

## Supplementary Information

### Auto-oxidation of a *trans*-1,2-Disiloxybenzocyclobutene: New Insights

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## Some answers to the comments

In the following section, some answers and lights were given to several comments.

*Page 2, ref 2: “Throughout the whole paper, the acronym TBS for the tert-butyl-dimethylsilyl group was used. This acronym indeed is frequently used in protective group chemistry, but should better read “TBDMS” in order not to be confused with “tributylsilyl”.*

Although TBDMS could be more adequate for the *tert*-butyl-dimethylsilyl group, the acronym TBS is well known and commonly used by the wide community of organic chemists as mentioned at least in three well recommended books: a) Philip J. Kocienski, *Protecting groups*, 3rd Edition, Georg Thieme Verlag, 2005, p. 109; b) K. C. Nicolaou and E. J. Sorensen, *Classics in Total Synthesis*, VCH, 1996 and c) Peter G. M. Wuts and Theodora W. Greene, *Greene’s Protective groups in Organic synthesis*, John Wiley & Sons, 4<sup>th</sup> Edition, 2007, p 189.

In comparison, tributylsilyl group is very scarcely employed as protecting group and does not appear in the books mentioned above. We thus think that no possible confusion might arise using OTBS acronym.

Moreover, their advice to use the alternative labeling “*rac-1*” or “*trans-1*” instead **1** is not really necessary. First of all, the relative configuration of the two stereogenic centers of **1** is, in our mind, sufficiently clear for an organic chemist without the need to specify it. In addition, the conditions of the reaction (*i.* NaBH<sub>4</sub>, *ii.* TBDMSCl, imidazole) clearly indicate that the product we obtained is in racemic form.

Beside our substantive comments, other issues in their comment may be confusing:

*Scheme 2:* only one arrow is required to describe the transformation from *meso-5* to *meso-6* + *rac-6*. Employing two arrows generally indicates a multistep synthesis !

*Scheme 3:* (Z,Z)-**7** and **8** are two mesomeric forms. Therefore, the mentioned double inversed arrows (which represents an equilibrium between these two molecules) are inappropriate. The readers should see, in place of an equilibrium arrow, a mesomeric form arrow.

*Comment 2 and beginning of the comment 3.*

We wrote “*This work elucidated for the first time each step of the mechanism of spin-forbidden addition of triplet oxygen  $O_2(^3\Sigma_g)$  to trans-1,2-disiloxybenzocyclobutene **1** to give the corresponding endoperoxide **7** by using both EPR/spin trapping and theoretical studies*” and not “*for the first time each step of the mechanism of spin-forbidden addition of triplet oxygen to trans-1,2-disiloxybenzocyclobutene*”. In our case, we have considered that no isomerization occurs, so each step of the mechanism was theoretically investigated.

*“In this context, we note that the formation of cyclic peroxides from reaction of  $^3O_2$  with o-quinodimethanes has been reported several times before.<sup>7</sup> This fact was ignored in ref. 1.”*

We wrote “*Moreover, to the best of our knowledge, only one example, using drastic conditions ( $T = 190$ - $240$  °C), was reported for the trapping of dioxygen by benzocyclobutene*”. While it is true that some *o*- and *p*-quinodimethanes are known to react with dioxygen, our argument relates to the specific case of benzocyclobutenes only and not to the general case of *o*-quinodimethanes.

## TURBOMOLE control sections

```

$atoms
c  1,3,5,7-9,11,13,19,23,27,31,35,39          \
    basis =c def2-TZVP                        \
    jbas  =c def2-TZVP
h  2,4,6,10,12,14,20-22,24-26,28-30,32-34,36-38,40-42  \
    basis =h def2-TZVP                        \
    jbas  =h def2-TZVP
o  15-16                                         \
    basis =o def2-TZVP                        \
    jbas  =o def2-TZVP
si 17-18                                         \
    basis =si def2-TZVP                      \
    jbas  =si def2-TZVP
$dft
    functional pbe
    gridsize   m3
$woelfling
ninter          50
riter    41
ncoord          2
align          0
tangtyp         1
nactive          50
nactive1         25
nactive2         26
maxit           40
dlst    3.0000000000000000
thr    1.0000000000000000E-004
hessinit model
tangents fixed
method q

```

## Geometries of the minimum energy pathway

```
*****
* Geometry 1
*****
```

```

42
Energy = -1276.5545399280
  c      4.399958325872686      1.600861561590533      -0.117554441840492
  h      5.485645118346339      1.607264289910578      -0.011594029376591
  c      3.716397233320422      2.805757548240310      -0.521958081548393
  h      4.294830167419888      3.701097738417799      -0.753818221100919
  c      2.357024598132256      2.838024895191578      -0.570655330999879
  h      1.836374954188092      3.768599065482992      -0.809823475239474
  c      1.551588520328518      1.684016632772797      -0.206263700006626
  c      2.260055437392701      0.390064099471857      -0.106599714671074
  c      3.699701289446150      0.452184468526684      0.086314992007666
  h      4.223152700760040     -0.476874759723672      0.325509954535556
  c      0.248625484328442      1.921414801524193      0.141207325222538
  h     -0.152687776891080      2.932463069224069      -0.004650545164747
  c      1.714905937635888     -0.849173822263804      -0.311309806351165
  h      2.359925547616388     -1.727956424112874      -0.183167848081869
  o     -0.574252630944350      1.020922492042261      0.725755218581731
  o      0.450539193434563     -1.081177632177748      -0.733620720834053
  si     -2.045854789566758      1.405805821197991      1.471885145462903
  si     -0.109851873776749     -2.575575752858967     -1.303022979852075
  c     -3.254076211197658      2.047048001440837      0.182089827596141
  h     -3.410939562571767      1.307987014031874     -0.616350053325628
  h     -4.231752018788082      2.263716692711104      0.639057664516965
  h     -2.896544480321165      2.976000897204223     -0.285704944484407
  c     -2.622045473855929     -0.212988392254005      2.216079983884501
  h     -2.779884382871486     -0.974651479553836      1.439963229571898
  h     -1.880371251060327     -0.602691217059078      2.927588968814249
  h     -3.571513002165272     -0.079457664929091      2.755409413535818
  c     -1.871408873876211     -2.234360196485761     -1.838550259491825
  h     -1.901713908353611     -1.447890757851961     -2.605809436304951
  h     -2.334662740516025     -3.138172441172141     -2.261421481990664
  h     -2.488334159596841     -1.904898994302244     -0.990987009842726
  c     -0.039109468081626     -3.842942601048608      0.084056698774806
  h     -0.433836467209447     -4.812380739045370     -0.256549995679741
  h      0.990255654853909     -4.011508782432374      0.432703934751365
  h     -0.637110318175758     -3.519352360774082      0.947823989301272
  c      0.949895475004525     -3.122604343150027     -2.755835814501659
  h      0.578300162302937     -4.070261129508963     -3.174150003900956
  h      0.934527876670783     -2.370333294272180     -3.557642667619461
  h      1.998344355027777     -3.278569093948704     -2.462744025917796
  c     -1.748498625751321      2.699174578930626      2.803027389492100
  h     -1.013910070451767      2.342470884266781      3.539382415546591
  h     -1.369956184644703      3.641858502671393      2.382003643892285
  h     -2.681733761414332      2.927088824074936      3.339924792638749
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*****
* Geometry 2
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42
Energy = -1276.5542536550
c      4.415832265005728      1.536369270029846      -0.090588137407996
h      5.502071780817294      1.534249817052535       0.014574223700406
c      3.739541540692037      2.751695534622766      -0.471128029190073
h      4.322216412377825      3.649983433820835      -0.681994911070236
c      2.380666363785057      2.790902911253573      -0.522322620235201
h      1.865194930995281      3.729171275325480      -0.743634737024013
c      1.566372120720462      1.636982960129745      -0.180145061577203
c      2.268020309182559      0.338760494391236      -0.097531786616812
c      3.708060777028042      0.389132273155483       0.092713962806196
h      4.226607907112123      -0.547758483402747      0.313255934665439
c      0.262948276877972      1.890561349135004      0.157308410722312
h      -0.115676363642590      2.910336050712698      0.007332681965443
c      1.717080790179672      -0.895464175694529      -0.319247999849925
h      2.362919987119261      -1.777514466461181      -0.213436181511671
o      -0.586597206708126      1.010474514046149      0.733301422725186
o      0.450258672739090      -1.116417343111275      -0.733505037314174
si      -2.045646346537286      1.455490152068708      1.477805636408515
si      -0.109847551066518      -2.599759774108790      -1.334365176376326
c      -3.273002565714474      2.070807949752104      0.194490543821989
h      -3.458809652345221      1.316817187201131      -0.583742178500580
h      -4.234182951527937      2.298387724831240      0.681808389049353
h      -2.929393913702928      2.991939340823347      -0.299034847694434
c      -2.649835846721867      -0.113400466852851      2.298703875586324
h      -2.831790940613835      -0.910317904890823      1.563894999296390
h      -1.915018993455619      -0.481514192692383      3.028981188776887
h      -3.593051924894962      0.076707609776030      2.833277680073738
c      -1.875034016853471      -2.252552973796338      -1.850239728491861
h      -1.910708772946337      -1.448296062716419      -2.599367966485106
h      -2.332476224504909      -3.149727723219776      -2.293627417306578
h      -2.490746000844042      -1.946707180065773      -0.992335414150820
c      -0.024789983982494      -3.898774028613962      0.021100338814910
h      -0.421693850653029      -4.860163345302541      -0.339508710307709
h      1.008327746896021      -4.073456700163566      0.356453163168812
h      -0.616746374165139      -3.594604834696397      0.896646442910300
c      0.940026265847601      -3.110843328195252      -2.806385456436389
h      0.564537842914241      -4.049595227706088      -3.241513568791755
h      0.918931260529279      -2.341246412224944      -3.592019902128171
h      1.990637630207996      -3.272969328158790      -2.523724012939055
c      -1.737455334524260      2.800678043467684      2.753373554688558
h      -1.001154874163838      2.481854042973276      3.505015862679341
h      -1.373315293735241      3.731925397835518      2.295861278513305
h      -2.676664217110959      3.035622731726650      3.278167350623619

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 \* Geometry 3  
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42
Energy = -1276.5536508560
  c      4.426287548354130      1.478020168068174      -0.063184651997943
  h      5.512771554259125      1.468968613361379      0.039836801301367
  c      3.755020972104713      2.701787402634307      -0.424487963649809
  h      4.340716372489756      3.602031092773504      -0.617773628592281
  c      2.396550390698202      2.746267243328079      -0.479179391267106
  h      1.886086709657051      3.690549038470009      -0.685983505371785
  c      1.573729554597303      1.592623511353621      -0.154109193353316
  c      2.271329046210825      0.290916324225212      -0.084318979829279
  c      3.712639930243196      0.332194668629564      0.103562054596621
  h      4.227287827491348      -0.610401445091819      0.308367339198487
  c      0.269270259098750      1.860501048126104      0.171813664132471
  h      -0.091312267257393      2.885122546646194      0.011131080757994
  c      1.718117246930660      -0.938591106782370      -0.324732688177319
  h      2.365027982831533      -1.822234526673937      -0.240528190935152
  o      -0.604405585951221      1.001376566778375      0.746877580075081
  o      0.449095204501995      -1.151946970491484      -0.735354870928314
  si     -2.048575700075856      1.504514932341942      1.489525543081262
  si     -0.106718195002036      -2.624981617375772      -1.367033972985068
  c      -3.290644305644464      2.091059325629463      0.206506871972229
  h      -3.502827569449650      1.319524922862933      -0.547052869139336
  h      -4.237685292457424      2.339657838894381      0.711802628874412
  h      -2.952463544489297      2.997277499122883      -0.317417064863889
  c      -2.678819653115454      -0.007628289940031      2.392670425282990
  h      -2.890490456825087      -0.838790538332596      1.705540984735534
  h      -1.949362377560487      -0.354457776339311      3.138428618402399
  h      -3.611699477348709      0.239886902433393      2.922591541940813
  c      -1.874699675832342      -2.275293677063401      -1.869781858458341
  h      -1.915841631771802      -1.456033763870036      -2.602148833846516
  h      -2.327874654691771      -3.165683247596074      -2.330918805148775
  h      -2.489790469093020      -1.990472189091121      -1.004284445278446
  c      -0.009661850855644      -3.953448799729595      -0.041276957105259
  h      -0.408120314925384      -4.906801119100102      -0.421064344388736
  h      1.025954112117541      -4.134789029210499      0.282580823279812
  h      -0.595715530634316      -3.670313365987503      0.845162144894122
  c      0.936166511334592      -3.102853851770104      -2.855391187216480
  h      0.556768273641667      -4.032415833344837      -3.306946001273771
  h      0.909058170409160      -2.317797204615111      -3.625365130623495
  h      1.988824209785660      -3.271605223929082      -2.584720242072928
  c      -1.720805533202608      2.899953567419285      2.705707469018718
  h      -0.981881884914519      2.613856702285186      3.467541337052230
  h      -1.364728325568653      3.815530830797537      2.212008436785773
  h      -2.660131336269433      3.150182329288563      3.224079515908260

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*****
* Geometry 4
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```

42
Energy = -1276.5528759480
c      4.432338551430036      1.422717366041364      -0.035258265600071
h      5.519111965048022      1.408025024190435      0.064581006753235
c      3.764293639700134      2.653123195170100      -0.378879122709153
h      4.352013634634677      3.555499720141499      -0.555237160855688
c      2.406148975042563      2.701430058473388      -0.436860764417522
h      1.899734030665078      3.650678527714109      -0.629574850744622
c      1.576562884327831      1.547849734321655      -0.127493529928258
c      2.272066852970795      0.244178499288275      -0.068729455222811
c      3.714380374742417      0.277818437200426      0.117118368114779
h      4.225985718519182      -0.669730405728390      0.307056786418451
c      0.270547554507838      1.826560419423992      0.186119220767128
h      -0.076334879187991      2.852977194449889      0.009798615536424
c      1.717638271548613      -0.980761465373250      -0.328247394359125
h      2.365653233409955      -1.865707885785927      -0.265695539795427
o      -0.622356701190135      0.988236819924173      0.764448832203254
o      0.446341629401196      -1.186022016681951      -0.737051129485838
si      -2.050954247989616      1.548286544221199      1.502372849410632
si      -0.104324040324357      -2.648366502581237      -1.399340779972835
c      -3.304390935068144      2.102400818134611      0.215742460947165
h      -3.543545613301304      1.309197685433229      -0.506250923155513
h      -4.237250747879325      2.382703279957379      0.731280755065789
h      -2.964296250906887      2.985628034432063      -0.344787772796361
c      -2.705683964709101      0.100453574426535      2.489884224138678
h      -2.948857460073490      -0.763275047944103      1.855566661128515
h      -1.980772788922681      -0.222543067421871      3.250535071812489
h      -3.626255119150847      0.406230722794560      3.011608038349279
c      -1.874867096314020      -2.294296912724908      -1.887850644799862
h      -1.920529865203930      -1.460588878863636      -2.603412232139086
h      -2.327019646794775      -3.176648303460154      -2.365035753863555
h      -2.486672715628961      -2.028318983510504      -1.014150871891487
c      0.005090594627269      -4.004136794771439      -0.102627059542516
h      -0.394211506225862      -4.949892070730490      -0.500096286387689
h      1.043471831012569      -4.190446931604098      0.209617320816271
h      -0.574952878221345      -3.741317360850410      0.793924081236041
c      0.932746110601565      -3.093192232749905      -2.902184742245178
h      0.550551910901773      -4.013882374770982      -3.369612059039999
h      0.900381933180462      -2.293487800876987      -3.656736609765220
h      1.987220375333311      -3.267431513341312      -2.642055323646753
c      -1.697095633203660      2.994379594913275      2.650958836429702
h      -0.955093475855556      2.740054561723192      3.420751655616018
h      -1.343213076228793      3.887052503911520      2.115900663647923
h      -2.632896110852364      3.269789156877525      3.163616763944940

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*****
* Geometry 5
*****
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```

42
Energy = -1276.5519784080
  c      4.435144318497046      1.370442577903815      -0.006891725142572
  h      5.522233203826094      1.351987630594613       0.089121409232044
  c      3.768582768588934      2.606236522352300      -0.332948425676932
  h      4.357009089760298      3.511196405937116      -0.492679969166632
  c      2.410598128162872      2.656568375727199      -0.395045291156504
  h      1.906783588806602      3.610096691559116      -0.573007953903588
  c      1.576453560882702      1.502070188123783      -0.100584546510242
  c      2.271609427791717      0.197792059791860      -0.050174246644311
  c      3.714587907539880      0.225806503071258       0.132668861227159
  h      4.224163316751145      -0.725484383413335      0.308822313138565
  c      0.267531887597922      1.787930010901351      0.198073048218118
  h     -0.069740475054878      2.813996390411999      0.002468801227002
  c      1.716467248163825      -1.022199524715240      -0.329118968477619
  h      2.364954362305243      -1.908016828245529      -0.287789265132521
  o     -0.640578270341523      0.969103421084874       0.783304808779219
  o      0.443644356957535      -1.218546280499210      -0.736978727343435
  si     -2.052398180174761      1.585162082110864       1.514802015650897
  si     -0.103639575239435      -2.668375781819942      -1.429557949570568
  c     -3.315784939957093      2.102226075794309      0.222671507595653
  h     -3.583765935105732      1.283827969710653      -0.459788772109487
  h     -4.233257806553171      2.423957708249194       0.741870268828801
  h     -2.968397545496895      2.953621846213166      -0.380984636145261
  c     -2.727825090393629      0.209229136923592       2.588171233318613
  h     -3.001774934764790      -0.685404280614647       2.012063910029543
  h     -2.006643009770848      -0.085389490539415       3.363676467988298
  h     -3.635245860712964      0.573007786149259       3.096259159967475
  c     -1.876524984489170      -2.306651432615490      -1.901912457293135
  h     -1.925464086309355      -1.458916724452104      -2.600548375964333
  h     -2.332189335441949      -3.179250105111010      -2.393251681088202
  h     -2.481895237431750      -2.056812461792370      -1.019044218371789
  c      0.017903808115422      -4.050184976908534      -0.161949365447957
  h     -0.381927853859925      -4.988706556580003      -0.575563975263787
  h      1.059157389232002      -4.240100307239348       0.138431921991358
  h     -0.555757340878429      -3.806894224125347       0.744083737434522
  c      0.927874747555987      -3.080640764633621      -2.945872155857670
  h      0.543889186659008      -3.992643335220118      -3.428876049213413
  h      0.890849976285630      -2.267059573467900      -3.685136669602809
  h      1.983842457309082      -3.259507024846390      -2.695102252006134
  c     -1.666434250619272      3.081553039683415       2.586626388571500
  h     -0.920654422462371      2.859118107943118       3.362520920339309
  h     -1.309959679675871      3.943692139118532       2.005326486146958
  h     -2.595491787020029      3.391195916808449       3.092393110749566
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*****
* Geometry 6
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42
Energy = -1276.5508879010
c      4.436444288699693      1.322373836135427      0.021378135907029
h      5.524003321453765      1.302257700363891      0.112545190185022
c      3.768807767683961      2.561889213721553     -0.287303424018365
h      4.356052336649089      3.470587449723089     -0.429142803128194
c      2.410729439819475      2.611962799532052     -0.352246926576340
h      1.907523170328162      3.568571022360346     -0.514830450097763
c      1.574665854698786      1.455022672312065     -0.073736841602745
c      2.272055239975310      0.151860668466697     -0.029453915346412
c      3.715542733605428      0.176775724053350      0.150191700792937
h      4.224967923105093     -0.777124356259966      0.312181993019198
c      0.261811530765882      1.744452144243078      0.208429153168602
h     -0.070688250961677      2.766553228312638     -0.012594639721701
c      1.716879403768179     -1.063113787036077     -0.327961949140661
h      2.365695382485674     -1.949301459681908     -0.308791428526605
o     -0.658353998761507      0.943598127067226      0.803039167551589
o      0.442521325975642     -1.249478617358369     -0.733895742011360
si     -2.052089572299032      1.614788814723503      1.526098111900238
si     -0.104837943481758     -2.684529616682914     -1.456718316446480
c     -3.326583481454648      2.089726775083330      0.228817199716755
h     -3.625995628113782      1.244616959648564     -0.406204108630696
h     -4.226456843114768      2.459760558414172      0.746677649455511
h     -2.970089456347940      2.901032061982154     -0.422784288947226
c     -2.743858843912104      0.318187310914850      2.685396809762592
h     -3.046038705561655     -0.605167627842906      2.172484275952193
h     -2.025794608171283      0.057654831879550      3.475730069820516
h     -3.638323411630306      0.738176199255081      3.173438085239562
c     -1.879539077639249     -2.310361745972064     -1.910352611592042
h     -1.930026601116828     -1.449080346245299     -2.592101965133426
h     -2.343289269886400     -3.171492887533826     -2.413872905235547
h     -2.475401766194750     -2.073857203683179     -1.017414790898337
c      0.027485819184217     -4.090834958129087     -0.217817301561199
h     -0.373293561590300     -5.022249528336600     -0.646060145565898
h      1.071602872844584     -4.283659630832132      0.070697873167868
h     -0.539299055013839     -3.865585253537451      0.697091890166239
c      0.920270473808036     -3.065389719569433     -2.985822716047303
h      0.534581989010368     -3.968742179639251     -3.483708934879557
h      0.879141949752776     -2.238582193885382     -3.709947482919828
h      1.977601717470463     -3.248517795810792     -2.743883429151866
c     -1.632159621992104      3.160532397245135      2.512287652631128
h     -0.881883104942908      2.971819097652485      3.292709602786428
h     -1.270934443007836      3.985021735343929      1.881481134400509
h     -2.552530782426684      3.509965356782604      3.008043817008187
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*****
* Geometry 7
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42
Energy = -1276.5495759160
c      4.436388919161073      1.279724735459037      0.050146295305302
h      5.524436872475123      1.260305055433657      0.134746206447656
c      3.764916271362930      2.521077147759605     -0.241099210153198
h      4.348833255633815      3.434405233669825     -0.364901782802749
c      2.406717965179756      2.568021946717069     -0.309248333010409
h      1.901823175886882      3.526549527588381     -0.455215335249913
c      1.571714685586847      1.407257036441236     -0.045484554542965
c      2.274251743906633      0.107131425376159     -0.006813686763767
c      3.718002949879116      0.131670177228874      0.168563509726886
h      4.229139661024050     -0.823449964541883      0.316564115433032
c      0.253792396558508      1.696236925671942      0.217367650545258
h     -0.078476634957059      2.710634358511094     -0.033566533759285
c      1.719625560902087     -1.102945431743941     -0.324432496916736
h      2.368697993492952     -1.988881236078578     -0.329525634207097
o     -0.675163987604278      0.912538832057264      0.824464139458374
o      0.443260337407369     -1.278283023500192     -0.727520002584984
si     -2.051107030049190      1.636980025229595      1.535824277986174
si     -0.108172160859720     -2.696226221099029     -1.480128411300176
c     -3.337076125439350      2.064206401350830      0.233981386270286
h     -3.669697151889065      1.192218677526229     -0.345713216176535
h     -4.217289020830978      2.488164184019837      0.744020779033220
h     -2.970244350635856      2.826497870769700     -0.469065910078682
c     -2.753175457027464      0.425619778798226      2.779334623186783
h     -3.079079331990793     -0.523438096715597      2.332423617249530
h     -2.036865097059083      0.204405365189954      3.583029155114378
h     -3.635771425544763      0.896743268351967      3.242263683253618
c     -1.883928662407858     -2.304014950671019     -1.912315504330809
h     -1.933593917170209     -1.429659942110446     -2.577332211365018
h     -2.360421410674016     -3.151777184994882     -2.426121679159443
h     -2.467324685475980     -2.077983559631865     -1.008445382435642
c      0.032960366990618     -4.125433714009879     -0.269181957557870
h     -0.369490737329211     -5.049838625397602     -0.710462903292740
h      1.079810503648402     -4.321023500448248      0.007446006993022
h     -0.526407724897665     -3.916439698915078      0.654044801898083
c      0.909492466651097     -3.047428882663546     -3.021331152319777
h      0.521632323903672     -3.942129301674793     -3.533052924772438
h      0.864987407732534     -2.208157368796695     -3.730622131075837
h      1.967934283428518     -3.235008644356730     -2.787760674595888
c     -1.595242389026731      3.230470933429504      2.426685418368042
h     -0.839344971649346      3.077446281925571      3.209553277105594
h     -1.227897243837546      4.009334492077344      1.743557870008356
h     -2.504580074820198      3.624644634790535      2.908753258519324

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* Geometry 8
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42
Energy = -1276.5481151710
  c      4.433956739558459      1.244789278115048      0.078632097829556
  h      5.522493317271862      1.229228134708340      0.156382629778643
  c      3.755593120274855      2.486340888830490     -0.194060544727097
  h      4.334126197119547      3.405194172455434     -0.299990302303095
  c      2.397052893809852      2.527080617901939     -0.264855450670145
  h      1.888010199590108      3.485653749634677     -0.392866706570472
  c      1.566944213718972      1.360174614146297     -0.016645198391757
  c      2.276977237787018      0.064939833172645      0.017581220432059
  c      3.720847815408809      0.092593145688512      0.188017544771547
  h      4.235970049864984     -0.862752982661135      0.322637613224985
  c      0.242892894624911      1.642635154582872      0.225690680694505
  h     -0.091508262738645      2.648399618559908     -0.055650079661261
  c      1.723737545412577     -1.140414526254512     -0.318361082790430
  h      2.372917276026367     -2.026271468600568     -0.348569153319973
  o     -0.690664291010856      0.874942717832770      0.847316096993344
  o      0.444856978529785     -1.303831333578529     -0.718539172351554
  si     -2.048886840787238      1.650694455839341      1.544178673058583
  si     -0.114185900519875     -2.702672417467846     -1.499289689749720
  c     -3.345471673031817      2.025123056755911      0.237350810963072
  h     -3.713217294241872      1.127436275931182     -0.278345475834724
  h     -4.204174364652930      2.509781723319876      0.729431581557400
  h     -2.965119478734902      2.726682496683734     -0.519660362188446
  c     -2.755573887300568      0.528792414133411      2.867978949962391
  h     -3.101091036806233     -0.441796226269654      2.487265550582340
  h     -2.038626546124918      0.349624279117646      3.681409078625494
  h     -3.627337042617876      1.044305030705997      3.303982728078697
  c     -1.889822205295160     -2.286868269123951     -1.908159483068796
  h     -1.935195095211544     -1.399793161153675     -2.556566747371678
  h     -2.384836607627163     -3.118651174711457     -2.429948021782376
  h     -2.457242531533729     -2.067344374587182     -0.992471643252486
  c      0.033505263060786     -4.153622784833776     -0.315789014594768
  h     -0.371448686051298     -5.071487737464637     -0.767840454975504
  h      1.083194097637174     -4.351675685859566     -0.050829253041498
  h     -0.517750077131086     -3.958489666593028      0.615423409625367
  c      0.895393982581176     -3.026945157108682     -3.052054509222227
  h      0.505196594317090     -3.912911180685526     -3.577068669442518
  h      0.848795061985702     -2.175986172888925     -3.747153816555835
  h      1.954874475149980     -3.219319192850707     -2.826062630070024
  c     -1.553543834333122      3.287329565414854      2.329999364543520
  h     -0.791303842680040      3.169511874402599      3.112782779852651
  h     -1.176810097557211      4.010465107296218      1.593139770082727
  h     -2.448089412440623      3.733285879032203      2.793690915443155
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*****
* Geometry 9
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42
Energy = -1276.5463190490
c      4.429881178498838      1.217912176273940      0.106061383059576
h      5.518880630291534      1.209351828444275      0.176780514051410
c      3.741254612299290      2.457523135935982     -0.146731598628861
h      4.311304763785020      3.383474551837618     -0.233595078083000
c      2.382391507629347      2.488467748400303     -0.218779144023118
h      1.865742014991856      3.445807898715172     -0.327832745607832
c      1.561499176605551      1.312972564839020      0.013494318593477
c      2.282248579651855      0.024684037190134      0.044954933325256
c      3.725819761710856      0.059611919479148      0.207943312391206
h      4.247558179754233     -0.893588641312023      0.328086432965411
c      0.229902677569637      1.584170204879956      0.233104759160050
h     -0.112527670399183      2.575995648232214     -0.083964547747682
c      1.731640142118118     -1.175294307353104     -0.312067889696960
h      2.380300987895275     -2.059271702140517     -0.368713523180231
o     -0.706009042002170      0.829441955781208      0.871780168677252
o      0.450723198179281     -1.326541055742956     -0.706299214373702
si     -2.046647222835033      1.656215909824692      1.550818853433114
si     -0.122140637333387     -2.703305694144517     -1.514377448286990
c     -3.352063309638245      1.975800854473606      0.239273264208558
h     -3.757442272131677      1.056264601394097     -0.204983183316079
h     -4.186488952084054      2.526170889162305      0.703022984008475
h     -2.956189108364525      2.604953214435755     -0.571847895598509
c     -2.753125416962632      0.626498005994104      2.948969368823112
h     -3.115786879156858     -0.361007830364406      2.633179406472677
h     -2.032354041363126      0.488855916571433      3.767154056201299
h     -3.614356856966774      1.180391055043368      3.358616172559991
c     -1.895928431854660     -2.256743426025477     -1.897396841687829
h     -1.933358477532545     -1.357882249932717     -2.530087413416171
h     -2.414811822296961     -3.070175628908529     -2.424347477722749
h     -2.444315208582981     -2.039904246230001     -0.969395224343940
c      0.028866778283954     -4.174050738061893     -0.356673073865484
h     -0.379793747456623     -5.085679008082216     -0.817302147718964
h      1.080877811386299     -4.374837655196720     -0.103393511507018
h     -0.513677467600334     -3.990404560250922      0.581874232552323
c      0.878464876535910     -3.003918153677379     -3.077765622426861
h      0.485023275345050     -3.881202466519715     -3.614761749613741
h      0.831337650885832     -2.142492629845084     -3.759597586573495
h      1.938266544138612     -3.201994279735628     -2.858570278015399
c     -1.508119216291889      3.328351759787926      2.226287550132851
h     -0.739008717759636      3.243166748467562      3.006831656815633
h     -1.118553590615889      3.986704266913935      1.437070289146485
h     -2.384239430717500      3.831402644268057      2.665136900955299
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*****
* Geometry 10
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42
Energy = -1276.5439881640
c      4.426621608089495      1.199898464022425      0.134313744078033
h      5.516369631900266      1.200795703784757      0.194612520134593
c      3.724284395285502      2.435860972832218     -0.096292893453604
h      4.283819090031139      3.369913030300268     -0.164124912208128
c      2.364495989630860      2.453131953807784     -0.170728172919338
h      1.838184487434537      3.407020727962384     -0.256696766310930
c      1.556446847965691      1.267007549938582      0.044662851306257
c      2.291126596385124     -0.012031049513289      0.070445157402387
c      3.734585495173078      0.033103852054013      0.225817160615807
h      4.265744586053907     -0.917092661731036      0.331363985547125
c      0.217117517158615      1.520861178616592      0.239372658514823
h     -0.134066418593485      2.495829158337176     -0.116128048845843
c      1.743262098497374     -1.208464157880281     -0.303029506590204
h      2.393875208930871     -2.088935905985744     -0.391983360507123
o     -0.716746363029646      0.782259338315067      0.897333730994455
o      0.458779426990521     -1.346598052025136     -0.691698315154600
si     -2.041650173388774      1.655529976336966      1.553429129304209
si     -0.132004584568031     -2.699400664383648     -1.524755621101810
c     -3.359500601904337      1.916794224587131      0.241333511107490
h     -3.801282726482514      0.980995220931746     -0.127611384378925
h     -4.168406865182444      2.528632782122547      0.671881688553097
h     -2.954031280216222      2.468687127267408     -0.619407880740971
c     -2.743493111960602      0.719587393156241      3.019145086057126
h     -3.119781188630063     -0.281346252487409      2.768545494595543
h     -2.017162011227989      0.624039144516254      3.838403776948171
h     -3.595090235580828      1.306361887007687      3.402840946973882
c     -1.901798393404017     -2.215694367944766     -1.880164485420001
h     -1.927917492957377     -1.306360404360793     -2.498240066449897
h     -2.447893802992051     -3.008783654533102     -2.410100537367789
h     -2.428900324888711     -1.998950640310433     -0.939928378518890
c      0.017787795269634     -4.188262810754562     -0.391278910316176
h     -0.396539344547704     -5.093587548375857     -0.858638339099195
h      1.071988917381526     -4.393167798267292     -0.149143653041631
h     -0.515308322544718     -4.012520032930013      0.554209661558473
c      0.857809024742473     -2.979801711655433     -3.098876536810821
h      0.459298179292263     -3.848141429177202     -3.646502914443587
h      0.811526469617512     -2.108379573160637     -3.767979216838552
h      1.918042245587705     -3.184992937320402     -2.886771960884474
c     -1.464275223686844      3.356714809949438      2.115079549876071
h     -0.686657617125331      3.305081450679057      2.890010703268518
h     -1.065206976461700      3.945753752418173      1.277954031215942
h     -2.320288646133937      3.914315946020890      2.525659259370833
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*****
* Geometry 11
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42
Energy = -1276.5412478670
c      4.427093083245863      1.186656877912054      0.160573319423634
h      5.516961954211427      1.199382221491312      0.211997268378686
c      3.710143486708102      2.417711027731762     -0.045221925798027
h      4.256852328999835      3.360275148133791     -0.092262672914664
c      2.350041718254032      2.419780105112745     -0.119942453674123
h      1.811727200291746      3.369334860498757     -0.181906634832003
c      1.556861330325620      1.221653527769325      0.078096401980015
c      2.306031600268070     -0.047492513718344      0.095772342882186
c      3.749010733922267      0.011041956575929      0.240827889147855
h      4.290999616145006     -0.934260893762111      0.329294003157252
c      0.209453816171671      1.458584406662766      0.246395058435062
h     -0.147622096685772      2.418862269922022     -0.142049915077468
c      1.762141137454792     -1.239155618225587     -0.297128709870884
h      2.412948606676134     -2.115000656168636     -0.417396752386445
o     -0.727902997550387      0.733009455869669      0.918810017930846
o      0.474036481385848     -1.366227462389396     -0.674805702333184
si     -2.037447324148405      1.652795207641852      1.550999867372092
si     -0.142194771591435     -2.692136638784994     -1.530134156533032
c     -3.372619352212403      1.850185436163083      0.246032951687728
h     -3.843391929887837      0.901726736954410     -0.047419729893525
h     -4.158709130911372      2.511722105035436      0.644017749306169
h     -2.968485745624835      2.327845359007912     -0.658770743612006
c     -2.725262815063915      0.812001269731716      3.080178614328014
h     -3.109738046374759     -0.200290993425715      2.895947842130581
h     -1.990262630879725      0.762677519113910      3.895908896374487
h     -3.569916709220103      1.425773463026136      3.436489830769705
c     -1.906167650137939     -2.168416022889671     -1.858192188958253
h     -1.919109788064763     -1.249570790460746     -2.462752921606637
h     -2.479636626765227     -2.940238978011589     -2.390273632984175
h     -2.412885580676834     -1.950698235178820     -0.906863914958507
c      0.000773026534879     -4.198868134014883     -0.420428492334222
h     -0.422645361302772     -5.096779442695362     -0.893236070668144
h      1.055894778240785     -4.411258361553708     -0.189137408134842
h     -0.522626299398374     -4.028744620826851      0.531474916411747
c      0.833667644842076     -2.956289906709889     -3.116019674655309
h      0.426966068816858     -3.814246247875800     -3.673736959225158
h      0.788827495911709     -2.075217020250122     -3.772336537491592
h      1.893753381126383     -3.170978034835607     -2.913219009759183
c     -1.429072517630108      3.377929674611420      1.996366627242677
h     -0.637408725276108      3.362429485428517      2.758913917928210
h     -1.031475188217896      3.899882258751156      1.115247404918489
h     -2.266781319152553      3.979969255757919      2.379847035481881
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*****
* Geometry 12
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42
Energy = -1276.5382324880
  c      4.430617389525603      1.177562901730916      0.185617470594188
  h      5.520593014786837      1.202782705741807      0.227459902441826
  c      3.697892598000841      2.402989422249937      0.006467665544005
  h      4.231331829925692      3.354220494317424     -0.017042619257139
  c      2.337807206645884      2.388527452641121     -0.064345437166382
  h      1.787054282431565      3.332520897249768     -0.102434044701903
  c      1.560474431544093      1.177590024391780      0.111143716041633
  c      2.325115245390010     -0.080985591208139      0.117538864928801
  c      3.767429452368079     -0.007792284939047      0.253790761190179
  h      4.321602838091241     -0.947554455559893      0.321517316868706
  c      0.206648185536106      1.398743734200263      0.256467960085274
  h     -0.152813568144410      2.345020764600663     -0.160509134123959
  c      1.785087663329348     -1.268736951515136     -0.293299841701048
  h      2.436536086648714     -2.138810117445495     -0.444993006210222
  o     -0.734937031981180      0.688233310631761      0.940929939717184
  o      0.492135058673833     -1.386099786897205     -0.656494823938487
  si     -2.032197830144189      1.648663808161553      1.545111399569314
  si     -0.151868300791717     -2.683447389028534     -1.533075620827855
  c     -3.389171312769950      1.777220777938373      0.254261141210851
  h     -3.879825883425316      0.819201640410638      0.033547831174365
  h     -4.157236050202780      2.476638315202424      0.621330829209725
  h     -2.994790778861913      2.187067862391840     -0.687299044062311
  c     -2.699519526812665      0.904477732060797      3.132563270843814
  h     -3.087516647125912     -0.116507866719918      3.016012697940031
  h     -1.954450814016297      0.904161300898469      3.940547694978717
  h     -3.539230807069381      1.540168641240179      3.461410701030054
  c     -1.908130924835973     -2.118436102831537     -1.834540807299309
  h     -1.906701723170753     -1.191578422199148     -2.427067703129799
  h     -2.507363464582575     -2.868997205445106     -2.368399901272122
  h     -2.396241490236162     -1.899614476696073     -0.873757742492357
  c     -0.020865448917985     -4.207180271981390     -0.445786576102840
  h     -0.456519884830862     -5.096326002354109     -0.923494582463404
  h      1.034329064154864     -4.430695811408617     -0.224856994981539
  h     -0.534188719781536     -4.040381695061677      0.512262958525750
  c      0.807516449928034     -2.934474768278938     -3.131060914480106
  h      0.389095280666963     -3.780867336085296     -3.697584941767880
  h      0.765362093439744     -2.043695607277769     -3.774403541489291
  h      1.867363013134451     -3.160973630745120     -2.939746445132550
  c     -1.403965962086720      3.393664136019984      1.871733930023048
  h     -0.594773156306087      3.417500091913181      2.615473684399771
  h     -1.019054955830159      3.851920935788895      0.950810748387866
  h     -2.226215763146074      4.030235845349979      2.231103700221298
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* Geometry 13
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42
Energy = -1276.5348995640
c      4.436874267654827      1.171060930687296      0.207794445140089
h      5.527108248715856      1.209620287925519      0.238687219196958
c      3.688052086517480      2.390827054827320      0.062621988717874
h      4.208253560034905      3.349668606972927      0.059030537190170
c      2.327018391849365      2.358929324568146     -0.007507698003864
h      1.764397276727715      3.295817412148816     -0.014805094401240
c      1.567061587173856      1.135436492985408      0.146384057264764
c      2.346249338271378     -0.113053028851211      0.138348485562693
c      3.788705923050764     -0.024328067284485      0.260400826563926
h      4.355786053571474     -0.957756175770957      0.308923589386802
c      0.207738644624146      1.340870126387321      0.271178140130453
h     -0.153593742904336      2.273323562128113     -0.174849922474049
c      1.809799246677486     -1.296742121161398     -0.289996497272183
h      2.463268639129838     -2.158245982652610     -0.477793554563957
o     -0.739196284517969      0.648569315381629      0.965570764942865
o      0.512853600711558     -1.405687783981110     -0.639127619754073
si     -2.027339790009159      1.643005745781053      1.537921076578442
si     -0.159950841545823     -2.673896218608776     -1.534140170360224
c     -3.407808813273282      1.699723011568085      0.267652687877043
h     -3.909908139008103      0.734531488171378      0.115322607441020
h     -4.162867480135541      2.427129648308449      0.606159227498591
h     -3.028387477331581      2.048648606037991     -0.704008105139616
c     -2.669068032641113      0.997522231883993      3.178507611746142
h     -3.056902099666457     -0.029005130374716      3.130129339461121
h     -1.913211773739876      1.047653168967488      3.974768633550309
h     -3.505568413341496      1.651013139841158      3.479814494424787
c     -1.907047693434408     -2.068635989637783     -1.811889866585920
h     -1.891051514839347     -1.135475557104855     -2.394147206410070
h     -2.529297215388024     -2.799027985080184     -2.347391919609025
h     -2.379130250369691     -1.849021219922377     -0.843495561885046
c     -0.044986077555859     -4.213346780731580     -0.468166311120432
h     -0.495422356570075     -5.092573890408469     -0.950195770826270
h      1.009307056572742     -4.450916931451117     -0.257268170047168
h     -0.548015976414027     -4.047915647937071      0.495583619328756
c      0.781612404580903     -2.914565477701876     -3.144412228144264
h      0.348213415312444     -3.748580523843014     -3.718065167066591
h      0.743372570753972     -2.014973245739108     -3.775614442715004
h      1.840640016024324     -3.155603712405403     -2.966584358265262
c     -1.390383960570234      3.404539444439349      1.743475043769735
h     -0.561738742710679      3.471486172642988      2.462748748427021
h     -1.027168663676663      3.801906441745947      0.786402753544422
h     -2.200817046706026      4.067419704815858      2.080589402621998

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*****
* Geometry 14
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42
Energy = -1276.5315772110
  c      4.444764722036961      1.165462529003210      0.227890120364225
  h      5.534502343627973      1.216345410013043      0.247989825726803
  c      3.681383405354830      2.378217064418624      0.115358571673774
  h      4.188288702650953      3.344084520284704      0.136625790749523
  c      2.321147205183412      2.330428130934205      0.055113309863436
  h      1.746390070469486      3.260132011867909      0.074862664024563
  c      1.576967224600430      1.095522854933784      0.184394988320824
  c      2.369536893792247     -0.142929178020180      0.157676576398275
  c      3.811512688472264     -0.038580255614988      0.265594294237231
  h      4.390704371103364     -0.965441503971641      0.289900930496391
  c      0.212358937131208      1.290184506012786      0.291227619229726
  h     -0.147688041488055      2.206822716383443     -0.179377754863350
  c      1.836704637493192     -1.321690655168974     -0.290571177724154
  h      2.490429346982773     -2.174390883386537     -0.512474725652596
  o     -0.741842552313700      0.614561414141275      0.992979117777232
  o      0.534273463297824     -1.424952192354173     -0.621990567755323
  si     -2.023500981774720      1.638004332361812      1.530538047934970
  si     -0.166583253391324     -2.664715804126489     -1.534711319299118
  c     -3.427916675291318      1.618831749389483      0.287075565809930
  h     -3.933004203834102      0.647272058294184      0.199802878283399
  h     -4.175682085028689      2.365585021707645      0.598726963441825
  h     -3.066877140957338      1.911770983024260     -0.709921303664413
  c     -2.634520756349934      1.093740075865045      3.219628787398402
  h     -3.018327342085892      0.064560461442246      3.239813386068128
  h     -1.866932513489714      1.194838864934526      3.999637778348143
  h     -3.469780300359958      1.760779955897993      3.493702199881143
  c     -1.903920464210387     -2.022314256517742     -1.792206832873804
  h     -1.873880391839624     -1.084023566380759     -2.365915195440864
  h     -2.545342298473823     -2.734527197860598     -2.329568303202576
  h     -2.363414708952313     -1.801896232505948     -0.817926071508149
  c     -0.070269804777078     -4.218534884856929     -0.488579705620632
  h     -0.537263705683575     -5.086666436997551     -0.974613759332352
  h      0.982210353085153     -4.472514865160172     -0.287457337336280
  h     -0.563367068915366     -4.053564882612189      0.480519054237315
  c      0.756953192285324     -2.896977164087939     -3.156677051497626
  h      0.306361997068658     -3.717702533852423     -3.736245425248317
  h      0.723516646155098     -1.989064244330696     -3.776253834802036
  h      1.814487886559543     -3.154298185780505     -2.993420175366190
  c     -1.389475710847729      3.412667130023904      1.613436375893168
  h     -0.540038806820298      3.525375936805685      2.302223493597615
  h     -1.055048249996230      3.752012040497336      0.623818764750645
  h     -2.192158676715386      4.094012093511206      1.930857013773883
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* Geometry 15
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42
Energy = -1276.5276905780
c      4.453801720673701      1.160443311821268      0.245292809785702
h      5.543205977490185      1.224525486476028      0.251392334409431
c      3.676618266365598      2.367124215335991      0.175026326877386
h      4.171315881775554      3.338536095889177      0.219918739221627
c      2.315174158480244      2.303362201324938      0.119886650745073
h      1.729725370744468      3.225562987412338      0.177175504670904
c      1.586747913684635      1.057516177016871      0.225447348116765
c      2.392340828892764      -0.171365002621161      0.175385568968442
c      3.833879225014888      -0.051890031759027      0.263882075264853
h      4.424535567556574      -0.970566148515843      0.260362739259171
c      0.217183361994264      1.239540765185716      0.312840763564579
h      -0.144899487152745      2.136308439013413      -0.190463972115158
c      1.862023589869605      -1.343955853531322      -0.293857072828594
h      2.516777001669688      -2.184154328170818      -0.551773037049775
o      -0.742008578319782      0.583757471056756      1.029025176482599
o      0.554749481850778      -1.443210138732052      -0.606648243504612
si     -2.018501950642370      1.637071471979242      1.527857426205345
si     -0.171118977597298      -2.655576433927270      -1.535461637386875
c      -3.444844146585012      1.539246526861906      0.314096641705933
h      -3.945407034083754      0.562018328130555      0.287544826946818
h      -4.190801029718232      2.298252185040286      0.600013765097682
h      -3.103183524689444      1.781985067521711      -0.703202879429159
c      -2.599266100930358      1.194412582177305      3.257360851109467
h      -2.975854752910482      0.165763259354583      3.342877220570859
h      -1.821093798954517      1.344375108585157      4.019006010386026
h      -3.435186953226731      1.870903149063498      3.505320999396163
c      -1.898949499445274      -1.981363667045789      -1.776636425426855
h      -1.856887249203807      -1.039527324260580      -2.343897829879916
h      -2.555756440368494      -2.678130175521864      -2.315903465398401
h      -2.349174762535510      -1.760585436162647      -0.798256796193795
c      -0.094294673266054      -4.222332189761569      -0.507432765217989
h      -0.578195970729930      -5.079122601039158      -0.996895970643656
h      0.955284008621554      -4.493229854162034      -0.315500269972014
h      -0.577863787852314      -4.057012781352975      0.466242197859770
c      0.734765446669431      -2.882435609250642      -3.168574592854622
h      0.266114478087279      -3.690029194217596      -3.752472117892641
h      0.707017722943220      -1.967674248916008      -3.778157631753761
h      1.789854691154593      -3.156590309004960      -3.020533152417625
c      -1.396062716141811      3.418493210067162      1.484243661420294
h      -0.528753626445918      3.580852520904844      2.140712480749441
h      -1.090553283210342      3.696024624455032      0.465632572733964
h      -2.195048512445322      4.114713258690417      1.777779041615409

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* Geometry 16
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42
Energy = -1276.5220314830
  c      4.460444946709198      1.161718334740581      0.258079764471003
  h      5.549232696775594      1.237583295813829      0.247377162679031
  c      3.669818501836200      2.358917237257167      0.241338202244407
  h      4.153803942013846      3.334105634495920      0.322102168837105
  c      2.307290986484860      2.279201875051866      0.199554712917935
  h      1.713378036362240      3.191225429994655      0.306853979549593
  c      1.596031187767138      1.023784377126461      0.267340455312335
  c      2.413273414330075     -0.193695942586696      0.187394309091625
  c      3.853846528942463     -0.058708467075322      0.252083468287951
  h      4.455845208758132     -0.969364472427156      0.207934542896471
  c      0.215987451509440      1.180441738141789      0.327288717188213
  h     -0.166385580248701      2.022583080595259     -0.250292175448801
  c      1.884431905977545     -1.362006216678119     -0.300391890388192
  h      2.540750550642711     -2.187612860937426     -0.597355167932153
  o     -0.733851663994336      0.563461461917673      1.089308831930026
  o      0.572299759730410     -1.460482667960577     -0.593689361135318
  si     -2.009779061435646      1.645784056330183      1.534116651411621
  si     -0.174118492248269     -2.649250210607297     -1.538665074029391
  c     -3.451235308546665      1.469983442858596      0.347076425715881
  h     -3.940599200252158      0.487394814514052      0.376099434392498
  h     -4.202232258615111      2.233359127796834      0.607543745869187
  h     -3.128342264827206      1.667214076063146     -0.685890499375944
  c     -2.569081091306834      1.297626732299867      3.292991079017850
  h     -2.935152866077160      0.270917449961882      3.432346335746487
  h     -1.783904907555874      1.489442985029673      4.037652257409542
  h     -3.408679148454306      1.977392931224440      3.518637729338283
  c     -1.893813972714480     -1.948618403629780     -1.766431064642413
  h     -1.842207574992833     -1.004286501210534     -2.328692983740158
  h     -2.563196344626572     -2.632596951403790     -2.306782116751879
  h     -2.336521340430379     -1.727840852156447     -0.784751689792472
  c     -0.115250380582844     -4.225571183123370     -0.524693713101596
  h     -0.614619236182630     -5.072516016455598     -1.015657694514131
  h      0.931655684254113     -4.511877625503392     -0.340346133337132
  h     -0.590259033853450     -4.058082558803423      0.452893444641363
  c      0.715454129131189     -2.873016123660094     -3.182047772159566
  h      0.230339632829982     -3.668841936874010     -3.769086436752122
  h      0.693446265122021     -1.952846301698785     -3.783813647407728
  h      1.768177317781372     -3.162971824794955     -3.047870256835082
  c     -1.402007771033762      3.426264870057091      1.363949831922844
  h     -0.525641458720610      3.642478088128243      1.991746111645457
  h     -1.116001090268661      3.632578048661724      0.322881503763820
  h     -2.201300717561706      4.137251371619791      1.620531328874732
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*****
* Geometry 17
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42
Energy = -1276.5107647150
c      4.465093573051416      1.175930376648984      0.262918625157923
h      5.553385301764759      1.258529707820118      0.237377582364360
c      3.667550864172668      2.360308165822406      0.317630065153039
h      4.145611022675780      3.335752672377762      0.429402454113203
c      2.298051220249652      2.265076542366405      0.296944970415643
h      1.700649303831876      3.163771469795814      0.469285783373540
c      1.604855760574613      1.006951677577153      0.307716232371043
c      2.428618573308174      -0.197993925877124      0.181363932531566
c      3.865970579400269      -0.050748006026935      0.217918383833615
h      4.475052035900363      -0.9530474444805346      0.124934963146342
c      0.200877380906287      1.111000365894767      0.318505872671606
h      -0.242530818846881      1.777707329229792      -0.425183419961443
c      1.900082802201496      -1.369967463829052      -0.313162364815887
h      2.558069832775472      -2.186752907551603      -0.632830630398800
o      -0.704318636510594      0.581420385321462      1.191355403931261
o      0.582318353314078      -1.471719281674206      -0.594424707046571
si      -1.998956176220843      1.676111660976011      1.555369974752516
si      -0.176132536520320      -2.650102758823584      -1.547341507047278
c      -3.440481891251816      1.432169586002269      0.376644246092968
h      -3.916681285241075      0.444823011180910      0.444005879542964
h      -4.202592939929757      2.192337405274177      0.615270066624040
h      -3.131680761714375      1.599175581355608      -0.665787743414175
c      -2.558735697481712      1.381714853467399      3.324310653817470
h      -2.911335759052015      0.352810193578406      3.483650288426024
h      -1.771475112343944      1.593716922213550      4.060966521606053
h      -3.405660003126459      2.054480646613092      3.542148972510165
c      -1.891177517337626      -1.932305042322167      -1.763927065267781
h      -1.833969755286295      -0.986156763133949      -2.322640179243376
h      -2.571053932647513      -2.606717624962961      -2.303516458463585
h      -2.327186894070792      -1.712197914539518      -0.778869004558550
c      -0.127644883088943      -4.228832856625578      -0.536923002382861
h      -0.636506972429596      -5.071767673258949      -1.025002180701939
h      0.917589514296165      -4.523465274457406      -0.356341950649394
h      -0.597051820001214      -4.056083027305049      0.442604343176073
c      0.702053524385502      -2.873952871515414      -3.197746479551240
h      0.208873678987709      -3.662375556045197      -3.788406751858663
h      0.684170979217689      -1.950045224949899      -3.793942358346162
h      1.753161408186314      -3.172435302947640      -3.070301243842469
c      -1.402622290456379      3.446955173034832      1.284038858608392
h      -0.528265344194641      3.705511829323288      1.897494423419074
h      -1.113965280169193      3.576336902922517      0.231077219190087
h      -2.201207109853411      4.176090704314197      1.490483614413244

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* Geometry 18
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```

42
Energy = -1276.4987982980
  c      4.472343196913340      1.201941997943160      0.267513074455533
  h      5.561291928488825      1.275689910239665      0.231477191195942
  c      3.689681270564961      2.367010366293422      0.387452143306484
  h      4.161922937087826      3.348211597105704      0.465124041971930
  c      2.300171615697462      2.254565053140188      0.433530773356752
  h      1.697996458385139      3.149437432940543      0.603581972161708
  c      1.631963249726500      1.021613453728784      0.332404265944930
  c      2.437764277303744     -0.162171374137498      0.120411820688911
  c      3.862857669817541     -0.031772529095565      0.166540652052926
  h      4.471496275108822     -0.931472590348711      0.046015379960486
  c      0.169482237294296      1.056356601038625      0.274258085994594
  h     -0.325354285279419      1.422170105380463     -0.628334692104852
  c      1.903713359214496     -1.369483584969095     -0.345657675163167
  h      2.562574960454062     -2.204339129282074     -0.608771476250958
  o     -0.659470594233293      0.688699376737875      1.305219539458941
  o      0.590417294226189     -1.478276531801193     -0.630071973525321
  si     -1.998799532276147      1.721027608355468      1.582631930801723
  si     -0.180364908076589     -2.660928011877683     -1.561438570418684
  c     -3.427727919583376      1.433087150070801      0.388799424505481
  h     -3.899719963604581      0.443824297698376      0.464379394497028
  h     -4.199597346798097      2.187832440281296      0.616796555433992
  h     -3.123626075905279      1.593722860170147     -0.656025222713398
  c     -2.572735911663250      1.415629349241192      3.342761422903689
  h     -2.911994308134650      0.379365435530353      3.487393019651005
  h     -1.781784025079103      1.621476857618978      4.077176100125141
  h     -3.425296330827872      2.075488383882097      3.571408967087795
  c     -1.892367484365792     -1.933586944580782     -1.766604979424931
  h     -1.832180522838043     -0.985549976257067     -2.322032897301165
  h     -2.579388944750914     -2.601459735756812     -2.304842353499596
  h     -2.322694903264124     -1.712745348080473     -0.779025497384222
  c     -0.129333870660281     -4.231993813936736     -0.540576202894794
  h     -0.639014747738564     -5.077791612903410     -1.022423992546539
  h      0.916184981461788     -4.525148466949680     -0.359607573247868
  h     -0.597502875605535     -4.052974682189856      0.438465458345073
  c      0.697201005341270     -2.883277912056689     -3.210674473725613
  h      0.207690574749488     -3.669191632710583     -3.806712641878510
  h      0.680584815382822     -1.955679733922341     -3.801269314776583
  h      1.748501644022814     -3.179008268191296     -3.078419275105496
  c     -1.409466275909196      3.479546424629298      1.268176790489880
  h     -0.535354956077455      3.739055120594776      1.881573226176753
  h     -1.106396346557462      3.554779556990816      0.212819510342412
  h     -2.197441433988843      4.226581389471657      1.442163217967253

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* Geometry 19
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42
Energy = -1276.4985724430
c      4.475664078686853      1.214844313269605      0.271151362821360
h      5.564276705914606      1.289514780107312      0.227343328063332
c      3.692734504413047      2.369153374525368      0.458764709861261
h      4.161308158033708      3.353346319409177      0.506459167148489
c      2.302975559420331      2.247856745368477      0.546018920969708
h      1.697818618081971      3.140543058385313      0.717268251486977
c      1.635985321898817      1.034067733747935      0.320968548699653
c      2.442774934544412      -0.130217718235216      0.032155435735106
c      3.864956286165703      -0.012086132230408      0.108396843707136
h      4.470232014380222      -0.911181646282660      -0.035373669374402
c      0.164944025637254      1.025868062325093      0.250204534772161
h      -0.354144789929948      1.010140526759112      -0.709895948566955
c      1.911495211630334      -1.357315513650784      -0.393440616572333
h      2.561188556303589      -2.226138434142948      -0.545564046507174
o      -0.609297467185269      0.841540255430649      1.371227339134189
o      0.605141186703798      -1.476149031298625      -0.691369952438404
si     -2.006031553601098      1.780101181656855      1.599441601749068
si     -0.183300857343600      -2.675152298848376      -1.577354716748697
c      -3.416697936666317      1.441597139198431      0.392814469530743
h      -3.878499156387920      0.447731569976074      0.475262377252283
h      -4.200670475550400      2.186987213803020      0.612293789057999
h      -3.114318678269162      1.599446083829011      -0.652764748769836
c      -2.583251133120048      1.434026723037738      3.350149733372296
h      -2.911680783503755      0.390671824330116      3.471384337642636
h      -1.791308489488638      1.628190312252154      4.086505106744724
h      -3.441567909702262      2.079182907330582      3.594588946694248
c      -1.894244594609285      -1.941178848795777      -1.770052239908740
h      -1.832644102942033      -0.992346256738159      -2.324270424381788
h      -2.586580250326947      -2.604375088958639      -2.306961085806411
h      -2.321212010301525      -1.719809896165496      -0.781090924320595
c      -0.129197633559323      -4.235975489973800      -0.541773231744519
h      -0.638107865757579      -5.085424841886471      -1.018065548956638
h      0.916482337514199      -4.527911686686796      -0.359250062510111
h      -0.597828570372255      -4.052203779495780      0.436243337057931
c      0.692989096185048      -2.896969708195354      -3.224278304053246
h      0.210726037421388      -3.680867553558505      -3.827285994156268
h      0.677321714872113      -1.964153224476932      -3.806872779851178
h      1.745134987125139      -3.186490710131867      -3.083696083611378
c      -1.428113394314028      3.531069158826876      1.271434198885624
h      -0.552065705883530      3.774202295929882      1.888966601169265
h      -1.108099032203919      3.567785871872634      0.217623806878573
h      -2.202203934278352      4.293712200165788      1.423962579599884
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* Geometry 20
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42
Energy = -1276.5081545510
c      4.472146565845715      1.211301096607946      0.272675692321685
h      5.559836012081728      1.304926545224946      0.248219914169720
c      3.656103553228716      2.360381068369135      0.515584200102484
h      4.116943353001050      3.350280265728329      0.542216749625784
c      2.292588285371112      2.219754350873667      0.651451716424986
h      1.683403931345264      3.109043467289929      0.823791621733733
c      1.616336691556754      1.004461757113827      0.301165312038942
c      2.458867250778668      -0.135092521800324      -0.090715402829783
c      3.887478705990835      0.001619682216088      0.042043509338559
h      4.495356519688626      -0.893734955719951      -0.106867961795058
c      0.201220021472915      0.901988439776091      0.283572888096976
h      -0.355197632691853      0.675575398729840      -0.625773590622958
c      1.947369757114627      -1.352254118854063      -0.470630703596437
h      2.565904246942317      -2.252326978860435      -0.513090226175925
o      -0.539721692205859      1.066547862338106      1.400852476020473
o      0.624895223690890      -1.468453255327798      -0.734035271753393
si      -2.028971820843608      1.853293674226683      1.602772565919522
si      -0.178714772993627      -2.675846728942123      -1.584037511806967
c      -3.410822792424372      1.442459400447367      0.390950570971183
h      -3.859123391827446      0.443891240333346      0.487437105448549
h      -4.206522842995902      2.178230981839100      0.603889254568846
h      -3.113494472549396      1.594970336067745      -0.656373291863438
c      -2.582025596774130      1.456800307141878      3.349158209578680
h      -2.900955721377283      0.408288243288472      3.455126483608395
h      -1.788289610841014      1.645503643347052      4.084803888791334
h      -3.445991336976417      2.087914764018699      3.609728422399535
c      -1.893781278986079      -1.941643247059695      -1.769919741527359
h      -1.833937237014124      -0.993252212308239      -2.325665919393290
h      -2.587193436261258      -2.604039615846043      -2.306568190199605
h      -2.322805841076839      -1.722095391123126      -0.781148084055986
c      -0.130016430875749      -4.234979210772866      -0.543830223616699
h      -0.639361601843193      -5.085074381371317      -1.018807803824828
h      0.915117189228395      -4.528083537548818      -0.360454056725498
h      -0.598565743350564      -4.050642599288794      0.434225276272793
c      0.688150930746147      -2.903707664205725      -3.233252115610686
h      0.207011374033760      -3.685796712122502      -3.838354350683064
h      0.675209632128092      -1.967760573153577      -3.810897506770714
h      1.740283356447307      -3.190303034146697      -3.088272031772316
c      -1.460796337537653      3.593837828851778      1.260371996186832
h      -0.579263364032824      3.814050153839292      1.879306904109503
h      -1.126144808392133      3.589376990306373      0.208617410670336
h      -2.215740275963913      4.374787191207017      1.389895172401801

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* Geometry 21
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42
Energy = -1276.5209976950
c      4.469310012239586      1.214473490254710      0.271716415460346
h      5.555216467923049      1.324599670766605      0.261305917155952
c      3.633561978295544      2.342649711719328      0.568933207415562
h      4.080895680011992      3.336393864279301      0.633391969552518
c      2.279414856150597      2.181129856681461      0.710122462297911
h      1.661281644009410      3.049446250656872      0.943906741942661
c      1.611961209220715      0.964487341995216      0.315946741381397
c      2.473393834660013      -0.148023832753244      -0.130868386933432
c      3.902407234702911      0.008800592189685      -0.008925139469643
h      4.522990482781032      -0.872931775045146      -0.187340404766989
c      0.218129879593364      0.830916328834254      0.359821071913653
h      -0.349047065418598      0.392559763119403      -0.457581871866277
c      1.980359477314810      -1.364504159549724      -0.526380725696584
h      2.604040313171757      -2.262646791398118      -0.565549676336057
o      -0.501637914337848      1.199805673799424      1.439254430037939
o      0.654191344589638      -1.499075035745138      -0.756877163807339
si      -2.027140068740386      1.914089724880884      1.600452244959098
si      -0.178887203493877      -2.687727336854164      -1.601368255317198
c      -3.399964021206987      1.418156273834287      0.407415585860850
h      -3.822464271487537      0.412276495075904      0.539776624201360
h      -4.214389239519730      2.137833895073514      0.605986465986030
h      -3.118447524255246      1.546804261216004      -0.647198227437402
c      -2.567477384045380      1.529598343531621      3.355600413319033
h      -2.868994111666993      0.475704724076315      3.464453670419596
h      -1.770110869820986      1.727815740277310      4.084396765266470
h      -3.439040268855475      2.145878150921424      3.624899257105296
c      -1.889045928543726      -1.934757578916794      -1.771785605443366
h      -1.828518752300490      -0.985591116329279      -2.326279698307419
h      -2.588235750141604      -2.592216942374016      -2.307441654723633
h      -2.316307591013417      -1.716841698377296      -0.781620117458996
c      -0.139159336865418      -4.240639800010840      -0.554276763337702
h      -0.654249847812449      -5.089899564294264      -1.023526525487609
h      0.905681874796556      -4.536335082114168      -0.371494271695871
h      -0.603733765852652      -4.047412748590488      0.424287123617769
c      0.677587523578529      -2.912566673871231      -3.253869726312582
h      0.194616912724386      -3.687608056548699      -3.865394333675270
h      0.668801193592424      -1.969919243583465      -3.821172022517932
h      1.729287756809801      -3.201533081487801      -3.107541276547412
c      -1.504696902450168      3.655576144535390      1.194206482248038
h      -0.618557493420478      3.897540668528297      1.797847228179727
h      -1.171546986839040      3.601136837792652      0.143362692744962
h      -2.255832844828737      4.444508837025077      1.290442346312862

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 \* Geometry 22  
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42
Energy = -1276.5279906920
  c      4.469512432395419      1.211019339984512      0.276971447542258
  h      5.554318960041450      1.333878086323744      0.264422203181390
  c      3.625104324766810      2.323269787967683      0.618188809978240
  h      4.066134190449628      3.317317917568786      0.720042527420134
  c      2.277156864256223      2.147322661794099      0.767709375155802
  h      1.651594114878563      2.998981101230371      1.044330667444590
  c      1.614027574416093      0.930492195690585      0.355453913522061
  c      2.482280711049834     -0.164339895421511     -0.128651903697321
  c      3.912164710504489      0.008534752444308     -0.028645331726926
  h      4.540883871688927     -0.859642200632856     -0.242862711183641
  c      0.230494231299165      0.783194196530479      0.437489385575713
  h     -0.339726778573891      0.240123410172446     -0.307739673596607
  c      2.001755056711386     -1.373388893495599     -0.556985185493891
  h      2.639278209887999     -2.259066795587402     -0.634197859714259
  o     -0.479491805239627      1.263782319529608      1.482013938788884
  o      0.675795685348232     -1.527749589626300     -0.765360098267125
si     -2.019248081008853      1.951980483020807      1.597832620726886
si     -0.180155069769303     -2.693979742906058     -1.616016654070498
  c     -3.391187474028233      1.361531748998518      0.445920789792539
  h     -3.783029855357866      0.351244475323856      0.629494524024792
  h     -4.223714003487809      2.065107492175131      0.627865917587264
  h     -3.132086235303350      1.452701007896032     -0.618263611098651
  c     -2.541900621342106      1.636726683015237      3.372215995271763
  h     -2.824824992800267      0.581421827195948      3.516133572806635
  h     -1.737679161618640      1.866801211493523      4.084126557134563
  h     -3.419526955415493      2.247185639832543      3.633473505244066
  c     -1.883076227801944     -1.920970986305143     -1.775124737549445
  h     -1.817909806891423     -0.970940276720460     -2.327490031977512
  h     -2.588783922665656     -2.571445466171534     -2.311208260425521
  h     -2.308831521179629     -1.703726056637127     -0.784117083402735
  c     -0.154466654949317     -4.247379908273800     -0.570377452229285
  h     -0.680208905239441     -5.091860274209718     -1.035912033380201
  h      0.888041608205113     -4.551990844578908     -0.390940159063983
  h     -0.613187972991634     -4.047242644022268      0.409554210572605
  c      0.665991039302574     -2.914578495113895     -3.273101867785165
  h      0.174481972272219     -3.679308094968400     -3.890442482669764
  h      0.662952268370151     -1.965919578063863     -3.830137582403731
  h      1.715465394372675     -3.212908726099160     -3.132376341813985
  c     -1.544433075479737      3.680191102627425      1.082597205466501
  h     -0.650578937907059      3.974820158793251      1.650386042859054
  h     -1.232132808802465      3.568958863300841      0.029589881385483
  h     -2.307170119132671      4.461973467828709      1.145829365101741

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 \* Geometry 23  
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42
Energy = -1276.5317408780
  c      4.473631122717938      1.204072891870942      0.286254808392857
  h      5.557266149581184      1.333431673826682      0.259334156032155
  c      3.628054511657135      2.306303311828865      0.657723811937835
  h      4.066283401453440      3.298895669072384      0.777875309600813
  c      2.282683849946859      2.122961632578856      0.819407186255942
  h      1.657700759006889      2.960410823073084      1.130938086681287
  c      1.621156704494508      0.905788209721982      0.403497910679674
  c      2.487704759024019     -0.176336992365568     -0.113997010425835
  c      3.918459480271521      0.002677280760852     -0.030868056858918
  h      4.549646547621703     -0.857425078585789     -0.268722718896332
  c      0.242348860621736      0.758411733574850      0.503088870971304
  h     -0.329365496621938      0.171289047175193     -0.208107933507139
  c      2.010433262176474     -1.378774924260610     -0.563345917255013
  h      2.657732204174066     -2.252465999281178     -0.685247271289721
  o     -0.463742564383071      1.293532454788864      1.524141045430869
  o      0.684944752247659     -1.538978219088511     -0.766927572130346
  si     -2.011056259767174      1.970418408210080      1.596514832545241
  si     -0.182174220575985     -2.691371010476296     -1.625469013358016
  c     -3.387246109341122      1.289465304529132      0.499519102941109
  h     -3.750263182183027      0.279570837595762      0.735958992399581
  h     -4.233160747293760      1.980672433548189      0.667541896518687
  h     -3.152260343053204      1.340268493929016     -0.572952109928118
  c     -2.512542074523215      1.754080228874112      3.391198962099027
  h     -2.778654842946227      0.703379636634297      3.590826274386477
  h     -1.700562199168933      2.027675093910676      4.078365719439434
  h     -3.394184257232840      2.365747093000167      3.633476054868925
  c     -1.879017693922500     -1.903667661285484     -1.780921957972023
  h     -1.807114063423098     -0.952732853722957     -2.330948950893306
  h     -2.589041877814377     -2.548083939786264     -2.318816906639061
  h     -2.304416904611840     -1.685695161675286     -0.789922743757922
  c     -0.170130689152842     -4.249314057654183     -0.586963603685149
  h     -0.707109538726694     -5.086557832862386     -1.052735793889816
  h      0.869904674622324     -4.564968101798334     -0.412282932731479
  h     -0.622591810017880     -4.046539773581708      0.395415924454287
  c      0.656796773810247     -2.908973572604530     -3.286477734402545
  h      0.154212777050331     -3.663718840821510     -3.907263993579482
  h      0.660743683807983     -1.956255106331538     -3.836685845909058
  h      1.703590641772220     -3.219766296093685     -3.153107689983962
  c     -1.579232736303700      3.668250543852014      0.954216704581450
  h     -0.675914973566879      4.019562469530279      1.471659198171198
  h     -1.298232807673448      3.494387859817795     -0.099058537517119
  h     -2.356500753471819      4.438121130185777      0.988454520384064

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 \* Geometry 24  
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      42
Energy = -1276.5348476720
  c      4.478291553946415      1.194266590335930      0.295515257215385
  h      5.561217060687274      1.327360223956661      0.254691859286624
  c      3.634975341163012      2.289542343184639      0.693945764591286
  h      4.074017597305135      3.279871246953742      0.829051455406620
  c      2.294045339866273      2.101405750642965      0.869804461997281
  h      1.669577548573401      2.931233289477578      1.205454263055929
  c      1.628377199775950      0.888265324241385      0.445946013512858
  c      2.490146320818900     -0.187276133032539     -0.094012244868641
  c      3.922223631085026     -0.004374224904620     -0.030593463573869
  h      4.553169477115397     -0.858240855912162     -0.289410516405479
  c      0.253977599609469      0.744430728839937      0.561568311535560
  h     -0.322259009171981      0.124143819524340     -0.121501596811317
  c      2.013791093972647     -1.379661774811116     -0.570232867699482
  h      2.667697819218898     -2.242399094569370     -0.728371888661914
  o     -0.447661116998665      1.322931143821253      1.561869310156948
  o      0.686982583817312     -1.546783873262409     -0.763188068992110
  si     -2.002874267278808      1.985433433036074      1.595567300597773
  si     -0.184641513512293     -2.687372592914336     -1.634042770482376
  c     -3.381179866920684      1.215148961321083      0.562231783211625
  h     -3.712064190374471      0.208408484069884      0.852491208077759
  h     -4.241807307232731      1.891236726191843      0.717506538221367
  h     -3.170527808252684      1.223387813554465     -0.516491120708298
  c     -2.481779752998073      1.875543214966062      3.405313891274668
  h     -2.730647235148113      0.833509610293220      3.664830639350748
  h     -1.662832733610416      2.194462498481083      4.064389176043533
  h     -3.367858858049543      2.488157496402066      3.626628641280961
  c     -1.876547240246892     -1.889623106772770     -1.790022317064775
  h     -1.798639998861177     -0.938579882160913     -2.338959940898631
  h     -2.588269719576366     -2.530290162074156     -2.330266610530736
  h     -2.303708260594539     -1.670861405757123     -0.800036371220136
  c     -0.184252031372612     -4.250458848880692     -0.603185574308846
  h     -0.731324738680319     -5.080094427205163     -1.070892884544240
  h      0.852940633411749     -4.576977729695700     -0.432967677983419
  h     -0.631854124554389     -4.047309493010749      0.381286942599659
  c      0.650846735826107     -2.902495766708716     -3.297300121816233
  h      0.137674351217952     -3.648255456433093     -3.920514704300347
  h      0.661659529224327     -1.946896021343339     -3.842179568475633
  h      1.694513180939317     -3.225327129867698     -3.170569628712420
  c     -1.617608898242821      3.644153064895029      0.828901301690154
  h     -0.706779150862337      4.049271817562009      1.290763250922792
  h     -1.368695017399062      3.410202789477968     -0.221045638735942
  h     -2.410988600322496      4.398825532490854      0.838706441595298

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 \* Geometry 25  
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42
Energy = -1276.5375576710
  c      4.483612438654720      1.182537766420663      0.301846465295648
  h      5.565379946224888      1.316777005484199      0.247808595671892
  c      3.645841472366327      2.273558530973003      0.725262794826120
  h      4.087899562826935      3.260449576328107      0.871259081427685
  c      2.307302167641745      2.084833277049036      0.914066691510325
  h      1.687206772993090      2.907228542319737      1.273644607563495
  c      1.636339845253375      0.875092959247278      0.487353134061606
  c      2.490293301821476     -0.196157380912893     -0.074068480704494
  c      3.923714144355077     -0.013285519593196     -0.026271791588989
  h      4.551709405457289     -0.863996029995034     -0.304284542930264
  c      0.264113591609825      0.735016182558267      0.615421273651535
  h     -0.313593916971372      0.092127460003934     -0.042955757877424
  c      2.011808726832465     -1.378625191346029     -0.571806910977650
  h      2.669524296553845     -2.232675691513464     -0.765435700436547
  o     -0.432556322439152      1.353876296122056      1.596799136994267
  o      0.683627207531484     -1.548048383134425     -0.760342696601204
  si     -1.994896878236661      2.000190055210709      1.596096841080738
  si     -0.187168846608931     -2.682123395059760     -1.642281421137967
  c     -3.373567602263351      1.143190511539912      0.634063684455040
  h     -3.669958963819423      0.142507391195816      0.977057965410123
  h     -4.249020627146650      1.802486670768680      0.778523147621393
  h     -3.187342283835547      1.108036522630692     -0.448530093084485
  c     -2.450438340297945      1.999767342350209      3.414559615384889
  h     -2.682010762892781      0.971243532005105      3.736198085167925
  h     -1.626119182930331      2.365037012484733      4.041695566437841
  h     -3.340854955589484      2.613446497115183      3.612719369145553
  c     -1.875917084254156     -1.879232345962367     -1.803043416233009
  h     -1.792977178405345     -0.928430626641233     -2.351737742966820
  h     -2.587017138767080     -2.518276804680614     -2.346023148372945
  h     -2.306511022461773     -1.659567328670081     -0.814798255734198
  c     -0.196033756724519     -4.250043950807746     -0.618926800320837
  h     -0.750982811885479     -5.073019732785069     -1.089181618557222
  h      0.839136875496030     -4.585794449216668     -0.452450070464665
  h     -0.639856568774771     -4.047889101811995      0.367619490296245
  c      0.647956309730357     -2.895687419479251     -3.306320325200809
  h      0.126051308779563     -3.634135083916242     -3.931312234785482
  h      0.665720782647853     -1.938134702991262     -3.847980430577876
  h      1.689052061630655     -3.229544753535869     -3.184515882398125
  c     -1.658490048069484      3.609421522936859      0.708600633060137
  h     -0.743192865872540      4.065241984168135      1.109336852617649
  h     -1.441701007841349      3.314379515430380     -0.332868427536702
  h     -2.468445422054348      4.346658816096365      0.696963942410944

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* Geometry 26
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42
Energy = -1276.5402954080
  c      4.488875333550832      1.167923720345643      0.308182439778828
  h      5.570087807432700      1.301697257759765      0.240026141003070
  c      3.658844535335609      2.256844546414475      0.753498236129311
  h      4.106038305386061      3.240157365658915      0.909517094729086
  c      2.321644659018516      2.070947204168825      0.952895260141273
  h      1.707846547898140      2.887809041187727      1.333625299516726
  c      1.643536765157583      0.864241294987959      0.526413385736007
  c      2.488333106798245     -0.204351931697008     -0.054738465535974
  c      3.922976013617374     -0.023679862078913     -0.023499824735529
  h      4.546350994141406     -0.871807268300739     -0.319856537734044
  c      0.274017777862036      0.727874279469444      0.668543186674831
  h     -0.306579299472487      0.065097384868940      0.037085021766089
  c      2.005663567071490     -1.375360497019660     -0.574284755909760
  h      2.665739900095882     -2.219531127320221     -0.800572668870790
  o     -0.418122254221490      1.388198347937527      1.627993927626886
  o      0.677313459215165     -1.547014927622166     -0.758390446827372
  si     -1.986863421601290      2.018887384789456      1.596602960393588
  si     -0.189303613554497     -2.677298221757437     -1.651510348175484
  c     -3.362549953191887      1.075929717646312      0.712280637584226
  h     -3.619667664196027      0.084067901987949      1.108598763965182
  h     -4.254612836524736      1.714585384691093      0.847861714152827
  h     -3.201082516114926      0.996302151849045     -0.371956352678911
  c     -2.419943388404257      2.127863334826191      3.417333529567018
  h     -2.633037244060713      1.116785450159840      3.801030683335585
  h     -1.590834473953232      2.538319019381424      4.009049014914750
  h     -3.315124418280460      2.741358374388769      3.592409405232197
  c     -1.876628491317097     -1.873833641779922     -1.819727632773971
  h     -1.790521090367733     -0.923755282036752     -2.369098990390564
  h     -2.584662048026152     -2.513614275271352     -2.365890581904826
  h     -2.312484513011986     -1.653523685269640     -0.834079077138751
  c     -0.205031171937011     -4.249178026178767     -0.634049615099759
  h     -0.765708384918365     -5.066551322995920     -1.107501167891672
  h      0.828071256126351     -4.592520557553844     -0.470514388133705
  h     -0.646683599096639     -4.049135822526507      0.353817781815153
  c      0.648409494463708     -2.889893267157293     -3.314413849526146
  h      0.119686298053179     -3.622598995703493     -3.940792643352361
  h      0.672355401258678     -1.931381625690669     -3.854095712875771
  h      1.686731355794349     -3.233089834105837     -3.195671908649969
  c     -1.703698387194918      3.570993312702604      0.595397127556687
  h     -0.788151496918647      4.074603650976360      0.933304602382574
  h     -1.515497529988729      3.215575192327508     -0.432531171002541
  h     -2.532671063981045      4.286856458229406      0.564254516922399
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 \* Geometry 27  
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                                42
Energy = -1276.5428308270
  c      4.493816047618883      1.151526387873273      0.311909184486723
  h      5.574695910359659      1.282711991837996      0.230526428572210
  c      3.672318181943197      2.239810228820180      0.775359761699071
  h      4.128029667138236      3.218652708345162      0.943936360354923
  c      2.337962776197711      2.058125229181140      0.989326737530052
  h      1.731513319359318      2.873269535861446      1.386419444772214
  c      1.650397166014530      0.855968967407749      0.563186546334449
  c      2.484222733029387      -0.211790467738580      -0.036066374966152
  c      3.919898437916924      -0.035798673018146      -0.020081355452611
  h      4.536985883883864      -0.882006316203099      -0.334687215008448
  c      0.282857195888007      0.727028412412324      0.717949831070285
  h      -0.301162098251535      0.043561363164286      0.112901845550912
  c      1.995629233006621      -1.370749543680408      -0.575499212798352
  h      2.656699438158820      -2.204690098831960      -0.832494746767422
  o      -0.404518205428220      1.425537464018927      1.656067642798853
  o      0.667380403700444      -1.542550953488345      -0.758388692625641
  si     -1.979941104861467      2.037269667186075      1.596962292291822
  si     -0.191259666848480      -2.673458290298121      -1.661098438364184
  c      -3.348929929660021      1.012477767626577      0.797046762014686
  h      -3.562007130650381      0.033269165487791      1.247294390863879
  h      -4.258158969490133      1.627850600557319      0.925968513101029
  h      -3.212157401107943      0.885619805729393      -0.286224609850521
  c      -2.390400525472860      2.258152669846291      3.412588694028889
  h      -2.584272420073117      1.269268877823105      3.859148306336245
  h      -1.557404158161317      2.712588032219296      3.965375519916271
  h      -3.290585482064985      2.870342397846189      3.564494022483232
  c      -1.878945867750448      -1.874085096646795      -1.840078424985503
  h      -1.791392116559451      -0.924862755470699      -2.390632750536517
  h      -2.581577263539951      -2.516970966421499      -2.389584440005672
  h      -2.321589922811622      -1.653199944319408      -0.857580093670901
  c      -0.211223079628940      -4.248766384658721      -0.648751721364284
  h      -0.775408980821682      -5.061779809721934      -1.125762010571657
  h      0.820153969118841      -4.597445422648447      -0.486918502228222
  h      -0.652305054480361      -4.051642205078042      0.339846981382763
  c      0.652016365522234      -2.885479461465093      -3.321462480158658
  h      0.118674045564214      -3.613998340072503      -3.949121240831195
  h      0.681291746368790      -1.926849009013472      -3.860430353308062
  h      1.687752675936659      -3.236041933310654      -3.203970926664669
  c      -1.753183899183306      3.527564704569582      0.490421089958441
  h      -0.843010924405518      4.077071318860450      0.765409943500438
  h      -1.590411514118188      3.114918521867936      -0.520077689588197
  h      -2.602799695418954      4.218825163623871      0.442595990486453

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* Geometry 28
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42
Energy = -1276.5451102600
c      4.498878906014647      1.133435320837721      0.313458839265872
h      5.579095361707861      1.259982156411569      0.219860995864989
c      3.687767385027758      2.223369736167607      0.792387096332667
h      4.152842951228035      3.196914859499143      0.969927711359484
c      2.356593430952792      2.047672765145431      1.020863707787482
h      1.757766665573426      2.864069081428690      1.431429314870163
c      1.656687826464663      0.851602696468674      0.595484284549119
c      2.477892471116478     -0.218243334914311     -0.018161490421684
c      3.914909230491146     -0.049142134718228     -0.017204345743916
h      4.523785286524497     -0.895526176886954     -0.346183273561898
c      0.291219905329180      0.731360249566440      0.763271195658653
h     -0.297310405634129      0.026708310052138      0.185616428085888
c      1.981737590962971     -1.365405736874511     -0.575090368927741
h      2.643462233652988     -2.189511793218816     -0.860026957941371
o     -0.390113198816021      1.468370858551183      1.677917378084676
o      0.653020428423425     -1.535723903422625     -0.757740171061821
si     -1.973634398375359      2.055992714700097      1.598035609158771
si     -0.193313865512254     -2.670111085891166     -1.670329311412547
c     -3.332825631553011      0.954089627171323      0.889604998192081
h     -3.499707889019580     -0.007772992707635      1.393323850356702
h     -4.258134342495231      1.545860370294080      1.013304952767202
h     -3.220211435042771      0.777288378024357     -0.189662693141622
c     -2.361889635274588      2.388818970826202      3.401174646209729
h     -2.536149137147321      1.427020405980164      3.910671505288863
h     -1.526165393660136      2.885933689643047      3.911971175180940
h     -3.266823568032338      2.999318564388514      3.529100769253059
c     -1.882705867601681     -1.879187364016181     -1.863851971520359
h     -1.795474273871159     -0.931072608062567     -2.416253409309581
h     -2.577634415809805     -2.527713825724657     -2.416660982089002
h     -2.333744896963117     -1.658126079629975     -0.885175790876237
c     -0.214445612676803     -4.248583253803341     -0.662813345633889
h     -0.779733271725978     -5.058726487077748     -1.143656015861569
h      0.816054604120498     -4.599561936052265     -0.501546903353767
h     -0.656422819727232     -4.054780342439330      0.325966092867821
c      0.658689573428241     -2.881594235478189     -3.327279123758371
h      0.123032719383612     -3.607916860282339     -3.955963246344637
h      0.692448974984856     -1.923760688480008     -3.867089138743911
h      1.692218511464840     -3.237589023970080     -3.209153797567692
c     -1.806436168753033      3.478238953618741      0.393834517129165
h     -0.905733152296257      4.069777975405074      0.606026840974022
h     -1.664129225670260      3.010960439117555     -0.595645048679402
h     -2.676935889563975      4.142613916766487      0.332234998615054
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 \* Geometry 29  
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42
Energy = -1276.5472136680
  c      4.503507715823185      1.113230961239038      0.315348742034041
  h      5.583360718722246      1.232806707806131      0.207284649655101
  c      3.706712018422294      2.207448483666181      0.808522878655036
  h      4.180024640043870      3.174846208105917      0.985376765245866
  c      2.373421284726489      2.043880875005164      1.041148207410367
  h      1.786624709659119      2.857536774837492      1.468085610055512
  c      1.662371180360601      0.850952611075436      0.624544169570126
  c      2.469268107342231     -0.222991229779906     -0.001131264739347
  c      3.908104979525701     -0.064465945118715     -0.013826039258372
  h      4.507614301183352     -0.913167498766489     -0.353748999913419
  c      0.299260170124412      0.742979273153307      0.803792275320660
  h     -0.293633971971627      0.014873268804336      0.256566289440890
  c      1.964175483339198     -1.359503792740695     -0.572597600303456
  h      2.625141293594985     -2.176340029555838     -0.881495016886259
  o     -0.375513696574557      1.514880127210261      1.692637764836991
  o      0.633694439007946     -1.526227720710498     -0.757077959851195
  si     -1.968488971549906      2.076447163946589      1.600110379759843
  si     -0.195102179075208     -2.667235492129564     -1.681010830667446
  c     -3.313719544483026      0.902616144098021      0.988679443470278
  h     -3.434479182227372     -0.036631111946756      1.545028166054825
  h     -4.253658259223572      1.471424191149413      1.108536688185571
  h     -3.223720378396361      0.674811009557682     -0.082996226466397
  c     -2.333965816755804      2.520285141931919      3.383643660589745
  h     -2.489001410664377      1.590625531476819      3.954769668929744
  h     -1.496919497598636      3.057489333732541      3.849522285215126
  h     -3.244385769960099      3.127295899874100      3.487015501914684
  c     -1.888028200158838     -1.889173789909164     -1.890359182893111
  h     -1.802961400168465     -0.942824748555772     -2.445872305053020
  h     -2.572395359909673     -2.545564053493858     -2.447098984833244
  h     -2.348948541427460     -1.668594484866310     -0.916340927113773
  c     -0.214367312785558     -4.247602431354388     -0.675881788934230
  h     -0.777716212220833     -5.056672060774041     -1.161142529173201
  h      0.815932322511357     -4.599073905291043     -0.514270200932993
  h     -0.658747157290917     -4.058620266348981      0.312649323453564
  c      0.668219627757112     -2.878432036300962     -3.332170983564675
  h      0.132593367918274     -3.604777448557503     -3.961248065576752
  h      0.705633857039725     -1.921918011458516     -3.874039514784589
  h      1.700290408064771     -3.2377044440877097     -3.211010746105323
  c     -1.862419014769931      3.425329744653647      0.305590267598635
  h     -0.974882966660790      4.054324359445832      0.455162787107087
  h     -1.737337179364866      2.905747384170578     -0.659534192524029
  h     -2.754358750539155      4.060221881517202      0.231612306483652

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 \* Geometry 30  
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42
Energy = -1276.5492591940
  c      4.507318385970312      1.091655620880929      0.315209882203091
  h      5.586884444044272      1.202359908606460      0.197329939474091
  c      3.723653832700785      2.191484509016636      0.817400122070544
  h      4.209566792687633      3.152093274471321      1.001820445174865
  c      2.391394759717405      2.040272798850148      1.058036065760558
  h      1.815172882490648      2.857714255804044      1.493543221183259
  c      1.666548089320274      0.852632558456147      0.648638233655706
  c      2.458391309103165     -0.227113513690074      0.013247261199694
  c      3.898709311612673     -0.079529535288004     -0.013063597996930
  h      4.487636866802505     -0.930994168663491     -0.363639785317074
  c      0.305764076695494      0.755951934513009      0.840874472700685
  h     -0.292656741428946      0.008386151697326      0.324845020301899
  c      1.943713667954004     -1.352811100966978     -0.570530061633595
  h      2.603853864489057     -2.161590008024609     -0.902146420715113
  o     -0.361509699022153      1.564332676770805      1.704207638858706
  o      0.613350277835932     -1.516229629491469     -0.757835581661677
  si     -1.963732695915691      2.098192391415095      1.602681206739146
  si     -0.196667712308071     -2.666353975335555     -1.690395832558956
  c     -3.290649983558040      0.857477728627694      1.093651342761439
  h     -3.364223372751306     -0.053673012079950      1.702313367888038
  h     -4.244772759517502      1.402574371545883      1.209629023104798
  h     -3.220835480330965      0.575612031057984      0.033377994211319
  c     -2.308104589994429      2.651550667795140      3.359757111594257
  h     -2.443399644776575      1.758548925250294      3.991075736124709
  h     -1.471253632365482      3.227565791867984      3.777408786695287
  h     -3.224132271584823      3.253899329406064      3.438204718848302
  c     -1.894240449321341     -1.905285910475755     -1.918919542906805
  h     -1.813148613548932     -0.960457279030747     -2.477490704841838
  h     -2.566297442499144     -2.571243084952370     -2.479392424797783
  h     -2.366366193491654     -1.685709947650522     -0.950035181689870
  c     -0.211644946548137     -4.248713349843943     -0.688261118379385
  h     -0.770779345994668     -5.058063634978914     -1.178181347141565
  h      0.819127714990753     -4.597609469661202     -0.524699177529394
  h     -0.660174708421597     -4.064815998900232      0.299277432034576
  c      0.680297118483756     -2.876572965279498     -3.335562328412661
  h      0.147311939941564     -3.604526089014898     -3.965470699628161
  h      0.719922032929007     -1.922072830780037     -3.880573180070408
  h      1.711385043505697     -3.236784542747865     -3.210049348452384
  c     -1.921526659545733      3.370053476016504      0.227174691767861
  h     -1.050872003204310      4.033518115042034      0.315613060538594
  h     -1.808581548361987      2.802349267525490     -0.711886624864407
  h     -2.834165097671289      3.974491469378144      0.144378919732748

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* Geometry 31
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42
Energy = -1276.5508274730
  c      4.510152946380793      1.068647644421983      0.311293898158599
  h      5.589723046970520      1.169479562092573      0.186061059595077
  c      3.741216517167995      2.175995501234703      0.820597088772740
  h      4.238853278397811      3.130478117615782      1.006227728781353
  c      2.409179887433167      2.039004005574645      1.069097059785485
  h      1.843837024839001      2.862853320567926      1.508712123273499
  c      1.669792427500150      0.856213841065891      0.669147934487023
  c      2.446498514744149     -0.231203507539557      0.027886612630463
  c      3.887916018729552     -0.095923041333391     -0.010061447888958
  h      4.465682113957652     -0.951845912299654     -0.368515978325449
  c      0.310713684413927      0.770070745929497      0.874970045264166
  h     -0.293145086319032      0.008112345006353      0.387823166667040
  c      1.922536026300876     -1.343982878134878     -0.571624275891502
  h      2.578823671819622     -2.149449841744981     -0.915009003564966
  o     -0.348420393162694      1.614379557763179      1.713421271534647
  o      0.591224273234806     -1.504559478250653     -0.758578142715716
  si     -1.959491455054157      2.121712711637032      1.606399758694529
  si     -0.197401121600678     -2.665343233997818     -1.699680700640172
  c     -3.265172271934351      0.820728175664443      1.204319168662425
  h     -3.292808487053199     -0.057135391438206      1.863654666498896
  h     -4.232237705162022      1.342631206402811      1.317367563253715
  h     -3.214181351602792      0.482242056017806      0.159529878276981
  c     -2.283909290145434      2.781321279094712      3.330301763010427
  h     -2.399192620063228      1.929709895301325      4.019926296774854
  h     -1.448961651876814      3.393613373204219      3.697192193131705
  h     -3.206085933392415      3.377197973178584      3.382770154017847
  c     -1.901018637331243     -1.925851334437443     -1.948515631350777
  h     -1.825893480637963     -0.982922000610390     -2.510972484458499
  h     -2.558749045947950     -2.602957858534969     -2.512679954236679
  h     -2.385755136976958     -1.708156601263179     -0.985517594408592
  c     -0.205659740507352     -4.249740994371791     -0.699408173912576
  h     -0.758019144142846     -5.060804304094847     -1.194355813316192
  h      0.826241788197885     -4.593929106527671     -0.532913080587973
  h     -0.659875780909319     -4.072131398647669      0.286558791130688
  c      0.694384585659931     -2.875340152782120     -3.337522875748926
  h      0.166263605990069     -3.606876521266778     -3.967724185434548
  h      0.734894079026418     -1.923408683360622     -3.886808634782281
  h      1.725267821797150     -3.234006057477442     -3.206006554039057
  c     -1.980884759498622      3.309837272807642      0.157803381812301
  h     -1.130145280637895      4.003896169802828      0.183657549465545
  h     -1.877103905275878      2.695409138448510     -0.752194111271044
  h     -2.913634139959388      3.882718583486253      0.069653465363805

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* Geometry 32
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42
Energy = -1276.5523372510
c      4.511816277954063      1.045873949980885      0.310058377095863
h      5.591316051630672      1.134144762712132      0.176878162614879
c      3.757325434055605      2.162607402374647      0.820002874454734
h      4.268050207738117      3.109638818601313      1.007392907862821
c      2.424589737865724      2.042276838594270      1.070880526009223
h      1.871158556666669      2.871803409593915      1.513587353827515
c      1.671356967560470      0.863477405384201      0.684066078681531
c      2.432058147210855      -0.232342676935840      0.038200078194064
c      3.875136233387201      -0.111732064159363      -0.008455905059710
h      4.441279985352323      -0.973312236664650      -0.372661858468221
c      0.315209581388591      0.791331436709917      0.903164598282775
h      -0.293612731069012      0.008247918721238      0.449652975551225
c      1.898166268963310      -1.337791507498663      -0.566490120011584
h      2.553444933183727      -2.138383882365441      -0.926957407750888
o      -0.335648382787957      1.662512659512136      1.717372617848074
o      0.565646954929813      -1.494523641539216      -0.758743915240626
si      -1.954525464890764      2.145039835027606      1.610453035107244
si      -0.198534803931734      -2.667531004352209      -1.709125052643937
c      -3.236728521132073      0.793040452908869      1.318244914379028
h      -3.217729985361490      -0.045162855221653      2.027847707668605
h      -4.216441162341976      1.290811270833554      1.428871200435854
h      -3.202125656099509      0.394706896642688      0.293981306038740
c      -2.261347089247038      2.910122682075173      3.293288435369241
h      -2.356048796902056      2.104999804341739      4.039204239985184
h      -1.430554043306348      3.556698249977031      3.606429399912226
h      -3.190920356399791      3.496388226667400      3.319815909434377
c      -1.908463627467020      -1.951115179420579      -1.978563991780417
h      -1.840214052013272      -1.010022456724765      -2.544920826351053
h      -2.550180701068475      -2.640397486666645      -2.546515350632868
h      -2.406146989797629      -1.736072582552692      -1.021602705952670
c      -0.197671681985208      -4.252428290163460      -0.709478031827944
h      -0.740776825232256      -5.066630879557772      -1.209737680444772
h      0.836103889496488      -4.589485495829873      -0.538676850342220
h      -0.658589511217570      -4.081418898305194      0.274561038900366
c      0.709909522616611      -2.874834128954053      -3.338813269362932
h      0.188880292330822      -3.611515071102305      -3.969328783267467
h      0.750068095143477      -1.925393286819241      -3.892589832928037
h      1.741352042669736      -3.229783299353538      -3.199913242835009
c      -2.038311813439124      3.248241307738758      0.097085588197703
h      -1.211026526469985      3.969475026703318      0.060928042417540
h      -1.942068728610177      2.589882778522081      -0.782138809939234
h      -2.990986434857289      3.787510893190027      0.005517595914267

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* Geometry 33
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42
Energy = -1276.5534049100
c      4.512725189959647      1.022502363449595      0.305490327746573
h      5.592610118562874      1.098329664272981      0.166297340276029
c      3.772355421238560      2.150463598137519      0.813042108255260
h      4.295627442326436      3.091739254033238      0.996491478307876
c      2.438576383270751      2.047121166957691      1.068183449294358
h      1.897143878540124      2.884221126625484      1.510925669258834
c      1.671629888705105      0.872301496631341      0.695759362982338
c      2.416616814918799      -0.233669540064091      0.047993904532192
c      3.861345372009423      -0.129832664906567      -0.004661798814773
h      4.415899250267477      -0.997984119260179      -0.370692775461060
c      0.317750222826299      0.810952843940327      0.927362512474063
h      -0.296661182764642      0.017638718321928      0.501998945792602
c      1.872591369824155      -1.332194065437979      -0.560301228564946
h      2.527162139557503      -2.129406701220389      -0.930067070493949
o      -0.324599799291797      1.710330977327339      1.718875376428481
o      0.540895692492559      -1.483588693151849      -0.760676473774935
si     -1.951536548100248      2.167038189687724      1.615289065268545
si     -0.198980620448053      -2.669164099177281      -1.717033795959446
c      -3.208682488138815      0.773152577530501      1.436407429174910
h      -3.144925107642626      -0.019898297460039      2.193747238213794
h      -4.199413694113840      1.248749827512295      1.544269545247408
h      -3.187750289584041      0.313970585053366      0.437549323932605
c      -2.241933059889661      3.035125589765745      3.250671108919569
h      -2.314981309657207      2.280680290092899      4.049973390370816
h      -1.416497585871284      3.712896231686457      3.507222107849138
h      -3.179086174193652      3.610135382398254      3.252008779456509
c      -1.915348388112530      -1.978478924577438      -2.008306013825067
h      -1.855421261778476      -1.039393899802472      -2.578638274685797
h      -2.539624405035152      -2.680955031034685      -2.579640742895418
h      -2.426767792000194      -1.766702711732313      -1.057973868729163
c      -0.187079150777114      -4.254512246929822      -0.718333872396867
h      -0.719589460008828      -5.072512941125298      -1.224011695499787
h      0.848627707898028      -4.582542182180512      -0.542658239913386
h      -0.655392561370491      -4.090884709300375      0.263265803641028
c      0.726098353821516      -2.874301042768404      -3.338785672246147
h      0.213579551819721      -3.617442362061938      -3.969065939694853
h      0.764743470061635      -1.928344777566554      -3.898248422990514
h      1.758237727201755      -3.223566242096620      -3.192069059654757
c      -2.096361051572789      3.179630654844170      0.043436243739340
h      -1.292848353985674      3.921739988322437      -0.054460103318676
h      -2.005294883688795      2.478279283692620      -0.802250509865669
h      -3.066561350319695      3.687092865145990      -0.049229422764853

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*****
* Geometry 34
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42
Energy = -1276.5543440730
c      4.511530808036656      1.000277681454254      0.301609831349953
h      5.591486465355815      1.062483548656886      0.158309717546113
c      3.785720458579626      2.139341353128386      0.804105400880847
h      4.320034521093789      3.074299219262752      0.982512715500634
c      2.450833599030697      2.054117662842003      1.059296630297907
h      1.920316972508500      2.898993249649635      1.498888334969178
c      1.670949783232952      0.882627233229977      0.702795954131186
c      2.400901537968192     -0.234004171214639      0.057163984137606
c      3.846804853133461     -0.145673212832623     -0.000564500244561
h      4.390047796992617     -1.021159572199158     -0.366685214343007
c      0.319488695111671      0.831215685296493      0.948351429901264
h     -0.299347079387411      0.026790040066367      0.551804198494124
c      1.848145105090053     -1.326160902954612     -0.555379706060448
h      2.500572886113509     -2.123348180605671     -0.930868563800111
o     -0.314690536563806      1.757430546769092      1.715832431574024
o      0.514682950534419     -1.474231686733444     -0.761401704053161
si     -1.949933041997111      2.188608630915118      1.620422703139650
si     -0.199552602001977     -2.672747340103009     -1.725460821352096
c     -3.177178908666112      0.759151559602442      1.558616608662627
h     -3.069883252141432      0.017639735758567      2.361681975911756
h     -4.178499097931668      1.212458857572290      1.662626645713976
h     -3.166097033712284      0.238925253310971      0.589992728778652
c     -2.224120743393966      3.156742627028663      3.201686346295790
h     -2.274048159772013      2.457433266867931      4.050917532149117
h     -1.405993595972310      3.862546185634483      3.398885867579576
h     -3.169925748742306      3.717232991812895      3.178825084261822
c     -1.922402934520233     -2.008274340557592     -2.036516629665856
h     -1.871128636812357     -1.071081086254347     -2.610737554104071
h     -2.528964484867884     -2.723464861104978     -2.611241537890602
h     -2.447026433373898     -1.800630423291693     -1.092510712500650
c     -0.175760039151306     -4.257872910372194     -0.726095068075128
h     -0.696084357659050     -5.080447487750339     -1.237254239501617
h      0.862257346248040     -4.576046520471100     -0.544875317104676
h     -0.652427375903291     -4.101867658538549      0.252728662589016
c      0.742318937909859     -2.874268454896007     -3.338386356044112
h      0.239565036980452     -3.624699506744429     -3.968220459592593
h      0.778308640207526     -1.931297223238384     -3.903164249211540
h      1.775819121086493     -3.216355411006186     -3.183046133686720
c     -2.154109950346789      3.107917290715325     -0.001830457303393
h     -1.375031812580367      3.865828554331373     -0.157970449130019
h     -2.065512187087896      2.367420214048856     -0.813486675368745
h     -3.140082128152545      3.584538341412261     -0.094289309926335

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*****
* Geometry 35
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42
Energy = -1276.5550542030
c      4.509693422736547      0.977771444112603      0.296019284393092
h      5.590217210504866      1.027230375275484      0.151360826497931
c      3.796978099805169      2.128976395955232      0.790855736777444
h      4.342637133937096      3.058857219053584      0.963763194564087
c      2.461302415906745      2.060935782098646      1.048032335226002
h      1.940521313814137      2.916079503803714      1.480705058879731
c      1.669124193320623      0.892168803404306      0.707856007160135
c      2.385066763852841     -0.235581285290763      0.065295074491692
c      3.831623614119106     -0.162027720648297      0.002456305861982
h      4.364176325258506     -1.044594026619688     -0.361146690866939
c      0.319592481324138      0.852097553940859      0.965652234924999
h     -0.304170153925798      0.038114537090215      0.597404278258833
c      1.824627374289045     -1.319941899609181     -0.553110955068621
h      2.474090559856788     -2.117875115693665     -0.928210853389252
o     -0.305948718580496      1.804619212325207      1.711524493477697
o      0.491929247870440     -1.465411535105202     -0.763701193197317
si     -1.948893506090677      2.210680319307219      1.625792791016783
si     -0.199475004789339     -2.676055998238804     -1.732239886739171
c     -3.143199461349718      0.754254578941634      1.682847083176787
h     -2.994834510853250      0.068500615267828      2.527813651901785
h     -4.154260086910385      1.185697316376997      1.782855181866661
h     -3.138198782220210      0.173755087111980      0.749080682366781
c     -2.208071098995071      3.275393591373285      3.146336108801427
h     -2.233457361594394      2.634930811716145      4.041494899982943
h     -1.399189428259612      4.006298899568698      3.281224633648716
h     -3.162982818833951      3.819285618483313      3.100727148448623
c     -1.928700234168838     -2.039463811235787     -2.062977824946242
h     -1.887084220750711     -1.104067905400696     -2.640749387047418
h     -2.517214229238058     -2.767031750481920     -2.641007104343082
h     -2.466675752347484     -1.836741200476500     -1.125499124936615
c     -0.163407783219602     -4.261673005425266     -0.733078539203636
h     -0.670700608557942     -5.088901042838760     -1.249905315096939
h      0.876677573823033     -4.568806120476594     -0.545340317149308
h     -0.648701109817720     -4.113769920956025      0.242633849277289
c      0.758249027249459     -2.874596856808853     -3.336985675048074
h      0.266344899741084     -3.632754562592310     -3.966390665761908
h      0.790573234993002     -1.935041184282855     -3.907377959961450
h      1.793220885672443     -3.207774493708048     -3.173131802124829
c     -2.210411841029520      3.032485341132908     -0.039932634762203
h     -1.456489861908581      3.801923516208313     -0.253303042882627
h     -2.121599655284053      2.254826227663188     -0.815910815317469
h     -3.210531770807272      3.479608909270427     -0.131138637561820
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*****
* Geometry 36
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42
Energy = -1276.5555896910
c      4.507217693489290      0.956866988335197      0.292109829255036
h      5.587949865921527      0.992682352862017      0.145552535645758
c      3.806698096804544      2.120477731108626      0.774442895641588
h      4.362821112322602      3.045317496900241      0.939944963507614
c      2.470032207673569      2.070372058863774      1.029849093858403
h      1.958821045840344      2.934681199208130      1.455147474647121
c      1.666411897044235      0.903948883333017      0.708336138429319
c      2.368744251313326     -0.234687502554948      0.070182911278817
c      3.816545545643501     -0.177500307478138      0.007850829834587
h      4.338705080877047     -1.067954958158240     -0.352227983600683
c      0.319730569331133      0.874651482947151      0.978967153131443
h     -0.309213762989390      0.051724215875746      0.638736381791158
c      1.800243052248657     -1.316319012734918     -0.546144309565589
h      2.449394474787544     -2.114822277612131     -0.922197968541563
o     -0.297640580337044      1.848791287893314      1.703545608737024
o      0.467888878894332     -1.458519478216927     -0.765340707758617
si     -1.947296879424245      2.231548387809060      1.630981212562002
si     -0.199236524457987     -2.680865225341217     -1.739160237783676
c     -3.107952276785544      0.758371265331597      1.808061830696659
h     -2.920575281870626      0.131943199158861      2.690742561898093
h     -4.127848600230602      1.168414525598828      1.904566899985847
h     -3.106865489050571      0.118106271832022      0.913901585051244
c     -2.194302193733987      3.389312694375853      3.084229071850747
h     -2.194286925503452      2.811154864017296      4.021120801068263
h     -1.396030988250356      4.140958542639877      3.154639957435237
h     -3.158610616828523      3.914591252971786      3.018795660027977
c     -1.934361288375311     -2.070950883144740     -2.087482223092285
h     -1.902469856155221     -1.137186754673880     -2.668381305036374
h     -2.504940275431448     -2.810226052159454     -2.668801299048955
h     -2.484768426406568     -1.874512469606157     -1.156021810277564
c     -0.150132354506396     -4.265486600261431     -0.738895089975840
h     -0.643511159561007     -5.097818320017844     -1.261213035185881
h      0.892034780294342     -4.561152280183815     -0.544711365030044
h     -0.644497262154605     -4.125792943146839      0.233320290961250
c      0.773713398232343     -2.874839548407272     -3.335710902449565
h      0.293320754767926     -3.641457451287598     -3.964020112907124
h      0.801566926618124     -1.938726608587924     -3.911748756644145
h      1.810344450345615     -3.198220821554806     -3.163272244957546
c     -2.265287268822561      2.952538985076161     -0.071570464018843
h     -1.536969423585117      3.728789741519159     -0.342417476126220
h     -2.175541794729893      2.138380698630258     -0.808838233147330
h     -3.278324952445074      3.370775931412740     -0.160741899533291
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 \* Geometry 37  
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42
Energy = -1276.5560565270
  c      4.503351361275432      0.938266015040771      0.287930338103388
  h      5.584627971727260      0.961194736078541      0.143701904035627
  c      3.813506456861042      2.114250017330887      0.755742175536657
  h      4.379620273831622      3.034307413178563      0.914999473750481
  c      2.476154849532884      2.080576070485288      1.008031259223568
  h      1.972608285191183      2.955058381669087      1.420961619892506
  c      1.662210895843260      0.916332658039277      0.704397784411240
  c      2.352739261984034     -0.234616120879106      0.075389288943048
  c      3.801446906179149     -0.191696414927802      0.012899274753578
  h      4.315001005083562     -1.090022096707663     -0.341130846387546
  c      0.318971080643136      0.895955892302861      0.989453968706712
  h     -0.312583224626794      0.063831681941372      0.678410329688756
  c      1.777948662843231     -1.313330833341047     -0.540877075277175
  h      2.425887290419348     -2.114484673709918     -0.914496847772436
  o     -0.290472885277852      1.890493930838294      1.691648488228685
  o      0.445014384370690     -1.452819544083706     -0.767290157061154
  si     -1.946221566046776      2.250643257755448      1.634783896339695
  si     -0.199443432777039     -2.686611905489224     -1.744695797660748
  c     -3.068939061563543      0.768385336917900      1.933423536674636
  h     -2.841754013523135      0.207836547420783      2.850405374131352
  h     -4.097378228328767      1.156096044942885      2.028332451652460
  h     -3.069732953419921      0.068305570393095      1.085205910495583
  c     -2.182524904969295      3.496533073289075      3.014871141044384
  h     -2.155115251705629      2.985226955104012      3.989119505019222
  h     -1.397545960501373      4.265178279008504      3.016918594264293
  h     -3.156935721370818      4.000769494748998      2.932491643781053
  c     -1.939890228615366     -2.102701935937538     -2.108565785732792
  h     -1.917557315686613     -1.169856875850251     -2.691279615491112
  h     -2.493520987616413     -2.852244130512011     -2.693173862148799
  h     -2.501206352415094     -1.913257093892082     -1.182318485501794
  c     -0.137363572033904     -4.270640067316526     -0.743677753817954
  h     -0.616263671961099     -5.108116849700369     -1.271456195323502
  h      0.906936080324360     -4.554439658049041     -0.542221946173356
  h     -0.641096597847707     -4.139292849058982      0.224854764514686
  c      0.787783276304468     -2.875151458312844     -3.333722787977702
  h      0.319809572577694     -3.650178645664538     -3.961360455371111
  h      0.810193761625957     -1.941934305969539     -3.914840904328035
  h      1.826649927134324     -3.187543781446304     -3.152918786471270
  c     -2.318175270757530      2.869479552495195     -0.096845465962134
  h     -1.616646484074156      3.648819350743716     -0.423673524195827
  h     -2.225826123636440      2.021886026530040     -0.794373434808536
  h     -3.342854996155765      3.259702559944122     -0.182187692232477

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* Geometry 38
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42
Energy = -1276.5563086480
c      4.499265936671349      0.920808575344117      0.283445399770944
h      5.580873732321065      0.932216965709955      0.140356199980250
c      3.819313788265550      2.109368712036999      0.733303092432781
h      4.392517217575991      3.026408525651709      0.880225519238895
c      2.480401864200690      2.091715803567205      0.981560429204666
h      1.983625721440989      2.976191952116956      1.381565070385081
c      1.658845944527945      0.926967160087637      0.700898808864836
c      2.338334305616793      -0.234207301071128      0.079027034285953
c      3.787681810808632      -0.205192311322125      0.018660310155181
h      4.293071619406378      -1.111360184083364      -0.325271249124510
c      0.318064071590035      0.916808121954033      0.996736892210576
h      -0.317574433347640      0.077396071710034      0.712254214615422
c      1.757587895608714      -1.311704186559103      -0.533394815439059
h      2.404743917573279      -2.116120188612471      -0.901211741137395
o      -0.284232332679067      1.931069366890324      1.679207077725614
o      0.426567572793019      -1.448138664127644      -0.769507975765300
si     -1.946113832230647      2.268010732510975      1.638792126947489
si     -0.198828767125165      -2.692141471931882      -1.748757455911125
c      -3.028874115490573      0.785962936104777      2.058013649243050
h      -2.763617347371193      0.295281136505138      3.004706066319881
h      -4.064849180294713      1.152411424079015      2.153269540303218
h      -3.029435213220496      0.029153729962428      1.259795007616810
c      -2.173699838827988      3.597783592569421      2.939735538479566
h      -2.115672632282183      3.156726362961927      3.946427263660595
h      -1.404117358219542      4.379071353657569      2.869754413492804
h      -3.158980702896519      4.078362273680325      2.844412767448842
c      -1.944480803055584      -2.132918625606061      -2.125079636960212
h      -1.932146085146211      -1.200400651193170      -2.708582534809572
h      -2.482535705911451      -2.891158853168985      -2.713119812296067
h      -2.515295111520570      -1.951176598039895      -1.203054602971554
c      -0.124042670116435      -4.275750563860323      -0.747077168924076
h      -0.588964713112244      -5.117866264725728      -1.280099361018967
h      0.921799894231156      -4.547967113162034      -0.538648196336638
h      -0.636522547749984      -4.152633073950098      0.217845491947201
c      0.800101500188719      -2.875824259998744      -3.331343126861342
h      0.344000141522025      -3.659093796306823      -3.957614838572034
h      0.816067407229816      -1.945799327111012      -3.917459651374347
h      1.840949375680245      -3.176467709278904      -3.143370236217426
c      -2.369096156253136      2.781112779332068      -0.115854414212811
h      -1.693692722997754      3.558468652704270      -0.498776372028551
h      -2.273172764708721      1.900937153519058      -0.771261532460846
h      -3.404293292777020      3.143876303702804      -0.196121306721599

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* Geometry 39
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42
Energy = -1276.5566082130
c      4.494399551146656      0.908024532260418      0.278921068795677
h      5.577037132374873      0.909025761183268      0.142223955228609
c      3.821003556313504      2.108458159671514      0.707735299637760
h      4.401186558235683      3.023049334197753      0.845565125056460
c      2.481087598793185      2.104207525598733      0.949534290426521
h      1.988379135861409      2.998783627132575      1.331213856635365
c      1.653566457073396      0.938636875800518      0.689572168525937
c      2.325639155404823     -0.234504644859664      0.082147502365631
c      3.775454726510734     -0.216035922198556      0.025840641857119
h      4.275741864368299     -1.129401215094181     -0.307299128890585
c      0.316895736390870      0.934813410665510      1.001426354374532
h     -0.319953876237443      0.086944335336293      0.747474167638983
c      1.740985816584318     -1.312059014146568     -0.526383728864850
h      2.387047986504210     -2.120833315383046     -0.887263330154303
o     -0.278954656679408      1.967760907198654      1.660376185449199
o      0.410162276564571     -1.447531586635378     -0.768287898255760
si     -1.945447499046677      2.284407742679718      1.640097899498767
si     -0.198643914878971     -2.699597286273025     -1.749471469084048
c     -2.985861429025388      0.811670283162030      2.180381215221407
h     -2.683754719871491      0.395559765947557      3.151361623105129
h     -4.029270517974274      1.155498750796609      2.276219897496728
h     -2.981664367440134      0.001126493370410      1.437134226752184
c     -2.165265230948659      3.693160710913119      2.856515786002228
h     -2.072233939296356      3.326195304373167      3.889709514726625
h     -1.415726423213392      4.483139469674895      2.710260026240651
h     -3.163012786401819      4.146286898184581      2.754108457634202
c     -1.948936289114676     -2.161502951653945     -2.134171120229464
h     -1.945969243905196     -1.228494097575373     -2.716838062051937
h     -2.473668863059147     -2.926422282192950     -2.725681186685603
h     -2.526901541484101     -1.988877215741046     -1.214987627702743
c     -0.112018616074064     -4.282987335706219     -0.748091608384466
h     -0.563904674423798     -5.129158640852546     -1.286102359271579
h      0.935345554354707     -4.544850068318279     -0.533472772856404
h     -0.632547285001340     -4.168010710120068      0.213452477019507
c      0.808941559325054     -2.876541099263654     -3.327672780619866
h      0.364220212451542     -3.667158310512185     -3.953040914288623
h      0.817724583317548     -1.948622400012448     -3.917313531094858
h      1.852254059681539     -3.165775349135827     -3.134405369782757
c     -2.418950966421347      2.690973214053078     -0.129699505695356
h     -1.770822903172151      3.462943684162506     -0.566808893366291
h     -2.318132524122242      1.781832495283426     -0.743035917748623
h     -3.463616073186733      3.027443469951127     -0.203085511323108
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*****
* Geometry 40
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42
Energy = -1276.5567903020
c      4.490051090088318      0.898258374896751      0.274334896202560
h      5.573307378732228      0.890594456460321      0.144094063867990
c      3.821469411248951      2.109791377062596      0.677993420452936
h      4.405557779013697      3.023454416883439      0.802827811067063
c      2.480672540295680      2.117154043977142      0.913302937971966
h      1.990019837887308      3.021336866549302      1.275127500545053
c      1.649535099831121      0.948716962220087      0.678390665247757
c      2.315547293708144      -0.234890047929754      0.084813101913481
c      3.766015158301768      -0.225047429192339      0.033895139260468
h      4.262411907764641      -1.145369063763352      -0.284946614464342
c      0.315628781290905      0.953132816476326      1.000162832377627
h      -0.322144557323252      0.095565461953235      0.777634269163804
c      1.727745511584837      -1.314520295880752      -0.516819688533526
h      2.373602680265687      -2.127253779047840      -0.868910181928305
o      -0.275007110269199      2.003839060987778      1.637672519872419
o      0.398722683752583      -1.449121360601791      -0.765701724051859
si      -1.945926217356866      2.299956526764932      1.639175207240903
si      -0.198263318257463      -2.707865473886479      -1.747039838465681
c      -2.940884872669945      0.845269199955414      2.299868983072104
h      -2.604686540776351      0.504760678492054      3.289137503979050
h      -3.990981733173839      1.166823659109449      2.397236625895991
h      -2.928867801112418      -0.014021866042077      1.613724222819582
c      -2.158619601743676      3.781956442931220      2.766533522721093
h      -2.026971860114366      3.489865441167073      3.819108421341512
h      -1.432654502746177      4.575682310124606      2.542156083932781
h      -3.169226341939178      4.205798384934570      2.663439099507884
c      -1.952921868478683      -2.188097314386507      -2.136064361967866
h      -1.959367753143038      -1.253671377381138      -2.716363701937621
h      -2.466629548274798      -2.957854751025920      -2.730997575984542
h      -2.535629373693275      -2.024501239203058      -1.218228578333980
c      -0.100185087702334      -4.291665379043270      -0.746943044512997
h      -0.541376055395296      -5.140737344702062      -1.289349240127428
h      0.948301851493699      -4.544378570144480      -0.527307138675442
h      -0.626898836006772      -4.184068647330736      0.212050255507188
c      0.814590315807032      -2.878261243384087      -3.323084386356611
h      0.379226890743633      -3.675006333144551      -3.947336261751835
h      0.815527167666170      -1.952105495385175      -3.915426217651049
h      1.860266479347961      -3.156409628157498      -3.126777807195254
c      -2.469408450255087      2.597243304243783      -0.138415394453904
h      -1.848489174389579      3.359752344038393      -0.628842836388420
h      -2.363303183520251      1.661091800819016      -0.708620041080726
h      -3.522185474035200      2.909302534611718      -0.202921823461846
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*****
* Geometry 41
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42
Energy = -1276.5569905110
c         4.485954376536730      0.892149166181468      0.269706398977103
h         5.570060431967027      0.877548153087314      0.146959764103787
c         3.819678197595341      2.114396076945136      0.644681644011180
h         4.406763250939496      3.027936969734007      0.755693391392395
c         2.477477100598310      2.131368484221473      0.871308219406124
h         1.987625648713307      3.044001762138075      1.211664154701933
c         1.645153574238196      0.958922426418316      0.662682948047669
c         2.307604678766396     -0.235617640995382      0.087444331364735
c         3.758597976312436     -0.232346766775953      0.043196036553293
h         4.253234507282855     -1.159337617909971     -0.258890612318787
c         0.314951165945965      0.969212729793086      0.997362061814944
h        -0.322348908132679      0.103532017982335      0.807035748465047
c         1.718095993623926     -1.318829999728938     -0.506205003907264
h         2.363858051206303     -2.135916561563161     -0.848822395034247
o        -0.271180726400562      2.037321218646662      1.608129952757593
o         0.389331494023194     -1.453652033733110     -0.759904056528320
si        -1.944950339997874      2.314681187316857      1.635504704713977
si        -0.197810593586762     -2.717415607825934     -1.741396598203159
c        -2.891854861154653      0.886946480315026      2.414011862844281
h        -2.523017638069788      0.622732430607878      3.415063880421453
h        -3.948061385243083      1.185708077592588      2.515457606093224
h        -2.869896017344534     -0.016494827832467      1.787432078486183
c        -2.152861680249622      3.863288092092397      2.670190837817737
h        -1.979383583365724      3.647341198851481      3.734776566556075
h        -1.454921341800203      4.655770649797373      2.366562324741373
h        -3.176327795695488      4.256986714581091      2.573400013972117
c        -1.956798399098081     -2.213249922335763     -2.130656873897963
h        -1.972403064655785     -1.277076089897140     -2.707870257521225
h        -2.461655284371777     -2.986460494072946     -2.728771155827765
h        -2.542191634415704     -2.059262121938379     -1.212941087590003
c        -0.088944452381375     -4.301983313222457     -0.743172543084060
h        -0.521218748924668     -5.153259689105886     -1.289448473889450
h         0.960624952031044     -4.547281567588610     -0.520185416189620
h        -0.620389285937877     -4.201364446805828      0.213954602043034
c         0.816872355880283     -2.880721090094295     -3.317299358555682
h         0.389412560512170     -3.682578832115866     -3.940521041977896
h         0.809536525665977     -1.955504042333684     -3.911100787949219
h         1.865133242088022     -3.148644734660417     -3.120115122101119
c        -2.519489795070829      2.502596981978227     -0.141403160021353
h        -1.927379585858089      3.252372088403698     -0.684440765714207
h        -2.407643067676720      1.542054834811908     -0.668004508612630
h        -3.579615893614847      2.791125901540450     -0.194460107749208

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*****
* Geometry 42
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42
Energy = -1276.5571683100
c      4.482456321350088      0.888570497000587      0.264427649742182
h      5.567525339614842      0.868585580507123      0.151082686923058
c      3.817055712198963      2.120324579303799      0.608793680485987
h      4.405538346900978      3.034708826886205      0.704504389984010
c      2.473396465224265      2.145487652586775      0.825550892884653
h      1.982627769754516      3.066490755832811      1.141634023159147
c      1.641382978957732      0.968239512107130      0.644963962337955
c      2.302141358352233      -0.236419319897180      0.089399210145263
c      3.753553193314928      -0.237940399367958      0.053185861960324
h      4.247520509013683      -1.170672619154062      -0.231093496278780
c      0.314366439070211      0.984135844773133      0.990470777700739
h      -0.322149862075874      0.111315576737020      0.832694466745039
c      1.711770503668735      -1.324540852882943      -0.494435278568443
h      2.357714247411786      -2.145975138326536      -0.825814525726689
o      -0.268904397102476      2.069787384924228      1.573001463385409
o      0.383952998008955      -1.460216012841044      -0.752247560234165
si     -1.944813593954033      2.329133774382577      1.628599141611508
si     -0.196804891008103      -2.727976111863078      -1.732875059533339
c      -2.840684269892695      0.936232545940191      2.521015699192843
h      -2.439600740574765      0.750570579602872      3.527640670318726
h      -3.902142756848975      1.212121252209977      2.629881777477740
h      -2.806728303986773      -0.007215544529403      1.956790880284505
c      -2.149688229586236      3.937405117681111      2.568392231428443
h      -1.931328533805582      3.798252633625594      3.637456709992390
h      -1.483093995231533      4.722640772295328      2.185154135250418
h      -3.185238926257063      4.301637248553972      2.484982072285576
c      -1.960442799432227      -2.237382492840498      -2.118652532608060
h      -1.985537809378182      -1.299178619872611      -2.692089988273574
h      -2.458242283639255      -3.013116166930526      -2.719518222739783
h      -2.546648310400063      -2.092845207879013      -1.199981777322720
c      -0.077528725760828      -4.313637798003541      -0.737126337387368
h      -0.502955008025630      -5.166212774529333      -1.286901338810282
h      0.972942785974807      -4.553010951125934      -0.512678526634088
h      -0.611929206291655      -4.219680588661030      0.218958246803901
c      0.816380130392434      -2.884275733691919      -3.310337873346032
h      0.394990763251270      -3.690294006631792      -3.932345025704634
h      0.800412075287123      -1.959724450636141      -3.904809685854602
h      1.867024646377546      -3.142974554537541      -3.114234065554123
c      -2.569845899618809      2.408598235743727      -0.139573558566094
h      -2.008104414905114      3.142075431414322      -0.734965979293288
h      -2.452377584520896      1.425334360739648      -0.621232105270642
h      -3.636725330586336      2.673876736138509      -0.177978562439722
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 \* Geometry 43  
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    42
Energy = -1276.5573254310
  c      4.478650809557301      0.888158839774745      0.259332749824141
  h      5.564671472771647      0.864082184146447      0.156436786285941
  c      3.812358649669520      2.128535429999868      0.569249584060523
  h      4.401437511796058      3.044090788256108      0.649478624408026
  c      2.467439438413309      2.160128283614029      0.775290341472386
  h      1.974602501828129      3.088488493233467      1.064900052325265
  c      1.637360294529745      0.977535925806107      0.624106148907402
  c      2.297936145822383     -0.237053721334076      0.090899601846341
  c      3.749744402315842     -0.241408029083225      0.064354296478803
  h      4.244661252119613     -1.179891697328231     -0.199498766065949
  c      0.313662263624648      0.998188450082594      0.980404578776811
  h     -0.319617083936132      0.117204524072181      0.857598378132637
  c      1.707788201542642     -1.331079941437775     -0.482241581686707
  h      2.353485089285015     -2.158010371465612     -0.800514559354664
  o     -0.268330454459391      2.099577660226251      1.533211302546285
  o      0.379770211638466     -1.468661972379478     -0.742220850934908
  si     -1.945228056244878      2.342061275327350      1.619052864184209
  si     -0.196049073612635     -2.739716983578747     -1.721983589370198
  c     -2.787030362617092      0.991026675089451      2.621374158490344
  h     -2.354639480944840      0.885019917190830      3.626600513406160
  h     -3.852869188775292      1.244122706314876      2.740635148793875
  h     -2.738533658005101      0.012761142698151      2.121166089850430
  c     -2.148308542156397      4.002683599195330      2.462731350608129
  h     -1.883100003633661      3.940881755086638      3.528330855670653
  h     -1.516988249291280      4.774274047207450      2.000026391638852
  h     -3.194653355797042      4.339194365545078      2.398996315343624
  c     -1.964376835302886     -2.261436450873280     -2.101185006420790
  h     -1.998926968597563     -1.321083044628688     -2.670482851224772
  h     -2.456793833236834     -3.038905277041842     -2.704326303272803
  h     -2.549660484538698     -2.126352976087007     -1.180524249174742
  c     -0.066157004623583     -4.326643599592107     -0.728696801837658
  h     -0.486366323643817     -5.180130867225763     -1.281241153412436
  h      0.985391115715908     -4.561390725399786     -0.504156184278573
  h     -0.602177706682110     -4.238772072032930      0.227082535602668
  c      0.813348012878872     -2.888806526600331     -3.302340201644601
  h      0.396770317508332     -3.698076843126815     -3.923337056219372
  h      0.788404153925933     -1.964184948121056     -3.896423358491305
  h      1.866657898061324     -3.138937362608305     -3.108874560040681
  c     -2.620501011084429      2.314876957117499     -0.132084546150463
  h     -2.090730288807287      3.028773911460382     -0.778582609946571
  h     -2.496525673684448      1.311737926134962     -0.568924102950846
  h     -3.693062136354405      2.558467884906396     -0.153045416349035

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*****
* Geometry 44
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42
Energy = -1276.5574590890
  c      4.475130750230213      0.890387971118158      0.253346518033867
  h      5.562137599103293      0.863708693832820      0.162414026962540
  c      3.806697705544171      2.138212340830021      0.527166740651479
  h      4.395116944527572      3.055538609776186      0.590291687271125
  c      2.460275467222300      2.174568202258814      0.721499009974749
  h      1.964342317405804      3.109423056772667      0.983297837933669
  c      1.633479732113632      0.986405818313102      0.600914957933451
  c      2.295369130771825      -0.237632727568440      0.091998059636212
  c      3.747594524749667      -0.243140851299116      0.075818425311770
  h      4.244632355335553      -1.186574805546969      -0.165708369208655
  c      0.313164565986854      1.011159020424225      0.967643568021679
  h      -0.316330881156231      0.123393330916468      0.879293750986677
  c      1.706089551422220      -1.338968504241679      -0.467932761244448
  h      2.352202673795058      -2.170680846899094      -0.773465595441200
  o      -0.268574726526782      2.127036591942744      1.489731973857632
  o      0.378499684227664      -1.478630591372629      -0.730848101788908
  si     -1.945259724727333      2.354544457353268      1.608911800583676
  si     -0.195120150810037      -2.752750576595230      -1.707891175115585
  c      -2.730793363690486      1.052662666234776      2.715705677101748
  h      -2.269930746010888      1.024946140998473      3.713368252264048
  h      -3.800133751481322      1.283607030448588      2.846853188728242
  h      -2.665491484869015      0.045377507392174      2.279267097066233
  c      -2.148782025489567      4.060987276619790      2.354871134240406
  h      -1.835853165706143      4.075807281631785      3.409095266739837
  h      -1.556639457055250      4.812820319697911      1.814312537727040
  h      -3.204452603432141      4.371113595704519      2.316503961014700
  c      -1.968234325699131      -2.284850843607710      -2.077899588982019
  h      -2.012269918103356      -1.342061470530101      -2.642448317080784
  h      -2.457131492773640      -3.063272322279115      -2.682706985326333
  h      -2.550764778222815      -2.158837446401281      -1.154220436353077
  c      -0.054536656761361      -4.341076767595330      -0.718088130462069
  h      -0.471559278248598      -5.194828201092451      -1.272783710427667
  h      0.998167705939759      -4.572127914942567      -0.495176819225994
  h      -0.590333598959296      -4.258549814511669      0.238328790348643
  c      0.807738204713720      -2.894482310252592      -3.293181714231093
  h      0.394324724494864      -3.706176437558610      -3.913136760527831
  h      0.773703744394403      -1.969469051641715      -3.886254052535681
  h      1.863668799375081      -3.137054607140672      -3.104184347688339
  c      -2.670014396803034      2.221948574129998      -0.117697956326977
  h      -2.173248719193852      2.912611946763386      -0.814037801802796
  h      -2.539312019578597      1.201112934662125      -0.508893357637806
  h      -3.747153112625374      2.445532291920828      -0.119184689917230
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*****
* Geometry 45
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42
Energy = -1276.5576115030
  c      4.471894365643876      0.895222025137933      0.247866994923034
  h      5.559938841365057      0.867722120650467      0.170163811056536
  c      3.800089328902602      2.149126674891837      0.483326106319243
  h      4.386668985872069      3.068602670545389      0.528710766596513
  c      2.451929969579877      2.188656776366320      0.663927732797524
  h      1.951393708863135      3.129150224728790      0.895572529966754
  c      1.629849067072050      0.994472107081756      0.574801525478510
  c      2.294730432094309      -0.238240366442615      0.091814458676424
  c      3.747122417913303      -0.242679516703481      0.086833480541772
  h      4.247474332798277      -1.190119895826364      -0.130202566537548
  c      0.312731288988167      1.022818652293140      0.951382380002203
  h      -0.312207862593023      0.128831402637526      0.898431765834031
  c      1.707185352934813      -1.347582035931518      -0.453468725218758
  h      2.353547313082116      -2.184161526323471      -0.744261302422821
  o      -0.269852781291304      2.152766819992022      1.442567527398140
  o      0.380418584134319      -1.490595608625525      -0.716924147715542
  si     -1.945274514075559      2.367406659185020      1.596223653476252
  si     -0.194042664138651      -2.766408385279737      -1.690893885229803
  c      -2.672308828133403      1.120729565790016      2.801527283692724
  h      -2.185248040848423      1.169614921049141      3.785990814638960
  h      -3.744167015581227      1.330131538681498      2.946505051093649
  h      -2.587593476437014      0.089551784942885      2.428833167648719
  c      -2.151014484841177      4.112962288472334      2.244084361105215
  h      -1.789147548248011      4.202327536824592      3.278758590927234
  h      -1.602143887189325      4.839075673597369      1.627891245708954
  h      -3.214149412572978      4.398740354099007      2.236559155008232
  c      -1.972120537752823      -2.307681423201567      -2.048566365538090
  h      -2.025728015989292      -1.362387364524871      -2.608003104671149
  h      -2.459189173341434      -3.086269087313665      -2.654687075634240
  h      -2.550457104460415      -2.190508787699204      -1.121102337849002
  c      -0.042863551060152      -4.356734640982632      -0.705137171766581
  h      -0.458432622950646      -5.210270704381773      -1.261376248614128
  h      1.010950070779540      -4.585329899625521      -0.485449470021318
  h      -0.576956795870288      -4.279386152457674      0.252661788421591
  c      0.799543996390564      -2.900960648210016      -3.282396244446581
  h      0.387729705267731      -3.714076518465196      -3.901490463613209
  h      0.756105607075649      -1.975076826947891      -3.873417101563002
  h      1.858026927318513      -3.136689776958476      -3.099539523324472
  c      -2.717892604939767      2.131279074113842      -0.098394463499934
  h      -2.255322576671297      2.795860792695377      -0.842333580809328
  h      -2.579486610280941      1.095136051663713      -0.443503960677725
  h      -3.798591877950259      2.336190574191332      -0.078174781662927

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 \* Geometry 46  
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42
Energy = -1276.5577533030
  c      4.468619008877056      0.902899296628798      0.242102946662303
  h      5.557645015403113      0.876142717184005      0.179649243214983
  c      3.792028237210403      2.161194678196692      0.437629488262757
  h      4.375977079275074      3.083052975150587      0.465506340164970
  c      2.442150630589851      2.202013347990485      0.603563735573686
  h      1.935998562842448      3.146858783378891      0.803566213556622
  c      1.626192752927442      1.001782765290257      0.546494636688779
  c      2.295608743016020     -0.238710856070572      0.091067323928823
  c      3.748069174556132     -0.240150897257565      0.098370730448945
  h      4.252911540551805     -1.190642584106382     -0.093140281159009
  c      0.312166104038205      1.032810512208012      0.932363634004743
  h     -0.306742880903975      0.133018471760892      0.915244581543236
  c      1.710629483207811     -1.356782512038557     -0.438536255621902
  h      2.357335304919355     -2.198015635028742     -0.714393309057031
  o     -0.272689097984105      2.174629154213544      1.392101203829012
  o      0.384038075702557     -1.503887401318190     -0.701215153406645
  si     -1.945556703777649      2.378415151358771      1.580993090521135
  si     -0.193074064882758     -2.780959020843510     -1.671336765490034
  c     -2.612833316621858      1.193221112372867      2.879137151620303
  h     -2.101111574381412      1.316955312055413      3.844568761424689
  h     -3.685834678782025      1.382840176418717      3.040632462829965
  h     -2.507521647072611      0.142936935160132      2.570197095125275
  c     -2.155423355023701      4.156681040819987      2.130497886757064
  h     -1.744347940695493      4.318209184679882      3.137651545959950
  h     -1.653235339929393      4.851347671813027      1.442334395326887
  h     -3.223411730058418      4.422121077472418      2.158481840104167
  c     -1.976161559296641     -2.329871220599432     -2.014087681359700
  h     -2.039173768471927     -1.381886247582170     -2.567895417103097
  h     -2.462943138612445     -3.108017482622963     -2.621078832462895
  h     -2.548853640260215     -2.221341446906490     -1.082078922635991
  c     -0.031342967483528     -4.373438827017165     -0.690052380136636
  h     -0.446871582941595     -5.226384459294619     -1.247362511825975
  h      1.023682786918901     -4.600416301222767     -0.474893097364174
  h     -0.562422111652656     -4.300739741245891      0.269787056677197
  c      0.789029138321926     -2.907916523556723     -3.270243548498442
  h      0.377693328128660     -3.721716257402102     -3.888671960218013
  h      0.736054870521216     -1.980588828387524     -3.858186492513608
  h      1.850108974882263     -3.137443475392355     -3.094879669684497
  c     -2.764609695303796      2.041470442786889     -0.074474379978092
  h     -2.337382701017760      2.677618862138616     -0.863194088866499
  h     -2.617510804551244      0.992642131015571     -0.373995216707516
  h     -3.847720913414859      2.229298671914965     -0.030488318578758

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 \* Geometry 47  
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42
Energy = -1276.5578390780
  c      4.465448787381056      0.913035217636874      0.236078193374369
  h      5.555315934289781      0.888716503441875      0.189138790255353
  c      3.783021295460205      2.174059716595432      0.390072348597256
  h      4.363355391338247      3.098549927373895      0.398704029743240
  c      2.431512784044970      2.214322819761004      0.540970701643208
  h      1.918943140425067      3.162071611966685      0.708248538647547
  c      1.622671755673036      1.008276277091441      0.516607134726515
  c      2.297917922942611     -0.239159667351417      0.090284179583995
  c      3.750363450670252     -0.235791666068224      0.110171887368265
  h      4.260679682646995     -1.188452433196131     -0.054025842051202
  c      0.311856250764660      1.041363581311675      0.911719782959258
  h     -0.300152788487132      0.136798153965305      0.929818713690502
  c      1.716154853203836     -1.366823696986558     -0.422060739242494
  h      2.363727410555615     -2.212494224550241     -0.682412510316350
  o     -0.276442031208284      2.193455688514847      1.339664456646521
  o      0.389995282477153     -1.518155708854306     -0.684484332662304
  si     -1.945465640973185      2.388034732138841      1.565231264738951
  si     -0.191830547710660     -2.796141661033193     -1.649701680473671
  c     -2.551929444017308      1.270491612769200      2.950069525150973
  h     -2.017641763527373      1.467175899257779      3.890903192992798
  h     -3.624854484927894      1.442522425719997      3.129762579948440
  h     -2.425782935503585      0.205833586837732      2.704108594994099
  c     -2.162266993313694      4.192817410283229      2.016379789628910
  h     -1.703367014169825      4.423766347065650      2.988717531451471
  h     -1.709305037404286      4.850951298398607      1.261277328143733
  h     -3.232447494794785      4.441971502034454      2.083010966369070
  c     -1.979775230534637     -2.350825298817224     -1.974987046658388
  h     -2.051964104632329     -1.399971608727931     -2.522684396599197
  h     -2.468116072450357     -3.127819634564105     -2.582233484721498
  h     -2.545162353645708     -2.250547599063405     -1.037578073751006
  c     -0.019638678547938     -4.390769956824475     -0.673409396009955
  h     -0.436981149281086     -5.242693592680377     -1.231056243641350
  h      1.036663587269580     -4.617294617555836     -0.464317503677729
  h     -0.546223494073351     -4.321938491744339      0.289221940910902
  c      0.776299480582425     -2.915892817080415     -3.257574556627722
  h      0.363799307185141     -3.729767964638684     -3.875054529778378
  h      0.713787069098992     -1.986942965634250     -3.842038969490727
  h      1.839942130457332     -3.140333864443563     -3.091368050737056
  c     -2.808973865907676      1.953045730924307     -0.044333394176645
  h     -2.417831278443235      2.558364240111591     -0.874975061367596
  h     -2.652355871377591      0.893944501229013     -0.298876731552444
  h     -3.893361882927357      2.125370779499071      0.024886175119391

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* Geometry 48
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42
Energy = -1276.5578858020
  c      4.462458104247014      0.925696776103876      0.230037508041451
  h      5.552987971455474      0.905567673103125      0.199510155332144
  c      3.773024764685591      2.187590536511219      0.340593747834947
  h      4.348897775874335      3.114841953049073      0.329878758926595
  c      2.419957282178799      2.225399959399600      0.475758113883105
  h      1.900072256586315      3.174523425020625      0.608936644366792
  c      1.619562587283662      1.013674740492980      0.485205395880204
  c      2.301924957602899     -0.239565665645261      0.089179889033930
  c      3.754200443220344     -0.229511279917907      0.122835511200682
  h      4.271030236651276     -1.183185776539753     -0.013051564312813
  c      0.311748519793585      1.048493446585935      0.888665777717077
  h     -0.292296025541929      0.139962073947736      0.942636906296265
  c      1.724241770616879     -1.377165824477399     -0.405337376331502
  h      2.372725891783605     -2.227191675980588     -0.649215413336621
  o     -0.281324360547138      2.209718089287428      1.282888704183295
  o      0.398145775907145     -1.533342026340981     -0.666156181335073
  si     -1.944949081884436      2.396926181565946      1.547174396894458
  si     -0.190387947869555     -2.811460562657241     -1.626125241060445
  c     -2.488915854233466      1.351805371160139      3.011810700553703
  h     -1.934608166617876      1.619554500739392      3.923027554754889
  h     -3.560754250246543      1.507213676180477      3.211348707939603
  h     -2.340156895726970      0.277538807112819      2.827785374111068
  c     -2.171020523825117      4.221949253957661      1.901266865073435
  h     -1.665849806115854      4.518713641658095      2.831885402263250
  h     -1.769673798232994      4.838943627880454      1.084554616257340
  h     -3.240546133742070      4.459078246154558      2.009284140782074
  c     -1.983156927049150     -2.370577963873820     -1.931143090942610
  h     -2.064387075277831     -1.416757568548924     -2.472360511493239
  h     -2.474542354547016     -3.145852838031100     -2.538157071710693
  h     -2.539864112069452     -2.278182374967421     -0.987694904687171
  c     -0.008086232074312     -4.408486153328636     -0.654984235211402
  h     -0.428919718859269     -5.258918891029754     -1.212404336261437
  h      1.049485642586924     -4.635681123689042     -0.453268898866098
  h     -0.528836849323937     -4.342970487699898      0.311110234286844
  c      0.761222309151501     -2.924514064680437     -3.243973695587466
  h      0.346065312879369     -3.737774340694556     -3.860389369702400
  h      0.689159355511844     -1.993559826903808     -3.824216361382337
  h      1.827412618781619     -3.144562223886997     -3.088381883240450
  c     -2.851251662541892      1.867651974319623     -0.009823796463803
  h     -2.497717744441433      2.440342337531264     -0.879583847136746
  h     -2.683961569334093      0.800714279650970     -0.220565140094104
  h     -3.935795045122668      2.025577534266669      0.086434493634696
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* Geometry 49
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42
Energy = -1276.5578699830
  c      4.458700609111028      0.939882732465230      0.224382297608613
  h      5.549656927140705      0.925430053254248      0.210858964233697
  c      3.761627756567949      2.200821501758102      0.290044323411981
  h      4.332394744534113      3.130786796032391      0.260247562086537
  c      2.407091916020143      2.234619686044867      0.408213624678617
  h      1.879244702510026      3.183611138671554      0.506459088983862
  c      1.615924772721863      1.017842491219788      0.452711195844306
  c      2.306316640979520     -0.240324285408600      0.088065059571213
  c      3.758273355389964     -0.222017587866068      0.136061194616525
  h      4.282371259302024     -1.175434841504903      0.029498822413298
  c      0.311650047961874      1.054753363920352      0.865771722344551
  h     -0.283530442682555      0.143391368293880      0.957623710260686
  c      1.733351636127467     -1.388170102581794     -0.388075169368457
  h      2.383059801733298     -2.242341636747303     -0.614017465444522
  o     -0.287103129905309      2.223843414798271      1.225159533210562
  o      0.407665103589061     -1.549271707444114     -0.648787381562748
  si     -1.944149090535458      2.405725840214028      1.528259100311666
  si     -0.188645308561719     -2.827648385814097     -1.602490908610277
  c     -2.425454126987872      1.437436207643373      3.065663302251912
  h     -1.854421772106549      1.773842957325952      3.943219501231730
  h     -3.495339608537988      1.576827415041268      3.285868684266702
  h     -2.251497015764050      0.358274644257361      2.942109433905504
  c     -2.182640029862243      4.245154588873591      1.785159926618483
  h     -1.634465397275991      4.604691845522991      2.667994980518726
  h     -1.834056350442239      4.815869983529732      0.912406669154419
  h     -3.248762805697401      4.474734665882749      1.934730079859866
  c     -1.985998024299277     -2.390067526200468     -1.885722210775197
  h     -2.076051073332003     -1.433123873450022     -2.419949800044300
  h     -2.481490129927159     -3.163153865095725     -2.492222859884990
  h     -2.533064688137485     -2.305507569213893     -0.935871301071651
  c      0.003422536626547     -4.426821791108807     -0.636355333867904
  h     -0.421689018559741     -5.275656806084499     -1.193099481171150
  h      1.062126649436885     -4.655322055172288     -0.442479274045821
  h     -0.511049467636730     -4.364051077870289      0.333339074391120
  c      0.745030312534610     -2.934098743049899     -3.230940362013255
  h      0.326631866729097     -3.746320856342642     -3.846432898419801
  h      0.663428404867979     -2.000872312856476     -3.806314137244615
  h      1.813622992095855     -3.150195775889375     -3.086722601657609
  c     -2.890534438608878      1.784985674170462      0.029933390066732
  h     -2.575799705394455      2.322851164158179     -0.876312168809471
  h     -2.711344068896812      0.712472576994591     -0.137603296162266
  h     -3.973986779664772      1.929999172357201      0.154685327197189
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 \* Geometry 50  
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42
Energy = -1276.5545870170
  c      4.446696995279054      0.950512913359915      0.215777440351608
  h      5.537561063479677      0.950512913359915      0.215777440351608
  c      3.734170634296316      2.205454583163631      0.215777440351608
  h      4.292591833244782      3.141794885525410      0.178221582628980
  c      2.376708837889298      2.221837074864993      0.307077223170987
  h      1.840760683946974      3.171669430762998      0.376530886478237
  c      1.603716995643461      0.996255390942845      0.424024877070331
  c      2.310907568432075     -0.262584940233154      0.105632108077557
  c      3.762824076932238     -0.224913015153902      0.170242339810625
  h      4.301572197760550     -1.173235840155534      0.100953512520691
  c      0.342082636005903      1.105606011814672      0.944724273439982
  h     -0.240976313024401      0.187611726617229      1.092612056959852
  c      1.741187381093350     -1.412969050654584     -0.370645260707866
  h      2.390434762676577     -2.280712281890327     -0.544510272118998
  o     -0.281756915008025      2.272198301499658      1.226833094708501
  o      0.440438724651167     -1.549471157759875     -0.717366543106053
si     -1.941908862826431      2.426456568061260      1.527785519885114
si     -0.181372483048235     -2.848592334600555     -1.610181089215190
  c     -2.378177698738701      1.520054511480211      3.116074413051686
  h     -1.797172008425085      1.906402307313121      3.965473072386104
  h     -3.446039927508266      1.643060980550634      3.353049092355582
  h     -2.180909347251907      0.440936568871239      3.037382584421027
  c     -2.211298877516951      4.272577965813290      1.687738072964411
  h     -1.635235792688385      4.688283702946048      2.526022806424463
  h     -1.900921358794204      4.794307514108412      0.771407105545892
  h     -3.273395249873705      4.499024416403832      1.863423655733833
  c     -1.984584457361831     -2.412720126265774     -1.864626724749173
  h     -2.084656801436646     -1.450677457428062     -2.386736528057390
  h     -2.492019887787573     -3.179997131592625     -2.468030462278794
  h     -2.514320516513043     -2.334259082682488     -0.905080724634423
  c      0.016328615626350     -4.438686009341788     -0.626448589068913
  h     -0.415299648760030     -5.289766229456852     -1.175076083697178
  h      1.073684590300502     -4.673229874519484     -0.435269282906175
  h     -0.493033313380256     -4.369823638687484      0.345260210769871
  c      0.729016451963262     -2.965980814911677     -3.250419421307895
  h      0.312989864080673     -3.774848601434409     -3.869917608801154
  h      0.640254158759790     -2.027354562958694     -3.816232233300517
  h      1.800043230243239     -3.173155971888988     -3.110945593700022
  c     -2.905147482449817      1.721379081492850      0.075825613511657
  h     -2.625467103239267      2.223739393627187     -0.861451643568373
  h     -2.722461398784355      0.644798464942599     -0.053838487328744
  h     -3.987131201773478      1.858605958720856      0.222867041132074

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