Supplementary Material

for

DFT Insights into the Adsorption of Organophosphate Pollutants on Mercaptobenzothiazole-Modified Graphene Surfaces

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XYZ coordinates for the systems used in this study. Charge and multiplicity included.

Graphene (G)

* xyz 0 1

C -0.316030000 0.418734000 -9.922702000

C -2.796482000 0.619200000 -9.891210000

C -5.278460000 0.821284000 -9.865616000

C -3.989769000 0.770940000 -7.747415000

C -4.001493000 0.734755000 -9.194480000

C -5.206727000 0.886580000 -7.021618000

C -6.451315000 0.935634000 -9.166217000

C -6.470963000 0.972743000 -7.721536000

C -7.656382000 1.088080000 -6.991996000

C -8.865969000 1.237674000 -4.822065000

C 4.646091000 0.012812000 -9.990164000

C 2.164353000 0.217104000 -9.953491000

C 0.948703000 0.372746000 -7.810548000

C 0.926099000 0.336484000 -9.254801000

C -0.274837000 0.490726000 -7.084015000

C -1.519090000 0.571555000 -7.779539000

C -1.538226000 0.535630000 -9.223845000

C -2.741910000 0.687820000 -7.052154000

C -2.722442000 0.722090000 -5.619990000

C -3.943800000 0.835649000 -4.891494000

C -5.191255000 0.919188000 -5.591068000

C -6.412294000 1.034561000 -4.860566000

C -7.670349000 1.121951000 -5.565687000

C -6.394934000 1.065495000 -3.433145000

C -7.615639000 1.181141000 -2.701519000

C -8.871947000 1.269075000 -3.409704000

C	-10.075048000	1.387410000	-2.651854000
C	-11.289645000	1.540997000	-0.483047000
C	5.838767000	-0.068028000	-9.320249000
C	4.656624000	0.089145000	-7.145409000
C	5.900004000	-0.034243000	-7.876666000
C	3.419332000	0.171972000	-7.840476000
C	3.389227000	0.135498000	-9.287297000
C	2.192099000	0.291336000	-7.114180000
C	2.213851000	0.325755000	-5.682017000
C	0.988559000	0.441992000	-4.952402000
C	-0.254305000	0.523943000	-5.650109000
C	-1.476703000	0.639255000	-4.921412000
C	-1.456643000	0.671867000	-3.492398000
C	-2.680263000	0.784772000	-2.762514000
C	-3.924532000	0.867889000	-3.461230000
C	-5.146664000	0.980811000	-2.731693000
C	-5.126816000	1.012244000	-1.304395000
C	-6.350993000	1.127372000	-0.572742000
C	-7.597179000	1.212009000	-1.274406000
C	-8.819323000	1.330063000	-0.539396000
C	-10.074247000	1.418863000	-1.255521000
C	-8.799034000	1.361826000	0.881805000
C	-10.033015000	1.484077000	1.628893000
C	-11.270069000	1.572001000	0.886775000
C	7.105905000	-0.116330000	-7.176867000
C	5.923573000	0.040029000	-5.015338000
C	7.160796000	-0.082874000	-5.751595000
C	4.682214000	0.123687000	-5.715026000
C	3.455439000	0.242809000	-4.984436000

C	3.477125000	0.276683000	-3.554214000
C	2.253200000	0.391972000	-2.824507000
C	1.009469000	0.476118000	-3.523416000
C	-0.213491000	0.589217000	-2.794073000
C	-0.193045000	0.622075000	-1.364819000
C	-1.415666000	0.735185000	-0.635494000
C	-2.660046000	0.816864000	-1.334635000
C	-3.882835000	0.930041000	-0.605034000
C	-3.862622000	0.960182000	0.823759000
C	-5.086200000	1.074859000	1.554138000
C	-6.330756000	1.158134000	0.853455000
C	-7.556402000	1.276104000	1.586054000
C	-7.534274000	1.307958000	3.013101000
C	-8.769814000	1.429797000	3.752370000
C	-9.994059000	1.515346000	3.024633000
C	8.377194000	-0.166032000	-5.038005000
C	7.187966000	-0.010817000	-2.887239000
C	8.423495000	-0.132755000	-3.626499000
C	5.946958000	0.073799000	-3.588050000
C	4.719348000	0.193015000	-2.855624000
C	4.740165000	0.225456000	-1.428378000
C	3.516806000	0.342623000	-0.698068000
C	2.273828000	0.425778000	-1.396664000
C	1.049820000	0.539561000	-0.666483000
C	1.070153000	0.571198000	0.761128000
C	-0.152468000	0.684247000	1.490448000
C	-1.395353000	0.766576000	0.792121000
C	-2.619491000	0.878861000	1.522331000
C	-2.599125000	0.909489000	2.950262000

C	-3.823168000	1.023215000	3.680029000
C	-5.065508000	1.105769000	2.981448000
C	-6.293251000	1.223586000	3.713929000
C	-6.269996000	1.255475000	5.141265000
C	-7.507346000	1.376887000	5.877553000
C	-8.723646000	1.461244000	5.163923000
C	9.647798000	-0.217700000	-2.898792000
C	8.452893000	-0.062721000	-0.756015000
C	9.686844000	-0.185370000	-1.503083000
C	7.210232000	0.022651000	-1.460246000
C	5.984712000	0.142205000	-0.727706000
C	6.004953000	0.172754000	0.698503000
C	4.780873000	0.289074000	1.430134000
C	3.537049000	0.373118000	0.730718000
C	2.314432000	0.488338000	1.460288000
C	2.334483000	0.518036000	2.888223000
C	1.110943000	0.631995000	3.618091000
C	-0.132153000	0.715538000	2.919735000
C	-1.355238000	0.827198000	3.649125000
C	-1.334516000	0.859153000	5.078183000
C	-2.559989000	0.973213000	5.807865000
C	-3.801650000	1.055165000	5.110306000
C	-5.028602000	1.172186000	5.840939000
C	-5.003200000	1.204322000	7.271378000
C	-6.246789000	1.325204000	8.002692000
C	-7.452625000	1.408153000	7.302876000
C	10.923916000	-0.273156000	-0.760978000
C	10.943503000	-0.242143000	0.608843000
C	8.473159000	-0.031434000	0.665201000

C	9.728086000	-0.120219000	1.381316000
C	7.251062000	0.087137000	1.400193000
C	7.269453000	0.117042000	2.827332000
C	6.048828000	0.233587000	3.558945000
C	4.800650000	0.319447000	2.857472000
C	3.578690000	0.434293000	3.586970000
C	3.597826000	0.464804000	5.017271000
C	2.376553000	0.579207000	5.745765000
C	1.130853000	0.662769000	5.047171000
C	-0.091671000	0.776713000	5.775914000
C	-0.071274000	0.808338000	7.209869000
C	-1.295070000	0.923225000	7.936465000
C	-2.538384000	1.005661000	7.240073000
C	-3.765868000	1.121971000	7.966435000
C	-3.736055000	1.154727000	9.413349000
C	-4.993099000	1.275185000	10.116260000
C	-6.185744000	1.356486000	9.446333000
C	9.728822000	-0.089666000	2.777672000
C	8.525691000	0.028214000	3.535533000
C	8.519646000	0.058746000	4.947919000
C	6.066097000	0.263321000	4.986394000
C	7.324062000	0.174799000	5.691535000
C	4.845098000	0.379116000	5.716890000
C	4.860460000	0.410387000	7.147479000
C	3.643506000	0.525920000	7.873292000
C	2.395748000	0.610404000	7.178005000
C	1.172831000	0.725586000	7.905425000
C	1.191769000	0.759061000	9.349795000
C	-0.030555000	0.874343000	10.048684000

C	-1.272661000	0.957026000	9.380778000
C	-2.511134000	1.073636000	10.079530000
C	7.309955000	0.206957000	7.117890000
C	6.124505000	0.321805000	7.847448000
C	6.104768000	0.357793000	9.292161000
C	3.655008000	0.559448000	9.320425000
C	4.931874000	0.471599000	9.991585000
C	2.449939000	0.674245000	10.017176000
H	11.863430000	-0.369645000	-1.327135000
H	11.898874000	-0.313166000	1.151780000
H	10.687458000	-0.161339000	3.315391000
H	9.478101000	-0.011748000	5.485862000
H	8.268353000	0.136944000	7.656223000
H	7.065381000	0.290236000	9.825765000
H	4.942786000	0.499104000	11.092757000
H	2.466862000	0.700659000	11.118880000
H	-0.014011000	0.901501000	11.150253000
H	-2.495082000	1.100037000	11.181245000
H	-4.971453000	1.300968000	11.217269000
H	-7.130908000	1.449610000	10.003023000
H	-8.395451000	1.502934000	7.864358000
H	-9.666508000	1.557012000	5.724953000
H	-10.937216000	1.611472000	3.585355000
H	-12.209588000	1.668528000	1.452918000
H	-12.245009000	1.612129000	-1.025982000
H	-11.033700000	1.458728000	-3.189591000
H	-9.824516000	1.306779000	-5.360024000
H	-8.614969000	1.155585000	-7.530312000
H	-7.412079000	1.001194000	-9.699798000

H -5.289422000 0.793085000 -10.966769000

H -2.813533000 0.591470000 -10.992879000

H -0.332738000 0.390099000 -11.024231000

H 2.147989000 0.187737000 -11.055127000

H 4.624169000 -0.015249000 -11.091112000

H 6.783787000 -0.163313000 -9.876818000

H 8.048677000 -0.212048000 -7.738283000

H 9.320118000 -0.261206000 -5.599034000

H 10.590929000 -0.314020000 -3.459525000

*

Mercaptobenzothiazole disulfide (MBTS)

* xyz 0 1

C	0.692666000	-2.310049000	-3.998027000
C	-0.666514000	-2.120869000	-4.285962000
C	1.146356000	-3.488227000	-3.364138000
H	-1.015922000	-1.201596000	-4.778166000
H	2.218687000	-3.607259000	-3.146748000
C	0.253297000	-4.503452000	-3.006043000
H	0.590049000	-5.425735000	-2.511433000
H	1.414084000	-1.525606000	-4.272459000
N	-2.117022000	-5.249874000	-2.980987000
C	-3.273909000	-4.812008000	-3.362996000
C	-1.119865000	-4.339104000	-3.284705000
C	-1.562334000	-3.140380000	-3.926520000
S	-3.302276000	-3.209859000	-4.153390000
S	-4.842911000	-5.626511000	-3.159050000
C	-3.268906000	-7.036378000	3.884091000
C	-3.206192000	-8.042771000	2.909905000
C	-3.643588000	-5.717297000	3.546532000
H	-2.912421000	-9.068105000	3.177154000
H	-3.686145000	-4.948727000	4.333133000
C	-3.959961000	-5.373447000	2.228247000
H	-4.253804000	-4.351569000	1.948762000
H	-3.018818000	-7.282419000	4.927196000
N	-4.180582000	-6.172586000	-0.114834000
C	-4.040027000	-7.274931000	-0.778099000
C	-3.901466000	-6.365760000	1.227339000
C	-3.524751000	-7.697110000	1.587284000
S	-3.538130000	-8.713330000	0.155114000

S -4.274671000 -7.511572000 -2.526956000

*

MBTS-modified Graphene (G-MBTS)

* xyz 0 1

C	-25.309982000	0.541301000	20.362306000
C	-23.939327000	0.537228000	20.363016000
C	-29.616686000	0.618845000	22.851682000
C	-28.206283000	0.637418000	22.829536000
C	-27.463465000	0.590040000	21.609440000
C	-26.067673000	0.595566000	21.593308000
C	-25.335324000	0.651187000	22.842573000
C	-23.915719000	0.647102000	22.843232000
C	-23.182467000	0.587279000	21.594696000
C	-21.786712000	0.574794000	21.612136000
C	-21.044788000	0.619054000	22.832895000
C	-19.634507000	0.595210000	22.856689000
C	-33.927930000	0.591905000	25.338443000
C	-32.484584000	0.640994000	25.299176000
C	-31.769905000	0.620151000	24.095603000
C	-30.345947000	0.655167000	24.065197000
C	-29.625449000	0.721929000	25.315766000
C	-28.198206000	0.747070000	25.314161000
C	-27.482250000	0.699128000	24.079896000
C	-26.055886000	0.705583000	24.079118000
C	-25.339680000	0.758779000	25.318569000
C	-23.913479000	0.753754000	25.319155000
C	-23.196112000	0.695983000	24.080491000
C	-21.769833000	0.683788000	24.082545000
C	-21.054829000	0.729377000	25.317394000
C	-19.627423000	0.705743000	25.320707000
C	-18.906261000	0.632896000	24.070884000

C	-17.482437000	0.593999000	24.102630000
C	-16.768677000	0.618278000	25.306746000
C	-15.325619000	0.561786000	25.347281000
C	-34.612955000	0.595977000	26.527350000
C	-33.924429000	0.652112000	27.795819000
C	-32.480987000	0.715055000	27.788265000
C	-31.768853000	0.706006000	26.554243000
C	-30.340334000	0.752535000	26.550969000
C	-29.625545000	0.817391000	27.792237000
C	-28.197215000	0.850619000	27.791514000
C	-27.482525000	0.809206000	26.555679000
C	-26.056292000	0.811721000	26.556078000
C	-23.198025000	0.800220000	26.557364000
C	-21.771916000	0.791103000	26.557988000
C	-21.057097000	0.833219000	27.794300000
C	-19.628430000	0.811781000	27.795976000
C	-18.913185000	0.743997000	26.556128000
C	-17.484944000	0.694117000	26.560901000
C	-16.773560000	0.704709000	27.795268000
C	-15.330679000	0.632592000	27.804287000
C	-14.641375000	0.567885000	26.536644000
C	-34.608792000	0.636035000	29.018641000
C	-33.922451000	0.675581000	30.263251000
C	-32.482732000	0.751385000	30.264161000
C	-31.769864000	0.772584000	29.027324000
C	-30.339078000	0.827725000	29.027379000
C	-29.626019000	0.861248000	30.266164000
C	-28.198899000	0.886657000	30.267168000
C	-27.483681000	0.886352000	29.029476000

C	-26.056207000	0.889738000	29.029990000
C	-25.341336000	0.896246000	30.267585000
C	-23.915003000	0.895281000	30.267231000
C	-23.200038000	0.878348000	29.030351000
C	-21.772058000	0.871448000	29.030426000
C	-21.057750000	0.877546000	30.267887000
C	-19.630608000	0.848281000	30.268679000
C	-18.915945000	0.821720000	29.031169000
C	-17.485180000	0.766596000	29.033148000
C	-16.773684000	0.738838000	30.270591000
C	-15.334079000	0.662868000	30.271568000
C	-14.646988000	0.617588000	29.027524000
C	-34.609534000	0.629244000	31.507221000
C	-33.925745000	0.641698000	32.730446000
C	-32.482736000	0.712696000	32.739461000
C	-31.771034000	0.777641000	31.501609000
C	-30.340383000	0.835016000	31.503702000
C	-29.627866000	0.823397000	32.738973000
C	-28.199167000	0.843244000	32.740735000
C	-27.484387000	0.879817000	31.504509000
C	-26.056549000	0.881991000	31.504515000
C	-25.342405000	0.851848000	32.740633000
C	-23.915032000	0.856752000	32.741154000
C	-23.200254000	0.887871000	31.505050000
C	-21.772995000	0.881049000	31.505743000
C	-21.059523000	0.843863000	32.743620000
C	-19.631151000	0.807172000	32.742799000
C	-18.917633000	0.814156000	31.507565000
C	-17.486742000	0.758374000	31.507425000

C	-16.775735000	0.701077000	32.746615000
C	-15.332291000	0.638119000	32.739097000
C	-14.647953000	0.622115000	31.516254000
C	-34.615045000	0.575385000	33.998004000
C	-33.930740000	0.567369000	35.187295000
C	-32.487680000	0.623395000	35.227889000
C	-31.771343000	0.700200000	33.973838000
C	-30.343046000	0.751784000	33.978631000
C	-29.629038000	0.712730000	35.214272000
C	-28.201682000	0.737009000	35.217784000
C	-27.484558000	0.799003000	33.977162000
C	-26.058508000	0.805347000	33.977849000
C	-25.343127000	0.758311000	35.216083000
C	-23.916937000	0.760635000	35.216620000
C	-23.200443000	0.811304000	33.979028000
C	-21.774196000	0.805224000	33.979427000
C	-21.058458000	0.743097000	35.221038000
C	-19.631255000	0.715749000	35.219342000
C	-18.916355000	0.742561000	33.984002000
C	-17.487878000	0.694986000	33.980667000
C	-16.772229000	0.629462000	35.235762000
C	-15.328931000	0.579259000	35.196495000
C	-14.643843000	0.582539000	34.007624000
C	-31.774066000	0.598380000	36.432055000
C	-30.350279000	0.637526000	36.463933000
C	-29.622171000	0.600331000	37.678207000
C	-28.211904000	0.624926000	37.702193000
C	-27.486773000	0.690010000	36.452634000
C	-26.060523000	0.702063000	36.454784000

C	-25.340990000	0.651835000	37.692025000
C	-23.921375000	0.654407000	37.692674000
C	-23.200783000	0.706874000	36.456099000
C	-21.774437000	0.698095000	36.455338000
C	-21.050442000	0.635896000	37.705711000
C	-19.640069000	0.615281000	37.683504000
C	-18.910780000	0.648943000	36.469934000
C	-17.486881000	0.611712000	36.439400000
C	-27.470086000	0.580477000	38.923006000
C	-26.074322000	0.592554000	38.940521000
C	-25.317544000	0.542715000	40.172265000
C	-23.946883000	0.545194000	40.172987000
C	-23.189110000	0.597892000	38.941964000
C	-21.793327000	0.591057000	38.925859000
C	-23.914198000	0.849219000	27.794375000
C	-25.341558000	0.856805000	27.793856000
H	-35.713228000	0.552354000	26.534595000
H	-35.708874000	0.580048000	29.019525000
H	-35.709495000	0.571013000	31.505675000
H	-35.715051000	0.525683000	33.990029000
H	-13.541418000	0.516932000	26.544439000
H	-13.547075000	0.558354000	29.029031000
H	-13.547826000	0.566943000	31.515445000
H	-13.543611000	0.537905000	34.000604000
H	-34.475552000	0.511946000	36.141806000
H	-32.323751000	0.537212000	37.383764000
H	-30.172381000	0.545027000	38.629856000
H	-28.020355000	0.530610000	39.875112000
H	-25.873218000	0.497913000	41.121440000

H	-23.392110000	0.503229000	41.122776000
H	-21.243965000	0.542932000	39.878557000
H	-19.090833000	0.563988000	38.635925000
H	-16.937988000	0.559585000	37.392094000
H	-14.784651000	0.532214000	36.151733000
H	-34.472115000	0.543580000	24.383230000
H	-32.318841000	0.567304000	23.142989000
H	-30.165860000	0.566497000	21.899300000
H	-25.864817000	0.498654000	19.412584000
H	-23.383715000	0.492618000	19.413797000
H	-14.780762000	0.507265000	24.392745000
H	-28.012968000	0.542543000	20.656809000
H	-19.084393000	0.540197000	21.904964000
H	-16.932822000	0.534263000	23.150787000
H	-21.236516000	0.524874000	20.659990000
C	-17.909062000	-2.468079000	29.476946000
C	-18.634772000	-2.491308000	30.676702000
C	-18.563504000	-2.460837000	28.225772000
H	-18.119819000	-2.485518000	31.647580000
H	-17.966902000	-2.427649000	27.302499000
C	-19.959709000	-2.466837000	28.142793000
H	-20.479356000	-2.443978000	27.174483000
H	-16.810009000	-2.441028000	29.517581000
N	-22.098886000	-2.483395000	29.418019000
C	-22.491219000	-2.491718000	30.662784000
C	-20.713997000	-2.486441000	29.333665000
C	-20.035105000	-2.502676000	30.590336000
S	-21.211746000	-2.523216000	31.896641000
S	-24.167327000	-2.473563000	31.188016000

C	-31.217267000	-2.450457000	30.861475000
C	-30.481169000	-2.481027000	29.668203000
C	-30.573052000	-2.424744000	32.117392000
H	-30.989102000	-2.490237000	28.693679000
H	-31.177530000	-2.382322000	33.035335000
C	-29.177560000	-2.420046000	32.211768000
H	-28.666399000	-2.382048000	33.183993000
H	-32.316063000	-2.432185000	30.812076000
N	-27.027534000	-2.439011000	30.955005000
C	-26.625125000	-2.463285000	29.713789000
C	-28.413169000	-2.448230000	31.027636000
C	-29.081544000	-2.483823000	29.765671000
S	-27.893908000	-2.521711000	28.469465000
S	-24.947224000	-2.453635000	29.196237000

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Azinphos-methyl (AZM)

* xyz 0 1

S	2.234795000	2.054647000	1.139438000
P	2.369467000	1.749785000	-0.977266000
S	1.849204000	3.207763000	-2.136637000
O	3.913687000	1.249078000	-1.157189000
C	4.804623000	0.880841000	-0.083940000
H	5.057214000	1.762931000	0.538777000
H	4.380203000	0.075376000	0.548133000
H	5.726721000	0.508663000	-0.566769000
O	1.454800000	0.421069000	-1.289581000
C	1.763465000	-0.842090000	-0.668527000
H	2.738006000	-1.228819000	-1.027735000
H	1.779728000	-0.753793000	0.438629000
H	0.961673000	-1.542456000	-0.966961000
C	0.493623000	2.662675000	1.201865000
H	0.336645000	2.923539000	2.264913000
H	0.378972000	3.554256000	0.560120000
N	-1.854194000	1.122685000	-0.973882000
N	-0.474223000	1.676922000	0.767297000
N	-1.092076000	1.976419000	-0.421057000
C	-2.050173000	-0.132265000	-0.404223000
C	-1.471986000	-0.491465000	0.842140000
C	-0.623237000	0.487693000	1.513709000
O	-0.050242000	0.348678000	2.597106000
C	-2.853304000	-1.065159000	-1.099453000
H	-3.292363000	-0.768773000	-2.061971000
C	-1.695424000	-1.772029000	1.387071000
C	-3.063099000	-2.330967000	-0.553628000

H	-1.236673000	-2.029763000	2.351751000
H	-3.682558000	-3.062414000	-1.093217000
C	-2.486479000	-2.685427000	0.688377000
H	-2.663956000	-3.687879000	1.103724000

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Diazinon (DIA)

* xyz 0 1

O	-0.716919000	-0.869075000	-0.321716000
P	0.503280000	-0.955344000	-1.485305000
S	0.440995000	0.290505000	-2.953846000
O	1.909362000	-0.907322000	-0.681932000
C	2.176379000	-1.742101000	0.481166000
H	1.285646000	-1.751798000	1.143648000
H	2.365512000	-2.779128000	0.131870000
O	0.263207000	-2.498397000	-1.923682000
C	-0.395531000	-3.522415000	-1.115807000
H	-0.023346000	-3.478792000	-0.073098000
H	-1.482264000	-3.303301000	-1.102300000
N	-1.298665000	2.416397000	2.044727000
N	0.037780000	1.148677000	0.529630000
C	-0.182920000	2.213620000	1.323904000
C	-2.274790000	1.478503000	1.970902000
C	-2.129654000	0.335062000	1.167909000
C	-0.921700000	0.235421000	0.464177000
H	-2.908180000	-0.435561000	1.087192000
C	-3.517215000	1.718543000	2.774141000
H	-3.261294000	1.840787000	3.846695000
H	-3.997119000	2.666718000	2.454562000
H	-4.247786000	0.894916000	2.668331000
C	0.938989000	3.223958000	1.451393000
H	0.453925000	4.202477000	1.649734000
C	1.794875000	3.312815000	0.186243000
C	1.793876000	2.867125000	2.682703000
H	1.177984000	2.814473000	3.602585000

H	2.288550000	1.882613000	2.544725000
H	2.586056000	3.626599000	2.840363000
H	2.268461000	2.336051000	-0.037053000
H	2.592791000	4.071913000	0.312561000
H	1.188395000	3.589731000	-0.699235000
C	3.380758000	-1.176030000	1.197246000
H	4.261782000	-1.144522000	0.525959000
H	3.178681000	-0.150441000	1.564652000
H	3.628133000	-1.815149000	2.067645000
C	-0.102772000	-4.863004000	-1.747588000
H	-0.619091000	-5.658595000	-1.175068000
H	-0.466990000	-4.897807000	-2.793426000
H	0.984261000	-5.079114000	-1.743192000

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Fenitrothion (FNT)

* xyz 0 1

O	-1.216102000	-0.043305000	-1.435513000
P	0.035920000	-0.587365000	-2.409996000
S	1.247311000	-1.844575000	-1.594093000
O	-0.858176000	-1.030452000	-3.684619000
C	-1.696238000	-2.203898000	-3.609174000
H	-2.044482000	-2.407308000	-4.636996000
H	-1.119937000	-3.072082000	-3.230633000
H	-2.565722000	-2.015150000	-2.948621000
O	0.753200000	0.752546000	-2.963472000
C	-0.022709000	1.816148000	-3.570005000
H	-0.438498000	1.482510000	-4.539841000
H	-0.843853000	2.137831000	-2.899185000
H	0.679126000	2.653891000	-3.729249000
C	-2.109654000	0.132720000	0.754792000
C	-2.000707000	0.590826000	2.064051000
C	-1.054200000	0.390706000	-0.137897000
H	-2.803768000	0.412578000	2.790332000
C	-0.845475000	1.277642000	2.484313000
C	0.089238000	1.093100000	0.277614000
H	0.891165000	1.309589000	-0.442798000
C	0.235473000	1.548167000	1.601751000
H	-2.993881000	-0.421181000	0.411680000
C	1.488896000	2.291675000	1.966507000
H	2.088201000	2.486807000	1.057643000
H	1.266286000	3.254592000	2.465665000
H	2.102463000	1.708930000	2.681984000
N	-0.820165000	1.706362000	3.884404000

O 0.257678000 2.054709000 4.381505000

O -1.884329000 1.695984000 4.518409000

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Glyphosate (GLY)

* xyz 0 1

P	1.734607000	-0.635172000	0.498769000
O	2.782787000	-1.510378000	1.143095000
O	1.239064000	0.575452000	1.434724000
O	2.253078000	0.193548000	-0.829774000
H	2.697237000	-0.409327000	-1.463696000
H	0.291935000	0.868290000	1.195118000
C	0.268326000	-1.548047000	-0.109263000
N	-0.592324000	-0.817396000	-1.032167000
H	-0.109533000	-0.004801000	-1.432645000
C	-1.924850000	-0.484740000	-0.601529000
C	-2.098113000	0.657927000	0.388011000
O	-1.186634000	1.279001000	0.937543000
O	-3.358099000	1.023457000	0.653571000
H	-3.990161000	0.473956000	0.140433000
H	-0.289888000	-1.901832000	0.781273000
H	-2.550152000	-0.217355000	-1.482128000
H	0.698213000	-2.462937000	-0.579160000
H	-2.421613000	-1.375159000	-0.159244000

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Malathion (MAL)

* xyz 0 1

C	0.276633000	-0.453800000	0.575049000
O	1.413741000	-0.832166000	0.824208000
O	-0.693357000	-0.703173000	1.478611000
C	-2.073043000	-0.286783000	1.289108000
H	-2.118829000	0.820853000	1.337393000
H	-2.436518000	-0.604906000	0.291036000
C	-2.898795000	-0.919110000	2.385756000
H	-2.529934000	-0.615817000	3.385629000
H	-2.878957000	-2.026079000	2.321691000
H	-3.950927000	-0.586422000	2.289713000
C	-0.054499000	0.270285000	-0.720371000
H	-1.017414000	0.811824000	-0.687080000
H	0.743532000	1.021343000	-0.879599000
C	-0.087039000	-0.670957000	-1.941728000
H	-0.280490000	-0.068980000	-2.849734000
C	-1.222610000	-1.685137000	-1.823364000
O	-2.274248000	-1.590745000	-2.437887000
O	-0.957636000	-2.626077000	-0.907528000
C	-2.013335000	-3.583669000	-0.619233000
H	-2.937694000	-3.021967000	-0.369584000
H	-2.217600000	-4.164229000	-1.542110000
C	-1.546204000	-4.453004000	0.523383000
H	-1.307386000	-3.840526000	1.415534000
H	-0.645265000	-5.037109000	0.247961000
H	-2.348353000	-5.166846000	0.794548000
S	1.575105000	-1.464065000	-2.154946000
P	1.154893000	-2.387873000	-4.037642000

S	0.291064000	-1.319679000	-5.403935000
O	2.606480000	-3.008008000	-4.458708000
C	3.772297000	-3.045229000	-3.609167000
H	4.117953000	-2.020336000	-3.366285000
H	3.585205000	-3.614420000	-2.676533000
H	4.558657000	-3.559563000	-4.191865000
O	0.225497000	-3.699251000	-3.689080000
C	0.727989000	-4.715917000	-2.797177000
H	1.583117000	-5.250284000	-3.258050000
H	1.033837000	-4.274441000	-1.826756000
H	-0.101058000	-5.428595000	-2.633546000

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Tokuthion (TOK)

* xyz 0 1

P	0.384984000	0.737108000	-1.480085000
O	1.329950000	0.162988000	-0.220267000
S	-0.477557000	2.460141000	-1.276286000
S	1.604667000	0.606146000	-3.207275000
C	3.170740000	-0.265261000	-2.744769000
H	3.668658000	0.326846000	-1.952398000
H	3.767348000	-0.115328000	-3.669761000
C	3.083120000	-1.742832000	-2.388567000
H	2.424163000	-1.875275000	-1.508433000
H	2.619946000	-2.300993000	-3.229060000
C	4.466397000	-2.310705000	-2.067355000
H	4.932902000	-1.776871000	-1.213444000
H	4.395703000	-3.381819000	-1.791849000
H	5.155434000	-2.226933000	-2.933519000
O	-0.725036000	-0.447736000	-1.483344000
C	-0.396085000	-1.855489000	-1.662104000
H	0.199410000	-2.191222000	-0.787668000
H	0.221526000	-1.960106000	-2.578650000
C	-1.691040000	-2.624037000	-1.781420000
H	-2.280202000	-2.277736000	-2.654249000
H	-2.307406000	-2.512084000	-0.867017000
H	-1.464146000	-3.700023000	-1.919408000
C	2.481683000	0.720757000	0.285263000
C	3.294136000	-0.118707000	1.081915000
C	2.889332000	2.043620000	0.046610000
C	4.495511000	0.352130000	1.626980000
C	4.091824000	2.524451000	0.581267000

C	4.886136000	1.675098000	1.366158000
H	2.257773000	2.704375000	-0.564471000
H	5.117540000	-0.312279000	2.240920000
H	4.406181000	3.557972000	0.385128000
Cl	2.796707000	-1.761357000	1.378935000
Cl	6.386976000	2.265897000	2.036073000

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Disulfoton (DST)

* xyz 0 1

P	-0.558071000	-0.331212000	-2.998293000
S	-0.849063000	1.011301000	-1.626645000
S	0.191143000	-2.230577000	-2.388108000
O	0.497370000	0.128686000	-4.155466000
C	1.430170000	-0.752309000	-4.850156000
H	0.886408000	-1.626639000	-5.262913000
H	2.181519000	-1.117575000	-4.118607000
C	2.087932000	0.049779000	-5.948799000
H	2.624018000	0.926078000	-5.533831000
H	1.339401000	0.404905000	-6.684605000
H	2.821272000	-0.589725000	-6.479348000
O	-1.974553000	-0.642902000	-3.764682000
C	-2.024784000	-1.530362000	-4.916873000
H	-1.377673000	-2.414102000	-4.724838000
H	-1.623282000	-0.984251000	-5.796478000
C	-3.462038000	-1.947478000	-5.129602000
H	-4.112312000	-1.066322000	-5.298487000
H	-3.846484000	-2.510208000	-4.254965000
H	-3.527645000	-2.602610000	-6.021310000
C	-1.160789000	-2.616106000	-1.188545000
H	-2.092219000	-2.807578000	-1.757393000
H	-1.307649000	-1.723123000	-0.547421000
C	-0.754643000	-3.831196000	-0.367055000
H	-0.578281000	-4.704376000	-1.028150000
H	0.176910000	-3.629329000	0.201485000
S	-2.109819000	-4.219389000	0.806781000
C	-1.431052000	-5.739179000	1.575454000

H -0.416769000 -5.506843000 1.962227000

H -2.080624000 -5.903623000 2.459491000

C -1.419200000 -6.964253000 0.671223000

H -0.764430000 -6.821334000 -0.212403000

H -2.438044000 -7.205738000 0.308568000

H -1.032927000 -7.845247000 1.225614000

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Parathion-methyl (PME)

* xyz 0 1

P	-0.978110000	-0.148671000	-2.506278000
S	-1.366692000	1.463664000	-1.524563000
O	-0.327312000	-1.434081000	-1.675774000
C	-0.824036000	-1.973140000	-0.510720000
C	-2.169930000	-1.837739000	-0.114044000
C	0.095859000	-2.698158000	0.272209000
C	-2.591280000	-2.427296000	1.079577000
C	-0.327091000	-3.294042000	1.459501000
C	-1.667908000	-3.148013000	1.852220000
H	-2.888461000	-1.288307000	-0.736313000
H	1.137796000	-2.782282000	-0.065812000
H	-3.632690000	-2.338410000	1.413981000
H	0.368713000	-3.863568000	2.088594000
N	-2.115246000	-3.767378000	3.101658000
O	-1.292590000	-4.416846000	3.758019000
O	-3.293816000	-3.611967000	3.442192000
O	0.158661000	0.043586000	-3.638142000
C	0.598306000	-1.074210000	-4.448761000
H	1.094505000	-0.639218000	-5.334624000
H	1.318069000	-1.694104000	-3.879208000
H	-0.260231000	-1.695284000	-4.770772000
O	-2.215462000	-0.940437000	-3.217871000
C	-3.147054000	-0.199325000	-4.037350000
H	-3.948153000	-0.907330000	-4.314766000
H	-3.576867000	0.649618000	-3.468525000
H	-2.648507000	0.178610000	-4.952072000

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Ethoprophos (ETH)

* xyz 0 1

P	0.538083000	-0.856354000	-1.672331000
O	0.583550000	-0.009780000	-2.923247000
S	-0.195421000	-2.817506000	-1.938358000
S	2.394803000	-1.167793000	-0.712600000
C	-1.837464000	-2.374325000	-2.679276000
H	-1.643132000	-1.710609000	-3.545780000
H	-2.411323000	-1.803802000	-1.921077000
C	-2.579017000	-3.640875000	-3.098279000
H	-1.954601000	-4.211794000	-3.818536000
H	-2.720846000	-4.296034000	-2.212272000
C	3.489826000	-0.915632000	-2.181250000
H	4.490982000	-0.774384000	-1.724555000
H	3.195262000	0.043034000	-2.651735000
C	3.483473000	-2.069102000	-3.177195000
H	3.722665000	-3.013913000	-2.644818000
H	2.458025000	-2.190271000	-3.586605000
C	4.474695000	-1.833794000	-4.315570000
H	5.513678000	-1.738480000	-3.937150000
H	4.455689000	-2.674578000	-5.038312000
H	4.236808000	-0.905200000	-4.875805000
C	-3.932723000	-3.309398000	-3.727580000
H	-3.812447000	-2.677138000	-4.631480000
H	-4.464107000	-4.233563000	-4.030863000
H	-4.585905000	-2.761202000	-3.017166000
O	-0.428734000	-0.144668000	-0.563936000
C	-0.620380000	-0.714974000	0.760050000
H	0.259612000	-0.448710000	1.383770000

H	-0.666931000	-1.822410000	0.674509000
C	-1.899317000	-0.156096000	1.340664000
H	-2.775028000	-0.446131000	0.726208000
H	-1.858744000	0.949599000	1.404283000
H	-2.045318000	-0.557112000	2.363034000

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MBTS-DIA

* xyz 0 1

C	6.147332000	-1.329922000	-2.260623000
C	5.624919000	-1.534640000	-0.974926000
C	5.310950000	-0.955463000	-3.335136000
H	6.281098000	-1.822277000	-0.141615000
H	5.748094000	-0.799761000	-4.332568000
C	3.935223000	-0.776272000	-3.151060000
H	3.278620000	-0.480943000	-3.981569000
H	7.225827000	-1.466018000	-2.430228000
N	2.049755000	-0.827898000	-1.525828000
C	1.861940000	-1.110913000	-0.266970000
C	3.384765000	-0.978885000	-1.868903000
C	4.244592000	-1.361931000	-0.793918000
S	3.298788000	-1.568888000	0.671242000
S	0.317988000	-1.064079000	0.564225000
C	-6.645470000	-2.072128000	1.417841000
C	-6.138455000	-1.833046000	0.131987000
C	-5.801272000	-2.053940000	2.549705000
H	-6.796898000	-1.856030000	-0.747779000
H	-6.227105000	-2.249136000	3.544937000
C	-4.431653000	-1.794309000	2.425750000
H	-3.767674000	-1.780488000	3.301674000
H	-7.718361000	-2.281657000	1.541473000
N	-2.560267000	-1.316304000	0.854773000
C	-2.376404000	-1.194781000	-0.431740000
C	-3.896916000	-1.554941000	1.143845000
C	-4.764652000	-1.580467000	0.010084000
S	-3.829380000	-1.314824000	-1.455181000

S	-0.839820000	-0.907269000	-1.224599000
O	0.142085000	-4.385427000	1.430978000
P	0.107788000	-5.111307000	-0.088982000
S	1.177935000	-4.339573000	-1.491743000
O	0.458884000	-6.673815000	0.167888000
C	-0.203452000	-7.452084000	1.207143000
H	-0.324933000	-6.826916000	2.116692000
H	-1.211438000	-7.737816000	0.839917000
O	-1.493115000	-5.024860000	-0.327985000
C	-2.496593000	-4.824924000	0.715156000
H	-2.361372000	-5.577435000	1.518669000
H	-2.337895000	-3.821576000	1.153906000
N	3.564752000	-3.645768000	3.535183000
N	2.364208000	-4.878591000	1.877285000
C	3.478296000	-4.591860000	2.589658000
C	2.459327000	-2.902269000	3.790937000
C	1.264293000	-3.115153000	3.087837000
C	1.292029000	-4.137820000	2.124615000
H	0.352444000	-2.534536000	3.279013000
C	2.577440000	-1.832813000	4.833075000
H	1.613756000	-1.324738000	5.018890000
H	2.952410000	-2.262928000	5.783504000
H	3.324820000	-1.076953000	4.513178000
C	4.711875000	-5.393586000	2.226953000
H	4.352252000	-6.423998000	2.018797000
C	5.761477000	-5.438082000	3.335860000
C	5.293600000	-4.836324000	0.912409000
H	4.525164000	-4.803213000	0.114355000
H	5.676817000	-3.806602000	1.064847000

H	6.138086000	-5.463987000	0.563185000
H	6.152447000	-4.425728000	3.558579000
H	6.614508000	-6.076012000	3.029792000
H	5.346103000	-5.849838000	4.276971000
C	0.651401000	-8.664074000	1.495040000
H	1.649324000	-8.359166000	1.867750000
H	0.162968000	-9.286492000	2.271282000
H	0.785112000	-9.282545000	0.585114000
C	-3.857761000	-4.950467000	0.071570000
H	-4.640998000	-4.700340000	0.814736000
H	-3.952915000	-4.250226000	-0.781145000
H	-4.038532000	-5.980227000	-0.295641000

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MBTS-AZM

* xyz 0 1

C	4.658285000	-5.155989000	-1.309830000
C	4.519081000	-4.543054000	-0.057199000
C	3.903253000	-4.723729000	-2.422498000
H	5.099530000	-4.889336000	0.809077000
H	4.026548000	-5.233008000	-3.389082000
C	2.991613000	-3.668625000	-2.313112000
H	2.389854000	-3.337678000	-3.170331000
H	5.356952000	-5.998116000	-1.421152000
N	1.961400000	-1.986295000	-0.793492000
C	2.040884000	-1.631383000	0.454281000
C	2.833012000	-3.033111000	-1.064439000
C	3.606907000	-3.481517000	0.050179000
S	3.209446000	-2.519659000	1.463385000
S	1.115081000	-0.364325000	1.283777000
C	-5.519546000	-2.494599000	-0.900981000
C	-4.461687000	-2.136933000	-1.745054000
C	-5.517018000	-2.145926000	0.471236000
H	-4.462095000	-2.425718000	-2.805342000
H	-6.356327000	-2.460698000	1.108659000
C	-4.462781000	-1.421037000	1.028732000
H	-4.443245000	-1.157370000	2.094328000
H	-6.365003000	-3.065969000	-1.312517000
N	-2.264302000	-0.345833000	0.609970000
C	-1.408713000	-0.224167000	-0.365251000
C	-3.380985000	-1.048681000	0.201680000
C	-3.390885000	-1.424761000	-1.180024000
S	-1.888527000	-0.928530000	-1.924919000

S	0.142604000	0.630824000	-0.279660000
C	-4.998308000	-5.622320000	1.216210000
S	-2.330182000	-4.355173000	0.175187000
P	-2.695560000	-4.616024000	2.268303000
S	-2.212842000	-3.173792000	3.468309000
O	-4.293313000	-4.955102000	2.285404000
H	-4.983538000	-5.012483000	0.289982000
H	-4.587054000	-6.630391000	1.013632000
H	-6.045258000	-5.722327000	1.557035000
O	-1.891923000	-5.975148000	2.707645000
C	-1.935769000	-7.204782000	1.962684000
H	-2.858756000	-7.772686000	2.197214000
H	-1.878241000	-7.017337000	0.869469000
H	-1.056452000	-7.797718000	2.277954000
C	-0.595750000	-3.755142000	0.303896000
H	-0.439353000	-3.123476000	-0.589256000
H	-0.472445000	-3.168668000	1.234765000
N	1.756293000	-6.076734000	1.625482000
N	0.369637000	-4.831695000	0.301387000
N	0.922470000	-5.120538000	1.519253000
C	2.111197000	-6.838605000	0.514085000
C	1.556486000	-6.603260000	-0.771877000
C	0.597092000	-5.515335000	-0.915862000
O	0.004055000	-5.173468000	-1.941055000
C	3.055584000	-7.875997000	0.689785000
H	3.476974000	-8.041496000	1.690902000
C	1.942980000	-7.397537000	-1.869725000
C	3.431564000	-8.654435000	-0.404006000
H	1.504948000	-7.191153000	-2.856024000

H	4.168857000	-9.460026000	-0.271184000
C	2.876117000	-8.418183000	-1.683340000
H	3.186461000	-9.040172000	-2.535367000

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MBTS-FNT

* xyz 0 1

C	5.380048000	-1.207770000	-1.393840000
C	4.011397000	-1.277206000	-1.106020000
C	5.858710000	-1.327224000	-2.720202000
H	3.649602000	-1.175798000	-0.073287000
H	6.940545000	-1.268707000	-2.911553000
C	4.979081000	-1.517072000	-3.787960000
H	5.339926000	-1.615632000	-4.821481000
H	6.093688000	-1.054464000	-0.570808000
N	2.607330000	-1.818966000	-4.466182000
C	1.427584000	-1.859831000	-3.903395000
C	3.593571000	-1.590864000	-3.524086000
C	3.122883000	-1.466836000	-2.178372000
S	1.377630000	-1.596234000	-2.146847000
S	-0.045567000	-2.042301000	-4.866600000
C	-4.587016000	-1.713470000	0.885228000
C	-4.640111000	-2.750173000	-0.056551000
C	-3.564361000	-0.739134000	0.845792000
H	-5.435339000	-3.508356000	-0.017624000
H	-3.540693000	0.050998000	1.611129000
C	-2.565696000	-0.780980000	-0.131666000
H	-1.754710000	-0.039111000	-0.157878000
H	-5.354398000	-1.663829000	1.672173000
N	-1.646449000	-2.026549000	-2.077226000
C	-1.920906000	-3.095506000	-2.765108000
C	-2.592388000	-1.817487000	-1.087841000
C	-3.639239000	-2.789669000	-1.039820000
S	-3.409038000	-3.959283000	-2.326865000

S	-0.923092000	-3.772076000	-4.062132000
O	0.401927000	-5.897831000	-1.296635000
P	1.848768000	-6.737518000	-1.268408000
S	2.309333000	-7.536193000	0.424378000
O	1.592324000	-7.663511000	-2.571912000
C	0.565451000	-8.676390000	-2.543553000
H	0.719155000	-9.306166000	-3.438334000
H	0.653818000	-9.300002000	-1.630311000
H	-0.437981000	-8.207447000	-2.582274000
O	2.962942000	-5.702341000	-1.823733000
C	2.795307000	-5.051321000	-3.106466000
H	2.915071000	-5.783564000	-3.927732000
H	1.798097000	-4.572872000	-3.176444000
H	3.594073000	-4.290976000	-3.166181000
C	-1.316560000	-5.209538000	0.198457000
C	-1.767705000	-4.338552000	1.186767000
C	-0.003829000	-5.061534000	-0.278010000
H	-2.783559000	-4.421302000	1.591378000
C	-0.925133000	-3.319991000	1.668300000
C	0.851560000	-4.077744000	0.241814000
H	1.882381000	-4.006181000	-0.133017000
C	0.413218000	-3.165240000	1.218903000
H	-1.961157000	-5.999747000	-0.208009000
C	1.370939000	-2.114424000	1.702661000
H	2.401425000	-2.371937000	1.391356000
H	1.110884000	-1.118516000	1.289665000
H	1.349972000	-2.000992000	2.802967000
N	-1.507050000	-2.415897000	2.660069000
O	-0.993547000	-1.301582000	2.819331000

O -2.511780000 -2.791812000 3.276449000

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MBTS-GLY

* xyz 0 1

C	4.227214000	-2.928934000	-1.970442000
C	3.490214000	-1.749784000	-1.799561000
C	3.686591000	-4.037473000	-2.662536000
H	3.908173000	-0.895249000	-1.250019000
H	4.290217000	-4.949926000	-2.778575000
C	2.396558000	-3.991301000	-3.199086000
H	1.964540000	-4.850100000	-3.732321000
H	5.243703000	-2.990555000	-1.555074000
N	0.336728000	-2.627992000	-3.489040000
C	-0.085856000	-1.439330000	-3.169936000
C	1.635006000	-2.813963000	-3.043028000
C	2.200437000	-1.698966000	-2.349880000
S	1.044375000	-0.387271000	-2.303049000
S	-1.680028000	-0.865898000	-3.698040000
C	-3.993144000	-4.513400000	2.129496000
C	-3.925593000	-4.389500000	0.734617000
C	-3.670895000	-3.431552000	2.979514000
H	-4.173297000	-5.237723000	0.081266000
H	-3.718109000	-3.563365000	4.070314000
C	-3.274675000	-2.196799000	2.453291000
H	-3.013524000	-1.348213000	3.102471000
H	-4.301522000	-5.474326000	2.566732000
N	-2.767607000	-0.917633000	0.380123000
C	-2.774238000	-1.112199000	-0.916540000
C	-3.201017000	-2.052791000	1.053553000
C	-3.527844000	-3.151418000	0.206492000
S	-3.309367000	-2.692333000	-1.473670000

S	-2.314290000	0.199560000	-2.006717000
P	0.389628000	-1.980174000	1.012095000
O	-0.114021000	-2.665029000	-0.230617000
O	1.980815000	-1.616954000	1.026004000
O	-0.291431000	-0.536366000	1.346037000
H	-1.242124000	-0.494241000	0.994733000
H	2.257859000	-1.665184000	1.977037000
C	0.235788000	-2.963928000	2.542413000
N	0.919584000	-2.271806000	3.631903000
H	0.487033000	-1.356076000	3.817484000
C	1.086018000	-3.058816000	4.843141000
C	-0.177814000	-3.577263000	5.530037000
O	-0.204469000	-4.588851000	6.211787000
O	-1.301401000	-2.834236000	5.385356000
H	-1.102738000	-2.030307000	4.857145000
H	0.748872000	-3.926618000	2.338778000
H	1.719419000	-3.945331000	4.640943000
H	-0.839765000	-3.208282000	2.708652000
H	1.624448000	-2.453184000	5.603701000

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MBTS-MAL

* xyz 0 1

C	4.137356000	-0.163198000	2.053639000
C	3.247584000	0.607504000	1.294822000
C	4.475603000	-1.482114000	1.668875000
H	2.979815000	1.627793000	1.602127000
H	5.172342000	-2.061641000	2.292701000
C	3.939698000	-2.058095000	0.514783000
H	4.194747000	-3.083485000	0.213010000
H	4.573433000	0.264069000	2.968271000
N	2.446510000	-1.728398000	-1.444588000
C	1.638587000	-0.817388000	-1.915519000
C	3.041380000	-1.303210000	-0.270977000
C	2.696641000	0.024147000	0.140518000
S	1.518498000	0.681160000	-0.970991000
S	0.714101000	-0.886407000	-3.419250000
C	-5.593186000	-0.959080000	0.078831000
C	-5.303209000	-1.290673000	-1.250374000
C	-4.582990000	-0.940935000	1.070334000
H	-6.094775000	-1.305890000	-2.013072000
H	-4.847895000	-0.678194000	2.104969000
C	-3.259910000	-1.255131000	0.754820000
H	-2.470014000	-1.262127000	1.518639000
H	-6.627849000	-0.707909000	0.355414000
N	-1.686731000	-1.951491000	-1.034259000
C	-1.714797000	-2.232284000	-2.310549000
C	-2.938632000	-1.591581000	-0.578367000
C	-3.970862000	-1.601095000	-1.572540000
S	-3.283743000	-2.063301000	-3.110220000

S	-0.304128000	-2.762981000	-3.244165000
C	2.135088000	-5.477128000	0.793282000
O	1.653213000	-5.779896000	1.878884000
O	3.427146000	-5.668220000	0.459870000
C	4.288181000	-6.268314000	1.469470000
H	3.695803000	-7.010169000	2.039178000
H	5.067101000	-6.797355000	0.889138000
C	4.889173000	-5.219905000	2.382968000
H	4.102427000	-4.661738000	2.928471000
H	5.516719000	-4.501088000	1.819389000
H	5.534242000	-5.716351000	3.135786000
C	1.349674000	-4.852836000	-0.334208000
H	1.841770000	-3.913252000	-0.662586000
H	1.368402000	-5.525988000	-1.215465000
C	-0.087829000	-4.567960000	0.074827000
H	-0.570032000	-3.997316000	-0.744795000
C	-0.242088000	-3.679837000	1.311989000
O	-1.203723000	-3.689757000	2.066259000
O	0.798895000	-2.844716000	1.421720000
C	0.823805000	-1.958768000	2.572522000
H	1.381502000	-1.069404000	2.228250000
H	-0.214599000	-1.660289000	2.815744000
C	1.503056000	-2.633003000	3.748147000
H	2.532475000	-2.946233000	3.484114000
H	0.934308000	-3.522713000	4.083600000
H	1.567517000	-1.921573000	4.595750000
S	-1.062769000	-6.116445000	0.326616000
P	-2.375177000	-5.925329000	-1.323698000
S	-1.588523000	-5.607890000	-3.083727000

O	-3.239958000	-7.301682000	-1.138861000
C	-2.707096000	-8.560093000	-1.599418000
H	-2.529704000	-8.531666000	-2.693533000
H	-1.760083000	-8.808819000	-1.078041000
H	-3.468143000	-9.325787000	-1.362137000
O	-3.481236000	-4.790487000	-0.966616000
C	-4.104448000	-4.737247000	0.338538000
H	-4.587141000	-5.704319000	0.582275000
H	-3.353032000	-4.477681000	1.109787000
H	-4.873982000	-3.946010000	0.275209000

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MBTS-TOK

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C	5.382567000	-2.371079000	1.640372000
C	4.316369000	-1.607306000	2.130244000
C	5.786576000	-2.284430000	0.286864000
H	4.000061000	-1.687333000	3.179689000
H	6.627816000	-2.898849000	-0.066071000
C	5.137392000	-1.429330000	-0.606290000
H	5.450561000	-1.351968000	-1.656882000
H	5.909794000	-3.056482000	2.320630000
N	3.334770000	0.259383000	-0.894445000
C	2.389485000	0.805948000	-0.179893000
C	4.058986000	-0.644574000	-0.138777000
C	3.657478000	-0.751644000	1.232083000
S	2.283127000	0.287813000	1.512320000
S	1.237544000	2.043776000	-0.712568000
C	-3.820986000	-3.259040000	0.021861000
C	-3.108859000	-3.056695000	-1.167901000
C	-3.740454000	-2.333756000	1.086838000
H	-3.152200000	-3.787953000	-1.987382000
H	-4.309902000	-2.520502000	2.009588000
C	-2.944048000	-1.188233000	0.990081000
H	-2.871428000	-0.467242000	1.817504000
H	-4.442341000	-4.160684000	0.129157000
N	-1.377578000	0.115341000	-0.437393000
C	-0.818366000	0.004882000	-1.606942000
C	-2.213992000	-0.962129000	-0.194913000
C	-2.310764000	-1.907604000	-1.262335000
S	-1.258830000	-1.418304000	-2.571100000

S	0.324195000	1.130746000	-2.364910000
P	0.865021000	-4.564481000	-0.163014000
O	1.540752000	-4.756174000	-1.706420000
S	0.677385000	-2.733024000	0.444909000
S	-0.915842000	-5.645798000	-0.190900000
C	-0.356569000	-7.276568000	-0.866936000
H	0.426443000	-7.070944000	-1.623597000
H	-1.247782000	-7.643119000	-1.417360000
C	0.096631000	-8.273298000	0.193728000
H	0.938996000	-7.831099000	0.763213000
H	-0.729001000	-8.440010000	0.917581000
C	0.520961000	-9.599684000	-0.437945000
H	0.837864000	-10.325482000	0.337661000
H	-0.309609000	-10.062389000	-1.011341000
H	1.372419000	-9.459685000	-1.136618000
O	1.880211000	-5.557749000	0.641050000
C	3.253727000	-5.126565000	0.896773000
H	3.485289000	-5.513524000	1.907970000
H	3.275851000	-4.017152000	0.947575000
C	4.216347000	-5.669820000	-0.137035000
H	5.253731000	-5.421366000	0.165251000
H	4.035778000	-5.233566000	-1.138383000
H	4.136155000	-6.772892000	-0.211599000
C	1.460284000	-3.797329000	-2.690300000
C	0.665068000	-4.014117000	-3.836498000
C	2.208147000	-2.614317000	-2.590862000
C	0.627637000	-3.067682000	-4.871075000
C	2.164256000	-1.647148000	-3.599778000
C	1.368948000	-1.884476000	-4.731355000

H	2.823724000	-2.456059000	-1.696202000
H	0.003574000	-3.243610000	-5.756708000
H	2.732763000	-0.714854000	-3.492189000
Cl	-0.294431000	-5.461377000	-3.967341000
Cl	1.270648000	-0.667075000	-5.981101000

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MBTS-DST

* xyz 0 1

C	7.277989000	-1.758251000	-1.754184000
C	6.604978000	-2.516077000	-0.784411000
C	6.630117000	-0.701470000	-2.431938000
H	7.112264000	-3.338818000	-0.260701000
H	7.183518000	-0.123157000	-3.186732000
C	5.296015000	-0.379141000	-2.158639000
H	4.784940000	0.442516000	-2.680461000
H	8.325925000	-1.995215000	-1.989816000
N	3.280111000	-0.928036000	-0.805626000
C	2.916580000	-1.786590000	0.108573000
C	4.597124000	-1.129555000	-1.190509000
C	5.265726000	-2.194230000	-0.514803000
S	4.161448000	-2.949983000	0.624679000
S	1.296173000	-1.852622000	0.810830000
C	-5.620718000	-2.961046000	-0.520131000
C	-4.795085000	-2.380433000	-1.493201000
C	-5.169281000	-3.138061000	0.807191000
H	-5.147874000	-2.244734000	-2.525190000
H	-5.838626000	-3.597781000	1.549017000
C	-3.884639000	-2.740998000	1.192174000
H	-3.529615000	-2.877959000	2.223011000
H	-6.632758000	-3.287221000	-0.800397000
N	-1.743506000	-1.698152000	0.466356000
C	-1.202323000	-1.232382000	-0.629600000
C	-3.030849000	-2.156417000	0.232898000
C	-3.501838000	-1.991432000	-1.107562000
S	-2.231323000	-1.285857000	-2.088851000

S	0.415528000	-0.585533000	-0.811291000
P	-1.368241000	-6.816417000	-0.325655000
S	-0.537582000	-8.543393000	-0.040204000
S	-1.611657000	-5.538073000	1.355505000
O	-2.922267000	-6.954762000	-0.808791000
C	-3.691022000	-5.810438000	-1.293353000
H	-3.261261000	-4.869082000	-0.891275000
H	-4.696425000	-5.924298000	-0.843631000
C	-3.752892000	-5.813300000	-2.804491000
H	-4.216414000	-6.747296000	-3.179197000
H	-2.742822000	-5.725095000	-3.252020000
H	-4.365614000	-4.958676000	-3.155246000
O	-0.548116000	-5.964393000	-1.461165000
C	-0.526006000	-4.521091000	-1.645453000
H	-0.797855000	-4.027580000	-0.688650000
H	-1.296033000	-4.258266000	-2.399536000
C	0.855375000	-4.119479000	-2.117366000
H	1.112997000	-4.630516000	-3.065817000
H	1.631532000	-4.363451000	-1.363345000
H	0.879869000	-3.024908000	-2.291252000
C	0.165592000	-5.281949000	1.774066000
H	0.711774000	-5.025427000	0.843556000
H	0.584479000	-6.224463000	2.175946000
C	0.261011000	-4.139352000	2.777808000
H	-0.334065000	-3.265923000	2.434313000
H	-0.088630000	-4.444174000	3.784505000
S	2.019569000	-3.650992000	2.892354000
C	2.018251000	-2.574626000	4.377635000
H	1.781132000	-3.235801000	5.236883000

H	3.082884000	-2.278924000	4.473908000
C	1.103065000	-1.362916000	4.326605000
H	0.036710000	-1.647835000	4.224704000
H	1.365716000	-0.688627000	3.488372000
H	1.204901000	-0.795769000	5.274894000

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MBTS-PME

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C	4.579047000	-2.880269000	-2.863566000
C	4.749067000	-2.254568000	-1.623663000
C	3.304164000	-2.973374000	-3.473386000
H	5.740414000	-2.192661000	-1.153548000
H	3.207826000	-3.473981000	-4.447170000
C	2.170632000	-2.438530000	-2.858106000
H	1.178270000	-2.498796000	-3.327184000
H	5.453916000	-3.313795000	-3.369413000
N	1.292925000	-1.198126000	-0.892464000
C	1.746446000	-0.685601000	0.220277000
C	2.312232000	-1.794763000	-1.607022000
C	3.610812000	-1.712444000	-1.003096000
S	3.486066000	-0.850967000	0.506946000
S	0.793670000	0.266083000	1.370867000
C	-5.826469000	-2.690574000	0.455555000
C	-4.640847000	-2.190634000	-0.100278000
C	-5.932562000	-2.945229000	1.841639000
H	-4.559988000	-2.000954000	-1.179786000
H	-6.874240000	-3.343309000	2.247450000
C	-4.857392000	-2.707350000	2.704073000
H	-4.930460000	-2.906701000	3.782843000
H	-6.684190000	-2.894428000	-0.202300000
N	-2.500831000	-1.921643000	2.887388000
C	-1.553624000	-1.513415000	2.090201000
C	-3.650746000	-2.212044000	2.168682000
C	-3.556206000	-1.966844000	0.762815000
S	-1.948672000	-1.388667000	0.365544000

S	0.065675000	-1.177431000	2.723316000
P	2.888638000	-5.206780000	1.500214000
S	2.438273000	-6.198544000	3.094277000
O	1.761296000	-4.100958000	0.946880000
C	0.436394000	-4.443605000	0.754559000
C	-0.413876000	-4.631037000	1.859858000
C	-0.042898000	-4.554258000	-0.562989000
C	-1.758458000	-4.938279000	1.644754000
C	-1.392583000	-4.837963000	-0.782079000
C	-2.230992000	-5.029402000	0.326614000
H	-0.014880000	-4.527698000	2.876664000
H	0.642664000	-4.403130000	-1.407312000
H	-2.448022000	-5.093920000	2.483420000
H	-1.801343000	-4.916291000	-1.797409000
N	-3.649242000	-5.326968000	0.103738000
O	-4.085802000	-5.261147000	-1.051111000
O	-4.343139000	-5.621563000	1.082081000
O	3.167072000	-6.151395000	0.218770000
C	3.602381000	-5.589724000	-1.042348000
H	3.046922000	-4.663719000	-1.278322000
H	4.686966000	-5.373549000	-1.006710000
H	3.391867000	-6.352241000	-1.814122000
O	4.179601000	-4.227921000	1.513617000
C	4.473887000	-3.441531000	2.686409000
H	3.666647000	-2.709173000	2.886385000
H	4.608847000	-4.098162000	3.569171000
H	5.416394000	-2.906110000	2.473990000

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MBTS-ETH

* xyz 0 1

C	1.014101000	-0.524847000	-2.966102000
C	2.247827000	-0.953788000	-2.457364000
C	-0.121916000	-0.413306000	-2.133812000
H	3.126868000	-1.049556000	-3.110162000
H	-1.077876000	-0.083658000	-2.566547000
C	-0.055616000	-0.728022000	-0.773286000
H	-0.938738000	-0.671015000	-0.123494000
H	0.931788000	-0.278646000	-4.034919000
N	1.411911000	-1.466164000	1.097052000
C	2.644472000	-1.832976000	1.271060000
C	1.176991000	-1.150041000	-0.232384000
C	2.315213000	-1.258783000	-1.089238000
S	3.688661000	-1.841993000	-0.165264000
S	3.414858000	-2.242952000	2.822955000
C	-0.536991000	2.787303000	6.215263000
C	0.582179000	2.397619000	5.465565000
C	-1.487081000	1.839019000	6.655821000
H	1.318629000	3.139238000	5.124782000
H	-2.355257000	2.175759000	7.241695000
C	-1.341428000	0.479680000	6.358154000
H	-2.075607000	-0.264585000	6.697766000
H	-0.673164000	3.850219000	6.464208000
N	0.059386000	-1.241633000	5.224176000
C	1.164498000	-1.285939000	4.541492000
C	-0.223968000	0.062557000	5.606418000
C	0.729424000	1.033362000	5.169110000
S	2.012136000	0.247026000	4.261812000

S	1.790910000	-2.844315000	3.971146000
P	-1.245543000	-4.553155000	-0.658646000
O	-1.717308000	-3.378372000	0.169466000
S	0.200379000	-3.885246000	-2.033163000
S	-0.571537000	-6.242566000	0.408409000
C	0.607810000	-5.464005000	-2.906714000
H	-0.243003000	-5.726406000	-3.564914000
H	0.713633000	-6.256398000	-2.135747000
C	1.894829000	-5.293600000	-3.713602000
H	2.037403000	-6.239820000	-4.279199000
H	1.746727000	-4.501737000	-4.479600000
C	0.646868000	-5.375710000	1.506314000
H	0.608316000	-5.956117000	2.450326000
H	0.232775000	-4.370313000	1.721146000
C	2.063176000	-5.310260000	0.942621000
H	2.057076000	-4.690431000	0.020973000
H	2.676934000	-4.753066000	1.684088000
C	2.701509000	-6.668369000	0.671182000
H	2.745261000	-7.286739000	1.592365000
H	2.127806000	-7.240137000	-0.088231000
H	3.737614000	-6.554217000	0.294925000
C	3.138767000	-4.993865000	-2.879484000
H	4.038190000	-4.917695000	-3.522570000
H	3.041141000	-4.033785000	-2.330674000
H	3.325575000	-5.789375000	-2.128582000
O	-2.384484000	-5.359454000	-1.517441000
C	-3.182360000	-4.611195000	-2.480743000
H	-2.522722000	-3.895675000	-3.018649000
H	-3.942263000	-4.025880000	-1.922922000

C	-3.818105000	-5.594924000	-3.433594000
H	-4.460257000	-6.317837000	-2.891275000
H	-3.048668000	-6.159378000	-3.998306000
H	-4.450092000	-5.049135000	-4.162467000

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G-MBTS-DIA

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C	-0.876205000	2.727469000	-9.882550000
C	0.493933000	2.742933000	-9.868331000
C	-5.200791000	2.422725000	-7.447176000
C	-3.792234000	2.489073000	-7.450745000
C	-3.039163000	2.596419000	-8.660036000
C	-1.644322000	2.634292000	-8.660705000
C	-0.924265000	2.572413000	-7.404526000
C	0.494608000	2.590227000	-7.389634000
C	1.238610000	2.668123000	-8.630828000
C	2.633514000	2.664086000	-8.601120000
C	3.363582000	2.581109000	-7.375992000
C	4.772703000	2.551472000	-7.343331000
C	-9.524441000	1.927753000	-5.035910000
C	-8.084730000	2.045698000	-5.050252000
C	-7.360903000	2.198147000	-6.238199000
C	-5.939805000	2.293219000	-6.246725000
C	-5.232091000	2.245645000	-4.987961000
C	-3.807144000	2.326711000	-4.969021000
C	-3.080687000	2.437505000	-6.192703000
C	-1.655469000	2.484244000	-6.176291000
C	-0.951545000	2.430759000	-4.929621000
C	0.474247000	2.451151000	-4.914282000
C	1.202236000	2.522652000	-6.146288000
C	2.628096000	2.516438000	-6.132302000
C	3.331700000	2.436638000	-4.892631000
C	4.758635000	2.403098000	-4.881478000
C	5.489680000	2.453682000	-6.126816000

C	6.911863000	2.390809000	-6.090343000
C	7.614724000	2.265342000	-4.886986000
C	9.055318000	2.167424000	-4.845603000
C	-10.217911000	1.759855000	-3.864163000
C	-9.542458000	1.699509000	-2.589124000
C	-8.103190000	1.827086000	-2.570374000
C	-7.381833000	1.994352000	-3.787344000
C	-5.956876000	2.104174000	-3.766499000
C	-5.254846000	2.061074000	-2.516909000
C	-3.829422000	2.162288000	-2.494753000
C	-3.103895000	2.283929000	-3.719193000
C	-1.678961000	2.341498000	-3.700482000
C	1.177944000	2.384488000	-3.669915000
C	2.603842000	2.376545000	-3.657648000
C	3.307435000	2.283189000	-2.417906000
C	4.735672000	2.234836000	-2.410422000
C	5.461941000	2.297118000	-3.644703000
C	6.888238000	2.214426000	-3.637526000
C	7.587641000	2.052424000	-2.407808000
C	9.027591000	1.931789000	-2.400250000
C	9.727915000	2.006178000	-3.660983000
C	-10.235057000	1.515376000	-1.385356000
C	-9.562869000	1.452380000	-0.134549000
C	-8.127917000	1.592080000	-0.105418000
C	-7.405227000	1.775824000	-1.323540000
C	-5.978130000	1.900189000	-1.297833000
C	-5.278388000	1.840570000	-0.052267000
C	-3.854388000	1.939477000	-0.029273000
C	-3.128538000	2.105035000	-1.250336000

C	-1.702532000	2.169586000	-1.230790000
C	-0.998880000	2.066762000	0.009982000
C	0.427392000	2.094252000	0.025145000
C	1.153190000	2.214364000	-1.200323000
C	2.581770000	2.197449000	-1.189807000
C	3.285055000	2.049045000	0.045299000
C	4.710817000	1.976875000	0.048844000
C	5.436381000	2.077616000	-1.179179000
C	6.865212000	1.976919000	-1.177140000
C	7.563909000	1.766214000	0.049637000
C	9.000602000	1.641303000	0.048591000
C	9.697884000	1.733429000	-1.186374000
C	-10.258545000	1.244924000	1.087484000
C	-9.588326000	1.165222000	2.314977000
C	-8.150595000	1.305373000	2.352212000
C	-7.430057000	1.526151000	1.137974000
C	-6.003204000	1.648284000	1.165219000
C	-5.302769000	1.538209000	2.401725000
C	-3.876087000	1.619213000	2.423901000
C	-3.151644000	1.828467000	1.210009000
C	-1.724206000	1.888588000	1.228995000
C	-1.020565000	1.732943000	2.462008000
C	0.406731000	1.764890000	2.478811000
C	1.131674000	1.947876000	1.261396000
C	2.559127000	1.923333000	1.271269000
C	3.262034000	1.724125000	2.500015000
C	4.689172000	1.644266000	2.501165000
C	5.412072000	1.767993000	1.277405000
C	6.840734000	1.658512000	1.276385000

C	7.539581000	1.428391000	2.502551000
C	8.979793000	1.309918000	2.492953000
C	9.673143000	1.418026000	1.280660000
C	-10.286089000	0.930042000	3.557424000
C	-9.612755000	0.821414000	4.747638000
C	-8.174458000	0.937412000	4.813200000
C	-7.450987000	1.193513000	3.587419000
C	-6.026786000	1.303635000	3.616446000
C	-5.322313000	1.144557000	4.846850000
C	-3.896729000	1.217654000	4.870318000
C	-3.171314000	1.457579000	3.655923000
C	-1.746189000	1.512736000	3.675529000
C	-1.040871000	1.331416000	4.907457000
C	0.385046000	1.366916000	4.925275000
C	1.111342000	1.575188000	3.709508000
C	2.537713000	1.562909000	3.720850000
C	3.243169000	1.351474000	4.952010000
C	4.668737000	1.276164000	4.951798000
C	5.392781000	1.414450000	3.729451000
C	6.818335000	1.308219000	3.724973000
C	7.522091000	1.066499000	4.965289000
C	8.961914000	0.957785000	4.924731000
C	9.655797000	1.073507000	3.747092000
C	-7.470522000	0.795968000	6.014287000
C	-6.050389000	0.887386000	6.068309000
C	-5.331791000	0.721577000	7.276597000
C	-3.924301000	0.790083000	7.320625000
C	-3.191540000	1.039388000	6.098683000
C	-1.766651000	1.095964000	6.120360000

C	-1.057095000	0.902171000	7.349342000
C	0.361572000	0.935449000	7.366717000
C	1.091276000	1.166943000	6.156010000
C	2.517462000	1.163802000	6.166822000
C	3.230235000	0.918867000	7.400901000
C	4.639009000	0.864312000	7.382634000
C	5.377612000	1.027902000	6.186337000
C	6.798355000	0.935469000	6.155643000
C	-3.192540000	0.609030000	8.534154000
C	-1.798625000	0.657221000	8.570325000
C	-1.052375000	0.458763000	9.793140000
C	0.317544000	0.485721000	9.809073000
C	1.083479000	0.716064000	8.604119000
C	2.478645000	0.713614000	8.598384000
C	0.450421000	2.306565000	-2.440327000
C	-0.976621000	2.286133000	-2.455648000
H	-11.314750000	1.663879000	-3.876654000
H	-11.331244000	1.409897000	-1.406259000
H	-11.354085000	1.133838000	1.063015000
H	-11.382172000	0.829927000	3.527174000
H	10.825691000	1.921153000	-3.652159000
H	10.794993000	1.635886000	-1.186599000
H	10.770311000	1.321184000	1.277155000
H	10.753114000	0.983196000	3.736956000
H	-10.161602000	0.633205000	5.682687000
H	-8.024143000	0.596140000	6.944478000
H	-5.886936000	0.524184000	8.206274000
H	-3.749180000	0.416836000	9.464202000
H	-1.615286000	0.274068000	10.720810000

H	0.865692000	0.321106000	10.749283000
H	3.020980000	0.530599000	9.538694000
H	5.178827000	0.668598000	8.321616000
H	7.336538000	0.742938000	7.096348000
H	9.495290000	0.772068000	5.869163000
H	-10.058761000	1.970585000	-5.997071000
H	-7.900234000	2.238070000	-7.197009000
H	-5.740752000	2.463196000	-8.405469000
H	-1.422747000	2.783668000	-10.836381000
H	1.058647000	2.811236000	-10.810741000
H	9.606705000	2.214975000	-5.796844000
H	-3.580005000	2.642845000	-9.617736000
H	5.330833000	2.596394000	-8.290985000
H	7.468423000	2.430002000	-7.039302000
H	3.192749000	2.721310000	-9.547632000
C	6.170254000	-1.160777000	-2.124056000
C	5.625253000	-1.306726000	-0.840087000
C	5.339696000	-0.990531000	-3.252968000
H	6.277082000	-1.425954000	0.037050000
H	5.795829000	-0.866088000	-4.245914000
C	3.946354000	-0.958787000	-3.126695000
H	3.294287000	-0.812055000	-3.999132000
H	7.263264000	-1.167534000	-2.247568000
N	2.016747000	-1.079417000	-1.555943000
C	1.812140000	-1.248228000	-0.279486000
C	3.372285000	-1.102658000	-1.847270000
C	4.228314000	-1.281001000	-0.715986000
S	3.258904000	-1.454280000	0.737230000
S	0.249070000	-1.306965000	0.509899000

C	-6.734630000	-1.759218000	1.415677000
C	-6.223980000	-1.581694000	0.121517000
C	-5.876895000	-1.839903000	2.534112000
H	-6.894451000	-1.516197000	-0.746715000
H	-6.309115000	-1.970956000	3.536657000
C	-4.488495000	-1.743911000	2.388393000
H	-3.813213000	-1.798894000	3.253865000
H	-7.823244000	-1.826785000	1.558362000
N	-2.600985000	-1.483472000	0.786234000
C	-2.422915000	-1.354397000	-0.500557000
C	-3.949764000	-1.565473000	1.098584000
C	-4.832863000	-1.486454000	-0.022218000
S	-3.898920000	-1.296790000	-1.500003000
S	-0.869985000	-1.242575000	-1.304811000
O	0.167218000	-4.501159000	1.439690000
P	0.122390000	-5.236781000	-0.075134000
S	1.195140000	-4.506123000	-1.497110000
O	0.454439000	-6.799301000	0.211445000
C	-0.193878000	-7.542176000	1.285274000
H	-0.331664000	-6.878690000	2.164585000
H	-1.194245000	-7.865765000	0.929510000
O	-1.476286000	-5.128693000	-0.317895000
C	-2.484736000	-4.897391000	0.714474000
H	-2.411154000	-5.684776000	1.492968000
H	-2.276271000	-3.917380000	1.184619000
N	3.593758000	-3.686567000	3.508434000
N	2.416126000	-4.913532000	1.830388000
C	3.532263000	-4.597715000	2.527586000
C	2.462823000	-3.000060000	3.806594000

C	1.270378000	-3.224797000	3.103266000
C	1.319993000	-4.222896000	2.115478000
H	0.342424000	-2.679275000	3.319305000
C	2.540983000	-1.997079000	4.914219000
H	1.640849000	-1.356930000	4.956348000
H	2.643466000	-2.517770000	5.889829000
H	3.442021000	-1.364176000	4.795854000
C	4.795789000	-5.321780000	2.107237000
H	4.490937000	-6.371768000	1.908437000
C	5.892617000	-5.304927000	3.170014000
C	5.287303000	-4.725206000	0.773226000
H	4.485260000	-4.736238000	0.008210000
H	5.609871000	-3.673605000	0.914463000
H	6.153103000	-5.299313000	0.386476000
H	6.228517000	-4.270652000	3.381227000
H	6.769893000	-5.886613000	2.823192000
H	5.545567000	-5.744292000	4.126066000
C	0.686059000	-8.720912000	1.631303000
H	1.676516000	-8.376871000	1.989568000
H	0.209914000	-9.315748000	2.436274000
H	0.834471000	-9.379482000	0.752234000
C	-3.837498000	-4.916141000	0.041023000
H	-4.621809000	-4.663309000	0.781911000
H	-3.880731000	-4.168766000	-0.776157000
H	-4.063679000	-5.914903000	-0.382442000

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C	-0.493455000	2.131402000	-9.899248000
C	0.874260000	2.051082000	-9.879973000
C	-4.835418000	2.165492000	-7.478645000
C	-3.426176000	2.120738000	-7.476950000
C	-2.663567000	2.164217000	-8.684009000
C	-1.269984000	2.097611000	-8.679732000
C	-0.560869000	1.986764000	-7.420642000
C	0.855588000	1.905337000	-7.400367000
C	1.607216000	1.929675000	-8.639275000
C	2.998341000	1.830887000	-8.604725000
C	3.716322000	1.701115000	-7.376777000
C	5.119460000	1.568877000	-7.340662000
C	-9.191926000	2.022774000	-5.083709000
C	-7.747491000	2.030079000	-5.091861000
C	-7.009997000	2.119048000	-6.277641000
C	-5.586091000	2.103171000	-6.280370000
C	-4.888886000	2.008459000	-5.018288000
C	-3.461911000	1.971803000	-4.994450000
C	-2.725135000	2.018553000	-6.216069000
C	-1.300649000	1.954538000	-6.194599000
C	-0.607199000	1.847191000	-4.945363000
C	0.816337000	1.767657000	-4.924967000
C	1.552308000	1.792515000	-6.153836000
C	2.974518000	1.691941000	-6.135274000
C	3.665960000	1.557835000	-4.894383000
C	5.084593000	1.406433000	-4.880431000
C	5.822599000	1.411384000	-6.122587000

C	7.235585000	1.238154000	-6.083219000
C	7.922021000	1.038865000	-4.880438000
C	9.351197000	0.833583000	-4.835605000
C	-9.900717000	1.913559000	-3.914252000
C	-9.236531000	1.801345000	-2.636939000
C	-7.792135000	1.817067000	-2.612476000
C	-7.055277000	1.931591000	-3.825859000
C	-5.626468000	1.932855000	-3.799726000
C	-4.934769000	1.820482000	-2.549057000
C	-3.506705000	1.792756000	-2.522311000
C	-2.768645000	1.868889000	-3.743233000
C	-1.344903000	1.806196000	-3.719928000
C	1.509098000	1.642432000	-3.679465000
C	2.930457000	1.533181000	-3.663241000
C	3.617937000	1.355597000	-2.424268000
C	5.037284000	1.188533000	-2.413445000
C	5.771441000	1.215859000	-3.644407000
C	7.187358000	1.018417000	-3.634690000
C	7.867580000	0.784930000	-2.405322000
C	9.295996000	0.565442000	-2.393999000
C	10.005150000	0.605874000	-3.651343000
C	-9.946289000	1.667218000	-1.436862000
C	-9.285889000	1.530347000	-0.186853000
C	-7.845066000	1.543078000	-0.153533000
C	-7.105416000	1.694735000	-1.364979000
C	-5.673467000	1.695753000	-1.334952000
C	-4.985306000	1.538006000	-0.091811000
C	-3.557534000	1.513816000	-0.063305000
C	-2.817463000	1.645726000	-1.278728000

C	-1.390556000	1.594749000	-1.254069000
C	-0.701962000	1.423796000	-0.011836000
C	0.721773000	1.341070000	0.008548000
C	1.460207000	1.427124000	-1.213822000
C	2.882331000	1.297579000	-1.200064000
C	3.566145000	1.069050000	0.034419000
C	4.983647000	0.897434000	0.043264000
C	5.718428000	0.955431000	-1.182454000
C	7.136621000	0.750332000	-1.176877000
C	7.815885000	0.493231000	0.052628000
C	9.239317000	0.261533000	0.052924000
C	9.945315000	0.309894000	-1.179489000
C	-10.000933000	1.346700000	1.026825000
C	-9.344625000	1.162692000	2.250276000
C	-7.900599000	1.172942000	2.292073000
C	-7.159681000	1.373181000	1.086445000
C	-5.727558000	1.370065000	1.118413000
C	-5.041913000	1.172740000	2.353460000
C	-3.612660000	1.162124000	2.386110000
C	-2.869852000	1.330442000	1.176690000
C	-1.442558000	1.290753000	1.204088000
C	-0.757553000	1.081013000	2.439322000
C	0.667199000	0.998500000	2.459426000
C	1.407154000	1.124251000	1.244675000
C	2.828234000	0.981278000	1.255873000
C	3.510105000	0.713687000	2.483326000
C	4.929388000	0.542080000	2.490806000
C	5.665950000	0.639369000	1.273142000
C	7.084470000	0.440667000	1.277719000

C	7.760655000	0.146327000	2.502251000
C	9.185983000	-0.087286000	2.493638000
C	9.889145000	-0.022612000	1.284214000
C	-10.063884000	0.942963000	3.482997000
C	-9.406610000	0.736804000	4.669515000
C	-7.963803000	0.733980000	4.741068000
C	-7.217391000	0.961319000	3.523216000
C	-5.787915000	0.962443000	3.559717000
C	-5.102403000	0.737572000	4.791191000
C	-3.674669000	0.729115000	4.826010000
C	-2.927004000	0.946761000	3.620894000
C	-1.501845000	0.903414000	3.648211000
C	-0.819673000	0.634702000	4.875708000
C	0.602821000	0.536712000	4.893566000
C	1.349261000	0.723960000	3.687254000
C	2.768525000	0.579461000	3.698044000
C	3.447810000	0.248872000	4.918560000
C	4.864700000	0.075308000	4.922637000
C	5.608466000	0.231278000	3.714973000
C	7.024543000	0.035695000	3.715607000
C	7.698096000	-0.315538000	4.945487000
C	9.125530000	-0.525769000	4.909115000
C	9.834932000	-0.415806000	3.740279000
C	-7.277626000	0.512107000	5.940249000
C	-5.854918000	0.502310000	6.002370000
C	-5.156558000	0.255741000	7.208405000
C	-3.748009000	0.224309000	7.259140000
C	-2.990856000	0.469056000	6.051291000
C	-1.567017000	0.418454000	6.078197000

C	-0.883577000	0.101330000	7.295409000
C	0.530062000	-0.013124000	7.310378000
C	1.281973000	0.202256000	6.110654000
C	2.700932000	0.057099000	6.119796000
C	3.383437000	-0.313567000	7.339723000
C	4.782755000	-0.478791000	7.322601000
C	5.542189000	-0.293293000	6.143844000
C	6.953688000	-0.473577000	6.119064000
C	-3.040376000	-0.064784000	8.465363000
C	-1.647866000	-0.137917000	8.503033000
C	-0.929096000	-0.469192000	9.713359000
C	0.436372000	-0.580987000	9.727188000
C	1.223096000	-0.368829000	8.532554000
C	2.610981000	-0.510350000	8.524529000
C	0.772411000	1.594188000	-2.454187000
C	-0.653575000	1.676576000	-2.474167000
H	-11.001821000	1.904499000	-3.930733000
H	-11.047470000	1.650277000	-1.462068000
H	-11.102060000	1.331895000	0.997947000
H	-11.164566000	0.938960000	3.449153000
H	11.093449000	0.440685000	-3.639747000
H	11.032047000	0.132399000	-1.176785000
H	10.974281000	-0.209807000	1.281607000
H	10.921536000	-0.592148000	3.729871000
H	-9.972743000	0.565476000	5.597585000
H	-7.848852000	0.330913000	6.863670000
H	-5.729311000	0.067118000	8.129264000
H	-3.615498000	-0.254477000	9.384732000
H	-1.510746000	-0.644470000	10.631337000

H	0.963539000	-0.846852000	10.656179000
H	3.129585000	-0.791634000	9.453905000
H	5.298764000	-0.768034000	8.250789000
H	7.467463000	-0.758670000	7.049883000
H	9.635228000	-0.792932000	5.847040000
H	-9.717380000	2.103741000	-6.047292000
H	-7.540855000	2.194352000	-7.239062000
H	-5.367077000	2.242531000	-8.439355000
H	-1.031632000	2.223212000	-10.855067000
H	1.446071000	2.076305000	-10.820299000
H	9.908746000	0.855418000	-5.784230000
H	-3.196191000	2.248384000	-9.643748000
H	5.682274000	1.574919000	-8.286608000
H	7.797093000	1.247891000	-7.030044000
H	3.563419000	1.845886000	-9.549410000
C	4.092014000	-1.855546000	-3.727964000
C	3.579196000	-1.979296000	-2.429287000
C	3.233249000	-1.685899000	-4.837020000
H	4.232430000	-2.103128000	-1.552375000
H	3.665460000	-1.574203000	-5.842379000
C	1.843190000	-1.642922000	-4.679704000
H	1.173532000	-1.502038000	-5.539645000
H	5.180969000	-1.878516000	-3.882412000
N	-0.047894000	-1.751344000	-3.053329000
C	-0.208529000	-1.873256000	-1.762000000
C	1.300498000	-1.769455000	-3.384265000
C	2.185667000	-1.932603000	-2.275336000
S	1.265335000	-2.050261000	-0.786310000
S	-1.765279000	-1.887487000	-0.937387000

C	-8.918442000	-1.762539000	-0.371422000
C	-8.308307000	-1.617489000	-1.625358000
C	-8.148187000	-1.957102000	0.794896000
H	-8.909855000	-1.455636000	-2.530573000
H	-8.653168000	-2.059623000	1.766309000
C	-6.751315000	-2.009679000	0.738618000
H	-6.157376000	-2.159367000	1.649650000
H	-10.014684000	-1.711326000	-0.297868000
N	-4.738704000	-1.884771000	-0.733364000
C	-4.468978000	-1.703050000	-1.997089000
C	-6.110327000	-1.863754000	-0.509033000
C	-6.907801000	-1.668133000	-1.678633000
S	-5.867458000	-1.501492000	-3.083506000
S	-2.882019000	-1.655833000	-2.746088000
C	-3.503380000	-2.239619000	2.532535000
S	0.642294000	-2.383395000	2.377778000
P	-1.103046000	-3.019800000	3.396144000
S	-1.185234000	-2.935679000	5.331674000
O	-2.073446000	-2.081481000	2.468600000
H	-3.791655000	-3.308480000	2.601804000
H	-3.912899000	-1.697585000	3.408176000
H	-3.891563000	-1.815525000	1.589602000
O	-1.430629000	-4.555479000	2.895119000
C	-1.438568000	-4.873685000	1.489173000
H	-2.312801000	-4.423624000	0.976811000
H	-0.505051000	-4.526052000	0.999029000
H	-1.497722000	-5.975391000	1.418106000
C	1.865218000	-2.809139000	3.674989000
H	1.809062000	-2.079345000	4.506726000

H	1.669049000	-3.817930000	4.087546000
N	4.381254000	-2.488232000	1.142283000
N	3.197898000	-2.784720000	3.078812000
N	3.264978000	-2.485287000	1.753707000
C	5.554202000	-2.792807000	1.824504000
C	5.561155000	-3.073945000	3.219255000
C	4.288133000	-3.057025000	3.933534000
O	4.099480000	-3.267967000	5.134043000
C	6.766981000	-2.819406000	1.097709000
H	6.745831000	-2.589419000	0.023272000
C	6.771634000	-3.374204000	3.875721000
C	7.955381000	-3.131336000	1.756755000
H	6.755814000	-3.581288000	4.954571000
H	8.900478000	-3.153767000	1.195251000
C	7.959977000	-3.407132000	3.143991000
H	8.907645000	-3.641794000	3.648704000

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C	-0.902794000	2.656662000	-9.676510000
C	0.462051000	2.777497000	-9.689693000
C	-5.120718000	1.820387000	-7.186384000
C	-3.725391000	2.018217000	-7.208885000
C	-3.016023000	2.271804000	-8.422237000
C	-1.628815000	2.417031000	-8.449027000
C	-0.874298000	2.319405000	-7.215524000
C	0.539182000	2.442910000	-7.229632000
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H	-10.876935000	1.026021000	-3.952889000
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H	-10.923381000	0.327256000	0.964769000
H	-10.956047000	-0.068051000	3.415226000
H	11.282053000	1.191467000	-3.665770000
H	11.246411000	0.899248000	-1.199108000
H	11.216143000	0.562454000	1.264396000
H	11.191226000	0.189171000	3.721145000
H	-9.741079000	-0.327141000	5.567470000
H	-7.607955000	-0.388575000	6.835234000
H	-5.475507000	-0.496785000	8.099242000
H	-3.343072000	-0.664642000	9.353748000
H	-1.215926000	-0.892586000	10.602100000

H	1.265457000	-0.875836000	10.636046000
H	3.423159000	-0.612039000	9.445816000
H	5.589071000	-0.397820000	8.250997000
H	7.756129000	-0.235174000	7.045160000
H	9.924596000	-0.105761000	5.837034000
H	-9.613831000	1.356513000	-6.065692000
H	-7.447867000	1.586191000	-7.260327000
H	-5.282580000	1.751225000	-8.465326000
H	-0.955344000	1.932792000	-10.893846000
H	1.526056000	1.917801000	-10.864351000
H	10.066725000	1.458976000	-5.815315000
H	-3.116853000	1.857784000	-9.676527000
H	5.792508000	1.735096000	-8.331171000
H	7.928492000	1.621727000	-7.069177000
H	3.656705000	1.827462000	-9.595801000
C	5.024653000	-1.766346000	-2.797624000
C	3.930318000	-1.882685000	-1.933386000
C	4.861585000	-1.823466000	-4.202611000
H	4.051981000	-1.833663000	-0.841918000
H	5.741181000	-1.702632000	-4.851194000
C	3.605572000	-2.035841000	-4.775295000
H	3.473399000	-2.093684000	-5.865271000
H	6.029585000	-1.619793000	-2.375437000
N	1.194747000	-2.474172000	-4.331895000
C	0.401356000	-2.589079000	-3.293861000
C	2.486603000	-2.193373000	-3.926684000
C	2.665605000	-2.085323000	-2.509603000
S	1.136211000	-2.322469000	-1.711308000
S	-1.241903000	-3.220906000	-3.443458000

C	-5.618030000	-2.804634000	2.721618000
C	-5.923918000	-2.644893000	1.366467000
C	-4.279129000	-2.771969000	3.181829000
H	-6.965105000	-2.657564000	1.016569000
H	-4.071235000	-2.890030000	4.255387000
C	-3.221644000	-2.578442000	2.294951000
H	-2.179479000	-2.511940000	2.629913000
H	-6.435023000	-2.947941000	3.443413000
N	-2.562703000	-2.201378000	-0.081070000
C	-3.137504000	-2.063528000	-1.257658000
C	-3.498607000	-2.427976000	0.916946000
C	-4.855775000	-2.462864000	0.470148000
S	-4.892357000	-2.236529000	-1.258748000
S	-2.435648000	-1.584534000	-2.807230000
P	0.640917000	-3.388232000	1.441949000
O	0.380684000	-4.511801000	0.474190000
O	2.178407000	-2.820572000	1.392999000
O	-0.260750000	-2.058637000	1.255819000
H	-1.048203000	-2.131723000	0.597113000
H	2.415326000	-2.481635000	2.288816000
C	0.436203000	-3.852467000	3.195106000
N	0.938785000	-2.813440000	4.083625000
H	0.551849000	-1.878975000	3.903793000
C	1.013041000	-3.142883000	5.493440000
C	-0.290620000	-3.229123000	6.291864000
O	-0.330523000	-3.562403000	7.461813000
O	-1.435596000	-2.908994000	5.632911000
H	-1.194047000	-2.593085000	4.735377000
H	1.041700000	-4.771628000	3.333505000

H 1.513264000 -4.125159000 5.617206000

H -0.627036000 -4.166422000 3.338737000

H 1.660312000 -2.416250000 6.025733000

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C	-1.053484000	2.941268000	-9.933150000
C	0.315160000	2.902368000	-9.987664000
C	-5.262486000	2.669108000	-7.300665000
C	-3.854369000	2.688699000	-7.371477000
C	-3.157740000	2.826431000	-8.611041000
C	-1.764253000	2.815129000	-8.680020000
C	-0.986951000	2.665278000	-7.465958000
C	0.430274000	2.624257000	-7.522460000
C	1.115195000	2.732665000	-8.794899000
C	2.508102000	2.663082000	-8.837006000
C	3.291817000	2.476838000	-7.657211000
C	4.696806000	2.366214000	-7.699971000
C	-9.479235000	2.232600000	-4.697918000
C	-8.038458000	2.299043000	-4.779428000
C	-7.367854000	2.467524000	-5.995995000
C	-5.946405000	2.515135000	-6.070941000
C	-5.180547000	2.395439000	-4.851395000
C	-3.754303000	2.424768000	-4.900151000
C	-3.084935000	2.557325000	-6.153808000
C	-1.660077000	2.549158000	-6.207378000
C	-0.898830000	2.411713000	-5.001105000
C	0.525161000	2.367320000	-5.058020000
C	1.193937000	2.463352000	-6.321324000
C	2.616279000	2.384282000	-6.381947000
C	3.374424000	2.196056000	-5.186848000
C	4.794610000	2.071879000	-5.253347000
C	5.465112000	2.152123000	-6.530662000

C	6.879712000	1.993401000	-6.573324000
C	7.630111000	1.745206000	-5.418688000
C	9.058989000	1.537950000	-5.461501000
C	-10.121026000	2.056109000	-3.498356000
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C	-7.277429000	2.181943000	-3.554993000
C	-5.849975000	2.238994000	-3.600990000
C	-5.090496000	2.128318000	-2.389703000
C	-3.662795000	2.166612000	-2.436041000
C	-2.993331000	2.306872000	-3.689904000
C	-1.568400000	2.302589000	-3.741173000
C	1.285481000	2.207903000	-3.855689000
C	2.706883000	2.112644000	-3.919712000
C	3.463925000	1.907210000	-2.725621000
C	4.883675000	1.762372000	-2.796832000
C	5.549656000	1.846342000	-4.063338000
C	6.965663000	1.671305000	-4.136367000
C	7.712085000	1.393263000	-2.956416000
C	9.135707000	1.161216000	-3.034983000
C	9.775106000	1.254102000	-4.326343000
C	-10.027652000	1.747151000	-1.028716000
C	-9.298345000	1.622594000	0.184896000
C	-7.858692000	1.698578000	0.145359000
C	-7.189241000	1.893354000	-1.100377000
C	-5.759201000	1.958983000	-1.141777000
C	-5.002313000	1.825772000	0.063741000
C	-3.575692000	1.856112000	0.017964000
C	-2.904456000	2.027938000	-1.232107000

C	-1.476954000	2.027352000	-1.282738000
C	-0.718117000	1.850019000	-0.082962000
C	0.705840000	1.799538000	-0.140564000
C	1.375396000	1.926058000	-1.398016000
C	2.797177000	1.810848000	-1.464834000
C	3.550681000	1.552497000	-0.277658000
C	4.966406000	1.382347000	-0.353990000
C	5.633950000	1.497091000	-1.613388000
C	7.050346000	1.303057000	-1.693073000
C	7.792034000	0.974096000	-0.518837000
C	9.209447000	0.729277000	-0.608259000
C	9.847499000	0.836025000	-1.873591000
C	-9.942285000	1.418586000	1.435510000
C	-9.217454000	1.277167000	2.625828000
C	-7.774174000	1.342775000	2.593215000
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C	-4.919269000	1.453442000	2.507380000
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C	-1.390631000	1.675110000	1.166998000
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C	0.790282000	1.387957000	2.299558000
C	1.461117000	1.555414000	1.049583000
C	2.881486000	1.420546000	0.979176000
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C	7.861437000	0.466298000	1.902978000
C	9.283193000	0.228007000	1.805328000
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C	-9.139720000	0.898434000	5.052467000
C	-7.695877000	0.942589000	5.048703000
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C	-5.593056000	1.223021000	3.751587000
C	-4.837945000	1.020875000	4.945740000
C	-3.411029000	1.035101000	4.901241000
C	-2.734905000	1.266656000	3.656945000
C	-1.309076000	1.255818000	3.606861000
C	-0.554803000	0.990292000	4.794602000
C	0.867198000	0.894625000	4.729678000
C	1.542190000	1.090884000	3.481667000
C	2.957668000	0.931135000	3.405133000
C	3.702326000	0.564851000	4.575801000
C	5.112043000	0.361433000	4.488653000
C	5.783924000	0.531971000	3.241406000
C	7.192922000	0.309734000	3.150693000
C	7.932770000	-0.085844000	4.328830000
C	9.353981000	-0.308703000	4.201718000
C	9.997060000	-0.159258000	2.999358000
C	-6.941772000	0.757310000	6.212742000
C	-5.517935000	0.780335000	6.197744000
C	-4.750477000	0.555264000	7.365439000
C	-3.341086000	0.541997000	7.337954000
C	-2.656825000	0.789418000	6.088002000
C	-1.232176000	0.754237000	6.035263000

C	-0.477626000	0.436628000	7.211184000
C	0.934846000	0.321721000	7.141692000
C	1.614550000	0.539991000	5.899894000
C	3.028367000	0.373095000	5.818999000
C	3.778465000	-0.015992000	6.992589000
C	5.170018000	-0.212290000	6.885603000
C	5.856849000	-0.035850000	5.661020000
C	7.259748000	-0.247705000	5.544667000
C	-2.562924000	0.265108000	8.503293000
C	-1.170307000	0.196709000	8.461415000
C	-0.380859000	-0.132814000	9.627333000
C	0.982342000	-0.250295000	9.558729000
C	1.697127000	-0.044179000	8.318757000
C	3.079415000	-0.203332000	8.223733000
C	0.617946000	2.114764000	-2.594348000
C	-0.808118000	2.162773000	-2.537203000
H	-11.220066000	2.002201000	-3.457870000
H	-11.127201000	1.690135000	-0.995822000
H	-11.042018000	1.363594000	1.465489000
H	-10.964132000	1.014298000	3.922423000
H	10.861133000	1.082662000	-4.383443000
H	10.930170000	0.646463000	-1.941651000
H	11.003899000	0.175108000	0.493730000
H	11.080255000	-0.339350000	2.921838000
H	-9.651645000	0.725833000	6.011224000
H	-7.458554000	0.573896000	7.167163000
H	-5.268880000	0.364313000	8.317379000
H	-3.083843000	0.075757000	9.454334000
H	-0.906997000	-0.304451000	10.578730000

H	1.562996000	-0.518670000	10.454362000
H	3.651332000	-0.494675000	9.117978000
H	5.737707000	-0.517114000	7.777886000
H	7.824930000	-0.554663000	6.437968000
H	9.914777000	-0.610317000	5.099268000
H	-10.056386000	2.324476000	-5.630387000
H	-7.950428000	2.560819000	-6.925327000
H	-5.846037000	2.768620000	-8.228592000
H	-1.642959000	3.068305000	-10.853981000
H	0.836113000	2.996771000	-10.952695000
H	9.565270000	1.601302000	-6.436799000
H	-3.742067000	2.938243000	-9.537255000
H	5.210414000	2.433486000	-8.671190000
H	7.391275000	2.051584000	-7.546324000
H	3.023513000	2.743228000	-9.806452000
C	7.167788000	-2.006812000	-2.049575000
C	6.416459000	-2.107081000	-0.869850000
C	6.546623000	-1.739949000	-3.288692000
H	6.904727000	-2.303611000	0.094886000
H	7.163704000	-1.649308000	-4.194642000
C	5.159540000	-1.576225000	-3.381841000
H	4.670136000	-1.360429000	-4.341857000
H	8.260612000	-2.122777000	-2.001172000
N	2.999416000	-1.545621000	-2.139334000
C	2.585870000	-1.671665000	-0.908990000
C	4.379504000	-1.680517000	-2.212536000
C	5.027002000	-1.938838000	-0.964734000
S	3.832614000	-1.994846000	0.323384000
S	0.922013000	-1.576540000	-0.361639000

C	-6.136286000	-1.497763000	-0.476861000
C	-5.426504000	-1.368801000	-1.679939000
C	-5.460337000	-1.651565000	0.753299000
H	-5.954690000	-1.231757000	-2.634481000
H	-6.042067000	-1.740054000	1.682603000
C	-4.062697000	-1.685500000	0.812257000
H	-3.530128000	-1.820548000	1.762305000
H	-7.235823000	-1.461296000	-0.495073000
N	-1.942762000	-1.544971000	-0.491496000
C	-1.574402000	-1.386586000	-1.733006000
C	-3.326134000	-1.556969000	-0.381953000
C	-4.025767000	-1.401561000	-1.618073000
S	-2.873137000	-1.241377000	-2.934841000
S	0.084769000	-1.298541000	-2.302128000
C	1.639254000	-5.142056000	2.390456000
O	0.924539000	-5.698466000	3.215225000
O	2.841135000	-4.595289000	2.649541000
C	3.278230000	-4.466388000	4.028322000
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H	4.171683000	-5.111631000	4.145634000
C	3.602937000	-3.008767000	4.292020000
H	2.713922000	-2.365253000	4.136452000
H	4.409003000	-2.647130000	3.623428000
H	3.939321000	-2.880620000	5.340210000
C	1.266873000	-4.953418000	0.935678000
H	1.853037000	-4.109273000	0.527923000
H	1.562122000	-5.853729000	0.358864000
C	-0.231035000	-4.684649000	0.743521000
H	-0.345366000	-4.154440000	-0.231675000

C	-0.847764000	-3.771432000	1.802830000
O	-2.017127000	-3.772586000	2.145824000
O	0.083177000	-2.934566000	2.292013000
C	-0.340714000	-1.999060000	3.315415000
H	0.436576000	-1.215355000	3.288223000
H	-1.304109000	-1.552204000	3.002553000
C	-0.433151000	-2.651247000	4.681389000
H	0.535796000	-3.091742000	4.987330000
H	-1.206250000	-3.443603000	4.696643000
H	-0.712694000	-1.888015000	5.434451000
S	-1.234689000	-6.216703000	0.587836000
P	-2.293614000	-5.721282000	-1.198458000
S	-1.267698000	-4.845072000	-2.596824000
O	-2.946921000	-7.193109000	-1.513506000
C	-2.128764000	-8.220426000	-2.105128000
H	-1.758844000	-7.900141000	-3.099897000
H	-1.264521000	-8.468948000	-1.454934000
H	-2.774234000	-9.110765000	-2.216026000
O	-3.626004000	-4.875621000	-0.815431000
C	-4.454530000	-5.232696000	0.312055000
H	-4.793790000	-6.285185000	0.237574000
H	-3.899207000	-5.068234000	1.255683000
H	-5.328296000	-4.557319000	0.271468000

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C	-1.420827000	1.788279000	-9.511621000
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C	-5.522480000	2.379807000	-6.765925000
C	-4.123699000	2.239854000	-6.873661000
C	-3.469376000	2.101861000	-8.135952000
C	-2.087144000	1.942049000	-8.237293000
C	-1.277490000	1.918709000	-7.035326000
C	0.126973000	1.734721000	-7.120824000
C	0.765752000	1.566906000	-8.410893000
C	2.144263000	1.361580000	-8.477267000
C	2.956911000	1.299883000	-7.303902000
C	4.346298000	1.066770000	-7.365626000
C	-9.649368000	2.827608000	-4.027194000
C	-8.214368000	2.719887000	-4.152343000
C	-7.580833000	2.621824000	-5.395989000
C	-6.166611000	2.501046000	-5.511392000
C	-5.367908000	2.492139000	-4.307205000
C	-3.949251000	2.358379000	-4.395231000
C	-3.321195000	2.226473000	-5.670294000
C	-1.906482000	2.070192000	-5.757687000
C	-1.112905000	2.048266000	-4.564758000
C	0.297724000	1.862459000	-4.650509000
C	0.921700000	1.698732000	-5.929575000
C	2.327089000	1.471581000	-6.013572000
C	3.112274000	1.397273000	-4.823826000
C	4.515809000	1.149757000	-4.907154000
C	5.142844000	0.984554000	-6.198327000

C	6.544060000	0.734717000	-6.253255000
C	7.323668000	0.635741000	-5.095343000
C	8.742242000	0.366842000	-5.142884000
C	-10.257504000	2.898837000	-2.799538000
C	-9.491820000	2.864654000	-1.575308000
C	-8.053043000	2.770728000	-1.669450000
C	-7.420515000	2.703915000	-2.943403000
C	-5.998775000	2.597078000	-3.032336000
C	-5.208519000	2.561274000	-1.837065000
C	-3.788047000	2.431163000	-1.923502000
C	-3.155770000	2.336366000	-3.200722000
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C	4.676004000	1.216253000	-2.435009000
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C	7.477938000	0.681665000	-2.610665000
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C	-9.341429000	2.854099000	0.887014000
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H	6.670151000	-2.084472000	-0.042073000
H	5.963588000	-1.596762000	-4.304340000
C	4.177230000	-1.647980000	-3.084503000
H	3.479644000	-1.518801000	-3.923776000
H	7.535017000	-1.871163000	-2.383119000
N	2.335726000	-1.762349000	-1.412453000
C	2.189800000	-1.925121000	-0.123093000
C	3.674655000	-1.761908000	-1.772269000
C	4.587266000	-1.924462000	-0.686441000
S	3.692393000	-2.083595000	0.818726000
S	0.635464000	-1.979838000	0.702349000

C	-6.366971000	-1.882271000	1.563926000
C	-5.847244000	-1.840236000	0.261542000
C	-5.515000000	-1.895136000	2.689651000
H	-6.515502000	-1.822553000	-0.610918000
H	-5.953082000	-1.919750000	3.698037000
C	-4.123913000	-1.861219000	2.541651000
H	-3.451892000	-1.856755000	3.411862000
H	-7.457664000	-1.895488000	1.706497000
N	-2.225422000	-1.761758000	0.936174000
C	-2.030873000	-1.717867000	-0.354545000
C	-3.575316000	-1.814668000	1.243496000
C	-4.452571000	-1.809113000	0.114416000
S	-3.504740000	-1.752898000	-1.364741000
S	-0.477178000	-1.619147000	-1.159561000
P	-0.564642000	-6.726892000	-0.934931000
S	-0.718311000	-8.582111000	-0.390858000
S	-1.052419000	-5.208084000	0.469574000
O	-1.518624000	-6.351035000	-2.208024000
C	-2.043446000	-5.023603000	-2.523242000
H	-1.404805000	-4.241197000	-2.064076000
H	-3.051041000	-4.949888000	-2.064870000
C	-2.109231000	-4.870517000	-4.024701000
H	-2.740743000	-5.657195000	-4.482532000
H	-1.100064000	-4.912636000	-4.481304000
H	-2.554065000	-3.885339000	-4.271732000
O	0.983844000	-6.413721000	-1.374623000
C	1.361544000	-5.178412000	-2.043740000
H	0.892707000	-4.313349000	-1.525487000
H	0.971157000	-5.210465000	-3.082460000

C	2.870248000	-5.090578000	-2.029239000
H	3.315709000	-6.023002000	-2.429310000
H	3.261161000	-4.922649000	-1.005392000
H	3.205490000	-4.251607000	-2.666988000
C	0.478499000	-5.262196000	1.496106000
H	1.311441000	-4.855215000	0.888998000
H	0.716070000	-6.310030000	1.762390000
C	0.205799000	-4.402455000	2.735109000
H	-0.634917000	-3.703701000	2.545925000
H	-0.049654000	-5.026981000	3.613430000
S	1.677279000	-3.381063000	3.111829000
C	1.096884000	-2.486781000	4.609613000
H	1.236838000	-3.167779000	5.474307000
H	1.831908000	-1.662633000	4.717590000
C	-0.327887000	-1.960648000	4.544561000
H	-1.070988000	-2.780723000	4.503869000
H	-0.486484000	-1.302853000	3.668474000
H	-0.541798000	-1.378611000	5.462553000

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C	-0.425063000	1.245014000	-10.001546000
C	0.943475000	1.297488000	-9.956109000
C	-4.806249000	1.099914000	-7.653015000
C	-3.399330000	1.193103000	-7.629252000
C	-2.616602000	1.190724000	-8.824495000
C	-1.223270000	1.261058000	-8.795575000
C	-0.535573000	1.345391000	-7.522741000
C	0.881701000	1.401243000	-7.475681000
C	1.656510000	1.372613000	-8.700133000
C	3.049815000	1.410640000	-8.636837000
C	3.748823000	1.477520000	-7.392742000
C	5.156934000	1.496660000	-7.323475000
C	-9.184552000	0.782677000	-5.310161000
C	-7.746806000	0.922911000	-5.301584000
C	-6.994174000	0.964433000	-6.480720000
C	-5.574786000	1.082411000	-6.464191000
C	-4.899666000	1.175567000	-5.190275000
C	-3.476890000	1.281913000	-5.144966000
C	-2.720326000	1.284141000	-6.355642000
C	-1.297148000	1.362539000	-6.309806000
C	-0.625097000	1.449172000	-5.047605000
C	0.798788000	1.509335000	-5.000450000
C	1.557521000	1.479487000	-6.215477000
C	2.982122000	1.518507000	-6.167006000
C	3.654426000	1.589534000	-4.909697000
C	5.080789000	1.607157000	-4.861151000
C	5.843555000	1.553121000	-6.086933000

C	7.265520000	1.547176000	-6.010504000
C	7.939313000	1.581064000	-4.784575000
C	9.380920000	1.552679000	-4.698881000
C	-9.905562000	0.720810000	-4.144714000
C	-9.262331000	0.796333000	-2.853857000
C	-7.826315000	0.951887000	-2.813301000
C	-7.076528000	1.011585000	-4.023173000
C	-5.654246000	1.145913000	-3.979006000
C	-4.984667000	1.238785000	-2.714608000
C	-3.561428000	1.363491000	-2.667681000
C	-2.805751000	1.375071000	-3.880656000
C	-1.383003000	1.462423000	-3.833567000
C	1.470893000	1.587046000	-3.739723000
C	2.895395000	1.628424000	-3.693278000
C	3.567937000	1.682688000	-2.434422000
C	4.996253000	1.691229000	-2.387650000
C	5.753409000	1.654812000	-3.604301000
C	7.180897000	1.633032000	-3.554379000
C	7.851364000	1.634047000	-2.298224000
C	9.294321000	1.585899000	-2.243622000
C	10.026186000	1.555479000	-3.488300000
C	-9.981845000	0.712803000	-1.654683000
C	-9.340304000	0.777018000	-0.387774000
C	-7.909339000	0.948273000	-0.338053000
C	-7.160041000	1.033692000	-1.550984000
C	-5.736629000	1.188170000	-1.503184000
C	-5.068467000	1.268362000	-0.241255000
C	-3.648235000	1.404315000	-0.193803000
C	-2.893242000	1.450266000	-1.407339000

C	-1.468548000	1.538445000	-1.360165000
C	-0.796239000	1.581838000	-0.099150000
C	0.629230000	1.638435000	-0.053070000
C	1.384776000	1.658803000	-1.267090000
C	2.812170000	1.694061000	-1.221043000
C	3.485805000	1.696917000	0.039618000
C	4.912533000	1.684128000	0.084607000
C	5.667652000	1.691881000	-1.130026000
C	7.098488000	1.655778000	-1.083460000
C	7.770399000	1.608969000	0.175446000
C	9.210850000	1.561832000	0.221731000
C	9.937929000	1.557736000	-0.999592000
C	-10.061870000	0.665098000	0.831734000
C	-9.421112000	0.709548000	2.076787000
C	-7.988202000	0.886600000	2.134984000
C	-7.241825000	1.011888000	0.922488000
C	-5.819796000	1.174460000	0.972242000
C	-5.149722000	1.202823000	2.230331000
C	-3.726793000	1.327077000	2.279325000
C	-2.975731000	1.434905000	1.067349000
C	-1.550672000	1.523282000	1.114513000
C	-0.875941000	1.500709000	2.373265000
C	0.550436000	1.551577000	2.419360000
C	1.303917000	1.630759000	1.207547000
C	2.730894000	1.653737000	1.253400000
C	3.405614000	1.587644000	2.511428000
C	4.834321000	1.575052000	2.555893000
C	5.586474000	1.623582000	1.344460000
C	7.017918000	1.588586000	1.389286000

C	7.690187000	1.520169000	2.649159000
C	9.134180000	1.486453000	2.686742000
C	9.856862000	1.509242000	1.486822000
C	-10.145110000	0.570850000	3.318767000
C	-9.500518000	0.590289000	4.529521000
C	-8.067896000	0.751790000	4.618250000
C	-7.318812000	0.911034000	3.391505000
C	-5.899507000	1.064627000	3.444326000
C	-5.224190000	1.044778000	4.700451000
C	-3.802234000	1.157610000	4.750818000
C	-3.050959000	1.302109000	3.537448000
C	-1.628148000	1.384588000	3.584753000
C	-0.949907000	1.322018000	4.843143000
C	0.474404000	1.374608000	4.890036000
C	1.227284000	1.485672000	3.677823000
C	2.652793000	1.505456000	3.723423000
C	3.331062000	1.424150000	4.984758000
C	4.757932000	1.426654000	5.028063000
C	5.510967000	1.496252000	3.817468000
C	6.939478000	1.476063000	3.859073000
C	7.616345000	1.399081000	5.134697000
C	9.060708000	1.379020000	5.140820000
C	9.782948000	1.420509000	3.975281000
C	-7.392355000	0.743019000	5.843559000
C	-5.977161000	0.880300000	5.922364000
C	-5.286750000	0.845922000	7.157503000
C	-3.882685000	0.951786000	7.228381000
C	-3.124466000	1.104197000	6.006107000
C	-1.701681000	1.186300000	6.055374000

C	-1.019742000	1.119211000	7.313005000
C	0.397427000	1.176722000	7.359954000
C	1.153280000	1.297418000	6.149294000
C	2.578348000	1.327469000	6.193972000
C	3.264369000	1.244873000	7.464402000
C	4.674261000	1.260284000	7.486640000
C	5.440086000	1.343745000	6.298921000
C	6.864318000	1.338495000	6.313369000
C	-3.178851000	0.901630000	8.470447000
C	-1.787410000	0.980658000	8.534478000
C	-1.068810000	0.918717000	9.787955000
C	0.299461000	0.976670000	9.833398000
C	1.091664000	1.100878000	8.629807000
C	2.486196000	1.139323000	8.657884000
C	0.713289000	1.606188000	-2.526405000
C	-0.712363000	1.544154000	-2.572825000
H	-11.000070000	0.604679000	-4.174584000
H	-11.075123000	0.584738000	-1.691586000
H	-11.153939000	0.528052000	0.791881000
H	-11.237118000	0.438826000	3.271730000
H	11.126074000	1.526045000	-3.444091000
H	11.038230000	1.519759000	-0.962279000
H	10.957435000	1.476757000	1.521556000
H	10.883614000	1.399319000	4.003549000
H	-10.068796000	0.474404000	5.464719000
H	-7.964913000	0.616076000	6.775132000
H	-5.861309000	0.722130000	8.088138000
H	-3.755512000	0.789099000	9.401394000
H	-1.651881000	0.817381000	10.716082000

H	0.826339000	0.921685000	10.798281000
H	3.007849000	1.075951000	9.625244000
H	5.194906000	1.193805000	8.454164000
H	7.383973000	1.275048000	7.281749000
H	9.575715000	1.324067000	6.111857000
H	-9.694584000	0.718363000	-6.283210000
H	-7.508625000	0.893729000	-7.451337000
H	-5.321389000	1.027837000	-8.623050000
H	-0.947081000	1.183408000	-10.968665000
H	1.531499000	1.279378000	-10.886519000
H	9.956306000	1.521293000	-5.636419000
H	-3.132941000	1.122228000	-9.794326000
H	5.738740000	1.458715000	-8.257104000
H	7.846012000	1.504886000	-6.944895000
H	3.632399000	1.383167000	-9.570521000
C	6.550236000	-1.637407000	-1.988089000
C	5.693930000	-1.609260000	-0.878729000
C	6.037722000	-1.706780000	-3.302486000
H	6.092984000	-1.545138000	0.143500000
H	6.733708000	-1.712885000	-4.153997000
C	4.660201000	-1.755072000	-3.541515000
H	4.255592000	-1.803955000	-4.562178000
H	7.637472000	-1.590941000	-1.827817000
N	2.391768000	-1.767558000	-2.510457000
C	1.873349000	-1.722838000	-1.314770000
C	3.775388000	-1.725809000	-2.444037000
C	4.312856000	-1.651070000	-1.120456000
S	3.005143000	-1.636689000	0.047415000
S	0.125241000	-1.742241000	-1.137238000

C	-6.367583000	-2.310330000	1.847606000
C	-5.523545000	-2.190219000	0.735988000
C	-5.852104000	-2.279611000	3.162692000
H	-5.926141000	-2.215229000	-0.286019000
H	-6.542576000	-2.359033000	4.015109000
C	-4.481911000	-2.139424000	3.400723000
H	-4.075687000	-2.111118000	4.421508000
H	-7.450772000	-2.418460000	1.689298000
N	-2.229485000	-1.904104000	2.365688000
C	-1.717913000	-1.823327000	1.170185000
C	-3.607959000	-2.024525000	2.300678000
C	-4.148648000	-2.048729000	0.976488000
S	-2.853286000	-1.881306000	-0.194195000
S	0.017647000	-1.611831000	0.988697000
P	2.460931000	-5.814210000	0.734707000
S	1.953613000	-7.375670000	1.745526000
O	1.210148000	-4.853119000	0.180097000
C	-0.130985000	-5.046257000	0.412899000
C	-0.649247000	-5.047426000	1.721907000
C	-0.976718000	-5.172411000	-0.704349000
C	-2.028369000	-5.147096000	1.914472000
C	-2.356458000	-5.267073000	-0.515134000
C	-2.866858000	-5.246130000	0.792937000
H	0.022120000	-4.942578000	2.584232000
H	-0.541033000	-5.178210000	-1.712446000
H	-2.462551000	-5.130609000	2.921821000
H	-3.041985000	-5.349204000	-1.367749000
N	-4.317586000	-5.301544000	0.991877000
O	-5.043209000	-5.306142000	-0.010288000

O	-4.749720000	-5.329947000	2.148775000
O	3.282387000	-6.132694000	-0.615850000
C	3.692546000	-5.078375000	-1.520413000
H	2.808187000	-4.533534000	-1.904159000
H	4.387180000	-4.381124000	-1.014309000
H	4.207750000	-5.577889000	-2.360063000
O	3.423832000	-4.699473000	1.422944000
C	3.001910000	-4.041067000	2.631463000
H	2.094969000	-3.427064000	2.451738000
H	2.802068000	-4.781437000	3.432374000
H	3.833002000	-3.380908000	2.939010000

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C	-0.113161000	-1.467728000	-9.805497000
C	1.235621000	-1.234387000	-9.739290000
C	-4.570040000	-1.588715000	-7.605377000
C	-3.193218000	-1.283059000	-7.579780000
C	-2.347542000	-1.496048000	-8.711405000
C	-0.977898000	-1.230724000	-8.670618000
C	-0.382516000	-0.716100000	-7.453336000
C	1.014619000	-0.476794000	-7.383976000
C	1.859661000	-0.740902000	-8.531384000
C	3.236053000	-0.530541000	-8.438550000
C	3.849889000	-0.063510000	-7.235929000
C	5.245013000	0.110274000	-7.125025000
C	-8.990550000	-1.936849000	-5.343909000
C	-7.586153000	-1.597612000	-5.343045000
C	-6.780682000	-1.747959000	-6.477976000
C	-5.394522000	-1.419022000	-6.466791000
C	-4.809388000	-0.911273000	-5.246865000
C	-3.420807000	-0.582629000	-5.205236000
C	-2.606643000	-0.767458000	-6.362527000
C	-1.210907000	-0.477187000	-6.308964000
C	-0.626560000	0.012788000	-5.096939000
C	0.774956000	0.262693000	-5.030334000
C	1.601963000	0.010021000	-6.171369000
C	3.011036000	0.217124000	-6.091500000
C	3.599374000	0.679150000	-4.875694000
C	5.013938000	0.844622000	-4.782137000
C	5.850292000	0.545933000	-5.921776000

C	7.262661000	0.676563000	-5.789534000
C	7.858878000	1.073486000	-4.587206000
C	9.291752000	1.181949000	-4.438471000
C	-9.764982000	-1.790201000	-4.220662000
C	-9.213631000	-1.288387000	-2.983272000
C	-7.811649000	-0.939278000	-2.952472000
C	-7.006560000	-1.091688000	-4.118312000
C	-5.619044000	-0.749671000	-4.082227000
C	-5.037716000	-0.250246000	-2.870397000
C	-3.649449000	0.086585000	-2.830067000
C	-2.838137000	-0.083932000	-3.993128000
C	-1.445843000	0.217158000	-3.942479000
C	1.363403000	0.726758000	-3.812396000
C	2.770547000	0.938749000	-3.734345000
C	3.362694000	1.369938000	-2.507375000
C	4.779451000	1.529257000	-2.413509000
C	5.606805000	1.263372000	-3.553570000
C	7.027053000	1.372589000	-3.442678000
C	7.621325000	1.742358000	-2.201872000
C	9.058802000	1.829456000	-2.079413000
C	9.863162000	1.542680000	-3.244302000
C	-9.989491000	-1.136467000	-1.826282000
C	-9.438284000	-0.646445000	-0.610520000
C	-8.039474000	-0.298036000	-0.570761000
C	-7.234060000	-0.445051000	-1.741512000
C	-5.843856000	-0.100885000	-1.702448000
C	-5.262660000	0.384056000	-0.489210000
C	-3.874845000	0.717522000	-0.447086000
C	-3.068042000	0.571088000	-1.617939000

C	-1.674370000	0.877798000	-1.568349000
C	-1.087206000	1.334337000	-0.346794000
C	0.314255000	1.592216000	-0.282186000
C	1.131828000	1.389167000	-1.438374000
C	2.541872000	1.599825000	-1.360287000
C	3.135684000	2.004707000	-0.124504000
C	4.551639000	2.156144000	-0.029940000
C	5.373867000	1.910423000	-1.174030000
C	6.798234000	2.013935000	-1.064698000
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C	8.830582000	2.447696000	0.298535000
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C	4.331589000	2.743707000	2.364093000
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