

SUPPLEMENTARY MATERIAL

DFT STUDY ON THE MECHANISTIC, ENERGETIC AND STRUCTURAL ASPECTS OF ADSORPTION OF TIRAPAZAMINE ONTO PRISTINE AND FUNCTIONALIZED CARBON NANOTUBES

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Cartesian coordinates, sum of electronic and zero-point energies (E), sum of electronic and thermal enthalpies (H) and Gibbs free energies (G) for the calculated structures.

In water

NTCOOH

C	-4.899397000	-2.146763000	-2.963260000
C	-4.899166000	-3.159030000	-2.035517000
C	-3.701830000	-3.494569000	-1.325958000
C	-3.702526000	-3.765140000	0.098873000
C	-2.476948000	-3.627792000	0.803484000
C	-2.477128000	-2.991279000	2.090512000
C	-1.230843000	-2.488745000	2.593937000
C	-1.229466000	-1.221036000	3.237048000
C	0.000006000	-0.519475000	3.365658000
C	-0.000004000	0.898416000	3.135210000
C	1.223742000	1.539153000	2.814654000
C	1.217941000	2.599525000	1.865479000
C	2.485670000	3.009147000	1.295816000
C	2.501168000	3.306701000	-0.121748000
C	3.730174000	3.187182000	-0.823237000
C	3.717802000	2.529042000	-2.105523000
C	4.912255000	2.021834000	-2.720980000
C	4.903886000	0.804858000	-3.350516000
C	-4.899296000	-3.711905000	0.879486000
C	-4.898040000	-3.101484000	2.111953000
C	-3.701864000	-2.519002000	2.631367000
C	-3.700494000	-1.221244000	3.290362000
C	-2.471666000	-0.511777000	3.354440000
C	-2.468250000	0.906911000	3.146812000

C	-1.223757000	1.539137000	2.814653000
C	-1.217971000	2.599508000	1.865478000
C	-0.000017000	2.995770000	1.286633000
C	-0.000020000	3.656055000	-0.097954000
C	1.270296000	3.230081000	-0.831771000
C	1.245788000	2.510334000	-2.026632000
C	2.484381000	1.996171000	-2.555492000
C	2.477073000	0.724238000	-3.220878000
C	3.701670000	0.025941000	-3.411470000
C	3.700996000	-1.408149000	-3.231191000
C	4.899435000	-2.146697000	-2.963257000
C	4.899217000	-3.158965000	-2.035514000
C	-4.888960000	-0.458031000	3.474312000
C	-4.882382000	0.909828000	3.291018000
C	-3.689025000	1.588159000	2.913349000
C	-3.688632000	2.679330000	1.941361000
C	-2.485704000	3.009113000	1.295814000
C	-2.501205000	3.306667000	-0.121750000
C	-1.270331000	3.230063000	-0.831772000
C	-1.245813000	2.510318000	-2.026633000
C	-0.000009000	2.000709000	-2.543015000
C	0.000000000	0.742457000	-3.175533000
C	1.235482000	0.025977000	-3.325768000
C	1.233238000	-1.380793000	-3.168892000
C	2.475149000	-2.040505000	-2.892150000
C	2.475281000	-3.103411000	-1.925460000
C	3.701885000	-3.494520000	-1.325956000
C	3.702584000	-3.765090000	0.098875000
C	4.899353000	-3.711838000	0.879489000
C	4.898088000	-3.101417000	2.111956000
C	-4.909600000	3.093561000	1.300156000
C	-4.931161000	3.326640000	-0.047879000
C	-3.730209000	3.187133000	-0.823240000
C	-3.717828000	2.528992000	-2.105526000
C	-2.484398000	1.996138000	-2.555495000
C	-2.477073000	0.724205000	-3.220880000
C	-1.235473000	0.025960000	-3.325769000
C	-1.233210000	-1.380809000	-3.168893000
C	0.000018000	-2.043028000	-2.883300000
C	0.000025000	-3.096650000	-1.926869000
C	1.233262000	-3.446715000	-1.298424000
C	1.231975000	-3.718328000	0.095465000
C	2.477004000	-3.627759000	0.803485000
C	2.477174000	-2.991245000	2.090513000
C	3.701903000	-2.518951000	2.631369000
C	3.700515000	-1.221194000	3.290364000
C	4.888971000	-0.457965000	3.474315000
C	4.882375000	0.909894000	3.291022000
C	-4.912272000	2.021768000	-2.720984000
C	-4.903887000	0.804792000	-3.350520000

C	-3.701661000	0.025892000	-3.411472000
C	-3.700967000	-1.408199000	-3.231193000
C	-2.475113000	-2.040538000	-2.892152000
C	-2.475231000	-3.103444000	-1.925461000
C	-1.233208000	-3.446731000	-1.298425000
C	-1.231917000	-3.718345000	0.095464000
C	0.000028000	-3.638324000	0.808584000
C	0.000023000	-3.001603000	2.092374000
C	1.230883000	-2.488728000	2.593938000
C	1.229488000	-1.221019000	3.237049000
C	2.471678000	-0.511743000	3.354442000
C	2.468243000	0.906945000	3.146815000
C	3.689009000	1.588209000	2.913352000
C	3.688602000	2.679381000	1.941364000
C	4.909565000	3.093628000	1.300160000
C	4.931124000	3.326706000	-0.047875000
H	-5.883959000	3.482254000	-0.542682000
H	-5.845021000	3.077940000	1.848607000
H	-5.831150000	1.435294000	3.292029000
H	-5.842218000	-0.958489000	3.606105000
H	-5.846665000	-2.932183000	2.610281000
H	-5.847791000	-4.005204000	0.442516000
H	-5.846336000	-3.598386000	-1.741249000
H	-5.845753000	-1.816509000	-3.377808000
H	-5.844169000	0.378695000	-3.683872000
H	-5.857450000	2.532289000	-2.570510000
H	5.844174000	0.378773000	-3.683868000
H	5.857425000	2.532367000	-2.570506000
H	5.883920000	3.482332000	-0.542678000
H	5.844985000	3.078019000	1.848612000
H	5.831136000	1.435373000	3.292034000
H	5.842236000	-0.958410000	3.606109000
H	5.846710000	-2.932103000	2.610285000
H	5.847852000	-4.005125000	0.442520000
H	5.846393000	-3.598307000	-1.741246000
H	5.845787000	-1.816431000	-3.377804000
C	-0.000032000	5.211032000	-0.062834000
O	-0.000119000	5.899911000	-1.061235000
O	-0.000187000	5.712920000	1.182516000
H	-0.000297000	6.684006000	1.103421000

E=-3630,141426,H=-3630,094310,G=-3630,206697 a.u.

TPZ

O	-1.475060000	-2.227516000	0.000010000
O	0.085026000	2.854522000	0.000262000
N	-1.017280000	-1.007000000	-0.000069000
N	-0.241326000	1.639586000	-0.000319000
N	-1.529603000	1.337311000	-0.000074000
N	-3.192799000	-0.281207000	0.000145000
C	0.327937000	-0.710857000	-0.000090000

C	0.737612000	0.641752000	-0.000149000
C	1.295912000	-1.734846000	0.000004000
C	2.106217000	0.975039000	-0.000019000
C	-1.894251000	0.043369000	0.000001000
C	2.631991000	-1.392875000	0.000077000
C	3.041854000	-0.036953000	0.000077000
H	0.954177000	-2.761344000	0.000043000
H	2.382157000	2.021286000	-0.000047000
H	3.382544000	-2.176434000	0.000161000
H	4.098645000	0.205688000	0.000142000
H	-3.412454000	-1.267170000	0.000159000
H	-3.901374000	0.433325000	0.000184000

E=-639,568885 , H=-639,558657, G=-639,603457 a.u.

NTCOOH/TPZ

C	-3.146242000	5.384826000	-2.533386000
C	-3.914532000	5.550775000	-1.407560000
C	-4.312745000	4.419050000	-0.626407000
C	-4.260509000	4.428653000	0.822937000
C	-4.212314000	3.178830000	1.495668000
C	-3.322901000	3.018849000	2.611283000
C	-2.973359000	1.684854000	3.008109000
C	-1.621102000	1.422260000	3.358047000
C	-1.159179000	0.078188000	3.347243000
C	0.148318000	-0.186318000	2.814315000
C	0.456286000	-1.499856000	2.378272000
C	1.268388000	-1.669026000	1.221671000
C	1.289934000	-2.974143000	0.592217000
C	1.261245000	-3.003146000	-0.855407000
C	0.756963000	-4.165237000	-1.497365000
C	-0.149151000	-3.989406000	-2.604433000
C	-0.998658000	-5.046164000	-3.077903000
C	-2.297945000	-4.786858000	-3.426484000
C	-3.809408000	5.569125000	1.557548000
C	-2.957181000	5.414476000	2.625970000
C	-2.517436000	4.114107000	3.020090000
C	-1.132606000	3.845171000	3.378564000
C	-0.677203000	2.502010000	3.302058000
C	0.635104000	2.233198000	2.790613000
C	0.929272000	0.900681000	2.346386000
C	1.739287000	0.719444000	1.189920000
C	1.758108000	-0.533608000	0.552569000
C	2.085206000	-0.617240000	-0.943395000
C	1.270438000	-1.758578000	-1.545873000
C	0.327516000	-1.563028000	-2.555362000
C	-0.518083000	-2.664080000	-2.943406000
C	-1.877952000	-2.394186000	-3.315124000
C	-2.823979000	-3.456393000	-3.332914000
C	-4.157380000	-3.186641000	-2.844196000
C	-5.038058000	-4.228990000	-2.406918000

C	-5.805792000	-4.062978000	-1.280733000
C	-0.132772000	4.859738000	3.375768000
C	1.135178000	4.596904000	2.898856000
C	1.472442000	3.307415000	2.398860000
C	2.307399000	3.126631000	1.213216000
C	2.250550000	1.902505000	0.527094000
C	2.227759000	1.903414000	-0.921283000
C	1.761495000	0.731258000	-1.579597000
C	0.808711000	0.882022000	-2.587809000
C	-0.032413000	-0.227389000	-2.961795000
C	-1.372503000	0.031600000	-3.306267000
C	-2.329123000	-1.039297000	-3.280917000
C	-3.640581000	-0.772799000	-2.820567000
C	-4.452567000	-1.873205000	-2.391701000
C	-5.261006000	-1.698688000	-1.216868000
C	-5.742275000	-2.845174000	-0.530561000
C	-5.690269000	-2.836824000	0.919052000
C	-5.700871000	-4.044058000	1.684841000
C	-4.848332000	-4.196281000	2.753377000
C	2.800051000	4.264337000	0.480855000
C	2.733641000	4.281193000	-0.885603000
C	2.198829000	3.153115000	-1.595579000
C	1.287061000	3.305930000	-2.701800000
C	0.441121000	2.211297000	-3.007286000
C	-0.921484000	2.467081000	-3.378605000
C	-1.851973000	1.385371000	-3.312490000
C	-3.164283000	1.647230000	-2.852259000
C	-3.974724000	0.555445000	-2.414250000
C	-4.776781000	0.728747000	-1.251813000
C	-5.214249000	-0.432889000	-0.546273000
C	-5.169148000	-0.421604000	0.873010000
C	-5.169080000	-1.681625000	1.560060000
C	-4.279552000	-1.841911000	2.675764000
C	-3.946858000	-3.149777000	3.116441000
C	-2.561731000	-3.415886000	3.475566000
C	-2.021073000	-4.733261000	3.504615000
C	-0.750464000	-4.982985000	3.027738000
C	0.898606000	4.593208000	-3.206246000
C	-0.404106000	4.836602000	-3.554162000
C	-1.394691000	3.807834000	-3.428117000
C	-2.728188000	4.075763000	-2.939530000
C	-3.496389000	2.983817000	-2.455379000
C	-4.304858000	3.158710000	-1.280844000
C	-4.737958000	1.987001000	-0.578193000
C	-4.693322000	1.995684000	0.841058000
C	-4.700157000	0.750572000	1.535233000
C	-3.810830000	0.590398000	2.647480000
C	-3.448679000	-0.730134000	3.040174000
C	-2.095892000	-0.989951000	3.390119000
C	-1.631834000	-2.347847000	3.366913000

C	-0.318331000	-2.609609000	2.855445000
C	0.047217000	-3.930756000	2.495686000
C	0.881993000	-4.110496000	1.309877000
C	0.902625000	-5.368329000	0.609443000
C	0.827329000	-5.393488000	-0.756359000
H	2.957844000	5.201190000	-1.414908000
H	3.083883000	5.169170000	1.006962000
H	1.821538000	5.427091000	2.772242000
H	-0.398643000	5.886877000	3.601470000
H	-2.503487000	6.298036000	3.062153000
H	-4.001647000	6.568889000	1.183299000
H	-4.089033000	6.555240000	-1.036857000
H	-2.737575000	6.262327000	-3.022782000
H	-0.702804000	5.850688000	-3.797275000
H	1.602221000	5.418557000	-3.182435000
H	-2.960221000	-5.617925000	-3.644592000
H	-0.660386000	-6.075605000	-3.028495000
H	0.682730000	-6.342917000	-1.260936000
H	0.825264000	-6.299525000	1.159903000
H	-0.430168000	-6.014235000	2.926546000
H	-2.656102000	-5.576458000	3.754135000
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H	-6.259388000	-4.905765000	1.335520000
H	-6.345117000	-4.917044000	-0.885092000
H	-4.994044000	-5.208301000	-2.871112000
C	3.584091000	-0.926745000	-1.260641000
O	4.004014000	-0.928642000	-2.404358000
O	4.319171000	-1.196290000	-0.191386000
H	5.291917000	-1.423980000	-0.455984000
O	6.722936000	-1.956271000	-0.451551000
O	10.274931000	0.785109000	2.397025000
N	7.606549000	-1.216264000	0.204580000
N	9.446284000	0.172113000	1.693918000
N	8.350897000	-0.283546000	2.270683000
N	6.368630000	-1.461727000	2.154336000
C	8.723891000	-0.720024000	-0.434221000
C	9.681623000	-0.010600000	0.320532000
C	8.928396000	-0.919231000	-1.810628000
C	10.841643000	0.503096000	-0.285555000
C	7.453427000	-0.966977000	1.528250000
C	10.070911000	-0.407387000	-2.395299000
C	11.030150000	0.302307000	-1.637596000
H	8.181850000	-1.466821000	-2.369514000
H	11.553208000	1.042244000	0.325606000
H	10.234146000	-0.553977000	-3.457882000
H	11.918161000	0.691968000	-2.122254000
H	5.546552000	-1.646354000	1.593973000
H	6.209907000	-1.131927000	3.096436000

E=-4269,723562,H=-4269,723562,G=-4269,807222a.u.

TS_{k1}

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C	5.423413000	-2.581517000	1.449135000
C	4.732097000	-1.499853000	2.056808000
C	3.695156000	-1.779807000	3.009826000
C	2.742179000	-0.744654000	3.291183000
C	1.372707000	-1.107355000	3.405753000
C	0.381941000	-0.098823000	3.263255000
C	-0.804830000	-0.410555000	2.516324000
C	-1.578746000	0.651770000	1.985049000
C	-2.194834000	0.489167000	0.711794000
C	-2.667781000	1.683290000	0.042005000
C	-2.423087000	1.770005000	-1.380630000
C	-2.379329000	3.055606000	-1.981636000
C	-1.326364000	3.326281000	-2.926551000
C	-0.955699000	4.661361000	-3.304715000
C	0.365057000	5.004039000	-3.429017000
C	5.400476000	-3.828919000	2.147818000
C	4.407412000	-4.095435000	3.061467000
C	3.390065000	-3.129106000	3.328231000
C	1.987669000	-3.500327000	3.448927000
C	1.014377000	-2.486637000	3.241232000
C	-0.180624000	-2.797115000	2.513123000
C	-0.948059000	-1.711065000	1.970866000
C	-1.566044000	-1.861339000	0.697282000
C	-2.046038000	-0.725950000	0.013751000
C	-2.137507000	-0.742164000	-1.520280000
C	-1.792334000	0.661806000	-2.013968000
C	-0.708717000	0.931819000	-2.853545000
C	-0.371271000	2.303335000	-3.145424000
C	1.011165000	2.664261000	-3.282963000
C	1.392267000	4.032044000	-3.193063000
C	2.611104000	4.352163000	-2.485334000
C	2.868549000	5.658008000	-1.954405000
C	3.440207000	5.803916000	-0.714384000
C	1.542717000	-4.847910000	3.329542000
C	0.383263000	-5.146880000	2.643771000
C	-0.391359000	-4.116178000	2.040620000
C	-1.013469000	-4.276784000	0.729488000
C	-1.385133000	-3.126908000	0.015146000
C	-1.140609000	-3.068235000	-1.413156000
C	-1.146473000	-1.784124000	-2.032191000
C	-0.070366000	-1.474011000	-2.867167000
C	0.255865000	-0.098193000	-3.144188000
C	1.613052000	0.262591000	-3.257918000
C	1.992789000	1.640067000	-3.121264000
C	3.197549000	1.954655000	-2.448036000
C	3.369869000	3.283001000	-1.938720000

C	3.974565000	3.437553000	-0.644606000
C	3.793301000	4.655169000	0.063676000
C	3.522400000	4.576324000	1.486423000
C	2.884972000	5.640906000	2.197115000
C	1.891878000	5.370489000	3.109525000
C	-0.837338000	-5.489424000	-0.026848000
C	-0.557442000	-5.429500000	-1.364474000
C	-0.464284000	-4.157716000	-2.025565000
C	0.581737000	-3.859718000	-2.969097000
C	0.903351000	-2.494707000	-3.169608000
C	2.282115000	-2.121018000	-3.307284000
C	2.626419000	-0.746422000	-3.133158000
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C	4.004772000	0.890815000	-1.941348000
C	4.606055000	1.043922000	-0.660587000
C	4.376514000	2.255384000	0.059091000
C	4.117367000	2.177903000	1.453235000
C	3.459977000	3.288263000	2.081589000
C	2.422518000	3.007581000	3.033828000
C	1.488106000	4.024111000	3.363340000
C	0.086947000	3.649006000	3.485111000
C	-0.969234000	4.598318000	3.378701000
C	-2.127306000	4.287843000	2.695324000
C	1.565208000	-4.830536000	-3.360344000
C	2.881816000	-4.471203000	-3.481383000
C	3.291902000	-3.120592000	-3.230029000
C	4.510813000	-2.800839000	-2.522134000
C	4.640268000	-1.501324000	-1.963341000
C	5.245553000	-1.347699000	-0.669425000
C	5.009683000	-0.128731000	0.046721000
C	4.750074000	-0.203578000	1.440927000
C	4.105207000	0.896611000	2.078308000
C	3.068439000	0.616444000	3.027426000
C	2.109890000	1.633297000	3.302928000
C	0.741235000	1.267253000	3.417552000
C	-0.255633000	2.287763000	3.266025000
C	-1.450599000	1.970025000	2.540688000
C	-2.290652000	3.014287000	2.080787000
C	-2.915213000	2.857138000	0.769814000
C	-3.365217000	4.005954000	0.026247000
C	-3.092313000	4.106828000	-1.310131000
H	-0.272297000	-6.336142000	-1.887523000
H	-0.779080000	-6.444604000	0.483271000
H	0.154802000	-6.188061000	2.443747000
H	2.187579000	-5.663535000	3.638590000
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H	6.063967000	-4.632933000	1.848000000
H	6.487159000	-4.507975000	-0.330980000
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H	3.625831000	-5.244703000	-3.638991000

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H	-3.296685000	5.040024000	-1.824303000
H	-3.789158000	4.858376000	0.545701000
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H	1.316037000	6.196701000	3.512868000
H	3.062195000	6.671304000	1.908109000
H	3.483974000	6.793494000	-0.272091000
H	2.479310000	6.536248000	-2.458092000
C	-3.556285000	-1.075568000	-2.207236000
O	-3.564680000	-1.170621000	-3.432420000
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H	-3.398021000	-3.196090000	-1.559327000
O	-4.836953000	-1.773359000	0.641841000
O	-8.901075000	1.213437000	-1.060992000
N	-5.886435000	-1.071951000	0.179930000
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C	-5.800590000	-0.296936000	-0.929531000
C	-8.428210000	-1.969515000	2.680382000
C	-9.509329000	-1.165218000	2.260861000
H	-6.381237000	-2.571720000	2.316963000
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C	3.693755000	2.777043000	-2.473468000
C	3.310354000	1.453849000	-2.874964000
C	1.994574000	1.260111000	-3.376380000
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C	-0.364401000	-1.501280000	-2.578930000
C	-1.321166000	-1.585927000	-1.528887000
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C	-1.649618000	-2.848329000	0.566865000
C	-1.299696000	-4.016394000	1.294677000
C	-0.523432000	-3.858122000	2.498684000
C	0.195090000	-4.946523000	3.100256000
C	1.458050000	-4.752405000	3.595087000
C	4.208331000	5.327614000	-1.433448000
C	3.483128000	5.188425000	-2.593534000
C	3.013159000	3.903818000	-3.004591000
C	1.666382000	3.705639000	-3.519262000
C	1.121179000	2.395286000	-3.462430000
C	-0.256526000	2.222824000	-3.106097000
C	-0.684489000	0.926180000	-2.665340000
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C	4.330133000	-4.391629000	2.897555000
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C	-2.309615000	2.107870000	0.389638000
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C	-1.169134000	1.056833000	2.242960000
C	-0.449078000	-0.086499000	2.744505000
C	0.856191000	0.104715000	3.238357000
C	1.740528000	-1.020580000	3.354594000
C	3.111671000	-0.847157000	3.049665000
C	3.898637000	-2.007036000	2.750623000
C	4.852976000	-1.918894000	1.680368000
C	5.341612000	-3.113492000	1.087882000
C	5.468507000	-3.149115000	-0.356520000
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C	4.769374000	-4.516420000	-2.244116000
C	-2.551628000	4.454500000	-1.130081000
C	-2.653022000	4.509510000	0.233090000
C	-2.282691000	3.374326000	1.031526000
C	-1.504710000	3.507705000	2.237249000
C	-0.770918000	2.375136000	2.669286000
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C	4.642896000	1.768375000	0.889740000
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C	-0.097690000	-3.954678000	-2.585250000
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H	-1.232012000	5.480968000	-3.313395000
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H	4.226950000	6.379077000	1.148745000
H	2.628883000	6.231191000	2.959913000
H	0.495913000	5.964329000	3.500736000
H	-1.743966000	5.649054000	2.628146000
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H	0.298195000	-6.075767000	-2.899042000
H	2.629642000	-5.797105000	-3.462051000
H	4.676820000	-5.501952000	-2.687951000
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H	4.169114000	-5.351046000	3.377132000
C	-3.878815000	-0.600594000	0.646645000
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C	-8.122110000	0.186521000	0.041030000
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C	-8.976984000	1.019039000	0.780048000
C	-10.051148000	-0.945648000	-0.947453000
C	-5.986983000	-0.545267000	-0.585285000
C	-10.343391000	0.853131000	0.653696000
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C	2.478488000	-2.913822000	-2.284288000
C	1.232018000	-2.377139000	-2.749990000
C	1.229890000	-1.066096000	-3.298558000
C	0.000109000	-0.357690000	-3.376089000
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C	-1.225162000	1.654780000	-2.677203000
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C	-3.717378000	2.278289000	2.302210000
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C	4.899421000	-3.021168000	-2.314444000
C	3.702845000	-2.403480000	-2.790196000
C	3.700536000	-1.061707000	-3.353696000
C	2.471547000	-0.349952000	-3.365589000
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C	1.223469000	1.656072000	-2.677479000

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C	-1.271873000	3.067130000	1.080875000
C	-1.245013000	2.264653000	2.222749000
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H	-5.856466000	2.248933000	2.768001000
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H	-5.848116000	3.110927000	-1.599616000
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C	-0.002142000	5.107084000	0.524330000
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N	-3.192722000	-0.281224000	0.000145000
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C	0.737610000	0.641712000	-0.000148000
C	1.295783000	-1.734929000	0.000004000

C	2.106204000	0.974926000	-0.000019000
C	-1.894119000	0.043537000	0.000001000
C	2.631871000	-1.393019000	0.000076000
C	3.041797000	-0.037128000	0.000077000
H	0.953766000	-2.761344000	0.000043000
H	2.382020000	2.021215000	-0.000047000
H	3.382377000	-2.176638000	0.000160000
H	4.098608000	0.205481000	0.000142000
H	-3.411851000	-1.267325000	0.000158000
H	-3.901233000	0.433326000	0.000183000

E=-639,568569,H=-639,558342,G=-639,603140a.u.

NTCOCI/TPZ

C	4.658424000	-4.960100000	-2.052978000
C	5.303076000	-4.954073000	-0.840451000
C	5.398274000	-3.749258000	-0.073532000
C	5.180955000	-3.731914000	1.360439000
C	4.830876000	-2.495973000	1.966139000
C	3.802817000	-2.474779000	2.968185000
C	3.172862000	-1.219046000	3.260320000
C	1.763172000	-1.201845000	3.440537000
C	1.070695000	0.032911000	3.313266000
C	-0.187986000	0.038060000	2.621563000
C	-0.677332000	1.261478000	2.097157000
C	-1.364772000	1.250644000	0.850326000
C	-1.540982000	2.513974000	0.164059000
C	-1.338225000	2.513656000	-1.268746000
C	-0.981196000	3.732011000	-1.904199000
C	0.066172000	3.698296000	-2.894736000
C	0.760735000	4.880709000	-3.320557000
C	2.117772000	4.855771000	-3.509545000
C	4.860687000	-4.917249000	2.092871000
C	3.875984000	-4.895486000	3.052705000
C	3.165484000	-3.689036000	3.334687000
C	1.722078000	-3.671540000	3.520680000
C	1.044075000	-2.438439000	3.328435000
C	-0.222349000	-2.430356000	2.657167000
C	-0.696198000	-1.187158000	2.119061000
C	-1.379448000	-1.188189000	0.871881000
C	-1.563152000	0.026717000	0.184996000
C	-1.700007000	0.019099000	-1.339225000
C	-1.038655000	1.273504000	-1.898577000
C	0.033054000	1.227625000	-2.789126000
C	0.705475000	2.456012000	-3.129818000
C	2.125345000	2.431084000	-3.336214000
C	2.859870000	3.648075000	-3.295654000
C	4.151176000	3.640156000	-2.645765000
C	4.770418000	4.837128000	-2.159578000
C	5.412846000	4.843120000	-0.945946000
C	0.930380000	-4.853744000	3.452208000

C	-0.295466000	-4.842648000	2.819157000
C	-0.796240000	-3.650892000	2.222734000
C	-1.497252000	-3.657545000	0.941558000
C	-1.583192000	-2.460445000	0.212248000
C	-1.396642000	-2.489656000	-1.222534000
C	-1.078423000	-1.267840000	-1.880114000
C	-0.000421000	-1.260462000	-2.770356000
C	0.667189000	-0.027778000	-3.100334000
C	2.065717000	-0.044871000	-3.275204000
C	2.804684000	1.183082000	-3.189614000
C	4.077188000	1.173605000	-2.569918000
C	4.619655000	2.414880000	-2.101596000
C	5.297600000	2.421407000	-0.835139000
C	5.478601000	3.653514000	-0.152688000
C	5.256302000	3.671959000	1.280602000
C	4.957185000	4.879316000	1.985420000
C	3.970277000	4.898284000	2.943184000
C	-1.686435000	-4.883458000	0.211104000
C	-1.461510000	-4.918475000	-1.137862000
C	-1.064683000	-3.727131000	-1.834718000
C	-0.018535000	-3.733800000	-2.826162000
C	0.647418000	-2.509461000	-3.083525000
C	2.068810000	-2.520466000	-3.284828000
C	2.776843000	-1.286194000	-3.163826000
C	4.049530000	-1.291782000	-2.543324000
C	4.591918000	-0.059801000	-2.066319000
C	5.264589000	-0.053556000	-0.811870000
C	5.398643000	1.185846000	-0.116195000
C	5.189006000	1.201975000	1.288194000
C	4.880142000	2.456896000	1.912101000
C	3.850591000	2.478234000	2.912629000
C	3.236676000	3.712467000	3.251692000
C	1.793397000	3.726995000	3.439991000
C	1.024283000	4.922578000	3.350146000
C	-0.204373000	4.922178000	2.722436000
C	0.650781000	-4.938828000	-3.228678000
C	2.008810000	-4.947378000	-3.411615000
C	2.776432000	-3.752590000	-3.217394000
C	4.066517000	-3.760168000	-2.565268000
C	4.563280000	-2.534279000	-2.047577000
C	5.242862000	-2.528449000	-0.782043000
C	5.372115000	-1.280191000	-0.089852000
C	5.163902000	-1.261509000	1.314782000
C	4.864696000	-0.019544000	1.947413000
C	3.835474000	0.001773000	2.944636000
C	3.196566000	1.241975000	3.232678000
C	1.786782000	1.256331000	3.413653000
C	1.090982000	2.503520000	3.275662000
C	-0.178393000	2.505873000	2.608939000
C	-0.730486000	3.728528000	2.151947000

C	-1.432067000	3.723726000	0.870789000
C	-1.592134000	4.938318000	0.115504000
C	-1.358806000	4.943433000	-1.232973000
H	-1.451260000	-5.875692000	-1.648089000
H	-1.859857000	-5.812750000	0.742270000
H	-0.800340000	-5.788208000	2.654183000
H	1.348730000	-5.807267000	3.755918000
H	3.541637000	-5.836007000	3.477447000
H	5.272842000	-5.873391000	1.788938000
H	5.606785000	-5.900134000	-0.405143000
H	4.473100000	-5.909953000	-2.542762000
H	2.510908000	-5.894949000	-3.575014000
H	0.108469000	-5.877893000	-3.251241000
H	2.639923000	5.788863000	-3.692258000
H	0.239296000	5.831049000	-3.358326000
H	-1.326453000	5.890845000	-1.760406000
H	-1.747487000	5.881331000	0.627770000
H	-0.691513000	5.873852000	2.540169000
H	1.462252000	5.873796000	3.632731000
H	3.653258000	5.854571000	3.345421000
H	5.387875000	5.820326000	1.660752000
H	5.738406000	5.791245000	-0.531395000
H	4.608137000	5.779721000	-2.671059000
C	-3.170302000	0.033040000	-1.891795000
O	-3.491938000	0.324559000	-2.996862000
O	-8.142557000	-1.008341000	-0.666900000
O	-11.728367000	2.474744000	1.138421000
N	-9.070192000	-0.213843000	-0.214768000
N	-10.909374000	1.617768000	0.717227000
N	-9.676270000	2.011041000	0.442777000
N	-7.524445000	1.488069000	-0.256443000
C	-10.350080000	-0.642328000	0.065291000
C	-11.300504000	0.286895000	0.544683000
C	-10.720494000	-1.988474000	-0.122456000
C	-12.616365000	-0.121448000	0.837439000
C	-8.788628000	1.107892000	-0.007798000
C	-12.012637000	-2.373531000	0.168118000
C	-12.964706000	-1.441709000	0.649068000
H	-9.972504000	-2.677665000	-0.491175000
H	-13.316835000	0.618014000	1.202425000
H	-12.304892000	-3.408770000	0.026036000
H	-13.974325000	-1.769692000	0.870189000
H	-6.946955000	0.813395000	-0.742466000
H	-7.313020000	2.472311000	-0.303197000
Cl	-4.470335000	-0.507290000	-0.700241000

E=-4654,079215,H=-4654,019535,G=-4654,167956 a.u.

TS_{k2}

C	-5.554529000	3.870231000	-2.510403000
C	-6.344535000	3.611561000	-1.416594000

C	-6.190047000	2.395072000	-0.680164000
C	-6.196619000	2.369833000	0.770975000
C	-5.589828000	1.262871000	1.420749000
C	-4.774056000	1.493110000	2.578737000
C	-3.852455000	0.465417000	2.969457000
C	-2.552080000	0.853368000	3.390555000
C	-1.510879000	-0.114927000	3.381893000
C	-0.214041000	0.287280000	2.915846000
C	0.694145000	-0.710597000	2.474874000
C	1.520722000	-0.436742000	1.349985000
C	2.155192000	-1.550281000	0.686322000
C	2.182286000	-1.529482000	-0.756018000
C	2.327189000	-2.757717000	-1.452784000
C	1.489333000	-2.983730000	-2.608054000
C	1.261560000	-4.293358000	-3.145441000
C	0.006885000	-4.662312000	-3.559331000
C	-6.364824000	3.556646000	1.549321000
C	-5.582381000	3.776154000	2.658626000
C	-4.598134000	2.819312000	3.052067000
C	-3.266092000	3.217129000	3.482065000
C	-2.227947000	2.251085000	3.408167000
C	-0.925894000	2.652518000	2.962861000
C	-0.021173000	1.634743000	2.510991000
C	0.806591000	1.900998000	1.387159000
C	1.430963000	0.823590000	0.720426000
C	1.694018000	0.924482000	-0.744572000
C	1.626602000	-0.396217000	-1.421279000
C	0.755781000	-0.625328000	-2.498166000
C	0.551657000	-1.976490000	-2.948630000
C	-0.757784000	-2.363129000	-3.389822000
C	-1.087554000	-3.743068000	-3.472391000
C	-2.406787000	-4.152663000	-3.040139000
C	-2.702169000	-5.501362000	-2.662798000
C	-3.490998000	-5.758839000	-1.567875000
C	-2.865646000	4.583454000	3.551303000
C	-1.609754000	4.967761000	3.132160000
C	-0.686372000	4.008294000	2.626544000
C	0.164255000	4.285241000	1.474997000
C	0.711175000	3.198832000	0.764712000
C	0.736941000	3.238496000	-0.677892000
C	0.892914000	2.005063000	-1.377009000
C	0.036704000	1.744680000	-2.457293000
C	-0.163227000	0.396429000	-2.908475000
C	-1.459836000	0.008871000	-3.321178000
C	-1.797104000	-1.382510000	-3.359736000
C	-3.093482000	-1.782442000	-2.951165000
C	-3.300044000	-3.150581000	-2.576468000
C	-4.128171000	-3.421489000	-1.435203000
C	-4.033030000	-4.684769000	-0.794317000
C	-4.039504000	-4.710582000	0.656772000
C	-3.510488000	-5.812358000	1.398140000

C	-2.728772000	-5.591014000	2.507940000
C	0.094626000	5.543511000	0.785658000
C	0.082601000	5.576013000	-0.583923000
C	0.165857000	4.358359000	-1.336832000
C	-0.667403000	4.114073000	-2.491435000
C	-0.888970000	2.766269000	-2.870085000
C	-2.196444000	2.371532000	-3.311449000
C	-2.514482000	0.977676000	-3.320144000
C	-3.810147000	0.575131000	-2.912174000
C	-4.024520000	-0.784581000	-2.535156000
C	-4.844719000	-1.052827000	-1.399470000
C	-4.703722000	-2.309111000	-0.738365000
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C	-4.147017000	-3.473178000	1.344575000
C	-3.331579000	-3.243645000	2.503144000
C	-2.441848000	-4.260022000	2.938897000
C	-1.110771000	-3.860740000	3.368670000
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C	1.236832000	-4.380501000	2.984358000
C	-1.591962000	5.090763000	-2.988744000
C	-2.843006000	4.711334000	-3.402842000
C	-3.239673000	3.335738000	-3.355350000
C	-4.560057000	2.927330000	-2.924290000
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C	-5.570057000	1.313233000	-1.358650000
C	-5.421822000	0.048569000	-0.700343000
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C	-4.877580000	-1.108104000	1.388140000
C	-4.058883000	-0.877207000	2.541884000
C	-3.135580000	-1.888868000	2.932046000
C	-1.835745000	-1.498909000	3.353281000
C	-0.787546000	-2.478199000	3.332877000
C	0.513320000	-2.072562000	2.887213000
C	1.464291000	-3.055110000	2.513287000
C	2.312073000	-2.779218000	1.359942000
C	2.946296000	-3.843075000	0.633799000
C	2.940264000	-3.837243000	-0.736795000
H	-0.129686000	6.513459000	-1.086660000
H	-0.102991000	6.456622000	1.336220000
H	-1.392258000	6.027369000	3.053649000
H	-3.593804000	5.353130000	3.782814000
H	-5.617060000	4.749642000	3.135717000
H	-6.991718000	4.362852000	1.184311000
H	-6.979654000	4.402663000	-1.032696000
H	-5.589622000	4.857038000	-2.958715000
H	-3.572532000	5.479145000	-3.636580000
H	-1.362200000	6.147315000	-2.905226000
H	-0.173341000	-5.698733000	-3.824048000
H	2.041886000	-5.044888000	-3.093365000
H	3.277875000	-4.720422000	-1.268253000
H	3.293005000	-4.728462000	1.155161000

H	2.007963000	-5.135800000	2.879220000
H	-0.188420000	-5.824099000	3.609600000
H	-2.210647000	-6.432116000	2.955837000
H	-3.584715000	-6.820027000	1.003992000
H	-3.573008000	-6.780152000	-1.212175000
H	-2.185333000	-6.326225000	-3.140973000
C	3.468985000	1.409632000	-1.008210000
O	4.203456000	1.231346000	-1.892273000
O	7.696887000	2.029399000	-0.348926000
O	10.610363000	-2.311864000	0.606030000
N	8.464791000	1.009616000	-0.118295000
N	9.958887000	-1.260382000	0.367200000
N	8.639540000	-1.334466000	0.340574000
N	6.576451000	-0.327099000	0.007880000
C	9.841375000	1.113499000	-0.061934000
C	10.616584000	-0.041823000	0.180515000
C	10.477121000	2.356300000	-0.250960000
C	12.021794000	0.038577000	0.240225000
C	7.919380000	-0.224686000	0.092495000
C	11.853674000	2.419792000	-0.191964000
C	12.630406000	1.261257000	0.054176000
H	9.857508000	3.223525000	-0.436438000
H	12.582616000	-0.866898000	0.430131000
H	12.350106000	3.373952000	-0.334971000
H	13.711248000	1.337524000	0.096961000
H	6.038534000	0.550378000	0.202013000
H	6.184673000	-1.221927000	0.257829000
Cl	4.315273000	2.181148000	0.757122000

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NTCOTPZ/HCl

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C	4.671677000	4.132289000	-0.470080000
C	4.601931000	2.890343000	-1.155603000
C	3.847345000	2.805846000	-2.374058000
C	3.435863000	1.506356000	-2.822306000
C	2.118387000	1.359897000	-3.334992000
C	1.545353000	0.060293000	-3.390122000
C	0.166692000	-0.089456000	-3.018834000
C	-0.305736000	-1.372540000	-2.640474000
C	-1.268229000	-1.471207000	-1.597063000
C	-1.478849000	-2.767422000	-0.986511000
C	-1.633258000	-2.795621000	0.453264000
C	-1.313142000	-3.995398000	1.142104000
C	-0.539763000	-3.895871000	2.354155000
C	0.150251000	-5.020393000	2.921568000
C	1.415078000	-4.872586000	3.427333000
C	4.414366000	5.306498000	-1.244366000

C	3.691565000	5.224070000	-2.411420000
C	3.194913000	3.965404000	-2.868905000
C	1.846558000	3.815511000	-3.395972000
C	1.271426000	2.516887000	-3.385843000
C	-0.111526000	2.363963000	-3.040951000
C	-0.570779000	1.063433000	-2.645537000
C	-1.531257000	0.956772000	-1.601498000
C	-1.745662000	-0.293778000	-0.987823000
C	-2.257733000	-0.349405000	0.462079000
C	-1.623675000	-1.554836000	1.149664000
C	-0.797421000	-1.437555000	2.267274000
C	-0.102788000	-2.606370000	2.746051000
C	1.219162000	-2.453403000	3.283628000
C	2.061216000	-3.593027000	3.407255000
C	3.462327000	-3.440098000	3.086388000
C	4.297184000	-4.555271000	2.750919000
C	5.209249000	-4.457732000	1.729063000
C	0.945242000	4.912827000	-3.508239000
C	-0.389065000	4.762046000	-3.191203000
C	-0.894683000	3.507780000	-2.746109000
C	-1.880277000	3.403179000	-1.673291000
C	-2.017094000	2.179577000	-0.996845000
C	-2.178400000	2.178159000	0.442414000
C	-1.900879000	0.971291000	1.143607000
C	-1.069573000	1.038552000	2.262897000
C	-0.379571000	-0.137727000	2.728885000
C	0.927418000	0.006217000	3.234058000
C	1.784909000	-1.142540000	3.315403000
C	3.160874000	-0.990728000	3.020907000
C	3.921744000	-2.157644000	2.684497000
C	4.881380000	-2.055274000	1.620361000
C	5.344302000	-3.240001000	0.988681000
C	5.476187000	-3.229050000	-0.455560000
C	5.479644000	-4.433906000	-1.225742000
C	4.755745000	-4.513935000	-2.392196000
C	-2.361076000	4.579868000	-0.997337000
C	-2.465203000	4.590983000	0.366692000
C	-2.124354000	3.421149000	1.126905000
C	-1.348478000	3.495229000	2.339013000
C	-0.643154000	2.331953000	2.735248000
C	0.680613000	2.470523000	3.272124000
C	1.516395000	1.313201000	3.310056000
C	2.892928000	1.460871000	3.015661000
C	3.654533000	0.302982000	2.670212000
C	4.606089000	0.404737000	1.617113000
C	5.027354000	-0.791313000	0.961122000
C	5.162334000	-0.778108000	-0.452391000
C	5.140116000	-2.034241000	-1.145817000
C	4.385151000	-2.119195000	-2.363977000
C	3.997847000	-3.394374000	-2.852837000

C	2.649117000	-3.541470000	-3.378668000
C	2.005657000	-4.807857000	-3.486081000
C	0.669956000	-4.947066000	-3.169851000
C	-0.917373000	4.744588000	2.901022000
C	0.349431000	4.875549000	3.406258000
C	1.256774000	3.765712000	3.390593000
C	2.657782000	3.917673000	3.070273000
C	3.383927000	2.763116000	2.674177000
C	4.344049000	2.866092000	1.610595000
C	4.759608000	1.660830000	0.956207000
C	4.894730000	1.671453000	-0.457335000
C	4.881593000	0.429170000	-1.156727000
C	4.125228000	0.344264000	-2.370672000
C	3.702983000	-0.941139000	-2.817083000
C	2.385025000	-1.084874000	-3.329242000
C	1.807371000	-2.397419000	-3.373966000
C	0.423819000	-2.544966000	-3.029473000
C	-0.095021000	-3.829554000	-2.730583000
C	-1.081246000	-3.935630000	-1.658466000
C	-1.296928000	-5.185544000	-0.977749000
C	-1.394859000	-5.213953000	0.386657000
H	-2.673528000	5.527072000	0.873730000
H	-2.497701000	5.505470000	-1.545561000
H	-1.012041000	5.648456000	-3.143069000
H	1.325256000	5.912125000	-3.691100000
H	3.372508000	6.142355000	-2.892854000
H	4.643111000	6.286361000	-0.839338000
H	4.450591000	6.268227000	1.373320000
H	2.843928000	6.095492000	3.174747000
H	0.701003000	5.860098000	3.695718000
H	-1.540559000	5.626837000	2.801618000
H	1.970816000	-5.756949000	3.720235000
H	-0.267744000	-6.016709000	2.825739000
H	-1.395343000	-6.171234000	0.897112000
H	-1.230324000	-6.120872000	-1.522299000
H	0.252750000	-5.946828000	-3.118851000
H	2.591953000	-5.702583000	-3.665337000
H	4.643463000	-5.481030000	-2.870690000
H	5.916156000	-5.339418000	-0.818324000
H	5.717923000	-5.355634000	1.394665000
H	4.112265000	-5.526510000	3.196907000
C	-3.807403000	-0.499994000	0.599187000
O	-4.308162000	-0.686756000	1.707264000
O	-6.046877000	1.396063000	0.791651000
O	-8.203933000	-2.056201000	-2.611613000
N	-6.604139000	0.540806000	0.021903000
N	-7.727887000	-1.257701000	-1.768271000
N	-6.428732000	-1.261005000	-1.547939000
N	-4.515111000	-0.393026000	-0.561411000
C	-7.995038000	0.518858000	-0.143043000

C	-8.569413000	-0.387701000	-1.054258000
C	-8.807569000	1.410240000	0.572895000
C	-9.959451000	-0.416341000	-1.252596000
C	-5.904417000	-0.389443000	-0.676442000
C	-10.174696000	1.374606000	0.371344000
C	-10.751538000	0.462080000	-0.539218000
H	-8.335622000	2.097038000	1.262545000
H	-10.368173000	-1.125928000	-1.959543000
H	-10.813261000	2.056713000	0.922054000
H	-11.826513000	0.450616000	-0.680418000
H	-5.769789000	-1.140621000	2.276312000
H	-3.986948000	-0.438056000	-1.427912000
Cl	-6.869003000	-1.597339000	2.891426000

E=-4654,090725,H=-4654,031977,G=-4654,175554a.u.

M06-2x

In water

TPZ

O	-1.467471000	-2.219711000	0.000000000
O	0.086954000	2.831101000	0.000021000
N	-1.015005000	-0.998737000	-0.000005000
N	-0.245813000	1.632682000	-0.000027000
N	-1.516195000	1.335958000	-0.000006000
N	-3.178392000	-0.273537000	0.000016000
C	0.323431000	-0.705854000	-0.000007000
C	0.734317000	0.636621000	-0.000012000
C	1.286879000	-1.732222000	0.000000000
C	2.099191000	0.976138000	-0.000002000
C	-1.882232000	0.037810000	0.000001000
C	2.617534000	-1.388600000	0.000006000
C	3.029602000	-0.033922000	0.000006000
H	0.939044000	-2.756685000	0.000003000
H	2.372463000	2.023293000	-0.000004000
H	3.368506000	-2.171406000	0.000013000
H	4.086341000	0.205568000	0.000012000
H	-3.409255000	-1.256422000	0.000002000
H	-3.877450000	0.450142000	0.000001000

E=-639,303379,H=-639,293318,G=-639,337767a.u.

NTCOOH

C	4.889808000	-2.134571000	2.940650000
C	4.888329000	-3.142648000	2.015587000
C	3.687925000	-3.485371000	1.320357000
C	3.688789000	-3.753665000	-0.106148000
C	2.472198000	-3.615621000	-0.807038000
C	2.472664000	-2.978810000	-2.089850000
C	1.225001000	-2.473808000	-2.590603000
C	1.223566000	-1.212178000	-3.231796000

C	0.000001000	-0.514627000	-3.366959000
C	0.000005000	0.905919000	-3.134025000
C	-1.217878000	1.539943000	-2.806239000
C	-1.212529000	2.589690000	-1.855332000
C	-2.480261000	3.006913000	-1.288263000
C	-2.495333000	3.301808000	0.129385000
C	-3.715359000	3.178219000	0.825308000
C	-3.705094000	2.518420000	2.104150000
C	-4.905385000	2.004581000	2.700782000
C	-4.897253000	0.792514000	3.326714000
C	4.887057000	-3.685424000	-0.875726000
C	4.885763000	-3.075443000	-2.104100000
C	3.688279000	-2.509529000	-2.627018000
C	3.687612000	-1.208954000	-3.285974000
C	2.467893000	-0.503611000	-3.350373000
C	2.464364000	0.910756000	-3.141379000
C	1.217890000	1.539936000	-2.806236000
C	1.212545000	2.589683000	-1.855329000
C	0.000008000	2.977018000	-1.273590000
C	0.000007000	3.632514000	0.104711000
C	-1.265270000	3.211850000	0.836599000
C	-1.244540000	2.499669000	2.026892000
C	-2.481149000	1.991095000	2.557176000
C	-2.474252000	0.718686000	3.220899000
C	-3.690165000	0.023212000	3.401774000
C	-3.688867000	-1.409120000	3.219738000
C	-4.889829000	-2.134545000	2.940639000
C	-4.888353000	-3.142622000	2.015576000
C	4.877623000	-0.451608000	-3.447978000
C	4.870842000	0.912159000	-3.262251000
C	3.675385000	1.588209000	-2.904232000
C	3.673113000	2.680628000	-1.930137000
C	2.480278000	3.006899000	-1.288258000
C	2.495347000	3.301796000	0.129390000
C	1.265282000	3.211844000	0.836601000
C	1.244544000	2.499663000	2.026895000
C	0.000001000	1.988172000	2.544200000
C	-0.000003000	0.737319000	3.170379000
C	-1.234011000	0.020430000	3.319715000
C	-1.230335000	-1.379074000	3.159046000
C	-2.471040000	-2.039269000	2.885245000
C	-2.470914000	-3.098569000	1.917839000
C	-3.687950000	-3.485351000	1.320348000
C	-3.688812000	-3.753645000	-0.106156000
C	-4.887078000	-3.685397000	-0.875737000
C	-4.885778000	-3.075417000	-2.104111000
C	4.897224000	3.079403000	-1.288678000
C	4.919514000	3.307095000	0.054464000
C	3.715370000	3.178200000	0.825316000
C	3.705099000	2.518402000	2.104158000

C	2.481150000	1.991083000	2.557181000
C	2.474245000	0.718673000	3.220904000
C	1.234000000	0.020424000	3.319718000
C	1.230318000	-1.379080000	3.159048000
C	-0.000010000	-2.040712000	2.875681000
C	-0.000012000	-3.089856000	1.917970000
C	-1.228370000	-3.435830000	1.288791000
C	-1.226482000	-3.703732000	-0.099592000
C	-2.472218000	-3.615608000	-0.807043000
C	-2.472678000	-2.978796000	-2.089856000
C	-3.688289000	-2.509509000	-2.627026000
C	-3.687614000	-1.208934000	-3.285982000
C	-4.877620000	-0.451581000	-3.447989000
C	-4.870832000	0.912186000	-3.262263000
C	4.905385000	2.004556000	2.700792000
C	4.897246000	0.792489000	3.326724000
C	3.690155000	0.023193000	3.401782000
C	3.688849000	-1.409139000	3.219745000
C	2.471020000	-2.039282000	2.885250000
C	2.470891000	-3.098583000	1.917845000
C	1.228346000	-3.435837000	1.288794000
C	1.226460000	-3.703739000	-0.099589000
C	-0.000010000	-3.628270000	-0.811111000
C	-0.000070000	-2.989141000	-2.095101000
C	-1.225011000	-2.473801000	-2.590606000
C	-1.223568000	-1.212172000	-3.231799000
C	-2.467890000	-0.503598000	-3.350378000
C	-2.464354000	0.910769000	-3.141384000
C	-3.675373000	1.588229000	-2.904241000
C	-3.673097000	2.680648000	-1.930146000
C	-4.897207000	3.079429000	-1.288690000
C	-4.919500000	3.307120000	0.054453000
H	5.871908000	3.456270000	0.551684000
H	5.831671000	3.060880000	-1.838309000
H	5.820399000	1.435580000	-3.245538000
H	5.832015000	-0.953093000	-3.565360000
H	5.835004000	-2.894009000	-2.596574000
H	5.836206000	-3.968128000	-0.433532000
H	5.835219000	-3.575959000	1.711995000
H	5.836748000	-1.797094000	3.347541000
H	5.837348000	0.361520000	3.653838000
H	5.850163000	2.512740000	2.541331000
H	-5.837358000	0.361550000	3.653826000
H	-5.850159000	2.512770000	2.541318000
H	-5.871894000	3.456300000	0.551670000
H	-5.831653000	3.060911000	-1.838323000
H	-5.820386000	1.435612000	-3.245553000
H	-5.832015000	-0.953061000	-3.565375000
H	-5.835016000	-2.893977000	-2.596587000
H	-5.836229000	-3.968096000	-0.433545000

H	-5.835245000	-3.575928000	1.711982000
H	-5.836768000	-1.797063000	3.347528000
C	0.000022000	5.176487000	0.060962000
O	-0.000099000	5.860868000	1.054665000
O	0.000203000	5.666024000	-1.179210000
H	0.000219000	6.636035000	-1.116804000

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C	-3.465395000	4.612288000	1.312166000
C	-3.414503000	3.354990000	1.949591000
C	-2.381660000	3.099392000	2.908731000
C	-2.083310000	1.730655000	3.225571000
C	-0.724597000	1.355982000	3.354598000
C	-0.380260000	-0.012376000	3.258362000
C	0.804603000	-0.363964000	2.520600000
C	0.924791000	-1.677937000	2.018455000
C	1.524610000	-1.878881000	0.751448000
C	1.354185000	-3.168338000	0.110559000
C	1.111829000	-3.159284000	-1.316593000
C	0.424533000	-4.251921000	-1.883504000
C	-0.622813000	-3.980111000	-2.832594000
C	-1.618564000	-4.959513000	-3.163687000
C	-2.926184000	-4.592729000	-3.296720000
C	-2.807708000	5.693683000	1.967827000
C	-1.818310000	5.446931000	2.885416000
C	-1.442897000	4.109661000	3.198421000
C	-0.042847000	3.723936000	3.331734000
C	0.283492000	2.361956000	3.165859000
C	1.470418000	2.006752000	2.452458000
C	1.579362000	0.666886000	1.947412000
C	2.178577000	0.455025000	0.680027000
C	1.989905000	-0.771400000	0.032324000
C	2.084759000	-0.839747000	-1.490953000
C	1.110146000	-1.900840000	-1.978707000
C	0.047055000	-1.611108000	-2.824809000
C	-0.930691000	-2.631507000	-3.093283000
C	-2.305721000	-2.247936000	-3.238943000
C	-3.317449000	-3.226437000	-3.115401000
C	-4.530755000	-2.867597000	-2.419161000
C	-5.401285000	-3.854810000	-1.859197000
C	-5.970915000	-3.656686000	-0.630539000
C	1.011077000	4.661229000	3.171299000
C	2.161314000	4.314615000	2.498949000
C	2.315333000	3.014663000	1.950179000
C	2.941224000	2.798548000	0.645014000
C	2.685386000	1.610260000	-0.037982000

C	2.445140000	1.649211000	-1.465448000
C	1.781501000	0.535587000	-2.052420000
C	0.710022000	0.787865000	-2.894571000
C	-0.266307000	-0.242392000	-3.149642000
C	-1.610501000	0.126383000	-3.271505000
C	-2.633632000	-0.865665000	-3.109276000
C	-3.825235000	-0.511148000	-2.446607000
C	-4.647580000	-1.554864000	-1.913187000
C	-5.248259000	-1.347958000	-0.627179000
C	-5.706855000	-2.461561000	0.105946000
C	-5.436288000	-2.493774000	1.532225000
C	-5.419227000	-3.719017000	2.260564000
C	-4.431300000	-3.962525000	3.180925000
C	3.390688000	3.921449000	-0.133074000
C	3.119577000	3.979288000	-1.468406000
C	2.410028000	2.905648000	-2.104416000
C	1.356169000	3.158199000	-3.053605000
C	0.393637000	2.148628000	-3.239631000
C	-0.984681000	2.518471000	-3.386383000
C	-1.974587000	1.510995000	-3.182115000
C	-3.167886000	1.858515000	-2.519868000
C	-3.986175000	0.825046000	-1.978308000
C	-4.581889000	1.030276000	-0.704255000
C	-4.993512000	-0.107415000	0.044099000
C	-4.735454000	-0.134360000	1.434124000
C	-4.735857000	-1.407352000	2.097411000
C	-3.704575000	-1.663334000	3.058052000
C	-3.416198000	-2.993862000	3.421913000
C	-2.015465000	-3.377997000	3.554193000
C	-1.599094000	-4.731641000	3.460822000
C	-0.446736000	-5.065741000	2.785840000
C	1.000848000	4.489078000	-3.456373000
C	-0.311246000	4.839986000	-3.588938000
C	-1.346679000	3.882478000	-3.336296000
C	-2.560593000	4.239240000	-2.639662000
C	-3.327731000	3.205720000	-2.060898000
C	-3.928342000	3.412442000	-0.774749000
C	-4.337372000	2.258485000	-0.029318000
C	-4.080162000	2.227674000	1.360746000
C	-4.086041000	0.977202000	2.032543000
C	-3.051332000	0.720703000	2.993673000
C	-2.738380000	-0.628173000	3.299511000
C	-1.379062000	-1.000122000	3.428497000
C	-1.036971000	-2.390704000	3.314432000
C	0.150291000	-2.739085000	2.599102000
C	0.345753000	-4.064568000	2.167033000
C	0.973351000	-4.277416000	0.862039000
C	0.772378000	-5.514903000	0.155780000
C	0.492265000	-5.500239000	-1.177098000
H	3.325991000	4.895026000	-2.012063000

H	3.814820000	4.791003000	0.357242000
H	2.878692000	5.094518000	2.268440000
H	0.860649000	5.701522000	3.438660000
H	-1.224455000	6.279474000	3.247107000
H	-2.966078000	6.712745000	1.632153000
H	-3.381751000	6.762034000	-0.509912000
H	-2.377759000	6.417187000	-2.679855000
H	-0.563581000	5.880369000	-3.763449000
H	1.764222000	5.256166000	-3.529336000
H	-3.680409000	-5.363092000	-3.414841000
H	-1.358778000	-6.012488000	-3.177153000
H	0.194263000	-6.420570000	-1.668058000
H	0.702854000	-6.449449000	0.701274000
H	-0.239327000	-6.115053000	2.607403000
H	-2.259900000	-5.528919000	3.783274000
H	-4.344909000	-4.958590000	3.601471000
H	-6.083351000	-4.529670000	1.981301000
H	-6.503460000	-4.477365000	-0.162180000
H	-5.500363000	-4.825614000	-2.332495000
C	3.494789000	-1.265898000	-1.979521000
O	3.914427000	-0.922919000	-3.069233000
O	4.131990000	-2.021263000	-1.123312000
H	5.123773000	-2.202827000	-1.444108000
O	6.538428000	-2.263493000	-1.625338000
O	8.352156000	-0.168060000	2.875492000
N	6.984722000	-1.666276000	-0.516656000
N	7.921439000	-0.628417000	1.816455000
N	8.082182000	-1.900501000	1.578931000
N	7.743837000	-3.704022000	0.185353000
C	6.804237000	-0.324881000	-0.297804000
C	7.275712000	0.225834000	0.901597000
C	6.162209000	0.495851000	-1.238472000
C	7.105071000	1.586758000	1.196932000
C	7.599478000	-2.406910000	0.419147000
C	5.991762000	1.829339000	-0.936079000
C	6.458674000	2.379823000	0.277498000
H	5.809412000	0.058074000	-2.164427000
H	7.482173000	1.969198000	2.136422000
H	5.478709000	2.471763000	-1.645322000
H	6.305607000	3.432794000	0.483738000
H	7.395899000	-4.065272000	-0.691366000
H	8.210978000	-4.289192000	0.859220000

E=-4268,203486,H=-4268,144925,G=-4268,284235a.u.

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C	-3.185263000	1.431692000	-3.697030000
C	-2.776122000	2.019059000	-2.473828000

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C	0.362977000	3.408865000	-1.225308000
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C	3.355940000	0.708235000	1.225278000
C	3.433564000	-0.002069000	2.473675000
C	3.132466000	-1.404821000	2.473730000
C	2.825877000	-2.051571000	3.696993000
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C	1.044901000	-3.388955000	4.886736000
C	-0.329371000	-3.530661000	4.886666000
C	-2.837566000	2.127513000	-4.886848000
C	-1.808990000	3.049888000	-4.886820000
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C	0.377662000	3.470512000	-3.696872000
C	1.062519000	3.263004000	-2.473684000
C	2.303884000	2.543723000	-2.473636000
C	2.778529000	2.009694000	-1.225253000
C	3.355940000	0.708235000	-1.225278000
C	3.451471000	0.000166000	0.000000000
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C	1.710820000	-2.971735000	1.225335000
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C	-1.078269000	-3.320307000	3.696899000
C	-2.346276000	-2.586059000	3.696749000
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C	2.824945000	2.052964000	3.696752000
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NT/TPZ1

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C	-4.373623000	-0.264427000	2.158336000
C	-4.021789000	1.006553000	1.579605000
C	-4.331325000	1.231163000	0.215164000
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C	-3.237293000	2.018324000	-1.837479000
C	-2.186702000	2.803771000	-2.360591000
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C	1.263718000	2.093452000	-3.287736000
C	2.496301000	2.741478000	-3.080934000
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C	4.473627000	2.858072000	-1.528108000
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C	-4.811224000	-2.857173000	3.080521000
C	-5.711983000	-2.264527000	2.222991000
C	-5.396045000	-1.041186000	1.580758000
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C	-4.982051000	0.176789000	-0.518648000
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C	-0.062158000	0.009401000	-3.348642000
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C	3.376761000	0.679133000	-0.181099000
C	4.059698000	1.671086000	0.550002000
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C	0.451486000	5.348523000	3.232099000
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H	3.100591000	4.771584000	3.692424000
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C	5.825380000	-1.055280000	-0.640599000
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C	0.933190000	-3.613716000	2.771531000
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H	-1.467834000	5.906454000	-3.513358000
H	0.712028000	6.061190000	-2.493699000
H	1.759366000	6.098402000	-0.594493000
H	1.468956000	6.008375000	1.796238000
H	2.742689000	-5.511217000	-0.911722000
H	2.452285000	-5.601294000	1.478861000
H	0.974496000	-5.769756000	3.064656000
H	-1.384403000	-5.979474000	3.519845000
H	-3.341383000	-6.119943000	2.599010000
H	-4.507450000	-6.159100000	0.489016000
H	-4.251527000	-6.078193000	-1.658125000
H	-2.614767000	-5.893666000	-3.418429000
H	-0.495306000	-5.704761000	-3.825618000
H	1.681944000	-5.550096000	-2.803203000

O	7.194347000	-2.073882000	0.781883000
O	7.997684000	2.648801000	-1.445783000
N	7.461719000	-0.916230000	0.251165000
N	7.842628000	1.534888000	-0.914973000
N	6.670295000	0.966565000	-0.983111000
N	5.305398000	-0.842541000	-0.504429000
C	8.700970000	-0.335411000	0.332528000
C	8.913407000	0.918886000	-0.261644000
C	9.757309000	-0.980855000	1.001800000
C	10.170352000	1.546071000	-0.199107000
C	6.496457000	-0.240479000	-0.407587000
C	10.981712000	-0.358863000	1.055878000
C	11.193697000	0.906210000	0.456464000
H	9.563237000	-1.946548000	1.449311000
H	10.290825000	2.513572000	-0.668755000
H	11.803362000	-0.846964000	1.568552000
H	12.170268000	1.371826000	0.517214000
H	5.183693000	-1.666975000	0.069060000
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E=-4079,127841,H=-4079,067911,G=-4079,197041a.u.

In DMF

TPZ

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N	-0.245743000	1.632884000	-0.000027000
N	-1.516191000	1.336072000	-0.000006000
N	-3.178308000	-0.273593000	0.000017000
C	0.323380000	-0.705839000	-0.000007000
C	0.734305000	0.636604000	-0.000012000
C	1.286737000	-1.732303000	0.000000000
C	2.099182000	0.976027000	-0.000002000
C	-1.882094000	0.037967000	0.000001000
C	2.617391000	-1.388751000	0.000006000
C	3.029530000	-0.034098000	0.000007000
H	0.938562000	-2.756664000	0.000003000
H	2.372336000	2.023222000	-0.000004000
H	3.368311000	-2.171618000	0.000013000
H	4.086289000	0.205348000	0.000012000
H	-3.408620000	-1.256624000	0.000002000
H	-3.877313000	0.450080000	0.000001000

E=-639,303042,H=-639,292982,G=-639,337428a.u.

NTCOCI

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C	3.836515000	-3.687032000	-0.331352000
C	2.610407000	-3.551652000	-1.015453000
C	2.578762000	-2.841323000	-2.258317000
C	1.309857000	-2.355191000	-2.722431000
C	1.257502000	-1.058820000	-3.287587000
C	0.008688000	-0.400000000	-3.374605000
C	-0.041249000	1.002862000	-3.057167000
C	-1.279512000	1.570573000	-2.685295000
C	-1.304323000	2.564061000	-1.677472000
C	-2.581684000	2.893591000	-1.077991000
C	-2.590988000	3.112331000	0.352133000
C	-3.798434000	2.907426000	1.049977000
C	-3.751816000	2.177796000	2.289256000
C	-4.927234000	1.590458000	2.866064000
C	-4.872103000	0.343326000	3.416343000
C	5.025186000	-3.529493000	-1.101296000
C	4.993214000	-2.848392000	-2.291936000
C	3.772425000	-2.297588000	-2.774867000
C	3.718450000	-0.962407000	-3.359148000
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C	2.420290000	1.100010000	-3.087345000
C	1.155550000	1.664609000	-2.707337000
C	1.121622000	2.662441000	-1.701107000
C	-0.099651000	2.976920000	-1.091315000
C	-0.100271000	3.531423000	0.331615000
C	-1.351410000	3.034038000	1.045220000
C	-1.291433000	2.250189000	2.192581000
C	-2.505363000	1.667786000	2.700071000
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C	-3.639733000	-0.386942000	3.435951000
C	-3.591133000	-1.805239000	3.168318000
C	-4.768357000	-2.553924000	2.854008000
C	-4.739529000	-3.505046000	1.870531000
C	4.878193000	-0.154259000	-3.491541000
C	4.823877000	1.196297000	-3.232250000
C	3.609221000	1.806986000	-2.825182000
C	3.578744000	2.837518000	-1.786902000
C	2.380837000	3.082976000	-1.117361000
C	2.400429000	3.279226000	0.315495000
C	1.180819000	3.101788000	1.023581000
C	1.193681000	2.325912000	2.171425000
C	-0.028618000	1.751682000	2.672407000
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C	-1.135690000	-1.687488000	3.096306000
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C	-3.533701000	-3.766299000	1.150740000
C	-3.536066000	-3.952216000	-0.289127000
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C	4.793580000	3.235887000	-1.129451000
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C	3.629468000	3.160091000	0.994928000
C	3.652677000	2.428130000	2.234756000
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C	2.493436000	0.529368000	3.259285000
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C	1.322042000	-1.602210000	3.083525000
C	0.113613000	-2.288823000	2.769330000
C	0.142752000	-3.279119000	1.749873000
C	-1.077324000	-3.629814000	1.108394000
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C	-2.362876000	-3.024080000	-2.232118000
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C	-3.650087000	-1.234995000	-3.317767000
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C	-4.910621000	0.834616000	-3.159152000
C	4.873981000	1.925810000	2.796051000
C	4.912135000	0.682037000	3.355925000
C	3.733708000	-0.131890000	3.395656000
C	3.780965000	-1.550956000	3.130197000
C	2.583048000	-2.201732000	2.765076000
C	2.612293000	-3.200382000	1.735956000
C	1.377376000	-3.543336000	1.094616000
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C	0.140475000	-3.654964000	-1.005938000
C	0.108365000	-2.942562000	-2.250747000
C	-1.138028000	-2.445810000	-2.709690000
C	-1.187410000	-1.149183000	-3.274055000
C	-2.457534000	-0.481955000	-3.344890000
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C	-3.738250000	1.531314000	-2.766624000
C	-3.767605000	2.561380000	-1.728308000
C	-4.998809000	2.879506000	-1.056159000
C	-5.014480000	3.033012000	0.297219000
H	5.772092000	3.526470000	0.724458000
H	5.723829000	3.281644000	-1.684497000
H	5.753901000	1.752836000	-3.198634000
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H	5.988874000	-3.545587000	1.481737000
H	5.941689000	-1.870708000	3.222897000
H	5.869297000	0.267443000	3.653462000
H	5.799761000	2.474058000	2.659449000
H	-5.794059000	-0.139180000	3.722650000
H	-5.890080000	2.074739000	2.745937000
H	-5.965949000	3.121367000	0.810516000

H	-5.937771000	2.857977000	-1.597919000
H	-5.878663000	1.320305000	-3.104760000
H	-5.804498000	-1.042612000	-3.572072000
H	-5.729261000	-3.034620000	-2.716488000
H	-5.676509000	-4.226636000	-0.617124000
H	-5.673621000	-3.951155000	1.546466000
H	-5.723395000	-2.273885000	3.284844000
C	-0.137670000	5.083114000	0.433364000
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E=-4013,235867,H=-4013,188117,G=-4013,302946a.u.

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C	-5.271397000	2.893780000	1.462674000
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C	-3.649526000	1.914889000	3.019786000
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C	-1.398517000	1.050677000	3.430706000
C	-0.486145000	-0.020033000	3.274751000
C	0.732605000	0.226865000	2.551173000
C	1.427713000	-0.868102000	1.992854000
C	2.062312000	-0.712661000	0.734167000
C	2.470439000	-1.910225000	0.025575000
C	2.228721000	-1.938008000	-1.399312000
C	2.097073000	-3.187880000	-2.037446000
C	1.039859000	-3.349914000	-3.002537000
C	0.578038000	-4.643784000	-3.416495000
C	-0.756938000	-4.876615000	-3.581253000
C	-5.161558000	4.113143000	2.192859000
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C	-3.253453000	3.215668000	3.392916000
C	-1.827698000	3.474897000	3.553753000
C	-0.934935000	2.405997000	3.325839000
C	0.285293000	2.649974000	2.623017000
C	0.971208000	1.525836000	2.050808000
C	1.599507000	1.671822000	0.790090000
C	1.994492000	0.527319000	0.084283000
C	2.099280000	0.572722000	-1.445062000
C	1.673378000	-0.774469000	-1.998961000
C	0.601253000	-0.930496000	-2.861451000
C	0.174508000	-2.259871000	-3.210715000
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C	-1.710003000	-3.832095000	-3.349265000
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C	0.597154000	3.953745000	2.192997000
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C	1.535052000	2.967072000	0.145718000
C	1.320625000	2.972569000	-1.283524000
C	1.237942000	1.719754000	-1.953728000
C	0.163221000	1.515642000	-2.814538000
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C	-1.638238000	-0.066732000	-3.291370000
C	-2.126728000	-1.413007000	-3.208087000
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C	-3.640480000	-2.978305000	-2.103181000
C	-4.267712000	-3.126992000	-0.821861000
C	-4.191353000	-4.369258000	-0.158341000
C	-3.931109000	-4.360745000	1.270371000
C	-3.378292000	-5.494891000	1.934131000
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C	0.901673000	5.359031000	-1.158842000
C	0.744186000	4.120004000	-1.866079000
C	-0.297787000	3.935932000	-2.840928000
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H	0.194792000	6.046925000	2.639183000
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H	-4.012034000	5.254631000	3.557527000
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H	-6.126911000	4.965095000	-0.246272000
H	-5.075221000	5.215490000	-2.406895000
H	-3.208136000	5.580771000	-3.488845000
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H	-4.031258000	-6.511819000	-0.549405000
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O	4.119919000	0.149988000	-2.759953000
O	8.032267000	2.278148000	-0.989302000
O	5.958590000	-2.347418000	0.500124000
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N	6.507925000	-0.933430000	-1.083205000
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C	7.518888000	0.824155000	0.771814000
C	6.964892000	-0.403759000	1.168500000
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C	7.048305000	0.250325000	-1.436214000
C	7.955406000	1.347595000	3.066495000
C	7.409382000	0.102600000	3.462877000
H	8.427941000	2.654674000	1.405890000
H	6.488172000	-1.730164000	2.786286000
H	8.337577000	2.023987000	3.823333000
H	7.382712000	-0.162001000	4.513351000
H	7.347414000	1.536859000	-2.913618000
H	6.509289000	0.081422000	-3.364428000
Cl	4.463662000	2.104385000	-1.097903000

E=-4652,545507,H=-4652,486729,G=-4652,635867a.u.