Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Molecular Structures of *Tris*(2-mercapto-1-*tert*-butylimidazolyl)hydroborato and *Tris*(2-mercapto-1-adamantylimidazolyl)hydroborato Sodium Complexes: Analysis of [Tm^R] Ligand Coordination Modes and Conformations

Ava Kreider-Mueller, Yi Rong, Jonathan S. Owen* and Gerard Parkin,*

Department of Chemistry,

Columbia University,

New York, New York 10027, USA.

Received xxxx xx, 2014.

Table 1. Cartesian coordinates for geometry optimized structure of [κ^3-S_2H-Tm^{But}]Na(THF)$_3$.

[κ^3-S_2H-Tm^{But}]Na(THF)$_3$ (3:0)

-2368.85447364002 Hartrees

Atom	x	y	z
B	7.582961172	10.11677453	4.8344907
H	6.529120026	10.00946773	5.371827248
S	7.100493733	12.79220259	6.747866054
S	5.233342128	9.920795475	2.487708684
S	7.619665094	7.364305913	6.705379632
N	7.861052116	11.60255065	4.393747723
N	8.047986548	13.80764788	4.33193702
N	7.669444608	9.221486081	3.542679598
N	7.242946972	8.191390466	1.63001792
N	8.763949985	9.683263732	5.782648738
N	10.04497637	8.623851775	7.245755209
C	7.659861553	12.73803829	5.139510648
C	8.365195653	11.95985802	3.157276061
H	8.579716883	11.22417982	2.401292002
C	8.485695032	13.30390083	3.105991028
H	8.820263188	13.93128446	2.300072577
C	8.022275348	15.25796603	4.68044524
C	6.577559432	15.68561115	5.000935176
H	6.186169717	15.10316947	5.836420055
H	5.933986293	15.52675868	4.129318053

H	6.557028514	16.75093588	5.258885232
C	8.963458699	15.52095272	5.872460792
H	8.656925703	14.9259328	6.734498071
H	8.937232205	16.58439954	6.137352266
H	9.993992806	15.25805316	5.607827475
C	8.517529347	16.08677196	3.480385076
H	7.881593092	15.95628488	2.599169408
H	9.550871397	15.8461738	3.209499954
H	8.486786039	17.1446297	3.75844908
C	6.719873019	9.091549953	2.558994175
C	8.755049712	8.426010288	3.227755646
H	9.611935126	8.359023628	3.875664217
C	8.508537167	7.791504181	2.061598242
H	9.112825135	7.081190494	1.527543696
C	6.599079976	7.716170839	0.370895509
C	5.278520252	6.997304194	0.705802836
H	4.600901542	7.673811183	1.228951856
H	5.472301528	6.129738637	1.345318006
H	4.803093618	6.64882095	-0.218548407
C	7.528831138	6.714620865	-0.339550528
H	8.482549079	7.168405823	-0.628412301
H	7.033184605	6.376403446	-1.254583564
H	7.729568373	5.83160274	0.275309719
C	6.364324546	8.911958372	-0.572848618
H	5.729199935	9.656179395	-0.089196436
H	5.882342713	8.567123198	-1.495076666
H	7.319631729	9.379092279	-0.838000233

C	8.814347111	8.573512084	6.590493934
C	9.936685747	10.40032448	5.93146229
H	10.10529623	11.32304833	5.403624258
C	10.72872644	9.764135445	6.821126389
H	11.69729048	10.04063073	7.195850465
C	10.57931285	7.646643806	8.238207921
C	9.634728745	7.579700318	9.453224412
H	8.636158258	7.270467477	9.140479548
H	9.564611669	8.562048029	9.931976723
H	10.02486941	6.862866134	10.18520357
C	11.96506146	8.109265289	8.72628921
H	12.69498767	8.160105156	7.91163236
H	12.33290711	7.379641906	9.454088489
H	11.92270743	9.082832495	9.224648141
C	10.73667455	6.265354808	7.57268874
H	9.775392133	5.918615845	7.189518111
H	11.11815017	5.54350325	8.304261939
H	11.44985789	6.322952628	6.742561566

$[\kappa^3\text{-}S_2H\text{-}Tm^{But}]Na(THF)_3$ (2:1)

-2368.85945934741 Hartrees

Atom	x	y	z
B	7.94805844	10.09132526	4.902672983
H	6.829683844	10.02439631	5.315311671
S	6.746449252	12.74335841	6.485672329
S	10.69949568	8.890298225	3.132557876
S	7.667846764	7.252540387	6.523446221

N	8.245529345	11.57649179	4.495267809
N	8.163330216	13.78205807	4.324872606
N	7.996841041	9.167169376	3.621737182
N	8.437646737	7.746277235	1.984362942
N	8.951732856	9.620407806	5.9872149
N	9.959659568	8.454728923	7.566921781
C	7.720943661	12.70275955	5.086010775
C	9.00707542	11.95156993	3.400933486
H	9.552797561	11.22119172	2.823489749
C	8.963538277	13.29631396	3.286574709
H	9.435721977	13.93616516	2.563665851
C	7.871920806	15.22768132	4.551608752
C	6.351769505	15.46936677	4.476448902
H	5.835080096	14.87181167	5.229274068
H	5.97300718	15.19481348	3.485786226
H	6.138289025	16.53134743	4.645626025
C	8.441782736	15.66357969	5.915638667
H	8.000191914	15.06994314	6.717800281
H	8.223373117	16.72428403	6.086243135
H	9.528899144	15.52866268	5.932391732
C	8.54769764	16.07021065	3.453251096
H	8.181034669	15.81464782	2.453956813
H	9.637587986	15.9692186	3.465902315
H	8.310874563	17.12309025	3.634496913
C	9.02411659	8.587469011	2.9226429
C	6.798339955	8.694315597	3.123023592
H	5.862844797	8.999140861	3.56091657

C	7.05033567	7.830201194	2.118133233
H	6.368623881	7.259013182	1.515417612
C	9.131918908	6.847481827	1.014813844
C	9.968333093	7.687695289	0.029979167
H	10.70792277	8.28127737	0.569537409
H	9.319728411	8.362341353	-0.539967255
H	10.48143404	7.024846708	-0.676621312
C	8.087010791	6.055793345	0.206606973
H	7.467849573	5.419858311	0.846696877
H	8.618587162	5.40485049	-0.494095579
H	7.434806974	6.711013838	-0.379901353
C	10.00858272	5.841343803	1.785171656
H	10.76640823	6.363775707	2.370467212
H	10.50078786	5.163828995	1.077502937
H	9.391095102	5.247055601	2.466339125
C	8.875302142	8.451661962	6.696916505
C	10.05163135	10.33731644	6.407900759
H	10.30196478	11.28898497	5.972095883
C	10.67758451	9.638241885	7.377855442
H	11.56595178	9.878916103	7.932083928
C	10.34065421	7.386218254	8.533658449
C	9.218344548	7.207790558	9.574187832
H	8.283817984	6.938366263	9.079161959
H	9.066197822	8.139165808	10.13030213
H	9.493795173	6.419859025	10.28525752
C	11.6286429	7.793647868	9.272787551
H	12.47238614	7.921113518	8.587223493

H	11.88824618	6.995405521	9.97495336
H	11.49904123	8.714740326	9.850045104
C	10.61525571	6.075009655	7.771687454
H	9.725873238	5.76280214	7.222033982
H	10.89927106	5.288160819	8.480683765
H	11.4354442	6.215928035	7.059996424

$[\kappa^3\text{-}S_2H\text{-}Tm^{But}]Na(THF)_3$ (0:3)

-2368.83340382509 Hartrees

Atom	x	y	z
B	8.138059698	10.09737583	4.579026309
H	7.063959305	9.963378235	5.141168132
S	9.113429274	11.36385328	1.444698293
S	10.65689787	7.842562985	3.60035182
S	11.06051915	11.89561506	5.363195053
N	8.098177181	11.54639513	4.00725234
N	8.237733744	13.49995995	2.982881691
N	8.144501933	8.98513597	3.486433694
N	8.455745446	7.410155092	1.967323237
N	9.194606523	9.887027969	5.705199228
N	10.87404769	9.771123504	7.137459736
C	8.49708825	12.1365862	2.832764376
C	7.59011474	12.5184858	4.850060641
H	7.226903837	12.26637539	5.832995261
C	7.674333869	13.71628651	4.239999433
H	7.39397738	14.68971005	4.598150192

C	8.53801686	14.58793046	2.007853523
C	10.05175178	14.61798881	1.721253178
H	10.37716058	13.66816439	1.29538309
H	10.60679266	14.78955913	2.648898297
H	10.27778138	15.42982458	1.01943518
C	7.720813115	14.37441495	0.718562277
H	7.958207808	13.40398324	0.279511992
H	7.952462342	15.1675209	-0.002277547
H	6.647643428	14.41160365	0.938630318
C	8.137333571	15.9473157	2.611569115
H	8.695164293	16.17106393	3.526131528
H	7.064956463	16.00590927	2.826303578
H	8.370757539	16.72738549	1.880577707
C	9.080063552	8.101066635	3.007538276
C	6.970505083	8.830191069	2.771616416
H	6.106658324	9.438600022	2.984356357
C	7.14802025	7.876462227	1.837321726
H	6.463642338	7.505993885	1.096493166
C	9.059388557	6.3709375	1.084030688
C	10.26653702	6.969708089	0.336530254
H	11.0212583	7.311856451	1.045578202
H	9.947843603	7.823946594	-0.269092067
H	10.70343682	6.211861034	-0.324910097
C	8.023948341	5.918124564	0.037228266
H	7.140408418	5.46315551	0.497569607
H	8.491409009	5.161012402	-0.599661753
H	7.703488994	6.742585352	-0.607157347

C	9.463797362	5.142604102	1.922779299
H	10.1776646	5.433233246	2.695271342
H	9.917141856	4.384068181	1.27363643
H	8.581466307	4.703032401	2.402062271
C	10.3753568	10.49609424	6.053735399
C	8.963134668	8.827991242	6.56441319
H	8.087503587	8.208486354	6.458688472
C	9.982973174	8.741932544	7.4398627
H	10.14857313	8.035961142	8.232693635
C	12.16345449	9.991854535	7.854084999
C	13.33334873	9.858691764	6.85990546
H	13.24493794	10.60165992	6.066431958
H	13.32803513	8.863544428	6.40418171
H	14.2838834	9.999832256	7.388393586
C	12.33767296	8.918763776	8.945455382
H	11.54733446	8.964544644	9.702289406
H	13.2906331	9.099067572	9.452118541
H	12.36972865	7.9082437	8.526535945
C	12.15304343	11.37413946	8.535867232
H	12.00080405	12.15850311	7.792625763
H	13.10649758	11.53989665	9.051392933
H	11.34712329	11.4261511	9.276962946

Table 2. Cartesian coordinates for geometry optimized structure of [κ^3-S_2H-Tm^{Ad}]$Na(THF)_3$.

[κ^3-S_2H-Tm^{Ad}]$Na(THF)_3$ (3:0)

-3065.67406542199 Hartrees

Atom	x	y	z
B	5.206327746	8.95037229	12.38390946
H	5.203614699	8.953562475	11.19609224
S	7.676705791	10.92642635	11.29204105
S	2.296134169	10.19597094	11.34498153
S	5.443931768	5.742399537	11.49112901
N	5.580816469	10.36356171	12.97534109
N	6.529275446	12.31599667	13.41856233
N	3.796893556	8.573753933	12.97527005
N	1.631729679	8.463382642	13.42434896
N	6.244707491	7.913912624	12.96998065
N	7.374049385	6.074170192	13.47381709
C	6.578165772	11.21293409	12.56251581
C	4.932165571	10.92636004	14.05925757
H	4.101065782	10.43733373	14.53702917
C	5.500135251	12.11724607	14.34036894
H	5.243516017	12.83536951	15.09712703
C	7.40853818	13.51374676	13.40640236
C	7.279859798	14.26534998	12.05750066
H	7.536332919	13.57880976	11.24656877
H	6.232225694	14.56232835	11.91755456
C	6.995224659	14.49357064	14.53535833

H	7.069434471	13.99770876	15.51159471
H	5.951452322	14.80409772	14.40199683
C	8.884121085	13.10726352	13.6533389
H	9.183843093	12.38830865	12.88643769
H	8.953157193	12.60181692	14.62647322
C	9.792333365	14.3539622	13.63181885
H	10.83324994	14.04015615	13.78589807
C	9.66215685	15.06288068	12.2662656
H	10.32949366	15.93588605	12.22986217
H	9.971446252	14.38430693	11.46225996
C	8.198841627	15.50435611	12.04793033
H	8.107377546	16.00820039	11.07695025
C	7.780808604	16.46968376	13.17541384
H	6.747121267	16.80713795	13.02038173
H	8.414970576	17.36742453	13.17139956
C	7.903828967	15.7432698	14.53015161
H	7.580970789	16.41099764	15.34055245
C	9.370158299	15.32203014	14.7550224
H	9.478503624	14.83590292	15.73432428
H	10.01873319	16.2093589	14.76491673
C	2.573558689	9.057442512	12.58187903
C	3.617868102	7.709841669	14.03946111
H	4.446303465	7.199786065	14.49907402
C	2.301302913	7.633175959	14.32489868
H	1.795651602	7.043254132	15.06690267
C	0.160552582	8.66273469	13.41934147
C	-0.437663303	8.240364266	12.05327998

H	-0.199952485	7.18346976	11.87560396
H	0.044293218	8.822080381	11.26357395
C	-0.186176422	10.14345271	13.7211876
H	0.303354083	10.77776162	12.97754556
H	0.224823358	10.40857281	14.70509838
C	-0.502375007	7.790009815	14.51649114
H	-0.275682674	6.73048909	14.34433109
H	-0.104359448	8.056480476	15.50391794
C	-2.034376819	7.992335071	14.51636267
H	-2.468226406	7.360695723	15.30354189
C	-2.6140177	7.588658722	13.14592229
H	-2.417742722	6.525715296	12.95094139
H	-3.705578261	7.717958346	13.14747266
C	-1.964799543	8.458297321	12.05078431
H	-2.363845783	8.174630856	11.06824789
C	-2.275192402	9.945909685	12.32511768
H	-1.826446112	10.57135227	11.54415908
H	-3.360907706	10.11681724	12.29520289
C	-1.714783282	10.3474733	13.70661307
H	-1.936308145	11.40528709	13.90097552
C	-2.363394191	9.472105716	14.79704176
H	-1.987678409	9.761542947	15.78816861
H	-3.452673004	9.618393658	14.81347228
C	6.371388726	6.584668069	12.64580364
C	7.155162509	8.220594811	13.96419529
H	7.250353331	9.218393605	14.3549276
C	7.848724948	7.107660198	14.28347729

H	8.648069302	6.978838426	14.98977615
C	7.838898369	4.66563627	13.57066115
C	6.672570776	3.743233532	14.01060181
H	6.300231478	4.086402854	14.98575937
H	5.855038423	3.842281547	13.29153286
C	8.962174281	4.542088246	14.63283142
H	8.594514593	4.872725547	15.61242507
H	9.808128863	5.187001778	14.36383933
C	8.416154938	4.187145888	12.21467786
H	9.255616307	4.838650659	11.93850585
H	7.647383755	4.300126018	11.44622354
C	8.884231021	2.721117813	12.32212612
H	9.267641407	2.397054198	11.34579499
C	9.99929205	2.609364497	13.38099118
H	10.35750571	1.5731011	13.45838363
H	10.86075611	3.225058257	13.08908022
C	9.447834291	3.079016926	14.74225987
H	10.24100348	3.031975713	15.50082603
C	8.273353523	2.170727775	15.1600334
H	8.616814745	1.130705613	15.25232383
H	7.89499008	2.471085022	16.14679541
C	7.153501424	2.280601337	14.10570024
H	6.307308747	1.644236277	14.39712111
C	7.694126454	1.826915313	12.73252347
H	6.900393727	1.892322308	11.97870371
H	8.010844657	0.775173716	12.78092557

$[\kappa^3\text{-}S_2H\text{-}Tm^{Ad}]Na(THF)_3$ (2:1)

-3065.67864759384 Hartrees

Atom	x	y	z
B	5.596587704	8.689579118	12.76705338
H	5.502035493	8.81375458	11.58451969
S	7.061572075	11.25457837	11.14723737
S	4.632564794	7.232022754	15.8019154
S	5.445470712	5.559216464	11.75403733
N	6.005123889	10.06415956	13.40056461
N	6.650084676	12.15190214	13.74975838
N	4.158708754	8.300526627	13.29473051
N	2.330713233	7.52827047	14.26769154
N	6.648372076	7.607922097	13.13464267
N	7.687661917	5.679270116	13.40860356
C	6.563184384	11.15627712	12.77765477
C	5.758232719	10.37481962	14.72922191
H	5.345758628	9.638389722	15.40525846
C	6.148126329	11.64624475	14.95285938
H	6.111763586	12.22133698	15.85955228
C	7.166527563	13.53556331	13.58801879
C	6.328431951	14.30658833	12.53648269
H	6.362222135	13.75990716	11.59064276
H	5.281551573	14.33056096	12.86778354
C	7.063487458	14.30459538	14.93113353
H	7.641922066	13.78816951	15.70728543
H	6.019603672	14.33979587	15.26685467

C	8.659380912	13.51546077	13.17078803
H	8.757244047	12.94682825	12.24258934
H	9.234730913	12.98832947	13.94379029
C	9.186235564	14.9551239	12.99811548
H	10.23693204	14.9149394	12.68200405
C	8.350146621	15.68478907	11.92428129
H	8.736451284	16.70282381	11.77210076
H	8.432655358	15.15910045	10.96542465
C	6.872425705	15.74006164	12.36930897
H	6.278426456	16.26046284	11.60640535
C	6.767879117	16.4934335	13.7100037
H	5.717759419	16.55869636	14.02589931
H	7.134133222	17.52436988	13.60398731
C	7.596751273	15.74617085	14.77353159
H	7.507131547	16.25809268	15.74128441
C	9.07541071	15.71123252	14.33735963
H	9.684377613	15.21348112	15.10422455
H	9.461497774	16.73543756	14.23678398
C	3.702969123	7.682363436	14.42855756
C	3.090571021	8.52538193	12.44965308
H	3.23960555	8.978497473	11.48386898
C	1.964699728	8.063402666	13.03163963
H	0.955304924	8.052459319	12.66451067
C	1.378704894	6.882878761	15.20845617
C	1.332107592	7.657524223	16.55109959
H	1.015876895	8.690581502	16.35224721
H	2.3399063	7.696174931	16.97159067

C	1.781185196	5.405218817	15.44970943
H	2.802285789	5.374125771	15.83656937
H	1.780318483	4.87780217	14.48736391
C	-0.052440104	6.890588117	14.61158356
H	-0.376391012	7.921276199	14.41932622
H	-0.063762626	6.356312397	13.65370049
C	-1.047553623	6.217304421	15.58379079
H	-2.047219675	6.239868522	15.12911273
C	-1.067183138	6.981174333	16.92339809
H	-1.405389357	8.014473571	16.76581885
H	-1.782734985	6.51167404	17.61317342
C	0.351785648	6.973701003	17.52633773
H	0.352487705	7.522842018	18.47736589
C	0.799715242	5.516026427	17.77017179
H	1.805166031	5.502544917	18.20808808

$[\kappa^3\text{-}S_2H\text{-}Tm^{Ad}]Na(THF)_3$ (1:2)

-3065.66779107288 Hartrees

Atom	x	y	z
B	8.210824372	14.95373636	12.06268731
H	8.349819708	14.69191905	10.90529067
S	10.28523125	16.95087894	14.18546916
S	6.034017435	16.15336653	14.55671262
S	10.17236701	12.59379925	10.7786413
N	8.411994825	16.49907251	12.20350663
N	8.640270325	18.63715687	12.72254105

N	6.678333021	14.59652751	12.37146406
N	4.603128954	14.28167548	13.07487332
N	9.087751802	14.00613324	12.89810171
N	10.24858865	12.23976584	13.53752599
C	9.081732439	17.35172648	13.04233644
C	7.616599842	17.24633686	11.3510254
H	7.018678177	16.77114949	10.5908036
C	7.736137455	18.5497398	11.66565599
H	7.26805757	19.40798301	11.22055919
C	8.910293244	19.89163547	13.47051787
C	10.41418466	20.26031828	13.41437899
H	10.99449751	19.42619775	13.81562332
H	10.7086343	20.39167125	12.36415508
C	8.113745793	21.0658137	12.84444208
H	7.040005626	20.843331	12.86172063
H	8.406885849	21.20465967	11.79566256
C	8.446339535	19.73924078	14.9422049
H	8.974415317	18.89604347	15.39391989
H	7.376954003	19.49464051	14.95039394
C	8.719193294	21.04036781	15.72218274
H	8.403500461	20.90417288	16.76493159
C	10.22883724	21.36062087	15.67678429
H	10.44113593	22.26899043	16.25924314
H	10.79735102	20.54168829	16.13391172
C	10.67402244	21.55543941	14.21105915
H	11.74756013	21.78469735	14.18001601
C	9.876944268	22.71597391	13.58370992

H	10.20076162	22.87907555	12.54656315
H	10.06329531	23.65268106	14.12818661
C	8.374248598	22.37406301	13.62368529
H	7.796984361	23.18120664	13.15200233
C	7.92819045	22.2019277	15.0893345
H	6.850817797	21.99322222	15.13485777
H	8.097871366	23.13486435	15.64576581
C	5.773163943	15.00194298	13.31743214
C	6.090973068	13.63172369	11.57293583
H	6.649464279	13.16348315	10.77778075
C	4.822864866	13.42909177	11.99111653
H	4.071961368	12.7610784	11.61093696
C	3.314431216	14.37906938	13.80999106
C	2.739791323	15.81491674	13.70220532
H	2.587299108	16.05485684	12.64120663
H	3.475826875	16.52004264	14.09671544
C	3.505180239	13.98818307	15.29814138
H	4.26400522	14.63880239	15.73946516
H	3.883904987	12.9585113	15.34706513
C	2.272256279	13.40723891	13.19888171
H	2.108971529	13.64476677	12.14013314
H	2.641963593	12.37553462	13.25174999
C	0.928866644	13.50629688	13.9561771
H	0.218099748	12.80636458	13.49627642
C	0.380951905	14.94422215	13.85928285
H	0.191275444	15.20730046	12.80969743
H	-0.581396135	15.01557885	14.38546989

C	1.407688337	15.91671442	14.47260489
H	1.031576864	16.94575109	14.40087346
C	1.639941025	15.55251034	15.9548619
H	2.36270402	16.24593866	16.40138014

$[\kappa^3\text{-}S_2H\text{-}Tm^{Ad}]Na(THF)_3$ (0:3)

-3065.65429831058 Hartrees

Atom	x	y	z
B	5.229144997	8.808148576	13.83115263
H	5.369465455	8.793903349	12.61945708
S	3.396391314	10.8741186	16.01448348
S	3.965282825	6.482905823	16.15155058
S	7.535818516	9.176204866	16.46936752
N	5.415531489	10.30642802	14.21672395
N	5.455280569	12.3958843	14.93628511
N	3.785354347	8.268435801	14.05218169
N	1.840383521	7.374643983	14.60050585
N	6.347687891	7.857018481	14.35387573
N	7.971910532	6.694306987	15.30072918
C	4.776671833	11.18090657	15.06068984
C	6.451443838	10.96732935	13.58127532
H	7.088092497	10.45549078	12.87824488
C	6.489959966	12.24142285	14.01379013
H	7.167316104	13.03288795	13.75255815
C	5.174444752	13.66540802	15.65300677
C	5.303175506	13.45860856	17.18373016

H	4.613375842	12.66932243	17.49197905
H	6.318755269	13.10846504	17.40714924
C	6.198991138	14.75342532	15.23769312
H	6.144733251	14.93078065	14.15586247
H	7.217807159	14.41728366	15.46623326
C	3.760830898	14.19391212	15.29776523
H	3.026137115	13.42475381	15.54972785
H	3.707875099	14.35982611	14.21283313
C	3.475261398	15.50667065	16.05578035
H	2.461455661	15.84934282	15.80832142
C	3.581143027	15.25753005	17.57606818
H	3.347003573	16.18048931	18.12626729
H	2.847501422	14.50194692	17.88186138
C	5.006200857	14.77714098	17.92632962
H	5.079696762	14.60179297	19.00754818
C	6.028048821	15.8520351	17.50407033
H	7.044902455	15.52981674	17.76584646
H	5.842493927	16.79502786	18.03795427
C	5.918996736	16.07776456	15.98258194
H	6.662810619	16.82058869	15.66285335
C	4.501647886	16.57908382	15.63909457
H	4.422139779	16.78002502	14.56173366
H	4.302490848	17.5279336	16.15736186
C	3.195944721	7.399292673	14.93664021
C	2.821563008	8.757427848	13.18871997
H	3.075679646	9.465341627	12.41697488
C	1.62925268	8.22459558	13.51504599

H	0.662860857	8.387196095	13.07555278
C	0.759015186	6.610618152	15.27036809
C	0.652480399	7.024348174	16.7605229
H	0.448226952	8.101057827	16.81282522
H	1.617508437	6.853862091	17.24350268
C	1.012582071	5.085750063	15.14934253
H	1.989278269	4.857943506	15.5839031
H	1.052147652	4.81708836	14.0845433
C	-0.605848061	6.915113358	14.59956124
H	-0.821864811	7.988979389	14.65684175
H	-0.575808885	6.639789807	13.53742283
C	-1.739260823	6.128003693	15.29495278
H	-2.687428835	6.367516901	14.79416699
C	-1.818521201	6.529989215	16.78167315
H	-2.051507286	7.599457039	16.87217309
H	-2.632779397	5.980873926	17.27580935
C	-0.46652155	6.223688624	17.45674668
H	-0.507512136	6.513747788	18.51476694
C	-0.166894862	4.712954719	17.34619456
H	0.789495061	4.486289702	17.83258966