

DFT-Based Mechanistic Study of Bifunctional Al-Porphyrin Catalyst for CO₂/PO and TsNCO Polymerizations toward Polycarbonates and Polyurethanes

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S1. Second-order NBO perturbation analysis of LP(O/N) → σ*(C–O) interactions in backbiting TS3a.

Table S1. Second-order NBO perturbation energies (E(2)) for LP(O/N) → σ*(C–O) donor–acceptor interactions in the relevant backbiting transition states (TS3a), computed at the ωB97XD/6-311G(d,p) level of theory.

Transition State	Donor NBO (i)	Acceptor NBO (j)	E(2), kcal/mol
TS3b_CO ₂	LP(O) on chain end (O114)	σ*(C–O) of carbonate (C113–O115)	9.43
TS3b_TsN	LP(N) on TsN-substituted chain end (N120)	σ*(C–O) of imidocarbonate/carbamate (C113–O114)	1.17

S2. Atomic coordinates (XYZ format) for all optimized structures

R

C	1.739000	1.395000	-1.249000
C	0.768000	1.595000	-2.296000
N	2.209000	0.105000	-1.291000
C	1.561000	-0.500000	-2.335000
C	0.654000	0.419000	-2.960000
C	2.140000	2.380000	-0.341000
H	0.250000	2.522000	-2.493000
C	5.554000	0.355000	2.448000
C	3.102000	2.170000	0.653000
H	0.024000	0.184000	-3.808000
N	3.812000	1.013000	0.848000
C	3.469000	3.144000	1.650000
C	4.635000	1.248000	1.917000
C	4.422000	2.573000	2.427000
C	5.778000	-0.936000	2.000000
N	5.107000	-1.539000	0.973000
C	5.616000	-2.803000	0.881000
C	6.741000	-1.843000	2.569000
C	6.643000	-3.002000	1.871000
C	1.747000	-1.808000	-2.759000
C	2.627000	-2.719000	-2.200000
N	3.465000	-2.461000	-1.150000
C	4.188000	-3.607000	-0.955000
C	2.804000	-4.071000	-2.661000
C	3.772000	-4.622000	-1.887000
C	5.193000	-3.773000	-0.015000
O	2.388000	-1.334000	1.179000
C	1.243000	-0.570000	1.654000
C	1.055000	-1.856000	0.991000

C	1.182000	-0.366000	3.134000
H	3.040000	4.131000	1.738000
H	4.940000	2.997000	3.277000
H	7.398000	-1.605000	3.395000
H	7.201000	-3.919000	2.004000
H	2.254000	-4.520000	-3.477000
H	4.186000	-5.621000	-1.934000
C	-6.252000	2.613000	-0.318000
C	-4.743000	2.737000	-0.509000
C	-4.134000	4.122000	-0.264000
C	-2.633000	3.914000	-0.168000
C	1.478000	3.715000	-0.422000
C	0.097000	3.790000	-0.211000
C	-0.570000	5.010000	-0.350000
C	0.157000	6.168000	-0.644000
C	1.531000	6.090000	-0.825000
C	2.199000	4.869000	-0.731000
C	-10.640000	-2.707000	-0.871000
C	-9.221000	-2.466000	-1.381000
C	-8.282000	-1.987000	-0.268000
H	-3.875000	-0.951000	1.879000
C	-5.709000	-2.013000	1.346000
C	-4.706000	-1.477000	2.363000
C	-4.112000	-2.599000	3.218000
C	-3.065000	-2.050000	4.186000
H	-4.904000	-3.125000	3.766000
H	-2.583000	-2.854000	4.749000
O	-1.917000	5.140000	-0.234000
H	-0.429000	2.879000	0.058000
H	3.268000	4.808000	-0.907000
H	2.089000	6.991000	-1.065000

H	-0.372000	7.110000	-0.741000
C	-6.719000	1.176000	-0.599000
C	-6.305000	0.225000	0.531000
N	-5.864000	-1.161000	0.102000
C	-4.539000	-1.035000	-0.650000
C	-1.500000	-3.226000	-1.583000
C	-2.411000	-2.002000	-1.530000
C	-3.698000	-2.299000	-0.751000
H	-0.565000	-2.999000	-2.104000
H	-2.656000	-1.673000	-2.548000
H	-3.405000	-2.635000	0.249000
H	-6.284000	0.872000	-1.556000
H	-7.806000	1.138000	-0.728000
H	-7.125000	0.088000	1.239000
H	-5.459000	0.629000	1.088000
C	-6.873000	-1.810000	-0.819000
H	-6.536000	2.909000	0.701000
H	-6.775000	3.294000	-0.999000
H	-4.218000	2.029000	0.145000
H	-4.494000	2.426000	-1.534000
H	-4.519000	4.562000	0.663000
H	-4.377000	4.808000	-1.083000
H	-2.307000	3.267000	-0.994000
H	-2.393000	3.383000	0.760000
H	-8.825000	-3.390000	-1.820000
H	-8.666000	-1.043000	0.135000
H	-11.067000	-1.791000	-0.449000
H	-11.294000	-3.042000	-1.681000
H	-10.652000	-3.475000	-0.089000
H	-9.239000	-1.719000	-2.185000
H	-8.297000	-2.719000	0.546000

H	-5.431000	-3.008000	0.995000
H	-6.702000	-2.089000	1.791000
H	-5.194000	-0.743000	3.015000
H	-3.642000	-3.341000	2.558000
H	-3.520000	-1.359000	4.904000
H	-2.298000	-1.496000	3.633000
H	-3.944000	-0.269000	-0.144000
H	-4.791000	-0.668000	-1.647000
H	-1.983000	-4.064000	-2.100000
H	-1.241000	-3.562000	-0.572000
H	-1.897000	-1.171000	-1.032000
H	-4.245000	-3.121000	-1.231000
H	-6.450000	-2.778000	-1.098000
H	-6.906000	-1.195000	-1.720000
H	1.038000	0.304000	1.046000
H	0.864000	-2.751000	1.576000
H	0.719000	-1.872000	-0.042000
H	0.200000	0.051000	3.379000
H	1.330000	-1.304000	3.677000
H	1.160000	-2.139000	-3.610000
H	6.149000	0.700000	3.288000
H	5.687000	-4.739000	0.022000
H	1.952000	0.349000	3.440000
Al	3.744000	-0.679000	-0.244000
Br	5.425000	0.058000	-1.827000
Br	-1.876000	0.617000	1.176000

TS1

C	1.913000	1.465000	-1.432000
C	1.018000	1.693000	-2.539000
N	2.371000	0.176000	-1.465000

C	1.799000	-0.411000	-2.559000
C	0.956000	0.532000	-3.240000
C	2.269000	2.435000	-0.486000
H	0.521000	2.628000	-2.752000
C	5.434000	0.331000	2.528000
C	3.206000	2.229000	0.531000
H	0.396000	0.322000	-4.143000
N	3.850000	1.048000	0.794000
C	3.593000	3.223000	1.504000
C	4.634000	1.272000	1.889000
C	4.488000	2.632000	2.334000
C	5.554000	-1.003000	2.176000
N	4.905000	-1.604000	1.138000
C	5.297000	-2.911000	1.144000
C	6.382000	-1.962000	2.867000
C	6.222000	-3.147000	2.227000
C	1.963000	-1.736000	-2.947000
C	2.708000	-2.694000	-2.279000
N	3.423000	-2.479000	-1.137000
C	4.023000	-3.664000	-0.830000
C	2.844000	-4.067000	-2.699000
C	3.657000	-4.670000	-1.797000
C	4.886000	-3.877000	0.237000
O	2.185000	-1.252000	0.977000
C	1.329000	-0.390000	1.683000
C	0.335000	-0.866000	0.720000
C	1.149000	-0.752000	3.138000
H	3.221000	4.236000	1.538000
H	5.002000	3.063000	3.183000
H	7.000000	-1.738000	3.726000
H	6.681000	-4.101000	2.449000

H	2.375000	-4.493000	-3.576000
H	3.998000	-5.697000	-1.777000
C	-6.247000	2.633000	0.369000
C	-4.747000	2.652000	0.085000
C	-4.062000	4.014000	0.216000
C	-2.563000	3.790000	0.115000
C	1.547000	3.741000	-0.537000
C	0.179000	3.745000	-0.238000
C	-0.545000	4.938000	-0.289000
C	0.108000	6.133000	-0.612000
C	1.466000	6.122000	-0.897000
C	2.192000	4.931000	-0.870000
C	-10.674000	-2.696000	-0.869000
C	-9.251000	-2.463000	-1.372000
C	-8.346000	-1.877000	-0.282000
H	-3.782000	-1.133000	1.753000
C	-5.589000	-2.184000	1.138000
C	-4.542000	-1.796000	2.177000
C	-3.814000	-3.024000	2.731000
C	-2.718000	-2.612000	3.712000
H	-4.524000	-3.708000	3.213000
H	-2.144000	-3.479000	4.053000
O	-1.880000	5.024000	-0.046000
H	-0.290000	2.805000	0.037000
H	3.250000	4.922000	-1.111000
H	1.964000	7.051000	-1.155000
H	-0.468000	7.053000	-0.643000
C	-6.900000	1.292000	-0.004000
C	-6.418000	0.119000	0.868000
N	-5.914000	-1.103000	0.123000
C	-4.672000	-0.714000	-0.668000

C	-1.644000	-2.299000	-2.450000
C	-2.668000	-1.249000	-2.028000
C	-3.780000	-1.845000	-1.157000
H	-0.873000	-1.851000	-3.082000
H	-3.109000	-0.778000	-2.916000
H	-3.312000	-2.348000	-0.303000
H	-6.703000	1.109000	-1.065000
H	-7.987000	1.374000	0.086000
H	-7.212000	-0.235000	1.527000
H	-5.587000	0.427000	1.503000
C	-6.950000	-1.642000	-0.843000
H	-6.434000	2.859000	1.427000
H	-6.743000	3.422000	-0.209000
H	-4.227000	1.953000	0.751000
H	-4.573000	2.282000	-0.935000
H	-4.310000	4.487000	1.174000
H	-4.394000	4.689000	-0.581000
H	-2.345000	3.140000	-0.745000
H	-2.200000	3.269000	1.008000
H	-8.826000	-3.410000	-1.728000
H	-8.783000	-0.935000	0.069000
H	-11.133000	-1.759000	-0.536000
H	-11.304000	-3.116000	-1.660000
H	-10.684000	-3.395000	-0.025000
H	-9.272000	-1.784000	-2.233000
H	-8.327000	-2.566000	0.568000
H	-5.259000	-3.046000	0.555000
H	-6.530000	-2.452000	1.619000
H	-5.013000	-1.249000	3.001000
H	-3.364000	-3.578000	1.895000
H	-3.144000	-2.120000	4.593000

H	-2.031000	-1.904000	3.234000
H	-4.073000	-0.062000	-0.033000
H	-5.026000	-0.123000	-1.514000
H	-2.114000	-3.115000	-3.011000
H	-1.141000	-2.732000	-1.579000
H	-2.170000	-0.461000	-1.452000
H	-4.338000	-2.598000	-1.726000
H	-6.536000	-2.574000	-1.236000
H	-7.005000	-0.935000	-1.673000
H	1.565000	0.670000	1.565000
H	-0.107000	-1.841000	0.879000
H	0.365000	-0.477000	-0.287000
H	0.356000	-0.143000	3.581000
H	0.888000	-1.811000	3.240000
H	1.450000	-2.050000	-3.851000
H	6.004000	0.672000	3.386000
H	5.290000	-4.878000	0.358000
H	2.085000	-0.571000	3.676000
Al	3.642000	-0.718000	-0.172000
Br	5.572000	-0.160000	-1.656000
Br	-1.725000	0.431000	1.191000

II

C	1.853000	1.438000	-1.387000
C	0.936000	1.653000	-2.482000
N	2.292000	0.144000	-1.402000
C	1.691000	-0.461000	-2.468000
C	0.840000	0.475000	-3.151000
C	2.245000	2.425000	-0.471000
H	0.450000	2.590000	-2.712000
C	5.405000	0.326000	2.552000

C	3.177000	2.221000	0.553000
H	0.260000	0.254000	-4.039000
N	3.805000	1.038000	0.831000
C	3.580000	3.224000	1.513000
C	4.596000	1.263000	1.920000
C	4.465000	2.631000	2.351000
C	5.553000	-1.005000	2.188000
N	4.910000	-1.614000	1.154000
C	5.346000	-2.904000	1.130000
C	6.425000	-1.946000	2.853000
C	6.297000	-3.125000	2.196000
C	1.856000	-1.789000	-2.848000
C	2.650000	-2.732000	-2.213000
N	3.404000	-2.506000	-1.101000
C	4.048000	-3.674000	-0.825000
C	2.808000	-4.099000	-2.650000
C	3.676000	-4.684000	-1.788000
C	4.948000	-3.870000	0.216000
O	2.176000	-1.269000	1.039000
C	1.157000	-0.463000	1.492000
C	-0.094000	-0.845000	0.690000
C	0.948000	-0.633000	2.997000
H	3.223000	4.243000	1.534000
H	4.986000	3.066000	3.194000
H	7.049000	-1.714000	3.706000
H	6.794000	-4.065000	2.394000
H	2.318000	-4.533000	-3.512000
H	4.049000	-5.700000	-1.791000
C	-6.220000	2.632000	0.390000
C	-4.719000	2.663000	0.102000
C	-4.050000	4.036000	0.201000

C	-2.549000	3.826000	0.107000
C	1.550000	3.744000	-0.544000
C	0.180000	3.770000	-0.259000
C	-0.534000	4.966000	-0.321000
C	0.130000	6.153000	-0.647000
C	1.491000	6.124000	-0.920000
C	2.207000	4.926000	-0.879000
C	-10.611000	-2.815000	-0.610000
C	-9.213000	-2.570000	-1.173000
C	-8.283000	-1.927000	-0.138000
H	-3.638000	-1.096000	1.695000
C	-5.461000	-2.162000	1.173000
C	-4.387000	-1.736000	2.168000
C	-3.650000	-2.944000	2.753000
C	-2.550000	-2.498000	3.715000
H	-4.355000	-3.611000	3.263000
H	-1.968000	-3.351000	4.075000
O	-1.873000	5.055000	-0.085000
H	-0.295000	2.834000	0.010000
H	3.268000	4.908000	-1.110000
H	2.000000	7.046000	-1.181000
H	-0.435000	7.079000	-0.689000
C	-6.864000	1.281000	0.037000
C	-6.351000	0.119000	0.906000
N	-5.851000	-1.103000	0.158000
C	-4.652000	-0.703000	-0.690000
C	-1.724000	-2.286000	-2.642000
C	-2.718000	-1.234000	-2.159000
C	-3.754000	-1.822000	-1.194000
H	-1.033000	-1.855000	-3.370000
H	-3.232000	-0.786000	-3.018000

H	-3.224000	-2.291000	-0.357000
H	-6.687000	1.094000	-1.027000
H	-7.950000	1.352000	0.149000
H	-7.124000	-0.238000	1.588000
H	-5.509000	0.442000	1.519000
C	-6.915000	-1.674000	-0.759000
H	-6.404000	2.871000	1.445000
H	-6.722000	3.408000	-0.198000
H	-4.196000	1.984000	0.789000
H	-4.540000	2.271000	-0.909000
H	-4.307000	4.532000	1.144000
H	-4.388000	4.683000	-0.615000
H	-2.326000	3.152000	-0.734000
H	-2.184000	3.338000	1.021000
H	-8.780000	-3.519000	-1.512000
H	-8.730000	-0.986000	0.201000
Br	-1.562000	0.460000	0.990000
H	-11.078000	-1.877000	-0.293000
H	-11.259000	-3.276000	-1.362000
H	-10.574000	-3.483000	0.258000
H	-9.280000	-1.922000	-2.056000
H	-8.214000	-2.590000	0.731000
H	-5.133000	-3.025000	0.591000
H	-6.375000	-2.445000	1.696000
H	-4.834000	-1.154000	2.981000
H	-3.205000	-3.523000	1.933000
H	-2.973000	-1.984000	4.585000
H	-1.865000	-1.801000	3.218000
H	-4.052000	-0.018000	-0.095000
H	-5.052000	-0.139000	-1.534000
H	-2.238000	-3.129000	-3.119000

H	-1.125000	-2.677000	-1.812000
H	-2.180000	-0.426000	-1.649000
H	-4.325000	-2.606000	-1.705000
H	-6.500000	-2.603000	-1.158000
H	-7.018000	-0.977000	-1.593000
H	1.339000	0.606000	1.301000
H	-0.496000	-1.819000	0.975000
H	0.101000	-0.804000	-0.380000
H	0.117000	-0.021000	3.366000
H	0.748000	-1.686000	3.229000
H	1.319000	-2.116000	-3.733000
H	5.980000	0.671000	3.406000
H	5.386000	-4.858000	0.314000
H	1.863000	-0.336000	3.519000
Al	3.545000	-0.759000	-0.082000
Br	5.493000	-0.153000	-1.634000

I2_CO2

C	-2.445000	2.609000	0.259000
C	-3.000000	3.646000	1.096000
N	-2.973000	1.395000	0.609000
C	-3.865000	1.640000	1.614000
C	-3.880000	3.043000	1.934000
C	-1.473000	2.824000	-0.722000
H	-2.746000	4.694000	1.036000
C	-0.677000	-1.455000	-2.838000
C	-0.921000	1.818000	-1.520000
H	-4.497000	3.495000	2.700000
N	-1.288000	0.504000	-1.499000
C	0.130000	2.018000	-2.489000
C	-0.537000	-0.128000	-2.446000

C	0.372000	0.808000	-3.058000
C	-1.582000	-2.369000	-2.316000
N	-2.399000	-2.145000	-1.250000
C	-3.120000	-3.286000	-1.067000
C	-1.808000	-3.695000	-2.840000
C	-2.758000	-4.267000	-2.060000
C	-4.656000	0.692000	2.250000
C	-4.729000	-0.653000	1.922000
N	-4.018000	-1.257000	0.928000
C	-4.466000	-2.543000	0.864000
C	-5.627000	-1.600000	2.540000
C	-5.467000	-2.772000	1.879000
C	-4.065000	-3.488000	-0.068000
C	0.296000	0.802000	1.336000
C	-1.207000	-0.123000	3.167000
H	0.602000	2.966000	-2.708000
H	1.074000	0.565000	-3.846000
H	-1.315000	-4.109000	-3.709000
H	-3.197000	-5.253000	-2.145000
H	-6.299000	-1.371000	3.357000
H	-5.979000	-3.713000	2.040000
C	3.482000	2.024000	-0.770000
C	4.334000	3.244000	-0.403000
C	3.612000	4.575000	-0.644000
C	2.938000	5.085000	0.631000
C	-0.920000	4.205000	-0.843000
C	0.292000	4.484000	-0.208000
C	0.835000	5.766000	-0.256000
C	0.155000	6.779000	-0.938000
C	-1.052000	6.498000	-1.566000
C	-1.594000	5.213000	-1.530000

C	8.890000	-1.088000	-0.624000
C	7.670000	-1.168000	0.290000
C	6.412000	-1.609000	-0.465000
H	1.698000	-3.413000	-1.086000
C	3.827000	-2.963000	-1.082000
C	2.510000	-3.224000	-1.794000
C	2.697000	-4.450000	-2.697000
C	1.424000	-4.837000	-3.439000
H	3.501000	-4.253000	-3.418000
H	1.588000	-5.723000	-4.060000
O	2.000000	6.118000	0.356000
H	0.780000	3.688000	0.342000
H	-2.535000	4.992000	-2.023000
H	-1.573000	7.288000	-2.097000
H	0.588000	7.773000	-0.967000
C	4.076000	0.752000	-0.166000
C	3.569000	-0.507000	-0.858000
N	3.866000	-1.804000	-0.115000
C	2.826000	-1.975000	0.984000
C	2.057000	-4.573000	3.767000
C	2.090000	-3.229000	3.044000
C	2.869000	-3.307000	1.727000
H	1.504000	-4.496000	4.707000
H	2.543000	-2.466000	3.688000
H	2.439000	-4.096000	1.100000
H	3.825000	0.751000	0.898000
H	5.168000	0.803000	-0.244000
H	4.022000	-0.599000	-1.848000
H	2.486000	-0.471000	-0.999000
C	5.247000	-1.765000	0.509000
H	2.454000	2.151000	-0.408000

H	3.412000	1.948000	-1.863000
H	4.628000	3.172000	0.655000
H	5.267000	3.204000	-0.977000
H	2.855000	4.445000	-1.426000
H	4.304000	5.343000	-1.003000
H	3.677000	5.546000	1.291000
H	2.476000	4.264000	1.195000
H	7.868000	-1.869000	1.111000
H	6.190000	-0.874000	-1.247000
Br	1.731000	1.467000	2.517000
H	8.724000	-0.377000	-1.441000
H	9.774000	-0.760000	-0.068000
H	9.114000	-2.064000	-1.068000
H	7.488000	-0.189000	0.751000
H	6.613000	-2.560000	-0.970000
H	4.130000	-3.844000	-0.511000
H	4.607000	-2.765000	-1.820000
H	2.213000	-2.361000	-2.400000
H	3.030000	-5.298000	-2.084000
H	1.089000	-4.025000	-4.094000
H	0.616000	-5.057000	-2.735000
H	1.850000	-1.850000	0.510000
H	2.966000	-1.136000	1.672000
H	3.070000	-4.924000	3.997000
H	1.568000	-5.336000	3.151000
H	1.064000	-2.895000	2.857000
H	3.893000	-3.608000	1.966000
H	5.367000	-2.694000	1.065000
H	5.231000	-0.952000	1.236000
H	-0.375000	1.649000	1.221000
H	0.777000	0.575000	0.384000

H	-0.530000	0.178000	3.974000
H	-1.932000	0.678000	3.001000
H	-5.301000	1.045000	3.049000
H	-0.059000	-1.789000	-3.666000
H	-4.539000	-4.464000	-0.023000
H	-1.750000	-1.020000	3.474000
O	-1.209000	-0.955000	0.873000
C	-0.435000	-0.428000	1.883000
H	0.350000	-1.157000	2.152000
Al	-2.590000	-0.406000	-0.233000
Br	-4.454000	0.154000	-1.918000
C	-0.904000	-3.554000	1.256000
O	-0.156000	-3.677000	0.368000
O	-1.601000	-3.552000	2.189000

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C	-2.492000	2.522000	0.317000
C	-3.020000	3.547000	1.183000
N	-3.023000	1.306000	0.658000
C	-3.894000	1.542000	1.684000
C	-3.885000	2.937000	2.032000
C	-1.534000	2.744000	-0.675000
H	-2.758000	4.594000	1.137000
C	-0.669000	-1.551000	-2.733000
C	-0.971000	1.735000	-1.463000
H	-4.479000	3.380000	2.820000
N	-1.323000	0.416000	-1.424000
C	0.099000	1.929000	-2.409000
C	-0.538000	-0.224000	-2.340000
C	0.375000	0.710000	-2.943000
C	-1.619000	-2.446000	-2.267000

N	-2.488000	-2.207000	-1.241000
C	-3.275000	-3.318000	-1.137000
C	-1.863000	-3.752000	-2.826000
C	-2.891000	-4.292000	-2.126000
C	-4.701000	0.595000	2.299000
C	-4.831000	-0.728000	1.908000
N	-4.147000	-1.316000	0.886000
C	-4.668000	-2.569000	0.750000
C	-5.789000	-1.653000	2.466000
C	-5.696000	-2.791000	1.737000
C	-4.288000	-3.498000	-0.206000
C	0.270000	0.681000	1.271000
C	-1.208000	-0.080000	3.200000
H	0.562000	2.879000	-2.637000
H	1.102000	0.460000	-3.705000
H	-1.327000	-4.176000	-3.664000
H	-3.365000	-5.256000	-2.259000
H	-6.452000	-1.430000	3.292000
H	-6.264000	-3.707000	1.841000
C	3.523000	1.992000	-0.860000
C	4.343000	3.256000	-0.583000
C	3.546000	4.549000	-0.800000
C	2.919000	5.042000	0.503000
C	-0.995000	4.130000	-0.808000
C	0.242000	4.415000	-0.225000
C	0.770000	5.703000	-0.288000
C	0.050000	6.714000	-0.932000
C	-1.181000	6.426000	-1.507000
C	-1.709000	5.136000	-1.455000
C	9.015000	-1.024000	-0.931000
C	7.857000	-1.103000	0.060000

C	6.558000	-1.567000	-0.606000
H	1.815000	-3.425000	-0.890000
C	3.948000	-2.999000	-0.989000
C	2.600000	-3.273000	-1.634000
C	2.724000	-4.534000	-2.497000
C	1.412000	-4.894000	-3.185000
H	3.511000	-4.393000	-3.250000
H	1.508000	-5.823000	-3.755000
O	1.956000	6.064000	0.274000
H	0.762000	3.620000	0.297000
H	-2.669000	4.909000	-1.907000
H	-1.733000	7.216000	-2.007000
H	0.473000	7.713000	-0.973000
C	4.209000	0.763000	-0.263000
C	3.682000	-0.535000	-0.864000
N	4.044000	-1.790000	-0.084000
C	3.070000	-1.891000	1.080000
C	2.530000	-3.961000	4.301000
C	2.244000	-2.971000	3.174000
C	3.342000	-2.984000	2.104000
H	1.727000	-3.946000	5.043000
H	2.149000	-1.957000	3.584000
H	3.369000	-3.973000	1.633000
H	4.047000	0.797000	0.819000
H	5.288000	0.840000	-0.429000
H	4.065000	-0.666000	-1.879000
H	2.591000	-0.521000	-0.928000
C	5.461000	-1.721000	0.444000
H	2.518000	2.083000	-0.431000
H	3.385000	1.880000	-1.943000
H	4.715000	3.226000	0.451000

H	5.232000	3.244000	-1.223000
H	2.756000	4.374000	-1.541000
H	4.183000	5.344000	-1.201000
H	3.680000	5.512000	1.133000
H	2.493000	4.214000	1.083000
H	8.114000	-1.790000	0.876000
H	6.280000	-0.847000	-1.384000
Br	1.723000	1.391000	2.395000
H	8.789000	-0.328000	-1.746000
H	9.929000	-0.680000	-0.439000
H	9.221000	-2.005000	-1.375000
H	7.694000	-0.119000	0.519000
H	6.738000	-2.523000	-1.109000
H	4.263000	-3.855000	-0.387000
H	4.699000	-2.848000	-1.766000
H	2.289000	-2.429000	-2.261000
H	3.044000	-5.371000	-1.864000
H	1.106000	-4.104000	-3.880000
H	0.611000	-5.023000	-2.450000
H	2.078000	-2.029000	0.643000
H	3.079000	-0.916000	1.572000
H	3.468000	-3.719000	4.812000
H	2.610000	-4.983000	3.914000
H	1.287000	-3.215000	2.703000
H	4.307000	-2.826000	2.599000
H	5.626000	-2.642000	1.002000
H	5.482000	-0.896000	1.159000
H	-0.378000	1.535000	1.107000
H	0.736000	0.373000	0.336000
H	-0.501000	0.207000	3.985000
H	-1.883000	0.760000	3.016000

H	-5.330000	0.937000	3.115000
H	-0.017000	-1.892000	-3.532000
H	-4.815000	-4.446000	-0.219000
H	-1.800000	-0.931000	3.547000
O	-1.312000	-1.071000	0.967000
C	-0.474000	-0.481000	1.925000
H	0.293000	-1.219000	2.202000
Al	-2.705000	-0.467000	-0.242000
Br	-4.485000	0.166000	-1.942000
C	-0.977000	-2.966000	1.115000
O	0.015000	-3.130000	0.473000
O	-1.815000	-3.367000	1.850000

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C	-3.356000	-0.435000	-0.212000
C	-4.465000	-0.997000	0.523000
N	-2.526000	-1.438000	-0.629000
C	-3.072000	-2.607000	-0.191000
C	-4.305000	-2.344000	0.505000
C	-3.168000	0.926000	-0.454000
H	-5.262000	-0.427000	0.979000
C	0.644000	1.297000	-3.422000
C	-2.168000	1.447000	-1.287000
H	-4.940000	-3.102000	0.944000
N	-1.196000	0.725000	-1.911000
C	-2.073000	2.835000	-1.678000
C	-0.476000	1.608000	-2.662000
C	-1.028000	2.930000	-2.539000
C	1.252000	0.053000	-3.498000
N	0.837000	-1.074000	-2.838000
C	1.687000	-2.073000	-3.217000

C	2.415000	-0.242000	-4.294000
C	2.687000	-1.561000	-4.114000
C	-2.502000	-3.867000	-0.320000
C	-1.276000	-4.141000	-0.904000
N	-0.471000	-3.225000	-1.517000
C	0.591000	-3.925000	-2.015000
C	-0.684000	-5.454000	-0.977000
C	0.480000	-5.318000	-1.658000
C	1.595000	-3.400000	-2.814000
C	0.515000	-2.005000	3.811000
C	-1.958000	-1.504000	3.435000
H	-2.739000	3.620000	-1.348000
H	-0.652000	3.805000	-3.053000
H	2.935000	0.475000	-4.916000
H	3.478000	-2.151000	-4.557000
H	-1.124000	-6.352000	-0.566000
H	1.198000	-6.083000	-1.928000
C	0.196000	3.648000	1.063000
C	-0.149000	5.044000	1.597000
C	-1.653000	5.342000	1.685000
C	-2.328000	4.673000	2.885000
C	-4.062000	1.900000	0.234000
C	-3.483000	2.729000	1.196000
C	-4.241000	3.702000	1.839000
C	-5.605000	3.817000	1.548000
C	-6.183000	2.975000	0.607000
C	-5.417000	2.023000	-0.067000
C	3.561000	3.810000	-4.415000
C	4.226000	3.691000	-3.045000
C	3.460000	2.734000	-2.128000
H	4.154000	-0.923000	1.457000

C	3.512000	0.263000	-0.257000
C	3.294000	-0.838000	0.781000
C	3.082000	-2.150000	0.025000
C	2.781000	-3.352000	0.907000
H	2.231000	-2.011000	-0.638000
H	2.709000	-4.253000	0.289000
O	-3.742000	4.582000	2.743000
H	-2.425000	2.614000	1.400000
H	-5.862000	1.389000	-0.827000
H	-7.240000	3.078000	0.377000
H	-6.186000	4.578000	2.058000
C	1.709000	3.468000	0.906000
C	2.005000	2.045000	0.449000
N	3.474000	1.702000	0.243000
C	4.209000	1.832000	1.559000
C	7.691000	0.910000	2.995000
C	6.208000	1.270000	2.962000
C	5.687000	1.450000	1.533000
H	8.038000	0.776000	4.024000
H	6.039000	2.191000	3.535000
H	5.849000	0.521000	0.977000
H	2.172000	3.668000	1.877000
H	2.084000	4.215000	0.196000
H	1.510000	1.826000	-0.499000
H	1.597000	1.330000	1.167000
C	4.142000	2.612000	-0.772000
H	-0.170000	2.864000	1.739000
H	-0.304000	3.485000	0.100000
H	0.308000	5.178000	2.587000
H	0.318000	5.787000	0.939000
H	-2.138000	5.008000	0.759000

H	-1.820000	6.422000	1.749000
H	-2.190000	5.282000	3.780000
H	-1.895000	3.688000	3.102000
H	5.261000	3.344000	-3.163000
H	2.436000	3.104000	-2.022000
Br	0.372000	-3.001000	5.500000
H	2.521000	4.144000	-4.320000
H	4.088000	4.529000	-5.050000
H	3.556000	2.845000	-4.935000
H	4.279000	4.680000	-2.572000
H	3.396000	1.750000	-2.606000
H	4.476000	0.131000	-0.755000
H	2.722000	0.192000	-1.007000
H	2.418000	-0.620000	1.400000
H	3.960000	-2.349000	-0.606000
H	1.804000	-3.223000	1.381000
H	3.544000	-3.518000	1.677000
H	3.659000	1.221000	2.276000
H	4.112000	2.872000	1.869000
H	8.299000	1.696000	2.534000
H	7.881000	-0.023000	2.453000
H	5.626000	0.482000	3.456000
H	6.277000	2.226000	1.034000
H	5.147000	2.213000	-0.916000
H	4.241000	3.593000	-0.299000
H	0.622000	-0.965000	4.097000
H	1.419000	-2.380000	3.337000
H	-2.169000	-1.754000	4.479000
H	-1.799000	-0.427000	3.350000
H	-3.051000	-4.704000	0.099000
H	1.089000	2.105000	-3.996000

H	2.357000	-4.086000	-3.172000
H	-2.818000	-1.782000	2.826000
C	-0.028000	-0.831000	1.125000
O	0.258000	0.056000	1.935000
O	0.133000	-0.724000	-0.136000
C	-0.728000	-2.264000	2.959000
H	-0.934000	-3.337000	2.988000
O	-0.446000	-2.051000	1.566000
Al	-0.846000	-1.261000	-1.721000
Br	-2.168000	-1.689000	-3.802000

TS3a_CO₂

C	-3.349000	-0.630000	0.247000
C	-4.293000	-1.172000	1.195000
N	-2.514000	-1.624000	-0.195000
C	-2.918000	-2.770000	0.427000
C	-4.043000	-2.501000	1.282000
C	-3.313000	0.702000	-0.166000
H	-5.052000	-0.602000	1.712000
C	0.109000	1.002000	-3.584000
C	-2.465000	1.190000	-1.170000
H	-4.549000	-3.242000	1.887000
N	-1.503000	0.474000	-1.820000
C	-2.521000	2.531000	-1.703000
C	-0.946000	1.317000	-2.738000
C	-1.583000	2.604000	-2.682000
C	0.806000	-0.195000	-3.601000
N	0.541000	-1.275000	-2.802000
C	1.436000	-2.242000	-3.161000
C	1.924000	-0.480000	-4.462000
C	2.322000	-1.748000	-4.180000

C	-2.299000	-4.008000	0.321000
C	-1.150000	-4.271000	-0.404000
N	-0.474000	-3.367000	-1.173000
C	0.571000	-4.050000	-1.731000
C	-0.495000	-5.554000	-0.451000
C	0.577000	-5.416000	-1.268000
C	1.471000	-3.533000	-2.649000
C	0.895000	-1.082000	3.597000
C	-1.381000	-2.180000	3.577000
H	-3.210000	3.299000	-1.381000
H	-1.338000	3.444000	-3.320000
H	2.331000	0.205000	-5.195000
H	3.123000	-2.318000	-4.631000
H	-0.831000	-6.437000	0.078000
H	1.307000	-6.161000	-1.556000
C	0.085000	3.720000	0.860000
C	-0.292000	5.147000	1.273000
C	-1.799000	5.352000	1.466000
C	-2.333000	4.741000	2.765000
C	-4.187000	1.692000	0.528000
C	-3.554000	2.650000	1.324000
C	-4.294000	3.632000	1.978000
C	-5.688000	3.639000	1.853000
C	-6.314000	2.677000	1.071000
C	-5.574000	1.704000	0.398000
C	2.453000	3.783000	-4.944000
C	3.354000	3.739000	-3.712000
C	2.823000	2.775000	-2.647000
H	4.464000	-0.572000	0.864000
C	3.383000	0.417000	-0.738000
C	3.475000	-0.603000	0.392000

C	3.210000	-2.009000	-0.149000
C	3.371000	-3.089000	0.915000
H	2.194000	-2.041000	-0.546000
H	3.127000	-4.072000	0.501000
O	-3.751000	4.607000	2.754000
H	-2.475000	2.610000	1.402000
H	-6.066000	0.970000	-0.231000
H	-7.395000	2.693000	0.974000
H	-6.258000	4.405000	2.368000
C	1.575000	3.595000	0.525000
C	1.886000	2.157000	0.134000
N	3.317000	1.875000	-0.295000
C	4.244000	2.135000	0.872000
C	7.994000	1.636000	1.710000
C	6.492000	1.804000	1.926000
C	5.725000	1.889000	0.603000
H	8.521000	1.567000	2.666000
H	6.302000	2.708000	2.518000
H	5.882000	0.961000	0.042000
H	2.160000	3.907000	1.396000
H	1.810000	4.289000	-0.291000
H	1.247000	1.840000	-0.693000
H	1.670000	1.483000	0.964000
C	3.739000	2.775000	-1.435000
H	-0.160000	3.004000	1.655000
H	-0.506000	3.428000	-0.018000
H	0.246000	5.422000	2.191000
H	0.055000	5.839000	0.495000
H	-2.328000	4.916000	0.612000
H	-2.036000	6.421000	1.466000
H	-2.123000	5.402000	3.609000

H	-1.866000	3.774000	2.989000
H	4.367000	3.439000	-4.007000
H	1.806000	3.077000	-2.372000
H	1.436000	4.093000	-4.677000
H	2.835000	4.492000	-5.685000
H	2.391000	2.801000	-5.425000
H	3.437000	4.745000	-3.283000
H	2.754000	1.768000	-3.068000
H	4.243000	0.324000	-1.405000
H	2.479000	0.235000	-1.324000
H	2.739000	-0.382000	1.171000
H	3.884000	-2.214000	-0.992000
H	2.694000	-2.913000	1.758000
H	4.394000	-3.125000	1.306000
H	3.886000	1.511000	1.692000
H	4.094000	3.176000	1.162000
H	8.410000	2.485000	1.157000
H	8.210000	0.725000	1.140000
H	6.106000	0.959000	2.511000
H	6.142000	2.701000	-0.002000
H	4.738000	2.449000	-1.728000
H	3.830000	3.781000	-1.019000
H	0.469000	-0.305000	4.209000
H	1.949000	-1.035000	3.369000
H	-1.364000	-2.235000	4.669000
H	-1.875000	-1.253000	3.267000
H	-2.737000	-4.830000	0.879000
H	0.429000	1.772000	-4.279000
H	2.243000	-4.198000	-3.021000
H	-1.949000	-3.024000	3.182000
C	0.204000	-0.921000	1.147000

O	0.472000	-0.031000	2.006000
O	0.137000	-0.733000	-0.087000
C	0.043000	-2.222000	3.058000
H	0.521000	-3.171000	3.292000
O	0.047000	-2.162000	1.616000
Al	-1.024000	-1.466000	-1.540000
Br	-2.509000	-2.154000	-3.380000
Br	1.521000	-2.188000	5.708000

I4a_CO₂

C	3.448000	0.110000	-0.453000
C	4.421000	0.405000	-1.472000
N	2.824000	-1.080000	-0.733000
C	3.388000	-1.541000	-1.893000
C	4.398000	-0.631000	-2.350000
C	3.152000	0.943000	0.627000
H	5.043000	1.288000	-1.499000
C	-0.132000	-1.393000	3.316000
C	2.247000	0.614000	1.639000
H	4.995000	-0.769000	-3.242000
N	1.490000	-0.524000	1.698000
C	2.008000	1.425000	2.807000
C	0.788000	-0.454000	2.869000
C	1.109000	0.755000	3.573000
C	-0.545000	-2.512000	2.615000
N	-0.092000	-2.878000	1.375000
C	-0.756000	-4.032000	1.056000
C	-1.537000	-3.446000	3.077000
C	-1.675000	-4.383000	2.105000
C	2.998000	-2.680000	-2.584000
C	1.976000	-3.533000	-2.210000

N	1.215000	-3.411000	-1.079000
C	0.360000	-4.479000	-1.087000
C	1.571000	-4.691000	-2.964000
C	0.567000	-5.277000	-2.267000
C	-0.562000	-4.776000	-0.096000
C	1.061000	1.784000	-2.512000
C	1.596000	0.450000	-4.646000
H	2.489000	2.370000	3.014000
H	0.695000	1.041000	4.531000
H	-2.048000	-3.384000	4.029000
H	-2.323000	-5.250000	2.091000
H	2.014000	-5.002000	-3.900000
H	0.010000	-6.173000	-2.509000
C	-0.946000	3.305000	0.962000
C	-0.891000	4.754000	1.454000
C	0.532000	5.319000	1.519000
C	1.140000	5.594000	0.143000
C	3.742000	2.313000	0.648000
C	2.868000	3.378000	0.407000
C	3.334000	4.692000	0.419000
C	4.692000	4.935000	0.654000
C	5.556000	3.874000	0.883000
C	5.091000	2.558000	0.889000
C	-3.056000	-0.455000	5.601000
C	-3.959000	0.004000	4.458000
C	-3.251000	-0.041000	3.101000
H	-4.133000	-0.946000	-1.885000
C	-3.329000	-0.907000	0.129000
C	-3.166000	-1.059000	-1.381000
C	-2.586000	-2.439000	-1.697000
C	-2.417000	-2.672000	-3.195000

H	-1.612000	-2.525000	-1.211000
H	-1.970000	-3.654000	-3.383000
O	2.552000	5.781000	0.207000
H	1.825000	3.148000	0.229000
H	5.766000	1.731000	1.088000
H	6.607000	4.074000	1.071000
H	5.046000	5.961000	0.659000
C	-2.350000	2.706000	1.069000
C	-2.307000	1.272000	0.569000
N	-3.618000	0.505000	0.615000
C	-4.630000	1.195000	-0.278000
C	-8.165000	0.521000	-1.700000
C	-6.775000	1.134000	-1.552000
C	-5.983000	0.503000	-0.402000
H	-8.709000	0.982000	-2.531000
H	-6.862000	2.215000	-1.384000
H	-5.872000	-0.569000	-0.597000
H	-3.023000	3.303000	0.446000
H	-2.697000	2.767000	2.108000
H	-1.580000	0.680000	1.129000
H	-2.007000	1.294000	-0.480000
C	-4.184000	0.463000	2.014000
H	-0.644000	3.244000	-0.090000
H	-0.240000	2.694000	1.542000
H	-1.519000	5.384000	0.810000
H	-1.329000	4.807000	2.459000
H	1.168000	4.610000	2.063000
H	0.543000	6.251000	2.093000
H	0.755000	6.532000	-0.264000
H	0.899000	4.807000	-0.581000
H	-4.857000	-0.626000	4.424000

H	-2.344000	0.571000	3.154000
H	-2.155000	0.166000	5.663000
H	-3.574000	-0.389000	6.562000
H	-2.741000	-1.495000	5.464000
H	-4.302000	1.028000	4.654000
H	-2.933000	-1.066000	2.888000
H	-4.143000	-1.541000	0.489000
H	-2.412000	-1.222000	0.633000
H	-2.516000	-0.283000	-1.799000
H	-3.229000	-3.219000	-1.267000
H	-1.753000	-1.916000	-3.627000
H	-3.377000	-2.625000	-3.723000
H	-4.147000	1.329000	-1.248000
H	-4.771000	2.193000	0.140000
H	-8.758000	0.662000	-0.790000
H	-8.101000	-0.555000	-1.896000
H	-6.211000	1.011000	-2.485000
H	-6.559000	0.602000	0.525000
H	-5.073000	-0.170000	1.967000
H	-4.516000	1.479000	2.241000
H	2.148000	1.893000	-2.471000
H	0.554000	2.745000	-2.588000
H	1.816000	1.347000	-5.235000
H	2.525000	0.088000	-4.196000
H	3.527000	-2.906000	-3.504000
H	-0.585000	-1.217000	4.286000
H	-1.166000	-5.668000	-0.225000
H	1.201000	-0.314000	-5.320000
C	0.293000	-0.080000	-1.511000
O	0.646000	1.167000	-1.278000
O	0.004000	-0.872000	-0.621000

C	0.584000	0.795000	-3.582000
H	-0.372000	1.125000	-3.992000
O	0.284000	-0.390000	-2.787000
Al	1.452000	-2.052000	0.392000
Br	3.124000	-3.340000	1.568000
Br	-2.275000	2.627000	-2.698000

I3b_CO₂

C	2.142000	0.367000	-2.166000
C	1.494000	0.002000	-3.400000
N	2.691000	-0.748000	-1.581000
C	2.401000	-1.794000	-2.415000
C	1.651000	-1.336000	-3.549000
C	2.192000	1.667000	-1.653000
H	0.991000	0.691000	-4.062000
C	4.863000	1.442000	2.389000
C	2.861000	2.011000	-0.475000
H	1.304000	-1.969000	-4.355000
N	3.577000	1.152000	0.318000
C	2.878000	3.334000	0.097000
C	4.064000	1.904000	1.352000
C	3.630000	3.266000	1.224000
C	5.271000	0.133000	2.570000
N	4.933000	-0.916000	1.760000
C	5.513000	-2.022000	2.313000
C	6.092000	-0.323000	3.662000
C	6.243000	-1.661000	3.502000
C	2.767000	-3.117000	-2.213000
C	3.503000	-3.593000	-1.141000
N	3.998000	-2.823000	-0.122000
C	4.694000	-3.679000	0.690000

C	3.870000	-4.971000	-0.951000
C	4.609000	-5.024000	0.185000
C	5.403000	-3.314000	1.823000
H	2.374000	4.194000	-0.317000
H	3.874000	4.059000	1.918000
H	6.490000	0.313000	4.441000
H	6.792000	-2.358000	4.122000
H	3.595000	-5.779000	-1.617000
H	5.070000	-5.886000	0.650000
C	-6.074000	0.693000	-2.062000
C	-4.666000	0.819000	-2.644000
C	-4.141000	2.247000	-2.768000
C	-2.700000	2.199000	-3.240000
C	1.419000	2.726000	-2.364000
C	0.033000	2.583000	-2.432000
C	-0.746000	3.552000	-3.065000
C	-0.132000	4.679000	-3.616000
C	1.250000	4.820000	-3.541000
C	2.034000	3.846000	-2.927000
C	-9.511000	-4.616000	0.491000
C	-8.143000	-4.524000	-0.180000
C	-7.281000	-3.408000	0.419000
H	-2.654000	-1.665000	1.744000
C	-4.713000	-2.336000	1.607000
C	-3.638000	-1.403000	2.150000
C	-3.615000	-1.512000	3.678000
C	-2.478000	-0.707000	4.303000
H	-4.575000	-1.162000	4.078000
H	-2.520000	-0.750000	5.396000
O	-2.106000	3.491000	-3.134000
H	-0.417000	1.731000	-1.936000

H	3.114000	3.950000	-2.885000
H	1.722000	5.695000	-3.979000
H	-0.749000	5.429000	-4.100000
C	-6.309000	-0.730000	-1.534000
C	-5.651000	-0.890000	-0.156000
N	-5.007000	-2.240000	0.126000
C	-3.728000	-2.314000	-0.688000
C	-0.553000	-4.491000	-0.986000
C	-1.534000	-3.348000	-1.237000
C	-2.839000	-3.528000	-0.452000
H	0.382000	-4.332000	-1.533000
H	-1.759000	-3.284000	-2.309000
H	-2.592000	-3.631000	0.610000
H	-5.896000	-1.428000	-2.271000
H	-7.378000	-0.956000	-1.465000
H	-6.390000	-0.731000	0.631000
H	-4.857000	-0.148000	-0.018000
C	-5.915000	-3.385000	-0.257000
H	-6.209000	1.414000	-1.245000
H	-6.826000	0.936000	-2.822000
H	-3.964000	0.279000	-1.997000
H	-4.639000	0.316000	-3.621000
H	-4.161000	2.715000	-1.778000
H	-4.758000	2.851000	-3.445000
H	-2.631000	1.865000	-4.286000
H	-2.170000	1.472000	-2.621000
H	-7.619000	-5.483000	-0.082000
H	-7.798000	-2.451000	0.290000
H	-10.065000	-3.677000	0.385000
H	-10.113000	-5.414000	0.045000
H	-9.411000	-4.828000	1.561000

H	-8.270000	-4.344000	-1.255000
H	-7.178000	-3.578000	1.496000
H	-4.450000	-3.379000	1.804000
H	-5.659000	-2.136000	2.115000
H	-3.824000	-0.366000	1.853000
H	-3.519000	-2.565000	3.975000
H	-2.530000	0.346000	4.005000
H	-1.505000	-1.097000	3.988000
H	-3.163000	-1.397000	-0.482000
H	-4.036000	-2.280000	-1.736000
H	-0.973000	-5.452000	-1.303000
H	-0.304000	-4.572000	0.079000
H	-1.084000	-2.387000	-0.961000
H	-3.326000	-4.460000	-0.764000
H	-5.371000	-4.302000	-0.024000
H	-6.033000	-3.339000	-1.341000
H	2.458000	-3.837000	-2.965000
H	5.189000	2.172000	3.123000
H	5.917000	-4.101000	2.366000
Al	3.921000	-0.809000	0.015000
Br	5.926000	-0.451000	-1.285000
C	1.099000	-1.912000	1.016000
C	0.946000	-0.459000	1.099000
H	1.066000	-2.394000	0.043000
H	0.791000	0.066000	0.161000
C	0.495000	0.252000	2.335000
H	-0.581000	0.426000	2.280000
H	0.993000	1.225000	2.401000
O	2.253000	-1.079000	1.218000
H	0.867000	-2.540000	1.873000
H	0.729000	-0.330000	3.231000

C	-2.019000	3.083000	2.431000
C	-1.722000	3.328000	0.953000
H	-2.760000	2.293000	2.535000
H	-2.644000	3.644000	0.456000
C	-0.607000	4.335000	0.727000
H	-0.872000	5.304000	1.158000
H	-0.426000	4.459000	-0.344000
O	-1.282000	2.095000	0.399000
Br	-2.803000	4.661000	3.286000
O	-1.758000	0.128000	-0.467000
C	-2.247000	1.135000	0.088000
O	-3.434000	1.383000	0.388000
H	-1.113000	2.849000	2.991000
H	0.319000	3.981000	1.193000

TS3b_CO₂

C	2.079000	0.613000	-1.884000
C	1.202000	0.331000	-2.996000
N	2.700000	-0.540000	-1.485000
C	2.251000	-1.532000	-2.313000
C	1.306000	-0.998000	-3.255000
C	2.272000	1.882000	-1.321000
H	0.602000	1.063000	-3.517000
C	5.520000	1.328000	2.241000
C	3.148000	2.146000	-0.261000
H	0.806000	-1.573000	-4.023000
N	3.932000	1.220000	0.370000
C	3.318000	3.437000	0.369000
C	4.598000	1.883000	1.361000
C	4.218000	3.270000	1.369000
C	5.928000	0.003000	2.269000

N	5.465000	-0.980000	1.447000
C	6.122000	-2.120000	1.798000
C	6.915000	-0.534000	3.177000
C	7.038000	-1.851000	2.883000
C	2.635000	-2.867000	-2.269000
C	3.555000	-3.424000	-1.394000
N	4.226000	-2.745000	-0.421000
C	5.055000	-3.646000	0.177000
C	3.958000	-4.810000	-1.401000
C	4.891000	-4.947000	-0.426000
C	5.939000	-3.365000	1.211000
H	2.809000	4.345000	0.081000
H	4.599000	4.012000	2.059000
H	7.438000	0.041000	3.931000
H	7.682000	-2.588000	3.344000
H	3.573000	-5.562000	-2.078000
H	5.434000	-5.836000	-0.133000
C	-6.277000	1.317000	-1.442000
C	-4.882000	1.507000	-2.048000
C	-4.211000	2.849000	-1.758000
C	-2.798000	2.823000	-2.312000
C	1.445000	3.009000	-1.842000
C	0.058000	2.951000	-1.693000
C	-0.751000	4.005000	-2.112000
C	-0.172000	5.134000	-2.689000
C	1.209000	5.192000	-2.848000
C	2.019000	4.136000	-2.436000
C	-10.089000	-4.170000	-0.104000
C	-8.734000	-3.999000	-0.788000
C	-7.759000	-3.179000	0.064000
H	-3.163000	-1.654000	1.523000

C	-5.116000	-2.568000	1.392000
C	-4.074000	-1.734000	2.118000
C	-3.705000	-2.346000	3.470000
C	-2.617000	-1.520000	4.157000
H	-4.591000	-2.414000	4.114000
H	-2.324000	-1.963000	5.113000
O	-2.106000	4.006000	-1.918000
H	-0.372000	2.078000	-1.217000
H	3.096000	4.183000	-2.569000
H	1.659000	6.067000	-3.307000
H	-0.812000	5.951000	-3.007000
C	-6.588000	-0.181000	-1.280000
C	-5.934000	-0.703000	0.005000
N	-5.409000	-2.129000	-0.029000
C	-4.145000	-2.128000	-0.881000
C	-0.978000	-4.218000	-1.561000
C	-2.047000	-3.142000	-1.733000
C	-3.239000	-3.347000	-0.788000
H	-0.136000	-4.040000	-2.236000
H	-2.400000	-3.129000	-2.772000
H	-2.851000	-3.457000	0.230000
H	-6.212000	-0.698000	-2.170000
H	-7.667000	-0.363000	-1.248000
H	-6.640000	-0.647000	0.836000
H	-5.068000	-0.092000	0.261000
C	-6.410000	-3.084000	-0.637000
H	-6.339000	1.813000	-0.464000
H	-7.036000	1.788000	-2.075000
H	-4.217000	0.730000	-1.657000
H	-4.944000	1.343000	-3.133000
H	-4.156000	3.011000	-0.675000

H	-4.777000	3.684000	-2.189000
H	-2.801000	2.761000	-3.410000
H	-2.293000	1.934000	-1.921000
H	-8.298000	-4.984000	-0.994000
H	-8.185000	-2.183000	0.231000
H	-10.554000	-3.199000	0.094000
H	-10.773000	-4.750000	-0.731000
H	-9.983000	-4.694000	0.852000
H	-8.869000	-3.506000	-1.758000
H	-7.657000	-3.657000	1.043000
H	-4.804000	-3.614000	1.330000
H	-6.067000	-2.536000	1.926000
H	-4.445000	-0.715000	2.278000
H	-3.345000	-3.372000	3.320000
H	-2.966000	-0.499000	4.351000
H	-1.727000	-1.453000	3.522000
H	-3.580000	-1.242000	-0.586000
H	-4.482000	-1.987000	-1.911000
H	-1.376000	-5.217000	-1.768000
H	-0.584000	-4.216000	-0.538000
H	-1.604000	-2.160000	-1.530000
H	-3.761000	-4.276000	-1.048000
H	-5.926000	-4.064000	-0.656000
H	-6.548000	-2.766000	-1.672000
H	2.189000	-3.529000	-3.005000
H	5.971000	1.999000	2.965000
H	6.539000	-4.187000	1.590000
Al	4.057000	-0.771000	0.005000
Br	5.907000	-0.323000	-1.652000
C	0.637000	-1.409000	0.802000
C	1.573000	-0.470000	1.531000

H	0.744000	-1.455000	-0.275000
H	1.551000	0.519000	1.059000
C	1.289000	-0.337000	3.018000
H	0.326000	0.148000	3.198000
H	2.083000	0.263000	3.474000
O	2.765000	-1.157000	1.306000
H	0.430000	-2.354000	1.293000
H	1.294000	-1.325000	3.492000
C	-2.489000	2.551000	2.420000
C	-1.370000	2.517000	1.380000
H	-3.203000	1.749000	2.252000
H	-1.779000	2.822000	0.413000
C	-0.178000	3.373000	1.757000
H	-0.489000	4.416000	1.853000
H	0.594000	3.306000	0.987000
O	-0.885000	1.167000	1.278000
Br	-3.515000	4.203000	2.235000
O	-1.265000	-0.941000	0.683000
C	-1.695000	0.268000	0.676000
O	-2.782000	0.606000	0.202000
H	-2.107000	2.525000	3.441000
H	0.249000	3.039000	2.708000

I4b_CO₂

C	2.079000	0.613000	-1.884000
C	1.202000	0.331000	-2.996000
N	2.700000	-0.540000	-1.485000
C	2.251000	-1.532000	-2.313000
C	1.306000	-0.998000	-3.255000
C	2.272000	1.882000	-1.321000
H	0.602000	1.063000	-3.517000

C	5.520000	1.328000	2.241000
C	3.148000	2.146000	-0.261000
H	0.806000	-1.573000	-4.023000
N	3.932000	1.220000	0.370000
C	3.318000	3.437000	0.369000
C	4.598000	1.883000	1.361000
C	4.218000	3.270000	1.369000
C	5.928000	0.003000	2.269000
N	5.465000	-0.980000	1.447000
C	6.122000	-2.120000	1.798000
C	6.915000	-0.534000	3.177000
C	7.038000	-1.851000	2.883000
C	2.635000	-2.867000	-2.269000
C	3.555000	-3.424000	-1.394000
N	4.226000	-2.745000	-0.421000
C	5.055000	-3.646000	0.177000
C	3.958000	-4.810000	-1.401000
C	4.891000	-4.947000	-0.426000
C	5.939000	-3.365000	1.211000
H	2.809000	4.345000	0.081000
H	4.599000	4.012000	2.059000
H	7.438000	0.041000	3.931000
H	7.682000	-2.588000	3.344000
H	3.573000	-5.562000	-2.078000
H	5.434000	-5.836000	-0.133000
C	-6.277000	1.317000	-1.442000
C	-4.882000	1.507000	-2.048000
C	-4.211000	2.849000	-1.758000
C	-2.798000	2.823000	-2.312000
C	1.445000	3.009000	-1.842000
C	0.058000	2.951000	-1.693000

C	-0.751000	4.005000	-2.112000
C	-0.172000	5.134000	-2.689000
C	1.209000	5.192000	-2.848000
C	2.019000	4.136000	-2.436000
C	-10.089000	-4.170000	-0.104000
C	-8.734000	-3.999000	-0.788000
C	-7.759000	-3.179000	0.064000
H	-3.163000	-1.654000	1.523000
C	-5.116000	-2.568000	1.392000
C	-4.074000	-1.734000	2.118000
C	-3.705000	-2.346000	3.470000
C	-2.617000	-1.520000	4.157000
H	-4.591000	-2.414000	4.114000
H	-2.324000	-1.963000	5.113000
O	-2.106000	4.006000	-1.918000
H	-0.372000	2.078000	-1.217000
H	3.096000	4.183000	-2.569000
H	1.659000	6.067000	-3.307000
H	-0.812000	5.951000	-3.007000
C	-6.588000	-0.181000	-1.280000
C	-5.934000	-0.703000	0.005000
N	-5.409000	-2.129000	-0.029000
C	-4.145000	-2.128000	-0.881000
C	-0.978000	-4.218000	-1.561000
C	-2.047000	-3.142000	-1.733000
C	-3.239000	-3.347000	-0.788000
H	-0.136000	-4.040000	-2.236000
H	-2.400000	-3.129000	-2.772000
H	-2.851000	-3.457000	0.230000
H	-6.212000	-0.698000	-2.170000
H	-7.667000	-0.363000	-1.248000

H	-6.640000	-0.647000	0.836000
H	-5.068000	-0.092000	0.261000
C	-6.410000	-3.084000	-0.637000
H	-6.339000	1.813000	-0.464000
H	-7.036000	1.788000	-2.075000
H	-4.217000	0.730000	-1.657000
H	-4.944000	1.343000	-3.133000
H	-4.156000	3.011000	-0.675000
H	-4.777000	3.684000	-2.189000
H	-2.801000	2.761000	-3.410000
H	-2.293000	1.934000	-1.921000
H	-8.298000	-4.984000	-0.994000
H	-8.185000	-2.183000	0.231000
H	-10.554000	-3.199000	0.094000
H	-10.773000	-4.750000	-0.731000
H	-9.983000	-4.694000	0.852000
H	-8.869000	-3.506000	-1.758000
H	-7.657000	-3.657000	1.043000
H	-4.804000	-3.614000	1.330000
H	-6.067000	-2.536000	1.926000
H	-4.445000	-0.715000	2.278000
H	-3.345000	-3.372000	3.320000
H	-2.966000	-0.499000	4.351000
H	-1.727000	-1.453000	3.522000
H	-3.580000	-1.242000	-0.586000
H	-4.482000	-1.987000	-1.911000
H	-1.376000	-5.217000	-1.768000
H	-0.584000	-4.216000	-0.538000
H	-1.604000	-2.160000	-1.530000
H	-3.761000	-4.276000	-1.048000
H	-5.926000	-4.064000	-0.656000

H	-6.548000	-2.766000	-1.672000
H	2.189000	-3.529000	-3.005000
H	5.971000	1.999000	2.965000
H	6.539000	-4.187000	1.590000
Al	4.057000	-0.771000	0.005000
Br	5.907000	-0.323000	-1.652000
C	0.637000	-1.409000	0.802000
C	1.573000	-0.470000	1.531000
H	0.744000	-1.455000	-0.275000
H	1.551000	0.519000	1.059000
C	1.289000	-0.337000	3.018000
H	0.326000	0.148000	3.198000
H	2.083000	0.263000	3.474000
O	2.765000	-1.157000	1.306000
H	0.430000	-2.354000	1.293000
H	1.294000	-1.325000	3.492000
C	-2.489000	2.551000	2.420000
C	-1.370000	2.517000	1.380000
H	-3.203000	1.749000	2.252000
H	-1.779000	2.822000	0.413000
C	-0.178000	3.373000	1.757000
H	-0.489000	4.416000	1.853000
H	0.594000	3.306000	0.987000
O	-0.885000	1.167000	1.278000
Br	-3.515000	4.203000	2.235000
O	-1.265000	-0.941000	0.683000
C	-1.695000	0.268000	0.676000
O	-2.782000	0.606000	0.202000
H	-2.107000	2.525000	3.441000
H	0.249000	3.039000	2.708000

I2_TsN

C	3.502000	2.443000	-0.643000
C	4.288000	3.103000	-1.659000
N	3.938000	1.159000	-0.480000
C	4.975000	0.990000	-1.348000
C	5.205000	2.202000	-2.089000
C	2.416000	3.022000	0.017000
H	4.149000	4.123000	-1.989000
C	0.661000	-0.338000	3.035000
C	1.644000	2.380000	0.991000
H	5.974000	2.331000	-2.840000
N	1.808000	1.089000	1.409000
C	0.531000	2.980000	1.684000
C	0.849000	0.858000	2.349000
C	0.043000	2.036000	2.531000
C	1.399000	-1.499000	2.875000
N	2.425000	-1.665000	1.992000
C	2.905000	-2.925000	2.195000
C	1.212000	-2.702000	3.653000
C	2.144000	-3.588000	3.228000
C	5.710000	-0.178000	-1.521000
C	5.521000	-1.367000	-0.834000
N	4.555000	-1.590000	0.102000
C	4.747000	-2.860000	0.556000
C	6.344000	-2.543000	-0.991000
C	5.867000	-3.468000	-0.124000
C	3.986000	-3.489000	1.531000
C	-0.043000	0.236000	-0.943000
C	1.780000	0.358000	-2.718000
H	0.187000	3.996000	1.546000
H	-0.772000	2.129000	3.238000
H	0.473000	-2.826000	4.434000

H	2.326000	-4.596000	3.578000
H	7.181000	-2.625000	-1.673000
H	6.226000	-4.473000	0.056000
C	-2.975000	3.396000	0.204000
C	-3.542000	4.537000	-0.645000
C	-2.472000	5.553000	-1.055000
C	-1.752000	5.118000	-2.330000
C	1.990000	4.383000	-0.424000
C	0.873000	4.487000	-1.258000
C	0.466000	5.735000	-1.728000
C	1.182000	6.880000	-1.372000
C	2.294000	6.771000	-0.547000
C	2.699000	5.528000	-0.064000
C	-7.891000	1.530000	4.421000
C	-7.474000	1.021000	3.043000
C	-5.992000	0.634000	2.998000
H	-2.195000	0.149000	3.399000
C	-3.508000	-1.096000	2.223000
C	-3.012000	-0.560000	3.560000
C	-2.497000	-1.738000	4.394000
C	-1.980000	-1.303000	5.763000
H	-3.304000	-2.468000	4.527000
H	-1.610000	-2.162000	6.330000
O	-0.592000	5.906000	-2.575000
H	0.355000	3.580000	-1.553000
H	3.565000	5.440000	0.585000
H	2.845000	7.664000	-0.269000
H	0.849000	7.842000	-1.748000
C	-3.929000	2.202000	0.243000
C	-3.443000	1.168000	1.242000
N	-4.208000	-0.137000	1.266000

C	-4.124000	-0.812000	-0.111000
C	-5.936000	-1.064000	-3.513000
C	-4.828000	-1.160000	-2.468000
C	-5.250000	-0.577000	-1.115000
H	-5.602000	-1.475000	-4.471000
H	-3.939000	-0.624000	-2.820000
H	-6.171000	-1.067000	-0.783000
H	-3.959000	1.780000	-0.765000
H	-4.939000	2.544000	0.497000
H	-3.475000	1.580000	2.250000
H	-2.403000	0.900000	1.031000
C	-5.663000	0.046000	1.632000
H	-2.015000	3.055000	-0.204000
H	-2.768000	3.764000	1.217000
H	-4.015000	4.123000	-1.547000
H	-4.343000	5.034000	-0.085000
H	-1.740000	5.660000	-0.245000
H	-2.909000	6.543000	-1.220000
H	-2.392000	5.282000	-3.201000
H	-1.510000	4.048000	-2.307000
H	-8.087000	0.153000	2.770000
H	-5.389000	1.524000	3.210000
Br	-1.440000	0.887000	-2.194000
H	-7.304000	2.410000	4.709000
H	-8.948000	1.814000	4.430000
H	-7.742000	0.761000	5.186000
H	-7.669000	1.793000	2.288000
H	-5.794000	-0.096000	3.789000
H	-2.655000	-1.498000	1.672000
H	-4.213000	-1.919000	2.370000
H	-3.788000	-0.035000	4.121000

H	-1.705000	-2.252000	3.834000
H	-2.777000	-0.831000	6.350000
H	-1.160000	-0.581000	5.680000
H	-4.039000	-1.883000	0.079000
H	-3.175000	-0.473000	-0.533000
H	-6.233000	-0.023000	-3.678000
H	-6.825000	-1.623000	-3.199000
H	-4.529000	-2.208000	-2.341000
H	-5.477000	0.484000	-1.247000
H	-6.116000	-0.944000	1.538000
H	-6.093000	0.680000	0.857000
H	0.289000	1.139000	-0.443000
H	-0.546000	-0.424000	-0.235000
H	1.112000	0.463000	-3.579000
H	2.033000	1.358000	-2.356000
H	6.515000	-0.149000	-2.248000
H	-0.115000	-0.353000	3.791000
H	4.259000	-4.505000	1.798000
H	2.702000	-0.132000	-3.043000
O	1.971000	-0.905000	-0.621000
C	1.128000	-0.491000	-1.623000
H	0.707000	-1.381000	-2.127000
Al	3.115000	-0.280000	0.677000
Br	4.724000	0.486000	2.538000
C	1.194000	-3.744000	-0.540000
O	2.194000	-3.996000	-1.064000
S	-1.312000	-4.250000	-0.262000
O	-2.299000	-3.475000	0.472000
O	-1.161000	-5.667000	0.018000
C	-1.537000	-4.014000	-2.001000
C	-1.821000	-3.594000	-4.736000

C	-1.641000	-2.714000	-2.488000
C	-1.575000	-5.111000	-2.852000
C	-1.771000	-2.510000	-3.851000
C	-1.729000	-4.889000	-4.218000
C	-1.947000	-3.356000	-6.218000
H	-1.612000	-1.865000	-1.816000
H	-1.486000	-6.116000	-2.456000
H	-1.822000	-1.491000	-4.223000
H	-1.767000	-5.740000	-4.891000
H	-2.212000	-4.272000	-6.751000
H	-2.707000	-2.598000	-6.431000
H	-0.998000	-2.991000	-6.627000
N	0.141000	-3.459000	0.033000

TS2_TsN

C	3.434000	2.554000	-0.549000
C	4.233000	3.264000	-1.517000
N	3.904000	1.278000	-0.401000
C	4.972000	1.165000	-1.243000
C	5.189000	2.401000	-1.942000
C	2.302000	3.079000	0.076000
H	4.073000	4.287000	-1.825000
C	0.547000	-0.426000	2.924000
C	1.512000	2.376000	0.990000
H	5.977000	2.573000	-2.664000
N	1.714000	1.081000	1.386000
C	0.344000	2.911000	1.641000
C	0.716000	0.789000	2.272000
C	-0.146000	1.925000	2.439000
C	1.352000	-1.541000	2.783000
N	2.434000	-1.637000	1.956000

C	2.950000	-2.887000	2.154000
C	1.169000	-2.769000	3.514000
C	2.161000	-3.606000	3.123000
C	5.749000	0.027000	-1.425000
C	5.581000	-1.179000	-0.767000
N	4.602000	-1.451000	0.145000
C	4.832000	-2.724000	0.579000
C	6.448000	-2.322000	-0.925000
C	5.986000	-3.278000	-0.086000
C	4.071000	-3.401000	1.519000
C	-0.118000	0.114000	-1.031000
C	1.787000	0.610000	-2.663000
H	-0.033000	3.916000	1.512000
H	-0.996000	1.967000	3.108000
H	0.385000	-2.945000	4.239000
H	2.359000	-4.618000	3.450000
H	7.302000	-2.360000	-1.589000
H	6.376000	-4.273000	0.085000
C	-3.090000	3.184000	0.146000
C	-3.678000	4.307000	-0.714000
C	-2.648000	5.378000	-1.082000
C	-1.880000	4.999000	-2.345000
C	1.837000	4.428000	-0.357000
C	0.740000	4.493000	-1.220000
C	0.288000	5.725000	-1.688000
C	0.941000	6.896000	-1.303000
C	2.035000	6.827000	-0.449000
C	2.484000	5.600000	0.035000
C	-8.151000	1.394000	4.133000
C	-7.671000	0.864000	2.784000
C	-6.192000	0.463000	2.817000

H	-2.351000	-0.073000	3.347000
C	-3.708000	-1.304000	2.213000
C	-3.207000	-0.730000	3.533000
C	-2.741000	-1.887000	4.425000
C	-2.195000	-1.402000	5.766000
H	-3.578000	-2.575000	4.598000
H	-1.855000	-2.244000	6.376000
O	-0.757000	5.849000	-2.559000
H	0.268000	3.567000	-1.533000
H	3.335000	5.544000	0.706000
H	2.538000	7.742000	-0.148000
H	0.576000	7.847000	-1.678000
C	-4.009000	1.964000	0.154000
C	-3.556000	0.947000	1.187000
N	-4.330000	-0.351000	1.197000
C	-4.169000	-1.038000	-0.165000
C	-5.719000	-1.232000	-3.694000
C	-4.695000	-1.344000	-2.569000
C	-5.218000	-0.779000	-1.243000
H	-5.312000	-1.626000	-4.630000
H	-3.783000	-0.800000	-2.843000
H	-6.165000	-1.266000	-0.985000
H	-3.994000	1.533000	-0.850000
H	-5.036000	2.287000	0.365000
H	-3.635000	1.380000	2.185000
H	-2.508000	0.671000	1.029000
C	-5.799000	-0.143000	1.476000
H	-2.106000	2.879000	-0.228000
H	-2.932000	3.559000	1.166000
H	-4.106000	3.882000	-1.634000
H	-4.516000	4.761000	-0.173000

H	-1.944000	5.511000	-0.251000
H	-3.129000	6.348000	-1.246000
H	-2.510000	5.141000	-3.227000
H	-1.583000	3.943000	-2.332000
H	-8.278000	-0.001000	2.491000
H	-5.592000	1.350000	3.049000
Br	-1.488000	0.711000	-2.317000
H	-7.571000	2.272000	4.440000
H	-9.204000	1.687000	4.086000
H	-8.047000	0.633000	4.914000
H	-7.820000	1.629000	2.011000
H	-6.039000	-0.260000	3.624000
H	-2.870000	-1.788000	1.712000
H	-4.463000	-2.077000	2.383000
H	-3.957000	-0.139000	4.065000
H	-1.974000	-2.462000	3.891000
H	-2.963000	-0.864000	6.331000
H	-1.345000	-0.723000	5.632000
H	-4.116000	-2.109000	0.032000
H	-3.184000	-0.727000	-0.519000
H	-6.006000	-0.188000	-3.864000
H	-6.628000	-1.796000	-3.459000
H	-4.401000	-2.392000	-2.436000
H	-5.428000	0.286000	-1.378000
H	-6.261000	-1.128000	1.368000
H	-6.180000	0.485000	0.670000
H	0.069000	0.985000	-0.409000
H	-0.573000	-0.687000	-0.451000
H	1.143000	0.729000	-3.540000
H	1.920000	1.590000	-2.203000
H	6.571000	0.099000	-2.130000

H	-0.274000	-0.499000	3.629000
H	4.366000	-4.415000	1.768000
H	2.763000	0.243000	-2.990000
O	2.008000	-0.886000	-0.704000
C	1.152000	-0.398000	-1.716000
H	0.865000	-1.260000	-2.340000
Al	3.127000	-0.198000	0.723000
Br	4.646000	0.599000	2.623000
C	1.467000	-2.823000	-0.620000
O	2.325000	-3.397000	-1.179000
S	-0.817000	-3.805000	-0.087000
O	-1.965000	-3.121000	0.518000
O	-0.440000	-5.115000	0.429000
C	-1.129000	-3.933000	-1.832000
C	-1.572000	-4.053000	-4.583000
C	-1.409000	-2.766000	-2.536000
C	-1.056000	-5.157000	-2.479000
C	-1.619000	-2.830000	-3.902000
C	-1.291000	-5.210000	-3.853000
C	-1.791000	-4.102000	-6.072000
H	-1.433000	-1.797000	-2.063000
H	-0.822000	-6.053000	-1.914000
H	-1.815000	-1.907000	-4.446000
H	-1.245000	-6.168000	-4.363000
H	-1.961000	-5.124000	-6.419000
H	-2.652000	-3.491000	-6.365000
H	-0.916000	-3.708000	-6.603000
N	0.370000	-2.690000	0.005000

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C	1.234000	3.461000	0.003000
C	1.457000	4.604000	-0.854000
N	2.304000	2.614000	-0.064000
C	3.196000	3.191000	-0.919000
C	2.668000	4.428000	-1.432000
C	0.063000	3.247000	0.738000
H	0.761000	5.418000	-0.998000
C	0.601000	-1.081000	2.868000
C	-0.191000	2.072000	1.460000
H	3.177000	5.071000	-2.139000
N	0.657000	1.002000	1.569000
C	-1.380000	1.827000	2.237000
C	0.048000	0.105000	2.401000
C	-1.238000	0.602000	2.804000
C	1.880000	-1.545000	2.612000
N	2.806000	-0.905000	1.841000
C	3.941000	-1.657000	1.905000
C	2.440000	-2.751000	3.166000
C	3.723000	-2.818000	2.729000
C	4.450000	2.698000	-1.239000
C	5.020000	1.546000	-0.716000
N	4.412000	0.685000	0.149000
C	5.350000	-0.285000	0.432000
C	6.361000	1.109000	-1.006000
C	6.567000	-0.019000	-0.284000
C	5.137000	-1.365000	1.267000
C	-1.835000	0.781000	-1.747000
C	-0.655000	2.599000	-3.089000
H	-2.203000	2.518000	2.350000
H	-1.919000	0.094000	3.475000
H	1.912000	-3.435000	3.818000

H	4.470000	-3.573000	2.940000
H	7.047000	1.619000	-1.670000
H	7.456000	-0.634000	-0.234000
C	-4.447000	0.725000	0.690000
C	-5.647000	1.587000	0.300000
C	-5.408000	3.074000	0.617000
C	-4.939000	3.864000	-0.606000
C	-0.940000	4.352000	0.769000
C	-2.224000	4.174000	0.238000
C	-3.156000	5.212000	0.267000
C	-2.800000	6.444000	0.824000
C	-1.528000	6.621000	1.349000
C	-0.597000	5.583000	1.331000
C	-7.389000	-4.783000	2.455000
C	-6.627000	-4.466000	1.170000
C	-5.216000	-3.940000	1.454000
H	-1.948000	-2.356000	2.856000
C	-2.175000	-3.665000	1.153000
C	-2.204000	-3.399000	2.653000
C	-1.151000	-4.286000	3.328000
C	-1.119000	-4.088000	4.842000
H	-1.356000	-5.339000	3.100000
H	-0.349000	-4.716000	5.301000
O	-4.414000	5.135000	-0.247000
H	-2.477000	3.220000	-0.207000
H	0.392000	5.720000	1.756000
H	-1.259000	7.577000	1.787000
H	-3.534000	7.243000	0.836000
C	-4.554000	-0.719000	0.199000
C	-3.383000	-1.523000	0.755000
N	-3.176000	-2.935000	0.247000

C	-2.494000	-2.961000	-1.121000
C	-3.074000	-2.219000	-4.859000
C	-2.374000	-2.693000	-3.588000
C	-3.289000	-2.583000	-2.361000
H	-2.426000	-2.353000	-5.731000
H	-1.469000	-2.101000	-3.419000
H	-4.157000	-3.237000	-2.497000
H	-4.581000	-0.714000	-0.891000
H	-5.503000	-1.143000	0.547000
H	-3.527000	-1.606000	1.830000
H	-2.431000	-1.006000	0.600000
C	-4.478000	-3.687000	0.146000
H	-3.530000	1.174000	0.292000
H	-4.333000	0.739000	1.782000
H	-5.849000	1.459000	-0.772000
H	-6.537000	1.225000	0.827000
H	-4.651000	3.160000	1.407000
H	-6.317000	3.543000	1.008000
H	-5.786000	4.084000	-1.261000
H	-4.218000	3.295000	-1.204000
H	-6.563000	-5.366000	0.546000
H	-5.294000	-3.022000	2.048000
Br	-3.544000	1.130000	-2.614000
H	-7.485000	-3.891000	3.084000
H	-8.396000	-5.148000	2.233000
H	-6.873000	-5.552000	3.039000
H	-7.180000	-3.719000	0.587000
H	-4.676000	-4.676000	2.058000
H	-1.184000	-3.399000	0.777000
H	-2.334000	-4.728000	0.950000
H	-3.184000	-3.590000	3.099000

H	-0.168000	-4.060000	2.899000
H	-2.081000	-4.351000	5.295000
H	-0.903000	-3.046000	5.107000
H	-2.118000	-3.981000	-1.233000
H	-1.620000	-2.317000	-1.016000
H	-3.321000	-1.155000	-4.780000
H	-4.002000	-2.775000	-5.039000
H	-2.034000	-3.729000	-3.699000
H	-3.654000	-1.557000	-2.308000
H	-4.242000	-4.635000	-0.344000
H	-5.112000	-3.116000	-0.533000
H	-1.810000	1.357000	-0.822000
H	-1.821000	-0.283000	-1.524000
H	-1.458000	2.755000	-3.812000
H	-0.803000	3.275000	-2.242000
H	5.052000	3.282000	-1.928000
H	-0.007000	-1.671000	3.545000
H	5.960000	-2.058000	1.409000
H	0.302000	2.841000	-3.560000
O	0.501000	1.030000	-1.760000
C	-0.640000	1.157000	-2.617000
H	-0.549000	0.461000	-3.454000
C	1.009000	-0.177000	-1.465000
O	1.939000	-0.191000	-0.627000
Al	2.565000	0.870000	0.911000
Br	3.415000	2.064000	2.905000
S	1.045000	-2.705000	-1.701000
O	0.481000	-3.626000	-2.690000
O	0.756000	-3.019000	-0.291000
C	2.818000	-2.710000	-1.902000
C	5.586000	-2.819000	-2.237000

C	3.413000	-2.018000	-2.959000
C	3.584000	-3.457000	-1.021000
C	4.788000	-2.069000	-3.110000
C	4.964000	-3.515000	-1.201000
C	7.081000	-2.863000	-2.421000
H	2.804000	-1.430000	-3.637000
H	3.113000	-3.957000	-0.182000
H	5.260000	-1.511000	-3.915000
H	5.566000	-4.090000	-0.504000
H	7.581000	-3.262000	-1.533000
H	7.354000	-3.496000	-3.272000
H	7.479000	-1.861000	-2.615000
N	0.502000	-1.223000	-2.108000

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C	1.234000	3.461000	0.003000
C	1.457000	4.604000	-0.854000
N	2.304000	2.614000	-0.064000
C	3.196000	3.191000	-0.919000
C	2.668000	4.428000	-1.432000
C	0.063000	3.247000	0.738000
H	0.761000	5.418000	-0.998000
C	0.601000	-1.081000	2.868000
C	-0.191000	2.072000	1.460000
H	3.177000	5.071000	-2.139000
N	0.657000	1.002000	1.569000
C	-1.380000	1.827000	2.237000
C	0.048000	0.105000	2.401000
C	-1.238000	0.602000	2.804000
C	1.880000	-1.545000	2.612000
N	2.806000	-0.905000	1.841000

C	3.941000	-1.657000	1.905000
C	2.440000	-2.751000	3.166000
C	3.723000	-2.818000	2.729000
C	4.450000	2.698000	-1.239000
C	5.020000	1.546000	-0.716000
N	4.412000	0.685000	0.149000
C	5.350000	-0.285000	0.432000
C	6.361000	1.109000	-1.006000
C	6.567000	-0.019000	-0.284000
C	5.137000	-1.365000	1.267000
C	-1.835000	0.781000	-1.747000
C	-0.655000	2.599000	-3.089000
H	-2.203000	2.518000	2.350000
H	-1.919000	0.094000	3.475000
H	1.912000	-3.435000	3.818000
H	4.470000	-3.573000	2.940000
H	7.047000	1.619000	-1.670000
H	7.456000	-0.634000	-0.234000
C	-4.447000	0.725000	0.690000
C	-5.647000	1.587000	0.300000
C	-5.408000	3.074000	0.617000
C	-4.939000	3.864000	-0.606000
C	-0.940000	4.352000	0.769000
C	-2.224000	4.174000	0.238000
C	-3.156000	5.212000	0.267000
C	-2.800000	6.444000	0.824000
C	-1.528000	6.621000	1.349000
C	-0.597000	5.583000	1.331000
C	-7.389000	-4.783000	2.455000
C	-6.627000	-4.466000	1.170000
C	-5.216000	-3.940000	1.454000

H	-1.948000	-2.356000	2.856000
C	-2.175000	-3.665000	1.153000
C	-2.204000	-3.399000	2.653000
C	-1.151000	-4.286000	3.328000
C	-1.119000	-4.088000	4.842000
H	-1.356000	-5.339000	3.100000
H	-0.349000	-4.716000	5.301000
O	-4.414000	5.135000	-0.247000
H	-2.477000	3.220000	-0.207000
H	0.392000	5.720000	1.756000
H	-1.259000	7.577000	1.787000
H	-3.534000	7.243000	0.836000
C	-4.554000	-0.719000	0.199000
C	-3.383000	-1.523000	0.755000
N	-3.176000	-2.935000	0.247000
C	-2.494000	-2.961000	-1.121000
C	-3.074000	-2.219000	-4.859000
C	-2.374000	-2.693000	-3.588000
C	-3.289000	-2.583000	-2.361000
H	-2.426000	-2.353000	-5.731000
H	-1.469000	-2.101000	-3.419000
H	-4.157000	-3.237000	-2.497000
H	-4.581000	-0.714000	-0.891000
H	-5.503000	-1.143000	0.547000
H	-3.527000	-1.606000	1.830000
H	-2.431000	-1.006000	0.600000
C	-4.478000	-3.687000	0.146000
H	-3.530000	1.174000	0.292000
H	-4.333000	0.739000	1.782000
H	-5.849000	1.459000	-0.772000
H	-6.537000	1.225000	0.827000

H	-4.651000	3.160000	1.407000
H	-6.317000	3.543000	1.008000
H	-5.786000	4.084000	-1.261000
H	-4.218000	3.295000	-1.204000
H	-6.563000	-5.366000	0.546000
H	-5.294000	-3.022000	2.048000
Br	-3.544000	1.130000	-2.614000
H	-7.485000	-3.891000	3.084000
H	-8.396000	-5.148000	2.233000
H	-6.873000	-5.552000	3.039000
H	-7.180000	-3.719000	0.587000
H	-4.676000	-4.676000	2.058000
H	-1.184000	-3.399000	0.777000
H	-2.334000	-4.728000	0.950000
H	-3.184000	-3.590000	3.099000
H	-0.168000	-4.060000	2.899000
H	-2.081000	-4.351000	5.295000
H	-0.903000	-3.046000	5.107000
H	-2.118000	-3.981000	-1.233000
H	-1.620000	-2.317000	-1.016000
H	-3.321000	-1.155000	-4.780000
H	-4.002000	-2.775000	-5.039000
H	-2.034000	-3.729000	-3.699000
H	-3.654000	-1.557000	-2.308000
H	-4.242000	-4.635000	-0.344000
H	-5.112000	-3.116000	-0.533000
H	-1.810000	1.357000	-0.822000
H	-1.821000	-0.283000	-1.524000
H	-1.458000	2.755000	-3.812000
H	-0.803000	3.275000	-2.242000
H	5.052000	3.282000	-1.928000

H	-0.007000	-1.671000	3.545000
H	5.960000	-2.058000	1.409000
H	0.302000	2.841000	-3.560000
O	0.501000	1.030000	-1.760000
C	-0.640000	1.157000	-2.617000
H	-0.549000	0.461000	-3.454000
C	1.009000	-0.177000	-1.465000
O	1.939000	-0.191000	-0.627000
Al	2.565000	0.870000	0.911000
Br	3.415000	2.064000	2.905000
S	1.045000	-2.705000	-1.701000
O	0.481000	-3.626000	-2.690000
O	0.756000	-3.019000	-0.291000
C	2.818000	-2.710000	-1.902000
C	5.586000	-2.819000	-2.237000
C	3.413000	-2.018000	-2.959000
C	3.584000	-3.457000	-1.021000
C	4.788000	-2.069000	-3.110000
C	4.964000	-3.515000	-1.201000
C	7.081000	-2.863000	-2.421000
H	2.804000	-1.430000	-3.637000
H	3.113000	-3.957000	-0.182000
H	5.260000	-1.511000	-3.915000
H	5.566000	-4.090000	-0.504000
H	7.581000	-3.262000	-1.533000
H	7.354000	-3.496000	-3.272000
H	7.479000	-1.861000	-2.615000
N	0.502000	-1.223000	-2.108000

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C	3.069000	2.518000	-0.541000
C	3.705000	3.297000	-1.565000
N	3.645000	1.268000	-0.463000
C	4.617000	1.258000	-1.433000
C	4.669000	2.515000	-2.113000
C	1.967000	2.944000	0.197000
H	3.426000	4.304000	-1.838000
C	0.928000	-0.646000	3.278000
C	1.348000	2.152000	1.159000
H	5.347000	2.749000	-2.922000
N	1.738000	0.883000	1.535000
C	0.222000	2.578000	1.939000
C	0.889000	0.534000	2.556000
C	-0.062000	1.574000	2.804000
C	1.797000	-1.686000	3.033000
N	2.757000	-1.690000	2.053000
C	3.338000	-2.929000	2.126000
C	1.791000	-2.934000	3.745000
C	2.747000	-3.708000	3.177000
C	5.419000	0.178000	-1.757000
C	5.368000	-1.049000	-1.131000
N	4.554000	-1.366000	-0.069000
C	4.871000	-2.664000	0.247000
C	6.187000	-2.169000	-1.497000
C	5.880000	-3.172000	-0.641000
C	4.330000	-3.393000	1.286000
H	-0.275000	3.532000	1.835000
H	-0.834000	1.535000	3.561000
H	1.129000	-3.170000	4.567000
H	3.037000	-4.719000	3.428000
H	6.899000	-2.167000	-2.312000

H	6.285000	-4.173000	-0.596000
C	-3.378000	2.860000	0.947000
C	-4.088000	4.141000	0.496000
C	-3.101000	5.256000	0.136000
C	-2.598000	5.104000	-1.297000
C	1.420000	4.306000	-0.070000
C	0.178000	4.450000	-0.699000
C	-0.318000	5.732000	-0.954000
C	0.436000	6.856000	-0.603000
C	1.671000	6.702000	0.012000
C	2.164000	5.430000	0.291000
C	-7.493000	-0.353000	5.019000
C	-7.264000	-0.491000	3.516000
C	-5.789000	-0.733000	3.178000
H	-1.932000	-1.012000	2.907000
C	-3.384000	-2.042000	1.687000
C	-2.679000	-1.803000	3.017000
C	-1.959000	-3.090000	3.446000
C	-1.604000	-3.076000	4.932000
H	-2.595000	-3.962000	3.245000
H	-1.036000	-3.969000	5.211000
O	-1.504000	5.981000	-1.572000
H	-0.377000	3.563000	-0.997000
H	3.122000	5.303000	0.784000
H	2.247000	7.580000	0.289000
H	0.029000	7.839000	-0.814000
C	-4.270000	1.630000	0.793000
C	-3.547000	0.407000	1.325000
N	-4.243000	-0.923000	1.103000
C	-4.320000	-1.229000	-0.401000
C	-6.560000	-0.758000	-3.511000

C	-5.326000	-1.071000	-2.668000
C	-5.565000	-0.809000	-1.176000
H	-6.364000	-0.940000	-4.572000
H	-4.482000	-0.453000	-2.995000
H	-6.443000	-1.376000	-0.847000
H	-4.458000	1.520000	-0.276000
H	-5.225000	1.786000	1.312000
H	-3.390000	0.506000	2.399000
H	-2.568000	0.315000	0.844000
C	-5.637000	-0.945000	1.677000
H	-2.491000	2.686000	0.328000
H	-3.037000	2.974000	1.984000
H	-4.713000	3.919000	-0.381000
H	-4.773000	4.478000	1.282000
H	-2.249000	5.228000	0.828000
H	-3.562000	6.244000	0.245000
H	-3.377000	5.410000	-2.001000
H	-2.347000	4.065000	-1.536000
H	-7.869000	-1.319000	3.125000
H	-5.201000	0.125000	3.522000
H	-6.914000	0.482000	5.430000
H	-8.549000	-0.171000	5.239000
H	-7.191000	-1.264000	5.549000
H	-7.607000	0.417000	3.005000
H	-5.440000	-1.613000	3.728000
H	-2.616000	-2.238000	0.939000
H	-4.046000	-2.910000	1.749000
H	-3.376000	-1.498000	3.801000
H	-1.055000	-3.213000	2.838000
H	-2.509000	-3.049000	5.549000
H	-1.004000	-2.198000	5.197000

H	-4.212000	-2.313000	-0.486000
H	-3.438000	-0.750000	-0.836000
H	-6.851000	0.293000	-3.401000
H	-7.414000	-1.377000	-3.214000
H	-5.037000	-2.121000	-2.813000
H	-5.791000	0.252000	-1.043000
H	-6.060000	-1.913000	1.396000
H	-6.199000	-0.177000	1.146000
H	6.128000	0.303000	-2.568000
H	0.208000	-0.764000	4.080000
H	4.692000	-4.404000	1.438000
Al	3.403000	-0.109000	0.995000
Br	4.954000	0.741000	2.536000
C	0.783000	-0.046000	-1.637000
C	1.384000	1.334000	-3.700000
H	1.376000	0.702000	-1.116000
H	-0.267000	0.112000	-1.397000
H	0.520000	1.988000	-3.544000
H	2.254000	1.761000	-3.196000
H	1.586000	1.269000	-4.773000
O	2.147000	-0.951000	-3.291000
C	1.039000	-0.018000	-3.135000
H	0.189000	-0.451000	-3.675000
C	2.109000	-1.865000	-2.312000
O	2.689000	-2.916000	-2.336000
S	0.231000	-2.464000	-0.487000
O	-0.638000	-1.603000	0.305000
O	1.012000	-3.504000	0.148000
C	-0.715000	-3.191000	-1.803000
C	-2.125000	-4.335000	-3.914000
C	-1.596000	-2.399000	-2.543000

C	-0.524000	-4.535000	-2.101000
C	-2.286000	-2.981000	-3.595000
C	-1.240000	-5.100000	-3.151000
C	-2.876000	-4.935000	-5.073000
H	-1.741000	-1.340000	-2.333000
H	0.175000	-5.125000	-1.518000
H	-2.963000	-2.367000	-4.183000
H	-1.099000	-6.152000	-3.384000
H	-2.823000	-6.027000	-5.064000
H	-3.929000	-4.639000	-5.055000
H	-2.456000	-4.585000	-6.023000
N	1.275000	-1.384000	-1.271000
Br	-2.333000	1.326000	-2.206000

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C	2.661000	1.310000	-1.736000
C	2.136000	1.042000	-3.050000
N	3.465000	0.273000	-1.330000
C	3.473000	-0.622000	-2.367000
C	2.628000	-0.161000	-3.432000
C	2.397000	2.465000	-1.001000
H	1.472000	1.696000	-3.596000
C	4.826000	2.038000	3.174000
C	2.881000	2.691000	0.291000
H	2.456000	-0.695000	-4.357000
N	3.747000	1.881000	0.975000
C	2.513000	3.818000	1.110000
C	3.955000	2.480000	2.188000
C	3.171000	3.679000	2.289000
C	5.634000	0.916000	3.092000
N	5.668000	0.046000	2.038000

C	6.572000	-0.921000	2.373000
C	6.551000	0.491000	4.118000
C	7.138000	-0.647000	3.669000
C	4.221000	-1.788000	-2.422000
C	5.094000	-2.232000	-1.443000
N	5.353000	-1.587000	-0.265000
C	6.299000	-2.338000	0.378000
C	5.878000	-3.435000	-1.535000
C	6.626000	-3.500000	-0.405000
C	6.877000	-2.032000	1.600000
H	1.831000	4.602000	0.813000
H	3.148000	4.331000	3.152000
H	6.712000	1.009000	5.054000
H	7.881000	-1.262000	4.160000
H	5.851000	-4.125000	-2.368000
H	7.346000	-4.255000	-0.116000
C	-5.947000	2.445000	-0.367000
C	-4.881000	2.396000	-1.464000
C	-3.963000	3.620000	-1.510000
C	-2.685000	3.284000	-2.265000
C	1.584000	3.551000	-1.626000
C	0.206000	3.394000	-1.799000
C	-0.556000	4.453000	-2.299000
C	0.076000	5.644000	-2.674000
C	1.448000	5.780000	-2.528000
C	2.210000	4.741000	-1.997000
C	-10.943000	-0.723000	2.083000
C	-10.038000	-1.040000	0.896000
C	-8.574000	-1.206000	1.314000
H	-3.685000	-1.591000	1.005000
C	-5.729000	-2.195000	1.433000

C	-4.298000	-1.878000	1.862000
C	-3.615000	-3.073000	2.527000
C	-2.194000	-2.715000	2.957000
H	-4.196000	-3.418000	3.392000
H	-1.678000	-3.578000	3.390000
O	-1.911000	4.468000	-2.408000
H	-0.240000	2.457000	-1.490000
H	3.282000	4.848000	-1.865000
H	1.929000	6.707000	-2.825000
H	-0.533000	6.452000	-3.068000
C	-6.733000	1.126000	-0.268000
C	-5.896000	0.081000	0.478000
N	-6.236000	-1.384000	0.251000
C	-5.532000	-1.940000	-0.983000
C	-5.076000	-1.204000	-4.742000
C	-5.001000	-1.955000	-3.415000
C	-5.710000	-1.191000	-2.292000
H	-4.566000	-1.759000	-5.535000
H	-3.951000	-2.108000	-3.140000
H	-6.767000	-1.064000	-2.556000
H	-6.993000	0.803000	-1.279000
H	-7.678000	1.293000	0.260000
H	-5.988000	0.258000	1.551000
H	-4.838000	0.171000	0.226000
C	-7.722000	-1.608000	0.112000
H	-5.470000	2.657000	0.600000
H	-6.646000	3.267000	-0.559000
H	-4.253000	1.512000	-1.315000
H	-5.370000	2.270000	-2.440000
H	-3.692000	3.933000	-0.493000
H	-4.462000	4.474000	-1.982000

H	-2.908000	2.890000	-3.265000
H	-2.146000	2.506000	-1.721000
H	-10.383000	-1.958000	0.404000
H	-8.220000	-0.268000	1.755000
H	-10.630000	0.203000	2.579000
H	-11.982000	-0.597000	1.762000
H	-10.915000	-1.528000	2.826000
H	-10.110000	-0.239000	0.150000
H	-8.514000	-1.967000	2.099000
H	-5.828000	-3.242000	1.132000
H	-6.415000	-2.014000	2.260000
H	-4.317000	-1.030000	2.554000
H	-3.577000	-3.898000	1.807000
H	-2.194000	-1.915000	3.708000
H	-1.614000	-2.371000	2.091000
H	-5.900000	-2.966000	-1.082000
H	-4.468000	-1.985000	-0.748000
H	-4.597000	-0.222000	-4.660000
H	-6.116000	-1.047000	-5.054000
H	-5.453000	-2.950000	-3.524000
H	-5.258000	-0.200000	-2.218000
H	-7.852000	-2.672000	-0.104000
H	-8.036000	-1.053000	-0.772000
H	4.130000	-2.390000	-3.320000
H	4.895000	2.636000	4.077000
H	7.619000	-2.722000	1.988000
Al	4.661000	0.224000	0.295000
Br	6.465000	1.431000	-0.780000
C	2.373000	-1.879000	0.883000
C	1.757000	-0.600000	1.220000
H	2.505000	-2.145000	-0.161000

H	1.468000	0.033000	0.389000
C	1.057000	-0.354000	2.520000
H	-0.009000	-0.555000	2.389000
H	1.182000	0.691000	2.823000
O	3.195000	-0.781000	1.332000
H	2.343000	-2.703000	1.590000
H	1.450000	-1.003000	3.308000
C	-2.326000	1.126000	2.379000
C	-1.942000	1.840000	1.083000
H	-2.528000	0.073000	2.199000
H	-2.844000	1.989000	0.486000
C	-1.237000	3.157000	1.341000
H	-1.846000	3.764000	2.018000
H	-1.086000	3.715000	0.415000
O	-1.052000	0.975000	0.375000
Br	-3.979000	1.865000	3.117000
C	-1.648000	-0.082000	-0.285000
O	-2.852000	-0.033000	-0.564000
H	-1.568000	1.235000	3.154000
H	-0.259000	2.983000	1.803000
N	-0.755000	-1.047000	-0.510000
S	-1.315000	-2.353000	-1.299000
C	0.076000	-3.450000	-1.103000
C	1.048000	-3.527000	-2.095000
C	0.168000	-4.232000	0.044000
C	2.126000	-4.388000	-1.922000
H	0.958000	-2.918000	-2.988000
C	1.257000	-5.081000	0.207000
H	-0.612000	-4.180000	0.796000
C	2.257000	-5.164000	-0.767000
H	2.885000	-4.456000	-2.696000

H	1.331000	-5.689000	1.104000
O	-2.445000	-3.006000	-0.609000
O	-1.486000	-2.119000	-2.741000
C	3.461000	-6.048000	-0.570000
H	3.771000	-6.512000	-1.511000
H	4.309000	-5.458000	-0.203000
H	3.262000	-6.841000	0.157000

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C	-2.557000	-1.551000	-1.703000
C	-2.091000	-1.368000	-3.058000
N	-3.340000	-0.489000	-1.339000
C	-3.390000	0.347000	-2.421000
C	-2.596000	-0.187000	-3.494000
C	-2.271000	-2.665000	-0.902000
H	-1.469000	-2.063000	-3.603000
C	-4.636000	-1.990000	3.284000
C	-2.753000	-2.832000	0.404000
H	-2.468000	0.280000	-4.461000
N	-3.585000	-1.970000	1.064000
C	-2.413000	-3.938000	1.269000
C	-3.799000	-2.507000	2.302000
C	-3.057000	-3.731000	2.445000
C	-5.414000	-0.845000	3.178000
N	-5.447000	-0.018000	2.096000
C	-6.323000	0.981000	2.398000
C	-6.305000	-0.357000	4.204000
C	-6.872000	0.775000	3.718000
C	-4.105000	1.535000	-2.504000
C	-4.936000	2.061000	-1.526000
N	-5.179000	1.491000	-0.313000

C	-6.085000	2.290000	0.317000
C	-5.700000	3.278000	-1.664000
C	-6.414000	3.419000	-0.519000
C	-6.627000	2.057000	1.575000
H	-1.759000	-4.755000	1.004000
H	-3.048000	-4.350000	3.333000
H	-6.464000	-0.833000	5.162000
H	-7.596000	1.424000	4.194000
H	-5.692000	3.918000	-2.537000
H	-7.112000	4.203000	-0.253000
C	5.428000	-2.476000	-0.376000
C	4.402000	-2.354000	-1.506000
C	3.453000	-3.546000	-1.616000
C	2.597000	-3.438000	-2.872000
C	-1.488000	-3.784000	-1.508000
C	-0.160000	-3.604000	-1.925000
C	0.523000	-4.651000	-2.549000
C	-0.108000	-5.888000	-2.720000
C	-1.413000	-6.065000	-2.292000
C	-2.111000	-5.018000	-1.694000
C	10.794000	0.069000	1.936000
C	9.897000	0.502000	0.779000
C	8.480000	0.850000	1.245000
H	3.655000	1.781000	1.079000
C	5.767000	2.155000	1.446000
C	4.323000	1.994000	1.917000
C	3.796000	3.248000	2.614000
C	2.355000	3.046000	3.082000
H	4.436000	3.512000	3.465000
H	1.960000	3.951000	3.553000
O	1.782000	-4.586000	-3.057000

H	0.307000	-2.638000	-1.761000
H	-3.142000	-5.147000	-1.382000
H	-1.900000	-7.025000	-2.437000
H	0.444000	-6.688000	-3.203000
C	6.355000	-1.251000	-0.285000
C	5.653000	-0.121000	0.476000
N	6.149000	1.300000	0.247000
C	5.482000	1.938000	-0.965000
C	4.787000	1.242000	-4.695000
C	4.877000	2.013000	-3.380000
C	5.534000	1.175000	-2.278000
H	4.323000	1.853000	-5.476000
H	3.870000	2.303000	-3.060000
H	6.562000	0.936000	-2.575000
H	6.636000	-0.956000	-1.299000
H	7.281000	-1.525000	0.229000
H	5.740000	-0.311000	1.546000
H	4.589000	-0.094000	0.236000
C	7.647000	1.359000	0.070000
H	4.921000	-2.627000	0.586000
H	6.042000	-3.369000	-0.545000
H	3.806000	-1.442000	-1.380000
H	4.946000	-2.244000	-2.455000
H	2.807000	-3.611000	-0.731000
H	4.019000	-4.484000	-1.663000
H	3.242000	-3.408000	-3.755000
H	2.001000	-2.518000	-2.875000
H	10.338000	1.370000	0.273000
H	8.025000	-0.038000	1.699000
H	10.383000	-0.812000	2.442000
H	11.797000	-0.184000	1.580000

H	10.892000	0.868000	2.679000
H	9.842000	-0.301000	0.032000
H	8.541000	1.611000	2.030000
H	5.972000	3.186000	1.145000
H	6.452000	1.896000	2.253000
H	4.272000	1.142000	2.604000
H	3.834000	4.085000	1.907000
H	2.285000	2.232000	3.813000
H	1.709000	2.796000	2.232000
H	5.959000	2.916000	-1.075000
H	4.437000	2.101000	-0.699000
H	4.181000	0.338000	-4.573000
H	5.780000	0.939000	-5.049000
H	5.448000	2.938000	-3.528000
H	4.980000	0.238000	-2.186000
H	7.890000	2.404000	-0.139000
H	7.875000	0.785000	-0.828000
H	-4.029000	2.084000	-3.437000
H	-4.706000	-2.550000	4.212000
H	-7.345000	2.781000	1.948000
Al	-4.367000	-0.225000	0.394000
Br	-6.301000	-1.488000	-0.610000
C	-1.274000	1.378000	0.178000
C	-1.675000	0.465000	1.296000
H	-1.604000	1.083000	-0.809000
H	-1.464000	-0.581000	1.057000
C	-1.099000	0.830000	2.653000
H	-0.009000	0.733000	2.667000
H	-1.527000	0.174000	3.417000
O	-3.020000	0.786000	1.205000
H	-1.397000	2.428000	0.416000

H	-1.360000	1.864000	2.901000
C	2.205000	-0.934000	2.513000
C	1.722000	-1.587000	1.217000
H	2.481000	0.106000	2.352000
H	2.574000	-1.776000	0.563000
C	0.924000	-2.848000	1.466000
H	1.541000	-3.558000	2.025000
H	0.619000	-3.313000	0.526000
O	0.856000	-0.636000	0.577000
Br	3.808000	-1.817000	3.186000
C	1.460000	0.375000	-0.078000
O	2.627000	0.318000	-0.452000
H	1.460000	-1.001000	3.305000
H	0.025000	-2.626000	2.049000
N	0.637000	1.442000	-0.235000
S	1.246000	2.663000	-1.211000
C	-0.110000	3.806000	-1.183000
C	-1.112000	3.684000	-2.141000
C	-0.173000	4.756000	-0.166000
C	-2.216000	4.527000	-2.063000
H	-1.038000	2.929000	-2.917000
C	-1.284000	5.590000	-0.100000
H	0.628000	4.827000	0.562000
C	-2.305000	5.469000	-1.042000
H	-3.013000	4.438000	-2.793000
H	-1.356000	6.330000	0.690000
O	2.389000	3.302000	-0.553000
O	1.415000	2.189000	-2.583000
C	-3.537000	6.335000	-0.947000
H	-3.767000	6.800000	-1.911000
H	-4.402000	5.723000	-0.664000

H -3.419000 7.126000 -0.202000

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C 2.967000 1.612000 -1.840000
C 2.639000 1.459000 -3.239000
N 3.670000 0.524000 -1.408000
C 3.797000 -0.309000 -2.480000
C 3.147000 0.264000 -3.631000
C 2.578000 2.695000 -1.047000
H 2.094000 2.181000 -3.832000
C 4.270000 1.841000 3.418000
C 2.866000 2.820000 0.318000
H 3.107000 -0.193000 -4.611000
N 3.576000 1.925000 1.066000
C 2.427000 3.914000 1.153000
C 3.616000 2.421000 2.336000
C 2.893000 3.664000 2.403000
C 4.999000 0.660000 3.398000
N 5.161000 -0.143000 2.310000
C 5.936000 -1.188000 2.710000
C 5.700000 0.105000 4.533000
C 6.285000 -1.041000 4.105000
C 4.461000 -1.530000 -2.488000
C 5.126000 -2.105000 -1.415000
N 5.214000 -1.570000 -0.165000
C 5.975000 -2.427000 0.572000
C 5.846000 -3.355000 -1.471000
C 6.375000 -3.554000 -0.238000
C 6.321000 -2.254000 1.906000
H 1.844000 4.759000 0.814000
H 2.773000 4.264000 3.296000

H	5.733000	0.551000	5.518000
H	6.898000	-1.735000	4.665000
H	5.935000	-3.979000	-2.352000
H	6.989000	-4.377000	0.108000
C	-5.764000	2.318000	-0.658000
C	-4.627000	2.210000	-1.678000
C	-3.783000	3.482000	-1.782000
C	-2.447000	3.195000	-2.449000
C	1.754000	3.771000	-1.675000
C	0.405000	3.514000	-1.943000
C	-0.418000	4.527000	-2.436000
C	0.129000	5.785000	-2.714000
C	1.475000	6.023000	-2.476000
C	2.293000	5.025000	-1.948000
C	-10.976000	-0.427000	1.684000
C	-10.004000	-0.886000	0.601000
C	-8.586000	-1.089000	1.145000
H	-3.652000	-1.983000	1.272000
C	-5.809000	-2.133000	1.573000
C	-4.392000	-1.875000	2.070000
C	-4.028000	-2.836000	3.204000
C	-2.621000	-2.558000	3.730000
H	-4.756000	-2.746000	4.020000
H	-2.352000	-3.252000	4.531000
O	-1.759000	4.423000	-2.640000
H	0.026000	2.524000	-1.719000
H	3.341000	5.216000	-1.742000
H	1.890000	7.002000	-2.696000
H	-0.522000	6.561000	-3.104000
C	-6.564000	1.012000	-0.529000
C	-5.810000	0.031000	0.374000

N	-6.188000	-1.439000	0.275000
C	-5.423000	-2.140000	-0.839000
C	-4.679000	-1.846000	-4.611000
C	-4.803000	-2.476000	-3.226000
C	-5.492000	-1.534000	-2.232000
H	-4.206000	-2.538000	-5.314000
H	-3.804000	-2.726000	-2.854000
H	-6.524000	-1.366000	-2.561000
H	-6.732000	0.609000	-1.530000
H	-7.551000	1.221000	-0.104000
H	-5.965000	0.324000	1.414000
H	-4.736000	0.064000	0.187000
C	-7.670000	-1.628000	0.048000
H	-5.354000	2.595000	0.323000
H	-6.444000	3.125000	-0.952000
H	-3.975000	1.370000	-1.410000
H	-5.045000	1.968000	-2.664000
H	-3.587000	3.894000	-0.783000
H	-4.318000	4.257000	-2.342000
H	-2.581000	2.709000	-3.424000
H	-1.879000	2.509000	-1.815000
H	-10.361000	-1.823000	0.155000
H	-8.216000	-0.136000	1.540000
H	-10.650000	0.520000	2.128000
H	-11.979000	-0.278000	1.272000
H	-11.049000	-1.168000	2.488000
H	-9.975000	-0.146000	-0.209000
H	-8.626000	-1.788000	1.987000
H	-5.975000	-3.200000	1.397000
H	-6.521000	-1.799000	2.328000
H	-4.326000	-0.849000	2.445000

H	-4.086000	-3.869000	2.839000
H	-2.545000	-1.540000	4.132000
H	-1.880000	-2.662000	2.930000
H	-5.806000	-3.164000	-0.851000
H	-4.378000	-2.170000	-0.532000
H	-4.065000	-0.940000	-4.569000
H	-5.661000	-1.573000	-5.015000
H	-5.370000	-3.414000	-3.289000
H	-4.971000	-0.572000	-2.244000
H	-7.826000	-2.702000	-0.083000
H	-7.901000	-1.147000	-0.903000
H	4.480000	-2.071000	-3.430000
H	4.219000	2.373000	4.363000
H	6.941000	-3.021000	2.361000
Al	4.335000	0.143000	0.474000
Br	6.491000	1.377000	-0.151000
C	-2.258000	1.200000	2.328000
C	-1.902000	1.861000	0.997000
H	-2.427000	0.131000	2.209000
H	-2.801000	1.936000	0.383000
C	-1.237000	3.209000	1.170000
H	-1.882000	3.847000	1.782000
H	-1.074000	3.698000	0.208000
O	-0.966000	0.993000	0.327000
Br	-3.934000	1.933000	3.004000
C	-1.483000	-0.125000	-0.208000
O	-2.676000	-0.304000	-0.394000
C	0.934000	-0.683000	-0.412000
C	1.521000	-0.462000	1.011000
H	1.102000	0.191000	-1.041000
H	1.377000	0.601000	1.268000

C	0.813000	-1.297000	2.079000
H	-0.251000	-1.053000	2.175000
H	1.296000	-1.110000	3.042000
O	2.854000	-0.800000	0.965000
H	1.501000	-1.507000	-0.836000
H	0.911000	-2.365000	1.854000
H	-1.500000	1.375000	3.091000
H	-0.269000	3.098000	1.668000
N	-0.504000	-1.034000	-0.502000
S	-1.068000	-2.470000	-1.272000
C	0.375000	-3.495000	-1.275000
C	1.203000	-3.499000	-2.395000
C	0.657000	-4.253000	-0.142000
C	2.358000	-4.270000	-2.362000
H	0.955000	-2.895000	-3.261000
C	1.821000	-5.013000	-0.123000
H	-0.019000	-4.243000	0.706000
C	2.671000	-5.013000	-1.226000
H	3.023000	-4.279000	-3.219000
H	2.066000	-5.598000	0.756000
O	-2.063000	-3.081000	-0.400000
O	-1.421000	-2.143000	-2.647000
C	3.869000	-5.929000	-1.205000
H	4.457000	-5.852000	-2.121000
H	4.523000	-5.700000	-0.360000
H	3.539000	-6.969000	-1.101000