

Electronic Supporting Information for
Mixed amidophenolate-catecholates of molybdenum(VI)

Sukesh Shekar, and Seth N. Brown*

251 Nieuwland Science Hall
Department of Chemistry and Biochemistry
University of Notre Dame
Notre Dame, Indiana 46556-5670 USA
E-mail: Seth.N.Brown.114@nd.edu

Contents:

DFT Calculations for isomers of (*t*-BuClip)Mo(3,5-*t*-Bu₂Cat)

Energy and Cartesian coordinates

1. <i>cis</i>-α, O1 trans to O2	S2
2. <i>cis</i>-β_1 O3 trans to N1/N2	S5
3. <i>cis</i>-β_2, O3 trans to O1/O2	S8

1. (^tBuClip)Mo(3,5-^tBu₂Cat) - *cis-α*, O1 trans to O2

Energy of optimized structure = -2891.987596 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Angstroms)		
	X	Y	Z
Mo	0.32637800	-0.55924800	-0.13137700
O	-1.00224700	-1.71771900	-1.11995100
O	1.38912700	-1.86605300	0.89778600
N	-1.25884000	-0.66128300	1.09028300
C	-4.09814300	-3.36969200	-0.14796900
C	-4.30321500	-2.80192300	1.13724600
C	-2.25369900	-1.58044900	0.81276400
C	-3.36815300	-1.89054200	1.61104200
C	-1.51320700	0.40107900	2.01338800
C	-1.10676800	0.28417800	3.34186700
C	-2.07885700	-2.15331100	-0.47295200
C	-3.02256400	-3.07714300	-0.98591500
C	-1.36982400	1.29322200	4.28375300
C	-2.05578900	2.42637200	3.82849700
C	-2.44675200	2.55474000	2.49337200
C	-2.18372900	1.55759300	1.54924600
H	-2.95048700	3.46156000	2.16956600
H	-0.58246000	-0.62208300	3.62863800
H	-4.83490100	-4.08067400	-0.50085300
H	-2.28341800	3.23826800	4.50977700
H	-3.46089500	-1.42571100	2.58469800
O	1.79859500	0.67238300	0.40497800
O	1.52293500	-1.30952400	-1.58989600
N	-0.31264000	1.31286300	-0.66054300
C	2.54588800	4.22437000	0.00638200
C	1.34512700	4.66019400	-0.59383300
C	0.55988300	2.37862500	-0.50644800
C	0.34314900	3.71900900	-0.84376500
C	-1.68757900	1.58608500	-0.94020900
C	-2.11114500	1.75414200	-2.26360300
C	1.77305200	1.97377900	0.10053400
C	2.80384100	2.89800600	0.37588500
C	-3.43781500	2.06895000	-2.58173900
C	-4.33489700	2.21355900	-1.50984100
C	-3.92601700	2.03816800	-0.19152400
C	-2.59930100	1.71472700	0.13046400
H	-4.65032900	2.13672800	0.61273600
H	-1.36437100	1.63309500	-3.03942800
H	3.31429300	4.95911100	0.19839800
H	-5.37570900	2.45690600	-1.70269400

H	-0.59741900	4.00582200	-1.30098700
C	2.58385000	-2.12997700	0.31687600
C	3.65384200	-2.70714200	1.00357000
C	2.65224000	-1.83213000	-1.06782600
C	4.82378200	-3.01032800	0.30761700
H	3.53538600	-2.90487500	2.06224400
C	3.82032000	-2.13816500	-1.80128600
C	4.86802800	-2.71722500	-1.07439400
H	5.77738000	-2.96258800	-1.60931700
C	3.90931100	-1.85963700	-3.31278900
C	6.05027600	-3.64717300	0.98728300
C	-2.84322800	-3.71191700	-2.37521700
C	-5.54155200	-3.21801100	1.95210200
C	4.11617400	2.46636100	1.05364800
C	1.10660700	6.13407800	-0.97886100
C	-3.92469900	2.25976000	-4.02932900
C	-0.90379500	1.11862100	5.73992500
C	5.27556700	-2.26269800	-3.90075000
H	5.28699600	-2.04340900	-4.97462900
H	6.10134700	-1.70617400	-3.44207200
H	5.47517300	-3.33415700	-3.78232700
C	2.81434800	-2.67138800	-4.04750000
H	2.96012900	-3.74725700	-3.89335500
H	1.81731900	-2.40471100	-3.68914100
H	2.85950700	-2.47506900	-5.12644600
C	3.70312400	-0.34975200	-3.58432600
H	2.73024200	-0.00994300	-3.22141800
H	4.48134500	0.24516300	-3.09159600
H	3.75728700	-0.15123900	-4.66235400
C	6.37005100	-5.00599100	0.31907600
H	7.24449600	-5.46977900	0.79291200
H	5.52450400	-5.69686400	0.41490300
H	6.59033500	-4.89508500	-0.74789100
C	7.27049300	-2.70628800	0.84315300
H	8.15384800	-3.14714900	1.32244100
H	7.51959200	-2.51911200	-0.20660000
H	7.07351700	-1.73739000	1.31645900
C	5.81642600	-3.89902100	2.48917100
H	5.61215000	-2.96841400	3.03096500
H	4.97916300	-4.58524600	2.66085800
H	6.71112300	-4.35104000	2.93259000
C	4.84572000	1.43037700	0.16461500
H	4.23604300	0.53988100	0.00006300
H	5.09490000	1.86409800	-0.81140800
H	5.78269900	1.11903500	0.64353900
C	3.80736000	1.83833400	2.43518100
H	3.30001500	2.56087100	3.08625900
H	3.17201300	0.95544500	2.33717100
H	4.74107700	1.53828300	2.92744000
C	5.07200500	3.65452200	1.27828400
H	5.98621100	3.29399900	1.76324800

H	5.36577300	4.13082800	0.33573500
H	4.63343600	4.41997900	1.92918500
C	2.30028000	7.04220600	-0.62577100
H	2.50977600	7.04287400	0.44997900
H	3.21280400	6.74125500	-1.15266300
H	2.07572700	8.07426400	-0.91841500
C	-0.13747400	6.66796200	-0.22900400
H	-1.03696300	6.09213200	-0.47053500
H	0.00939300	6.61865600	0.85615200
H	-0.32765800	7.71413800	-0.49968200
C	0.86584700	6.23488200	-2.50455000
H	1.73449900	5.86698400	-3.06267300
H	-0.00458300	5.64949100	-2.81890700
H	0.69028800	7.27788500	-2.79653300
C	0.63552400	0.96261700	5.77019100
H	0.96989400	0.09358600	5.19422400
H	1.12748100	1.84857800	5.35305400
H	0.98376500	0.83348700	6.80225800
C	-1.55993300	-0.14674900	6.34288000
H	-2.65277100	-0.06033100	6.34420500
H	-1.29517600	-1.05004500	5.78335000
H	-1.22951200	-0.28905700	7.37889200
C	-1.28336500	2.32362700	6.62144900
H	-0.93394500	2.15411700	7.64592400
H	-0.82164000	3.25149200	6.26504200
H	-2.36835100	2.47381100	6.66403300
C	-5.05379200	1.24517300	-4.32977700
H	-5.41630200	1.37402300	-5.35694900
H	-4.69351700	0.21577000	-4.22265400
H	-5.90816100	1.37300900	-3.65665400
C	-2.79952600	2.04623400	-5.05992100
H	-1.97929200	2.76051800	-4.92428000
H	-2.38473700	1.03335100	-5.00725400
H	-3.19564500	2.18918800	-6.07162100
C	-4.47037200	3.69810100	-4.19906700
H	-4.83445100	3.84862500	-5.22269300
H	-5.30178300	3.90210100	-3.51600400
H	-3.68749500	4.44044300	-4.00497900
C	-2.84705600	-2.60254000	-3.45536200
H	-3.79959100	-2.05841100	-3.44845300
H	-2.03863100	-1.88626800	-3.29209000
H	-2.71868400	-3.04722500	-4.45010100
C	-1.50008200	-4.48135700	-2.42724600
H	-0.65173100	-3.81852900	-2.24231600
H	-1.48244400	-5.28323200	-1.67931200
H	-1.37035200	-4.93926100	-3.41574700
C	-3.97375600	-4.70429500	-2.70908800
H	-3.80035500	-5.12750900	-3.70482100
H	-4.01239200	-5.53928800	-1.99957700
H	-4.95721300	-4.21965400	-2.72482400
C	-6.82427800	-2.85211800	1.16694100

H	-6.87850700	-1.77190500	0.98902400
H	-6.86488400	-3.35302300	0.19414600
H	-7.71612100	-3.14981400	1.73229000
C	-5.51073900	-4.74531100	2.20100900
H	-6.39041400	-5.05561800	2.77840900
H	-5.51153300	-5.31249200	1.26439400
H	-4.61518700	-5.03209000	2.76398400
C	-5.60149200	-2.51231700	3.32041900
H	-4.73133500	-2.75380100	3.94154600
H	-5.65568700	-1.42257400	3.21534700
H	-6.49579700	-2.83650000	3.86467300

2. (^tBuClip)Mo(3,5-^tBu₂Cat) - *cis*-β₁, O3 trans to N1/N2

Energy of optimized structure = -2891.995836 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Angstroms)		
	X	Y	Z
Mo	-0.11664700	-0.13285500	0.77032700
O	1.23035400	-0.67715200	2.16803700
N	1.18806900	-1.30946400	-0.17355300
N	0.54729800	1.43721300	-0.30499500
O	-0.45899900	1.36891400	2.06743900
O	-1.37287400	-1.52851200	1.56294300
O	-1.76733800	0.02599100	-0.31271500
C	2.29525400	-1.80256300	0.47222700
C	2.26743500	-1.43868100	1.84248800
C	3.26831700	-1.90075000	2.73210100
C	4.26721700	-2.68620100	2.15770200
H	5.05767100	-3.04937300	2.80299800
C	4.32923700	-3.04563400	0.78394600
C	3.32460500	-2.59511700	-0.06320500
H	3.30948000	-2.83500600	-1.11930400
C	1.09514200	-0.62441700	-2.51314100
C	0.85390800	-1.59916200	-1.52446500
C	0.24334500	-2.82441800	-1.83151100
H	0.08340500	-3.51582200	-1.01274400
C	-0.16700600	-3.13004300	-3.13077800
C	0.06529800	-2.15277700	-4.11713600
H	-0.24758700	-2.33374600	-5.14129600
C	0.68234200	-0.94324100	-3.81866300
H	0.83835100	-0.21427800	-4.60883100
C	1.86793700	0.61724600	-2.25247100
C	1.62089900	1.56058100	-1.22377700
C	2.48037100	2.67076200	-1.08241500
H	2.27380000	3.34636700	-0.26287800

C	3.56264700	2.90982800	-1.92734800
C	3.77513400	1.98759800	-2.96684900
H	4.60204100	2.11955600	-3.65825400
C	2.95278900	0.88052800	-3.11186000
H	3.16292000	0.16596000	-3.90251400
C	-0.19039800	2.57358900	0.06506200
C	-0.73484900	2.49405500	1.38073500
C	-1.48323300	3.56979100	1.91347800
C	-1.67427900	4.67201900	1.07338000
H	-2.24685700	5.50327200	1.45963900
C	-1.17597000	4.76664900	-0.24474000
C	-0.42550500	3.70079800	-0.73553700
H	-0.02198100	3.71496500	-1.74216000
C	-2.60365200	-1.61252400	1.05496700
C	-2.84636500	-0.73038000	-0.01886300
C	-4.09108400	-0.69532600	-0.68207900
C	-5.05225600	-1.59418500	-0.20274100
H	-6.02490200	-1.60206500	-0.67790200
C	-4.83724000	-2.49114700	0.86783100
C	-3.59118200	-2.49401400	1.50146600
H	-3.35986200	-3.15238500	2.32992400
C	-5.97905600	-3.43119200	1.30076400
C	-4.36710500	0.28107800	-1.83876000
C	-5.57633700	-4.33746400	2.48000700
H	-4.72871300	-4.98415100	2.22592000
H	-5.30705800	-3.75497900	3.36829100
H	-6.41723000	-4.98609200	2.75164400
C	-7.20373800	-2.59221100	1.73871000
H	-7.57528000	-1.95736300	0.92759200
H	-8.02506000	-3.24889600	2.05202600
H	-6.94825000	-1.94042800	2.58202700
C	-6.37881300	-4.34062800	0.11403100
H	-7.19246700	-5.01620900	0.40671300
H	-6.72187500	-3.75973800	-0.74845600
H	-5.52964400	-4.95281500	-0.21125700
C	-5.78998600	0.12019600	-2.40863500
H	-6.56020400	0.32798800	-1.65703700
H	-5.93260300	0.82983200	-3.23165700
H	-5.96131100	-0.88661800	-2.80709900
C	-3.36406300	0.03175300	-2.99048300
H	-2.33155800	0.16281100	-2.65914500
H	-3.47000000	-0.98543600	-3.38625300
H	-3.55403700	0.73422800	-3.81221300
C	-4.21916400	1.73583100	-1.32970000
H	-4.92949000	1.93757600	-0.51901700
H	-3.21041800	1.93028800	-0.95818400
H	-4.42633300	2.44181800	-2.14441300
C	-2.04506200	3.51411200	3.34666000
C	-0.87720500	3.36059000	4.35255800
H	-0.30584000	2.44939500	4.16212500
H	-0.19533600	4.21759200	4.29023800

H	-1.26800300	3.31509900	5.37689700
C	-3.01544700	2.31581400	3.48872800
H	-3.85756300	2.41280700	2.79300800
H	-2.51309900	1.36667400	3.29124700
H	-3.42175000	2.28327600	4.50748700
C	-2.82173800	4.79336300	3.71521500
H	-3.19279700	4.70598300	4.74252400
H	-2.18996600	5.68822900	3.66903700
H	-3.68999400	4.94974800	3.06432200
C	-1.43848100	5.99249000	-1.14282200
C	-2.29583400	7.06575700	-0.44461700
H	-1.80774900	7.45956400	0.45422700
H	-2.45739800	7.90768600	-1.12737700
H	-3.28049500	6.67892200	-0.15874000
C	-2.18403700	5.54519000	-2.42325000
H	-1.60506900	4.81440100	-2.99755900
H	-3.14728100	5.08546000	-2.17438900
H	-2.37522200	6.40641100	-3.07563000
C	-0.09033800	6.64066800	-1.53889100
H	-0.25799300	7.51080200	-2.18595800
H	0.45729000	6.97856100	-0.65121800
H	0.55241400	5.94030800	-2.08347500
C	4.50702900	4.11186300	-1.74990400
C	4.47651200	4.97927900	-3.03136400
H	3.46904600	5.36851300	-3.21868200
H	5.15613900	5.83370300	-2.92691100
H	4.78670700	4.41312800	-3.91610000
C	5.94793500	3.59913100	-1.51359800
H	6.30795700	2.99160200	-2.35061100
H	6.63663000	4.44447500	-1.39436400
H	6.00174400	2.98586900	-0.60688200
C	4.11140100	5.00166400	-0.55661900
H	3.10486400	5.41923800	-0.67286700
H	4.14742700	4.45314000	0.39142300
H	4.81023700	5.84209500	-0.47775800
C	-0.86008900	-4.45374400	-3.49610300
C	-0.02877700	-5.18675600	-4.57596100
H	-0.51701600	-6.12804200	-4.85565900
H	0.08154400	-4.58650500	-5.48538300
H	0.97569600	-5.42277200	-4.20593900
C	-2.27366300	-4.15347600	-4.05012700
H	-2.88454900	-3.63518300	-3.30231600
H	-2.23605800	-3.52587600	-4.94697700
H	-2.78204500	-5.08782700	-4.31787100
C	-1.00787500	-5.39083200	-2.28214800
H	-0.03589700	-5.65861500	-1.85182700
H	-1.62204700	-4.94372800	-1.49243800
H	-1.49731700	-6.32042400	-2.59384200
C	3.23764100	-1.53259200	4.22457000
C	3.29626100	0.00703900	4.38111500
H	4.22256100	0.40723200	3.95094500

H	2.44918700	0.49043300	3.88865100
H	3.27465700	0.27651200	5.44450100
C	4.42811700	-2.13638300	4.99379800
H	4.36010500	-1.84951800	6.04917500
H	4.43294900	-3.23195300	4.95040100
H	5.39045900	-1.77226800	4.61483800
C	1.93120400	-2.06953400	4.86003300
H	1.04792400	-1.64918300	4.37348700
H	1.88151900	-3.16222100	4.78115000
H	1.89732500	-1.80612500	5.92457900
C	5.49796000	-3.91718600	0.28873400
C	5.41411000	-4.19797000	-1.22372900
H	4.49862000	-4.73949300	-1.48837200
H	5.44733000	-3.27305500	-1.81090700
H	6.26437800	-4.81658300	-1.53242900
C	5.48292000	-5.27554600	1.03075800
H	6.31482300	-5.90525300	0.69142400
H	5.58085000	-5.15168500	2.11435900
H	4.54805300	-5.81524700	0.84034800
C	6.83888900	-3.19600900	0.56685900
H	6.98822300	-3.00560000	1.63469400
H	7.67993800	-3.80781700	0.21757100
H	6.87922300	-2.23233300	0.04632000

3. (^tBuClip)Mo(3,5-^tBu₂Cat) - *cis*-β₂, O3 *trans* to O1/O2

Energy of optimized structure = -2891.997496 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Angstroms)		
	X	Y	Z
Mo	-0.13494400	0.06213900	0.66170300
O	0.90623200	-0.94165300	2.05525100
N	0.65690200	-1.50766700	-0.29252100
N	1.05027600	1.29590200	-0.39591800
O	0.05548300	1.59346500	1.96437700
O	-1.84399000	-0.66515200	1.51691500
O	-1.57079100	0.62317700	-0.57182600
C	1.50974400	-2.36768200	0.36054600
C	1.60743900	-2.02399400	1.73120000
C	2.37591400	-2.81020200	2.62257500
C	3.03662300	-3.89688600	2.04856100
H	3.64715200	-4.51575300	2.69453600
C	2.97097500	-4.25203700	0.67517600
C	2.19384400	-3.47255600	-0.17336100
H	2.09960700	-3.68996700	-1.23012600
C	0.89815900	-0.81797100	-2.62312100

C	0.29697200	-1.65326000	-1.66242700
C	-0.69366300	-2.58043600	-2.01387300
H	-1.11120000	-3.18502700	-1.21755400
C	-1.15133700	-2.70013100	-3.32819200
C	-0.56227300	-1.85411500	-4.28594100
H	-0.89220700	-1.89418500	-5.31999000
C	0.43759200	-0.95065700	-3.94478900
H	0.86579700	-0.31328400	-4.71332800
C	2.05089800	0.07067300	-2.32255400
C	2.11970300	1.04175500	-1.29363200
C	3.30173800	1.79311400	-1.12495800
H	3.31712300	2.50170600	-0.30722900
C	4.42019400	1.64742200	-1.94366000
C	4.33117300	0.70119600	-2.97905800
H	5.16980600	0.54027000	-3.64985700
C	3.18322700	-0.05826000	-3.15048500
H	3.15539900	-0.80300400	-3.94067400
C	0.73067300	2.61354900	-0.04378100
C	0.16936000	2.73356800	1.26097900
C	-0.19535600	4.00710300	1.77089300
C	0.01208400	5.09311800	0.92266900
H	-0.25679800	6.07740200	1.28545600
C	0.54515200	5.00236600	-0.38827500
C	0.90363100	3.74767500	-0.85925900
H	1.30575000	3.60921900	-1.85457900
C	-3.00190300	-0.44118300	0.88578100
C	-2.84911800	0.28412100	-0.31238900
C	-5.20992500	0.21742200	-0.74468400
C	-4.28378800	-0.85846100	1.30619000
C	-0.78117900	4.15767100	3.18671600
C	0.24159500	3.64077200	4.22828200
H	0.48330100	2.58912200	4.05991000
H	1.17016600	4.22281100	4.18259800
H	-0.17066800	3.74266500	5.23995300
C	-2.09631700	3.34809300	3.30017900
H	-2.84146400	3.71418500	2.58355200
H	-1.93176800	2.28500900	3.11286600
H	-2.51624700	3.45717700	4.30802400
C	-1.10263300	5.62628100	3.52737900
H	-1.51359300	5.67834100	4.54179300
H	-0.20972200	6.26216100	3.50194900
H	-1.85019000	6.05321600	2.84840400
C	0.70008400	6.28188900	-1.23036500
C	-0.68231700	6.95231900	-1.41663200
H	-1.13816300	7.22322900	-0.45856200
H	-0.58467300	7.86992000	-2.00994900
H	-1.37453500	6.28120400	-1.93786900
C	1.28248900	5.99335300	-2.62704900
H	2.28014900	5.54246200	-2.56816400
H	0.63779900	5.32314900	-3.20699900
H	1.37685700	6.92955600	-3.18894300

C	1.65281300	7.26406000	-0.50686900
H	1.76521300	8.18682300	-1.08950400
H	1.27999000	7.54057600	0.48492300
H	2.64706700	6.82055200	-0.37755600
C	5.70772600	2.46679500	-1.74783300
C	5.98229800	3.29362600	-3.02704500
H	5.16099600	3.99185500	-3.22648200
H	6.90391700	3.87720200	-2.91264300
H	6.09964000	2.65497700	-3.90896000
C	6.89400700	1.50667100	-1.49298800
H	7.04743000	0.81493400	-2.32804500
H	7.82154800	2.07622600	-1.35766500
H	6.72669800	0.90917400	-0.58964600
C	5.61251600	3.43978400	-0.55742200
H	4.80651100	4.17103800	-0.68884400
H	5.44517200	2.91293300	0.38886900
H	6.55102600	3.99750300	-0.46302600
C	-2.26632000	-3.67930200	-3.73399700
C	-1.74115500	-4.63350600	-4.83294600
H	-2.53142200	-5.32909100	-5.13987600
H	-1.41218900	-4.09013300	-5.72508900
H	-0.89242300	-5.22363800	-4.46823700
C	-3.46978600	-2.87441200	-4.28197400
H	-3.85950900	-2.18900500	-3.52054400
H	-3.19572100	-2.27972700	-5.15997700
H	-4.27847800	-3.55387300	-4.57779800
C	-2.75532800	-4.53197700	-2.54809200
H	-1.94755900	-5.13756700	-2.12095700
H	-3.18179100	-3.91508100	-1.74935000
H	-3.53874000	-5.21896200	-2.88717200
C	2.46915700	-2.46006700	4.11680900
C	3.05594400	-1.03672100	4.28432200
H	4.06399600	-0.97844900	3.85582000
H	2.42899400	-0.28633400	3.79682400
H	3.12737500	-0.78511200	5.34984400
C	3.37338100	-3.44176400	4.88653700
H	3.40283700	-3.15317400	5.94323400
H	2.99948800	-4.47123500	4.83735000
H	4.40441800	-3.43124100	4.51352100
C	1.05516100	-2.51458600	4.74614700
H	0.37457700	-1.81280000	4.25846300
H	0.63107000	-3.52249800	4.66307100
H	1.10916400	-2.25801700	5.81153600
C	3.75736000	-5.47986300	0.17873800
C	3.56549500	-5.72185700	-1.33057400
H	2.51432900	-5.90297500	-1.58268600
H	3.92027100	-4.87373000	-1.92735400
H	4.13639200	-6.60497400	-1.63916400
C	3.27679300	-6.74400300	0.93109500
H	3.83419600	-7.62559500	0.59090800
H	3.42156900	-6.65667800	2.01288200

H	2.21093000	-6.92506200	0.75052200
C	5.26790500	-5.26905100	0.44245200
H	5.48221000	-5.13355400	1.50768700
H	5.84081700	-6.13790500	0.09520100
H	5.63704800	-4.38358900	-0.08771100
C	-5.34549100	-0.50605600	0.46203700
C	-3.92822300	0.61465600	-1.13323200
H	-3.73704000	1.17467100	-2.04080500
H	-6.34396200	-0.80755700	0.75522300
C	-6.46483500	0.54397700	-1.57667800
C	-4.47654100	-1.64966700	2.61111300
C	-7.16991000	-0.76813400	-1.99596500
H	-7.47832100	-1.36144400	-1.12878100
H	-8.06858600	-0.54941000	-2.58656200
H	-6.50561700	-1.39074500	-2.60680900
C	-6.12540800	1.33138200	-2.85696900
H	-5.65052200	2.29270200	-2.62994000
H	-5.45623100	0.76710200	-3.51670800
H	-7.04390600	1.54052900	-3.41748100
C	-7.43950700	1.40059500	-0.73333500
H	-8.34034400	1.64005900	-1.31253800
H	-7.75671100	0.87974500	0.17604700
H	-6.96870900	2.34304300	-0.43085100
C	-5.95571100	-1.99091200	2.87384000
H	-6.03731600	-2.55231400	3.81167200
H	-6.57315800	-1.09056400	2.97382000
H	-6.38223800	-2.61361000	2.07853400
C	-3.95787100	-0.81279200	3.80563100
H	-2.90155500	-0.56124200	3.68377800
H	-4.52630600	0.12000700	3.90182200
H	-4.07295900	-1.37697400	4.73992800
C	-3.68561000	-2.97824100	2.53017000
H	-4.04912400	-3.59743300	1.70076500
H	-2.61852700	-2.79383200	2.38310000
H	-3.81154900	-3.54991100	3.45838400