

Supplementary Information

Fragment Molecular Orbital Study of the cAMP-Dependent Protein Kinase Catalyzed Phosphoryl Transfer: A Comparison with the Differential Transition State Stabilization Method

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Structures used in the FMO calculations:

Initial state

H	3.180000	10.170000	7.271000
N	4.076000	10.443000	7.701000
H	4.320000	9.696000	8.335000
C	5.051000	10.737000	6.642000
H	4.565000	11.294000	5.840000
C	6.222000	11.586000	7.180000
H	6.939000	11.753000	6.375000
C	5.777000	12.952000	7.703000
H	6.652000	13.553000	7.947000
H	5.210000	13.471000	6.931000
H	5.159000	12.840000	8.594000
O	6.874000	10.911000	8.238000
H	7.361000	11.593000	8.742000
C	5.602000	9.444000	6.036000
O	5.448000	8.356000	6.607000
N	6.281000	9.582000	4.901000
H	6.322000	10.506000	4.485000
C	7.115000	8.567000	4.258000
H	7.456000	7.835000	4.991000
H	6.539000	8.053000	3.496000
C	8.340000	9.218000	3.613000
O	8.737000	10.318000	4.007000
N	8.968000	8.550000	2.647000
H	8.598000	7.636000	2.390000
C	10.127000	9.075000	1.908000
H	10.916000	9.335000	2.614000
C	10.666000	8.004000	0.956000
H	9.835000	7.521000	0.440000
H	11.325000	8.462000	0.215000
O	11.403000	7.042000	1.679000
H	11.503000	6.264000	1.094000
C	9.827000	10.328000	1.080000
O	10.750000	11.103000	0.808000
N	8.571000	10.539000	0.671000
H	7.857000	9.872000	0.951000
C	8.221000	11.498000	-0.381000
H	9.122000	12.011000	-0.717000
C	7.663000	10.733000	-1.593000
H	6.656000	10.384000	-1.357000
H	7.578000	11.422000	-2.436000
C	8.508000	9.542000	-2.017000

C	9.754000	9.731000	-2.641000
H	10.089000	10.732000	-2.861000
C	10.559000	8.625000	-2.977000
H	11.522000	8.771000	-3.445000
C	10.107000	7.321000	-2.706000
H	10.718000	6.467000	-2.964000
C	8.858000	7.131000	-2.090000
H	8.491000	6.140000	-1.869000
C	8.070000	8.238000	-1.733000
H	7.129000	8.082000	-1.226000
C	7.256000	12.591000	0.087000
O	7.443000	13.746000	-0.295000
N	6.254000	12.259000	0.911000
H	6.171000	11.280000	1.176000
C	5.193000	13.193000	1.315000
H	5.422000	14.199000	0.961000
H	4.266000	12.885000	0.832000
C	4.922000	13.294000	2.818000
O	5.518000	12.593000	3.644000
H	4.169000	14.013000	3.142000
C	-0.340000	13.291000	5.232000
H	-0.762000	13.810000	4.377000
C	-0.743000	11.809000	5.112000
H	-0.372000	11.263000	5.979000
C	-2.269000	11.652000	5.040000
H	-2.667000	12.219000	4.197000
H	-2.525000	10.601000	4.912000
H	-2.731000	12.001000	5.961000
C	-0.163000	11.188000	3.837000
H	0.925000	11.165000	3.890000
H	-0.516000	10.166000	3.726000
H	-0.468000	11.761000	2.968000
H	-0.732000	13.744000	6.137000
H	0.738000	13.419000	5.221000
C	-1.440000	13.891000	1.181000
H	-0.855000	13.775000	2.091000
C	-1.259000	12.620000	0.324000
H	-1.670000	11.776000	0.879000
H	-1.819000	12.720000	-0.606000
C	0.223000	12.322000	0.001000
H	0.590000	13.055000	-0.718000
H	0.811000	12.409000	0.916000
C	0.425000	10.908000	-0.572000
H	0.052000	10.186000	0.156000
H	-0.147000	10.801000	-1.496000
C	1.909000	10.613000	-0.851000
H	2.282000	11.314000	-1.603000
H	2.474000	10.762000	0.073000
N	2.115000	9.222000	-1.321000
H	1.651000	9.051000	-2.216000
H	3.103000	8.995000	-1.430000
H	1.760000	8.563000	-0.627000
H	-2.480000	14.031000	1.448000
H	-1.096000	14.779000	0.662000
C	9.354000	10.601000	-8.675000
H	9.346000	9.561000	-9.000000
C	8.923000	10.623000	-7.192000
H	8.940000	11.650000	-6.830000
H	7.899000	10.255000	-7.115000
C	9.779000	9.781000	-6.236000

H	10.748000	10.253000	-6.106000
H	9.281000	9.776000	-5.269000
C	9.949000	8.333000	-6.683000
O	8.992000	7.571000	-6.755000
N	11.146000	7.914000	-7.033000
H	11.285000	6.955000	-7.332000
H	11.927000	8.564000	-6.982000
H	8.663000	11.167000	-9.289000
H	10.353000	11.004000	-8.815000
C	-0.178000	7.928000	-8.581000
H	-0.320000	6.881000	-8.308000
C	0.718000	8.570000	-7.501000
H	1.680000	8.064000	-7.538000
H	0.877000	9.622000	-7.736000
C	0.167000	8.461000	-6.067000
H	-0.740000	9.063000	-5.993000
H	-0.105000	7.421000	-5.880000
C	1.166000	8.916000	-4.982000
O	2.318000	9.297000	-5.306000
O	0.816000	8.851000	-3.780000
H	-1.159000	8.395000	-8.641000
H	0.280000	7.971000	-9.566000
C	4.735000	-1.253000	-2.206000
H	5.701000	-1.715000	-2.010000
C	4.930000	0.272000	-2.102000
H	5.394000	0.739000	-2.991000
H	3.978000	0.828000	-1.957000
C	5.848000	0.677000	-0.931000
O	6.406000	-0.180000	-0.215000
O	5.944000	1.939000	-0.779000
H	4.352000	-1.573000	-3.180000
H	4.053000	-1.603000	-1.437000
H	3.153000	-2.987000	2.679000
H	2.875000	-2.722000	4.404000
C	3.586000	-3.079000	3.668000
H	3.800000	-4.131000	3.863000
C	4.940000	-2.303000	3.768000
H	5.381000	-2.404000	4.774000
H	5.693000	-2.698000	3.060000
C	4.752000	-0.820000	3.484000
H	4.327000	-0.702000	2.477000
H	4.025000	-0.403000	4.192000
C	6.060000	-0.031000	3.563000
H	6.400000	0.037000	4.605000
H	6.820000	-0.581000	3.004000
C	5.880000	1.347000	2.948000
H	5.576000	1.249000	1.907000
H	5.123000	1.927000	3.484000
N	7.108000	2.194000	2.903000
H	7.764000	1.896000	2.152000
H	6.799000	3.157000	2.598000
H	7.589000	2.237000	3.813000
C	0.842000	1.512000	3.523000
H	0.627000	2.582000	3.566000
C	1.603000	1.235000	2.206000
H	1.961000	0.206000	2.218000
H	0.905000	1.334000	1.375000
C	2.776000	2.143000	1.853000
O	3.000000	3.237000	2.372000
N	3.543000	1.716000	0.880000

H	4.335000	2.262000	0.553000
H	3.391000	0.793000	0.478000
H	-0.082000	0.947000	3.543000
H	1.438000	1.251000	4.389000
N	-1.081000	4.667000	-0.610000
H	-1.563000	5.489000	-0.261000
C	0.254000	4.875000	-1.187000
H	0.352000	5.945000	-1.373000
C	1.322000	4.530000	-0.146000
H	1.005000	4.914000	0.824000
H	1.402000	3.447000	-0.067000
C	2.690000	5.121000	-0.480000
O	2.966000	5.671000	-1.565000
O	3.650000	5.067000	0.325000
C	0.468000	4.187000	-2.548000
O	1.254000	3.250000	-2.710000
H	-0.128000	4.562000	-3.381000
H	-1.055000	3.984000	0.118000
C	5.012000	3.219000	-7.368000
H	5.646000	3.828000	-8.012000
C	5.914000	2.237000	-6.616000
H	5.268000	1.542000	-6.078000
H	6.489000	1.663000	-7.343000
C	6.892000	2.835000	-5.624000
C	7.439000	4.126000	-5.779000
H	7.153000	4.758000	-6.605000
C	8.356000	4.621000	-4.834000
H	8.769000	5.615000	-4.941000
C	8.710000	3.841000	-3.721000
H	9.405000	4.227000	-2.990000
C	8.146000	2.566000	-3.558000
H	8.375000	1.961000	-2.696000
C	7.274000	2.052000	-4.525000
H	6.898000	1.046000	-4.426000
H	4.305000	2.687000	-7.994000
H	4.465000	3.868000	-6.694000
H	13.116000	0.754000	-6.676000
N	12.194000	0.536000	-6.997000
H	12.185000	-0.458000	-7.175000
C	11.185000	1.033000	-6.067000
H	11.664000	1.723000	-5.372000
C	10.122000	1.814000	-6.856000
H	9.350000	2.156000	-6.171000
H	10.590000	2.697000	-7.293000
S	9.376000	0.811000	-8.179000
H	10.532000	0.375000	-8.706000
C	10.581000	-0.115000	-5.234000
O	10.636000	-1.285000	-5.626000
N	10.006000	0.226000	-4.082000
H	10.036000	1.206000	-3.828000
C	9.470000	-0.689000	-3.067000
H	8.391000	-0.555000	-2.995000
H	9.670000	-1.724000	-3.338000
C	10.066000	-0.414000	-1.684000
O	10.648000	0.647000	-1.458000
N	9.939000	-1.367000	-0.761000
H	9.454000	-2.217000	-1.039000
C	10.492000	-1.290000	0.604000
H	11.043000	-0.359000	0.702000
C	9.351000	-1.229000	1.628000

H	8.694000	-2.091000	1.511000
C	9.843000	-1.166000	3.075000
H	10.470000	-0.286000	3.213000
H	8.989000	-1.095000	3.747000
H	10.402000	-2.066000	3.332000
O	8.629000	-0.035000	1.419000
H	7.935000	-0.192000	0.745000
C	11.441000	-2.475000	0.858000
O	11.072000	-3.600000	0.519000
H	12.407000	-2.325000	1.339000
H	13.213000	2.346000	5.198000
H	12.827000	2.152000	3.803000
O	13.239000	1.624000	4.524000
H	-1.771000	7.447000	0.430000
H	-0.310000	7.811000	0.277000
O	-1.159000	7.801000	-0.230000
H	5.364000	11.652000	-5.984000
H	5.234000	10.185000	-5.896000
O	5.517000	10.937000	-5.339000
H	3.440000	9.339000	-4.063000
H	4.758000	10.014000	-3.895000
O	4.213000	9.337000	-3.443000
H	7.039000	5.147000	6.333000
H	7.119000	3.797000	5.716000
O	6.495000	4.540000	5.783000
H	6.426000	-1.857000	0.099000
H	5.913000	-3.194000	0.633000
O	6.618000	-2.825000	0.074000
H	5.870000	6.890000	-3.649000
H	4.970000	7.806000	-2.927000
O	5.328000	6.885000	-2.822000
H	4.784000	3.628000	-2.763000
H	5.553000	3.313000	-1.533000
O	5.169000	4.112000	-1.998000
H	3.689000	5.236000	4.956000
H	5.127000	4.878000	4.742000
O	4.294000	5.020000	4.222000
H	14.246000	6.901000	-1.041000
H	13.421000	6.069000	-0.104000
O	14.212000	6.648000	-0.097000
MG	4.829000	5.902000	-1.186000
MG	3.940000	5.001000	2.259000
O	5.821000	4.388000	1.955000
P	6.579000	5.641000	1.379000
O	6.527000	5.720000	-0.154000
O	7.842000	6.021000	2.082000
O	5.312000	6.775000	1.835000
P	4.889000	8.149000	1.038000
O	5.880000	9.254000	1.207000
O	4.416000	7.756000	-0.367000
O	3.533000	8.521000	1.906000
P	2.129000	7.677000	2.096000
O	1.215000	7.875000	0.927000
O	2.442000	6.244000	2.518000
O	1.524000	8.467000	3.370000
C	2.276000	8.485000	4.623000
H	2.540000	9.550000	4.752000
H	3.199000	7.909000	4.477000
H	1.685000	8.102000	5.445000
N	10.062000	4.099000	1.937000

H	9.159000	4.543000	1.991000
C	10.370000	3.353000	0.707000
H	10.533000	2.310000	0.970000
C	9.133000	3.414000	-0.188000
H	8.893000	4.450000	-0.482000
H	9.301000	2.812000	-1.093000
O	8.027000	2.893000	0.525000
H	7.308000	2.539000	-0.066000
C	11.615000	3.854000	-0.040000
O	12.028000	5.009000	0.111000
H	12.104000	3.166000	-0.729000
H	10.166000	3.524000	2.745000

Transition state

H	3.180000	10.170000	7.271000
N	4.067000	10.418000	7.664000
H	4.308000	9.672000	8.300000
C	5.027000	10.675000	6.582000
H	4.536000	11.219000	5.774000
C	6.220000	11.516000	7.082000
H	6.931000	11.648000	6.266000
C	5.808000	12.904000	7.575000
H	6.698000	13.492000	7.797000
H	5.248000	13.416000	6.794000
H	5.194000	12.828000	8.472000
O	6.871000	10.858000	8.152000
H	7.346000	11.549000	8.654000
C	5.555000	9.359000	6.005000
O	5.417000	8.294000	6.621000
N	6.203000	9.449000	4.848000
H	6.233000	10.352000	4.390000
C	7.040000	8.410000	4.246000
H	7.360000	7.693000	5.003000
H	6.479000	7.881000	3.484000
C	8.285000	9.038000	3.619000
O	8.733000	10.098000	4.065000
N	8.878000	8.392000	2.616000
H	8.467000	7.513000	2.306000
C	10.048000	8.928000	1.900000
H	10.824000	9.178000	2.624000
C	10.608000	7.874000	0.945000
H	9.789000	7.361000	0.438000
H	11.247000	8.348000	0.197000
O	11.384000	6.949000	1.676000
H	11.522000	6.173000	1.096000
C	9.772000	10.200000	1.091000
O	10.716000	10.946000	0.811000
N	8.518000	10.461000	0.706000
H	7.779000	9.819000	0.988000
C	8.189000	11.449000	-0.326000
H	9.099000	11.961000	-0.640000
C	7.636000	10.719000	-1.561000
H	6.628000	10.364000	-1.338000
H	7.555000	11.431000	-2.384000
C	8.481000	9.540000	-2.015000
C	9.740000	9.745000	-2.608000
H	10.085000	10.752000	-2.775000

C	10.541000	8.648000	-2.980000
H	11.515000	8.808000	-3.422000
C	10.071000	7.338000	-2.781000
H	10.678000	6.492000	-3.073000
C	8.808000	7.132000	-2.198000
H	8.423000	6.135000	-2.043000
C	8.027000	8.228000	-1.797000
H	7.075000	8.062000	-1.313000
C	7.230000	12.540000	0.156000
O	7.448000	13.708000	-0.172000
N	6.194000	12.190000	0.928000
H	6.093000	11.201000	1.154000
C	5.125000	13.119000	1.317000
H	5.321000	14.112000	0.911000
H	4.192000	12.770000	0.874000
C	4.893000	13.283000	2.820000
H	4.150000	14.016000	3.133000
O	5.510000	12.616000	3.660000
C	-0.346000	13.287000	5.233000
H	-0.723000	13.849000	4.383000
C	-0.747000	11.804000	5.121000
H	-0.362000	11.259000	5.983000
C	-2.273000	11.641000	5.068000
H	-2.683000	12.208000	4.231000
H	-2.526000	10.589000	4.942000
H	-2.725000	11.987000	5.995000
C	-0.183000	11.187000	3.838000
H	0.906000	11.175000	3.870000
H	-0.527000	10.161000	3.736000
H	-0.511000	11.753000	2.973000
H	-0.747000	13.739000	6.135000
H	0.734000	13.402000	5.256000
C	-1.428000	13.877000	1.167000
H	-0.843000	13.767000	2.078000
C	-1.233000	12.606000	0.312000
H	-1.653000	11.761000	0.858000
H	-1.777000	12.707000	-0.628000
C	0.256000	12.308000	0.016000
H	0.641000	13.049000	-0.686000
H	0.824000	12.382000	0.944000
C	0.469000	10.901000	-0.572000
H	0.058000	10.174000	0.129000
H	-0.067000	10.814000	-1.519000
C	1.960000	10.585000	-0.794000
H	2.376000	11.288000	-1.520000
H	2.487000	10.711000	0.155000
N	2.162000	9.195000	-1.269000
H	1.754000	9.040000	-2.193000
H	3.150000	8.935000	-1.296000
H	1.748000	8.544000	-0.602000
H	-2.469000	14.009000	1.433000
H	-1.090000	14.767000	0.647000
C	9.358000	10.593000	-8.675000
H	9.283000	9.593000	-9.087000
C	8.930000	10.618000	-7.191000
H	8.943000	11.646000	-6.832000
H	7.907000	10.246000	-7.112000
C	9.791000	9.783000	-6.234000
H	10.759000	10.260000	-6.108000
H	9.296000	9.780000	-5.265000

C	9.966000	8.335000	-6.677000
O	9.012000	7.571000	-6.754000
N	11.165000	7.916000	-7.023000
H	11.303000	6.958000	-7.323000
H	11.945000	8.568000	-6.971000
H	8.717000	11.243000	-9.260000
H	10.382000	10.937000	-8.800000
C	-0.180000	7.950000	-8.566000
H	-0.296000	6.885000	-8.376000
C	0.715000	8.608000	-7.495000
H	1.685000	8.120000	-7.545000
H	0.853000	9.663000	-7.731000
C	0.186000	8.491000	-6.052000
H	-0.724000	9.087000	-5.963000
H	-0.078000	7.449000	-5.865000
C	1.201000	8.947000	-4.981000
O	2.343000	9.337000	-5.327000
O	0.876000	8.874000	-3.772000
H	-1.178000	8.385000	-8.588000
H	0.250000	8.063000	-9.560000
C	4.753000	-1.189000	-2.171000
H	5.707000	-1.675000	-1.976000
C	4.986000	0.338000	-2.062000
H	5.414000	0.802000	-2.968000
H	4.048000	0.910000	-1.885000
C	5.956000	0.738000	-0.925000
O	6.404000	-0.111000	-0.125000
O	6.211000	1.991000	-0.891000
H	4.365000	-1.492000	-3.143000
H	4.063000	-1.527000	-1.405000
H	3.114000	-2.980000	2.673000
H	2.847000	-2.731000	4.402000
C	3.549000	-3.091000	3.660000
H	3.749000	-4.144000	3.844000
C	4.914000	-2.344000	3.766000
H	5.373000	-2.490000	4.758000
H	5.650000	-2.719000	3.029000
C	4.730000	-0.854000	3.546000
H	4.264000	-0.693000	2.563000
H	4.042000	-0.453000	4.300000
C	6.050000	-0.092000	3.601000
H	6.446000	-0.088000	4.624000
H	6.769000	-0.615000	2.964000
C	5.853000	1.314000	3.071000
H	5.459000	1.271000	2.058000
H	5.171000	1.906000	3.688000
N	7.111000	2.109000	2.948000
H	7.756000	1.673000	2.270000
H	6.817000	3.046000	2.561000
H	7.597000	2.217000	3.852000
C	0.865000	1.546000	3.527000
H	0.483000	2.558000	3.572000
C	1.629000	1.305000	2.202000
H	1.997000	0.280000	2.191000
H	0.929000	1.414000	1.375000
C	2.793000	2.235000	1.866000
O	2.999000	3.329000	2.391000
N	3.585000	1.834000	0.903000
H	4.345000	2.439000	0.619000
H	3.468000	0.915000	0.481000

H	0.035000	0.852000	3.590000
H	1.510000	1.393000	4.384000
N	-1.128000	4.684000	-0.601000
H	-1.605000	5.501000	-0.237000
C	0.205000	4.901000	-1.179000
H	0.294000	5.972000	-1.366000
C	1.276000	4.570000	-0.137000
H	0.965000	4.965000	0.829000
H	1.359000	3.488000	-0.047000
C	2.639000	5.160000	-0.491000
O	2.894000	5.715000	-1.579000
O	3.624000	5.085000	0.282000
C	0.425000	4.213000	-2.538000
O	1.187000	3.254000	-2.689000
H	-0.145000	4.606000	-3.380000
H	-1.098000	3.991000	0.117000
C	5.000000	3.223000	-7.347000
H	5.567000	3.851000	-8.026000
C	5.895000	2.243000	-6.584000
H	5.246000	1.567000	-6.024000
H	6.454000	1.646000	-7.305000
C	6.899000	2.842000	-5.619000
C	7.452000	4.128000	-5.796000
H	7.145000	4.760000	-6.614000
C	8.404000	4.618000	-4.884000
H	8.821000	5.608000	-5.009000
C	8.789000	3.839000	-3.781000
H	9.514000	4.221000	-3.076000
C	8.218000	2.571000	-3.593000
H	8.472000	1.967000	-2.738000
C	7.308000	2.062000	-4.528000
H	6.927000	1.060000	-4.410000
H	4.276000	2.676000	-7.941000
H	4.456000	3.871000	-6.667000
H	13.122000	0.725000	-6.678000
N	12.203000	0.495000	-6.998000
H	12.198000	-0.499000	-7.182000
C	11.190000	0.988000	-6.072000
H	11.663000	1.687000	-5.382000
C	10.121000	1.756000	-6.866000
H	9.350000	2.104000	-6.184000
H	10.584000	2.634000	-7.316000
S	9.374000	0.734000	-8.172000
H	10.529000	0.314000	-8.713000
C	10.595000	-0.158000	-5.230000
O	10.660000	-1.332000	-5.607000
N	10.015000	0.190000	-4.083000
H	10.036000	1.174000	-3.844000
C	9.469000	-0.713000	-3.062000
H	8.387000	-0.599000	-3.025000
H	9.700000	-1.749000	-3.300000
C	10.011000	-0.385000	-1.670000
O	10.524000	0.711000	-1.446000
N	9.916000	-1.326000	-0.732000
H	9.472000	-2.203000	-0.999000
C	10.475000	-1.210000	0.629000
H	11.061000	-0.297000	0.683000
C	9.341000	-1.064000	1.654000
H	8.671000	-1.922000	1.598000
C	9.851000	-0.916000	3.088000

H	10.496000	-0.041000	3.164000
H	9.005000	-0.788000	3.763000
H	10.397000	-1.809000	3.395000
O	8.627000	0.126000	1.384000
H	7.908000	-0.086000	0.747000
C	11.389000	-2.416000	0.920000
O	10.984000	-3.538000	0.616000
H	12.361000	-2.281000	1.393000
N	10.082000	3.980000	1.978000
H	9.173000	4.389000	2.110000
C	10.312000	3.325000	0.684000
H	10.370000	2.249000	0.848000
C	9.099000	3.626000	-0.194000
H	9.086000	4.675000	-0.521000
H	9.090000	2.969000	-1.067000
O	7.840000	3.420000	0.484000
H	7.221000	2.783000	-0.048000
C	11.599000	3.790000	-0.025000
O	12.044000	4.929000	0.155000
H	12.083000	3.098000	-0.713000
H	10.272000	3.371000	2.744000
M	4.761000	5.925000	-1.195000
M	4.011000	5.141000	2.204000
O	5.798000	4.175000	1.783000
P	6.803000	5.161000	1.111000
O	6.541000	5.580000	-0.325000
O	7.914000	5.747000	1.912000
O	5.243000	6.737000	1.797000
P	4.899000	8.080000	1.056000
O	5.875000	9.207000	1.239000
O	4.451000	7.764000	-0.399000
O	3.478000	8.562000	1.833000
P	2.114000	7.708000	2.087000
O	1.152000	7.875000	0.947000
O	2.431000	6.277000	2.527000
O	1.516000	8.503000	3.372000
C	2.275000	8.509000	4.611000
H	2.533000	9.573000	4.762000
H	3.203000	7.943000	4.453000
H	1.685000	8.102000	5.445000
H	13.308000	2.317000	5.190000
H	12.921000	2.118000	3.794000
O	13.318000	1.588000	4.522000
H	-1.801000	7.494000	0.436000
H	-0.337000	7.833000	0.272000
O	-1.189000	7.822000	-0.236000
H	5.400000	11.651000	-6.003000
H	5.277000	10.184000	-5.908000
O	5.576000	10.938000	-5.362000
H	3.464000	9.357000	-4.077000
H	4.792000	10.017000	-3.911000
O	4.250000	9.329000	-3.476000
H	7.110000	5.100000	6.269000
H	7.231000	3.726000	5.713000
O	6.604000	4.468000	5.709000
H	6.400000	-1.823000	0.168000
H	5.897000	-3.181000	0.656000
O	6.612000	-2.785000	0.129000
H	5.833000	6.861000	-3.680000
H	4.955000	7.784000	-2.936000

O	5.291000	6.851000	-2.854000
H	4.630000	3.604000	-2.775000
H	5.558000	3.310000	-1.649000
O	5.051000	4.081000	-2.025000
H	3.785000	5.287000	4.884000
H	5.224000	4.901000	4.696000
O	4.404000	5.062000	4.165000
H	14.234000	6.863000	-1.023000
H	13.431000	6.011000	-0.083000
O	14.211000	6.603000	-0.080000