

Electronic Supporting Information

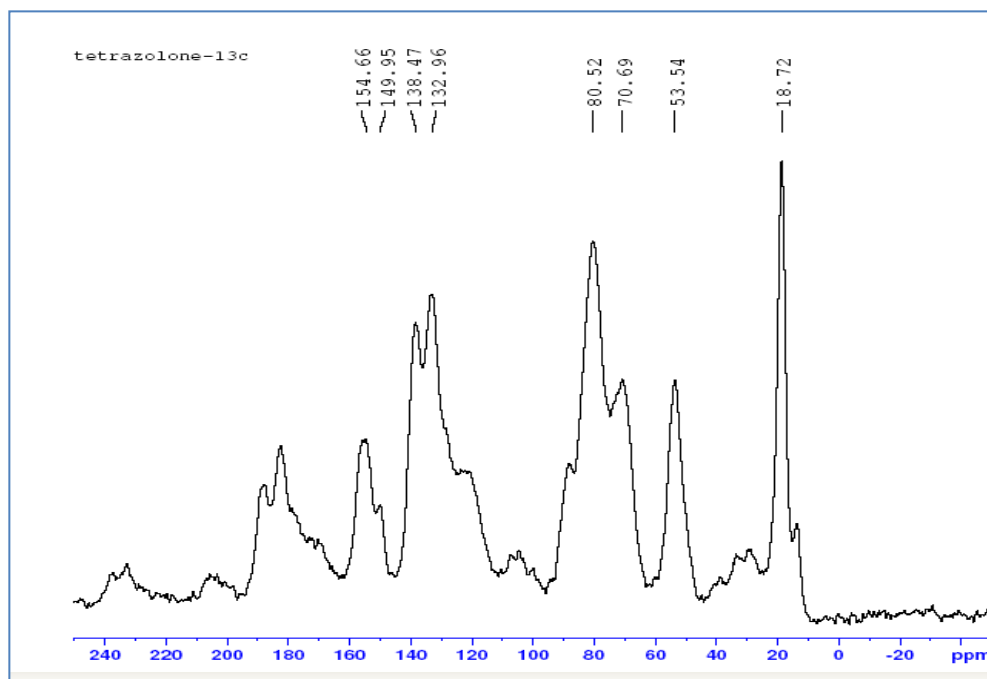
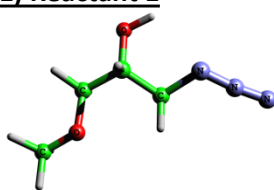


Figure .1. ^{13}C NMR (solid state) spectrum of GAP-TDI (cured)

Optimized geometries of the molecules at B3LYP/6-31g(d,p) level DFT

1) Reactant 1



Number of imaginary frequency = 0

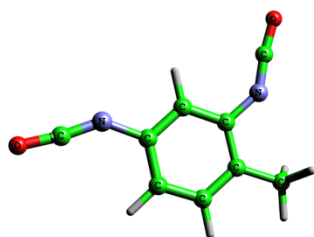
Total energy = -472.464988785 au

X,Y,Z coordinates in Å.

O	0.030326000	2.096785000	0.182281000
C	0.364635000	0.810309000	-0.310196000
H	0.374584000	0.797094000	-1.411406000
C	1.772575000	0.510192000	0.191782000
H	2.451572000	1.303472000	-0.157018000
H	1.781789000	0.527832000	1.294469000
O	2.159172000	-0.756511000	-0.304650000
C	-0.639105000	-0.237683000	0.168556000
N	-1.973671000	0.205274000	-0.309250000
N	-2.925066000	-0.527899000	-0.026153000
N	-3.878611000	-1.124134000	0.173382000

H	-0.628663000	-0.283672000	1.265734000
H	-0.379940000	-1.222756000	-0.233092000
C	3.464939000	-1.125645000	0.090175000
H	3.556811000	-1.192062000	1.185385000
H	3.669599000	-2.107309000	-0.343035000
H	4.217570000	-0.410569000	-0.275842000
H	-0.896134000	2.250053000	-0.053997000

2) Reactant 2



Number of imaginary frequency = 0

Total energy = -606.542627946 au

X,Y,Z coordinates in Å.

C	-1.122410000	0.109149000	-0.000014000
C	-1.058017000	1.515723000	-0.000038000
C	0.038266000	-0.671719000	0.000100000
H	-0.025122000	-1.754129000	0.000146000
C	0.212492000	2.100544000	0.000022000
C	1.291584000	-0.056218000	0.000202000
H	0.288524000	3.184118000	-0.000040000
C	1.379557000	1.342230000	0.000139000
H	2.351774000	1.824478000	0.000182000
C	-2.314605000	2.346169000	-0.000105000
H	-2.932793000	2.133210000	0.878677000
H	-2.076517000	3.412556000	-0.000540000
H	-2.933095000	2.132535000	-0.878504000
N	-2.388303000	-0.485279000	-0.000054000
N	2.422898000	-0.876075000	0.000280000
C	3.629487000	-0.785507000	-0.000034000
C	-2.905207000	-1.578802000	-0.000060000
O	4.805877000	-0.841878000	-0.000324000
O	-3.533604000	-2.574710000	-0.000022000

3) Pre-reaction complex for TS1

This complex is 8.8 kJ/mol more stable than the infinitely separated reactants.

Number of imaginary frequency = 0

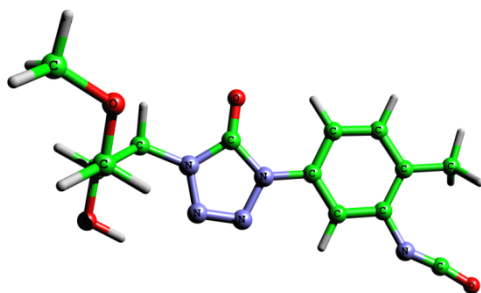
Total energy = -1079.01094872 au

X,Y,Z coordinates in Å.

C	-4.099147000	-0.322917000	-0.096460000
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C	-4.419116000	1.052882000	-0.128812000
C	-2.771150000	-0.756081000	-0.067112000
H	-2.561360000	-1.819273000	-0.043247000
C	-3.354069000	1.958755000	-0.130879000
C	-1.733109000	0.180557000	-0.069668000
H	-3.575346000	3.021788000	-0.155151000
C	-2.024173000	1.547345000	-0.102898000
H	-1.212934000	2.266670000	-0.102914000
C	-5.848771000	1.524253000	-0.159712000
H	-6.409584000	1.183410000	0.718885000
H	-5.896336000	2.615277000	-0.178620000
H	-6.381230000	1.154111000	-1.044118000
N	-5.084069000	-1.310171000	-0.092020000
N	-0.396954000	-0.217394000	-0.043078000
C	0.352592000	-1.152136000	0.047754000
C	-6.278748000	-1.486799000	-0.109141000
O	1.180867000	-1.993966000	0.123707000
O	-7.413584000	-1.804881000	-0.122199000
O	3.893218000	-1.549085000	1.495119000
C	4.666979000	-0.573408000	0.825624000
H	5.644443000	-0.576228000	1.323462000
C	4.855813000	-0.949789000	-0.654551000
H	3.884495000	-0.915414000	-1.159728000
O	5.705675000	-0.049755000	-1.351073000
C	4.096165000	0.837265000	0.995418000
N	2.713303000	0.848391000	0.454018000
N	2.181301000	1.948689000	0.311866000
N	1.580718000	2.905504000	0.135156000
H	4.725475000	1.556071000	0.458423000
H	4.072559000	1.095636000	2.060689000
C	7.086040000	-0.334751000	-1.214049000
H	7.624245000	0.393433000	-1.825519000
H	7.439350000	-0.246530000	-0.176165000
H	7.325853000	-1.346641000	-1.573525000
H	5.231582000	-1.981479000	-0.707760000
H	3.023454000	-1.595509000	1.066172000

4) Product from TS1



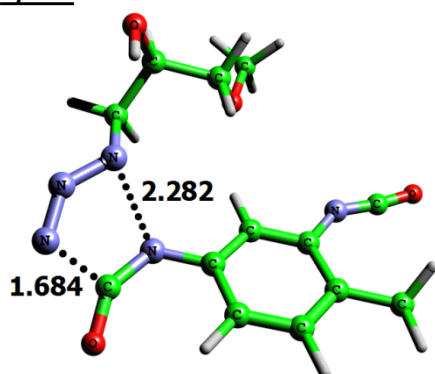
Number of imaginary frequency = 0

Total energy = -1079.04336083 au

X,Y,Z coordinates in Å.

C	3.593366000	-0.218019000	0.128805000
C	3.971182000	1.138868000	0.021537000
C	2.267808000	-0.619161000	-0.048952000
H	2.011557000	-1.666237000	0.038808000
C	2.961491000	2.059099000	-0.268755000
C	1.292154000	0.336380000	-0.338100000
H	3.224390000	3.109328000	-0.356330000
C	1.630495000	1.687901000	-0.450512000
H	0.869081000	2.422071000	-0.675356000
C	5.399748000	1.574421000	0.211216000
H	6.070418000	1.099743000	-0.515132000
H	5.493867000	2.655830000	0.089939000
H	5.774843000	1.318837000	1.209552000
N	4.520026000	-1.220311000	0.414909000
N	-0.054014000	-0.084697000	-0.517936000
C	-1.175273000	0.690795000	-0.841258000
C	5.688153000	-1.425083000	0.641665000
O	-1.282327000	1.887431000	-1.044579000
O	6.791723000	-1.768293000	0.874549000
O	-4.450752000	-2.237623000	-0.422343000
C	-4.518454000	-0.832329000	-0.249468000
H	-5.530937000	-0.548544000	-0.560514000
C	-4.325947000	-0.460118000	1.231425000
H	-3.325600000	-0.765501000	1.558504000
O	-4.420273000	0.933561000	1.471670000
C	-3.569589000	-0.071680000	-1.188824000
N	-2.159877000	-0.284897000	-0.878357000
N	-1.645837000	-1.513825000	-0.615247000
N	-0.397166000	-1.401197000	-0.393139000
H	-3.723054000	1.005823000	-1.100410000
H	-3.761374000	-0.379867000	-2.221618000
C	-5.745668000	1.410025000	1.629230000
H	-5.673987000	2.475054000	1.860497000
H	-6.352931000	1.291598000	0.719989000
H	-6.260411000	0.899347000	2.456594000
H	-5.056696000	-1.026194000	1.826454000
H	-3.524834000	-2.504003000	-0.305024000

5) TS2



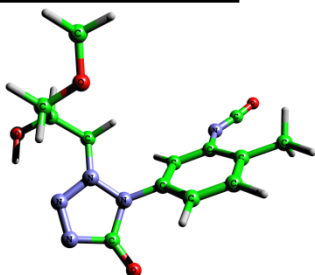
Number of imaginary frequency = 1

Total energy = -1078.93591162 au

X,Y,Z coordinates in Å.

C	2.270419000	-0.364738000	-0.137381000
C	2.888720000	-1.453630000	0.520763000
C	0.924832000	-0.406217000	-0.500741000
H	0.485968000	0.452948000	-0.993097000
C	2.091466000	-2.570442000	0.794826000
C	0.149065000	-1.543139000	-0.220956000
H	2.543349000	-3.419723000	1.299794000
C	0.746452000	-2.629257000	0.449251000
H	0.164418000	-3.516710000	0.667567000
C	4.340616000	-1.413054000	0.913034000
H	4.555296000	-0.584317000	1.598817000
H	4.633694000	-2.339761000	1.411333000
H	4.994018000	-1.283429000	0.041585000
N	2.979932000	0.795312000	-0.449935000
N	-1.176930000	-1.563179000	-0.651166000
C	-1.905999000	-2.639447000	-0.596740000
C	4.055888000	1.335437000	-0.389326000
O	-1.837900000	-3.828489000	-0.800068000
O	5.045000000	1.979727000	-0.396347000
O	-3.241765000	2.275001000	1.679900000
C	-2.525818000	2.351053000	0.459568000
H	-2.852253000	3.279523000	-0.022774000
C	-1.012328000	2.428361000	0.714403000
H	-0.661316000	1.481923000	1.143643000
O	-0.282896000	2.624610000	-0.488295000
C	-2.891307000	1.199293000	-0.484319000
N	-2.697031000	-0.093656000	0.206956000
N	-3.537743000	-0.997536000	0.005623000
N	-3.474641000	-2.180363000	-0.190329000
H	-2.237244000	1.204819000	-1.363037000
H	-3.930396000	1.280285000	-0.812621000
C	-0.100152000	3.983596000	-0.853210000
H	0.485937000	3.987916000	-1.774430000
H	-1.051284000	4.502434000	-1.039475000
H	0.450607000	4.534204000	-0.077651000
H	-0.813286000	3.225543000	1.442976000
H	-3.073243000	1.396603000	2.052775000

6) Product from TS2



Number of imaginary frequency = 0

Total energy = -1079.00205805 au

X,Y,Z coordinates in Å

C	-2.654483000	-0.036352000	-0.307422000
C	-3.130213000	0.278132000	0.984651000
C	-1.385442000	0.377857000	-0.724339000
H	-1.064741000	0.157659000	-1.735570000
C	-2.285691000	1.011552000	1.824651000
C	-0.561781000	1.083137000	0.152502000
H	-2.637986000	1.270901000	2.818521000
C	-1.011582000	1.412689000	1.432582000
H	-0.380044000	1.989464000	2.097231000
C	-4.500002000	-0.150257000	1.438912000
H	-4.614103000	-1.240512000	1.412708000
H	-4.689094000	0.178537000	2.462822000
H	-5.287922000	0.271772000	0.803809000
N	-3.419050000	-0.752092000	-1.226940000
N	0.724289000	1.519160000	-0.276672000
C	1.265581000	2.814693000	-0.100004000
C	-4.493210000	-1.283599000	-1.383559000
O	0.647975000	3.813703000	0.199324000
O	-5.490533000	-1.839665000	-1.672383000
O	4.141986000	-0.978191000	-1.458341000
C	3.024158000	-1.481695000	-0.757961000
H	2.823541000	-2.469306000	-1.191168000
C	3.333627000	-1.659830000	0.740594000
H	3.519739000	-0.683993000	1.200499000
O	2.252078000	-2.248074000	1.448042000
C	1.732215000	-0.681142000	-1.000684000
N	1.809553000	0.676173000	-0.451277000
N	2.900476000	1.421059000	-0.559357000
N	2.650688000	2.662764000	-0.337287000
H	0.908819000	-1.183048000	-0.490479000
H	1.522881000	-0.627140000	-2.075411000
C	2.261372000	-3.666082000	1.448930000
H	1.403012000	-3.989227000	2.042223000
H	2.168681000	-4.093708000	0.439826000
H	3.179464000	-4.060714000	1.907692000
H	4.251760000	-2.255761000	0.831969000
H	4.254959000	-0.051176000	-1.190186000

7) X,Y,Z coordinates in Å for TS3

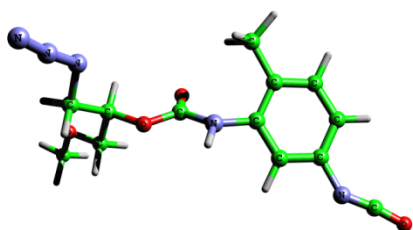
Number of imaginary frequency = 1

Total energy = -1078.99682995 au

O	1.713712000	0.025188000	-0.900878000
C	2.946185000	0.026242000	-0.153547000

H	2.764227000	-0.362755000	0.856561000
C	3.933333000	-0.882639000	-0.885641000
H	3.490797000	-1.882851000	-0.988111000
H	4.124482000	-0.487386000	-1.896824000
O	5.127238000	-0.925479000	-0.123900000
C	3.444496000	1.460581000	-0.053572000
N	2.453995000	2.236119000	0.726520000
N	2.700572000	3.439073000	0.858341000
N	2.822167000	4.558390000	1.048207000
H	3.557930000	1.882184000	-1.061310000
H	4.420462000	1.456170000	0.444441000
H	0.734888000	0.541781000	-0.458727000
C	6.094694000	-1.818722000	-0.655369000
H	6.397439000	-1.521494000	-1.670244000
H	6.962939000	-1.777286000	0.005008000
H	5.710508000	-2.848450000	-0.685514000
C	-1.644216000	-0.534375000	0.147791000
C	-2.003393000	-1.447153000	1.162914000
C	-2.616139000	0.229018000	-0.508921000
H	-2.317382000	0.935622000	-1.274864000
C	-3.369024000	-1.578917000	1.453789000
C	-3.966951000	0.078854000	-0.190424000
H	-3.670835000	-2.276740000	2.230195000
C	-4.349444000	-0.839335000	0.797043000
H	-5.397354000	-0.963197000	1.051887000
C	-0.974501000	-2.233625000	1.936672000
H	-0.178434000	-1.579977000	2.311656000
H	-1.437047000	-2.726413000	2.795804000
H	-0.496452000	-3.002750000	1.320725000
N	-0.294386000	-0.289656000	-0.209784000
N	-4.899941000	0.860355000	-0.880999000
C	-6.088689000	1.061086000	-0.951102000
C	0.586395000	-1.182718000	-0.565259000
O	-7.221614000	1.348136000	-1.115251000
O	0.868228000	-2.328620000	-0.732839000

8) Product from TS3



Number of imaginary frequency = 0

Total energy = -1079.03766735 au

X,Y,Z coordinates in Å.

O	-1.676057000	0.073746000	-0.524044000
C	-2.912992000	0.474754000	0.099177000

H	-2.901715000	0.163430000	1.145917000
C	-3.022963000	1.998157000	0.024212000
H	-2.175753000	2.436733000	0.571369000
H	-2.956950000	2.327403000	-1.027138000
O	-4.256577000	2.374556000	0.601000000
C	-4.039523000	-0.221938000	-0.644753000
N	-3.968987000	-1.671397000	-0.358865000
N	-4.693957000	-2.389277000	-1.052271000
N	-5.312515000	-3.159011000	-1.628055000
H	-3.946925000	-0.029597000	-1.721879000
H	-4.989395000	0.197621000	-0.295829000
H	0.318365000	-0.559439000	-1.427768000
C	-4.433002000	3.777129000	0.660180000
H	-4.423773000	4.231059000	-0.342663000
H	-5.404552000	3.960499000	1.123693000
H	-3.650793000	4.257982000	1.266137000
C	1.814281000	-0.555793000	0.036540000
C	2.173302000	-1.338207000	1.151217000
C	2.778680000	0.144717000	-0.692487000
H	2.487120000	0.744894000	-1.547986000
C	3.527533000	-1.347882000	1.512979000
C	4.123435000	0.094626000	-0.321871000
H	3.830424000	-1.940566000	2.371512000
C	4.498861000	-0.652442000	0.801485000
H	5.540716000	-0.693959000	1.103325000
C	1.170412000	-2.160097000	1.917101000
H	0.505089000	-2.701406000	1.236138000
H	1.676875000	-2.889820000	2.553825000
H	0.536256000	-1.524777000	2.541751000
N	0.470056000	-0.502175000	-0.430370000
N	5.046909000	0.810295000	-1.089695000
C	6.232061000	1.049099000	-1.127166000
C	-0.585262000	-0.009954000	0.293909000
O	7.357933000	1.360518000	-1.282027000
O	-0.573358000	0.302165000	1.467726000

9) X,Y,Z coordinates in Å for TS4

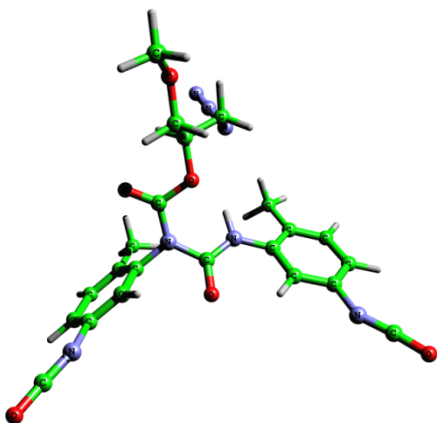
Number of imaginary frequency = 1

Total energy = -1685.51908848 au

O	-0.580604000	1.882712000	0.440707000
C	-0.941985000	3.236643000	0.807849000
H	-1.975350000	3.240697000	1.162107000
C	0.003678000	3.632251000	1.939665000
H	-0.117291000	2.924777000	2.774422000
H	1.049659000	3.565573000	1.596958000
O	-0.332246000	4.949237000	2.319159000
C	-0.790900000	4.133654000	-0.421740000
N	-1.667299000	3.720371000	-1.537792000

N	-2.827601000	4.152477000	-1.497250000
N	-3.913118000	4.490684000	-1.590346000
H	0.230329000	4.053230000	-0.802249000
H	-0.968029000	5.170853000	-0.119480000
C	0.456809000	5.433114000	3.392066000
H	1.524807000	5.459093000	3.129510000
H	0.117368000	6.448138000	3.606911000
H	0.334082000	4.815116000	4.293464000
C	-1.964323000	-1.316520000	-0.386020000
C	-2.625843000	-1.485954000	-1.612461000
C	-2.176192000	-2.165552000	0.696554000
H	-1.646930000	-2.010807000	1.628616000
C	-3.515345000	-2.562906000	-1.707657000
C	-3.069090000	-3.233399000	0.568553000
H	-4.046770000	-2.722837000	-2.641261000
C	-3.741346000	-3.430928000	-0.644328000
H	-4.436941000	-4.257678000	-0.748745000
C	-2.406678000	-0.549083000	-2.774261000
H	-1.369887000	-0.575760000	-3.130459000
H	-3.048114000	-0.823346000	-3.614802000
H	-2.633681000	0.487402000	-2.503568000
N	-1.013177000	-0.224897000	-0.240464000
N	-3.256881000	-4.068405000	1.670621000
C	-3.889427000	-5.046916000	1.996164000
C	-1.579322000	1.016332000	0.214528000
O	-4.441280000	-5.987455000	2.440528000
O	-2.760115000	1.218273000	0.340536000
C	2.501368000	-0.655153000	-0.905020000
C	3.017898000	-0.435717000	-2.202230000
C	3.352838000	-1.026335000	0.145200000
H	2.956581000	-1.195634000	1.138139000
C	4.391746000	-0.600473000	-2.396833000
C	4.721372000	-1.181838000	-0.085434000
H	4.802372000	-0.435661000	-3.389369000
C	5.249950000	-0.968232000	-1.364087000
H	6.313554000	-1.089619000	-1.542380000
C	2.114365000	-0.037943000	-3.341670000
H	1.582790000	0.896678000	-3.129757000
H	2.688275000	0.102126000	-4.261258000
H	1.351651000	-0.801539000	-3.535088000
N	1.118105000	-0.480400000	-0.725650000
N	5.528553000	-1.551752000	0.996180000
C	6.683360000	-1.789538000	1.260161000
C	0.469368000	-0.635819000	0.416382000
O	7.766191000	-2.044085000	1.652330000
O	0.609285000	-0.940025000	1.569967000
H	-0.152204000	-0.124727000	-1.116903000

Product from TS4



Number of imaginary frequency = 0

Total energy = -1685.59368844 au

X,Y,Z coordinates in Å.

O	-0.019195000	1.795841000	0.435786000
C	0.020278000	3.193899000	0.806018000
H	-0.666671000	3.749581000	0.163336000
C	-0.434162000	3.327493000	2.260144000
H	-1.465645000	2.955656000	2.345199000
H	0.207348000	2.709179000	2.910602000
O	-0.350360000	4.694856000	2.602990000
C	1.457416000	3.665077000	0.606304000
N	1.881123000	3.590532000	-0.810028000
N	1.631246000	4.586948000	-1.501409000
N	1.471055000	5.439267000	-2.243210000
H	2.138507000	3.011240000	1.156586000
H	1.549041000	4.678796000	1.006966000
C	-0.812560000	4.965057000	3.914637000
H	-0.216454000	4.433936000	4.671773000
H	-0.714279000	6.040549000	4.074322000
H	-1.867293000	4.678810000	4.036940000
C	-2.411511000	-0.634625000	-0.718508000
C	-2.912978000	-0.522244000	-2.024260000
C	-3.088180000	-1.341146000	0.270776000
H	-2.669565000	-1.425304000	1.265171000
C	-4.134788000	-1.151143000	-2.294926000
C	-4.303851000	-1.961416000	-0.027368000
H	-4.551737000	-1.080626000	-3.295433000
C	-4.828786000	-1.862868000	-1.322286000
H	-5.772663000	-2.343105000	-1.561179000
C	-2.190347000	0.264288000	-3.087581000
H	-1.135370000	-0.020607000	-3.155424000
H	-2.646993000	0.104310000	-4.067187000
H	-2.228133000	1.336887000	-2.867043000
N	-1.145615000	-0.008388000	-0.387703000
N	-4.955076000	-2.661734000	0.990833000
C	-5.953995000	-3.316429000	1.178443000

C	-1.202802000	1.339291000	-0.058660000
O	-6.883178000	-3.967635000	1.496938000
O	-2.193944000	2.026968000	-0.186070000
C	2.445565000	-1.030552000	-0.553095000
C	3.481909000	-0.530381000	-1.372778000
C	2.673952000	-2.102603000	0.315449000
H	1.873292000	-2.497752000	0.922392000
C	4.739436000	-1.132542000	-1.271213000
C	3.942593000	-2.683238000	0.383101000
H	5.546093000	-0.759895000	-1.896299000
C	4.987758000	-2.195842000	-0.409727000
H	5.972199000	-2.649352000	-0.356646000
C	3.247345000	0.599342000	-2.346055000
H	3.005100000	1.546206000	-1.846459000
H	4.140431000	0.772745000	-2.951014000
H	2.422394000	0.372537000	-3.032620000
N	1.182157000	-0.393197000	-0.635592000
N	4.120970000	-3.751236000	1.267769000
C	4.976595000	-4.519218000	1.640215000
C	-0.017878000	-0.908625000	-0.232733000
O	5.711933000	-5.323260000	2.090454000
O	-0.201982000	-2.047771000	0.149414000
H	1.187129000	0.569404000	-0.940080000