

Exploring the factors controlling the mechanism and the high stereoselectivity of the polar [3+2] cycloaddition reaction of the *N,N'*-cyclic azomethine imine with 3-nitro-2-phenyl-2*H*-chromene. A molecular electron density theory study

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S3. Cartesian coordinates of the stationary points involved in the 32CA reaction between **1** and chromene **2**.

Table S1. Total energies (a.u) in gas phase of the stationary points involved in the 32CA reaction of the azomethine imine **1** with chromene **2**.

System	<i>E</i> (a.u)
Chromene 2	-858.74377
Azomethine imine 1	-571.90804
TS-ox	-1430.63884
TS-on	-1430.62862
TS-mn	-1430.56559
TS-mx	-1430.62305
3ox	-1430.66445
3on	-1430.67198
3mn	-1430.67162
3mx	-1430.65346

Table S2. Total energies (a.u) in isopropanol solvent of the stationary points involved in the 32CA reaction of the azomethine imine **1** with chromene **2**.

System	<i>E</i> (a.u)
Chromene 2	-858.7538373
Azomethine imine 1	-571.9260006
TS-ox	-1430.66001
TS-on	-1430.650963
TS-mn	-1430.584528
TS-mx	-1430.642416
3ox	-1430.679159
3on	-1430.686535
3mn	-1430.685198
3mx	-1430.667409

**Cartesian coordinates of the stationary points involved in the 32CA reaction between
azomethine imine 1 and chromene 2**

Azomethine imine 1

C	0.01822200	-0.91302100	-0.08825200
N	-1.15383900	-0.32199800	-0.06071400
N	-2.28132000	-1.04502300	-0.12288300
C	-3.36041500	-0.20362400	0.00498000
C	-2.88846900	1.25434500	0.20601400
C	-1.38538300	1.16677100	0.04428600
O	-4.52338700	-0.54482100	-0.01941600
C	1.35934700	-0.36455700	-0.04898000
C	1.74247400	0.99020200	-0.14846100
C	3.08269900	1.35606700	-0.09768100
C	4.08150200	0.39647500	0.04916300
C	3.72563800	-0.94886500	0.13754600
C	2.39142200	-1.32123600	0.08583300
H	-3.19220700	1.58870200	1.19936800
H	-3.36882900	1.89835900	-0.53007700
H	-0.80986400	1.54473000	0.88806200
H	-1.02331000	1.62544300	-0.87602600
H	-0.07172200	-1.99098500	-0.13349300
H	1.00928100	1.76954800	-0.28272900
H	3.34745100	2.40419300	-0.17923000
H	5.12315000	0.69235200	0.08838500
H	4.49029700	-1.70943000	0.24550100
H	2.12674100	-2.37053500	0.15404800

Chromene 2

C	-1.17700900	1.51503600	0.44699300
C	0.01583000	1.54403200	-0.16470000
C	0.53678200	0.39127700	-0.98237700
O	-0.58033600	-0.40015700	-1.48934700
C	-1.68002300	-0.57267100	-0.71328200
C	-2.03566000	0.36668500	0.27743000
N	0.87488700	2.71589800	-0.04679500
O	0.51019200	3.64401500	0.66632400
O	1.92703700	2.69090000	-0.68203100
C	-3.22219700	0.17777300	1.00261900
C	-4.03550900	-0.91769100	0.75448500
C	-3.67313900	-1.83248800	-0.23941200
C	-2.50444800	-1.66491600	-0.97447100
H	-1.49208300	2.36104500	1.04582200
H	-3.49397100	0.90468300	1.76051700
H	-4.30722600	-2.68834000	-0.44109400
H	-2.21401700	-2.36403100	-1.74846400
H	-4.94748400	-1.06023700	1.32087900
H	1.01279600	0.77533200	-1.88276400
C	1.52589600	-0.50760000	-0.25816600
C	2.51209200	-1.15703800	-1.00636900
C	1.45118500	-0.74609500	1.11636600
C	3.40555900	-2.03096500	-0.39600900
H	2.58034800	-0.97154300	-2.07311100
C	2.34425500	-1.62222900	1.72928700
H	0.70125400	-0.24287800	1.71518400

C	3.32195300	-2.26634900	0.97537400
H	4.16974400	-2.52259100	-0.98723600
H	2.27829600	-1.79749700	2.79710100
H	4.01960000	-2.94386100	1.45455000

TS-ox

C	3.47056500	2.27748300	2.34806600
C	2.81825800	1.04991600	2.40658400
C	1.88492300	0.72382500	1.42630800
C	1.58638100	1.61947900	0.39205000
C	2.25805100	2.84365700	0.34357800
C	3.19988500	3.17276600	1.31267500
H	4.20199600	2.53018300	3.10756600
H	3.02531400	0.33267200	3.19123300
C	0.51622800	1.26146700	-0.58484400
H	2.00516800	3.54522800	-0.44267900
H	3.71513000	4.12477300	1.26590700
C	0.25007900	-0.15085700	-0.64956500
C	0.96571200	-1.12927000	0.24062500
C	-1.93051300	0.26122100	0.80987000
H	-1.11338200	0.26390900	1.52018800
C	-2.89501800	-0.82629100	0.85591700
C	-3.55782500	-1.30806300	-0.28700100
C	-3.10199100	-1.46911600	2.09024700
C	-4.43933700	-2.37704400	-0.17797500
H	-3.32938200	-0.89827700	-1.26180900
C	-3.99456600	-2.52698300	2.19168800

H	-2.56378700	-1.12581500	2.96691600
C	-4.67098600	-2.97819300	1.05782500
H	-4.93047600	-2.75520500	-1.06663600
H	-4.15658400	-3.00670600	3.14976900
H	-5.36031700	-3.81122200	1.13439900
C	-1.24771500	3.24455300	-0.83279400
C	-2.76476500	3.26642600	-1.01739000
H	-3.20637700	3.94666600	-0.28390500
H	-3.00429000	3.62716600	-2.01598600
C	-3.16361800	1.81250700	-0.77898600
H	-4.08664900	1.66944000	-0.21967000
H	-3.18407500	1.25054100	-1.70812000
O	1.22846100	-0.48173600	1.52053800
O	-0.44837500	4.03608900	-1.26689700
N	-0.90800900	2.11899600	-0.07385700
N	-2.02464600	1.33477700	0.06136000
N	-0.55952200	-0.64031400	-1.65690400
O	-0.67984800	-1.87178700	-1.80408300
H	0.60450200	1.75675500	-1.54848600
O	-1.20262300	0.18799800	-2.36211400
C	2.25958100	-1.73458000	-0.30382400
C	2.70206000	-1.51331800	-1.60661900
C	3.00939100	-2.56903600	0.53280900
C	3.87910200	-2.10467300	-2.06475700
H	2.12834300	-0.87902600	-2.27114200
C	4.18445100	-3.15772000	0.07907700
H	2.67124900	-2.74517100	1.54802500

C	4.62374900	-2.92618600	-1.22445100
H	4.21057200	-1.92247000	-3.08096400
H	4.75708100	-3.79924500	0.73996800
H	5.53871900	-3.38602800	-1.58103000
H	0.28905600	-1.94872400	0.48804100

TS-on

C	-3.64349200	1.76756900	-1.81470900
C	-2.57721800	0.90795200	-2.07175100
C	-1.64196700	0.66824000	-1.07212100
C	-1.74186100	1.29126100	0.18010400
C	-2.83088800	2.13138100	0.42726200
C	-3.78002900	2.36721300	-0.56381400
H	-4.37962700	1.95243700	-2.58892300
H	-2.46987700	0.40125700	-3.02296000
C	-0.66374700	1.03868300	1.18273400
H	-2.91306300	2.62057000	1.38979400
H	-4.61776600	3.02401600	-0.36263500
C	-0.00977100	-0.24820100	1.00500300
C	-0.29294300	-1.08837200	-0.21670600
C	2.13697400	0.71016900	0.63532900
C	0.16113500	3.54773700	0.52763700
C	1.04084900	3.90254000	-0.68027500
H	0.42606300	4.36598200	-1.45050600
H	1.81119000	4.61533600	-0.37422000
C	1.63599500	2.55175500	-1.08508600
H	1.01391300	2.03950900	-1.82457300

H	2.66636600	2.59331900	-1.43408300
O	-0.58658600	-0.17808600	-1.32490100
O	-0.72779600	4.21111200	0.99546100
N	0.54538700	2.28298800	0.99802500
N	1.58314900	1.83977700	0.20927300
N	0.48163100	-0.91948200	2.13887400
O	0.80683700	-2.11198300	2.01377300
H	-0.93751600	1.24634300	2.21060500
O	0.66467800	-0.26905300	3.18772200
C	-1.39798000	-2.13389900	-0.10679400
C	-2.34500900	-2.13900600	0.91677700
C	-1.47685800	-3.11194700	-1.10345000
C	-3.35554300	-3.09843800	0.94182100
H	-2.29368700	-1.39963700	1.70687400
C	-2.48464500	-4.07007200	-1.08270600
H	-0.74085100	-3.11807300	-1.90091700
C	-3.42947300	-4.06471500	-0.05717700
H	-4.08183200	-3.09205300	1.74678800
H	-2.52975100	-4.82444300	-1.86046400
H	-4.21338900	-4.81346400	-0.03458300
H	0.61736300	-1.59659100	-0.53508200
C	3.02799900	-0.16316300	-0.10948900
C	3.04961300	-0.27623700	-1.51269100
C	3.86792500	-1.00213400	0.64736500
C	3.91921100	-1.16558600	-2.13102300
H	2.36573600	0.29890100	-2.12045500
C	4.73461200	-1.88859400	0.02218200

H	3.82478400	-0.95743700	1.72895700
C	4.76977200	-1.96631100	-1.36869000
H	3.92418900	-1.24470800	-3.21194600
H	5.37525300	-2.52539100	0.62044600
H	5.44462800	-2.65943500	-1.85753800
H	2.14367500	0.62770300	1.71741100

TS-mn

C	1.49711700	3.72186400	-2.37146300
C	0.28617200	4.41379400	-2.31574700
C	1.57726600	2.43814800	-1.84293700
C	0.46053000	1.83370700	-1.27592600
C	-0.78374900	2.53810700	-1.23255700
C	-0.84356800	3.83549600	-1.74982500
C	0.29162200	0.57236700	-0.52490200
C	-0.88692100	-0.07250000	-0.91296600
C	-2.06990700	0.60086800	-0.30139500
O	-1.92288900	2.05261700	-0.65390100
N	0.30589800	-2.49141700	-0.10748600
N	1.37001900	-2.03913100	-0.72265500
C	2.08755000	-0.99485600	-0.28789700
C	-0.28883200	-3.47824600	-0.91992900
C	0.46363500	-3.57934100	-2.25425900
C	1.69449200	-2.72545500	-2.02988000
O	-1.26490600	-4.10336000	-0.59280100
H	0.21691500	5.41502600	-2.72573700
H	2.50829500	1.88518100	-1.88317000

H	-1.78806900	4.36369400	-1.71100100
H	2.84058800	-0.68839600	-1.00404700
H	-0.17778400	-3.17317000	-3.03912300
H	0.68195900	-4.62211300	-2.48114000
H	1.87044500	-1.96890600	-2.78768300
H	2.59904300	-3.31151400	-1.85466800
N	-1.03298100	-0.38435600	-2.32121600
O	0.00751500	-0.60303900	-2.96155500
O	-2.15769200	-0.52372400	-2.79901400
H	-2.97376100	0.30472800	-0.83151500
C	-2.25106600	0.43438600	1.19377000
C	-2.35981300	1.52917700	2.05108200
C	-2.58259400	1.33301900	3.41397300
C	-2.70532000	0.04544400	3.92726600
C	-2.60095900	-1.05068300	3.07091700
C	-2.37443000	-0.86078900	1.71131800
H	-2.27814100	2.52970300	1.64783700
H	-2.66442400	2.19128700	4.07162400
H	-2.88375300	-0.10530900	4.98614700
H	-2.69661400	-2.05805600	3.46038700
H	-2.27883700	-1.71883500	1.05546100
H	0.36045900	0.70258100	0.55310300
C	2.36142800	-0.65712800	1.11300600
C	3.44817000	0.20439300	1.35181200
C	1.63661400	-1.14976700	2.21185000
C	3.80886100	0.55457400	2.64580900
H	4.01596300	0.59428500	0.51337000

C	2.01083600	-0.79885600	3.50522800
H	0.78609000	-1.79351800	2.04277000
C	3.09119600	0.05141000	3.73030100
H	4.65113300	1.21718600	2.80850000
H	1.44254600	-1.18677800	4.34261400
H	3.36929100	0.32495700	4.74157700
H	2.36819500	4.17988300	-2.82406800

TS-mx

C	1.81279700	3.45985700	-0.47475300
C	0.75880900	3.86361900	-1.29340000
C	1.89590500	2.13423300	-0.05755700
C	0.93527200	1.19535500	-0.44902500
C	-0.14164400	1.63353400	-1.23693700
C	-0.22714700	2.95371200	-1.66749000
C	1.00661600	-0.23712700	-0.06259000
C	-0.22230600	-0.95118500	-0.20572800
C	-1.48678200	-0.25636700	-0.64416200
O	-1.11804500	0.75196000	-1.63187600
N	0.31416800	-2.11499200	-1.95694400
N	1.45799600	-1.48914300	-2.27655100
C	2.23063200	-1.23157800	-1.16481500
C	-0.56639500	-1.98095900	-3.05082100
C	0.17410700	-1.31595500	-4.21381200
C	1.37760300	-0.68369600	-3.52816400
O	-1.71803600	-2.33626300	-3.03328100
H	0.68837600	4.89408700	-1.62252400

H	2.71862700	1.81506500	0.57244000
H	-1.07631500	3.25001400	-2.27105400
H	-0.48297600	-0.59975400	-4.70360500
H	0.46051700	-2.08138000	-4.94015100
H	1.19777100	0.36785000	-3.29676900
H	2.31784600	-0.78015600	-4.06917800
N	-0.39711000	-2.14016400	0.60906000
O	0.60802800	-2.63705400	1.12457500
O	-1.52783200	-2.59990900	0.70575100
H	-2.11074700	-0.95464900	-1.19988500
C	-2.33247000	0.36419400	0.45989300
C	-1.80705900	0.81317700	1.67325600
C	-2.63137800	1.41749000	2.62053400
C	-3.98987700	1.58063400	2.36509100
C	-4.52388000	1.13214300	1.15799200
C	-3.69991400	0.52678400	0.21538900
H	-0.75352600	0.68864000	1.89183100
H	-2.21003200	1.75746900	3.55988600
H	-4.63090600	2.04729900	3.10457400
H	-5.58299300	1.24541900	0.95557300
H	-4.11798000	0.17018500	-0.71986100
H	1.54478100	-0.44628700	0.85640700
H	2.56648900	4.17310900	-0.16298600
C	3.58879400	-0.63500400	-1.26167100
C	4.59568200	-1.22587600	-0.48161300
C	3.92219800	0.48843700	-2.03310000
C	5.89470400	-0.72986100	-0.48782500

H	4.35354600	-2.08834600	0.12986200
C	5.22516900	0.97913900	-2.04497600
H	3.16864200	1.00310300	-2.61101300
C	6.21576800	0.37287700	-1.27645300
H	6.65558600	-1.20750400	0.11864100
H	5.46202300	1.84673200	-2.65020800
H	7.22818000	0.76002900	-1.28778000
H	2.20315100	-2.09999500	-0.51188100

3ox

C	3.64022400	2.03115100	2.43867700
C	2.91736600	0.84816600	2.51810400
C	1.92261000	0.58648300	1.57590600
C	1.64279500	1.49660600	0.55769100
C	2.38676300	2.67827800	0.48496500
C	3.38117900	2.94780500	1.41724400
H	4.41422000	2.23515200	3.16980700
H	3.10464200	0.11494400	3.29283100
C	0.52977800	1.24433300	-0.44586300
H	2.16046700	3.38662700	-0.30517100
H	3.95027800	3.86735600	1.35110900
C	-0.16184100	-0.12244300	-0.23352400
C	0.69755900	-1.17468200	0.50884300
C	-1.42459500	0.28823000	0.64258200
H	-0.98183900	0.33934300	1.64057400
C	-2.60185200	-0.66090900	0.75579400
C	-3.37795900	-1.09796200	-0.32730400

C	-2.94276200	-1.10957600	2.03838000
C	-4.45828700	-1.95176500	-0.12495700
H	-3.14926300	-0.79029400	-1.33836800
C	-4.02309900	-1.96363200	2.24138300
H	-2.35507600	-0.77908500	2.88810600
C	-4.78651700	-2.38603600	1.15711500
H	-5.04196400	-2.28153400	-0.97664500
H	-4.26647900	-2.29517100	3.24428500
H	-5.62927000	-3.05100700	1.30791200
C	-0.84192500	3.18718000	-1.24623700
C	-2.35147600	3.40980400	-1.16058400
H	-2.55796500	4.21438400	-0.44802800
H	-2.74741900	3.68879800	-2.13539200
C	-2.84801600	2.05275600	-0.64642200
H	-3.78793000	2.10298500	-0.09841500
H	-2.95348800	1.36501200	-1.48988900
O	1.20094800	-0.57635700	1.72217300
O	-0.02545700	3.72798300	-1.96395400
N	-0.55888800	2.21402300	-0.32233500
N	-1.75452400	1.67696300	0.28563100
N	-0.63289100	-0.70371000	-1.55536500
O	-0.74359500	-1.91584900	-1.62020300
H	0.91489400	1.34085500	-1.46333100
O	-0.95041000	0.07614500	-2.44565000
C	1.81885700	-1.86226600	-0.25574300
C	2.61725900	-1.23822300	-1.21866300
C	2.09622200	-3.19152600	0.08153600

C	3.66376800	-1.92860000	-1.82749100
H	2.44088600	-0.21125700	-1.50865500
C	3.14150900	-3.88147400	-0.52219800
H	1.48153000	-3.69015300	0.82329600
C	3.93016100	-3.24970600	-1.48156500
H	4.26960000	-1.42857000	-2.57442300
H	3.33567100	-4.91254000	-0.24931500
H	4.74303100	-3.78503100	-1.95888200
H	0.02139200	-1.94907200	0.86812000

3on

C	1.50054200	2.92377500	2.98272800
C	1.33317000	1.55286400	2.83050100
C	0.85388100	1.05040000	1.62139000
C	0.53797300	1.90390600	0.56519900
C	0.72664000	3.28036400	0.72788600
C	1.20423000	3.79105800	1.92982400
H	1.87426400	3.31559300	3.92197200
H	1.57101200	0.85638700	3.62502200
C	-0.05068200	1.36062700	-0.72557600
H	0.46347700	3.94472400	-0.08769900
H	1.34264600	4.85930500	2.04593900
C	-0.06291900	-0.19324100	-0.79640200
C	0.87923800	-0.88810900	0.22127200
C	-1.60772900	-0.59556200	-0.66561000
C	-2.16337700	2.79707400	-1.12782500
C	-3.61797200	2.45408300	-0.78321700

H	-3.85737900	2.94773400	0.16373200
H	-4.30070300	2.82673400	-1.54569300
C	-3.60758400	0.92481900	-0.64410000
H	-4.32447000	0.53377600	0.07637700
H	-3.79095500	0.45534900	-1.62265300
O	0.67490600	-0.30715000	1.52145200
O	-1.70695400	3.84943200	-1.53040100
N	-1.46493000	1.66126900	-0.85751000
N	-2.22789900	0.64756400	-0.19040200
N	0.35897700	-0.69037000	-2.19585600
O	0.32059000	-1.90270200	-2.34310300
H	0.46463800	1.77318300	-1.59155900
O	0.68064500	0.10990800	-3.05300000
C	2.35779300	-0.96361500	-0.13042500
C	3.09367200	0.09207000	-0.68031800
C	3.02345100	-2.15835600	0.16702800
C	4.45913000	-0.04723900	-0.92022100
H	2.61825700	1.03161200	-0.92565000
C	4.38661000	-2.29823900	-0.07015300
H	2.46366800	-2.98679400	0.58760100
C	5.10932600	-1.23956400	-0.61570500
H	5.01246600	0.78009500	-1.34940500
H	4.88176700	-3.23348600	0.16500100
H	6.17120900	-1.34507200	-0.80680200
H	0.51956000	-1.90755900	0.33903700
C	-1.96895500	-1.78512000	0.19727800
C	-2.19548400	-1.64624700	1.57074300

C	-2.10008500	-3.04810300	-0.39036100
C	-2.54448300	-2.75356700	2.33931100
H	-2.09708700	-0.66954300	2.02476000
C	-2.44139000	-4.15535600	0.38184700
H	-1.92313300	-3.16366500	-1.45336200
C	-2.66575600	-4.01016100	1.74915600
H	-2.72031800	-2.63392800	3.40249600
H	-2.53837300	-5.12837400	-0.08624800
H	-2.93743000	-4.87041100	2.35065100
H	-1.94508100	-0.80217600	-1.69222800

3mn

C	2.43895300	3.71112200	0.15288300
C	1.37178200	4.56379000	0.43131900
C	2.20984300	2.34645400	-0.00481900
C	0.92302700	1.82606000	0.11866500
C	-0.14478200	2.69824700	0.38615300
C	0.07858800	4.06444900	0.54195400
C	0.52201900	0.38630500	0.01395400
C	-0.79796900	0.28919800	-0.78047900
C	-1.92640000	1.02059400	-0.01970300
O	-1.43127500	2.25300100	0.55399200
N	-0.88589500	-1.09602000	-1.03804000
N	0.37010700	-1.79231400	-0.76084600
C	1.39220600	-0.73047500	-0.60431900
C	-1.66888500	-1.75764400	-1.95603200
C	-0.93500100	-3.05961600	-2.25841600

C	0.51856300	-2.72244500	-1.90045600
O	-2.72152800	-1.34606200	-2.39446100
H	1.54369200	5.62712200	0.55346900
H	3.03827100	1.67974100	-0.20820100
H	-0.76711900	4.71049300	0.74128700
H	1.77270000	-0.40278600	-1.57930800
H	-1.08532200	-3.34672000	-3.29772200
H	-1.33973800	-3.84713500	-1.61468000
H	1.01022100	-2.22939400	-2.74994100
H	1.10794300	-3.58589700	-1.59280000
N	-0.61875400	1.03446000	-2.19986200
O	0.06979200	0.46127400	-3.02800000
O	-1.16897300	2.10313700	-2.35861800
H	-2.69379900	1.30775400	-0.73843900
C	-2.55589600	0.18027600	1.07795700
C	-2.15544300	0.30273900	2.41008800
C	-2.75336800	-0.47730600	3.39883600
C	-3.75996700	-1.37950200	3.06655100
C	-4.17228300	-1.49441100	1.73980900
C	-3.57768600	-0.71673400	0.75080300
H	-1.39978700	1.02989700	2.67885500
H	-2.43804400	-0.36920600	4.43061000
H	-4.22886200	-1.98114900	3.83707600
H	-4.96554800	-2.18425400	1.47452400
H	-3.90015600	-0.80874800	-0.28025200
H	0.24649600	0.03142000	1.01575200
C	2.54677700	-1.21606100	0.24894800

C	3.86213400	-1.03087000	-0.18298300
C	2.32050100	-1.86219300	1.46901900
C	4.93505600	-1.46036900	0.59678000
H	4.04915200	-0.55233300	-1.13917200
C	3.39016900	-2.29272800	2.24762000
H	1.30266000	-2.04563800	1.79219500
C	4.70079900	-2.08942400	1.81613100
H	5.95019000	-1.30909900	0.24751500
H	3.20154200	-2.79247000	3.19120000
H	5.53274900	-2.42678000	2.42385000
H	3.44398100	4.10477100	0.06054200

3mx

C	-1.43583800	4.08299900	-0.70125400
C	-0.48333300	4.68615600	0.11990100
C	-1.36622300	2.71455000	-0.94289700
C	-0.35518100	1.93819200	-0.37473300
C	0.60567700	2.56112600	0.43752700
C	0.53321400	3.93134500	0.69105900
C	-0.12100800	0.48240900	-0.64030600
C	0.51412500	-0.24206400	0.56457900
C	1.83850700	0.47332000	0.95514800
O	1.65867000	1.90134200	1.00961600
N	0.54698500	-1.56784700	0.10050500
N	-0.38143800	-1.79860100	-1.01325600
C	-1.14238600	-0.51982900	-1.23565000
C	0.81672800	-2.72625500	0.79803700

C	0.04648600	-3.82645600	0.07853700
C	-1.06664100	-3.05410500	-0.64098900
O	1.54038200	-2.80399500	1.76695000
H	-0.53227800	5.75059400	0.31931100
H	-2.10717300	2.24102000	-1.57574000
H	1.28103200	4.37723200	1.33479700
H	-0.31267600	-4.56433400	0.79395800
H	0.72192900	-4.31929300	-0.62837000
H	-1.90679800	-2.88226500	0.04043900
H	-1.42838400	-3.55362200	-1.54021100
N	-0.43080300	-0.20360800	1.86724400
O	-1.09493100	-1.19411700	2.10506500
O	-0.42832100	0.81954500	2.52694300
H	2.09984300	0.18219400	1.97296000
C	3.00065300	0.13491600	0.03263400
C	3.34074800	0.96474000	-1.03889400
C	4.41689300	0.64373700	-1.86450600
C	5.16915700	-0.50197400	-1.62128900
C	4.84376000	-1.32355300	-0.54351500
C	3.76881400	-1.00673100	0.28161200
H	2.78664300	1.87852000	-1.21396100
H	4.67231400	1.29796600	-2.69051100
H	6.00997800	-0.74757600	-2.26020300
H	5.43244300	-2.21067100	-0.33859200
H	3.51492400	-1.65153300	1.11481500
H	0.70506600	0.43186500	-1.36283000
H	-2.22781300	4.67203300	-1.14760600

H	-1.13701100	-0.37468500	-2.31929500
C	-2.61491800	-0.49897100	-0.82856000
C	-3.50724500	-1.15603700	-1.68933500
C	-3.14289600	0.14146800	0.29657400
C	-4.87119900	-1.20530500	-1.42234400
H	-3.12562200	-1.63359200	-2.58673400
C	-4.51114200	0.10303000	0.56173300
H	-2.51203600	0.70603900	0.96684800
C	-5.37874700	-0.57563200	-0.28800200
H	-5.53609800	-1.72466400	-2.10329000
H	-4.89454800	0.61083600	1.43922000
H	-6.44136900	-0.60431800	-0.07543600