000	-1.744123000
O	1.349751000	-0.038289000	-1.423300000
O	-1.077160000	-0.063633000	-0.794923000
H	1.936688000	-0.041551000	-2.201507000
O	-0.089050000	1.771419000	-3.236857000
H	-0.819736000	2.349885000	-3.507902000
Hf	2.530351000	-0.080990000	0.675313000
Hf	-0.011516000	-1.870276000	2.482783000
Hf	0.042219000	1.707307000	2.495527000
Hf	-0.028489000	1.707455000	-1.077578000
Hf	-2.523951000	-0.080469000	0.701461000
Hf	0.028556000	-1.901986000	-1.101922000
F	-2.880458000	4.367592000	-3.410656000
F	2.831178000	5.132205000	-2.116541000
F	-2.850794000	-3.913256000	-3.963932000
F	2.792153000	-3.770334000	-4.006718000
C	-0.715874000	-0.311782000	-4.754709000
C	0.385785000	-1.050736000	-4.291328000
C	1.747672000	-0.800067000	-4.875717000
H	2.049019000	-1.710841000	-5.426641000
H	-0.701004000	0.101812000	-5.771594000
H	1.686426000	0.028511000	-5.603082000
H	3.538074000	-0.374927000	-4.196790000
H	-1.867397000	-1.406732000	-3.678369000
H	-0.302090000	0.716390000	-4.032541000
O	2.657478000	-0.516034000	-3.832234000
O	0.250834000	-1.801094000	-3.282376000
O	-1.966889000	-0.678512000	-4.323474000
C	-3.723006000	0.915218000	-5.398587000
C	-4.825831000	0.298354000	-4.574616000
C	-6.054899000	1.184393000	-4.583962000
H	-3.415846000	0.292462000	-6.279537000
H	-7.781904000	1.136395000	-3.702337000
H	-6.450148000	1.239038000	-5.618221000
H	-5.767987000	2.206853000	-4.280104000
H	-5.844396000	-1.327907000	-4.577177000

H	-4.454799000	0.250483000	-3.525815000
O	-3.235773000	1.993327000	-5.163806000
O	-6.986219000	0.595208000	-3.705684000
O	-5.103136000	-0.975073000	-5.088471000

Hf-NU-1000 (-F) Prod

C	-3.248311000	-2.182821000	-1.650063000
C	-3.229666000	-2.386625000	2.899972000
C	-3.232277000	2.034295000	3.104012000
C	3.276906000	2.142007000	2.939220000
C	3.226918000	2.366311000	-1.338686000
C	3.259354000	-2.277905000	-1.561501000
C	-3.265329000	2.236142000	-1.457370000
C	3.257205000	-2.506602000	2.716416000
H	4.087811000	2.690608000	3.466023000
H	4.060966000	-3.138163000	3.156024000
H	-4.031876000	2.544692000	3.684988000
H	-4.030767000	-2.970487000	3.403148000
C	5.679721000	-2.858075000	-1.782318000
C	-5.667770000	-2.553662000	-2.175007000
C	4.372030000	-2.968485000	-2.281785000
C	-4.329415000	-2.948546000	-2.335484000
C	4.196886000	-3.733334000	-3.442647000
C	-4.083348000	-4.048973000	-3.169941000
C	5.257212000	-4.368831000	-4.078503000
C	-5.107333000	-4.713140000	-3.836432000
C	6.539201000	-4.250065000	-3.550053000
C	-6.419318000	-4.281976000	-3.674117000
C	6.752203000	-3.492293000	-2.397532000
C	-6.703304000	-3.201876000	-2.835289000
C	5.569261000	2.699424000	-2.144323000
C	-5.615419000	3.076011000	-1.489342000
C	4.288311000	3.227765000	-1.929965000
C	-4.345608000	3.043235000	-2.084805000
C	4.069184000	4.562062000	-2.296850000
C	-4.161736000	3.785798000	-3.260099000
C	5.069062000	5.340714000	-2.867630000
C	-5.188764000	4.540147000	-3.816303000
C	6.324607000	4.781641000	-3.089989000
C	-6.432598000	4.568053000	-3.192607000
C	6.577921000	3.457945000	-2.726953000
C	-6.648800000	3.834698000	-2.024707000
H	5.821398000	-2.256124000	-0.882993000
H	-5.868729000	-1.707439000	-1.516597000
H	5.057570000	-4.946192000	-4.982407000
H	-4.851432000	-5.559090000	-4.475385000

H	7.756226000	-3.395076000	-1.980820000
H	-7.732825000	-2.866405000	-2.698605000
H	5.741958000	1.664045000	-1.844361000
H	-5.762277000	2.487150000	-0.581690000
H	4.845785000	6.377134000	-3.124684000
H	-4.993744000	5.090394000	-4.737828000
H	7.563323000	3.020241000	-2.896342000
H	-7.624499000	3.852510000	-1.536006000
H	-7.224485000	-4.796991000	-4.202582000
H	7.373924000	-4.751201000	-4.044944000
H	-7.238345000	5.163922000	-3.627028000
H	7.110340000	5.389343000	-3.544238000
H	-1.925533000	-2.936011000	0.580108000
H	-0.874602000	1.354693000	5.080872000
H	-0.011142000	0.055545000	4.774782000
H	0.052601000	4.025453000	0.571307000
H	0.654789000	4.299113000	2.660463000
H	0.849645000	4.353416000	-0.770930000
H	1.966169000	-0.193813000	3.562017000
H	-1.918200000	2.810532000	0.831321000
H	-0.599277000	-2.024602000	5.077760000
H	0.893382000	-4.450301000	2.103962000
H	0.645303000	-4.404834000	-1.244056000
H	0.030697000	-4.131961000	0.806317000
O	-1.057274000	-0.101171000	2.179363000
O	-3.619424000	1.295174000	2.159547000
O	-3.630718000	1.333432000	-0.634801000
O	-3.609870000	-1.507540000	2.083141000
O	-2.045809000	-2.667953000	3.212160000
O	0.044357000	-4.079649000	1.826538000
O	2.073194000	-2.843128000	2.970857000
O	2.071074000	-2.582252000	-1.845859000
O	3.634811000	-1.531243000	2.019033000
O	3.608912000	-1.427318000	-0.694578000
O	3.642810000	1.287708000	2.093237000
O	3.613294000	1.370381000	-0.654563000
O	2.027274000	2.669936000	-1.556789000
O	2.098191000	2.442222000	3.255638000
O	1.075211000	1.406396000	0.740094000
O	1.413594000	-0.132293000	2.773097000
O	0.042688000	-1.537265000	4.549808000
O	-0.025902000	1.073082000	4.712550000
O	1.065139000	-1.542401000	0.671221000
O	-1.396690000	-2.131472000	0.648115000
O	-2.056108000	-2.367698000	-2.000750000
O	-0.025192000	-3.897788000	-0.772980000

O	-3.619591000	-1.372572000	-0.739092000
O	-0.002394000	3.780840000	2.183124000
O	0.030222000	3.956780000	-0.440367000
O	-1.388838000	2.005334000	0.774420000
O	-2.047957000	2.245995000	3.459670000
O	-2.073963000	2.492418000	-1.756289000
O	1.368669000	-0.014403000	-1.360903000
O	-1.093714000	-0.027194000	-0.785080000
H	1.869044000	-0.005795000	-2.203323000
O	0.048979000	1.676342000	-3.151535000
H	-0.708001000	1.970341000	-3.670054000
Hf	2.527341000	-0.061877000	0.681254000
Hf	-0.010249000	-1.876448000	2.476754000
Hf	0.045074000	1.710538000	2.506639000
Hf	-0.024404000	1.749986000	-1.080776000
Hf	-2.522210000	-0.062303000	0.719423000
Hf	0.017417000	-1.813212000	-1.100625000
F	-2.994059000	3.764640000	-3.907120000
F	2.886298000	5.147585000	-2.067318000
F	-2.843743000	-4.513359000	-3.339501000
F	2.984240000	-3.863754000	-4.000248000
C	0.274907000	-2.759239000	-5.427534000
C	0.657397000	-1.667829000	-4.473913000
C	1.724009000	-0.701440000	-4.891319000
H	2.610114000	-1.318567000	-5.136072000
H	1.125417000	-3.473778000	-5.405008000
H	1.392984000	-0.276338000	-5.859654000
H	1.289258000	0.880248000	-3.822409000
H	-1.082159000	-3.330880000	-4.170705000
H	0.247079000	-2.360181000	-6.453506000
O	2.071727000	0.260301000	-3.966851000
O	0.121837000	-1.646994000	-3.369368000
O	-0.938294000	-3.358188000	-5.132597000
C	-2.270850000	-0.824363000	-6.008406000
C	-3.252559000	-0.991441000	-4.889165000
C	-3.272512000	0.196252000	-3.924814000
H	-2.617184000	-1.252488000	-6.985589000
H	-4.296833000	0.111270000	-2.247239000
H	-3.230101000	1.144356000	-4.493179000
H	-2.383576000	0.164637000	-3.269731000
H	-5.139656000	-1.118753000	-4.708011000
H	-2.875320000	-1.880227000	-4.335227000
O	-1.190133000	-0.290295000	-5.895859000
O	-4.480599000	0.141382000	-3.197907000
O	-4.515043000	-1.237062000	-5.439361000

4.3 -CH₃Hf-NU-1000 (-CH₃)

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086617000	2.685633000	3.472621000
H	4.063472000	-3.157106000	3.122082000
H	-4.031806000	2.545073000	3.684455000
H	-4.030274000	-2.992662000	3.377237000
C	5.650624000	-2.839767000	-1.765647000
C	-5.622733000	-2.461838000	-2.256163000
C	4.347573000	-3.014969000	-2.260786000
C	-4.297022000	-2.890522000	-2.430331000
C	4.125810000	-3.865333000	-3.373387000
C	-4.009896000	-3.961146000	-3.313253000
C	5.242342000	-4.503146000	-3.932373000
C	-5.089959000	-4.546590000	-3.989256000
C	6.527658000	-4.329876000	-3.427595000
C	-6.398819000	-4.103387000	-3.822948000
C	6.736560000	-3.491353000	-2.334368000
C	-6.671051000	-3.051849000	-2.949479000
C	5.596817000	3.063085000	-1.439435000
C	-5.670598000	2.607593000	-1.890940000
C	4.299268000	3.191010000	-1.958694000
C	-4.349007000	3.036735000	-2.092677000
C	4.048112000	4.075235000	-3.036983000
C	-4.093246000	4.194198000	-2.870998000
C	5.137294000	4.801703000	-3.539483000
C	-5.199632000	4.861478000	-3.416419000
C	6.417554000	4.684209000	-3.005681000
C	-6.505028000	4.420087000	-3.221304000
C	6.652967000	3.809405000	-1.946143000
C	-6.746085000	3.283480000	-2.451609000
H	5.785773000	-2.173650000	-0.912288000
H	-5.805874000	-1.643609000	-1.558016000
H	5.089327000	-5.156150000	-4.795938000
H	-4.888265000	-5.380799000	-4.666926000
H	7.739846000	-3.343694000	-1.929648000
H	-7.694001000	-2.697269000	-2.807213000
H	5.751555000	2.360984000	-0.617973000

H	-5.829534000	1.720243000	-1.276597000
H	4.967277000	5.478414000	-4.381579000
H	-5.021262000	5.760365000	-4.013081000
H	7.654085000	3.705729000	-1.522374000
H	-7.765645000	2.928678000	-2.287034000
H	-7.208984000	-4.586217000	-4.374946000
H	7.367950000	-4.849954000	-3.893826000
H	-7.336177000	4.970274000	-3.669304000
H	7.235808000	5.274728000	-3.425196000
H	-1.933392000	-2.946392000	0.622385000
H	-0.872462000	1.405884000	5.083239000
H	-0.012158000	0.101779000	4.804644000
H	0.011135000	4.019623000	0.574413000
H	0.654151000	4.301601000	2.643620000
H	0.866464000	4.307955000	-0.725457000
H	1.960937000	-0.173563000	3.587556000
H	-1.942950000	2.793687000	0.835584000
H	-0.605411000	-1.987816000	5.138200000
H	0.897098000	-4.436466000	2.198151000
H	0.713302000	-4.421388000	-1.139024000
H	0.031412000	-4.153032000	0.900607000
O	-1.064758000	-0.101125000	2.191429000
O	-3.618502000	1.286215000	2.168249000
O	-3.611733000	1.333450000	-0.630034000
O	-3.607042000	-1.507546000	2.086662000
O	-2.048946000	-2.649361000	3.245838000
O	0.044341000	-4.079097000	1.913547000
O	2.076107000	-2.827217000	3.002223000
O	2.043920000	-2.537445000	-1.863228000
O	3.631123000	-1.525522000	2.025034000
O	3.590878000	-1.429581000	-0.686758000
O	3.650255000	1.284659000	2.096561000
O	3.586653000	1.355774000	-0.649869000
O	2.025361000	2.697913000	-1.513158000
O	2.098430000	2.448304000	3.240468000
O	1.067917000	1.379544000	0.734089000
O	1.410384000	-0.122173000	2.796388000
O	0.035102000	-1.510372000	4.599397000
O	-0.024946000	1.114064000	4.719466000
O	1.070968000	-1.550838000	0.712710000
O	-1.387605000	-2.154098000	0.700681000
O	-2.022327000	-2.343052000	-1.966289000
O	0.000152000	-3.934903000	-0.711096000
O	-3.620192000	-1.436564000	-0.691837000
O	-0.005600000	3.781661000	2.171803000
O	0.006736000	3.966903000	-0.441119000

O	-1.394927000	2.001584000	0.775698000
O	-2.047153000	2.255473000	3.454601000
O	-2.068467000	2.482086000	-1.767193000
O	1.328926000	-0.042810000	-1.417165000
O	-1.074112000	-0.048756000	-0.749482000
H	1.878484000	0.031433000	-2.207197000
O	0.096645000	1.699265000	-3.132846000
H	-0.695125000	1.849908000	-3.657505000
C	-2.729701000	4.756638000	-3.130154000
H	-2.162513000	4.923937000	-2.205106000
H	-2.107188000	4.076703000	-3.728014000
H	-2.807382000	5.709137000	-3.670194000
C	2.707806000	4.255462000	-3.681032000
H	2.197825000	3.305259000	-3.885782000
H	2.013560000	4.814362000	-3.035675000
H	2.807948000	4.816776000	-4.619099000
C	2.788126000	-4.113205000	-3.999267000
H	2.096225000	-4.623095000	-3.314951000
H	2.283711000	-3.181692000	-4.287237000
H	2.895689000	-4.736614000	-4.896019000
C	-2.638508000	-4.512732000	-3.550281000
H	-2.000429000	-3.796543000	-4.086964000
H	-2.106568000	-4.733399000	-2.615615000
H	-2.695192000	-5.430696000	-4.149762000
Hf	2.537563000	-0.051457000	0.699804000
Hf	-0.023561000	-1.859405000	2.537570000
Hf	0.034014000	1.710684000	2.498048000
Hf	-0.043271000	1.751306000	-1.101302000
Hf	-2.541206000	-0.063100000	0.711795000
Hf	0.021359000	-1.846099000	-0.993248000

Hf-NU-1000 (-CH₃) Ads

C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086407000	2.705396000	3.453047000
H	4.063495000	-3.149737000	3.133567000
H	-4.033233000	2.559493000	3.669431000
H	-4.035009000	-2.977460000	3.388436000
C	5.488798000	-2.110214000	-2.596145000
C	-5.391841000	-1.716465000	-2.756186000

C	4.326985000	-2.874218000	-2.411056000
C	-4.348634000	-2.634545000	-2.549387000
C	4.190238000	-4.127689000	-3.052836000
C	-4.356090000	-3.879929000	-3.214143000
C	5.245880000	-4.555637000	-3.868789000
C	-5.420182000	-4.140898000	-4.089446000
C	6.386979000	-3.781696000	-4.066575000
C	-6.431214000	-3.213492000	-4.318486000
C	6.511961000	-2.549593000	-3.427529000
C	-6.420924000	-1.990440000	-3.647059000
C	5.578684000	3.116495000	-1.430715000
C	-5.670484000	2.600171000	-1.876320000
C	4.289599000	3.189675000	-1.980725000
C	-4.347730000	2.984623000	-2.152725000
C	4.043745000	4.018933000	-3.102123000
C	-4.096151000	4.039795000	-3.066093000
C	5.125330000	4.749044000	-3.614835000
C	-5.206929000	4.651779000	-3.664994000
C	6.396231000	4.686751000	-3.050138000
C	-6.512717000	4.256201000	-3.391918000
C	6.628153000	3.864809000	-1.948608000
C	-6.750422000	3.222082000	-2.488020000
H	5.559373000	-1.149598000	-2.081424000
H	-5.358851000	-0.769851000	-2.211383000
H	5.165736000	-5.530643000	-4.357764000
H	-5.446198000	-5.104871000	-4.605075000
H	7.402807000	-1.935326000	-3.573528000
H	-7.212800000	-1.256862000	-3.813451000
H	5.731663000	2.455718000	-0.575235000
H	-5.826549000	1.793546000	-1.158243000
H	4.957620000	5.383293000	-4.489823000
H	-5.030939000	5.468124000	-4.370812000
H	7.621788000	3.803804000	-1.499688000
H	-7.770283000	2.905875000	-2.258790000
H	-7.236114000	-3.450660000	-5.018345000
H	7.184222000	-4.148240000	-4.717831000
H	-7.346800000	4.761648000	-3.884981000
H	7.209226000	5.278316000	-3.478185000
H	-1.916814000	-2.940455000	0.607161000
H	-0.879891000	1.343947000	5.117561000
H	-0.014377000	0.044736000	4.807592000
H	0.021974000	4.012254000	0.629916000
H	0.653777000	4.288436000	2.682429000
H	0.902530000	4.298483000	-0.657292000
H	1.968389000	-0.197823000	3.588804000
H	-1.939159000	2.783813000	0.834871000

H	-0.611485000	-2.024295000	5.104078000
H	0.898228000	-4.459293000	2.174774000
H	0.622829000	-4.455311000	-1.213843000
H	0.037689000	-4.164675000	0.870914000
O	-1.056099000	-0.105660000	2.198100000
O	-3.613243000	1.286582000	2.166691000
O	-3.609158000	1.344318000	-0.618302000
O	-3.604418000	-1.506402000	2.083683000
O	-2.049878000	-2.663188000	3.231309000
O	0.048920000	-4.095135000	1.889736000
O	2.076035000	-2.838113000	2.987450000
O	2.052766000	-2.592662000	-1.797945000
O	3.632937000	-1.523919000	2.029845000
O	3.613765000	-1.436826000	-0.686292000
O	3.646751000	1.281502000	2.103061000
O	3.598728000	1.401150000	-0.606221000
O	2.014941000	2.671220000	-1.547598000
O	2.098627000	2.436166000	3.263753000
O	1.070559000	1.399560000	0.773264000
O	1.413113000	-0.134801000	2.801912000
O	0.036868000	-1.540903000	4.580169000
O	-0.031963000	1.064130000	4.745936000
O	1.072007000	-1.547480000	0.699440000
O	-1.372360000	-2.147873000	0.686285000
O	-2.056039000	-2.516987000	-1.915304000
O	-0.023407000	-3.949569000	-0.707823000
O	-3.576551000	-1.412959000	-0.699794000
O	-0.010064000	3.773113000	2.210980000
O	0.037844000	3.957032000	-0.389754000
O	-1.383895000	1.995346000	0.799231000
O	-2.049400000	2.240402000	3.473961000
O	-2.056653000	2.493045000	-1.739760000
O	1.397811000	-0.009392000	-1.322466000
O	-1.069248000	-0.052080000	-0.766004000
H	1.917282000	-0.015495000	-2.150926000
O	0.000919000	1.495968000	-3.137006000
H	-0.823220000	1.841231000	-3.512808000
C	-2.733561000	4.541712000	-3.428868000
H	-2.138184000	4.816365000	-2.548242000
H	-2.152890000	3.774523000	-3.959477000
H	-2.814011000	5.417472000	-4.085777000
C	2.715023000	4.137133000	-3.783856000
H	2.249063000	3.161808000	-3.973186000
H	1.983953000	4.689365000	-3.175136000
H	2.820488000	4.668164000	-4.738752000
C	3.003707000	-5.023228000	-2.870463000

H	2.764681000	-5.164841000	-1.806468000
H	2.092359000	-4.616445000	-3.332410000
H	3.195318000	-6.013045000	-3.304147000
C	-3.305790000	-4.932022000	-3.029666000
H	-2.545224000	-4.874460000	-3.824918000
H	-2.779552000	-4.867119000	-2.070088000
H	-3.747742000	-5.933999000	-3.111911000
Hf	2.536487000	-0.071494000	0.700388000
Hf	-0.009635000	-1.880581000	2.505793000
Hf	0.036075000	1.697588000	2.545157000
Hf	-0.017723000	1.735794000	-1.014623000
Hf	-2.520533000	-0.072040000	0.723946000
Hf	0.038429000	-1.865067000	-1.065450000
C	-1.754366000	-2.452275000	-5.187578000
C	-0.310731000	-2.814303000	-4.792857000
C	0.307394000	-1.441995000	-4.528745000
C	-1.665228000	-0.997700000	-5.666282000
C	1.814206000	-1.279381000	-4.645603000
C	-2.539617000	-0.005204000	-4.918065000
H	2.308924000	-2.133585000	-4.163315000
H	0.204208000	-3.266246000	-5.662077000
H	-2.367825000	-2.493300000	-4.274199000
H	-1.235460000	1.301375000	-5.420280000
H	2.084084000	-1.289797000	-5.715943000
H	1.655229000	0.623443000	-4.175145000
H	-2.445051000	-0.178540000	-3.825518000
H	-3.598451000	-0.166091000	-5.175805000
H	-0.983812000	-3.593867000	-3.146540000
H	-0.116318000	-0.035697000	-3.192639000
H	-1.847987000	-3.362465000	-6.894252000
H	-1.871588000	-0.927302000	-6.747935000
O	-2.365484000	-3.342775000	-6.080134000
O	2.272749000	-0.110675000	-4.001124000
O	-2.190634000	1.315713000	-5.258566000
O	-0.134815000	-1.063059000	-3.238024000
O	-0.196003000	-3.694735000	-3.713721000
O	-0.286650000	-0.606659000	-5.494459000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000

C	3.257200000	-2.506600000	2.716400000
H	4.086277000	2.708634000	3.449805000
H	4.063084000	-3.145748000	3.140316000
H	-4.032575000	2.563095000	3.666998000
H	-4.034522000	-2.975028000	3.392214000
C	5.492209000	-2.122681000	-2.592692000
C	-5.396423000	-1.733048000	-2.754946000
C	4.329203000	-2.883362000	-2.402303000
C	-4.349651000	-2.645694000	-2.542830000
C	4.193742000	-4.144307000	-3.029411000
C	-4.354640000	-3.896602000	-3.197182000
C	5.251594000	-4.582640000	-3.837054000
C	-5.419664000	-4.168197000	-4.068085000
C	6.393870000	-3.811970000	-4.040410000
C	-6.434355000	-3.246156000	-4.302521000
C	6.517738000	-2.572524000	-3.415445000
C	-6.426694000	-2.017689000	-3.641086000
C	5.583160000	3.098708000	-1.428361000
C	-5.666439000	2.581173000	-1.910690000
C	4.290277000	3.201664000	-1.965580000
C	-4.343666000	2.984808000	-2.158007000
C	4.046006000	4.071231000	-3.056891000
C	-4.088597000	4.058611000	-3.048073000
C	5.131738000	4.806260000	-3.553648000
C	-5.195501000	4.667891000	-3.656668000
C	6.406556000	4.710710000	-3.002952000
C	-6.501044000	4.251699000	-3.414655000
C	6.637261000	3.850761000	-1.930730000
C	-6.742499000	3.200186000	-2.532074000
H	5.561776000	-1.156121000	-2.089132000
H	-5.365016000	-0.782008000	-2.217955000
H	5.172152000	-5.563301000	-4.314720000
H	-5.443551000	-5.136488000	-4.575656000
H	7.409632000	-1.960778000	-3.565776000
H	-7.221420000	-1.288164000	-3.811696000
H	5.735400000	2.410536000	-0.594848000
H	-5.825787000	1.762039000	-1.207697000
H	4.963775000	5.472351000	-4.404550000
H	-5.016861000	5.499099000	-4.344229000
H	7.633425000	3.763755000	-1.491874000
H	-7.762447000	2.868352000	-2.326605000
H	-7.239942000	-3.491725000	-4.998680000
H	7.192885000	-4.186767000	-4.684774000
H	-7.332183000	4.755244000	-3.914560000
H	7.222712000	5.306884000	-3.418303000
H	-1.915490000	-2.939453000	0.601234000

H	-0.878853000	1.328065000	5.126084000
H	-0.014575000	0.028800000	4.804585000
H	0.027261000	4.007732000	0.643488000
H	0.655432000	4.282472000	2.690410000
H	0.916790000	4.290999000	-0.638962000
H	1.966977000	-0.204507000	3.586503000
H	-1.936876000	2.787099000	0.838417000
H	-0.609719000	-2.033926000	5.091785000
H	0.895203000	-4.463447000	2.162880000
H	0.606305000	-4.453326000	-1.225498000
H	0.038271000	-4.159886000	0.855782000
O	-1.057383000	-0.106130000	2.198615000
O	-3.613723000	1.287199000	2.166758000
O	-3.611014000	1.347005000	-0.617774000
O	-3.606734000	-1.505592000	2.084993000
O	-2.049484000	-2.665956000	3.225255000
O	0.047746000	-4.095572000	1.877563000
O	2.075740000	-2.840509000	2.980896000
O	2.055018000	-2.594758000	-1.794935000
O	3.634399000	-1.525104000	2.028391000
O	3.615564000	-1.430445000	-0.691347000
O	3.645621000	1.281286000	2.103369000
O	3.596613000	1.408632000	-0.599440000
O	2.011396000	2.658428000	-1.567402000
O	2.098415000	2.433413000	3.267716000
O	1.069434000	1.402712000	0.777647000
O	1.413084000	-0.137807000	2.798923000
O	0.038640000	-1.547777000	4.570450000
O	-0.032503000	1.050470000	4.749450000
O	1.069340000	-1.544108000	0.690216000
O	-1.375367000	-2.143818000	0.678936000
O	-2.056934000	-2.513802000	-1.917356000
O	-0.026998000	-3.942203000	-0.708583000
O	-3.577609000	-1.407403000	-0.704203000
O	-0.010280000	3.769976000	2.218393000
O	0.049104000	3.952783000	-0.377647000
O	-1.383852000	1.996949000	0.805350000
O	-2.049610000	2.236575000	3.477542000
O	-2.052879000	2.491102000	-1.736930000
O	1.404289000	-0.002541000	-1.314692000
O	-1.068079000	-0.047357000	-0.757126000
H	1.914484000	-0.018848000	-2.148598000
O	-0.037316000	1.374675000	-3.141077000
H	-0.864923000	1.693470000	-3.537754000
C	-2.725775000	4.585900000	-3.371629000
H	-2.154772000	4.851411000	-2.472219000

H	-2.120484000	3.837903000	-3.901449000
H	-2.804036000	5.473789000	-4.012300000
C	2.714612000	4.233180000	-3.724420000
H	2.246214000	3.271459000	-3.969214000
H	1.987677000	4.752063000	-3.082762000
H	2.818099000	4.816975000	-4.648165000
C	3.006179000	-5.036875000	-2.839527000
H	2.765351000	-5.166928000	-1.774453000
H	2.095603000	-4.634074000	-3.306506000
H	3.197473000	-6.031273000	-3.262739000
C	-3.301271000	-4.944368000	-3.005852000
H	-2.542766000	-4.891911000	-3.803438000
H	-2.773518000	-4.869891000	-2.047757000
H	-3.740934000	-5.948125000	-3.077976000
Hf	2.535688000	-0.078646000	0.699708000
Hf	-0.008616000	-1.884796000	2.492209000
Hf	0.034251000	1.692663000	2.554439000
Hf	-0.016127000	1.729507000	-0.994489000
Hf	-2.523256000	-0.075312000	0.726635000
Hf	0.034701000	-1.859233000	-1.093758000
C	-1.728605000	-2.490163000	-5.169571000
C	-0.291732000	-2.846683000	-4.752565000
C	0.330534000	-1.474440000	-4.488144000
C	-1.630643000	-1.038971000	-5.657490000
C	1.841202000	-1.346540000	-4.630414000
C	-2.506432000	-0.045551000	-4.911117000
H	2.324425000	-2.204944000	-4.146004000
H	0.231211000	-3.309601000	-5.611762000
H	-2.358057000	-2.524858000	-4.267287000
H	-1.198746000	1.234813000	-5.474922000
H	2.102131000	-1.370495000	-5.702644000
H	1.785231000	0.571498000	-4.254888000
H	-2.425526000	-0.228998000	-3.819892000
H	-3.563957000	-0.192643000	-5.183358000
H	-0.987260000	-3.619326000	-3.112240000
H	-0.086880000	0.092918000	-3.201667000
H	-1.784316000	-3.424836000	-6.864588000
H	-1.841706000	-0.975870000	-6.739014000
O	-2.325315000	-3.387777000	-6.066546000
O	2.337582000	-0.184365000	-3.998153000
O	-2.134893000	1.278647000	-5.228442000
O	-0.095126000	-1.056658000	-3.225991000
O	-0.189227000	-3.718835000	-3.663963000
O	-0.253735000	-0.653005000	-5.491858000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086795000	2.713452000	3.443828000
H	4.062910000	-3.137200000	3.153237000
H	-4.031332000	2.569761000	3.662445000
H	-4.033386000	-2.973426000	3.395985000
C	5.426840000	-2.016925000	-2.712782000
C	-5.387398000	-1.717466000	-2.768258000
C	4.322297000	-2.840353000	-2.445698000
C	-4.353421000	-2.640808000	-2.540860000
C	4.220788000	-4.112793000	-3.054557000
C	-4.372100000	-3.899741000	-3.179011000
C	5.247132000	-4.495575000	-3.929219000
C	-5.438481000	-4.168646000	-4.049267000
C	6.324523000	-3.660632000	-4.215528000
C	-6.440153000	-3.236713000	-4.299343000
C	6.418809000	-2.411252000	-3.604142000
C	-6.418424000	-1.999668000	-3.654338000
C	5.567828000	3.144318000	-1.443183000
C	-5.661091000	2.574511000	-1.939325000
C	4.284419000	3.172291000	-2.010666000
C	-4.336389000	2.978814000	-2.174954000
C	4.041158000	3.935430000	-3.178510000
C	-4.073342000	4.047699000	-3.068689000
C	5.119975000	4.650558000	-3.717927000
C	-5.174640000	4.651639000	-3.692623000
C	6.384442000	4.636358000	-3.135461000
C	-6.482056000	4.234572000	-3.462266000
C	6.613779000	3.878065000	-1.988496000
C	-6.731301000	3.187921000	-2.576129000
H	5.481479000	-1.050409000	-2.204032000
H	-5.345784000	-0.760486000	-2.242693000
H	5.193212000	-5.482900000	-4.396436000
H	-5.472916000	-5.142920000	-4.544646000
H	7.264979000	-1.752951000	-3.812176000
H	-7.202979000	-1.262034000	-3.837272000
H	5.718817000	2.531326000	-0.552251000
H	-5.826740000	1.759016000	-1.233574000
H	4.955042000	5.233647000	-4.628330000
H	-4.990096000	5.479530000	-4.382655000

H	7.602489000	3.855207000	-1.525407000
H	-7.752793000	2.855288000	-2.379994000
H	-7.246627000	-3.480846000	-4.995071000
H	7.098351000	-3.993162000	-4.911588000
H	-7.308562000	4.733750000	-3.974063000
H	7.194835000	5.215363000	-3.585076000
H	-1.928290000	-2.924770000	0.593902000
H	-0.876095000	1.305573000	5.144622000
H	-0.016190000	0.004854000	4.802886000
H	0.026565000	4.012031000	0.668669000
H	0.663772000	4.270704000	2.706417000
H	0.908050000	4.301998000	-0.621223000
H	1.962963000	-0.212167000	3.590038000
H	-1.935377000	2.794020000	0.846461000
H	-0.610745000	-2.047145000	5.072913000
H	0.893667000	-4.467786000	2.110465000
H	0.656128000	-4.426983000	-1.210709000
H	0.023370000	-4.145843000	0.814180000
O	-1.058314000	-0.105109000	2.196168000
O	-3.614327000	1.287992000	2.167293000
O	-3.616030000	1.358169000	-0.610370000
O	-3.609637000	-1.502099000	2.089846000
O	-2.048382000	-2.670766000	3.216158000
O	0.046303000	-4.091063000	1.837420000
O	2.075585000	-2.844649000	2.970858000
O	2.069935000	-2.649102000	-1.741231000
O	3.636924000	-1.529241000	2.021945000
O	3.621640000	-1.403016000	-0.716650000
O	3.643879000	1.281059000	2.103167000
O	3.601103000	1.417980000	-0.592368000
O	2.008517000	2.670323000	-1.548686000
O	2.098964000	2.428840000	3.275085000
O	1.065534000	1.402803000	0.786094000
O	1.413867000	-0.140742000	2.799505000
O	0.039285000	-1.557018000	4.557339000
O	-0.033833000	1.030173000	4.757719000
O	1.070405000	-1.533141000	0.682058000
O	-1.382391000	-2.133297000	0.672223000
O	-2.062843000	-2.523711000	-1.911798000
O	-0.038328000	-3.937393000	-0.754941000
O	-3.576837000	-1.395518000	-0.708427000
O	-0.007911000	3.765051000	2.235285000
O	0.044093000	3.958203000	-0.354253000
O	-1.384130000	2.002385000	0.818270000
O	-2.050016000	2.230039000	3.484333000
O	-2.047995000	2.488648000	-1.730699000

O	1.400600000	0.014516000	-1.329465000
O	-1.074910000	-0.029614000	-0.762542000
H	1.888074000	-0.052788000	-2.173211000
O	-0.039199000	1.395367000	-3.175517000
H	-0.864335000	1.600204000	-3.667493000
C	-2.708086000	4.576879000	-3.379960000
H	-2.147337000	4.846276000	-2.475293000
H	-2.094231000	3.829996000	-3.901764000
H	-2.781960000	5.463260000	-4.023294000
C	2.719442000	3.992014000	-3.881264000
H	2.276620000	2.997884000	-4.026162000
H	1.972654000	4.562740000	-3.310298000
H	2.827654000	4.473319000	-4.861835000
C	3.097346000	-5.065615000	-2.785135000
H	2.915950000	-5.182820000	-1.707175000
H	2.144354000	-4.723940000	-3.217830000
H	3.322470000	-6.057170000	-3.197861000
C	-3.332275000	-4.956360000	-2.969885000
H	-2.560740000	-4.911974000	-3.754916000
H	-2.815056000	-4.879300000	-2.006259000
H	-3.781039000	-5.956120000	-3.041877000
Hf	2.535462000	-0.086383000	0.698741000
Hf	-0.008280000	-1.887598000	2.472928000
Hf	0.030159000	1.685329000	2.572228000
Hf	-0.016739000	1.734677000	-0.957896000
Hf	-2.529870000	-0.078642000	0.725601000
Hf	0.022613000	-1.846094000	-1.128981000
C	-1.710525000	-2.573088000	-5.157045000
C	-0.285600000	-3.016588000	-4.807265000
C	0.400864000	-1.688884000	-4.444710000
C	-1.534682000	-1.117705000	-5.609304000
C	1.911245000	-1.703672000	-4.620812000
C	-2.377430000	-0.115515000	-4.840123000
H	2.289173000	-2.646468000	-4.188806000
H	0.197410000	-3.426319000	-5.715366000
H	-2.306689000	-2.596054000	-4.232791000
H	-1.111137000	1.133245000	-5.587918000
H	2.150014000	-1.693935000	-5.698103000
H	3.434115000	-0.625292000	-4.069639000
H	-2.285677000	-0.314466000	-3.754380000
H	-3.441677000	-0.222066000	-5.107042000
H	-0.829017000	-3.787409000	-3.113458000
H	0.075950000	0.408122000	-3.301374000
H	-1.855031000	-3.495623000	-6.852343000
H	-1.751900000	-1.024854000	-6.689296000
O	-2.393620000	-3.405432000	-6.057085000

O	2.476002000	-0.582265000	-3.961579000
O	-1.956204000	1.214663000	-5.119756000
O	0.031454000	-1.290567000	-3.196889000
O	-0.191203000	-3.998067000	-3.818467000
O	-0.148663000	-0.796357000	-5.439173000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087782000	2.699081000	3.458062000
H	4.064807000	-3.139272000	3.147279000
H	-4.032737000	2.554118000	3.675619000
H	-4.031747000	-2.980523000	3.390618000
C	5.423638000	-1.952098000	-2.714141000
C	-5.559063000	-2.181370000	-2.533592000
C	4.305020000	-2.775814000	-2.508499000
C	-4.302062000	-2.802229000	-2.502142000
C	4.164962000	-3.975306000	-3.246780000
C	-4.058437000	-3.955389000	-3.286390000
C	5.168919000	-4.286125000	-4.175124000
C	-5.105885000	-4.416564000	-4.095852000
C	6.260925000	-3.450121000	-4.393758000
C	-6.340500000	-3.775174000	-4.147418000
C	6.392464000	-2.272540000	-3.659324000
C	-6.574407000	-2.650252000	-3.358047000
C	5.583165000	3.107435000	-1.453664000
C	-5.583152000	2.267555000	-2.317951000
C	4.293751000	3.166847000	-2.004118000
C	-4.346364000	2.925154000	-2.224917000
C	4.047788000	3.952669000	-3.156199000
C	-4.154151000	4.170777000	-2.874523000
C	5.132425000	4.657170000	-3.698729000
C	-5.232610000	4.688610000	-3.607134000
C	6.403905000	4.611623000	-3.133350000
C	-6.447197000	4.016415000	-3.714977000
C	6.634866000	3.831817000	-2.001037000
C	-6.627823000	2.796270000	-3.065438000
H	5.506823000	-1.043479000	-2.110822000
H	-5.713362000	-1.313340000	-1.890194000
H	5.082673000	-5.216114000	-4.744026000

H	-4.941148000	-5.312618000	-4.700909000
H	7.248918000	-1.612885000	-3.814250000
H	-7.543574000	-2.147030000	-3.380329000
H	5.734242000	2.477648000	-0.574366000
H	-5.696620000	1.322656000	-1.784192000
H	4.965826000	5.257745000	-4.597500000
H	-5.107358000	5.654218000	-4.104640000
H	7.628908000	3.785408000	-1.551066000
H	-7.578405000	2.263599000	-3.136330000
H	-7.126536000	-4.163968000	-4.799525000
H	7.014909000	-3.724812000	-5.135259000
H	-7.257500000	4.453156000	-4.303596000
H	7.218625000	5.183481000	-3.584538000
H	-1.939277000	-2.930663000	0.600038000
H	-0.882199000	1.343014000	5.101167000
H	-0.015633000	0.043295000	4.793863000
H	0.025936000	4.004809000	0.612730000
H	0.657679000	4.281601000	2.670976000
H	0.913303000	4.262599000	-0.673486000
H	1.961444000	-0.196397000	3.582027000
H	-1.930895000	2.785011000	0.827902000
H	-0.609215000	-2.023253000	5.088184000
H	0.894558000	-4.447703000	2.149056000
H	0.611177000	-4.454658000	-1.175755000
H	0.013071000	-4.152052000	0.854923000
O	-1.063561000	-0.104530000	2.187969000
O	-3.615616000	1.291395000	2.163054000
O	-3.619991000	1.346500000	-0.628504000
O	-3.611406000	-1.504022000	2.089630000
O	-2.048596000	-2.662832000	3.225005000
O	0.039333000	-4.087517000	1.877432000
O	2.076211000	-2.840471000	2.982378000
O	2.084402000	-2.700309000	-1.697190000
O	3.632188000	-1.531362000	2.016917000
O	3.619371000	-1.398659000	-0.721603000
O	3.643785000	1.284274000	2.097716000
O	3.598266000	1.384059000	-0.626665000
O	2.020617000	2.691956000	-1.522835000
O	2.098518000	2.439139000	3.261157000
O	1.069201000	1.397575000	0.758362000
O	1.411838000	-0.134059000	2.791175000
O	0.039094000	-1.537656000	4.566319000
O	-0.032404000	1.063570000	4.733650000
O	1.058263000	-1.537212000	0.687605000
O	-1.395422000	-2.137251000	0.675629000
O	-2.044889000	-2.408771000	-1.940933000

O	-0.059841000	-3.946579000	-0.707229000
O	-3.625782000	-1.413626000	-0.707408000
O	-0.011294000	3.771283000	2.201348000
O	0.036774000	3.951309000	-0.405247000
O	-1.385042000	1.990504000	0.790212000
O	-2.048930000	2.241962000	3.470353000
O	-2.067774000	2.545889000	-1.709511000
O	1.357706000	-0.014579000	-1.364155000
O	-1.095365000	-0.041854000	-0.788952000
H	1.868926000	-0.027421000	-2.197003000
O	-0.036182000	1.748310000	-3.168211000
H	-0.800559000	2.253275000	-3.493263000
C	-2.884411000	4.962466000	-2.806030000
H	-2.489173000	5.037773000	-1.785431000
H	-2.078902000	4.499796000	-3.394981000
H	-3.044006000	5.975654000	-3.196103000
C	2.716596000	4.043303000	-3.836336000
H	2.243259000	3.062787000	-3.976989000
H	1.992342000	4.624930000	-3.247037000
H	2.818630000	4.531854000	-4.814127000
C	3.019977000	-4.926449000	-3.079342000
H	2.831091000	-5.157269000	-2.022305000
H	2.078077000	-4.516082000	-3.473265000
H	3.222219000	-5.868924000	-3.603985000
C	-2.771695000	-4.720860000	-3.261191000
H	-1.945218000	-4.175357000	-3.739724000
H	-2.415406000	-4.908431000	-2.239744000
H	-2.890050000	-5.685482000	-3.772959000
Hf	2.526186000	-0.077934000	0.690365000
Hf	-0.014224000	-1.878033000	2.488844000
Hf	0.035043000	1.695268000	2.531207000
Hf	-0.022207000	1.722598000	-1.034501000
Hf	-2.532282000	-0.080858000	0.715537000
Hf	0.014763000	-1.865643000	-1.095934000
C	-1.578027000	-1.677715000	-5.360148000
C	-0.162503000	-2.207803000	-5.528505000
C	0.628745000	-1.520914000	-4.426958000
C	-1.451792000	-0.152550000	-5.378159000
C	2.082461000	-1.242207000	-4.705128000
C	-2.491433000	0.504353000	-4.501430000
H	2.585351000	-2.228093000	-4.629141000
H	0.231655000	-1.882634000	-6.516234000
H	-1.936369000	-2.017383000	-4.372779000
H	-3.191202000	2.299657000	-4.229732000
H	2.193755000	-0.891683000	-5.744381000
H	3.577062000	-0.426608000	-3.756245000

H	-2.293864000	0.234221000	-3.440907000
H	-3.474826000	0.073334000	-4.772642000
H	-0.910368000	-3.953970000	-5.758307000
H	-0.019853000	0.855609000	-4.147062000
H	-2.254415000	-1.869458000	-7.166066000
H	-1.603853000	0.205061000	-6.418260000
O	-2.472639000	-2.225342000	-6.294406000
O	2.616831000	-0.320058000	-3.788663000
O	-2.455102000	1.897554000	-4.710849000
O	0.214989000	-1.692484000	-3.256291000
O	-0.089621000	-3.598348000	-5.388017000
O	-0.110490000	0.145684000	-5.009672000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087969000	2.685450000	3.471962000
H	4.065926000	-3.150436000	3.128325000
H	-4.030563000	2.549653000	3.681942000
H	-4.031670000	-2.993404000	3.374274000
C	5.402097000	-1.906139000	-2.739829000
C	-5.439927000	-1.701567000	-2.651305000
C	4.299343000	-2.750340000	-2.528796000
C	-4.349369000	-2.585542000	-2.573613000
C	4.171178000	-3.945304000	-3.276704000
C	-4.324894000	-3.744866000	-3.378635000
C	5.168242000	-4.229910000	-4.220965000
C	-5.409788000	-3.959649000	-4.241860000
C	6.242724000	-3.373064000	-4.445506000
C	-6.468903000	-3.064541000	-4.335884000
C	6.363790000	-2.200859000	-3.700705000
C	-6.486129000	-1.921889000	-3.535412000
C	5.491190000	3.321425000	-1.096584000
C	-5.650458000	2.540423000	-2.013390000
C	4.311490000	3.254682000	-1.852859000
C	-4.339352000	3.031912000	-2.107650000
C	4.186200000	4.018112000	-3.037433000
C	-4.084424000	4.235357000	-2.810419000
C	5.265859000	4.833527000	-3.402039000
C	-5.179257000	4.880460000	-3.401455000

C	6.422964000	4.915421000	-2.631276000
C	-6.472836000	4.372333000	-3.323812000
C	6.539601000	4.154392000	-1.469742000
C	-6.714648000	3.193031000	-2.621749000
H	5.479150000	-1.003243000	-2.127464000
H	-5.429136000	-0.820951000	-2.006774000
H	5.091914000	-5.156785000	-4.796266000
H	-5.408600000	-4.859620000	-4.863252000
H	7.207669000	-1.525976000	-3.858767000
H	-7.312354000	-1.210079000	-3.597397000
H	5.558329000	2.705246000	-0.197095000
H	-5.813056000	1.624657000	-1.443370000
H	5.191564000	5.417857000	-4.323474000
H	-5.001769000	5.814510000	-3.941713000
H	7.444431000	4.205700000	-0.860493000
H	-7.726073000	2.788302000	-2.544088000
H	-7.286840000	-3.262194000	-5.033045000
H	6.992027000	-3.627967000	-5.198626000
H	-7.295011000	4.905453000	-3.807729000
H	7.238638000	5.570981000	-2.945600000
H	-1.950246000	-2.933080000	0.624432000
H	-0.874523000	1.384367000	5.088828000
H	-0.011611000	0.081038000	4.796553000
H	0.034754000	3.985708000	0.576298000
H	0.649195000	4.298280000	2.639142000
H	0.904279000	4.258716000	-0.720671000
H	1.964249000	-0.169310000	3.577564000
H	-1.944835000	2.773963000	0.799535000
H	-0.609156000	-1.988205000	5.119796000
H	0.894550000	-4.450961000	2.185804000
H	0.727507000	-4.443110000	-1.087546000
H	0.007975000	-4.167922000	0.898228000
O	-1.059190000	-0.100962000	2.182061000
O	-3.617798000	1.286155000	2.168738000
O	-3.618688000	1.319744000	-0.644767000
O	-3.607897000	-1.501494000	2.092969000
O	-2.049877000	-2.652486000	3.242680000
O	0.038913000	-4.091634000	1.913884000
O	2.077748000	-2.831527000	3.001008000
O	2.082859000	-2.703690000	-1.702345000
O	3.629762000	-1.528234000	2.020238000
O	3.619701000	-1.414537000	-0.708950000
O	3.644494000	1.288011000	2.092308000
O	3.585525000	1.381933000	-0.628121000
O	2.026899000	2.647535000	-1.620654000
O	2.098362000	2.448774000	3.247166000

O	1.064962000	1.400690000	0.731570000
O	1.409663000	-0.119968000	2.789197000
O	0.037272000	-1.511984000	4.587030000
O	-0.026903000	1.097965000	4.721315000
O	1.065167000	-1.555533000	0.714351000
O	-1.384015000	-2.155932000	0.702860000
O	-2.057430000	-2.503246000	-1.919859000
O	-0.026918000	-3.981445000	-0.705532000
O	-3.583753000	-1.448686000	-0.667043000
O	-0.010134000	3.777677000	2.167437000
O	0.044432000	3.917001000	-0.440166000
O	-1.394396000	1.981746000	0.774205000
O	-2.046182000	2.251825000	3.457579000
O	-2.059163000	2.483074000	-1.739063000
O	1.364717000	-0.055567000	-1.343068000
O	-1.100628000	-0.074144000	-0.801689000
H	1.843087000	-0.086591000	-2.191395000
O	0.043120000	1.774351000	-3.188636000
H	0.897106000	2.106610000	-3.491134000
C	-2.733879000	4.867724000	-2.935926000
H	-2.225654000	4.971046000	-1.968404000
H	-2.057270000	4.265478000	-3.557104000
H	-2.819775000	5.861985000	-3.393396000
C	2.990482000	3.959141000	-3.938749000
H	2.737612000	2.923033000	-4.209410000
H	2.090293000	4.386412000	-3.475394000
H	3.180129000	4.505105000	-4.871441000
C	3.047488000	-4.920468000	-3.102480000
H	2.862626000	-5.149466000	-2.044614000
H	2.097452000	-4.535415000	-3.502754000
H	3.269681000	-5.861595000	-3.621165000
C	-3.220826000	-4.756198000	-3.372959000
H	-2.542086000	-4.573377000	-4.221963000
H	-2.621412000	-4.754068000	-2.455938000
H	-3.624306000	-5.766279000	-3.527143000
Hf	2.518925000	-0.078185000	0.695619000
Hf	-0.019497000	-1.870880000	2.518344000
Hf	0.030653000	1.707077000	2.509161000
Hf	-0.043068000	1.694717000	-1.073522000
Hf	-2.540117000	-0.076401000	0.713973000
Hf	0.012581000	-1.890794000	-1.041956000
C	-1.738897000	-1.828365000	-5.258452000
C	-0.327843000	-2.424613000	-5.356094000
C	0.548823000	-1.644268000	-4.399553000
C	-1.645593000	-0.301264000	-5.396299000
C	1.971729000	-1.343740000	-4.767152000

C	-2.580802000	0.419427000	-4.439791000
H	2.490828000	-2.322765000	-4.703278000
H	0.054237000	-2.355281000	-6.388890000
H	-2.097406000	-2.076730000	-4.243030000
H	-1.760370000	2.106601000	-4.026453000
H	2.020888000	-1.014635000	-5.818208000
H	3.495310000	-0.544364000	-3.859236000
H	-2.349679000	0.082954000	-3.404278000
H	-3.610286000	0.084474000	-4.655166000
H	-0.669211000	-3.853072000	-4.105547000
H	-0.210907000	0.727033000	-4.412878000
H	-2.406403000	-2.208382000	-7.033493000
H	-1.904998000	-0.020391000	-6.435612000
O	-2.660807000	-2.420484000	-6.126887000
O	2.539312000	-0.400975000	-3.892360000
O	-2.515470000	1.806781000	-4.564091000
O	0.180975000	-1.650906000	-3.214362000
O	-0.275934000	-3.782452000	-4.990596000
O	-0.285225000	0.084494000	-5.187263000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.086730000	2.697232000	3.461302000
H	4.062881000	-3.142265000	3.146333000
H	-4.031718000	2.553262000	3.677610000
H	-4.031248000	-2.968578000	3.405269000
C	5.603252000	-2.262825000	-2.337905000
C	-5.599330000	-2.323162000	-2.415060000
C	4.336109000	-2.861868000	-2.414656000
C	-4.326028000	-2.914881000	-2.380939000
C	4.121104000	-3.941756000	-3.307392000
C	-4.087623000	-4.141792000	-3.048378000
C	5.207303000	-4.364700000	-4.086593000
C	-5.160760000	-4.710124000	-3.750538000
C	6.457664000	-3.757165000	-4.009385000
C	-6.410956000	-4.100445000	-3.810697000
C	6.659910000	-2.697062000	-3.128294000
C	-6.637186000	-2.899225000	-3.137770000
C	5.607800000	3.010423000	-1.493988000

C	-5.663152000	2.655383000	-1.871397000
C	4.300599000	3.182675000	-1.974812000
C	-4.335510000	3.048033000	-2.099586000
C	4.049537000	4.099807000	-3.025140000
C	-4.062175000	4.168111000	-2.923881000
C	5.145120000	4.808047000	-3.539760000
C	-5.158633000	4.837911000	-3.486856000
C	6.435783000	4.641798000	-3.045756000
C	-6.471281000	4.434963000	-3.260651000
C	6.672248000	3.736342000	-2.013048000
C	-6.728885000	3.334778000	-2.444363000
H	5.731622000	-1.432532000	-1.641606000
H	-5.739845000	-1.387051000	-1.869807000
H	5.059950000	-5.203289000	-4.773013000
H	-5.001954000	-5.662456000	-4.263802000
H	7.634998000	-2.210709000	-3.057323000
H	-7.619234000	-2.422136000	-3.168278000
H	5.763191000	2.287814000	-0.690900000
H	-5.831422000	1.784514000	-1.236290000
H	4.971202000	5.511569000	-4.358964000
H	-4.966382000	5.708792000	-4.119899000
H	7.680321000	3.594186000	-1.617717000
H	-7.754488000	3.009182000	-2.257476000
H	-7.216178000	-4.572139000	-4.379122000
H	7.275516000	-4.117149000	-4.638395000
H	-7.294894000	4.986429000	-3.721179000
H	7.259072000	5.219268000	-3.473601000
H	-1.939254000	-2.931885000	0.583688000
H	-0.881818000	1.347141000	5.091467000
H	-0.016392000	0.048294000	4.785249000
H	0.010785000	4.012864000	0.600492000
H	0.657240000	4.289573000	2.657660000
H	0.882886000	4.286918000	-0.692601000
H	1.958995000	-0.199135000	3.569373000
H	-1.950817000	2.786979000	0.826537000
H	-0.604493000	-2.028934000	5.083934000
H	0.905142000	-4.435596000	2.103913000
H	0.641266000	-4.412356000	-1.222599000
H	0.017383000	-4.138618000	0.821227000
O	-1.065132000	-0.104729000	2.176681000
O	-3.617014000	1.286089000	2.168219000
O	-3.618993000	1.353575000	-0.614837000
O	-3.609302000	-1.508768000	2.083811000
O	-2.046395000	-2.672420000	3.212764000
O	0.042810000	-4.086795000	1.838127000
O	2.073532000	-2.848371000	2.968484000

O	2.059163000	-2.604184000	-1.798470000
O	3.631552000	-1.520908000	2.033580000
O	3.605311000	-1.441264000	-0.677845000
O	3.644681000	1.284491000	2.098213000
O	3.590815000	1.380362000	-0.626444000
O	2.022254000	2.693081000	-1.526647000
O	2.097422000	2.439885000	3.257019000
O	1.062209000	1.404147000	0.753354000
O	1.405710000	-0.134620000	2.781180000
O	0.037290000	-1.540278000	4.557036000
O	-0.032523000	1.066612000	4.723693000
O	1.056429000	-1.550611000	0.680207000
O	-1.395843000	-2.137366000	0.648235000
O	-2.053683000	-2.358638000	-2.013165000
O	-0.055015000	-3.919053000	-0.775510000
O	-3.618641000	-1.411842000	-0.713183000
O	-0.012435000	3.777663000	2.190889000
O	0.013775000	3.961872000	-0.417622000
O	-1.395804000	1.999058000	0.778043000
O	-2.047700000	2.247051000	3.463301000
O	-2.062377000	2.453989000	-1.782742000
O	1.377196000	-0.018779000	-1.333545000
O	-1.085233000	-0.039224000	-0.792002000
H	1.923028000	0.001528000	-2.144863000
O	0.140294000	1.728346000	-3.141449000
H	-0.607607000	1.849867000	-3.734893000
C	-2.689281000	4.690212000	-3.220728000
H	-2.103470000	4.875452000	-2.310786000
H	-2.090219000	3.977155000	-3.805237000
H	-2.753573000	5.625512000	-3.792217000
C	2.700740000	4.342010000	-3.630274000
H	2.177061000	3.412437000	-3.885371000
H	2.024594000	4.868806000	-2.940906000
H	2.793908000	4.957336000	-4.534894000
C	2.821844000	-4.674322000	-3.453343000
H	2.463116000	-5.064090000	-2.490810000
H	2.011771000	-4.036333000	-3.833867000
H	2.935812000	-5.524825000	-4.137720000
C	-2.768844000	-4.849454000	-3.030483000
H	-2.026298000	-4.349496000	-3.669955000
H	-2.307631000	-4.864773000	-2.034728000
H	-2.881544000	-5.880753000	-3.388595000
Hf	2.523223000	-0.067861000	0.692558000
Hf	-0.020066000	-1.876588000	2.481626000
Hf	0.032777000	1.703084000	2.518555000
Hf	-0.032509000	1.742036000	-1.059121000

Hf	-2.534384000	-0.065270000	0.703964000
Hf	0.026972000	-1.828793000	-1.096768000
C	-1.440449000	-0.450491000	-5.898425000
C	-0.321077000	-1.517637000	-5.735467000
C	0.520996000	-1.154582000	-4.522408000
C	-2.494781000	-0.517417000	-4.801851000
C	1.786637000	-0.394531000	-4.816894000
C	-3.489877000	0.633797000	-4.844793000
H	2.533580000	-1.185567000	-5.039676000
H	0.337550000	-1.426412000	-6.623787000
H	-1.960447000	-0.682650000	-6.849905000
H	-5.079915000	-0.348037000	-4.353861000
H	1.641809000	0.128477000	-5.784404000
H	1.512641000	1.086562000	-3.643688000
H	-3.828153000	0.805024000	-5.885761000
H	-3.013685000	1.564047000	-4.501946000
H	-1.737511000	-2.768507000	-5.388382000
H	-3.601574000	-2.021918000	-4.196684000
H	-0.469556000	1.019005000	-6.744978000
H	-2.020858000	-0.527784000	-3.800837000
O	-0.912829000	0.857787000	-5.905254000
O	2.265166000	0.438452000	-3.831684000
O	-4.564191000	0.377060000	-3.978734000
O	0.165327000	-1.502334000	-3.404598000
O	-0.807400000	-2.815469000	-5.682403000
O	-3.182617000	-1.747254000	-5.026474000

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C	-3.248200000	-2.182800000	-1.650100000
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C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087747000	2.715414000	3.440542000
H	4.062236000	-3.146245000	3.141053000
H	-4.032007000	2.572449000	3.659352000
H	-4.032756000	-2.984663000	3.383685000
C	5.627133000	-2.361045000	-2.267761000
C	-5.262102000	-1.596473000	-2.931155000
C	4.328098000	-2.872088000	-2.416009000
C	-4.325514000	-2.584783000	-2.595668000
C	4.078030000	-3.891085000	-3.370433000
C	-4.376330000	-3.857443000	-3.200277000

C	5.163668000	-4.341602000	-4.135228000
C	-5.379781000	-4.078982000	-4.153408000
C	6.447034000	-3.824781000	-3.982073000
C	-6.282979000	-3.082921000	-4.516215000
C	6.683764000	-2.826142000	-3.039851000
C	-6.228856000	-1.832623000	-3.900792000
C	5.527922000	3.251801000	-1.262535000
C	-5.671365000	2.403936000	-1.998172000
C	4.290978000	3.229206000	-1.924452000
C	-4.358332000	2.787611000	-2.316251000
C	4.096975000	4.010091000	-3.088753000
C	-4.126190000	3.605216000	-3.449534000
C	5.171430000	4.794338000	-3.529479000
C	-5.237423000	3.996462000	-4.210771000
C	6.387962000	4.829855000	-2.853068000
C	-6.534021000	3.606395000	-3.887322000
C	6.570725000	4.053443000	-1.710323000
C	-6.755253000	2.802842000	-2.770192000
H	5.782391000	-1.576252000	-1.526181000
H	-5.191079000	-0.627737000	-2.428662000
H	4.987446000	-5.128457000	-4.874032000
H	-5.447106000	-5.064202000	-4.623523000
H	7.685043000	-2.410510000	-2.908798000
H	-6.930974000	-1.043725000	-4.181487000
H	5.644946000	2.623385000	-0.377197000
H	-5.816600000	1.769654000	-1.122366000
H	5.044515000	5.390469000	-4.437503000
H	-5.070098000	4.628473000	-5.087823000
H	7.522412000	4.067584000	-1.175006000
H	-7.766344000	2.491083000	-2.499582000
H	-7.038000000	-3.287538000	-5.279138000
H	7.262793000	-4.205685000	-4.601430000
H	-7.371764000	3.936885000	-4.506644000
H	7.197984000	5.460757000	-3.226917000
H	-1.929718000	-2.923513000	0.605241000
H	-0.883058000	1.316289000	5.144480000
H	-0.017421000	0.016415000	4.814964000
H	0.054170000	4.010324000	0.667221000
H	0.669083000	4.272801000	2.715130000
H	0.985489000	4.245314000	-0.595891000
H	1.966553000	-0.204618000	3.599493000
H	-1.918144000	2.795439000	0.841370000
H	-0.614607000	-2.034333000	5.089335000
H	0.879558000	-4.466832000	2.175747000
H	0.685078000	-4.445533000	-1.124293000
H	0.027272000	-4.150259000	0.863138000

O	-1.056818000	-0.101540000	2.200145000
O	-3.614901000	1.284665000	2.170515000
O	-3.604272000	1.383470000	-0.580967000
O	-3.611137000	-1.501204000	2.091656000
O	-2.049893000	-2.659171000	3.229117000
O	0.036957000	-4.088391000	1.890645000
O	2.076319000	-2.836107000	2.982912000
O	2.069112000	-2.643349000	-1.734414000
O	3.638818000	-1.528084000	2.024957000
O	3.615565000	-1.402594000	-0.708061000
O	3.643660000	1.280706000	2.103520000
O	3.589241000	1.415518000	-0.593424000
O	2.009475000	2.645619000	-1.595281000
O	2.100463000	2.429152000	3.279672000
O	1.081736000	1.405797000	0.790107000
O	1.415232000	-0.136819000	2.810259000
O	0.037171000	-1.546085000	4.574128000
O	-0.036941000	1.041441000	4.765469000
O	1.066294000	-1.525912000	0.697077000
O	-1.382047000	-2.133368000	0.686753000
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O	-0.010300000	-3.948520000	-0.680812000
O	-3.580669000	-1.410841000	-0.696740000
O	-0.000129000	3.767400000	2.240174000
O	0.096384000	3.949677000	-0.353757000
O	-1.368757000	2.002295000	0.831663000
O	-2.051026000	2.231433000	3.485879000
O	-2.065208000	2.578347000	-1.676312000
O	1.368607000	-0.002395000	-1.346488000
O	-1.089696000	-0.025694000	-0.769109000
H	1.845334000	-0.023867000	-2.198843000
O	-0.098759000	1.646611000	-3.198182000
H	-0.299424000	2.523415000	-3.551543000
C	-2.771596000	4.049027000	-3.908894000
H	-2.207628000	4.569619000	-3.124135000
H	-2.160367000	3.183474000	-4.206405000
H	-2.858049000	4.711699000	-4.779960000
C	2.831837000	4.008832000	-3.891531000
H	2.487241000	2.988757000	-4.107203000
H	2.005947000	4.507263000	-3.362867000
H	2.982869000	4.530136000	-4.845638000
C	2.742470000	-4.528749000	-3.606164000
H	2.353852000	-5.010495000	-2.698288000
H	1.970001000	-3.807183000	-3.905690000
H	2.818465000	-5.297439000	-4.386127000
C	-3.428911000	-4.962585000	-2.847623000

H	-2.503528000	-4.906017000	-3.439401000
H	-3.118205000	-4.939976000	-1.795582000
H	-3.881263000	-5.941538000	-3.053169000
Hf	2.542839000	-0.096020000	0.696157000
Hf	-0.006611000	-1.882428000	2.491434000
Hf	0.036401000	1.687392000	2.578145000
Hf	-0.009982000	1.716925000	-0.939914000
Hf	-2.530875000	-0.079641000	0.732846000
Hf	0.016488000	-1.870004000	-1.103669000
C	-1.874495000	0.034754000	-5.080046000
C	-0.697012000	-2.150396000	-5.272981000
C	0.241287000	-1.552135000	-4.459488000
C	-3.040831000	-0.519953000	-5.824008000
C	1.487710000	-0.883173000	-4.983667000
C	-4.191010000	0.481523000	-5.757105000
H	2.290748000	-1.638357000	-5.052163000
H	-0.624518000	-2.175738000	-6.361330000
H	-1.098635000	0.540801000	-5.692061000
H	-5.904922000	0.615115000	-6.658085000
H	1.321028000	-0.530477000	-6.020871000
H	1.263058000	0.765281000	-3.961532000
H	-3.843123000	1.470895000	-6.119112000
H	-4.513583000	0.603374000	-4.705844000
H	-1.669802000	-2.818219000	-3.781033000
H	-3.492356000	-0.901614000	-7.634019000
H	-1.019187000	0.991415000	-3.459919000
H	-3.375114000	-1.450730000	-5.316769000
O	-1.993871000	0.287420000	-3.852812000
O	1.985157000	0.132593000	-4.147480000
O	-5.204756000	-0.040735000	-6.581690000
O	0.064995000	-1.591196000	-3.180397000
O	-1.663372000	-2.933957000	-4.758193000
O	-2.666065000	-0.752762000	-7.154993000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000
C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.087733000	2.718672000	3.436833000
H	4.061701000	-3.145111000	3.143524000
H	-4.031972000	2.575215000	3.656541000

H	-4.032601000	-2.982587000	3.386548000
C	5.610384000	-2.299345000	-2.326141000
C	-5.342591000	-1.652771000	-2.830793000
C	4.330571000	-2.869175000	-2.414600000
C	-4.351400000	-2.607066000	-2.562783000
C	4.097290000	-3.939243000	-3.315763000
C	-4.396569000	-3.879113000	-3.173350000
C	5.179605000	-4.379689000	-4.090908000
C	-5.449317000	-4.130366000	-4.065165000
C	6.442926000	-3.802153000	-4.000325000
C	-6.417461000	-3.170395000	-4.353577000
C	6.663160000	-2.753049000	-3.110376000
C	-6.369689000	-1.921168000	-3.730126000
C	5.527050000	3.252582000	-1.270401000
C	-5.674337000	2.464472000	-1.948728000
C	4.290830000	3.222815000	-1.933445000
C	-4.358609000	2.815165000	-2.293719000
C	4.098844000	3.989857000	-3.107089000
C	-4.129998000	3.634058000	-3.426972000
C	5.173841000	4.768658000	-3.555752000
C	-5.246233000	4.054560000	-4.163982000
C	6.389409000	4.812004000	-2.878021000
C	-6.544886000	3.696279000	-3.814540000
C	6.570499000	4.048857000	-1.726126000
C	-6.763340000	2.896064000	-2.694907000
H	5.753190000	-1.477039000	-1.623611000
H	-5.278882000	-0.687427000	-2.321181000
H	5.017307000	-5.207483000	-4.786883000
H	-5.512379000	-5.115289000	-4.536008000
H	7.648791000	-2.290081000	-3.028642000
H	-7.128678000	-1.162130000	-3.939334000
H	5.643086000	2.634238000	-0.377857000
H	-5.817536000	1.831594000	-1.071570000
H	5.048391000	5.353738000	-4.471102000
H	-5.082340000	4.683064000	-5.043789000
H	7.521496000	4.068976000	-1.189818000
H	-7.776498000	2.610075000	-2.404454000
H	-7.225130000	-3.408078000	-5.051606000
H	7.256501000	-4.176074000	-4.626765000
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H	7.200022000	5.438343000	-3.258119000
H	-1.929358000	-2.920799000	0.604842000
H	-0.879060000	1.304836000	5.160041000
H	-0.017844000	0.003719000	4.815711000
H	0.052891000	4.012477000	0.678207000
H	0.670398000	4.270355000	2.722200000

H	0.982426000	4.253944000	-0.585926000
H	1.965962000	-0.209176000	3.601317000
H	-1.916450000	2.799837000	0.845774000
H	-0.614853000	-2.041740000	5.081374000
H	0.879775000	-4.467858000	2.161844000
H	0.656201000	-4.451285000	-1.150564000
H	0.028618000	-4.146522000	0.847493000
O	-1.055593000	-0.100361000	2.199793000
O	-3.613937000	1.284930000	2.170224000
O	-3.603986000	1.385119000	-0.579679000
O	-3.612035000	-1.500710000	2.091938000
O	-2.049504000	-2.661379000	3.224831000
O	0.038363000	-4.086775000	1.876961000
O	2.075976000	-2.837427000	2.978731000
O	2.070826000	-2.642261000	-1.739193000
O	3.640063000	-1.527415000	2.026262000
O	3.613915000	-1.399569000	-0.708865000
O	3.643043000	1.280662000	2.103802000
O	3.588290000	1.421008000	-0.588129000
O	2.007430000	2.647375000	-1.594429000
O	2.100756000	2.426386000	3.284290000
O	1.081754000	1.409419000	0.799463000
O	1.415279000	-0.138115000	2.811903000
O	0.036844000	-1.550922000	4.568482000
O	-0.037056000	1.030744000	4.771780000
O	1.068579000	-1.521637000	0.693630000
O	-1.384632000	-2.128334000	0.682070000
O	-2.075390000	-2.544323000	-1.914921000
O	-0.019041000	-3.943749000	-0.688409000
O	-3.577399000	-1.404309000	-0.700406000
O	0.000098000	3.765706000	2.247868000
O	0.095352000	3.952432000	-0.343753000
O	-1.368438000	2.005633000	0.837528000
O	-2.051541000	2.228570000	3.489826000
O	-2.058703000	2.559042000	-1.688041000
O	1.369606000	0.011786000	-1.346913000
O	-1.089046000	-0.018230000	-0.769800000
H	1.842978000	-0.003569000	-2.203761000
O	-0.075883000	1.694341000	-3.238894000
H	-0.296733000	2.578490000	-3.564301000
C	-2.775384000	4.055969000	-3.908047000
H	-2.185878000	4.554317000	-3.127413000
H	-2.190479000	3.182977000	-4.235529000
H	-2.866347000	4.733582000	-4.766859000
C	2.835011000	3.978287000	-3.911928000
H	2.492299000	2.955023000	-4.115532000

H	2.008975000	4.484266000	-3.390539000
H	2.987303000	4.487243000	-4.872435000
C	2.783538000	-4.641011000	-3.480700000
H	2.423686000	-5.060743000	-2.531181000
H	1.982843000	-3.973584000	-3.830665000
H	2.879323000	-5.467118000	-4.197150000
C	-3.403150000	-4.960208000	-2.881707000
H	-2.510960000	-4.868920000	-3.517945000
H	-3.042749000	-4.938725000	-1.845971000
H	-3.839079000	-5.948239000	-3.078075000
Hf	2.544925000	-0.099518000	0.697202000
Hf	-0.004904000	-1.884365000	2.483138000
Hf	0.034499000	1.685320000	2.590438000
Hf	-0.002884000	1.716826000	-0.917810000
Hf	-2.529550000	-0.079236000	0.733091000
Hf	0.017169000	-1.864130000	-1.119550000
C	-2.032788000	0.018236000	-5.125153000
C	-0.482003000	-2.351195000	-5.259962000
C	0.351988000	-1.654753000	-4.434890000
C	-3.116435000	-0.735518000	-5.809859000
C	1.663489000	-1.059498000	-4.869981000
C	-4.414878000	0.081640000	-5.821957000
H	2.472376000	-1.794693000	-4.712458000
H	-0.336054000	-2.454293000	-6.335808000
H	-1.233057000	0.436695000	-5.782628000
H	-5.683013000	-1.358499000	-5.987601000
H	1.649100000	-0.847576000	-5.956208000
H	1.302927000	0.692276000	-4.067653000
H	-4.251262000	1.034191000	-6.351290000
H	-4.723648000	0.322172000	-4.787797000
H	-1.582658000	-2.876373000	-3.802515000
H	-3.540422000	-1.271319000	-7.583977000
H	-0.904338000	1.128384000	-3.462662000
H	-3.302496000	-1.652462000	-5.205474000
O	-2.101593000	0.294845000	-3.927545000
O	2.051525000	0.074581000	-4.116080000
O	-5.396373000	-0.617064000	-6.542208000
O	0.049874000	-1.581818000	-3.160648000
O	-1.522972000	-3.061392000	-4.765576000
O	-2.723956000	-1.042557000	-7.117336000

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C	-3.248200000	-2.182800000	-1.650100000
C	-3.229700000	-2.386600000	2.900000000
C	-3.232300000	2.034300000	3.104000000
C	3.276900000	2.142000000	2.939200000

C	3.226900000	2.366300000	-1.338700000
C	3.259300000	-2.277900000	-1.561500000
C	-3.265300000	2.236100000	-1.457300000
C	3.257200000	-2.506600000	2.716400000
H	4.085775000	2.687888000	3.472374000
H	4.064598000	-3.142654000	3.142407000
H	-4.032753000	2.536427000	3.690595000
H	-4.031839000	-2.985569000	3.383976000
C	5.456255000	-2.000165000	-2.674769000
C	-5.606543000	-2.205406000	-2.379751000
C	4.268419000	-2.743397000	-2.565499000
C	-4.322882000	-2.758805000	-2.506071000
C	4.039281000	-3.836140000	-3.438850000
C	-4.083085000	-3.790050000	-3.447200000
C	5.027778000	-4.121230000	-4.392956000
C	-5.171142000	-4.226266000	-4.216273000
C	6.194058000	-3.369158000	-4.503715000
C	-6.439732000	-3.666453000	-4.091985000
C	6.413364000	-2.298722000	-3.638208000
C	-6.662731000	-2.643345000	-3.170165000
C	5.549962000	3.208059000	-1.305896000
C	-5.678278000	2.697529000	-1.685640000
C	4.293180000	3.222069000	-1.929609000
C	-4.364747000	3.093575000	-1.983920000
C	4.077080000	4.022805000	-3.077159000
C	-4.135108000	4.284430000	-2.720209000
C	5.156404000	4.788520000	-3.540844000
C	-5.261073000	5.003514000	-3.147048000
C	6.394096000	4.787480000	-2.903168000
C	-6.560963000	4.594974000	-2.857558000
C	6.596101000	3.992463000	-1.775960000
C	-6.774238000	3.436581000	-2.112663000
H	5.600791000	-1.168637000	-1.980827000
H	-5.750472000	-1.401515000	-1.654890000
H	4.869318000	-4.966099000	-5.069088000
H	-5.008078000	-5.029025000	-4.940482000
H	7.325771000	-1.702962000	-3.709402000
H	-7.648108000	-2.183336000	-3.072190000
H	5.679444000	2.565579000	-0.432244000
H	-5.816851000	1.780658000	-1.111033000
H	5.013844000	5.401920000	-4.435058000
H	-5.103222000	5.923076000	-3.717197000
H	7.563915000	3.980587000	-1.270091000
H	-7.787163000	3.110831000	-1.862855000
H	-7.256815000	-4.031103000	-4.719569000
H	6.934163000	-3.623971000	-5.266026000

H	-7.406705000	5.194157000	-3.205045000
H	7.205719000	5.406193000	-3.293972000
H	-1.941279000	-2.941478000	0.625159000
H	-0.874402000	1.380848000	5.079533000
H	-0.014015000	0.075077000	4.785619000
H	0.025855000	3.993444000	0.558566000
H	0.650498000	4.294702000	2.619704000
H	0.902632000	4.246001000	-0.737803000
H	1.962100000	-0.174709000	3.576626000
H	-1.932016000	2.778491000	0.793719000
H	-0.612258000	-1.993556000	5.100050000
H	0.902964000	-4.444461000	2.171240000
H	0.598394000	-4.494190000	-1.137901000
H	-0.000002000	-4.170189000	0.889938000
O	-1.060799000	-0.099441000	2.180812000
O	-3.613274000	1.295481000	2.157950000
O	-3.597608000	1.288374000	-0.674895000
O	-3.607961000	-1.501723000	2.091571000
O	-2.048397000	-2.658833000	3.231328000
O	0.043922000	-4.087978000	1.906794000
O	2.076761000	-2.829106000	2.997608000
O	2.106522000	-2.768371000	-1.593098000
O	3.632365000	-1.538739000	2.005951000
O	3.628477000	-1.368493000	-0.754886000
O	3.646037000	1.281868000	2.099947000
O	3.594586000	1.386081000	-0.623324000
O	2.018073000	2.651759000	-1.576687000
O	2.096480000	2.451981000	3.240320000
O	1.067337000	1.388338000	0.727062000
O	1.413541000	-0.122847000	2.784268000
O	0.035751000	-1.513388000	4.572776000
O	-0.026508000	1.093243000	4.713635000
O	1.063752000	-1.539530000	0.698018000
O	-1.386242000	-2.154365000	0.683868000
O	-2.042502000	-2.375550000	-1.981928000
O	-0.086942000	-3.983671000	-0.692801000
O	-3.607904000	-1.472235000	-0.662469000
O	-0.009999000	3.773349000	2.150269000
O	0.032628000	3.926741000	-0.458294000
O	-1.387355000	1.982587000	0.755314000
O	-2.046061000	2.255924000	3.454776000
O	-2.068973000	2.496044000	-1.764098000
O	1.351032000	-0.050919000	-1.409956000
O	-1.072085000	-0.075831000	-0.788763000
H	1.939206000	-0.035452000	-2.189873000
O	-0.062239000	1.744125000	-3.230197000

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C	-2.781697000	4.827728000	-3.050637000
H	-2.145248000	4.931194000	-2.162200000
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H	-2.873325000	5.809792000	-3.532397000
C	2.784289000	4.067042000	-3.831739000
H	2.367443000	3.068279000	-4.014676000
H	1.999320000	4.602623000	-3.277839000
H	2.919273000	4.577470000	-4.794212000
C	2.821787000	-4.708223000	-3.397768000
H	2.667304000	-5.143122000	-2.400842000
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C	-2.750848000	-4.439184000	-3.659947000
H	-2.039559000	-3.753857000	-4.143741000
H	-2.270148000	-4.738607000	-2.719704000
H	-2.855594000	-5.323478000	-4.301918000
Hf	2.530446000	-0.079588000	0.684918000
Hf	-0.014219000	-1.869783000	2.501302000
Hf	0.036165000	1.703350000	2.502960000
Hf	-0.031020000	1.697280000	-1.072332000
Hf	-2.526780000	-0.085814000	0.704156000
Hf	0.030134000	-1.909550000	-1.071450000
C	-0.538861000	-0.352501000	-4.775460000
C	0.515485000	-1.134443000	-4.270189000
C	1.918870000	-0.934297000	-4.783227000
H	2.325608000	-1.931118000	-5.030748000
H	-0.480608000	0.031179000	-5.801777000
H	1.900300000	-0.339303000	-5.712876000
H	3.613408000	-0.639364000	-3.828085000
H	-1.776421000	-1.302193000	-3.644508000
H	-0.139390000	0.668242000	-4.064781000
O	2.710598000	-0.294112000	-3.798389000
O	0.304007000	-1.872846000	-3.263843000
O	-1.817149000	-0.658228000	-4.379690000
C	-3.382956000	1.108201000	-5.405875000
C	-4.564527000	0.481236000	-4.710734000
C	-5.773897000	1.394588000	-4.786431000
H	-3.069460000	0.562997000	-6.335213000
H	-7.556398000	1.357899000	-4.027688000
H	-6.062781000	1.521617000	-5.849285000
H	-5.507578000	2.390501000	-4.387766000
H	-5.574134000	-1.146395000	-4.853092000
H	-4.289921000	0.379322000	-3.636592000
O	-2.838962000	2.121188000	-5.037699000
O	-6.795786000	0.768497000	-4.045557000

O -4.814412000 -0.758556000 -5.309018000

Hf-NU-1000 (-CH₃) Prod

C -3.248214000 -2.182818000 -1.650130000
C -3.229699000 -2.386590000 2.899991000
C -3.232291000 2.034307000 3.103971000
C 3.276893000 2.142007000 2.939200000
C 3.226919000 2.366292000 -1.338712000
C 3.259351000 -2.277925000 -1.561498000
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H 4.085536000 2.695774000 3.464275000
H 4.062608000 -3.145637000 3.141596000
H -4.032324000 2.545255000 3.683474000
H -4.032028000 -2.968031000 3.403695000
C 5.411144000 -1.957560000 -2.720137000
C -5.658424000 -2.609566000 -2.006798000
C 4.307401000 -2.791167000 -2.490056000
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C -5.204901000 -5.034803000 -3.244896000
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C -4.316470000 3.133674000 -2.013768000
C 4.042404000 4.074091000 -3.050867000
C -4.033991000 4.152757000 -2.959695000
C 5.134378000 4.784436000 -3.570519000
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C -6.679712000 3.725427000 -2.030668000
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H 5.121064000 -5.297653000 -4.638265000
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H 7.229578000 -1.630146000 -3.832242000
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H	7.666286000	3.646735000	-1.597291000
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H	-7.341205000	-5.153254000	-3.496589000
H	7.031043000	-3.788917000	-5.078233000
H	-7.221962000	5.354429000	-3.345166000
H	7.241978000	5.224208000	-3.493004000
H	-1.942728000	-2.933948000	0.581938000
H	-0.875464000	1.361084000	5.094206000
H	-0.012791000	0.060745000	4.790383000
H	0.007353000	4.010463000	0.590463000
H	0.642022000	4.298977000	2.649975000
H	0.862991000	4.310001000	-0.709059000
H	1.960178000	-0.192676000	3.576046000
H	-1.939519000	2.796566000	0.830683000
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H	0.895861000	-4.434671000	2.108113000
H	0.633866000	-4.412205000	-1.210521000
H	0.004444000	-4.136700000	0.828617000
O	-1.063062000	-0.103608000	2.181036000
O	-3.617650000	1.294553000	2.159411000
O	-3.638221000	1.317547000	-0.656798000
O	-3.607221000	-1.513310000	2.075744000
O	-2.046768000	-2.665955000	3.218808000
O	0.034530000	-4.081589000	1.844467000
O	2.073387000	-2.846883000	2.971847000
O	2.059077000	-2.623323000	-1.781559000
O	3.631674000	-1.519668000	2.036277000
O	3.615676000	-1.457390000	-0.670890000
O	3.646629000	1.282958000	2.100837000
O	3.594328000	1.383220000	-0.622768000
O	2.020850000	2.686743000	-1.529756000
O	2.096745000	2.443249000	3.251169000
O	1.065641000	1.403142000	0.753687000
O	1.407559000	-0.131605000	2.787067000
O	0.040688000	-1.533341000	4.565882000
O	-0.028731000	1.077526000	4.722880000
O	1.057702000	-1.552740000	0.695520000
O	-1.407796000	-2.132966000	0.644955000
O	-2.057250000	-2.354723000	-2.037734000
O	-0.066204000	-3.915740000	-0.773082000
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O	0.007893000	3.956001000	-0.427193000

O	-1.401315000	1.997604000	0.769526000
O	-2.048105000	2.245571000	3.461638000
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O	1.399008000	-0.029846000	-1.313562000
O	-1.070211000	-0.033147000	-0.783743000
H	1.928159000	-0.012743000	-2.136833000
O	0.158905000	1.695313000	-3.147483000
H	-0.581628000	1.532136000	-3.746784000
C	-2.672338000	4.455422000	-3.504814000
H	-1.961065000	4.731949000	-2.714981000
H	-2.215133000	3.590723000	-4.006831000
H	-2.727337000	5.279066000	-4.228328000
C	2.696413000	4.283254000	-3.673394000
H	2.186489000	3.341485000	-3.910874000
H	2.007771000	4.817468000	-3.002301000
H	2.788951000	4.877288000	-4.591868000
C	3.059567000	-4.981080000	-2.965900000
H	2.868361000	-5.148656000	-1.896921000
H	2.110069000	-4.621711000	-3.389736000
H	3.284745000	-5.952481000	-3.424492000
C	-2.736757000	-4.912926000	-2.977660000
H	-2.225945000	-4.471372000	-3.846074000
H	-2.071500000	-4.764718000	-2.117578000
H	-2.825725000	-5.988770000	-3.178403000
Hf	2.528961000	-0.066509000	0.698449000
Hf	-0.019615000	-1.873691000	2.494373000
Hf	0.035882000	1.705634000	2.514076000
Hf	-0.014605000	1.741392000	-1.074930000
Hf	-2.526029000	-0.059209000	0.706166000
Hf	0.027796000	-1.820423000	-1.074287000
C	0.184681000	-2.364043000	-5.524772000
C	0.717694000	-1.444330000	-4.467061000
C	1.882602000	-0.562149000	-4.806171000
H	2.727431000	-1.246257000	-5.025455000
H	0.923436000	-3.194636000	-5.592793000
H	1.642299000	-0.086543000	-5.778781000
H	1.471740000	0.970361000	-3.683063000
H	-1.280097000	-2.704078000	-4.304073000
H	0.212549000	-1.866148000	-6.508271000
O	2.256998000	0.346235000	-3.842458000
O	0.188367000	-1.491448000	-3.360933000
O	-1.097816000	-2.809167000	-5.257140000
C	-2.133366000	-0.240633000	-5.675585000
C	-3.044221000	-0.531609000	-4.523305000
C	-3.986081000	0.640061000	-4.224813000
H	-2.454211000	-0.691733000	-6.649436000

H	-4.474446000	0.229697000	-2.373079000
H	-4.569585000	0.892628000	-5.124352000
H	-3.395420000	1.531951000	-3.949053000
H	-4.569698000	-1.655146000	-4.248227000
H	-2.391712000	-0.652963000	-3.628328000
O	-1.137889000	0.448959000	-5.588120000
O	-4.908499000	0.253153000	-3.243945000
O	-3.778697000	-1.683847000	-4.809755000

5. Hf-MOF-808 case

Hf-MOF-808

C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000
C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.266356000	2.583476000	-0.404248000
H	2.433138000	-1.482337000	-4.219102000
H	0.958139000	-4.277098000	-1.437952000
H	1.606867000	-3.993742000	-2.849297000
H	0.319932000	-1.014248000	-4.070243000
H	-2.136947000	2.338032000	-3.112646000
H	0.148187000	-4.895692000	1.479586000
H	5.367970000	0.323372000	4.021999000
C	6.917650000	1.826390000	4.227467000
C	5.753894000	1.287712000	3.686316000
H	-5.354373000	2.482501000	1.705743000
C	-7.353018000	2.163830000	0.928946000
C	-5.963556000	2.102362000	0.882917000
O	-3.068195000	-0.783036000	2.385518000
H	-5.458336000	-0.274918000	2.694356000
H	5.527896000	-0.483985000	-3.836953000
C	-4.853239000	-2.327448000	2.490503000
C	-5.793847000	-1.314177000	2.713912000
C	5.136144000	1.446180000	-2.973523000
C	5.882253000	0.544541000	-3.743245000
O	-2.734898000	-2.856642000	1.599408000
O	-0.179495000	-4.113873000	1.946680000
O	1.047039000	-2.150722000	0.228536000
O	3.309043000	1.834462000	-1.541149000
O	0.881896000	2.933017000	-2.195034000
O	-0.818125000	1.738692000	-0.282607000
Hf	-0.966141000	-2.739649000	0.234429000
Hf	1.498973000	1.729042000	-0.260176000

H	-8.640026000	-3.160772000	-2.629562000
C	-6.901679000	-3.557370000	-1.410764000
C	-7.563087000	-3.015356000	-2.513689000
O	3.181205000	2.098612000	1.259099000
O	1.176274000	3.682724000	0.254956000
O	-0.506714000	-4.615724000	-0.599417000
H	8.412325000	2.603437000	-4.716162000
C	7.056401000	0.959024000	-4.365367000
C	7.491349000	2.277961000	-4.226320000
H	8.303571000	3.483050000	4.204478000
C	6.694059000	3.758689000	2.790499000
C	7.389089000	3.061564000	3.779995000
H	9.249396000	-4.661595000	0.602003000
C	7.591816000	-3.803601000	1.689063000
C	8.243637000	-4.239766000	0.534563000
O	-3.289126000	1.083433000	-1.342295000
H	-4.915515000	-1.487064000	-4.030886000
C	-6.852204000	-2.284367000	-3.468206000
C	-5.484355000	-2.080745000	-3.311761000
H	-8.581528000	-3.227482000	3.109566000
C	-7.131835000	-1.637355000	2.923089000
C	-7.532346000	-2.974158000	2.938348000
H	-5.568402000	0.577703000	-2.135453000
H	5.785996000	-2.916760000	2.495471000
C	-5.321789000	1.537933000	-0.227141000
C	-6.085470000	1.026250000	-1.284037000
C	5.672005000	-3.160035000	0.361892000
C	6.310088000	-3.267523000	1.604233000
O	-3.225765000	1.529902000	0.856811000
O	0.695778000	0.632923000	1.366179000
O	3.819887000	-2.409912000	-0.890330000
O	1.754230000	-3.887793000	-1.899504000
O	-0.319842000	-2.056876000	-1.901541000
Hf	-1.381685000	0.491533000	1.529324000
Hf	1.901042000	-1.537804000	-1.622358000
O	3.478805000	-0.174441000	-2.530369000
O	1.714608000	-1.867207000	-3.703561000
O	-1.220899000	1.200968000	3.445185000
H	-0.609391000	-2.617158000	-2.630432000
H	2.557583000	-3.222973000	3.273173000
H	0.369352000	0.436647000	3.903664000
H	0.977765000	-0.848230000	4.579086000
H	0.581171000	-3.714773000	2.466310000
H	-1.154474000	-5.005977000	-1.195964000
H	4.986531000	3.456990000	-2.230744000
C	6.751845000	3.181132000	-3.461093000

C	5.579739000	2.767623000	-2.834563000
O	3.713098000	-2.277332000	1.346378000
O	1.735154000	-2.724369000	3.202613000
O	-1.350933000	1.783929000	-3.161808000
H	-0.792644000	-1.891470000	2.972538000
H	1.637715000	4.048394000	1.015846000
H	0.051123000	2.617362000	-2.644927000
H	0.715526000	3.816401000	-1.835593000
H	-1.886665000	1.273025000	4.133962000
H	-0.461271000	0.301502000	-4.543991000
H	5.821711000	-3.505042000	-1.753862000
C	7.612573000	-4.136256000	-0.706055000
C	6.332669000	-3.596414000	-0.793621000
H	-4.989800000	-3.793294000	-0.410706000
H	4.971032000	3.751592000	1.473958000
C	-4.813777000	-2.634663000	-2.213842000
C	-5.527736000	-3.381290000	-1.268093000
C	5.051008000	1.983790000	2.694604000
C	5.528439000	3.223462000	2.250138000
O	-2.870337000	-1.356896000	-2.587652000
O	-0.565689000	-0.538246000	-4.074847000
O	0.759062000	0.228042000	-1.620855000
O	3.464993000	0.249576000	2.497594000
O	1.181879000	-0.128740000	3.968571000
O	-0.449639000	-1.474138000	2.173615000
H	-9.201479000	1.675188000	-0.076873000
C	-7.475775000	1.066095000	-1.223852000
C	-8.110148000	1.639194000	-0.120746000
H	-4.518040000	-4.444357000	2.306747000
C	-6.595033000	-3.988931000	2.732834000
C	-5.261794000	-3.667253000	2.496363000
O	-2.748254000	-3.088994000	-1.165171000
H	3.655679000	-0.087489000	0.015110000
O	-1.647414000	-0.785379000	-0.072042000
O	2.699281000	-0.198082000	0.009743000
H	7.461974000	1.281970000	5.002513000
H	7.064750000	4.724476000	2.439600000
H	7.092808000	4.213336000	-3.353274000
H	7.637501000	0.251697000	-4.961521000
H	8.123281000	-4.478343000	-1.609092000
H	8.087704000	-3.881573000	2.659285000
H	-8.067457000	0.645146000	-2.040087000
H	-7.851585000	2.614045000	1.790743000
H	-7.459180000	-4.118934000	-0.657416000
H	-7.371599000	-1.863444000	-4.332661000
H	-7.866529000	-0.843037000	3.074545000

H	-6.909731000	-5.035204000	2.748423000
Hf	-1.291558000	0.068670000	-1.951502000
Hf	1.818955000	-1.090305000	1.880572000

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C	-3.448800000	-1.965700000	2.156799000
C	3.881700000	1.003300000	-2.299800000
C	-3.841599000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356801000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.245098000	2.573274000	-0.381660000
H	2.415248000	-1.481441000	-4.229997000
H	0.924914000	-4.273138000	-1.437022000
H	1.569718000	-4.006135000	-2.856855000
H	0.293702000	-0.992560000	-4.056028000
H	-2.051676000	2.410308000	-3.027840000
H	0.135039000	-4.900363000	1.444649000
H	5.436804000	0.289681000	3.939066000
C	6.839551000	1.899005000	4.317686000
C	5.737430000	1.312311000	3.703094000
H	-5.300997000	2.358378000	1.801091000
C	-7.308570000	2.248261000	0.985534000
C	-5.924733000	2.105466000	0.939356000
O	-3.069412000	-0.786052000	2.391539000
H	-5.437287000	-0.265174000	2.741852000
H	5.527029000	-0.460025000	-3.856654000
C	-4.861390000	-2.318738000	2.462262000
C	-5.788158000	-1.299686000	2.717531000
C	5.130781000	1.459978000	-2.972743000
C	5.877518000	0.568948000	-3.754339000
O	-2.724554000	-2.860079000	1.618270000
O	-0.175218000	-4.129974000	1.942694000
O	1.057648000	-2.157762000	0.229004000
O	3.296198000	1.830684000	-1.542462000
O	0.883610000	2.965980000	-2.143112000
O	-0.795273000	1.707515000	-0.327836000
Hf	-0.969144000	-2.715430000	0.260050000
Hf	1.495180000	1.668458000	-0.269189000
H	-8.544966000	-3.426325000	-2.939789000
C	-6.834108000	-3.830424000	-1.685113000
C	-7.485881000	-3.225169000	-2.760683000
O	3.190103000	2.081297000	1.233287000
O	1.066494000	3.598166000	0.506982000
O	-0.515602000	-4.594547000	-0.595098000
H	8.396014000	2.647132000	-4.715837000

C	7.047282000	0.994302000	-4.377084000
C	7.478094000	2.313285000	-4.225971000
H	8.061803000	3.671827000	4.487266000
C	6.453148000	3.934933000	3.070094000
C	7.197973000	3.210742000	4.002091000
H	9.291599000	-4.560035000	0.590417000
C	7.630729000	-3.707960000	1.676976000
C	8.277304000	-4.158861000	0.525167000
O	-3.297097000	1.087116000	-1.347959000
H	-4.886085000	-1.396322000	-4.003303000
C	-6.788457000	-2.359977000	-3.606365000
C	-5.444191000	-2.088840000	-3.369453000
H	-8.607983000	-3.183601000	3.012283000
C	-7.132129000	-1.610463000	2.905065000
C	-7.553373000	-2.940299000	2.861136000
H	-5.597090000	0.860905000	-2.214122000
H	5.817841000	-2.836048000	2.484143000
C	-5.311165000	1.612792000	-0.220911000
C	-6.094432000	1.256137000	-1.325703000
C	5.683751000	-3.132529000	0.358170000
C	6.337928000	-3.198753000	1.595166000
O	-3.223598000	1.484275000	0.857029000
O	0.714322000	0.641068000	1.405308000
O	3.810487000	-2.430919000	-0.889377000
O	1.723076000	-3.892901000	-1.909010000
O	-0.334577000	-2.035798000	-1.879989000
Hf	-1.374567000	0.549860000	1.605603000
Hf	1.901958000	-1.559902000	-1.628261000
O	3.491680000	-0.178655000	-2.524885000
O	1.703716000	-1.867842000	-3.706227000
O	-1.321934000	0.703403000	3.740130000
H	-0.640717000	-2.592050000	-2.605246000
H	2.592786000	-3.272358000	3.215720000
H	0.343309000	0.206779000	4.014231000
H	1.195385000	-0.979388000	4.602307000
H	0.598207000	-3.748784000	2.453546000
H	-1.175462000	-4.979624000	-1.181607000
H	4.979044000	3.463120000	-2.207674000
C	6.738765000	3.205639000	-3.448094000
C	5.570442000	2.781443000	-2.821666000
O	3.717392000	-2.279754000	1.347651000
O	1.772305000	-2.766169000	3.189676000
O	-1.309600000	1.805466000	-3.141079000
H	-0.734759000	-1.927293000	2.984536000
H	1.778802000	3.899939000	1.093429000
H	0.073569000	2.602057000	-2.612066000

H	0.658779000	3.860845000	-1.861577000
H	-1.850374000	0.011153000	4.156383000
H	-0.489987000	0.326566000	-4.511143000
H	5.816396000	-3.522898000	-1.751022000
C	7.630375000	-4.096127000	-0.710015000
C	6.339630000	-3.582392000	-0.794893000
H	-4.955403000	-4.033287000	-0.618343000
H	4.754168000	3.902523000	1.725566000
C	-4.783508000	-2.700334000	-2.296380000
C	-5.483775000	-3.578381000	-1.459285000
C	4.989055000	2.033285000	2.763132000
C	5.353203000	3.349296000	2.450494000
O	-2.880972000	-1.331792000	-2.551669000
O	-0.589657000	-0.518650000	-4.050139000
O	0.784437000	0.222260000	-1.630841000
O	3.487150000	0.237361000	2.476203000
O	1.244501000	-0.218006000	4.008788000
O	-0.423512000	-1.493595000	2.182096000
H	-9.173780000	1.983620000	-0.071792000
C	-7.479403000	1.382178000	-1.268156000
C	-8.086515000	1.882059000	-0.114869000
H	-4.555654000	-4.431823000	2.201659000
C	-6.630405000	-3.960864000	2.622508000
C	-5.289904000	-3.651401000	2.413148000
O	-2.758890000	-3.064744000	-1.134983000
H	3.654395000	-0.086266000	0.022613000
O	-1.603644000	-0.739993000	-0.007202000
O	2.700703000	-0.217506000	0.005701000
H	7.422272000	1.333785000	5.048673000
H	6.730785000	4.963210000	2.828068000
H	7.077106000	4.237477000	-3.329582000
H	7.628401000	0.295341000	-4.982920000
H	8.137165000	-4.449627000	-1.610840000
H	8.139410000	-3.753301000	2.642610000
H	-8.090007000	1.086052000	-2.124441000
H	-7.786334000	2.637564000	1.887819000
H	-7.382573000	-4.498206000	-1.016540000
H	-7.300433000	-1.889050000	-4.449002000
H	-7.855337000	-0.811232000	3.083424000
H	-6.962054000	-5.001572000	2.591823000
Hf	-1.299339000	0.091883000	-1.911248000
Hf	1.826630000	-1.111758000	1.885869000
C	-1.038285000	3.918314000	4.723364000
C	-2.248429000	3.902697000	3.769793000
C	-1.551266000	4.072078000	2.421458000
C	-0.023707000	4.811872000	3.999859000

C	-2.357400000	4.534968000	1.225644000
C	1.370285000	4.243365000	3.821130000
H	-3.267857000	3.925903000	1.146160000
H	-2.845675000	4.820439000	3.939985000
H	-0.654630000	2.886784000	4.783588000
H	1.481046000	5.424957000	2.319880000
H	-2.657543000	5.584419000	1.390822000
H	-0.684484000	4.555879000	0.203787000
H	1.295435000	3.200577000	3.450365000
H	1.893068000	4.202095000	4.789246000
H	-2.516790000	2.014957000	3.937685000
H	-0.116273000	3.076715000	1.538274000
H	-1.777330000	5.143206000	6.024291000
H	0.038420000	5.799170000	4.490714000
O	-1.318405000	4.294974000	6.042752000
O	-1.630288000	4.385777000	0.022077000
O	2.122986000	5.046514000	2.938483000
O	-0.897618000	2.836462000	2.124965000
O	-3.091415000	2.813817000	3.883328000
O	-0.571837000	5.049497000	2.681258000

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C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000
C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.253024000	2.561214000	-0.313686000
H	2.398617000	-1.444879000	-4.233076000
H	0.916446000	-4.257780000	-1.462653000
H	1.553662000	-3.978842000	-2.885745000
H	0.274186000	-0.951015000	-4.044128000
H	-1.983376000	2.468094000	-2.980071000
H	0.109747000	-4.920784000	1.402819000
H	5.345538000	0.362195000	4.055333000
C	6.820381000	1.926841000	4.338576000
C	5.701081000	1.347405000	3.747761000
H	-5.322013000	2.190757000	1.846148000
C	-7.282912000	2.402095000	0.937544000
C	-5.919950000	2.118583000	0.933351000
O	-3.054958000	-0.794705000	2.409631000
H	-5.307189000	-0.332148000	3.204495000
H	5.556608000	-0.441767000	-3.842085000
C	-4.839849000	-2.325795000	2.544485000
C	-5.692952000	-1.345237000	3.068267000

C	5.120691000	1.478675000	-2.978218000
C	5.885599000	0.595300000	-3.750757000
O	-2.747562000	-2.852455000	1.579502000
O	-0.193581000	-4.158928000	1.918231000
O	1.065288000	-2.168818000	0.224471000
O	3.281271000	1.822570000	-1.543562000
O	0.881562000	3.062453000	-1.994725000
O	-0.795645000	1.698205000	-0.303349000
Hf	-0.972009000	-2.708104000	0.256266000
Hf	1.492784000	1.645417000	-0.222609000
H	-8.369486000	-3.790405000	-3.334650000
C	-6.665850000	-4.208229000	-2.074418000
C	-7.348203000	-3.506275000	-3.069372000
O	3.196900000	2.076518000	1.222267000
O	0.882413000	3.500593000	0.763772000
O	-0.509622000	-4.581193000	-0.628380000
H	8.358211000	2.716313000	-4.737968000
C	7.045786000	1.038732000	-4.378968000
C	7.448114000	2.368321000	-4.243361000
H	8.131704000	3.642383000	4.390215000
C	6.560746000	3.872081000	2.925135000
C	7.251936000	3.188730000	3.927191000
H	9.297788000	-4.552674000	0.555116000
C	7.638991000	-3.713958000	1.655226000
C	8.282495000	-4.152883000	0.497133000
O	-3.286135000	1.105938000	-1.350939000
H	-4.931198000	-1.235053000	-3.873302000
C	-6.729459000	-2.439375000	-3.723325000
C	-5.431578000	-2.071431000	-3.381129000
H	-8.510080000	-3.217022000	3.453625000
C	-7.008141000	-1.666037000	3.391530000
C	-7.477104000	-2.966679000	3.199688000
H	-5.533035000	1.291695000	-2.347920000
H	5.827402000	-2.853885000	2.477004000
C	-5.291273000	1.724513000	-0.256152000
C	-6.039147000	1.612111000	-1.434852000
C	5.686028000	-3.130162000	0.348716000
C	6.344930000	-3.206436000	1.582589000
O	-3.249913000	1.411010000	0.867888000
O	0.724066000	0.605730000	1.427754000
O	3.803113000	-2.435426000	-0.885583000
O	1.714680000	-3.876046000	-1.938059000
O	-0.339572000	-2.011273000	-1.881448000
Hf	-1.373687000	0.556483000	1.656681000
Hf	1.900348000	-1.553947000	-1.627452000
O	3.509475000	-0.185748000	-2.518265000

O	1.687216000	-1.831800000	-3.709644000
O	-1.265367000	0.598185000	3.808817000
H	-0.640592000	-2.564584000	-2.611016000
H	2.593792000	-3.338846000	3.177391000
H	0.364361000	0.115219000	4.049415000
H	1.220806000	-1.092134000	4.595259000
H	0.586584000	-3.789965000	2.427730000
H	-1.172700000	-4.956984000	-1.217167000
H	4.924569000	3.486433000	-2.237341000
C	6.689827000	3.253396000	-3.475436000
C	5.531581000	2.810975000	-2.842936000
O	3.727019000	-2.280890000	1.353195000
O	1.775950000	-2.828042000	3.167670000
O	-1.241293000	1.861583000	-3.086025000
H	-0.717972000	-1.976861000	2.987605000
H	1.493193000	3.926961000	1.398392000
H	0.108440000	2.653603000	-2.501063000
H	0.550791000	3.906294000	-1.664448000
H	-1.765340000	-0.130148000	4.197313000
H	-0.490725000	0.389354000	-4.462406000
H	5.811690000	-3.502438000	-1.764152000
C	7.630853000	-4.080376000	-0.735021000
C	6.338640000	-3.568824000	-0.810545000
H	-4.815479000	-4.375192000	-0.954219000
H	4.881137000	3.814815000	1.554169000
C	-4.741042000	-2.774598000	-2.385856000
C	-5.365293000	-3.846597000	-1.735587000
C	5.004296000	2.028296000	2.741436000
C	5.439988000	3.295909000	2.334935000
O	-2.902706000	-1.300245000	-2.508957000
O	-0.605727000	-0.471064000	-4.033001000
O	0.796746000	0.240208000	-1.609162000
O	3.474963000	0.248589000	2.493447000
O	1.271801000	-0.306066000	4.034558000
O	-0.415880000	-1.531599000	2.188202000
H	-9.095509000	2.505691000	-0.232885000
C	-7.402696000	1.890588000	-1.424726000
C	-8.024716000	2.287379000	-0.239585000
H	-4.636483000	-4.378635000	1.941571000
C	-6.629629000	-3.948058000	2.682266000
C	-5.315492000	-3.629119000	2.353080000
O	-2.759446000	-3.062067000	-1.132762000
H	3.659811000	-0.089857000	0.028268000
O	-1.577498000	-0.730005000	0.012361000
O	2.706857000	-0.226765000	0.017944000
H	7.360775000	1.393497000	5.123975000

H	6.899994000	4.859697000	2.604021000
H	7.005318000	4.293909000	-3.370128000
H	7.641425000	0.345645000	-4.977400000
H	8.134940000	-4.424880000	-1.640847000
H	8.150901000	-3.767493000	2.618743000
H	-7.986476000	1.795727000	-2.343268000
H	-7.772290000	2.710483000	1.864425000
H	-7.153690000	-5.038514000	-1.558369000
H	-7.265217000	-1.890987000	-4.501682000
H	-7.673469000	-0.898202000	3.793089000
H	-6.998494000	-4.965744000	2.533797000
Hf	-1.303548000	0.114013000	-1.881345000
Hf	1.830677000	-1.144946000	1.894595000
C	-1.202641000	3.769243000	4.826776000
C	-2.375792000	3.705630000	3.834725000
C	-1.662745000	3.900138000	2.494352000
C	-0.149299000	4.612305000	4.086079000
C	-2.506230000	4.427996000	1.346688000
C	1.198715000	3.916957000	3.980672000
H	-3.405750000	3.808030000	1.242200000
H	-3.016979000	4.595533000	3.994890000
H	-0.827731000	2.742305000	4.965531000
H	2.146204000	5.493149000	3.325004000
H	-2.823889000	5.460181000	1.576642000
H	-0.894463000	4.664932000	0.299743000
H	1.069040000	2.894237000	3.594072000
H	1.631745000	3.822818000	4.994629000
H	-2.569539000	1.813107000	4.001234000
H	-0.033377000	3.119050000	1.452507000
H	-2.015016000	5.054101000	6.021021000
H	-0.020494000	5.584191000	4.598834000
O	-1.528001000	4.226738000	6.113121000
O	-1.801771000	4.367468000	0.118762000
O	2.089646000	4.559450000	3.089823000
O	-0.984742000	2.737376000	2.126041000
O	-3.180800000	2.580536000	3.926993000
O	-0.697143000	4.904145000	2.796712000

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C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000
C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.284824000	2.541993000	-0.225909000

H	2.388808000	-1.433659000	-4.232534000
H	0.906388000	-4.253961000	-1.467587000
H	1.542541000	-3.975297000	-2.892941000
H	0.259788000	-0.941091000	-4.032790000
H	-1.972316000	2.455037000	-3.016629000
H	0.106425000	-4.932202000	1.386073000
H	5.346380000	0.377191000	4.060947000
C	6.799480000	1.959584000	4.357782000
C	5.691760000	1.367411000	3.758015000
H	-5.385782000	2.081190000	1.840477000
C	-7.269231000	2.540366000	0.863707000
C	-5.933608000	2.148603000	0.896528000
O	-3.032333000	-0.814470000	2.455002000
H	-5.295306000	-0.303209000	3.168248000
H	5.575658000	-0.434860000	-3.827360000
C	-4.862563000	-2.295324000	2.483556000
C	-5.706581000	-1.300753000	2.995407000
C	5.118800000	1.486136000	-2.975515000
C	5.895048000	0.605548000	-3.739883000
O	-2.751134000	-2.856187000	1.579820000
O	-0.192223000	-4.175454000	1.911642000
O	1.070901000	-2.174664000	0.224643000
O	3.272411000	1.818773000	-1.545570000
O	0.873680000	3.114642000	-1.911075000
O	-0.785898000	1.704513000	-0.272606000
Hf	-0.971405000	-2.703918000	0.265796000
Hf	1.493000000	1.622311000	-0.207806000
H	-8.287275000	-3.911895000	-3.497654000
C	-6.600085000	-4.311887000	-2.209628000
C	-7.283603000	-3.601032000	-3.197379000
O	3.192557000	2.074959000	1.221387000
O	0.932109000	3.563842000	0.776038000
O	-0.509895000	-4.574513000	-0.636298000
H	8.352931000	2.743751000	-4.726813000
C	7.054168000	1.056215000	-4.364929000
C	7.443672000	2.390161000	-4.234618000
H	8.088087000	3.691812000	4.422923000
C	6.524323000	3.905275000	2.947846000
C	7.217486000	3.228061000	3.952646000
H	9.311490000	-4.522091000	0.534028000
C	7.649648000	-3.699940000	1.642025000
C	8.293518000	-4.128564000	0.480295000
O	-3.263469000	1.148417000	-1.353627000
H	-4.930893000	-1.220661000	-3.865271000
C	-6.688322000	-2.491157000	-3.799411000
C	-5.412687000	-2.089942000	-3.413386000

H	-8.590862000	-3.094417000	3.224060000
C	-7.042613000	-1.588618000	3.258529000
C	-7.541503000	-2.869930000	3.017369000
H	-5.426956000	1.612468000	-2.427383000
H	5.834462000	-2.856033000	2.472206000
C	-5.268604000	1.822049000	-0.294023000
C	-5.956783000	1.885342000	-1.512218000
C	5.690059000	-3.121878000	0.342745000
C	6.352246000	-3.200262000	1.574728000
O	-3.299083000	1.316775000	0.881374000
O	0.737711000	0.597518000	1.448414000
O	3.798300000	-2.441448000	-0.884110000
O	1.705908000	-3.873827000	-1.945573000
O	-0.343703000	-2.002451000	-1.873803000
Hf	-1.369637000	0.561774000	1.710847000
Hf	1.900298000	-1.559399000	-1.626117000
O	3.516072000	-0.188444000	-2.516538000
O	1.680296000	-1.824435000	-3.708072000
O	-1.216058000	0.521857000	3.869418000
H	-0.646208000	-2.554083000	-2.603958000
H	2.607675000	-3.370807000	3.156590000
H	0.394653000	0.063803000	4.080032000
H	1.270994000	-1.144820000	4.597777000
H	0.592121000	-3.812681000	2.419038000
H	-1.177471000	-4.943491000	-1.224290000
H	4.900133000	3.495975000	-2.246870000
C	6.673665000	3.272484000	-3.475220000
C	5.516628000	2.822926000	-2.845544000
O	3.732006000	-2.283573000	1.355498000
O	1.789930000	-2.859902000	3.158353000
O	-1.203485000	1.876892000	-3.064375000
H	-0.694583000	-2.002802000	2.996779000
H	1.495428000	3.990877000	1.464509000
H	0.119539000	2.698686000	-2.438643000
H	0.490048000	3.898344000	-1.494430000
H	-1.691453000	-0.231336000	4.240518000
H	-0.490595000	0.415906000	-4.415579000
H	5.813646000	-3.482717000	-1.772321000
C	7.638730000	-4.053830000	-0.750052000
C	6.342989000	-3.550479000	-0.820129000
H	-4.772315000	-4.452938000	-1.050739000
H	4.854940000	3.830352000	1.565484000
C	-4.720440000	-2.802407000	-2.425913000
C	-5.321782000	-3.916517000	-1.826861000
C	4.993111000	2.041987000	2.748718000
C	5.415084000	3.316256000	2.348559000

O	-2.915338000	-1.282019000	-2.483744000
O	-0.617707000	-0.458756000	-4.017900000
O	0.801125000	0.243339000	-1.597989000
O	3.486568000	0.245158000	2.487233000
O	1.309467000	-0.349359000	4.049183000
O	-0.397965000	-1.553725000	2.197604000
H	-8.998791000	2.908338000	-0.377265000
C	-7.292981000	2.275052000	-1.540939000
C	-7.949365000	2.604411000	-0.353743000
H	-4.695040000	-4.338050000	1.838426000
C	-6.703390000	-3.864688000	2.510305000
C	-5.368083000	-3.578610000	2.241538000
O	-2.761344000	-3.060743000	-1.131200000
H	3.663110000	-0.093213000	0.029569000
O	-1.565357000	-0.725682000	0.032825000
O	2.710786000	-0.234717000	0.020336000
H	7.341231000	1.431255000	5.145616000
H	6.852711000	4.898181000	2.631844000
H	6.979026000	4.316450000	-3.374342000
H	7.658979000	0.365413000	-4.956771000
H	8.143077000	-4.390275000	-1.658760000
H	8.163824000	-3.755382000	2.604223000
H	-7.829132000	2.318173000	-2.491839000
H	-7.785588000	2.793285000	1.792707000
H	-7.069413000	-5.176355000	-1.734168000
H	-7.225129000	-1.935174000	-4.571579000
H	-7.700989000	-0.810389000	3.651673000
H	-7.096371000	-4.866645000	2.321888000
Hf	-1.304851000	0.120451000	-1.853184000
Hf	1.837032000	-1.161374000	1.901794000
C	-1.218879000	3.680330000	4.885407000
C	-2.437868000	3.595270000	3.959122000
C	-1.801141000	3.780021000	2.571020000
C	-0.221224000	4.535867000	4.084764000
C	-2.780876000	4.294256000	1.529718000
C	1.128603000	3.854270000	3.942262000
H	-3.700354000	3.690086000	1.615961000
H	-3.090548000	4.469846000	4.155988000
H	-0.821467000	2.659886000	5.007922000
H	2.021230000	5.471541000	3.293282000
H	-3.027811000	5.346486000	1.752628000
H	-2.890592000	4.441440000	-0.404711000
H	0.997907000	2.845339000	3.519812000
H	1.579380000	3.732004000	4.944540000
H	-2.579592000	1.699370000	4.114419000
H	0.086092000	3.349374000	1.272319000

H	-1.983138000	4.958229000	6.117611000
H	-0.082380000	5.511633000	4.590062000
O	-1.476390000	4.140668000	6.187424000
O	-2.217595000	4.171226000	0.229603000
O	2.013459000	4.534375000	3.063711000
O	-1.164273000	2.648205000	2.157093000
O	-3.213412000	2.450673000	4.089618000
O	-0.823895000	4.807544000	2.820934000

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C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000
C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.239457000	2.579980000	-0.284107000
H	2.426088000	-1.493242000	-4.226921000
H	0.921299000	-4.266444000	-1.435945000
H	1.566189000	-3.996274000	-2.855207000
H	0.287869000	-1.008347000	-4.053207000
H	-2.058361000	2.382447000	-3.079803000
H	0.124766000	-4.905862000	1.435634000
H	5.401166000	0.376104000	4.025724000
C	6.772423000	2.018334000	4.379986000
C	5.699022000	1.390831000	3.754903000
H	-5.361146000	2.201410000	1.821248000
C	-7.265941000	2.574550000	0.852863000
C	-5.925152000	2.201271000	0.885618000
O	-3.054559000	-0.798029000	2.419168000
H	-5.330282000	-0.336664000	3.168942000
H	5.615909000	-0.437041000	-3.780933000
C	-4.846869000	-2.327821000	2.520097000
C	-5.712674000	-1.349568000	3.025965000
C	5.188123000	1.457023000	-2.855775000
C	5.977679000	0.578800000	-3.609790000
O	-2.742713000	-2.852967000	1.585723000
O	-0.180598000	-4.137958000	1.940411000
O	1.068081000	-2.162035000	0.232469000
O	3.208886000	1.853331000	-1.636281000
O	0.837142000	2.983123000	-2.205588000
O	-0.788631000	1.719982000	-0.364180000
Hf	-0.966861000	-2.707378000	0.267578000
Hf	1.463458000	1.688531000	-0.233066000
H	-8.326952000	-3.870175000	-3.409735000
C	-6.638078000	-4.256874000	-2.119825000

C	-7.315397000	-3.568170000	-3.127388000
O	3.188445000	2.066350000	1.224234000
O	1.213461000	3.725943000	0.315768000
O	-0.517746000	-4.587821000	-0.600532000
H	8.609749000	2.631394000	-4.277013000
C	7.202006000	1.000881000	-4.119396000
C	7.647589000	2.301513000	-3.877770000
H	7.961959000	3.815760000	4.519238000
C	6.399003000	3.997057000	3.038716000
C	7.122153000	3.322266000	4.023501000
H	9.267845000	-4.625847000	0.569034000
C	7.614166000	-3.772861000	1.665924000
C	8.258666000	-4.211217000	0.508194000
O	-3.284531000	1.096018000	-1.346146000
H	-4.922985000	-1.258376000	-3.894679000
C	-6.703504000	-2.492072000	-3.772549000
C	-5.417899000	-2.101710000	-3.409020000
H	-8.533949000	-3.225249000	3.356191000
C	-7.033793000	-1.671497000	3.322885000
C	-7.496540000	-2.973142000	3.122984000
H	-5.464304000	1.468737000	-2.404846000
H	5.810000000	-2.893558000	2.483665000
C	-5.274595000	1.806643000	-0.291209000
C	-5.983740000	1.787786000	-1.498939000
C	5.677832000	-3.150313000	0.352532000
C	6.327994000	-3.246096000	1.589550000
O	-3.275431000	1.387818000	0.878272000
O	0.727420000	0.630759000	1.413212000
O	3.809806000	-2.426110000	-0.887727000
O	1.721431000	-3.887830000	-1.907267000
O	-0.338724000	-2.032298000	-1.873967000
Hf	-1.363036000	0.552443000	1.647545000
Hf	1.899636000	-1.552216000	-1.617600000
O	3.523546000	-0.185753000	-2.521387000
O	1.706438000	-1.860127000	-3.701076000
O	-1.266509000	0.651421000	3.793984000
H	-0.637716000	-2.591969000	-2.599408000
H	2.604949000	-3.300569000	3.183379000
H	0.355184000	0.153993000	4.043104000
H	1.248564000	-1.015945000	4.609626000
H	0.598316000	-3.759873000	2.446546000
H	-1.178944000	-4.964674000	-1.190637000
H	5.023520000	3.428875000	-2.011389000
C	6.868289000	3.179268000	-3.122727000
C	5.643026000	2.759985000	-2.612304000
O	3.727007000	-2.273651000	1.349987000

O	1.785530000	-2.792253000	3.174994000
O	-1.318738000	1.774983000	-3.187359000
H	-0.710660000	-1.928978000	3.002962000
H	0.894985000	4.236187000	-0.440123000
H	0.027885000	2.575127000	-2.644238000
H	1.556130000	2.889891000	-2.842178000
H	-1.844493000	0.004666000	4.216707000
H	-0.545780000	0.279090000	-4.523481000
H	5.811031000	-3.506667000	-1.762350000
C	7.615738000	-4.119145000	-0.727234000
C	6.331300000	-3.588775000	-0.806265000
H	-4.802949000	-4.392786000	-0.970676000
H	4.744440000	3.888065000	1.643637000
C	-4.732136000	-2.791808000	-2.401490000
C	-5.349469000	-3.873118000	-1.760236000
C	4.972837000	2.063182000	2.763340000
C	5.329474000	3.370161000	2.406010000
O	-2.905926000	-1.302384000	-2.513832000
O	-0.607079000	-0.556983000	-4.040682000
O	0.790627000	0.225217000	-1.620084000
O	3.500383000	0.236488000	2.485261000
O	1.268542000	-0.254411000	4.015003000
O	-0.412252000	-1.509264000	2.188409000
H	-9.020627000	2.842513000	-0.378424000
C	-7.325098000	2.159022000	-1.529092000
C	-7.967112000	2.553359000	-0.354081000
H	-4.628391000	-4.380003000	1.922103000
C	-6.636635000	-3.953022000	2.623705000
C	-5.316750000	-3.631856000	2.320271000
O	-2.764001000	-3.054083000	-1.123728000
H	3.659807000	-0.079427000	0.031413000
O	-1.577436000	-0.731136000	0.007182000
O	2.705802000	-0.204920000	0.001529000
H	7.337655000	1.492754000	5.153136000
H	6.666429000	5.020405000	2.765253000
H	7.220649000	4.194692000	-2.928278000
H	7.815340000	0.313062000	-4.705856000
H	8.120593000	-4.463215000	-1.632854000
H	8.119134000	-3.841658000	2.632137000
H	-7.876385000	2.137475000	-2.472014000
H	-7.770025000	2.880023000	1.772792000
H	-7.120117000	-5.094942000	-1.610911000
H	-7.235075000	-1.954058000	-4.560970000
H	-7.708623000	-0.904143000	3.709498000
H	-7.000397000	-4.971588000	2.468761000
Hf	-1.298054000	0.092345000	-1.894410000

Hf	1.837869000	-1.118038000	1.890819000
C	0.081856000	4.030678000	4.330547000
C	-1.394341000	4.068125000	3.929952000
C	-1.406449000	3.833444000	2.424138000
C	0.777364000	5.003427000	3.381048000
C	-2.391864000	4.578102000	1.562848000
C	2.266549000	4.760945000	3.271265000
H	-3.390748000	4.210259000	1.870789000
H	-1.792791000	5.077534000	4.159301000
H	0.455587000	3.007786000	4.135891000
H	2.852906000	6.571502000	2.931581000
H	-2.344769000	5.660042000	1.771537000
H	-2.873418000	4.592761000	-0.320521000
H	2.436440000	3.788629000	2.784070000
H	2.672090000	4.683502000	4.299244000
H	-1.842119000	2.237868000	4.366585000
H	0.682751000	4.344043000	1.342453000
H	-0.221753000	5.031078000	5.954436000
H	0.608945000	6.031898000	3.773082000
O	0.329052000	4.286793000	5.683931000
O	-2.128607000	4.287203000	0.207869000
O	2.944291000	5.717204000	2.495682000
O	-1.102066000	2.666716000	2.064649000
O	-2.197991000	3.138325000	4.576198000
O	0.106966000	4.900949000	2.134423000

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C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000
C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.254137000	2.552390000	-0.398565000
H	2.439651000	-1.500954000	-4.225242000
H	0.941468000	-4.279104000	-1.425605000
H	1.596662000	-4.015823000	-2.839900000
H	0.313135000	-1.020398000	-4.070580000
H	-2.107003000	2.365239000	-3.069042000
H	0.138436000	-4.894182000	1.460003000
H	5.179664000	0.488149000	4.234013000
C	6.811299000	1.911551000	4.355433000
C	5.650356000	1.375570000	3.806574000
H	-5.279475000	2.361561000	1.814375000
C	-7.256353000	2.508148000	0.933411000
C	-5.894426000	2.220012000	0.921961000

O	-3.078429000	-0.780143000	2.366335000
H	-5.359762000	-0.343121000	3.124893000
H	5.562806000	-0.470760000	-3.809827000
C	-4.826211000	-2.351061000	2.570679000
C	-5.711914000	-1.373461000	3.042326000
C	5.128229000	1.463479000	-2.977130000
C	5.895387000	0.566231000	-3.731004000
O	-2.737401000	-2.853036000	1.589570000
O	-0.175125000	-4.120104000	1.950282000
O	1.059157000	-2.158049000	0.228460000
O	3.300516000	1.830566000	-1.538780000
O	0.882292000	2.873137000	-2.283738000
O	-0.810175000	1.683376000	-0.394547000
Hf	-0.971204000	-2.722824000	0.249386000
Hf	1.457761000	1.701516000	-0.299044000
H	-8.519881000	-3.528360000	-2.965379000
C	-6.782391000	-3.964796000	-1.758838000
C	-7.467627000	-3.300931000	-2.777775000
O	3.172930000	2.121683000	1.270767000
O	1.138642000	3.709963000	0.185639000
O	-0.512399000	-4.607088000	-0.588083000
H	8.384179000	2.662853000	-4.730038000
C	7.062577000	0.995724000	-4.356142000
C	7.469082000	2.325610000	-4.237195000
H	8.309401000	3.461189000	4.214844000
C	6.816901000	3.641091000	2.664843000
C	7.395905000	3.043533000	3.784907000
H	9.221785000	-4.724960000	0.612127000
C	7.586796000	-3.815213000	1.691306000
C	8.222009000	-4.289485000	0.542566000
O	-3.315145000	1.033606000	-1.338635000
H	-4.947425000	-1.288749000	-3.894769000
C	-6.812765000	-2.342946000	-3.554130000
C	-5.475598000	-2.044478000	-3.309636000
H	-8.469385000	-3.310591000	3.522154000
C	-7.017652000	-1.717742000	3.379621000
C	-7.444196000	-3.041011000	3.256759000
H	-5.574069000	1.159474000	-2.296465000
H	5.801293000	-2.882291000	2.490837000
C	-5.290246000	1.734486000	-0.245817000
C	-6.062585000	1.541614000	-1.397976000
C	5.665176000	-3.175911000	0.364650000
C	6.312201000	-3.262743000	1.604026000
O	-3.224796000	1.486126000	0.857251000
O	0.710169000	0.658084000	1.388077000
O	3.820409000	-2.414237000	-0.890529000

O	1.741981000	-3.899287000	-1.891129000
O	-0.326778000	-2.055521000	-1.889534000
Hf	-1.371200000	0.539857000	1.576108000
Hf	1.903739000	-1.553970000	-1.629611000
O	3.495564000	-0.179627000	-2.524339000
O	1.726187000	-1.888308000	-3.704819000
O	-1.371037000	0.753557000	3.713758000
H	-0.624071000	-2.615678000	-2.615448000
H	2.590218000	-3.232471000	3.235330000
H	0.299788000	0.241772000	3.995472000
H	1.167623000	-0.924349000	4.596355000
H	0.594977000	-3.733530000	2.459922000
H	-1.161885000	-4.996533000	-1.183085000
H	4.932520000	3.483374000	-2.269889000
C	6.707903000	3.224994000	-3.488910000
C	5.543278000	2.796189000	-2.858624000
O	3.720544000	-2.260930000	1.345484000
O	1.767585000	-2.730276000	3.200756000
O	-1.380002000	1.747585000	-3.206115000
H	-0.734536000	-1.911103000	2.987128000
H	1.622320000	4.107698000	0.921459000
H	0.045530000	2.544868000	-2.719724000
H	0.734148000	3.795021000	-2.037130000
H	-1.918307000	0.080079000	4.136319000
H	-0.500986000	0.270930000	-4.556608000
H	5.791604000	-3.574543000	-1.743131000
C	7.581906000	-4.206813000	-0.694970000
C	6.309617000	-3.649644000	-0.785270000
H	-4.888137000	-4.172519000	-0.719911000
H	5.191601000	3.567112000	1.238218000
C	-4.781742000	-2.712380000	-2.292738000
C	-5.441981000	-3.676075000	-1.519752000
C	5.057307000	1.977708000	2.689274000
C	5.649826000	3.113310000	2.120585000
O	-2.881947000	-1.341257000	-2.564482000
O	-0.577014000	-0.560665000	-4.067913000
O	0.783556000	0.210498000	-1.649204000
O	3.463925000	0.256933000	2.492122000
O	1.209268000	-0.166645000	3.997292000
O	-0.431117000	-1.484570000	2.177899000
H	-9.093151000	2.527848000	-0.203165000
C	-7.425448000	1.822826000	-1.380855000
C	-8.022989000	2.306953000	-0.215928000
H	-4.557881000	-4.425808000	2.074940000
C	-6.563594000	-4.020657000	2.793991000
C	-5.259923000	-3.677314000	2.448133000

O	-2.753370000	-3.067567000	-1.140741000
H	3.646959000	-0.075136000	0.003600000
O	-1.597258000	-0.755462000	-0.026876000
O	2.691398000	-0.190970000	0.009166000
H	7.265738000	1.445052000	5.232318000
H	7.278751000	4.521887000	2.213739000
H	7.025551000	4.266277000	-3.398242000
H	7.660226000	0.291514000	-4.939433000
H	8.079417000	-4.579089000	-1.593423000
H	8.089920000	-3.876669000	2.658988000
H	-8.027258000	1.661725000	-2.278373000
H	-7.725361000	2.888743000	1.843809000
H	-7.298654000	-4.706162000	-1.144348000
H	-7.351573000	-1.823823000	-4.350365000
H	-7.708408000	-0.950734000	3.737339000
H	-6.898416000	-5.056557000	2.701063000
Hf	-1.301037000	0.072777000	-1.938539000
Hf	1.810383000	-1.097123000	1.871820000
C	-0.635057000	3.961286000	4.629619000
C	-1.903748000	4.091334000	3.758444000
C	-1.603386000	3.828591000	2.301345000
C	0.584291000	4.675901000	4.025648000
C	-2.058075000	4.725055000	1.190989000
C	1.636410000	3.696059000	3.532177000
H	-3.152176000	4.567770000	1.113211000
H	-2.332063000	5.101171000	3.883474000
H	-0.420363000	2.879741000	4.680110000
H	3.052156000	3.786913000	2.209338000
H	-1.921017000	5.779423000	1.491891000
H	-0.484440000	4.295797000	0.114541000
H	1.165539000	2.887252000	2.940652000
H	2.128725000	3.217938000	4.400256000
H	-2.439633000	2.276825000	4.104223000
H	0.960475000	5.700165000	2.443798000
H	-1.147927000	5.269604000	5.959834000
H	1.030627000	5.309688000	4.817219000
O	-0.902250000	4.336631000	5.955912000
O	-1.465599000	4.410750000	-0.028053000
O	2.551333000	4.430023000	2.741211000
O	-1.068964000	2.760326000	2.022624000
O	-2.878512000	3.158646000	4.141735000
O	0.157396000	5.500383000	2.950221000

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C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000

C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.232542000	2.590703000	-0.350310000
H	2.418034000	-1.477301000	-4.215699000
H	0.932311000	-4.265835000	-1.430513000
H	1.587229000	-3.992831000	-2.844259000
H	0.296877000	-0.998576000	-4.050841000
H	-2.046386000	2.409004000	-3.037777000
H	0.119773000	-4.903289000	1.440710000
H	5.515424000	0.199290000	3.799915000
C	7.085114000	1.686973000	3.987194000
C	5.884211000	1.181512000	3.497545000
H	-5.380083000	2.250509000	1.790271000
C	-7.327359000	2.378179000	0.844721000
C	-5.958791000	2.126146000	0.872472000
O	-3.061560000	-0.791888000	2.408268000
H	-5.337511000	-0.352726000	3.189950000
H	5.496929000	-0.445443000	-3.900115000
C	-4.837140000	-2.340706000	2.541972000
C	-5.707943000	-1.371054000	3.055624000
C	5.113047000	1.468951000	-2.999880000
C	5.845134000	0.584775000	-3.802565000
O	-2.743431000	-2.847816000	1.577900000
O	-0.188116000	-4.131914000	1.938706000
O	1.060427000	-2.149513000	0.238391000
O	3.313139000	1.823018000	-1.518129000
O	0.913984000	2.897445000	-2.225208000
O	-0.785349000	1.725959000	-0.342817000
Hf	-0.969358000	-2.711793000	0.256803000
Hf	1.475906000	1.691170000	-0.240636000
H	-8.419683000	-3.713310000	-3.223898000
C	-6.714191000	-4.120987000	-1.962807000
C	-7.387835000	-3.446662000	-2.982453000
O	3.167435000	2.115541000	1.279945000
O	1.243116000	3.730804000	0.364678000
O	-0.512255000	-4.591246000	-0.600957000
H	8.330166000	2.678385000	-4.816930000
C	6.997721000	1.017953000	-4.451650000
C	7.426101000	2.338258000	-4.306089000
H	8.462398000	3.352873000	3.983964000
C	6.756902000	3.713202000	2.708555000
C	7.521151000	2.955531000	3.596750000
H	9.224019000	-4.726468000	0.579005000
C	7.577576000	-3.858652000	1.675251000

C	8.223855000	-4.290884000	0.516132000
O	-3.273522000	1.096054000	-1.339951000
H	-4.918168000	-1.284048000	-3.914670000
C	-6.746444000	-2.429726000	-3.692000000
C	-5.435528000	-2.082599000	-3.379172000
H	-8.502973000	-3.278124000	3.426336000
C	-7.021406000	-1.707584000	3.369987000
C	-7.471488000	-3.014956000	3.179623000
H	-5.493211000	1.192985000	-2.366209000
H	5.782681000	-2.958467000	2.491197000
C	-5.298198000	1.701556000	-0.287671000
C	-6.023399000	1.530977000	-1.473636000
C	5.665727000	-3.177013000	0.355161000
C	6.302891000	-3.305194000	1.596048000
O	-3.266340000	1.432094000	0.876000000
O	0.704657000	0.656202000	1.424457000
O	3.816104000	-2.408375000	-0.887994000
O	1.733434000	-3.882645000	-1.894897000
O	-0.333623000	-2.031303000	-1.876744000
Hf	-1.380793000	0.541116000	1.619549000
Hf	1.900091000	-1.544421000	-1.615215000
O	3.490897000	-0.177912000	-2.522420000
O	1.704701000	-1.863727000	-3.694472000
O	-1.253534000	0.746751000	3.730483000
H	-0.627825000	-2.589242000	-2.605606000
H	2.593788000	-3.287654000	3.190758000
H	0.324815000	0.179683000	4.040174000
H	1.154550000	-1.047773000	4.593242000
H	0.586987000	-3.752524000	2.448523000
H	-1.167437000	-4.971075000	-1.195982000
H	4.970000000	3.468037000	-2.224538000
C	6.701489000	3.224088000	-3.507108000
C	5.550614000	2.791622000	-2.854603000
O	3.726599000	-2.265770000	1.349674000
O	1.773281000	-2.781091000	3.179392000
O	-1.322768000	1.786523000	-3.171308000
H	-0.747571000	-1.904976000	2.996752000
H	2.103465000	4.132240000	0.538903000
H	0.088953000	2.545292000	-2.673866000
H	0.754391000	3.833174000	-2.059655000
H	-1.890800000	0.227311000	4.234057000
H	-0.509676000	0.304767000	-4.520191000
H	5.810175000	-3.504375000	-1.763753000
C	7.593821000	-4.166814000	-0.723071000
C	6.320495000	-3.610575000	-0.804707000
H	-4.856666000	-4.289679000	-0.855210000

H	4.948032000	3.784133000	1.515387000
C	-4.753791000	-2.758031000	-2.358932000
C	-5.399864000	-3.781948000	-1.654792000
C	5.107989000	1.941835000	2.612807000
C	5.556587000	3.206660000	2.214734000
O	-2.897622000	-1.311645000	-2.526081000
O	-0.591518000	-0.533473000	-4.043333000
O	0.787406000	0.231013000	-1.613472000
O	3.461898000	0.258021000	2.504729000
O	1.224542000	-0.262640000	4.033650000
O	-0.429665000	-1.500003000	2.181948000
H	-9.121678000	2.392723000	-0.357875000
C	-7.393290000	1.775783000	-1.497114000
C	-8.046102000	2.200647000	-0.338875000
H	-4.602889000	-4.392845000	1.947670000
C	-6.606516000	-3.986538000	2.672818000
C	-5.294434000	-3.651026000	2.352295000
O	-2.757071000	-3.063190000	-1.135370000
H	3.647728000	-0.069956000	0.033719000
O	-1.591980000	-0.735255000	-0.006269000
O	2.692867000	-0.193679000	0.029940000
H	7.686245000	1.091913000	4.678601000
H	7.100186000	4.702781000	2.398573000
H	7.037489000	4.257325000	-3.393654000
H	7.567165000	0.323976000	-5.074080000
H	8.099830000	-4.506360000	-1.629693000
H	8.071947000	-3.954345000	2.644688000
H	-7.957395000	1.631555000	-2.421571000
H	-7.839408000	2.711486000	1.750478000
H	-7.219263000	-4.911264000	-1.402326000
H	-7.274914000	-1.903551000	-4.490492000
H	-7.700287000	-0.947102000	3.762754000
H	-6.960049000	-5.009883000	2.525915000
Hf	-1.297761000	0.096577000	-1.908844000
Hf	1.817750000	-1.106215000	1.901684000
C	0.341693000	4.560780000	3.972480000
C	-1.187293000	4.352507000	3.734525000
C	-1.354762000	3.969681000	2.285945000
C	1.159561000	3.291976000	4.193103000
C	-1.604367000	5.003485000	1.223988000
C	2.633843000	3.664490000	4.320373000
H	-2.691340000	5.210016000	1.254404000
H	-1.661025000	5.338968000	3.886952000
H	0.444700000	5.176192000	4.881856000
H	4.222235000	2.719376000	4.940151000
H	-1.113075000	5.946588000	1.528482000

H	-0.273295000	4.407381000	-0.005050000
H	2.735264000	4.538314000	4.994253000
H	3.046855000	3.952494000	3.335795000
H	-1.463160000	2.541309000	4.394332000
H	1.423812000	2.007213000	5.569557000
H	1.021268000	4.698606000	2.147449000
H	1.048203000	2.615767000	3.310568000
O	0.896250000	5.305519000	2.903701000
O	-1.248849000	4.580680000	-0.052277000
O	3.282358000	2.531345000	4.847686000
O	-1.255152000	2.794003000	1.977168000
O	-1.811220000	3.445444000	4.571483000
O	0.732214000	2.654390000	5.367470000

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C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000
C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.209637000	2.581974000	-0.237084000
H	2.396966000	-1.445497000	-4.237217000
H	0.903228000	-4.260079000	-1.464538000
H	1.545133000	-3.989669000	-2.889190000
H	0.262418000	-0.959055000	-4.042799000
H	-1.953607000	2.466960000	-2.988841000
H	0.105158000	-4.929486000	1.391776000
H	5.191784000	0.459499000	4.212753000
C	6.572231000	2.086703000	4.604503000
C	5.542140000	1.450248000	3.917515000
H	-5.373737000	2.291399000	1.771246000
C	-7.300692000	2.510332000	0.799078000
C	-5.945005000	2.198861000	0.844420000
O	-3.036212000	-0.810126000	2.450129000
H	-5.359429000	-0.269476000	2.971839000
H	5.609310000	-0.452977000	-3.768598000
C	-4.867245000	-2.297815000	2.460369000
C	-5.747390000	-1.284276000	2.861047000
C	5.131668000	1.480003000	-2.956874000
C	5.925470000	0.589178000	-3.690785000
O	-2.744052000	-2.857409000	1.591103000
O	-0.195462000	-4.171109000	1.913647000
O	1.068640000	-2.174426000	0.222405000
O	3.260311000	1.824113000	-1.560005000
O	0.860432000	3.088242000	-1.980019000

O	-0.770661000	1.712629000	-0.290157000
Hf	-0.971689000	-2.703936000	0.266548000
Hf	1.475553000	1.610131000	-0.223535000
H	-8.319302000	-3.873244000	-3.428066000
C	-6.634061000	-4.260060000	-2.133526000
C	-7.308041000	-3.572099000	-3.143788000
O	3.234225000	2.058859000	1.184869000
O	1.207330000	3.684974000	0.688726000
O	-0.513836000	-4.575817000	-0.633203000
H	8.401130000	2.715781000	-4.658664000
C	7.097322000	1.031929000	-4.297558000
C	7.482216000	2.368351000	-4.180290000
H	7.806629000	3.853716000	4.747914000
C	6.387401000	3.989934000	3.124756000
C	6.996321000	3.356279000	4.209280000
H	9.321136000	-4.496612000	0.536984000
C	7.656576000	-3.677610000	1.643242000
C	8.301290000	-4.108049000	0.482642000
O	-3.258859000	1.125027000	-1.345425000
H	-4.912588000	-1.264771000	-3.908036000
C	-6.693486000	-2.497555000	-3.789156000
C	-5.408905000	-2.107293000	-3.422348000
H	-8.611931000	-3.106379000	3.105725000
C	-7.089730000	-1.574186000	3.087403000
C	-7.558123000	-2.879151000	2.926714000
H	-5.471887000	1.269977000	-2.394619000
H	5.838236000	-2.838446000	2.471745000
C	-5.285786000	1.755403000	-0.309521000
C	-5.999817000	1.624704000	-1.507022000
C	5.692819000	-3.114762000	0.343654000
C	6.356660000	-3.184542000	1.575283000
O	-3.291966000	1.368098000	0.882456000
O	0.746711000	0.602857000	1.436296000
O	3.797580000	-2.446641000	-0.884484000
O	1.704466000	-3.882417000	-1.941796000
O	-0.343165000	-2.010353000	-1.878063000
Hf	-1.363127000	0.559167000	1.696336000
Hf	1.899493000	-1.567584000	-1.631617000
O	3.518896000	-0.188726000	-2.516821000
O	1.689663000	-1.837949000	-3.712455000
O	-1.178247000	0.589061000	3.848373000
H	-0.646633000	-2.565383000	-2.605258000
H	2.605215000	-3.375877000	3.147630000
H	0.417878000	0.088925000	4.069808000
H	1.255497000	-1.148088000	4.584145000
H	0.587537000	-3.806617000	2.422926000

H	-1.182732000	-4.944991000	-1.219600000
H	4.895914000	3.500853000	-2.265017000
C	6.694833000	3.261165000	-3.451596000
C	5.525551000	2.819035000	-2.839572000
O	3.731063000	-2.283872000	1.354631000
O	1.789138000	-2.862451000	3.151235000
O	-1.221712000	1.848478000	-3.095155000
H	-0.704797000	-1.964753000	3.002554000
H	2.033717000	4.173236000	0.568496000
H	0.131387000	2.631630000	-2.512347000
H	0.429085000	3.889379000	-1.657235000
H	-1.771759000	-0.027582000	4.293374000
H	-0.507433000	0.379131000	-4.453197000
H	5.815953000	-3.483463000	-1.770072000
C	7.644975000	-4.041475000	-0.747383000
C	6.346728000	-3.544732000	-0.818171000
H	-4.802666000	-4.395372000	-0.978691000
H	4.870937000	3.834001000	1.585607000
C	-4.726897000	-2.796085000	-2.411267000
C	-5.346174000	-3.876828000	-1.770997000
C	4.926083000	2.081046000	2.829668000
C	5.355749000	3.355466000	2.438946000
O	-2.911327000	-1.291695000	-2.499767000
O	-0.618993000	-0.485031000	-4.029768000
O	0.799380000	0.235547000	-1.617936000
O	3.497188000	0.239153000	2.473358000
O	1.318668000	-0.354307000	4.035813000
O	-0.397600000	-1.542835000	2.192498000
H	-9.074398000	2.612743000	-0.429814000
C	-7.357738000	1.928615000	-1.548102000
C	-8.008759000	2.373039000	-0.396336000
H	-4.644677000	-4.380271000	1.975362000
C	-6.683641000	-3.894147000	2.533714000
C	-5.343429000	-3.604544000	2.295233000
O	-2.763014000	-3.054398000	-1.124869000
H	3.654692000	-0.083235000	0.019017000
O	-1.565542000	-0.723575000	0.023073000
O	2.704555000	-0.238208000	0.007432000
H	7.048225000	1.591654000	5.454045000
H	6.722347000	4.981894000	2.812560000
H	6.996265000	4.307256000	-3.361316000
H	7.715635000	0.332852000	-4.865198000
H	8.150017000	-4.379367000	-1.655171000
H	8.172048000	-3.726508000	2.605105000
H	-7.913994000	1.816980000	-2.481725000
H	-7.810899000	2.860108000	1.699703000

H	-7.118331000	-5.096311000	-1.623716000
H	-7.222298000	-1.960452000	-4.580030000
H	-7.776487000	-0.778767000	3.386336000
H	-7.052529000	-4.915048000	2.409048000
Hf	-1.311032000	0.112735000	-1.870855000
Hf	1.840159000	-1.161314000	1.898686000
C	0.465201000	4.729722000	3.493345000
C	-1.981213000	3.983071000	3.843781000
C	-1.783573000	3.725887000	2.508622000
C	0.460434000	5.112162000	4.934494000
C	-2.220142000	4.671522000	1.417395000
C	1.888244000	5.323221000	5.422498000
H	-3.258875000	4.442302000	1.122508000
H	-2.385061000	4.934188000	4.199232000
H	0.187249000	5.531383000	2.776474000
H	2.637662000	6.065251000	7.057324000
H	-2.223821000	5.717360000	1.781348000
H	-0.512541000	4.413290000	0.508224000
H	2.393701000	6.071478000	4.779536000
H	2.447770000	4.373825000	5.339282000
H	-1.495003000	2.199614000	4.402985000
H	-0.095597000	6.601257000	5.983182000
H	1.135007000	3.612836000	1.816760000
H	0.032576000	4.267625000	5.515531000
O	1.084565000	3.707583000	3.119751000
O	-1.443732000	4.523386000	0.242492000
O	1.772512000	5.777621000	6.751024000
O	-1.217712000	2.623623000	2.121384000
O	-1.776782000	3.072074000	4.801252000
O	-0.291332000	6.287962000	5.089929000

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C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000
C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.229285000	2.571378000	-0.258482000
H	2.385224000	-1.422755000	-4.240158000
H	0.907324000	-4.251106000	-1.479018000
H	1.540561000	-3.970643000	-2.905402000
H	0.257714000	-0.923847000	-4.038113000
H	-1.931242000	2.500264000	-2.961710000
H	0.102369000	-4.936471000	1.378086000
H	5.521351000	0.252705000	3.830941000

C	6.785365000	1.926761000	4.384752000
C	5.742336000	1.314148000	3.696554000
H	-5.376709000	2.267838000	1.780447000
C	-7.296799000	2.517030000	0.802605000
C	-5.943830000	2.194170000	0.849175000
O	-3.030685000	-0.815260000	2.466336000
H	-5.352520000	-0.269747000	2.993151000
H	5.574707000	-0.432365000	-3.830836000
C	-4.870534000	-2.292483000	2.449676000
C	-5.745911000	-1.280211000	2.863847000
C	5.122877000	1.485163000	-2.968192000
C	5.898078000	0.606116000	-3.735540000
O	-2.747394000	-2.854698000	1.584222000
O	-0.199136000	-4.180245000	1.902693000
O	1.068043000	-2.176654000	0.218625000
O	3.265394000	1.819922000	-1.553079000
O	0.874468000	3.131441000	-1.875225000
O	-0.780230000	1.706418000	-0.275441000
Hf	-0.972166000	-2.706440000	0.260063000
Hf	1.495066000	1.618604000	-0.206935000
H	-8.316728000	-3.874339000	-3.434797000
C	-6.627733000	-4.269345000	-2.147660000
C	-7.306076000	-3.572651000	-3.148980000
O	3.221949000	2.068427000	1.199272000
O	0.934138000	3.500848000	0.947136000
O	-0.506918000	-4.572585000	-0.647924000
H	8.367665000	2.740471000	-4.701158000
C	7.060854000	1.056024000	-4.354232000
C	7.455533000	2.387460000	-4.213921000
H	7.848353000	3.771807000	4.751321000
C	6.242853000	4.034802000	3.330513000
C	7.033661000	3.289220000	4.206046000
H	9.315927000	-4.512868000	0.526157000
C	7.648819000	-3.707961000	1.638941000
C	8.297222000	-4.121101000	0.474094000
O	-3.255057000	1.137887000	-1.345984000
H	-4.920451000	-1.248157000	-3.891863000
C	-6.696715000	-2.488655000	-3.783392000
C	-5.412811000	-2.097895000	-3.414770000
H	-8.623345000	-3.087298000	3.064182000
C	-7.091035000	-1.565251000	3.079602000
C	-7.567276000	-2.864030000	2.893834000
H	-5.463511000	1.311795000	-2.402302000
H	5.828699000	-2.879109000	2.473577000
C	-5.282872000	1.764165000	-0.309164000
C	-5.992474000	1.657348000	-1.511713000

C	5.691448000	-3.119138000	0.340746000
C	6.350550000	-3.210327000	1.573533000
O	-3.296817000	1.348028000	0.885253000
O	0.737164000	0.590477000	1.442355000
O	3.795867000	-2.444085000	-0.882974000
O	1.705813000	-3.869678000	-1.958320000
O	-0.342883000	-1.997520000	-1.881936000
Hf	-1.371120000	0.550573000	1.701357000
Hf	1.899591000	-1.558114000	-1.632426000
O	3.518748000	-0.189796000	-2.515619000
O	1.676157000	-1.811957000	-3.715256000
O	-1.159927000	0.604951000	3.855690000
H	-0.645309000	-2.548533000	-2.612650000
H	2.607093000	-3.396145000	3.117836000
H	0.377737000	0.032659000	4.053804000
H	1.287925000	-1.136510000	4.617454000
H	0.583676000	-3.817795000	2.413814000
H	-1.174641000	-4.941574000	-1.235807000
H	4.911621000	3.490978000	-2.225695000
C	6.687148000	3.267982000	-3.450813000
C	5.526092000	2.819345000	-2.827940000
O	3.733875000	-2.283737000	1.356517000
O	1.793561000	-2.879195000	3.140561000
O	-1.181978000	1.898801000	-3.043469000
H	-0.708738000	-1.984187000	3.000009000
H	1.530547000	3.644094000	1.711342000
H	0.124997000	2.705271000	-2.411874000
H	0.500533000	3.955676000	-1.540452000
H	-1.777187000	0.028814000	4.322241000
H	-0.485124000	0.438553000	-4.417414000
H	5.821629000	-3.456504000	-1.777750000
C	7.645643000	-4.033674000	-0.757060000
C	6.348647000	-3.533207000	-0.824959000
H	-4.793770000	-4.410766000	-0.997729000
H	4.575004000	3.986677000	1.945391000
C	-4.726288000	-2.795610000	-2.412887000
C	-5.340557000	-3.885511000	-1.783334000
C	4.947573000	2.057268000	2.814031000
C	5.207395000	3.420246000	2.631597000
O	-2.913085000	-1.286085000	-2.490706000
O	-0.617529000	-0.436739000	-4.022566000
O	0.802549000	0.246477000	-1.599586000
O	3.489368000	0.240546000	2.477219000
O	1.301121000	-0.370060000	4.028607000
O	-0.401089000	-1.555513000	2.193525000
H	-9.063799000	2.652682000	-0.432459000

C	-7.347720000	1.972290000	-1.553778000
C	-8.000276000	2.404002000	-0.397974000
H	-4.659430000	-4.367294000	1.928969000
C	-6.697808000	-3.877724000	2.486633000
C	-5.354661000	-3.592921000	2.259527000
O	-2.759966000	-3.060027000	-1.131004000
H	3.661422000	-0.094746000	0.026485000
O	-1.569140000	-0.726711000	0.024358000
O	2.709445000	-0.238427000	0.016256000
H	7.409912000	1.342774000	5.065066000
H	6.436086000	5.101096000	3.193315000
H	6.996884000	4.309777000	-3.341532000
H	7.664399000	0.366703000	-4.949069000
H	8.153371000	-4.358220000	-1.668164000
H	8.160166000	-3.774694000	2.601960000
H	-7.900807000	1.879593000	-2.491295000
H	-7.808307000	2.856599000	1.706327000
H	-7.108038000	-5.113022000	-1.646389000
H	-7.229067000	-1.944651000	-4.567113000
H	-7.773928000	-0.770771000	3.389642000
H	-7.072958000	-4.893652000	2.341784000
Hf	-1.306376000	0.125753000	-1.860865000
Hf	1.834595000	-1.170427000	1.897759000
C	1.355896000	3.596390000	4.651079000
C	-2.042777000	3.977319000	3.811638000
C	-1.928206000	3.688001000	2.497909000
C	1.494033000	2.586543000	5.752711000
C	-2.585773000	4.444567000	1.387388000
C	2.842145000	1.897006000	5.725625000
H	-3.484159000	3.922701000	1.020376000
H	-2.571694000	4.862740000	4.174295000
H	0.814132000	4.530335000	4.935283000
H	3.722385000	0.632563000	6.908847000
H	-2.916241000	5.441927000	1.730368000
H	-0.883824000	4.874768000	0.540264000
H	3.641346000	2.654700000	5.850900000
H	2.982873000	1.399119000	4.752925000
H	-1.329225000	2.303365000	4.405323000
H	1.463518000	2.569922000	7.655662000
H	0.077558000	3.185999000	1.421932000
H	0.719031000	1.816657000	5.537898000
O	1.810192000	3.421751000	3.540254000
O	-1.738378000	4.535652000	0.237635000
O	2.831189000	0.978968000	6.801069000
O	-1.172181000	2.639737000	2.111252000
O	-1.514600000	3.201596000	4.783628000

O 1.257076000 3.225119000 6.976874000

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C -3.448800000 -1.965700000 2.156800000
C 3.881700000 1.003300000 -2.299800000
C -3.841600000 1.392100000 -0.254600000
C 4.304100000 -2.576300000 0.267700000
C -3.369500000 -2.356800000 -1.985400000
C 3.808500000 1.407600000 2.107100000
H -1.256448000 2.628094000 -0.259698000
H 2.370950000 -1.402368000 -4.223476000
H 0.917346000 -4.239639000 -1.482650000
H 1.551326000 -3.937891000 -2.902023000
H 0.254196000 -0.928589000 -4.027845000
H -2.018461000 2.461577000 -2.943972000
H 0.074115000 -4.950642000 1.377580000
H 4.978221000 0.767572000 4.449678000
C 6.677275000 2.118262000 4.468903000
C 5.531572000 1.546645000 3.921147000
H -5.427073000 2.221355000 1.765293000
C -7.282480000 2.635771000 0.724564000
C -5.952420000 2.234570000 0.807502000
O -3.014850000 -0.824824000 2.493074000
H -5.330849000 -0.258542000 3.020245000
H 5.549975000 -0.431155000 -3.862620000
C -4.880241000 -2.271220000 2.418589000
C -5.742558000 -1.255551000 2.850914000
C 5.114184000 1.483012000 -2.983988000
C 5.876461000 0.606353000 -3.766532000
O -2.752025000 -2.851492000 1.578531000
O -0.213627000 -4.181915000 1.891159000
O 1.062187000 -2.158881000 0.227239000
O 3.290805000 1.815434000 -1.528965000
O 0.887113000 3.016650000 -2.023800000
O -0.791188000 1.779650000 -0.164876000
Hf -0.965961000 -2.716403000 0.262524000
Hf 1.495662000 1.681550000 -0.192725000
H -8.251567000 -3.966758000 -3.552556000
C -6.582786000 -4.335778000 -2.231723000
C -7.255189000 -3.644228000 -3.240605000
O 3.218433000 2.082619000 1.217568000
O 1.269504000 3.734188000 0.521573000
O -0.511078000 -4.573148000 -0.657893000
H 8.338027000 2.740746000 -4.751974000
C 7.032188000 1.057230000 -4.397799000
C 7.431566000 2.386985000 -4.254706000

H	8.269086000	3.552748000	4.197842000
C	6.909403000	3.531367000	2.518813000
C	7.367204000	3.109468000	3.768855000
H	9.233318000	-4.710455000	0.514922000
C	7.615608000	-3.809516000	1.626856000
C	8.230917000	-4.278333000	0.465169000
O	-3.235365000	1.147655000	-1.334418000
H	-4.909195000	-1.256805000	-3.906067000
C	-6.657989000	-2.539101000	-3.849492000
C	-5.391841000	-2.122687000	-3.448698000
H	-8.659554000	-3.007200000	2.935158000
C	-7.096896000	-1.519440000	3.032669000
C	-7.595983000	-2.800742000	2.792790000
H	-5.371594000	1.526984000	-2.469080000
H	5.843326000	-2.883987000	2.462455000
C	-5.262389000	1.837109000	-0.345151000
C	-5.921303000	1.844524000	-1.580854000
C	5.668018000	-3.172664000	0.337774000
C	6.337969000	-3.260633000	1.564948000
O	-3.336737000	1.296834000	0.897470000
O	0.724980000	0.633600000	1.474268000
O	3.792956000	-2.425764000	-0.879489000
O	1.713724000	-3.848510000	-1.953125000
O	-0.349118000	-1.994930000	-1.871100000
Hf	-1.368691000	0.514134000	1.716093000
Hf	1.892599000	-1.528792000	-1.616607000
O	3.501510000	-0.184501000	-2.519710000
O	1.659768000	-1.792803000	-3.702140000
O	-0.889145000	0.592542000	3.823958000
H	-0.641353000	-2.544622000	-2.606909000
H	2.611847000	-3.450189000	3.008306000
H	0.488248000	-0.104255000	4.173214000
H	1.317690000	-1.413913000	4.538281000
H	0.582660000	-3.820398000	2.393210000
H	-1.174777000	-4.930374000	-1.257505000
H	4.915308000	3.486241000	-2.227520000
C	6.675341000	3.265008000	-3.476470000
C	5.521486000	2.815994000	-2.840598000
O	3.748956000	-2.254011000	1.357741000
O	1.797676000	-2.937334000	3.070077000
O	-1.264259000	1.869956000	-3.045427000
H	-0.735119000	-1.906358000	3.024750000
H	2.123439000	4.207274000	0.592976000
H	0.087955000	2.650274000	-2.513811000
H	0.627416000	3.879244000	-1.675172000
H	-1.589795000	0.774414000	4.457686000

H	-0.526926000	0.406416000	-4.440049000
H	5.756601000	-3.565179000	-1.773396000
C	7.567899000	-4.194273000	-0.760194000
C	6.292288000	-3.641337000	-0.825392000
H	-4.771692000	-4.447597000	-1.043287000
H	5.370744000	3.303315000	1.007366000
C	-4.710780000	-2.815912000	-2.440012000
C	-5.313369000	-3.926073000	-1.834882000
C	5.056213000	1.984610000	2.680192000
C	5.751759000	2.978047000	1.978390000
O	-2.919877000	-1.277331000	-2.477426000
O	-0.630218000	-0.453719000	-4.007352000
O	0.775947000	0.263806000	-1.568464000
O	3.437475000	0.277725000	2.534092000
O	1.390399000	-0.550380000	4.106742000
O	-0.398434000	-1.548085000	2.194994000
H	-8.980141000	2.948536000	-0.573935000
C	-7.253465000	2.240006000	-1.661007000
C	-7.934798000	2.636987000	-0.509490000
H	-4.701154000	-4.330493000	1.830199000
C	-6.739893000	-3.817815000	2.366317000
C	-5.387028000	-3.553953000	2.174807000
O	-2.762667000	-3.056473000	-1.126203000
H	3.651342000	-0.077693000	0.037262000
O	-1.564672000	-0.721541000	0.041275000
O	2.697503000	-0.210176000	0.037932000
H	7.036941000	1.789581000	5.446565000
H	7.458273000	4.297209000	1.965117000
H	6.988100000	4.305800000	-3.366100000
H	7.626580000	0.370036000	-5.004225000
H	8.050108000	-4.562016000	-1.668786000
H	8.136675000	-3.871605000	2.584886000
H	-7.765808000	2.238784000	-2.625781000
H	-7.816095000	2.948055000	1.625311000
H	-7.053678000	-5.196568000	-1.751018000
H	-7.185796000	-1.998820000	-4.638763000
H	-7.769760000	-0.722122000	3.357186000
H	-7.133126000	-4.819568000	2.177671000
Hf	-1.303626000	0.121260000	-1.850164000
Hf	1.840943000	-1.155528000	1.910123000
C	3.985414000	5.994810000	1.642316000
C	0.131282000	3.960666000	2.916557000
C	-1.127218000	3.768799000	2.330800000
C	3.131702000	6.020790000	2.874470000
C	-1.759097000	4.825951000	1.457224000
C	3.259785000	4.696833000	3.633280000

H	-2.442840000	5.440518000	2.077229000
H	0.412405000	4.988563000	3.183773000
H	4.927126000	6.600125000	1.699730000
H	1.836340000	4.077578000	4.777880000
H	-1.000778000	5.510311000	1.050851000
H	-2.913563000	3.465636000	0.785408000
H	4.326181000	4.539751000	3.880851000
H	2.940728000	3.865494000	2.983377000
H	0.096097000	2.198774000	3.791307000
H	3.131960000	6.891712000	4.562514000
H	0.721193000	3.846111000	1.699318000
H	2.079459000	6.114980000	2.524409000
O	3.707500000	5.346817000	0.657613000
O	-2.438541000	4.217928000	0.387807000
O	2.505134000	4.785061000	4.810235000
O	-1.710009000	2.645590000	2.335673000
O	0.628780000	3.032614000	3.813460000
O	3.502779000	7.092134000	3.690854000

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C	-3.448800000	-1.965700000	2.156800000
C	3.881700000	1.003300000	-2.299800000
C	-3.841600000	1.392100000	-0.254600000
C	4.304100000	-2.576300000	0.267700000
C	-3.369500000	-2.356800000	-1.985400000
C	3.808500000	1.407600000	2.107100000
H	-1.204040000	2.593645000	-0.369606000
H	2.407019000	-1.457607000	-4.230301000
H	0.939993000	-4.259129000	-1.449815000
H	1.576069000	-3.974104000	-2.868643000
H	0.286982000	-0.980091000	-4.056213000
H	-2.059020000	2.419568000	-3.030311000
H	0.135151000	-4.903661000	1.436861000
H	5.223497000	0.481578000	4.209825000
C	6.839694000	1.921955000	4.316144000
C	5.677280000	1.377125000	3.780914000
H	-5.426244000	1.842442000	1.876763000
C	-7.354033000	2.150769000	0.931490000
C	-5.984203000	1.902346000	0.939002000
O	-3.053698000	-0.792632000	2.406029000
H	-5.252194000	-0.385211000	3.374866000
H	5.549464000	-0.461889000	-3.834532000
C	-4.830126000	-2.334299000	2.568393000
C	-5.654434000	-1.382757000	3.183625000
C	5.125361000	1.465406000	-2.980186000
C	5.885314000	0.573391000	-3.747489000

O	-2.750797000	-2.847034000	1.568011000
O	-0.177538000	-4.133062000	1.933284000
O	1.060178000	-2.153846000	0.226361000
O	3.297258000	1.827457000	-1.540043000
O	0.878354000	2.963091000	-2.147605000
O	-0.801037000	1.707869000	-0.313328000
Hf	-0.968904000	-2.718515000	0.245864000
Hf	1.483152000	1.718524000	-0.239973000
H	-8.391665000	-3.754917000	-3.291242000
C	-6.660802000	-4.219372000	-2.085631000
C	-7.366627000	-3.477115000	-3.033882000
O	3.201881000	2.085347000	1.235324000
O	1.178841000	3.675791000	0.408276000
O	-0.507109000	-4.595161000	-0.607935000
H	8.374512000	2.672734000	-4.739597000
C	7.049878000	1.005884000	-4.375454000
C	7.461186000	2.333229000	-4.244992000
H	8.312334000	3.496123000	4.171795000
C	6.790574000	3.674746000	2.650403000
C	7.398289000	3.070268000	3.751010000
H	9.235830000	-4.696711000	0.580984000
C	7.600114000	-3.802050000	1.671528000
C	8.232957000	-4.267428000	0.517879000
O	-3.281869000	1.105765000	-1.343942000
H	-4.975871000	-1.160164000	-3.784653000
C	-6.766478000	-2.378187000	-3.651015000
C	-5.462793000	-2.020146000	-3.320534000
H	-8.475841000	-3.252431000	3.547000000
C	-6.960286000	-1.713503000	3.533426000
C	-7.449693000	-2.994777000	3.273607000
H	-5.457316000	1.564595000	-2.406697000
H	5.813097000	-2.882916000	2.483184000
C	-5.300063000	1.698200000	-0.267249000
C	-6.003266000	1.740726000	-1.477661000
C	5.668565000	-3.169052000	0.356361000
C	6.321776000	-3.257022000	1.592422000
O	-3.260632000	1.434126000	0.874106000
O	0.710578000	0.652358000	1.434318000
O	3.811980000	-2.415168000	-0.886357000
O	1.734251000	-3.872283000	-1.920208000
O	-0.336327000	-2.027317000	-1.883174000
Hf	-1.367521000	0.527489000	1.611687000
Hf	1.900501000	-1.532147000	-1.627669000
O	3.497671000	-0.182341000	-2.521866000
O	1.694838000	-1.844007000	-3.707391000
O	-1.231127000	0.685129000	3.751032000

H	-0.632230000	-2.579797000	-2.615514000
H	2.598402000	-3.263242000	3.214810000
H	0.285735000	0.141530000	4.032020000
H	1.234000000	-1.004000000	4.605965000
H	0.593136000	-3.750933000	2.445018000
H	-1.158459000	-4.979753000	-1.204059000
H	4.940822000	3.477826000	-2.249064000
C	6.707578000	3.227022000	-3.482468000
C	5.545202000	2.795525000	-2.849934000
O	3.725488000	-2.265649000	1.350346000
O	1.777590000	-2.757148000	3.194063000
O	-1.322590000	1.809577000	-3.148063000
H	-0.735050000	-1.928243000	2.989245000
H	1.811898000	4.011379000	1.066951000
H	0.067373000	2.614399000	-2.619064000
H	0.683878000	3.869905000	-1.878845000
H	-1.852958000	0.094786000	4.194205000
H	-0.513677000	0.330335000	-4.512482000
H	5.788028000	-3.557287000	-1.753798000
C	7.586754000	-4.183389000	-0.716403000
C	6.310648000	-3.633803000	-0.798553000
H	-4.788072000	-4.425633000	-1.010745000
H	5.132045000	3.595023000	1.255140000
C	-4.748914000	-2.763081000	-2.371578000
C	-5.355770000	-3.865250000	-1.756250000
C	5.059235000	1.982023000	2.679356000
C	5.623022000	3.134919000	2.116304000
O	-2.901184000	-1.303324000	-2.511241000
O	-0.601351000	-0.513598000	-4.046457000
O	0.783815000	0.239627000	-1.620071000
O	3.445726000	0.264496000	2.525261000
O	1.231718000	-0.219720000	4.038792000
O	-0.421816000	-1.508807000	2.180033000
H	-9.123690000	2.391832000	-0.283268000
C	-7.371965000	1.993141000	-1.482448000
C	-8.048174000	2.198804000	-0.278577000
H	-4.666623000	-4.346874000	1.834118000
C	-6.630734000	-3.947619000	2.665194000
C	-5.324765000	-3.619550000	2.313476000
O	-2.754847000	-3.071442000	-1.142685000
H	3.647699000	-0.068390000	0.023817000
O	-1.593054000	-0.741040000	-0.005731000
O	2.693415000	-0.196071000	0.021280000
H	7.314756000	1.452197000	5.180328000
H	7.229043000	4.570987000	2.206130000
H	7.029593000	4.266021000	-3.381829000

H	7.641894000	0.305990000	-4.969612000
H	8.082638000	-4.548332000	-1.618750000
H	8.108162000	-3.864090000	2.636578000
H	-7.918022000	2.024771000	-2.428111000
H	-7.886263000	2.300997000	1.873823000
H	-7.133776000	-5.075784000	-1.599314000
H	-7.321136000	-1.797236000	-4.391606000
H	-7.602410000	-0.969208000	4.010212000
H	-7.015230000	-4.950302000	2.464085000
Hf	-1.291441000	0.106100000	-1.907071000
Hf	1.822074000	-1.110124000	1.878535000
C	0.502656000	5.322866000	3.194164000
C	-3.235710000	3.752093000	3.144481000
C	-2.195816000	3.720920000	2.076320000
C	1.655330000	4.503585000	3.701083000
C	-2.163268000	4.782364000	1.010677000
C	1.260843000	3.055871000	3.939339000
H	-3.185514000	4.881584000	0.604176000
H	-4.220569000	3.874889000	2.655265000
H	0.734507000	5.914846000	2.266462000
H	2.243003000	1.440089000	4.340527000
H	-1.952904000	5.750491000	1.511193000
H	-0.367424000	4.303019000	0.305639000
H	0.908170000	2.614221000	2.988400000
H	0.416075000	3.026839000	4.653345000
H	-2.379706000	2.183967000	3.938853000
H	3.338461000	3.917051000	2.975374000
H	-3.065866000	4.703759000	3.694086000
H	1.952789000	4.939001000	4.680780000
O	-0.584636000	5.362244000	3.717869000
O	-1.295817000	4.487666000	-0.029068000
O	2.406237000	2.397023000	4.413701000
O	-1.350368000	2.831833000	2.058185000
O	-3.248440000	2.643798000	3.964937000
O	2.702159000	4.619723000	2.768977000

6. Hf-UIO-66 case

Hf-UIO-66

C	10.500304000	13.573387000	3.164252000
C	13.590710000	10.499150000	3.218816000
C	7.259476000	10.315372000	3.225519000
C	13.586689000	13.569289000	0.091792000
C	7.226103000	7.224727000	0.091424000
C	10.347298000	13.576508000	-3.149301000
C	10.494316000	7.256216000	-3.139784000

C	13.586899000	10.339498000	-3.142396000
C	7.268501000	10.493894000	-3.141496000
C	7.267313000	13.569007000	-0.062020000
C	13.640791000	7.253253000	-0.115407000
H	6.480796000	14.352396000	-0.118725000
H	14.373555000	14.352482000	0.146590000
H	10.551911000	14.360928000	3.946796000
H	10.294903000	14.355689000	-3.939692000
H	10.550598000	6.488156000	-3.941806000
H	14.370154000	10.294241000	-3.929266000
H	6.486963000	10.556791000	-3.929142000
C	6.623882000	10.218865000	5.647670000
C	14.267354000	10.666816000	5.625413000
C	5.658873000	10.169368000	6.649006000
C	15.247364000	10.772038000	6.607668000
C	5.468677000	3.874086000	0.169697000
C	6.473141000	4.835501000	0.111947000
C	16.962368000	10.768287000	4.901400000
C	3.913727000	10.204159000	4.973700000
C	4.804616000	6.584912000	0.250388000
C	15.985060000	10.663927000	3.916616000
C	4.875769000	10.255272000	3.970092000
C	3.802105000	5.621224000	0.309255000
C	6.237721000	10.262146000	4.301351000
C	14.630782000	10.610405000	4.273292000
C	4.304065000	10.161362000	6.313219000
C	16.594833000	10.822039000	6.246946000
C	4.132707000	4.265746000	0.269280000
C	6.147604000	6.197841000	0.152289000
H	7.687723000	10.226448000	5.891025000
H	13.208682000	10.630191000	5.887945000
H	5.962491000	10.136249000	7.697615000
H	14.961281000	10.816447000	7.660821000
H	5.726668000	2.813236000	0.136402000
H	7.523154000	4.547971000	0.030294000
H	18.017067000	10.808463000	4.620570000
H	2.853227000	10.197173000	4.712683000
H	4.565736000	7.649628000	0.279075000
H	16.251660000	10.622290000	2.859019000
H	4.591473000	10.289070000	2.916802000
H	2.756193000	5.926610000	0.386439000
H	8.438465000	12.380029000	2.001122000
O	8.492885000	10.271347000	3.573462000
O	12.370785000	10.419450000	3.598691000
O	10.465303000	12.389045000	3.581853000
O	10.478400000	13.977883000	1.978332000

O	8.414076000	6.816277000	0.033577000
O	12.400890000	13.985177000	0.058746000
O	6.862165000	8.442345000	0.096995000
O	13.990886000	12.381365000	0.065712000
O	13.963489000	10.484845000	2.015426000
O	6.862042000	10.400438000	2.030867000
O	9.005479000	11.843558000	1.436486000
O	11.779140000	8.930562000	1.530599000
O	9.372227000	9.355676000	1.090981000
O	11.474702000	11.473307000	1.063050000
Hf	10.422157000	12.948090000	-0.010359000
Hf	10.417341000	7.804110000	0.060490000
Hf	10.438268000	10.465396000	2.469064000
Hf	12.954427000	10.373936000	0.024076000
Hf	7.906731000	10.386329000	0.031724000
H	15.098819000	2.847779000	-0.464678000
H	13.314761000	4.596913000	-0.297036000
H	16.313219000	7.662996000	-0.148074000
H	18.108879000	5.929850000	-0.318433000
H	8.444033000	8.438408000	-1.938215000
H	12.403534000	12.382244000	-1.957930000
C	15.368257000	3.904182000	-0.396673000
C	14.371449000	4.870751000	-0.304477000
C	16.062791000	6.602839000	-0.217736000
C	17.057418000	5.633663000	-0.313079000
C	16.711377000	4.284350000	-0.401883000
C	14.713551000	6.226355000	-0.214052000
O	8.457066000	10.460112000	-3.542059000
O	12.399616000	10.369175000	-3.544831000
O	10.485978000	8.450683000	-3.532710000
O	10.375648000	12.386778000	-3.540750000
O	10.377431000	13.999078000	-1.963913000
O	10.438442000	6.824520000	-1.966249000
O	8.452824000	13.986341000	-0.039622000
O	12.450862000	6.873358000	-0.182600000
O	14.011424000	8.466979000	0.034764000
O	6.861894000	12.382750000	-0.021285000
O	14.000976000	10.360699000	-1.954966000
O	6.854505000	10.458759000	-1.954527000
O	11.846259000	11.834065000	-1.395269000
O	9.005186000	8.988472000	-1.381125000
O	11.475887000	9.376485000	-0.984508000
O	9.377261000	11.458176000	-1.011219000
H	12.296675000	8.319867000	2.071386000
Hf	10.432865000	10.393666000	-2.468836000
O	10.499637000	6.592059000	1.698193000

H	9.758480000	6.024547000	1.926689000
H	17.363329000	10.904111000	7.019301000
H	17.493304000	3.524520000	-0.475271000
H	3.344591000	3.510278000	0.315007000
H	3.547566000	10.121604000	7.100590000

Hf-UIO-66 Ads

C	10.500300000	13.573400000	3.164300000
C	13.590800000	10.499200000	3.218800000
C	7.259400000	10.315400000	3.225500000
C	13.586700000	13.569300000	0.091800000
C	7.226100000	7.224700000	0.091400000
C	10.347300000	13.576500000	-3.149300000
C	10.494300000	7.256200000	-3.139800000
C	13.586900000	10.339500000	-3.142400000
C	7.268500000	10.493900000	-3.141500000
C	7.267300000	13.569000000	-0.062000000
C	13.640800000	7.253200000	-0.115400000
H	6.481009000	14.351625000	-0.128761000
H	14.372619000	14.354072000	0.137377000
H	10.552827000	14.362837000	3.945223000
H	10.293509000	14.360666000	-3.934877000
H	10.545097000	6.480834000	-3.934939000
H	14.370862000	10.281611000	-3.928319000
H	6.483305000	10.555189000	-3.925795000
C	6.414391000	10.426801000	5.596950000
C	14.221259000	10.731110000	5.629151000
C	5.402532000	10.240221000	6.533402000
C	15.181830000	10.796463000	6.634569000
C	5.505774000	3.875285000	0.459935000
C	6.501433000	4.836976000	0.319646000
C	16.933263000	10.543713000	4.984043000
C	3.914461000	9.498808000	4.777028000
C	4.813185000	6.572650000	0.268775000
C	15.976757000	10.482532000	3.975134000
C	4.921801000	9.693600000	3.837595000
C	3.819313000	5.608455000	0.406793000
C	6.183693000	10.152008000	4.242473000
C	14.615669000	10.572016000	4.292894000
C	4.153435000	9.772715000	6.125006000
C	16.536999000	10.700845000	6.313311000
C	4.164818000	4.259307000	0.503420000
C	6.161487000	6.192657000	0.223771000
H	7.394520000	10.787429000	5.917272000
H	13.155342000	10.810687000	5.858421000
H	5.594978000	10.449313000	7.587369000

H	14.874202000	10.926301000	7.674646000
H	5.775735000	2.820022000	0.538883000
H	7.554494000	4.553163000	0.289596000
H	17.994159000	10.469578000	4.735031000
H	2.936902000	9.130309000	4.458538000
H	4.563696000	7.632438000	0.189706000
H	16.264340000	10.362462000	2.929027000
H	4.755378000	9.485535000	2.778819000
H	2.769244000	5.907829000	0.438642000
H	8.451227000	12.361782000	2.001342000
O	8.459402000	10.419240000	3.638279000
O	12.375597000	10.466752000	3.583005000
O	10.464246000	12.390453000	3.583288000
O	10.476604000	13.978411000	1.977296000
O	8.424988000	6.828705000	0.041394000
O	12.400411000	13.982424000	0.061079000
O	6.855858000	8.438074000	0.052489000
O	13.993122000	12.381973000	0.072601000
O	13.984587000	10.467090000	2.019230000
O	6.902366000	10.333445000	2.017054000
O	9.015539000	11.821030000	1.438608000
O	11.821585000	8.952601000	1.458047000
O	9.372523000	9.329863000	1.099210000
O	11.472028000	11.454732000	1.067431000
Hf	10.429689000	12.929147000	0.009879000
Hf	10.439999000	7.855941000	0.010028000
Hf	10.444851000	10.414594000	2.524876000
Hf	12.950678000	10.382978000	0.037448000
Hf	7.921998000	10.388523000	0.028589000
H	15.072171000	2.825481000	-0.314697000
H	13.297528000	4.588913000	-0.241285000
H	16.311103000	7.639585000	-0.096522000
H	18.099042000	5.890986000	-0.172494000
H	8.442309000	8.436385000	-1.935687000
H	12.408496000	12.386348000	-1.949262000
C	15.347370000	3.881570000	-0.266929000
C	14.355645000	4.857111000	-0.226232000
C	16.056030000	6.579391000	-0.144716000
C	17.045762000	5.601692000	-0.187056000
C	16.692839000	4.252624000	-0.247730000
C	14.704425000	6.212486000	-0.164480000
O	8.455131000	10.460632000	-3.550062000
O	12.400126000	10.370535000	-3.553063000
O	10.482007000	8.445698000	-3.539306000
O	10.378004000	12.389027000	-3.553883000
O	10.375846000	13.986667000	-1.961934000

O	10.448409000	6.828670000	-1.962471000
O	8.453488000	13.980432000	-0.034514000
O	12.443268000	6.868884000	-0.154146000
O	14.016881000	8.463799000	-0.028114000
O	6.861571000	12.380548000	-0.014278000
O	13.997068000	10.373804000	-1.956780000
O	6.860469000	10.459608000	-1.953667000
O	11.846795000	11.833085000	-1.396201000
O	9.013677000	8.991104000	-1.393857000
O	11.478102000	9.376190000	-1.021676000
O	9.380928000	11.452196000	-1.020106000
H	12.345017000	8.399246000	2.074337000
Hf	10.434800000	10.410694000	-2.492682000
O	10.440110000	6.614658000	1.757576000
H	9.644450000	6.062186000	1.773828000
H	17.289614000	10.751235000	7.103942000
H	17.470889000	3.485990000	-0.280353000
H	3.383997000	3.502842000	0.613588000
H	3.361679000	9.618469000	6.861864000
C	8.697497000	7.915282000	5.921535000
C	10.129555000	8.474441000	5.932949000
C	10.763076000	7.724194000	4.761936000
C	8.833259000	6.536382000	5.267493000
C	12.273591000	7.567540000	4.721210000
C	7.955359000	6.302407000	4.049782000
H	12.744697000	8.522099000	4.987925000
H	10.641515000	8.158228000	6.861623000
H	8.103281000	8.562573000	5.258107000
H	9.302800000	5.073790000	3.477870000
H	12.564705000	6.822479000	5.481813000
H	12.162914000	6.526947000	3.055259000
H	8.015162000	7.189920000	3.384232000
H	6.900901000	6.202689000	4.353615000
H	9.464478000	10.185672000	5.324294000
H	10.306483000	7.639699000	2.828232000
H	8.544490000	7.421838000	7.785269000
H	8.667314000	5.732144000	6.004968000
O	8.032756000	7.940319000	7.152735000
O	12.739130000	7.214424000	3.437801000
O	8.340692000	5.130052000	3.376290000
O	10.288368000	8.356231000	3.584916000
O	10.221202000	9.864007000	5.844815000
O	10.210041000	6.430469000	4.853528000

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C	10.500300000	13.573400000	3.164300000
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C	13.590800000	10.499200000	3.218800000
C	7.259400000	10.315400000	3.225500000
C	13.586700000	13.569300000	0.091800000
C	7.226100000	7.224700000	0.091400000
C	10.347300000	13.576500000	-3.149300000
C	10.494300000	7.256200000	-3.139800000
C	13.586900000	10.339500000	-3.142400000
C	7.268500000	10.493900000	-3.141500000
C	7.267300000	13.569000000	-0.062000000
C	13.640800000	7.253200000	-0.115400000
H	6.481418000	14.351971000	-0.129496000
H	14.372411000	14.354341000	0.135785000
H	10.553930000	14.363014000	3.945030000
H	10.293101000	14.361228000	-3.934295000
H	10.543110000	6.479219000	-3.933426000
H	14.370870000	10.280657000	-3.928286000
H	6.483203000	10.554788000	-3.925756000
C	6.407578000	10.443671000	5.594057000
C	14.220655000	10.753374000	5.626694000
C	5.392791000	10.263715000	6.528730000
C	15.180355000	10.822340000	6.632714000
C	5.513240000	3.870639000	0.450025000
C	6.507333000	4.835075000	0.317628000
C	16.931668000	10.532304000	4.988202000
C	3.911329000	9.505480000	4.774071000
C	4.814359000	6.565786000	0.249862000
C	15.976095000	10.468238000	3.978540000
C	4.921372000	9.694060000	3.836277000
C	3.822174000	5.598804000	0.380037000
C	6.181416000	10.157581000	4.241160000
C	14.615551000	10.574371000	4.293094000
C	4.145598000	9.791078000	6.120425000
C	16.535007000	10.709736000	6.314796000
C	4.170805000	4.250785000	0.481004000
C	6.164094000	6.189605000	0.217093000
H	7.385867000	10.808193000	5.915744000
H	13.155041000	10.845264000	5.853089000
H	5.581449000	10.482316000	7.581463000
H	14.872448000	10.968116000	7.670604000
H	5.785460000	2.816213000	0.532452000
H	7.561577000	4.554831000	0.297610000
H	17.992175000	10.444775000	4.741834000
H	2.935324000	9.132892000	4.455556000
H	4.562505000	7.624793000	0.167639000
H	16.264001000	10.332919000	2.934381000
H	4.758543000	9.477147000	2.778686000

H	2.770995000	5.895089000	0.402332000
H	8.451820000	12.361708000	2.001738000
O	8.457528000	10.422140000	3.639471000
O	12.376804000	10.473300000	3.582025000
O	10.463181000	12.390601000	3.583139000
O	10.476288000	13.978761000	1.977109000
O	8.428070000	6.832173000	0.050009000
O	12.400356000	13.981494000	0.061325000
O	6.854254000	8.436889000	0.048625000
O	13.993855000	12.382036000	0.073999000
O	13.986590000	10.462318000	2.019197000
O	6.903414000	10.327012000	2.016291000
O	9.014817000	11.818816000	1.439780000
O	11.826884000	8.956629000	1.452160000
O	9.374332000	9.333296000	1.094048000
O	11.470966000	11.451889000	1.068757000
Hf	10.429983000	12.925811000	0.013490000
Hf	10.440922000	7.867726000	0.005978000
Hf	10.443909000	10.404908000	2.534858000
Hf	12.950531000	10.386225000	0.040190000
Hf	7.921300000	10.390341000	0.028920000
H	15.068627000	2.825044000	-0.344317000
H	13.295123000	4.588138000	-0.251594000
H	16.310229000	7.637832000	-0.112846000
H	18.097130000	5.889177000	-0.207651000
H	8.442387000	8.435558000	-1.936988000
H	12.408190000	12.386895000	-1.947962000
C	15.344426000	3.880806000	-0.293090000
C	14.353258000	4.856406000	-0.241348000
C	16.054588000	6.577908000	-0.163648000
C	17.043725000	5.600173000	-0.216591000
C	16.690078000	4.251458000	-0.280889000
C	14.702710000	6.211462000	-0.175720000
O	8.454998000	10.461020000	-3.550884000
O	12.400015000	10.370102000	-3.553636000
O	10.480698000	8.444905000	-3.540651000
O	10.378580000	12.389200000	-3.555677000
O	10.375788000	13.984765000	-1.961677000
O	10.452277000	6.830646000	-1.961035000
O	8.453593000	13.979247000	-0.033874000
O	12.440697000	6.867705000	-0.136135000
O	14.016945000	8.462849000	-0.036769000
O	6.860568000	12.380641000	-0.014194000
O	13.996519000	10.375225000	-1.956883000
O	6.860639000	10.459657000	-1.953865000
O	11.846664000	11.832470000	-1.395883000

O	9.013548000	8.991330000	-1.396012000
O	11.477890000	9.375996000	-1.024759000
O	9.380444000	11.451714000	-1.021625000
H	12.345840000	8.405037000	2.073579000
Hf	10.434111000	10.413394000	-2.495490000
O	10.422606000	6.667628000	1.810615000
H	9.621793000	6.121915000	1.856153000
H	17.286939000	10.762739000	7.105916000
H	17.467684000	3.484806000	-0.322043000
H	3.391256000	3.492124000	0.584841000
H	3.351711000	9.642040000	6.856062000
C	8.715265000	7.954468000	5.929515000
C	10.144681000	8.517379000	5.924758000
C	10.776768000	7.762182000	4.754803000
C	8.850293000	6.573502000	5.279101000
C	12.289493000	7.606510000	4.739542000
C	7.971300000	6.345234000	4.060686000
H	12.754660000	8.562697000	5.009000000
H	10.662260000	8.211081000	6.854006000
H	8.110224000	8.595805000	5.270839000
H	9.313791000	5.087707000	3.535961000
H	12.573433000	6.865006000	5.506160000
H	12.242967000	6.524829000	3.104187000
H	8.028913000	7.235429000	3.399242000
H	6.917154000	6.240815000	4.364793000
H	9.465378000	10.224307000	5.318439000
H	10.330620000	7.585298000	2.776739000
H	8.589937000	7.475557000	7.799136000
H	8.675738000	5.772283000	6.018098000
O	8.063239000	7.980945000	7.168335000
O	12.779139000	7.252213000	3.464050000
O	8.362315000	5.178576000	3.375618000
O	10.312312000	8.363277000	3.572740000
O	10.233170000	9.907268000	5.824578000
O	10.226352000	6.459914000	4.872273000

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C	10.500297000	13.573398000	3.164325000
C	13.590817000	10.499225000	3.218820000
C	7.259410000	10.315411000	3.225499000
C	13.586705000	13.569298000	0.091799000
C	7.226092000	7.224705000	0.091370000
C	10.347297000	13.576490000	-3.149302000
C	10.494281000	7.256195000	-3.139807000
C	13.586902000	10.339497000	-3.142403000
C	7.268500000	10.493887000	-3.141503000

C	7.267299000	13.568992000	-0.061996000
C	13.640800000	7.253202000	-0.115402000
H	6.482554000	14.353447000	-0.126349000
H	14.372334000	14.354457000	0.133744000
H	10.557575000	14.365428000	3.942413000
H	10.293063000	14.362944000	-3.932618000
H	10.542973000	6.476869000	-3.931124000
H	14.371550000	10.282434000	-3.927906000
H	6.482920000	10.556145000	-3.925522000
C	6.385393000	10.432648000	5.584974000
C	14.251481000	10.796431000	5.614206000
C	5.367113000	10.237937000	6.513102000
C	15.221385000	10.861914000	6.610677000
C	5.529283000	3.848348000	0.292286000
C	6.517254000	4.822703000	0.191531000
C	16.947449000	10.464164000	4.962633000
C	3.909631000	9.452616000	4.750335000
C	4.823209000	6.548749000	0.301292000
C	15.981550000	10.404374000	3.962382000
C	4.923077000	9.656276000	3.818898000
C	3.836596000	5.572195000	0.406720000
C	6.172584000	10.140173000	4.231221000
C	14.628208000	10.566365000	4.283239000
C	4.130358000	9.744064000	6.097679000
C	16.568708000	10.693848000	6.286379000
C	4.188338000	4.221716000	0.402081000
C	6.170391000	6.179856000	0.195091000
H	7.358520000	10.808949000	5.908289000
H	13.191543000	10.927147000	5.848472000
H	5.544355000	10.462154000	7.566719000
H	14.926522000	11.047106000	7.646070000
H	5.802535000	2.790595000	0.283315000
H	7.571241000	4.552074000	0.107910000
H	18.002229000	10.332827000	4.710820000
H	2.941229000	9.065113000	4.425926000
H	4.568047000	7.610134000	0.295952000
H	16.256154000	10.229762000	2.920485000
H	4.770355000	9.436845000	2.760203000
H	2.787124000	5.863675000	0.489279000
H	8.450930000	12.351928000	2.001358000
O	8.442756000	10.461056000	3.649802000
O	12.384746000	10.523928000	3.585760000
O	10.456585000	12.392060000	3.584362000
O	10.478115000	13.976690000	1.975225000
O	8.433172000	6.839010000	0.053397000
O	12.400550000	13.979459000	0.058971000

O	6.847425000	8.432726000	0.050961000
O	13.995323000	12.381576000	0.078174000
O	13.983838000	10.431115000	2.015483000
O	6.908256000	10.307291000	2.010505000
O	9.012175000	11.812079000	1.434787000
O	11.819537000	8.936828000	1.458498000
O	9.369046000	9.319229000	1.088866000
O	11.471769000	11.440293000	1.065265000
Hf	10.432005000	12.915148000	0.022437000
Hf	10.440261000	7.893345000	-0.013352000
Hf	10.434101000	10.380027000	2.559728000
Hf	12.949871000	10.391310000	0.051390000
Hf	7.917907000	10.392835000	0.033196000
H	15.068100000	2.825564000	-0.389678000
H	13.294063000	4.586979000	-0.281038000
H	16.307788000	7.635969000	-0.105213000
H	18.095428000	5.888780000	-0.213990000
H	8.441934000	8.431999000	-1.941465000
H	12.408082000	12.385503000	-1.947670000
C	15.343473000	3.880764000	-0.325676000
C	14.352000000	4.855579000	-0.264761000
C	16.052717000	6.576483000	-0.166838000
C	17.042164000	5.599567000	-0.227878000
C	16.689027000	4.251514000	-0.306956000
C	14.700823000	6.209996000	-0.184060000
O	8.454650000	10.462103000	-3.553611000
O	12.399760000	10.367417000	-3.555683000
O	10.479868000	8.443244000	-3.541544000
O	10.378866000	12.389656000	-3.561171000
O	10.375605000	13.979037000	-1.961132000
O	10.453431000	6.831808000	-1.959446000
O	8.454145000	13.975584000	-0.034683000
O	12.436211000	6.865059000	-0.118777000
O	14.014809000	8.460600000	-0.048187000
O	6.857431000	12.380790000	-0.017456000
O	13.994049000	10.375376000	-1.956589000
O	6.861038000	10.456648000	-1.954475000
O	11.846662000	11.828768000	-1.397848000
O	9.011617000	8.991202000	-1.402465000
O	11.475260000	9.372038000	-1.029317000
O	9.379699000	11.446513000	-1.024976000
H	12.328716000	8.404363000	2.104207000
Hf	10.431978000	10.421925000	-2.502335000
O	10.422592000	6.644399000	1.871360000
H	9.657645000	6.068646000	2.095904000
H	17.328714000	10.743874000	7.070005000

H	17.466886000	3.485541000	-0.355000000
H	3.413192000	3.455587000	0.481171000
H	3.334011000	9.583826000	6.828393000
C	8.692844000	7.925032000	5.963560000
C	10.116742000	8.483893000	6.074308000
C	10.780688000	7.900744000	4.819503000
C	8.859275000	6.635405000	5.143765000
C	12.290557000	7.732773000	4.868117000
C	7.944158000	6.607553000	3.929219000
H	12.748795000	8.691914000	5.136237000
H	10.608706000	8.063316000	6.971434000
H	8.110044000	8.644778000	5.369373000
H	8.146529000	4.700129000	3.531742000
H	12.557228000	6.999541000	5.648619000
H	12.437556000	6.504790000	3.362030000
H	8.093462000	7.523053000	3.333618000
H	6.889311000	6.606435000	4.264505000
H	9.636526000	10.250601000	5.483474000
H	10.420680000	7.323703000	2.604974000
H	8.538580000	7.278971000	7.778298000
H	8.649715000	5.754857000	5.781196000
O	7.991215000	7.788438000	7.169089000
O	12.821190000	7.358647000	3.609165000
O	8.210203000	5.531770000	3.047117000
O	10.370552000	8.594656000	3.716491000
O	10.195954000	9.872971000	6.181653000
O	10.233025000	6.566431000	4.773840000

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C	10.500300000	13.573400000	3.164300000
C	13.590800000	10.499200000	3.218800000
C	7.259400000	10.315400000	3.225500000
C	13.586700000	13.569300000	0.091800000
C	7.226100000	7.224700000	0.091400000
C	10.347300000	13.576500000	-3.149300000
C	10.494300000	7.256200000	-3.139800000
C	13.586900000	10.339500000	-3.142400000
C	7.268500000	10.493900000	-3.141500000
C	7.267300000	13.569000000	-0.062000000
C	13.640800000	7.253200000	-0.115400000
H	6.481651000	14.353134000	-0.121624000
H	14.373055000	14.353552000	0.140912000
H	10.558947000	14.364990000	3.942901000
H	10.294893000	14.359717000	-3.936045000
H	10.551632000	6.477572000	-3.931490000
H	14.370792000	10.287625000	-3.928909000

H	6.484579000	10.564338000	-3.926475000
C	6.506934000	10.093890000	5.615534000
C	14.287717000	10.557938000	5.626496000
C	5.521835000	9.822462000	6.559983000
C	15.271166000	10.527343000	6.611137000
C	5.423166000	3.889335000	0.052580000
C	6.419717000	4.851550000	-0.090191000
C	16.976165000	10.346523000	4.905041000
C	3.898823000	9.552732000	4.787956000
C	4.873757000	6.560866000	0.658179000
C	15.995061000	10.376635000	3.918083000
C	4.883491000	9.821040000	3.842289000
C	3.884126000	5.593689000	0.813823000
C	6.198631000	10.087662000	4.249011000
C	14.644316000	10.481444000	4.272789000
C	4.217758000	9.549577000	6.147366000
C	16.615829000	10.421621000	6.251343000
C	4.156845000	4.258862000	0.509954000
C	6.150957000	6.194095000	0.214100000
H	7.530417000	10.304473000	5.931483000
H	13.230883000	10.642323000	5.891156000
H	5.777508000	9.812589000	7.621251000
H	14.989204000	10.588660000	7.664675000
H	5.634135000	2.845883000	-0.191199000
H	7.419890000	4.579931000	-0.435874000
H	18.028643000	10.263549000	4.624794000
H	2.876134000	9.343158000	4.466015000
H	4.679768000	7.611872000	0.881655000
H	16.255497000	10.317945000	2.859760000
H	4.654885000	9.826767000	2.774985000
H	2.892947000	5.880871000	1.171641000
H	8.444949000	12.355176000	2.001930000
O	8.453392000	10.416845000	3.627485000
O	12.390450000	10.542150000	3.601755000
O	10.454083000	12.392726000	3.585795000
O	10.479346000	13.977365000	1.976349000
O	8.412043000	6.809925000	-0.008713000
O	12.400905000	13.983247000	0.057672000
O	6.854661000	8.433688000	0.099577000
O	13.992685000	12.381777000	0.071764000
O	13.970895000	10.455005000	2.011950000
O	6.883743000	10.364649000	2.016356000
O	9.012329000	11.824136000	1.433099000
O	11.800331000	8.948530000	1.469406000
O	9.352123000	9.316264000	1.111556000
O	11.468524000	11.454191000	1.062458000

Hf	10.430366000	12.928422000	0.011481000
Hf	10.434493000	7.859516000	0.037003000
Hf	10.435352000	10.411284000	2.530272000
Hf	12.945241000	10.384118000	0.041696000
Hf	7.916952000	10.396965000	0.037368000
H	15.077164000	2.827958000	-0.350300000
H	13.300432000	4.588499000	-0.256066000
H	16.309827000	7.642730000	-0.112694000
H	18.100288000	5.897159000	-0.210192000
H	8.448998000	8.429784000	-1.929616000
H	12.406378000	12.380583000	-1.952874000
C	15.351111000	3.884214000	-0.298342000
C	14.358305000	4.858211000	-0.245864000
C	16.056447000	6.582348000	-0.165562000
C	17.047354000	5.606334000	-0.219715000
C	16.696151000	4.257071000	-0.285681000
C	14.705346000	6.213707000	-0.178839000
O	8.455256000	10.458133000	-3.548149000
O	12.399213000	10.365235000	-3.552181000
O	10.473862000	8.444416000	-3.543006000
O	10.376282000	12.387992000	-3.552230000
O	10.376023000	13.987428000	-1.962374000
O	10.448933000	6.835103000	-1.958734000
O	8.453204000	13.979531000	-0.035835000
O	12.443197000	6.867521000	-0.143164000
O	14.014933000	8.463202000	-0.023926000
O	6.858265000	12.381675000	-0.022086000
O	13.996160000	10.372029000	-1.956514000
O	6.857808000	10.451059000	-1.953904000
O	11.844972000	11.829400000	-1.397474000
O	9.009451000	8.989048000	-1.381494000
O	11.472322000	9.367793000	-1.015048000
O	9.377856000	11.449849000	-1.018470000
H	12.324783000	8.393465000	2.083619000
Hf	10.433541000	10.406790000	-2.486857000
O	10.409671000	6.427905000	1.668906000
H	9.784638000	5.720468000	1.451269000
H	17.387306000	10.398325000	7.024858000
H	17.475104000	3.491792000	-0.327530000
H	3.378193000	3.501992000	0.629368000
H	3.445104000	9.332489000	6.888826000
C	8.749523000	7.448106000	5.653344000
C	10.195336000	7.812001000	6.012573000
C	10.925842000	7.834703000	4.677062000
C	8.817012000	6.267671000	4.679216000
C	12.356428000	7.361992000	4.579222000

C	7.764102000	6.330938000	3.603058000
H	12.987964000	8.158525000	5.006897000
H	10.626005000	7.051168000	6.687030000
H	8.339004000	8.323438000	5.121174000
H	7.156687000	5.169085000	2.166251000
H	12.493192000	6.464471000	5.204919000
H	12.206368000	6.503156000	2.821409000
H	7.923461000	7.256002000	3.005121000
H	6.777950000	6.427029000	4.099308000
H	10.019300000	9.724629000	6.027940000
H	10.171239000	6.361225000	3.059087000
H	8.268799000	6.527747000	7.283172000
H	8.696799000	5.321463000	5.240157000
O	7.901814000	7.238373000	6.743044000
O	12.787454000	7.153185000	3.259234000
O	7.867176000	5.169563000	2.820628000
O	10.501868000	8.737837000	3.900436000
O	10.315102000	9.048705000	6.657360000
O	10.135905000	6.262194000	4.125878000

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C	10.500300000	13.573400000	3.164300000
C	13.590800000	10.499200000	3.218800000
C	7.259400000	10.315400000	3.225500000
C	13.586700000	13.569300000	0.091800000
C	7.226100000	7.224700000	0.091400000
C	10.347300000	13.576500000	-3.149300000
C	10.494300000	7.256200000	-3.139800000
C	13.586900000	10.339500000	-3.142400000
C	7.268500000	10.493900000	-3.141500000
C	7.267300000	13.569000000	-0.062000000
C	13.640800000	7.253200000	-0.115400000
H	6.480633000	14.351875000	-0.120338000
H	14.372874000	14.353244000	0.145841000
H	10.557732000	14.364801000	3.942967000
H	10.298158000	14.358509000	-3.937183000
H	10.553060000	6.475910000	-3.929181000
H	14.370840000	10.291503000	-3.928808000
H	6.484961000	10.564425000	-3.926306000
C	6.489963000	10.133872000	5.612179000
C	14.282731000	10.522971000	5.628401000
C	5.508637000	9.837812000	6.552668000
C	15.265194000	10.481599000	6.613581000
C	5.453537000	3.900800000	-0.252015000
C	6.464256000	4.852594000	-0.178024000
C	16.973713000	10.344682000	4.906728000

C	3.931941000	9.409862000	4.769095000
C	4.808521000	6.583738000	0.166210000
C	15.993691000	10.385122000	3.919180000
C	4.911678000	9.707685000	3.827419000
C	3.798390000	5.628144000	0.101757000
C	6.201837000	10.066260000	4.243220000
C	14.641658000	10.473197000	4.273975000
C	4.229835000	9.472980000	6.131756000
C	16.611044000	10.392346000	6.253646000
C	4.119494000	4.286754000	-0.109007000
C	6.148779000	6.201117000	0.029694000
H	7.494909000	10.416254000	5.931764000
H	13.225286000	10.596184000	5.893760000
H	5.747501000	9.878524000	7.617073000
H	14.981552000	10.521820000	7.667638000
H	5.704507000	2.850581000	-0.416075000
H	7.512444000	4.564372000	-0.277239000
H	18.027122000	10.275021000	4.626533000
H	2.930733000	9.121779000	4.441087000
H	4.575972000	7.638651000	0.323088000
H	16.256097000	10.347599000	2.860367000
H	4.702195000	9.654629000	2.757250000
H	2.754492000	5.929708000	0.213525000
H	8.441338000	12.351344000	2.001904000
O	8.458733000	10.408999000	3.626171000
O	12.386643000	10.525597000	3.602719000
O	10.457528000	12.392799000	3.587220000
O	10.477758000	13.976359000	1.976889000
O	8.427192000	6.827658000	0.071079000
O	12.400766000	13.983178000	0.056500000
O	6.864151000	8.439998000	0.124320000
O	13.992444000	12.381843000	0.067261000
O	13.969576000	10.473145000	2.012570000
O	6.886432000	10.384824000	2.018053000
O	9.014234000	11.826153000	1.432909000
O	11.808346000	8.970450000	1.467387000
O	9.360806000	9.311072000	1.128997000
O	11.468771000	11.465708000	1.063083000
Hf	10.426187000	12.934656000	0.005747000
Hf	10.433738000	7.857500000	0.048368000
Hf	10.437975000	10.430865000	2.521843000
Hf	12.942443000	10.388168000	0.037136000
Hf	7.911626000	10.390203000	0.042036000
H	15.123966000	2.852033000	-0.507421000
H	13.331308000	4.590385000	-0.410648000
H	16.301774000	7.656239000	0.029129000

H	18.109351000	5.929453000	-0.066102000
H	8.440239000	8.424457000	-1.918053000
H	12.405320000	12.376865000	-1.954972000
C	15.385989000	3.905637000	-0.386936000
C	14.383766000	4.869555000	-0.331213000
C	16.059973000	6.598216000	-0.086566000
C	17.060816000	5.632472000	-0.140653000
C	16.725460000	4.286013000	-0.290463000
C	14.713875000	6.222427000	-0.179605000
O	8.455958000	10.455911000	-3.546976000
O	12.398790000	10.364466000	-3.550349000
O	10.471683000	8.444038000	-3.543345000
O	10.373791000	12.387239000	-3.548970000
O	10.374999000	13.989613000	-1.962750000
O	10.449043000	6.838822000	-1.956087000
O	8.453164000	13.981731000	-0.036615000
O	12.445268000	6.859682000	-0.158132000
O	14.006474000	8.464076000	-0.012757000
O	6.861553000	12.381040000	-0.022719000
O	13.995704000	10.368248000	-1.955678000
O	6.859286000	10.453033000	-1.953217000
O	11.842738000	11.828240000	-1.398098000
O	9.003886000	8.983939000	-1.372849000
O	11.467757000	9.364179000	-1.012407000
O	9.379618000	11.444343000	-1.012268000
H	12.349527000	8.433573000	2.081566000
Hf	10.429147000	10.403087000	-2.485641000
O	10.559646000	6.382018000	1.661817000
H	10.904753000	5.552851000	1.305148000
H	17.381650000	10.360665000	7.027658000
H	17.512152000	3.528876000	-0.333452000
H	3.326066000	3.537327000	-0.162175000
H	3.460927000	9.232911000	6.869923000
C	8.749286000	7.468917000	5.682959000
C	10.210523000	7.789146000	6.038107000
C	10.978615000	7.898733000	4.739150000
C	8.686948000	6.285779000	4.700627000
C	12.348180000	7.310697000	4.575500000
C	7.772108000	6.577671000	3.523347000
H	13.047367000	8.025745000	5.050774000
H	10.638929000	6.999485000	6.677104000
H	8.370001000	8.371324000	5.170018000
H	8.425178000	5.711048000	1.928285000
H	12.413235000	6.375005000	5.156311000
H	11.990440000	6.709366000	2.748163000
H	8.102174000	7.525585000	3.047213000

H	6.750681000	6.752916000	3.906075000
H	9.895915000	9.686789000	6.227397000
H	10.052385000	6.043034000	3.258077000
H	8.205169000	6.529341000	7.282032000
H	8.309133000	5.396368000	5.240791000
O	7.929293000	7.322299000	6.806016000
O	12.728251000	7.144625000	3.243414000
O	7.753300000	5.524461000	2.604786000
O	10.516589000	8.695624000	3.909763000
O	10.337682000	8.998422000	6.746207000
O	10.002479000	5.986531000	4.250617000

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C	10.500300000	13.573400000	3.164300000
C	13.590800000	10.499200000	3.218800000
C	7.259400000	10.315400000	3.225500000
C	13.586700000	13.569300000	0.091800000
C	7.226100000	7.224700000	0.091400000
C	10.347300000	13.576500000	-3.149300000
C	10.494300000	7.256200000	-3.139800000
C	13.586900000	10.339500000	-3.142400000
C	7.268500000	10.493900000	-3.141500000
C	7.267300000	13.569000000	-0.062000000
C	13.640800000	7.253200000	-0.115400000
H	6.482518000	14.352037000	-0.137090000
H	14.372087000	14.354286000	0.136937000
H	10.568123000	14.363458000	3.942995000
H	10.298745000	14.359794000	-3.935737000
H	10.562238000	6.479262000	-3.931626000
H	14.370448000	10.287804000	-3.928783000
H	6.484922000	10.565985000	-3.926160000
C	6.586262000	10.720439000	5.602210000
C	14.281868000	10.521428000	5.626127000
C	5.613230000	10.838279000	6.588875000
C	15.265712000	10.504966000	6.610449000
C	5.523792000	3.849637000	-0.091575000
C	6.512270000	4.826139000	-0.023662000
C	16.977066000	10.437025000	4.902053000
C	3.890269000	10.395439000	4.947515000
C	4.811433000	6.548276000	-0.024882000
C	15.995720000	10.452668000	3.915404000
C	4.860548000	10.289972000	3.954806000
C	3.824313000	5.570775000	-0.097161000
C	6.215092000	10.444279000	4.278541000
C	14.641706000	10.494223000	4.271896000
C	4.265500000	10.670099000	6.263538000

C	16.613514000	10.462787000	6.249421000
C	4.178775000	4.221368000	-0.128358000
C	6.162870000	6.182588000	0.012003000
H	7.646929000	10.828812000	5.838844000
H	13.222513000	10.558144000	5.889169000
H	5.904835000	11.053955000	7.618938000
H	14.982303000	10.527449000	7.665134000
H	5.800848000	2.793471000	-0.115771000
H	7.569234000	4.553927000	0.007335000
H	18.032063000	10.404003000	4.621105000
H	2.836215000	10.262583000	4.694963000
H	4.549434000	7.607480000	0.008746000
H	16.258577000	10.431550000	2.856256000
H	4.584444000	10.075352000	2.920770000
H	2.771784000	5.860652000	-0.124466000
H	8.439700000	12.355521000	2.016099000
O	8.467896000	10.322800000	3.599387000
O	12.384911000	10.513211000	3.601440000
O	10.454091000	12.391368000	3.583293000
O	10.468603000	13.975820000	1.976150000
O	8.423017000	6.836553000	0.058801000
O	12.399003000	13.980059000	0.063284000
O	6.844584000	8.435721000	0.149233000
O	13.991646000	12.381372000	0.070481000
O	13.966680000	10.471733000	2.011561000
O	6.865741000	10.268549000	2.021711000
O	8.996164000	11.806503000	1.452915000
O	11.804043000	8.951068000	1.477763000
O	9.371949000	9.313726000	1.117385000
O	11.457340000	11.451134000	1.071189000
Hf	10.424870000	12.926232000	0.013385000
Hf	10.431547000	7.855650000	0.039193000
Hf	10.442485000	10.408640000	2.540449000
Hf	12.942232000	10.384196000	0.040488000
Hf	7.913557000	10.383433000	0.045922000
H	15.111563000	2.840786000	-0.381711000
H	13.322932000	4.586881000	-0.318100000
H	16.305303000	7.657267000	-0.017455000
H	18.108401000	5.924322000	-0.083712000
H	8.438798000	8.425954000	-1.929082000
H	12.402919000	12.380139000	-1.946467000
C	15.377015000	3.897363000	-0.301416000
C	14.377336000	4.864752000	-0.265010000
C	16.060085000	6.596753000	-0.097466000
C	17.058378000	5.627548000	-0.134625000
C	16.718395000	4.277710000	-0.235995000

C	14.712452000	6.220919000	-0.162271000
O	8.455783000	10.457892000	-3.546254000
O	12.398286000	10.367349000	-3.549851000
O	10.472125000	8.445631000	-3.539247000
O	10.374574000	12.387230000	-3.550106000
O	10.373470000	13.985682000	-1.961043000
O	10.437808000	6.834707000	-1.958655000
O	8.453761000	13.977434000	-0.031113000
O	12.446100000	6.865069000	-0.175956000
O	14.007233000	8.465505000	-0.009529000
O	6.859345000	12.380432000	-0.008405000
O	13.994952000	10.369846000	-1.955412000
O	6.858326000	10.449481000	-1.952628000
O	11.841045000	11.828240000	-1.392065000
O	8.995112000	8.983412000	-1.374368000
O	11.467729000	9.367890000	-1.012972000
O	9.375270000	11.443769000	-1.008211000
H	12.347483000	8.403099000	2.080836000
Hf	10.430007000	10.405946000	-2.483991000
O	10.529610000	6.397416000	1.637017000
H	10.441312000	5.509423000	1.267366000
H	17.385169000	10.450537000	7.022982000
H	17.503067000	3.517758000	-0.264449000
H	3.402285000	3.454459000	-0.180791000
H	3.502733000	10.753004000	7.041383000
C	8.822505000	6.180054000	4.837349000
C	9.917034000	7.013253000	5.585610000
C	10.850632000	7.560494000	4.526781000
C	7.756800000	7.073410000	4.213192000
C	12.106058000	6.776441000	4.275707000
C	6.765537000	6.360877000	3.315739000
H	12.806268000	7.093788000	5.074115000
H	10.497642000	6.288869000	6.189642000
H	8.318249000	5.563198000	5.601851000
H	6.100977000	7.886295000	2.276180000
H	11.876954000	5.716946000	4.503114000
H	12.034623000	6.577549000	2.387090000
H	6.271318000	5.543294000	3.863156000
H	7.277276000	5.913930000	2.447137000
H	8.500696000	8.191683000	6.186400000
H	6.252893000	8.074623000	4.914279000
H	9.680464000	5.812242000	3.104931000
H	8.252170000	7.851116000	3.590165000
O	9.399081000	5.310414000	3.907621000
O	12.701514000	6.939547000	3.036168000
O	5.753682000	7.276656000	2.947142000

O	10.553660000	8.579144000	3.912596000
O	9.432758000	8.016036000	6.414789000
O	7.052960000	7.672531000	5.289002000

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C	10.500300000	13.573400000	3.164300000
C	13.590800000	10.499200000	3.218800000
C	7.259400000	10.315400000	3.225500000
C	13.586700000	13.569300000	0.091800000
C	7.226100000	7.224700000	0.091400000
C	10.347300000	13.576500000	-3.149300000
C	10.494300000	7.256200000	-3.139800000
C	13.586900000	10.339500000	-3.142400000
C	7.268500000	10.493900000	-3.141500000
C	7.267300000	13.569000000	-0.062000000
C	13.640800000	7.253200000	-0.115400000
H	6.481366000	14.352926000	-0.119068000
H	14.372528000	14.354017000	0.139343000
H	10.557134000	14.367834000	3.940239000
H	10.293386000	14.361470000	-3.934149000
H	10.530315000	6.474210000	-3.929013000
H	14.371381000	10.281593000	-3.927961000
H	6.482865000	10.550018000	-3.925925000
C	6.278201000	10.241305000	5.553162000
C	14.279028000	10.513757000	5.626713000
C	5.290232000	9.811631000	6.435430000
C	15.257636000	10.464306000	6.615133000
C	5.590853000	3.926420000	0.984189000
C	6.545408000	4.862523000	0.596428000
C	16.969569000	10.300052000	4.914495000
C	4.127710000	8.727066000	4.609903000
C	4.859494000	6.596982000	0.634064000
C	15.992871000	10.349007000	3.923952000
C	5.106691000	9.171228000	3.724432000
C	3.906361000	5.660551000	1.025212000
C	6.191042000	9.924962000	4.192911000
C	14.641093000	10.455439000	4.274242000
C	4.217901000	9.049529000	5.967645000
C	16.603500000	10.357460000	6.260050000
C	4.271524000	4.325236000	1.205079000
C	6.188513000	6.206044000	0.424290000
H	7.125362000	10.826672000	5.916116000
H	13.220796000	10.599478000	5.883667000
H	5.358694000	10.067679000	7.494622000
H	14.972118000	10.511374000	7.668535000
H	5.874690000	2.880054000	1.118262000

H	7.582524000	4.567757000	0.421744000
H	18.022948000	10.216398000	4.637743000
H	3.289995000	8.128724000	4.240120000
H	4.593270000	7.645430000	0.485871000
H	16.258344000	10.304724000	2.866174000
H	5.061183000	8.930117000	2.659807000
H	2.871679000	5.970718000	1.189259000
H	8.447685000	12.354835000	1.994782000
O	8.427140000	10.493000000	3.671346000
O	12.394435000	10.582355000	3.591927000
O	10.451963000	12.396302000	3.587718000
O	10.483433000	13.976078000	1.974514000
O	8.415908000	6.825187000	-0.055203000
O	12.401466000	13.981391000	0.056869000
O	6.846584000	8.433649000	0.035828000
O	13.996174000	12.382389000	0.073950000
O	13.977503000	10.442674000	2.010062000
O	6.906159000	10.378147000	2.013014000
O	9.018271000	11.823384000	1.429639000
O	11.799599000	8.942915000	1.485046000
O	9.352008000	9.317366000	1.102297000
O	11.471462000	11.447741000	1.058379000
Hf	10.432617000	12.924764000	0.015830000
Hf	10.438548000	7.907177000	-0.001535000
Hf	10.432717000	10.413705000	2.551723000
Hf	12.955249000	10.394727000	0.053174000
Hf	7.916884000	10.399349000	0.029081000
H	15.077590000	2.835306000	-0.477144000
H	13.300557000	4.587195000	-0.303416000
H	16.305049000	7.646792000	-0.162930000
H	18.095964000	5.908985000	-0.337671000
H	8.453560000	8.430921000	-1.928364000
H	12.409679000	12.386983000	-1.952234000
C	15.350248000	3.890810000	-0.407359000
C	14.357165000	4.860708000	-0.309786000
C	16.052358000	6.587213000	-0.231832000
C	17.043868000	5.615396000	-0.329540000
C	16.694355000	4.266985000	-0.416990000
C	14.701879000	6.215399000	-0.220480000
O	8.454867000	10.466614000	-3.552632000
O	12.399929000	10.366873000	-3.555518000
O	10.478712000	8.443145000	-3.544547000
O	10.378790000	12.389567000	-3.558918000
O	10.375222000	13.983146000	-1.962362000
O	10.469792000	6.839296000	-1.956309000
O	8.453414000	13.978473000	-0.036463000

O	12.435694000	6.864660000	-0.099030000
O	14.011140000	8.461698000	-0.040060000
O	6.858717000	12.381243000	-0.024237000
O	13.994914000	10.376629000	-1.956668000
O	6.860240000	10.459192000	-1.954527000
O	11.847914000	11.832581000	-1.400398000
O	9.021280000	9.004730000	-1.402957000
O	11.482622000	9.377084000	-1.022753000
O	9.381089000	11.450595000	-1.024495000
H	12.281004000	8.377184000	2.121748000
Hf	10.434979000	10.421120000	-2.501577000
O	10.314829000	6.504099000	1.749068000
H	10.096919000	5.613563000	1.445356000
H	17.371289000	10.319294000	7.036663000
H	17.473767000	3.504960000	-0.493481000
H	3.524161000	3.591541000	1.515837000
H	3.444033000	8.713204000	6.663059000
C	8.566836000	6.439573000	4.266158000
C	9.793099000	7.812717000	5.849606000
C	10.692873000	7.917951000	4.805086000
C	7.396810000	6.407104000	5.181846000
C	11.929788000	7.061270000	4.691499000
C	6.190751000	5.749002000	4.502442000
H	12.725910000	7.535010000	5.292229000
H	9.896040000	7.097505000	6.666440000
H	9.280361000	5.595975000	4.333234000
H	4.792502000	6.560200000	5.552489000
H	11.750192000	6.075907000	5.166552000
H	11.718196000	6.597772000	2.810726000
H	6.440573000	4.716887000	4.210438000
H	5.922308000	6.302424000	3.584043000
H	8.871302000	9.369032000	5.281609000
H	6.883623000	5.472586000	6.756116000
H	9.346138000	6.853674000	2.457342000
H	7.110607000	7.461708000	5.399184000
O	8.455530000	7.100469000	3.184537000
O	12.431849000	6.945668000	3.388877000
O	5.130814000	5.662270000	5.422415000
O	10.470190000	8.807821000	3.904376000
O	8.876070000	8.775687000	6.063426000
O	7.729805000	5.709957000	6.350337000

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C	10.500580000	13.573437000	3.164344000
C	13.590787000	10.499198000	3.218836000
C	7.259454000	10.315342000	3.225492000

C	13.586652000	13.569378000	0.091861000
C	7.226119000	7.224678000	0.091325000
C	10.347288000	13.576517000	-3.149278000
C	10.494069000	7.256236000	-3.139806000
C	13.586896000	10.339553000	-3.142334000
C	7.268497000	10.493795000	-3.141594000
C	7.267289000	13.568916000	-0.062138000
C	13.640768000	7.253250000	-0.115308000
H	6.483903000	14.354690000	-0.129006000
H	14.371849000	14.354941000	0.133023000
H	10.569938000	14.370161000	3.937214000
H	10.296761000	14.364113000	-3.931704000
H	10.537256000	6.473284000	-3.927787000
H	14.371716000	10.277517000	-3.927361000
H	6.482055000	10.554738000	-3.924970000
C	6.488017000	10.229677000	5.618546000
C	14.306357000	10.633258000	5.615236000
C	5.480671000	10.101074000	6.571920000
C	15.294088000	10.619384000	6.595529000
C	5.524064000	3.885114000	0.632711000
C	6.515393000	4.846179000	0.454442000
C	16.983523000	10.317547000	4.891156000
C	3.831242000	9.957788000	4.808399000
C	4.816935000	6.544174000	0.163510000
C	15.997846000	10.333773000	3.908280000
C	4.839518000	10.076570000	3.853369000
C	3.826274000	5.581881000	0.333768000
C	6.176326000	10.207030000	4.252897000
C	14.652766000	10.490695000	4.264659000
C	4.152041000	9.962092000	6.169336000
C	16.633268000	10.460849000	6.234508000
C	4.178326000	4.252582000	0.573576000
C	6.169162000	6.183797000	0.226745000
H	7.529635000	10.346296000	5.923836000
H	13.252700000	10.754420000	5.877145000
H	5.733187000	10.111472000	7.634152000
H	15.020633000	10.733130000	7.646991000
H	5.798617000	2.844225000	0.818114000
H	7.572767000	4.576129000	0.495610000
H	18.031672000	10.192705000	4.610000000
H	2.788242000	9.870488000	4.492082000
H	4.561845000	7.591896000	-0.008641000
H	16.250938000	10.223688000	2.852321000
H	4.610899000	10.070630000	2.785229000
H	2.773435000	5.868357000	0.287991000
H	8.444105000	12.353706000	1.999257000

O	8.442091000	10.383898000	3.642132000
O	12.400537000	10.586445000	3.600463000
O	10.442973000	12.397242000	3.589676000
O	10.478104000	13.974511000	1.973010000
O	8.433179000	6.837510000	0.037391000
O	12.400438000	13.977618000	0.058279000
O	6.845149000	8.430338000	0.042092000
O	13.996902000	12.381837000	0.079551000
O	13.972275000	10.421586000	2.008467000
O	6.883304000	10.334031000	2.015721000
O	9.005971000	11.804742000	1.442230000
O	11.803395000	8.939145000	1.466401000
O	9.359749000	9.308661000	1.096956000
O	11.466532000	11.436368000	1.066411000
Hf	10.430600000	12.909288000	0.029528000
Hf	10.447092000	7.932456000	-0.012066000
Hf	10.438738000	10.368992000	2.589958000
Hf	12.947444000	10.400421000	0.058396000
Hf	7.916135000	10.392860000	0.041674000
H	15.084648000	2.840376000	-0.527572000
H	13.303855000	4.587328000	-0.356164000
H	16.302173000	7.647224000	-0.117960000
H	18.097471000	5.913272000	-0.288438000
H	8.449962000	8.425099000	-1.934295000
H	12.406426000	12.387278000	-1.945491000
C	15.355217000	3.894686000	-0.435219000
C	14.359976000	4.862490000	-0.338078000
C	16.051940000	6.588600000	-0.207043000
C	17.045674000	5.618964000	-0.302627000
C	16.698930000	4.271804000	-0.416398000
C	14.701768000	6.215903000	-0.222085000
O	8.454120000	10.464646000	-3.556081000
O	12.399597000	10.368310000	-3.557327000
O	10.474767000	8.442000000	-3.545276000
O	10.377725000	12.390036000	-3.564562000
O	10.372460000	13.975414000	-1.960638000
O	10.465028000	6.838917000	-1.955115000
O	8.454234000	13.973139000	-0.031125000
O	12.432858000	6.858266000	-0.078603000
O	14.005848000	8.460513000	-0.055621000
O	6.854841000	12.381288000	-0.018849000
O	13.992559000	10.379818000	-1.956467000
O	6.862454000	10.455235000	-1.954228000
O	11.844110000	11.829044000	-1.398093000
O	9.014712000	8.996570000	-1.403163000
O	11.481136000	9.372182000	-1.040137000

O	9.378352000	11.441830000	-1.022770000
H	12.324929000	8.362437000	2.071143000
Hf	10.429700000	10.427799000	-2.509200000
O	10.393294000	6.412030000	1.803115000
H	10.211521000	5.525042000	1.463040000
H	17.408270000	10.449070000	7.004809000
H	17.480133000	3.511548000	-0.491834000
H	3.400458000	3.498789000	0.715663000
H	3.361166000	9.866819000	6.917240000
C	7.647952000	6.294015000	4.055952000
C	10.158437000	7.361063000	5.668868000
C	10.980218000	7.850736000	4.711179000
C	6.284804000	6.540007000	4.623693000
C	12.413190000	7.452488000	4.586201000
C	5.215109000	6.625366000	3.540657000
H	13.076434000	8.281165000	4.881551000
H	10.425920000	6.600304000	6.401484000
H	8.259355000	5.538624000	4.606184000
H	3.858816000	7.624826000	4.485553000
H	12.628535000	6.616239000	5.275546000
H	12.113734000	6.543391000	2.882210000
H	5.215350000	5.695262000	2.950063000
H	5.441047000	7.457198000	2.848343000
H	8.845102000	8.571035000	5.125931000
H	5.035421000	5.557078000	5.663378000
H	9.576889000	6.625729000	2.345237000
H	6.347051000	7.534250000	5.124207000
O	8.050011000	6.829794000	3.039609000
O	12.796192000	7.127180000	3.251353000
O	3.943779000	6.726941000	4.132595000
O	10.483170000	8.769805000	3.889389000
O	8.889370000	7.852124000	5.789828000
O	5.994963000	5.523800000	5.540750000

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C	10.500300000	13.573400000	3.164300000
C	13.590800000	10.499200000	3.218800000
C	7.259400000	10.315400000	3.225500000
C	13.586700000	13.569300000	0.091800000
C	7.226100000	7.224700000	0.091400000
C	10.347300000	13.576500000	-3.149300000
C	10.494300000	7.256200000	-3.139800000
C	13.586900000	10.339500000	-3.142400000
C	7.268500000	10.493900000	-3.141500000
C	7.267300000	13.569000000	-0.062000000
C	13.640800000	7.253200000	-0.115400000

H	6.483293000	14.353557000	-0.131224000
H	14.372520000	14.354052000	0.134312000
H	10.566250000	14.367215000	3.939727000
H	10.296210000	14.361476000	-3.934058000
H	10.545211000	6.478439000	-3.932383000
H	14.371314000	10.285733000	-3.928069000
H	6.483343000	10.559095000	-3.925390000
C	6.566655000	10.166134000	5.629108000
C	14.287870000	10.495801000	5.623205000
C	5.582869000	10.065462000	6.607972000
C	15.269982000	10.431826000	6.607365000
C	5.481379000	3.870009000	0.287481000
C	6.477523000	4.831622000	0.148076000
C	16.973966000	10.264944000	4.898735000
C	3.875016000	10.058954000	4.894716000
C	4.834397000	6.580226000	0.463564000
C	15.993979000	10.327862000	3.912359000
C	4.856259000	10.159227000	3.913435000
C	3.840398000	5.616959000	0.608208000
C	6.208761000	10.214759000	4.275064000
C	14.644589000	10.443892000	4.269179000
C	4.237076000	10.012115000	6.242003000
C	16.613479000	10.316638000	6.246135000
C	4.162080000	4.261844000	0.519845000
C	6.161159000	6.193571000	0.234386000
H	7.624303000	10.208378000	5.897452000
H	13.231426000	10.589048000	5.883795000
H	5.864900000	10.027522000	7.662432000
H	14.989254000	10.474063000	7.662265000
H	5.732225000	2.809397000	0.214605000
H	7.513176000	4.541021000	-0.039393000
H	18.025558000	10.174497000	4.617437000
H	2.821439000	10.015511000	4.609970000
H	4.602800000	7.644801000	0.529351000
H	16.254619000	10.287058000	2.853240000
H	4.594466000	10.195186000	2.854422000
H	2.807941000	5.922638000	0.791485000
H	8.440681000	12.351614000	2.000996000
O	8.465458000	10.324767000	3.610354000
O	12.395719000	10.595868000	3.596098000
O	10.437682000	12.395486000	3.589232000
O	10.485999000	13.972456000	1.974388000
O	8.420722000	6.823676000	-0.008377000
O	12.399988000	13.979103000	0.059486000
O	6.859219000	8.437551000	0.076992000
O	13.993169000	12.380860000	0.077157000

O	13.968638000	10.432449000	2.008784000
O	6.875670000	10.372935000	2.021231000
O	9.012217000	11.810236000	1.445842000
O	11.786858000	8.915229000	1.500882000
O	9.362641000	9.305799000	1.117038000
O	11.461101000	11.434297000	1.064770000
Hf	10.428326000	12.919235000	0.017653000
Hf	10.429708000	7.876786000	0.009217000
Hf	10.442579000	10.404042000	2.564454000
Hf	12.946720000	10.386755000	0.047925000
Hf	7.916034000	10.388536000	0.044306000
H	15.087354000	2.832528000	-0.375032000
H	13.306466000	4.587839000	-0.282756000
H	16.308111000	7.648052000	-0.092023000
H	18.102568000	5.906869000	-0.188820000
H	8.444754000	8.429931000	-1.924591000
H	12.405430000	12.381839000	-1.947315000
C	15.358489000	3.888906000	-0.312623000
C	14.363509000	4.860545000	-0.260458000
C	16.057234000	6.587662000	-0.154995000
C	17.050403000	5.614039000	-0.208747000
C	16.702537000	4.264599000	-0.286974000
C	14.707047000	6.216319000	-0.180990000
O	8.455679000	10.460730000	-3.550938000
O	12.399251000	10.367092000	-3.552668000
O	10.478788000	8.444761000	-3.539845000
O	10.377556000	12.388415000	-3.555568000
O	10.373580000	13.981931000	-1.960856000
O	10.452069000	6.832985000	-1.959339000
O	8.454740000	13.976467000	-0.028461000
O	12.442600000	6.865457000	-0.142324000
O	14.010204000	8.463230000	-0.020270000
O	6.859433000	12.381214000	-0.018130000
O	13.994506000	10.372070000	-1.955570000
O	6.862238000	10.454651000	-1.953136000
O	11.844412000	11.827445000	-1.394595000
O	9.014083000	8.993276000	-1.389464000
O	11.475091000	9.367543000	-1.016092000
O	9.378158000	11.444188000	-1.015080000
H	12.344726000	8.352154000	2.075813000
Hf	10.431331000	10.413977000	-2.492842000
O	10.445598000	6.271373000	1.560310000
H	9.892983000	5.553464000	1.221902000
H	17.384026000	10.267382000	7.019378000
H	17.483359000	3.501276000	-0.328360000
H	3.380445000	3.506695000	0.632080000

H	3.465497000	9.932619000	7.011577000
C	9.510743000	6.659893000	4.027300000
C	10.645885000	7.471978000	4.180889000
C	12.011658000	6.837141000	4.300151000
H	12.600824000	7.405880000	5.034233000
H	9.492188000	5.657419000	4.469656000
H	11.921820000	5.801874000	4.673499000
H	12.223112000	6.356183000	2.423003000
H	8.427399000	8.204404000	3.897126000
H	9.993218000	6.433555000	2.785607000
O	12.728060000	6.877396000	3.078835000
O	10.549310000	8.719891000	3.959518000
O	8.275314000	7.242605000	3.923475000

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C	10.500300000	13.573400000	3.164300000
C	13.590800000	10.499200000	3.218800000
C	7.259400000	10.315400000	3.225500000
C	13.586700000	13.569300000	0.091800000
C	7.226100000	7.224700000	0.091400000
C	10.347300000	13.576500000	-3.149300000
C	10.494300000	7.256200000	-3.139800000
C	13.586900000	10.339500000	-3.142400000
C	7.268500000	10.493900000	-3.141500000
C	7.267300000	13.569000000	-0.062000000
C	13.640800000	7.253200000	-0.115400000
H	6.481786000	14.352567000	-0.129116000
H	14.372643000	14.353788000	0.144523000
H	10.565672000	14.362954000	3.944304000
H	10.295774000	14.358546000	-3.937204000
H	10.554950000	6.481373000	-3.934928000
H	14.370072000	10.288774000	-3.929542000
H	6.485476000	10.562827000	-3.927408000
C	6.543944000	10.365750000	5.630731000
C	14.283806000	10.511712000	5.627581000
C	5.551083000	10.309998000	6.604383000
C	15.266250000	10.469218000	6.612663000
C	5.450406000	3.882377000	0.204044000
C	6.459168000	4.837594000	0.102082000
C	16.974056000	10.336938000	4.905218000
C	3.869195000	10.096365000	4.879149000
C	4.802303000	6.597125000	0.254023000
C	15.993659000	10.379991000	3.918230000
C	4.859179000	10.151055000	3.904549000
C	3.796949000	5.640317000	0.357368000
C	6.204361000	10.280011000	4.273767000

C	14.641672000	10.466438000	4.273665000
C	4.213717000	10.172557000	6.229309000
C	16.612039000	10.381223000	6.252412000
C	4.120189000	4.282088000	0.340086000
C	6.141554000	6.201204000	0.137718000
H	7.592659000	10.481299000	5.911973000
H	13.226090000	10.587389000	5.888431000
H	5.819426000	10.379049000	7.660904000
H	14.984290000	10.508534000	7.667398000
H	5.701487000	2.819159000	0.178405000
H	7.506451000	4.545392000	0.001048000
H	18.027353000	10.268132000	4.624352000
H	2.822458000	9.987320000	4.587510000
H	4.571472000	7.663927000	0.277642000
H	16.255617000	10.345189000	2.859233000
H	4.611418000	10.081739000	2.843793000
H	2.754982000	5.952611000	0.456378000
H	8.441285000	12.368398000	2.002243000
O	8.472356000	10.275660000	3.613108000
O	12.385694000	10.536061000	3.600064000
O	10.444603000	12.391759000	3.585119000
O	10.480735000	13.977530000	1.977385000
O	8.414433000	6.811787000	0.049691000
O	12.400545000	13.984080000	0.057276000
O	6.861379000	8.439893000	0.098126000
O	13.992381000	12.382255000	0.068352000
O	13.970628000	10.471346000	2.013295000
O	6.882165000	10.376526000	2.023517000
O	9.007963000	11.822524000	1.446780000
O	11.812118000	8.955789000	1.484589000
O	9.371064000	9.334257000	1.103592000
O	11.470240000	11.464313000	1.062361000
Hf	10.428054000	12.934191000	0.004222000
Hf	10.423988000	7.832418000	0.047563000
Hf	10.448831000	10.427298000	2.509246000
Hf	12.947922000	10.379450000	0.034365000
Hf	7.917955000	10.389156000	0.035301000
H	15.073712000	2.828117000	-0.336122000
H	13.298837000	4.590138000	-0.234525000
H	16.311599000	7.643324000	-0.139337000
H	18.099944000	5.896288000	-0.245494000
H	8.440766000	8.434654000	-1.934830000
H	12.404955000	12.380635000	-1.954978000
C	15.348803000	3.884504000	-0.293918000
C	14.356979000	4.859168000	-0.237620000
C	16.056877000	6.582859000	-0.183812000

C	17.046781000	5.606036000	-0.242547000
C	16.694123000	4.256657000	-0.297165000
C	14.705669000	6.214717000	-0.182299000
O	8.455925000	10.457020000	-3.545325000
O	12.399137000	10.366102000	-3.549559000
O	10.476969000	8.446632000	-3.539878000
O	10.375956000	12.387561000	-3.547751000
O	10.375164000	13.991435000	-1.962495000
O	10.442321000	6.831219000	-1.961779000
O	8.453344000	13.981219000	-0.030622000
O	12.445463000	6.870275000	-0.152338000
O	14.016613000	8.464364000	-0.014701000
O	6.860423000	12.381709000	-0.017982000
O	13.998393000	10.370292000	-1.956579000
O	6.856778000	10.454516000	-1.953802000
O	11.844923000	11.830895000	-1.396752000
O	9.004605000	8.983795000	-1.379735000
O	11.471867000	9.369712000	-1.005174000
O	9.377237000	11.452546000	-1.014128000
H	12.338749000	8.391988000	2.084391000
Hf	10.434468000	10.399378000	-2.478768000
O	10.491407000	6.524537000	1.685715000
H	9.825877000	5.831166000	1.784843000
H	17.382971000	10.348477000	7.026108000
H	17.472247000	3.490680000	-0.342369000
H	3.331135000	3.531643000	0.427714000
H	3.435167000	10.127062000	6.994602000
C	9.533346000	6.888759000	5.089078000
C	10.683699000	7.489521000	4.357588000
C	11.960975000	6.698709000	4.258753000
H	12.594327000	7.067309000	5.089095000
H	9.886860000	6.418189000	6.024702000
H	11.734893000	5.641346000	4.503241000
H	11.984004000	6.511875000	2.383246000
H	8.648104000	8.583663000	4.792939000
H	9.222826000	6.044739000	4.430259000
O	12.643543000	6.838265000	3.064772000
O	10.544279000	8.615966000	3.897472000
O	8.499466000	7.782639000	5.337827000
C	7.468599000	4.116563000	3.090359000
C	6.717684000	4.906737000	4.120404000
C	6.382829000	6.318439000	3.628513000
H	6.933603000	3.214258000	2.696251000
H	6.486096000	7.381590000	5.216205000
H	5.658983000	6.233114000	2.802924000
H	7.288903000	6.816555000	3.231201000

H	5.010203000	4.877601000	4.955129000
H	7.413217000	5.019603000	4.984108000
O	8.575058000	4.424236000	2.707719000
O	5.768217000	7.033660000	4.660971000
O	5.555149000	4.227037000	4.489707000