Sensory Perception of Non-Deuterated and Deuterated Organic Compounds

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W.P. Conceptualization: Supporting; Data curation: Equal; Methodology: Equal.
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**Table S1:** Molecular parameters: $P_s$ = vapor pressure; $D_{\text{air}}$ = diffusion coefficient in air; $D_{\text{water}}$ = diffusion coefficient in water; $K_{\text{OW}}$ = octanol/water distribution coefficient; $K_{\text{OA}}$ = octanol/air distribution coefficient; $K_{\text{HdA}}$ = n-hexadecane/air distribution coefficient; $H$ = Henry constant; $S_{\text{water}}$ = solubility in water; $\Delta H_{\text{vap}}$ = enthalpy of evaporation; $\Delta H_{\text{Diss}}$ = bond dissociation enthalpy. All data for $T = 298$ K and $p = 1013$ mbar.

| Parameter                  | octanoic acid | D15-octanoic acid | acetone | D6-acetone |
|----------------------------|---------------|-------------------|---------|------------|
| Molecular formula          | $\text{C}_8\text{H}_{16}\text{O}_2$ | $\text{C}_8\text{D}_{15}\text{H}_1\text{O}_2$ | $\text{C}_3\text{H}_6\text{O}$ | $\text{C}_3\text{D}_3\text{O}$ |
| CAS-No.                    | 124-07-2      | 69974-55-6        | 67-64-1 | 666-52-4   |
| Molar weight (g/mol)       | 144.2         | 159.30            | 58.1    | 64.1       |
| Melting point (°C)         | 16.3          | -94               |         |            |
| Boiling point (°C)         | 237           | 239               | 56      |            |
| $P_s$ (Pa)                 | 0.63          | 30867             |         |            |
| $D_{\text{air}}$ (cm²/s)   | 0.053         | 0.108             |         |            |
| $D_{\text{water}}$ (cm²/s) | $6.9 \cdot 10^{-6}$ | $1.1 \cdot 10^{-5}$ |         |            |
| Molar volume (cm³/mol)     | 160.3         | 71.4              |         |            |
| log $K_{\text{OW}}$        | 2.78          | -0.24             |         |            |
| log $K_{\text{OA}}$        | 7.30          | 2.55              |         |            |
| log $K_{\text{HdA}}$       | 4.68          | 1.70              |         |            |
| $H$ (mol/(m³ Pa))          | 13            | 0.25              |         |            |
| log $S_{\text{water}}$ (mol/l) | -2.2          | soluble           |         |            |
| $\Delta H_{\text{vap}}$ (kcal/mol) | 19.98 | 7.0              |         |            |
| $\Delta H_{\text{Diss}}$ (kcal/mol) | (CH₃) 95.5 | (CD₃) 98.1       | (CH₃)  | (CD₃) 91.4 |
|                             | (CH₂) 89.8    | (CD₂) 92.4        |         |            |

1) Chemspider
2) SPARC (298 K)
3) Ambrose et al. (1974)
4) Mackay et al. (2006)
5) Calculated from $K_{\text{OA}} = K_{\text{OW}} \cdot R \cdot T \cdot H$ (for 298 K)
6) UFZ-LSER Database (Ulrich et al., 2017)
7) Sander (2015)
8) This work (B97-3c)
**Table S2:** Presentation of D15-octanoic acid/octanoic acid and D6-acetone/acetone to trained and untrained subjects: portion of men and women, age structure of the panel and responses.

| Sample A | octanoic acid | D6-acetone |
|----------|---------------|------------|
| Sample B | D15-octanoic acid | acetone |
| Probands (total) | 69 | 100% | 69 | 100% |
| Probands (male) | 34 | 49% | 33 | 48% |
| Probands (female) | 35 | 51% | 36 | 52% |
| Age 15-20 | 5 | 7% | 4 | 6% |
| Age 21-25 | 8 | 12% | 14 | 20% |
| Age 26-30 | 13 | 19% | 15 | 22% |
| Age 31-35 | 8 | 12% | 10 | 14% |
| Age 36-40 | 12 | 17% | 7 | 10% |
| Age 41-45 | 5 | 7% | 5 | 7% |
| Age 46-50 | 4 | 6% | 0 | 0% |
| Age 51-55 | 8 | 12% | 6 | 9% |
| Age 56-60 | 4 | 6% | 4 | 6% |
| Age 61-65 | 1 | 1% | 4 | 6% |
| Age 66-70 | 0 | 0% | 0 | 0% |
| Age 71-75 | 1 | 1% | 0 | 0% |
| Sample A first | 34 | 49% | 34 | 49% |
| Sample B first | 35 | 51% | 35 | 51% |
| Q1: Differences in the hedonic tone? | No: 23 | 33% | No: 17 | 24% |
| Q2: Odor type of A and B different? | No: 31 | 45% | No: 40 | 58% |
**Table S3:** Presentation of octanoic acid/octanoic acid and acetone/acetone to trained and untrained subjects: portion of men and women, age structure of the panel and responses.

| Sample A | octanoic acid | acetone |
|----------|---------------|---------|
| Sample B | octanoic acid | acetone |
| Probands (total) | 58 | 100% | 54 | 100% |
| Probands (male) | 33 | 57% | 31 | 57% |
| Probands (female) | 25 | 43% | 23 | 43% |
| Age 15-20 | 0 | 0% | 0 | 0% |
| Age 21-25 | 5 | 9% | 6 | 11% |
| Age 26-30 | 9 | 16% | 14 | 26% |
| Age 31-35 | 8 | 14% | 4 | 7% |
| Age 36-40 | 7 | 12% | 13 | 24% |
| Age 41-45 | 7 | 12% | 4 | 7% |
| Age 46-50 | 4 | 7% | 3 | 6% |
| Age 51-55 | 6 | 10% | 2 | 4% |
| Age 56-60 | 9 | 16% | 8 | 15% |
| Age 61-65 | 2 | 3% | 0 | 0% |
| Age 66-70 | 1 | 1% | 0 | 0% |
| Age 71-75 | 0 | 0% | 0 | 0% |
| Sample A first | 27 | 47% | 27 | 50% |
| Sample B first | 31 | 53% | 27 | 50% |
| Q1: Differences in the hedonic tone? | No: 31 | 53% | No: 27 | 50% |
| Q2: Odor type of A and B different? | No: 37 | 64% | No: 41 | 76% |
Figure S1: Measured IR spectrum of acetone.

Figure S2: Measured IR spectrum of D6-acetone.
**Figure S3:** Measured IR spectrum of octanoic acid.

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Figure S5: Retention times (ion extraction mode) of acetone (Ion 57.70 - 58.70) and D6-acetone (Ion 63.70 - 64.70) on the non-polar SPB®-Octyl column at 35 °C.

Figure S6: Retention times (ion extraction mode) of acetone (Ion 57.70 - 58.70) and D6-acetone (Ion 63.70 - 64.70) on the slightly polar DB5 column at 35 °C.
**Figure S7:** Retention times (scan mode) of acetone, D6-acetone, octanoic acid, D15-octanoic acid, dimethyl carbonate, DMSO and 3-methoxy benzaldehyde on the non-polar SPB®-Octyl column at 150 °C.

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Quantum chemical calculations

The Cartesian coordinates (xyz-files) of the peptides and the protein cut-out are available at the end of this Supporting Information.

Non-polar and polar model homodimers

![Structures of homodimers of model systems.](image)

**Figure S15:** Structures of homodimers of model systems.

The computed $\Delta \Delta G$ and $\Delta G_H$ values for the alkane dimers are summarized in Table S4 and S5, respectively, and the respective structures are depicted in Figure S15.

**Table S4:** $\Delta \Delta G$ values of alkane dimers. Computed with GFN2-xTB on unconstrained (xTB) and constrained (2% shortened C-D bonds) geometries (scaled xTB) and B97-3c (values in kcal/mol).

| Method   | C₂  | C₃  | C₄  | C₅  | C₆  | C₇  | C₈  |
|----------|-----|-----|-----|-----|-----|-----|-----|
| xTB      | -0.26 | -0.25 | -0.12 | -0.18 | -0.12 | -0.08 | -0.10 |
| scaled xTB | -0.90 | -0.19 | -0.19 | -0.21 | -0.14 | -0.08 | -0.09 |
| B97-3c   | 0.20 | 0.24 | 0.23 | 0.30 | 0.26 | -0.11 | -0.12 |
The sign of the $\Delta\Delta G$ values for the alkane dimers, computed by GFN2-xTB, indicates that the non-deuterated complexes are favored by 0.26 to 0.08 kcal/mol. Generally, chromatographic experiments with non-polar and slightly polar columns show earlier retention times for perdeuterated compounds (Wade, 1999; see also Figure S5 – S8), which is in agreement with the computed values, since a shorter retention time correlates with a weaker interaction of the compound with the chromatographic phase. The positive $\Delta G_H$ values show that none of the alkane dimers is bound in gas-phase. Upon deuteration of one monomer, the free association energy ($\Delta G_D$) changes by values between 1.1 and 3.6%.

In order to investigate the isotope effect on the bond lengths for $\Delta\Delta G$, all deuterium containing bonds were shortened by 2%. Table S4 shows that the $\Delta\Delta G$ values only differ for smaller alkanes ($<C_5$) between relaxed and constrained structures. For larger alkanes, the differences in $\Delta\Delta G$ values are small and can be neglected. In addition to the semiempirical method GFN2-
xtB, DFT calculations were performed. The ΔΔG values of GFN2-xTB and B97-3c differ in sign except for heptane and octane. This discrepancy is difficult to explain but we note that for the two largest systems (which are most similar to the experimentally investigated octanoic acid) the DFT and GFN2-xTB values are very similar. Furthermore, the ΔG_H values of both methods are similar. The largest difference is observed for the ethane dimer, whereas the difference of the remaining values is between 0.3 and 1.1 kcal/mol.

The interaction energy of the alkane dimers is dominated by non-polar dispersion forces. This type of non-covalent interaction is probably also dominating the interaction of a typical organic odorant in an olfactory receptor. However, polar non-covalent interactions may also be important. To access this type of interaction, three model dimers with solely polar interaction motifs are constructed and ΔΔG values are computed. The ΔΔG and ΔG_H values for the hydrogen-bonded dimers are shown in Table S5 and S6, respectively, and the structures in Figure S15. The order of magnitude of the ΔΔG values is similar to the non-polar dimers and the sign also indicates for the formic acid (ΔΔG = -0.11) and ethylene glycol (ΔΔG = -0.02) dimer a stronger interaction of the non-deuterated dimer. In the case of the water dimer (ΔΔG = 0.04), the deuterated dimer shows a higher binding affinity. The relative change in binding affinities upon deuteration is similar to the non-polar homodimers (1.4 to 2.5%). The ΔΔG and ΔG_H values of the polar dimers, computed with GFN2-xTB are in excellent agreement with the B97-3c results, which justifies the sole application of the GFN2-xTB method in further studies.

Complexes of model peptides with octanoic acid and acetone

The structures of the three model peptides (A: PNSIT, B: SCTYP, C: PIHDK) with octanoic acid as ligand are depicted in Figure S16 and the ΔΔG and ΔG_H values of the complexes of the peptides with octanoic acid and acetone are shown in Table S7.

Figure S16: Structure of complexes of model peptides with octanoic acid (green carbon atoms).
**Table S7**: $\Delta\Delta G$ and $\Delta G_H$ values of peptide complexes with octanoic acid and acetone, computed with GFN2-xTB (values in kcal/mol).

| Peptide | $\Delta\Delta G$ octanoic acid | $\Delta\Delta G$ acetone | $\Delta G_H$ peptide octanoic acid | $\Delta G_H$ acetone |
|---------|---------------------------------|--------------------------|-----------------------------------|----------------------|
| A       | 0.06                            | -0.07                    | A                                 | 2.38                 |
| B       | -0.04                           | -0.18                    | B                                 | 2.86                 |
| C       | -0.20                           | -0.04                    | C                                 | 6.69                 |

The $\Delta\Delta G$ values for complexes of the three model peptides with octanoic acid and acetone are of similar magnitude than those of the homodimers (-0.18 to 0.06 kcal/mol). Except for one case (peptide A with octanoic acid) the non-deuterated complexes are more strongly bound. The $\Delta G_H$ values show that except for the complex of peptide C with acetone, all complexes are repulsive and the relative change in association free energy upon deuteration is on average slightly larger (values between 0.6 and 9.0%), compared to all homodimers. Note that the model cases are not constructed to simulate any experiments. The aim is rather to show for a variety of bonding situations that the deuteration has a noticeable effect on association free energies. Furthermore, the $\Delta\Delta G$ values of all model systems indicate no clear tendency, whether the deuterated or non-deuterated complex is more stable.

**Figure S17**: Cartoon representation of bovine rhodopsin with bound retinal (red) (PDB: 1F88).
Olfactory receptor model: cut-out from bovine rhodopsin

To model the interaction of an odor molecule (e.g., octanoic acid or acetone) with a typical olfactory receptor, the X-ray structure of bovine rhodopsin (member of the GPCR family) is taken as substitute. The structure of 1F88 from the PDB is depicted in Figure S17.

As described in the main text, a cut-out is constructed with octanoic acid as replacement for the retinal ligand. The ΔΔG and ΔG_H values for three different ligand variants are summarized in Table S8. For a discussion, see main text.

The absolute binding affinities (ΔG_H) for the two protonation states (OA- and OA-H) differ largely (16.14 and 0.73 kcal/mol, respectively) due to additional strong electrostatic interactions in the former. In contrast, the ΔΔG values are similar for all ligand protonation/deuteration states (ranging from 0.52 to 0.60 kcal/mol). Due to limitations of the model system, the significance of the calculated ΔG_H values in comparison to experimental data is difficult to assess. For a further discussion of the ΔΔG values, see main text.

**Table S8**: ΔΔG and ΔG_H values for the complexes of the cut-out from bovine rhodopsin with octanoic acid as anion (OA-), perdeuterated excluding carboxylic hydrogen (OA-H) and perdeuterated including carboxylic hydrogen (OA-D), computed with GFN2-xTB (values in kcal/mol).

| Ligand | ΔΔG | ΔG_H |
|--------|-----|------|
| OA-    | 0.52| 16.14|
| OA-H   | 0.59| 0.73 |
| OA-D   | 0.60| 0.73 |

Additionally, the complex of acetone with the OR model is studied. The choice of the bovine rhodopsin as olfactory receptor model is motivated by the structural similarity between retinal and octanoic acid. This premise does not hold in the case for acetone as ligand and the complex of acetone and bovine rhodopsin may not fully represent a natural olfactory receptor system. However, the computation of ΔΔG values for acetone bound to the same olfactory receptor model may provide some fundamental understanding of the molecular olfactory mechanism. For this purpose, the acetone ligand is manually placed at three different positions in the OR pocket, resulting in three different binding modes (equilibrium structures), for which the ΔΔG and ΔG_H values are summarized in Table S9.
Table S9: ΔΔG and ΔGH values for the complexes of the cut-out from bovine rhodopsin with acetone in three different binding modes, computed with GFN2-xTB (values in kcal/mol).

| Binding mode | ΔΔG   | ΔGH   |
|--------------|-------|-------|
| 1            | -1.71 | 3.82  |
| 2            | -1.51 | 9.46  |
| 3            | -0.87 | 0.88  |

The ΔΔG values have the same sign for all three binding modes, but differ somewhat in magnitude (from -0.87 to -1.71 kcal/mol). The ΔGH values show a larger spreads from 0.88 to 9.46 kcal/mol). For further discussion, see main text.

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Wade, D., 1999. Deuterium isotope effects on noncovalent interactions between molecules. Chemico-Biological Interactions 117, 191-217.
APPENDIX: Cartesian coordinates (xyz-files):

101 
./peptides/A/OA/coord.xyz
N  4.1926353  0.6514565 -2.0801178
H  3.5653815  1.1607512 -2.6900891
C  3.7957628  -0.7443377 -1.9151053
C  3.2917707  -0.9801739 -0.4939584
O  2.9555078  -2.0921685  0.0821416
N  3.2823955  0.1090352  0.2725263
H  3.4948454  0.9802195 -0.2151805
C  2.7571288  0.1099444  1.6202527
C  3.2820607  1.3099438  2.4075428
C  2.4696841  1.5003890  3.6786057
O  1.4829467  0.8186656  3.9335671
N  2.9006968  2.4723387  4.4843320
H  3.7066325  3.0292742  4.2551812
H  2.3983810  2.6648859  5.3372114
H  4.3342014  1.1651331  2.6506748
H  3.1873563  2.2102271  1.7955508
C  1.2248464  0.1572378  1.5516967
O  0.6381139  1.1989724  1.2388881
N  0.6037301  -0.9936550  1.7641991
C  -0.8419567  -1.1393963  1.7718895
C  -1.4217076  -0.8381120  3.1697341
O  -1.3457604  0.5142265  3.5427579
H  -0.4175031  0.7350621  3.7316998
H  -2.4823706  -1.1038049  3.1771228
H  -0.8935601  -1.4720299  3.8903767
H  -1.0394049  -2.1916043  1.5445783
C  -1.4385627  -0.3265437  0.6200267
C  -1.1757808  -0.6372374  -0.5448699
O  -2.2586160  0.6688881  0.9385302
H  -2.3072926  0.9557484  1.9135352
C  -3.0041624  1.4247508  -0.0491916
C  -2.1396584  1.9301747  -1.2080716
O  -2.6203769  2.1394663  -2.3122003
N  -0.8478346  2.1601424  -0.9172956
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C  0.0987734  2.6101963  -1.9040076
C  0.8221941  1.4784016  -2.6376603
O  1.6405211  1.7318162  -3.4947544
O  0.5781569  0.2286756  -2.3038394
H  -0.1504168  0.0615771  -1.6456195
H  -0.4510550  3.1746001  -2.6672656
C  1.1913648  3.5248827  -1.2814473
O  2.0656461  2.7932160  -0.4596407
H  1.5434554  2.3725127  0.2562318
C  0.5698686  4.7025127  -0.5363689
H  0.0182303  4.3495340  0.3306671
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H  1.3599607  5.3683434  -0.2014745
H  1.8099328  3.8844418  -2.1113016
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C  -2.3174468  3.4702130  -1.0477518
C  -2.8741824  2.1707817  -1.6164127
O   -2.3895976  1.6593591  -2.6100200
O   -2.9552455  1.6790178  -1.0668055
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H   -2.7438917  3.6596296  -0.0553492
H   -1.1442300  6.2713188  -2.4631522
H    0.5582387  4.9203874  -0.8009131
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C    1.6853438  1.6198896  -1.8522736
C    3.1602521  1.3406853  -1.7697402
C    3.6266802  0.0483726  -1.5632501
C    4.9754758  -0.2028513  -1.4066521
C    5.8887046  0.8464257  -1.4470301
C    5.4305326  2.1413566  -1.6623249
C    4.0784115  2.3803636  -1.8196807
C    3.7355984  3.3912236  -1.9817891
C    6.1307309  2.9634986  -1.7014468
O    7.2056090  0.5605067  -1.2694582
H    7.7342950  1.3685378  -1.3252299
H    5.3405180  -1.2044593  -1.2446028
H    2.9251633  -0.7726010  -1.5247102
H    1.4704316  2.3565941  -2.6252255
H    1.1387787  0.7033739  -2.0824295
H    2.6572713  0.9152434  3.6468647
C    3.8490054  -0.1739374  2.1593301
O    4.0201291  -1.4116765  2.8040493
H    4.3531719  -1.2652418  3.7001441
C    5.0376544  0.7576783  2.3422570
H    4.8554832  1.6910153  1.8178169
H    5.9329035  0.2924872  1.9390016
H    5.1905811  0.9781616  3.3966779
H    3.7308334  -0.4198644  1.0973956
C   -0.2419342  -2.4780453  1.4701593
H    0.5603974  -3.0628885  1.9165250
H   -1.0600434  -3.1454939  1.2013136
S    0.4342149  -1.7979492  -0.0847392
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O   -4.4345010  2.6248609  1.3568149
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C    1.8081938  -5.9107391  0.2637903
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C    0.6278206  -5.3638386  -1.9265731
C   -0.8028223  -5.2785258  -1.4007017
C   -1.6238010  -4.2543191  -2.1806599
C   -3.0066229  -4.0353169  -1.5696107
C   -3.7852822  -2.9459319  -2.3058233
C   -3.1843219  -1.5744206  -2.1044543
O   -2.6235027  -1.2208078  -1.0839471
O   -3.3493634  -0.7937309  -3.1486859
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -2.9852737 | 0.1299025 | -3.0103469 |
| H    | -3.8336430 | -3.1433539 | -3.3764703 |
| H    | -4.8079957 | -2.8957714 | -1.9233675 |
| H    | -3.5733287 | -4.9667063 | -1.6021325 |
| H    | -2.9022297 | -3.7391711 | -0.5231506 |
| H    | -1.7324631 | -4.5848053 | -3.2159320 |
| H    | -1.0845006 | -3.3042855 | 0.7333913  |
| H    | -0.7837301 | -4.9891628 | 0.3492755  |
| H    | -1.2812609 | -6.2581829 | -1.4673491 |
| H    | 1.0887777  | -4.3795866 | -1.8709880 |
| H    | 0.5975657  | -5.6614956 | -2.9787152 |
| H    | 0.9934534  | -7.3359771 | -1.1284118 |
| H    | 0.9080070  | -5.8815849 | 0.8722398  |
| H    | 2.2511016  | -4.9171134 | 0.2510339  |

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O  0.3080799 -1.9513201 1.9905136
N -1.4530000 -2.7752674 0.8545376
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C  2.0664166 -0.5619528 1.7116880
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C -0.2315514  3.6317957  1.7589469
H  0.2620845  4.2251605  0.9832839
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H -2.2176222  4.7959138  2.9808036
C  2.5427543  4.1794362  1.5021826
H -2.4600588  4.7917017  0.6029072
H -3.5001235  4.3663316  1.9803935
C -2.3708361  2.7048248  1.1237188
C -2.8867218  2.4235194 -0.2873437
O -2.3435289  2.8957867 -1.2611015
O -3.9933713  1.7221930 -0.3961095
H -4.3108306  1.3107325  0.4621599
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| Atom | X            | Y            | Z            |
|------|--------------|--------------|--------------|
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| C    | -2.4952760   | 3.2405940    | -0.5076840   |
| N    | -2.6351910   | 3.4336810    | 0.8319700    |
| C    | -1.4417340   | 3.7474050    | 1.2645820    |
| N    | -0.5313960   | 3.7709230    | 0.2703650    |
| H    | 0.4589160    | 3.9875270    | 0.3396950    |
| H    | 1.2063110    | 3.9664560    | 2.2863120    |
| H    | -3.3477700   | 3.0007900    | -1.1122440   |
| H    | -1.2417210   | 3.5201650    | -2.9920550   |
| H    | 0.3137400    | 3.9955000    | -2.844960    |
| C    | -2.8330360   | -1.6965530   | -2.6134200   |
| C    | -3.3480600   | -0.5121130   | -3.4285560   |
| H    | -3.8165300   | 0.2279730    | -2.7850950   |
| H    | -2.5390270   | -0.0435500   | -3.9831350   |
| H    | -4.0912420   | -0.8599100   | -4.1409920   |
| C    | -2.0897360   | -2.7010470   | -3.5046760   |
| C    | -2.0261760   | -4.0989010   | -2.8979170   |
| C    | -1.4783450   | -4.7676960   | -3.5564730   |
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| H    | -3.0278130   | -4.4982220   | -2.7579170   |
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| H    | -1.0784360   | -2.3367210   | -3.6958590   |
| H    | -3.6908640   | -2.2091940   | -2.1647970   |
| H    | -1.5047400   | -2.1429990   | -0.9724970   |
| H    | -3.3882860   | 1.4582410    | 1.5747280    |
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| C    | 3.1863920    | -4.1180190   | -4.2100550   |
| C    | 3.5813760    | -2.6468390   | -4.3156160   |
| C    | 2.3913270    | -1.7537170   | -4.6592160   |
| C    | 2.7865540    | -0.2815040   | -4.7465940   |
| C    | 1.5932050    | 0.6096690    | -5.0804170   |
| C    | 1.9912360    | 2.0808790    | -5.1454180   |
| C    | 0.8294970    | 2.9856050    | -5.4497220   |
| O    | -0.3185150   | 2.6387470    | -5.6048930   |
| O    | 1.2056250    | 4.2607570    | -5.5314700   |
| H    | 0.4575780    | 4.8534530    | -5.7244240   |
| H    | 2.4196190    | 2.4077690    | -4.1952040   |
| H    | 2.7501870    | 2.2467570    | -5.9127940   |
| H    | 1.1640970    | 0.3115120    | -6.0389340   |
| H    | 0.8141390    | 0.4840100    | -4.3260320   |
| H    | 3.5552280    | -0.1597390   | -5.5126640   |
| H    | 3.2155060    | 0.0317210    | -3.7923630   |
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| H    | 1.9640860    | -2.0707750   | -5.6132950   |
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| H    | 4.3507960    | -2.5351810   | -5.0831420   |
| H    | 2.4138760    | -4.2291640   | -3.4455360   |
| H    | 2.7589190    | -4.4457380   | -5.1605260   |
| H    | 5.1480890    | -4.9244020   | -4.6224220   |
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H     6.3469604    -0.9258864    -2.6927150
H     6.5322295    -0.0056421    -3.3084082
C     4.6452740    -0.9258864    -2.6927150
H     4.4038704    -1.0158944    -3.7512078
H     4.8294947    -1.9249215    -2.3002257
C     3.4741447    -0.5838088    -0.8867123
N     3.4273187    -0.5838088    0.4102551
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H    -2.0710052    2.7219309    -0.4643944
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H    -0.3055939    2.4928334    -2.9322232
H     0.1099187    -2.2183986    -2.9952024
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C    -2.2154874    -3.5122688    -2.4919542
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| Atom | X     | Y     | Z     |
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| C    | -1.4023662  | -1.0361263  | 2.4758917 |
| C    | -1.8505470  | 0.3687220   | 2.2730764 |
| C    | -1.1859948  | 1.5458708   | 2.0613232 |
| N    | -2.0854260  | 2.5660791   | 1.9508549 |
| C    | -2.7162044  | 2.0204113   | 2.0956051 |
| N    | -3.1765504  | 0.6985751   | 2.2995380 |
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| H    | -4.1952428  | 2.5604028   | 2.0641391 |
| H    | -0.1351766  | 1.7203300   | 1.9614683 |
| H    | -0.8268161  | -1.1253426  | 3.4078688 |
| C    | 3.5622734   | -0.2085858  | 2.8543025 |
| C    | 2.5652210   | 0.9477383   | 2.2730764 |
| C    | 1.1859948   | 1.5458708   | 2.0613232 |
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| N    | 3.1765504   | 0.6985751   | 2.2995380 |
| H    | 3.9272448   | 0.0184637   | 2.4002928 |
| H    | 4.1952428   | 2.5604028   | 2.0641391 |
| H    | 0.1351766   | 1.7203300   | 1.9614683 |
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| H    | -0.8268161  | -1.1253426  | 3.4078688 |
| C    | 3.5622734   | -0.2085858  | 2.8543025 |
| C    | 2.5652210   | 0.9477383   | 2.2730764 |
| C    | 1.1859948   | 1.5458708   | 2.0613232 |
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| At. | X     | Y     | Z     | At. | X     | Y     | Z     |
|-----|-------|-------|-------|-----|-------|-------|-------|
| C   | 56.7489362 | 15.3120832 | -8.6109519 | C   | 58.0981322 | 14.5867907 | -8.6665305 |
| O   | 58.6183542 | 14.0827941 | -7.6800043 | C   | 55.6705038 | 14.2752993 | -8.9330257 |
| N   | 58.6131115 | 14.5216625 | -9.9022191 | C   | 59.9058174 | 13.9316142 | -10.1948015 |
| C   | 60.9713872 | 14.6759502 | -9.4353416 | O   | 62.0606311 | 14.2465809 | -9.1604921 |
| O   | 59.1846175 | 13.3957366 | -12.4680589 | C   | 61.5085169 | 13.3063851 | -11.7196055 |
| N   | 61.1485002 | 14.4916220 | -6.1798562 | C   | 65.4370683 | 15.0563538 | -6.892735 |
| O   | 66.5474374 | 15.3109749 | -6.493907 | C   | 65.322169 | 13.2364308 | -8.5488463 |
| C   | 65.5704131 | 11.7393033 | -8.7741322 | C   | 66.8455828 | 11.5049118 | -9.6224297 |
| O   | 66.9319881 | 12.1418707 | -10.703435 | O   | 67.6985784 | 10.7160938 | -9.1895614 |
| N   | 66.4953484 | 12.6391836 | -3.502897 | C   | 67.1980523 | 11.3570698 | -3.5171194 |
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| C   | 56.2989955 | 13.3693982 | -16.2234624 | C   | 56.7761365 | 15.3732747 | -17.4300360 |
| C   | 57.3590063 | 13.6154749 | -15.3735645 | C   | 57.8311435 | 15.6395622 | -16.5782613 |
| C   | 58.1367814 | 14.7569885 | -15.5447805 | O   | 59.1724345 | 15.0449897 | -14.7247327 |
| N   | 47.4698622 | 11.6701203 | -12.1007435 | C   | 48.9082567 | 11.7579991 | -11.9659713 |
| C   | 49.5574032 | 11.6016764 | -13.3438084 | O   | 49.0519021 | 10.9056396 | -14.2120287 |
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|   | X       | Y       | Z       |
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| O| 52.8710798| 10.6933979| -13.0212321|
| N| 52.0918919| 13.3482538| -15.1568014|
| S| 51.0795149| 13.9682605| -16.5408690|
| N| 53.7106478| 10.9005852| -15.1094053|
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| C| 55.5849298| 9.7450008| -16.1489214|
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| O| 56.4165423| 6.6198190| -17.0737967|
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| C| 56.7672501| 1.9678273| -20.3522735|
| O| 57.3494930| 0.9071269| -20.4316466|
| N| 57.4550409| 2.1525403| -17.9275254|
| C| 57.5113988| 3.1056208| -16.0375924|
| C| 58.9438042| 3.8200103| -16.7669973|
| O| 56.8050604| 3.3494575| -15.8199221|
| N| 56.1281562| 4.7699638| -15.7932515|
| C| 55.0174275| 4.2986002| -14.8405300|
| O| 58.2025865| 5.0365282| -14.8352466|
| N| 58.4320151| 6.0189943| -13.9227037|
| C| 67.6326450| 6.7824074| -16.2437711|
| C| 66.7745932| 6.9745661| -15.0733074|
| C| 67.1643860| 5.8613527| -14.1025796|
| C| 68.1842620| 5.9402154| -13.4219368|
| C| 65.3137426| 6.9674636| -15.5342519|
| C| 64.3195647| 7.1223277| -14.3937079|
| S| 62.6284910| 6.8119360| -15.0017157|
| C| 61.7829880| 6.6850883| -13.4055066|
| N| 66.4165344| 4.7577776| -14.0829066|
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| C| 68.1994171| 3.5564603| -12.9286054|
| O| 68.6848126| 3.5262509| -11.8173829|
| C| 66.0392922| 2.3990943| -13.5798341|
| C| 64.5505303| 2.5875904| -13.6961607|
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| C| 63.9761093| 2.9431696| -14.9125278|
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| C| 61.8130680| 3.0728277| -13.8846616|
| N| 69.9626730| 7.3535531| -11.2276990|
| C| 68.7918947| 8.1229296| -10.8294807|
| C| 67.8500348| 7.2087787| -10.0361735|
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| C| 68.9647015| 9.8415076| -12.6011765|
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| H | 55.8779922 | 2.7932643 | -17.6370986 |
| H | 60.1043601 | 5.3239096 | -15.7673077 |
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| H | 67.4900533 | 7.5471606 | -16.8951665 |
| H | 66.9722208 | 7.9300773 | -14.5562058 |
| H | 65.1101018 | 6.0543472 | -16.0973016 |
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| H | 66.5791705 | 0.0800126 | -7.3946071 |
| H | 64.8235961 | 0.7631743 | -5.8001735 |
| H | 63.2186035 | 7.0654480 | 3.0480787 |
| H | 61.7161609 | 8.3715520 | 0.9100192 |
| H | 64.4781491 | 7.0604273 | 0.8316044 |
| H | 64.1977097 | 8.7948033 | 1.0708918 |
| H | 63.2162386 | 10.1673484 | -0.7346442 |
| H | 64.2411939 | 6.0714515 | -1.3744282 |
| H | 63.0935787 | 10.5153070 | -3.1709952 |
| H | 64.0837458 | 6.4158408 | -3.8021793 |
| H | 63.4997361 | 8.6374031 | -4.7042217 |
| H   | X        | Y        | Z        | H   | X        | Y        | Z        |
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| 3   | 60.6258900 | 6.5773894 | -4.8959949 | 4   | 61.2644994 | 6.4473389 | -3.2421270 |
| 5   | 60.5377307 | 8.3209141 | -1.4376587 | 6   | 59.4226186 | 10.5748221 | -1.6151127 |
| 7   | 58.9254400 | 7.9966790 | -6.2953420 | 8   | 61.2644994 | 6.4473389 | -3.2421270 |
| 9   | 57.7375815 | 6.5773894 | -4.8959949 | 10  | 59.4226186 | 10.5748221 | -1.6151127 |
| 11  | 57.3335261 | 11.9476589 | -5.9061592 | 12  | 58.9254400 | 7.9966790 | -6.2953420 |
| 13  | 57.1602910 | 3.1657662 | -5.2188160 | 14  | 55.0596916 | 3.1897223 | -7.2608121 |
| 15  | 55.3292943 | 5.4823590 | -6.3897354 | 16  | 53.9972465 | 5.7433765 | -10.9750286 |
| 17  | 53.9065844 | 5.7433765 | -10.9750286 | 18  | 55.0596916 | 3.1897223 | -7.2608121 |
| 19  | 57.0926822 | 5.3600992 | -6.5119215 | 20  | 55.3292943 | 5.4823590 | -6.3897354 |
| 21  | 55.0936110 | 6.4439377 | -12.7723291 | 22  | 58.1720239 | 5.9832516 | -8.5274939 |
| 23  | 58.0891546 | 6.5967204 | -10.9105466 | 24  | 55.0936110 | 6.4439377 | -12.7723291 |
| 25  | 51.4140369 | 5.2721490 | -7.3748341 | 26  | 52.9952966 | 7.3012337 | -7.2582191 |
| 27  | 52.9952966 | 7.3012337 | -7.2582191 | 28  | 51.6582309 | 8.4207623 | -9.0461823 |
| 29  | 51.7915603 | 6.682985  | -9.3160875 | 30  | 50.284589  | 7.3608844 | -8.6749293 |
| 31  | 49.866937 | 7.2903650 | -5.8389835 | 32  | 50.0408855 | 10.1726218 | -5.1468187 |
| 33  | 47.6887981 | 9.6452541 | -4.1077436 | 34  | 47.7510115 | 8.1608725 | -5.0750759 |
| 35  | 47.7510115 | 8.1608725 | -5.0750759 | 36  | 48.0310389 | 11.8679102 | -5.2920334 |
| 37  | 47.1439719 | 8.2562414 | -7.3862644 | 38  | 47.2588093 | 13.1791562 | -7.2249862 |
| 39  | 46.3622960 | 9.5612573 | -9.3095652 | 40  | 46.4089232 | 12.0365757 | -9.2329886 |
| 41  | 53.2470764 | 7.2477801 | -2.7090265 | 42  | 55.3007119 | 8.4696766 | -2.3533930 |
| 43  | 55.3007119 | 8.4696766 | -2.3533930 | 44  | 55.7532352 | 9.0092491 | -4.7297511 |
| 45  | 54.9403483 | 7.4480106 | -4.5881414 | 46  | 54.0267394 | 8.8802441 | -5.1031947 |
| 47  | 52.4973116 | 10.3518979 | -3.3399281 | 48  | 54.0317332 | 12.8595096 | -3.3446583 |
| 49  | 51.8051692 | 13.8863323 | -3.8629444 | 50  | 51.0642183 | 12.2830110 | -3.7748860 |
| 51  | 52.4396437 | 11.5188653 | -5.6716705 | 52  | 53.2637594 | 13.0741108 | -5.7354088 |
| 53  | 51.4938310 | 14.0916573 | -6.8529878 | 54  | 50.309271 | 13.2879874 | -5.8408143 |
| 55  | 49.9469899 | 12.5331126 | -8.0710227 | 56  | 50.6752740 | 11.1795016 | -7.1797728 |
| 57  | 52.1195253 | 13.1172718 | -8.9685793 | 58  | 51.6405764 | 11.5326381 | -9.3788442 |
| 59  | 61.6229408 | 8.0259353 | -8.7889364 |
| Element | X         | Y         | Z         |
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| H       | 70.1633224| 12.9948225| -4.2803741|
| H       | 69.1240606| 12.2393105| -5.5018649|
| H       | 68.4522623| 13.5067034| -4.4987218|
| H       | 60.0630192| -0.1107554| -6.1605128|
| H       | 59.6687371| 1.5709366 | -5.7099421|
| H       | 58.4790546| 0.6038007 | -6.5677377|
| H       | 64.0196535| 15.8482238| -14.1023210|
| H       | 65.3779908| 15.5571452| -12.9861660|
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| H       | 68.5151375| 3.6419977 | -15.0577101|
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481
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| C   | 49.7991553 | 9.1718066 | -4.812868 |
| C   | 50.2090571 | 8.9636576 | -3.3499462 |
| O   | 50.6612410 | 9.8868752 | -2.709598 |
| C   | 48.2610566 | 9.1171890 | -4.9212586 |
| C   | 47.7612083 | 9.8652208 | -6.1259868 |
| C   | 47.6856170 | 11.2532115 | -6.0950746 |
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| C   | 54.6421890 | 10.3611738 | -2.8995170 |
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| C   | 52.3563475 | 12.535754 | -5.428953 |
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|  | x   | y   | z   |
|---|-----|-----|-----|
| C | 63.776939 | 8.1131315 | -3.6763476 |
| N | 58.8828985 | 5.6259238 | -2.0836684 |
| C | 59.3486778 | 5.6561409 | -3.4576530 |
| C | 60.0652659 | 4.3816478 | -3.8403650 |
| O | 59.8578230 | 3.8643031 | -4.9256143 |
| C | 59.4843042 | 8.092887 | -3.9283563 |
| C | 58.9551997 | 8.387733 | -2.9403541 |
| C | 58.9983161 | 8.6276373 | 5.1637396 |
| N | 58.1856827 | 9.8766811 | -3.4795717 |
| C | 58.1838787 | 9.7394569 | -4.8345310 |
| C | 59.1664810 | 8.28025 | -6.5042384 |
| C | 57.5373881 | 10.4891586 | -5.8108967 |
| C | 58.5188767 | 9.0218703 | -7.4660492 |
| N | 57.7100486 | 10.115180 | -7.1243847 |
| C | 56.2862272 | 2.9907858 | -5.5175843 |
| C | 56.1093741 | 3.5227935 | -6.8570847 |
| O | 55.7728543 | 2.3676139 | -8.8601976 |
| C | 56.2142782 | 5.0706718 | -6.9528561 |
| C | 56.3365971 | 5.4843612 | -8.3898572 |
| C | 55.2370385 | 5.4606263 | -9.2356685 |
| C | 57.5775218 | 5.8053014 | -8.9249650 |
| C | 55.3728254 | 5.718544 | -10.586142 |
| C | 57.7301588 | 6.053674 | -10.272222 |
| C | 56.6261778 | 5.9975147 | -11.147880 |
| O | 56.8207823 | 6.1998503 | -12.4491009 |
| N | 58.4203448 | 3.0558047 | -7.4778118 |
| C | 59.5149835 | 2.5579527 | -8.2821063 |
| C | 60.0725316 | 1.2208455 | -7.7840034 |
| O | 60.7928273 | 0.5587645 | -8.4962028 |
| C | 60.6603641 | 3.572852 | -8.3033972 |
| N | 51.5753870 | 6.0591033 | -6.5159923 |
| C | 51.9688082 | 7.2846380 | -7.209627 |
| C | 51.4600694 | 8.4936704 | -6.4306704 |
| O | 52.0150632 | 9.5801770 | -6.4968770 |
| C | 51.3354704 | 7.3205432 | -8.6035770 |
| N | 50.3456437 | 8.2645442 | -5.7237203 |
| C | 49.7280719 | 9.2419618 | -4.8554363 |
| C | 50.1318323 | 9.0192087 | -3.3926238 |
| O | 50.6175008 | 9.9261100 | -2.7535120 |
| C | 48.1907273 | 9.2175359 | -4.9697876 |
| C | 47.7100248 | 9.9682165 | -6.1808363 |
| C | 47.6583596 | 11.3573394 | -6.1574770 |
| C | 47.3090335 | 9.2991965 | -7.3288160 |
| C | 47.2007707 | 12.0637575 | -7.2546741 |
| C | 46.8478195 | 10.0050038 | -8.4279155 |
| C | 46.7878275 | 11.3883555 | -8.3919398 |
| N | 53.3236822 | 8.3700875 | -2.4357407 |
| C | 54.5716022 | 8.8875939 | -2.9876338 |
| C | 54.5757115 | 10.4217047 | -2.9451406 |
| O | 55.6154134 | 11.0501680 | -2.7784712 |
| C | 54.7152341 | 8.4476882 | -4.4456774 |
| N | 53.3850744 | 11.0006865 | -3.1292731 |
| C | 53.1868085 | 12.4341594 | -3.0923627 |
| C | 52.8569588 | 12.9633160 | -1.6929291 |
| Atoms | Coordinates |
|-------|-------------|
| H 50.1102091 | 10.2244636 -5.1551349 |
| H 47.7762236 | 9.6851997 -4.0748416 |
| H 47.8528891 | 8.1819024 -5.0127570 |
| H 47.9668007 | 11.8865352 -5.2682390 |
| H 47.3415909 | 8.2203690 -7.36266 |
| H 47.1560146 | 13.1417115 -7.2225421 |
| H 45.5249295 | 9.4692263 -3.089553 |
| H 46.4163699 | 11.9434643 -9.2405022 |
| H 53.3462017 | 7.3557180 -2.4550478 |
| H 55.4638852 | 8.5568547 -2.4281085 |
| H 55.6283385 | 8.8539054 -4.8719186 |
| H 54.7609224 | 7.3625568 -4.5015858 |
| H 53.8678291 | 8.8043671 -5.0247519 |
| H 52.5629299 | 10.4097734 -3.1575950 |
| H 54.1287767 | 12.9020770 -3.4036274 |
| H 51.8971319 | 13.942762 -3.8724620 |
| H 51.1438532 | 12.349536 -3.7295149 |
| H 52.4169011 | 11.5298115 -5.6617484 |
| H 53.3041631 | 13.0485222 -5.7625352 |
| H 51.5486472 | 14.1420575 -6.8268431 |
| H 50.3455436 | 13.3717125 -5.8014143 |
| H 49.9575116 | 12.6756695 -8.0583992 |
| H 50.5761056 | 11.2755875 -7.1588735 |
| H 52.1515008 | 13.0907096 -8.9559585 |
| H 51.6071884 | 11.5272045 -9.3351894 |
| H 57.8756014 | 11.0179993 -10.3548821 |
| H 52.8109985 | 18.6729764 -14.1061819 |
| C 56.6674041 | 16.5923300 -12.9722744 |
| H 56.9010735 | 17.2683137 -9.2832539 |
| H 60.8887156 | 15.6881586 -9.3007249 |
| H 61.2855377 | 15.0431371 -4.7751332 |
| C 65.9470965 | 15.2357606 -5.4284073 |
| H 66.3881195 | 12.9248951 -2.5977775 |
| C 69.2113795 | 12.8421036 -4.3916312 |
| H 68.3819742 | 13.5321167 -13.8410778 |
| C 65.2199616 | 15.4424994 -14.0585267 |
| H 57.1308734 | 13.2660359 -19.3192061 |
| C 52.9481998 | 11.4493768 -19.2912942 |
| H 47.1296518 | 11.2340543 -11.2846705 |
| H 49.9953281 | 13.8983677 -15.9664009 |
| C 56.6801726 | 7.3491248 -19.0926297 |
| H 56.2402757 | 4.3597270 -18.0466494 |
| C 55.3965251 | 2.2709202 -21.0220903 |
| H 68.1431238 | 6.2010894 -16.4829017 |
| C 69.0598797 | 3.2442062 -14.1372294 |
| H 70.6360285 | 7.8704403 -11.8102879 |
| C 70.2300535 | 3.9488895 -8.7077550 |
| H 62.7214538 | 8.6535530 3.0079797 |
| C 61.9983964 | 5.1768234 1.6395009 |
| H 58.3416879 | 6.4672491 -1.9120770 |
| C 61.0170208 | 3.8223042 -2.8411989 |
| H 55.5920434 | 3.3799189 -4.8897568 |
| C 59.7093718 | 0.8337168 -6.3862986 |
| H 52.2025900 | 5.8724714 -5.7410120 |
| C 49.8767467 | 7.6616226 -2.8285859 |
| H 53.2218893 | 8.6515530 -1.4691618 |
C  52.4206553  11.9491947  -0.6820216
H  52.7277953  11.6887603  -8.0931268
H  55.3470598  1.7272522  -21.780385
H  66.6024742  16.0902987  -5.2900821
H  64.9318312  15.487137  -5.1307593
H  66.2725852  14.3947194  -4.8123316
H  50.1205146  7.6485515  -1.7705985
H  48.8377519  7.3792696  -2.9742948
H  50.4988824  6.9377652  -3.3493622
H  57.6610339  16.5630904  -13.458557
H  56.0181571  17.2456574  -13.5418764
H  56.7828021  16.9659901  -11.9534829
H  52.7609822  11.0800680  -20.0604377
H  53.3604845  10.6282802  -18.7116925
H  52.3824522  12.1017578  -18.6273142
H  50.0718266  12.4492203  0.2168250
H  51.6392283  11.3205645  -1.1030047
H  53.2717956  11.3173971  -0.4358557
H  61.5286132  4.3107546  1.1831331
H  63.0404763  4.9550327  1.8589390
H  61.5068608  5.4308332  2.5757258
H  60.1819725  4.7366920  -8.7252356
H  60.903002  3.059855  -8.3039688
H  69.8820362  3.7820996  -9.7241193
H  70.2682732  13.0475491  -4.2487878
H  69.0234629  12.5560429  -5.4242358
H  68.6148550  13.7270779  -4.1886739
H  60.2316357  -0.0750577  -6.1026459
H  59.9656789  1.6489097  -5.7124135
H  58.6338057  0.6790952  -6.3262840
H  64.2433779  15.9068927  -14.1585946
H  65.732145  15.5402375  -13.0335817
H  65.9567704  15.9223195  -14.6943046
H  69.2175370  2.1680478  -14.1866700
H  68.5508029  3.5800168  -15.0370355
H  70.0253063  3.7255965  -14.0484517
H  56.3195320  6.3745996  -19.4103839
H  55.9058468  8.0981414  -19.2558999
H  57.5507193  7.6458997  -19.6705607
H  61.640122  3.0778082  -3.2962086
H  61.5992243  4.6188674  -2.3842233
H  60.4242208  3.3535121  -2.0565936
O  57.5512719  9.6100020  -13.2341283
H  57.1502130  11.9586966  -11.6616191
C  59.5985814  10.3027309  -12.2327151
H  60.0896560  9.6312743  -12.9318457
H  56.3625544  10.4778362  -11.1338668
H  59.9349129  10.0913916  -11.2217872
H  59.8806913  11.3293306  -12.4705660

481
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N  52.0988018  17.9242786  -13.8504568
C  52.2418575  17.5219790  -12.4556516

55
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 53.4925517| 16.6404693| -12.3098936|
| O       | 54.1333050| 16.579354 | -11.2712363|
| C       | 51.0081278| 16.7202588| -12.024770 |
| C       | 51.1454089| 16.1514564| -10.6172048|
| C       | 51.8826774| 14.7961142| -10.569992 |
| O       | 52.3142739| 14.4617773| -9.437836  |
| O       | 51.9497413| 14.105265| -11.5984737|
| N       | 53.8346110| 15.9869498| -13.4327808|
| C       | 54.8377799| 14.9394118| -13.4701345|
| C       | 56.1694035| 15.3869437| -12.8910923|
| O       | 56.8390687| 14.6199511| -12.2291959|
| N       | 56.8253860| 16.390770 | -10.184734 |
| C       | 56.8966650| 15.3232604| -8.5925940 |
| C       | 58.2845910| 14.6689899| -8.6504214 |
| O       | 58.8813896| 14.2825764| -7.6540693 |
| N       | 55.8318759| 14.5247711| -5.5921579 |
| C       | 56.1988012| 13.0190337| -4.7709935 |
| C       | 56.836512 | 12.4765768| -4.7703723 |
| N       | 57.297560 | 13.5014174| -6.7948582 |
| C       | 65.1368139| 13.6117344| -7.1058178 |
| C       | 65.6713389| 15.0197522| -6.7970728 |
| O       | 66.6841466| 15.4355319| -7.3097861 |
| C       | 65.4600795| 13.2203149| -8.5485540 |
| C       | 65.6022476| 11.7117775| -8.7798071 |
| O       | 66.8281615| 11.4126132| -9.6746973 |
| O       | 66.8708522| 11.9803042| -10.7971448|
| C       | 67.7006579| 10.6488267| -9.2320688 |
| N       | 66.664926 | 12.6618464| -3.5593343 |
| C       | 67.3624751| 11.3757372| -3.5236906|
| C       | 68.8567965| 11.6492249| -3.4021287|
| O       | 69.5341044| 11.0655421| -2.5780230 |
| C       | 67.0041322| 10.6041551| -4.8065850 |
| C       | 67.6288933| 9.2134750 | -5.0011358 |
| C       | 69.0493358| 9.2861747 | -5.5590904 |
| C       | 67.5946067| 8.3715202 | -3.7268776 |
| N       | 67.4336571| 13.9556272| -13.5345209|
| C       | 66.5361320| 13.3461375| -14.5030048|
| C       | 65.1507865| 13.9805545| -14.3660632|
| O       | 64.1320139| 13.3428451| -14.5226663|
| C       | 66.4891828| 11.8158143| -14.3566615|
| S       | 65.6980811| 10.9652325| -15.7514278|
| N       | 56.4935234| 12.6800578| -19.7826562|
| C       | 55.3001683| 12.5737303| -18.9611209|
| C       | 54.0967663| 12.2823932| -19.8477983|
| O       | 54.0494239| 12.6733779| -20.9941878|
| C       | 54.9803778| 13.8756396| -18.1707184|
| C       | 56.1039786| 14.2067354| -17.2305517|

56
| Atom | X          | Y          | Z            |
|------|------------|------------|--------------|
| C    | 56.4288175 | 13.3326986 | -16.1986723 |
| C    | 56.8754764 | 15.3521182 | -17.3905346 |
| C    | 57.4935888 | 13.5813761 | -15.356481  |
| C    | 57.9347958 | 15.6211706 | -16.5449953 |
| O    | 59.2981349 | 15.0234423 | -14.709044  |
| N    | 49.0392925 | 11.7624869 | -11.901602  |
| C    | 49.6844732 | 11.6034228 | -13.2810745 |
| O    | 49.1705931 | 10.9105633 | -14.147430  |
| C    | 49.6153154 | 10.5944655 | -11.0515517 |
| O    | 50.9755782 | 10.7277958 | -10.7198661 |
| N    | 50.8708123 | 12.2115082 | -13.4249563 |
| C    | 51.7445256 | 11.9884740 | -14.560061  |
| O    | 52.9711480 | 10.6538751 | -12.978582  |
| C    | 52.2320132 | 13.3335199 | -15.0975287 |
| S    | 51.2190082 | 13.9727033 | -16.4793501 |
| N    | 53.8271893 | 10.8835011 | -15.0590262 |
| C    | 55.0340373 | 10.1458887 | -14.7987385 |
| O    | 55.6974919 | 9.7211964  | -16.1009464 |
| O    | 55.1829150 | 9.9668306  | -17.1820880 |
| N    | 56.8846921 | 9.1350032  | -15.9403455 |
| C    | 57.6837297 | 8.6951738  | -17.068049  |
| C    | 56.9708827 | 7.5323460  | -17.7741013 |
| O    | 56.4396589 | 6.6436972  | -17.1459292 |
| C    | 59.0830299 | 8.2906266  | -16.5640543 |
| O    | 59.8550916 | 9.5073227  | -16.0275907 |
| C    | 59.8776204 | 7.5479366  | -17.6342565 |
| C    | 60.3378403 | 10.4866600 | -17.0935257 |
| N    | 55.9884887 | 3.8224632  | -19.1244992 |
| C    | 57.1067909 | 2.8958946  | -19.1264833 |
| C    | 57.0115345 | 1.9003938  | -20.2773643 |
| O    | 57.6716063 | 0.8826772  | -20.2848779 |
| C    | 57.3364022 | 2.1487232  | -17.7861308 |
| C    | 57.4727591 | 3.1394747  | -16.6681772 |
| C    | 58.6655397 | 3.8221394  | -16.4597764 |
| C    | 56.3800512 | 3.4640963  | -15.8753991 |
| C    | 58.7584172 | 4.8249213  | -15.5155411 |
| C    | 56.4594502 | 4.4671392  | -14.9299634 |
| C    | 57.6406930 | 5.1771449  | -14.7645704 |
| O    | 57.7308295 | 6.2249161  | -13.9013188 |
| N    | 66.9643957 | 6.3694248  | -16.4020961 |
| C    | 66.8872644 | 6.9416845  | -15.0585701 |
| C    | 67.3469848 | 5.8479906  | -14.0885509 |
| O    | 68.3868264 | 5.9192523  | -13.4425071 |
| C    | 65.4391621 | 7.3663423  | -14.7838876 |
| C    | 65.2613371 | 7.9495379  | -13.3884274 |
| S    | 63.5486799 | 7.8076931  | -12.8014221 |
| C    | 63.6794254 | 6.2624696  | -11.8583867 |
| N    | 66.5711256 | 4.7623373  | -14.0489575 |
| C    | 66.8081723 | 3.7016647  | -13.0892315 |
| C    | 68.3150306 | 3.4960012  | -12.9138838 |
| O    | 68.8094861 | 3.4540336  | -11.8079284 |
| C    | 66.1303479 | 2.4046488  | -13.5666639 |
| C    | 64.6482387 | 2.622945   | -13.7084911 |
| X    | Y    | Z         |
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| H    | 54.8605106 | 14.6343772 | -8.8094086 |
| H    | 56.0161291 | 13.8411746 | -9.8776976 |
| H    | 58.1804588 | 14.9450288 | -10.6276766 |
| H    | 60.0547285 | 12.8810447 | -9.8678828 |
| H    | 60.4932365 | 13.6945316 | -12.2035233 |
| H    | 61.9166776 | 13.4497139 | -13.0830241 |
| H    | 62.4706590 | 13.6573713 | -11.4226664 |
| H    | 61.5464008 | 12.2221454 | -11.8724999 |
| H    | 60.4216007 | 14.6089278 | -6.4058857 |
| H    | 61.2170200 | 12.5238333 | -6.2910656 |
| H    | 61.3477771 | 12.9614663 | -4.5788839 |
| H    | 63.0873977 | 12.9614663 | -7.4572648 |
| H    | 65.6754759 | 12.9508877 | -6.4103365 |
| H    | 66.4030379 | 13.7045394 | -8.8065243 |
| H    | 64.6925405 | 13.6303963 | -9.2055083 |
| H    | 64.7160313 | 11.3069799 | -9.2702316 |
| H    | 65.7545893 | 11.1763720 | -7.8414366 |
| H    | 65.7090399 | 12.5282979 | -3.8813160 |
| H    | 67.0680200 | 10.7590607 | -2.6579632 |
| H    | 67.2574286 | 11.2265564 | -5.6674811 |
| H    | 65.9154872 | 10.4945626 | -4.7916500 |
| H    | 67.0128484 | 8.7140109 | -5.7593830 |
| H    | 69.4279113 | 8.2821913 | -5.7388248 |
| H    | 69.0569454 | 9.8254435 | -6.5050669 |
| H    | 69.7183229 | 9.7796454 | -4.8596498 |
| H    | 67.8907546 | 7.3493437 | -3.9511265 |
| H    | 68.2850047 | 8.7736855 | -2.9895326 |
| H    | 66.5912094 | 8.3573559 | -3.3072006 |
| H    | 67.1971832 | 13.6248403 | -12.6015134 |
| H    | 66.8989219 | 13.5987668 | -15.505778 |
| H    | 65.9760698 | 11.5447727 | -13.4319247 |
| H    | 67.5059577 | 11.4225214 | -14.3195011 |
| H    | 64.4977344 | 11.5047279 | -15.5741169 |
| H    | 56.2608765 | 13.1585690 | -20.647624 |
| H    | 55.4438562 | 11.7483129 | -18.2610319 |
| H    | 54.0476009 | 13.7373475 | -17.6211547 |
| H    | 54.8325582 | 14.6891389 | -18.8845467 |
| H    | 55.8470246 | 12.4350200 | -16.0665957 |
| H    | 56.6461218 | 16.0439946 | -18.1878741 |
| H    | 57.7475467 | 12.8900003 | -14.5662215 |
| H    | 58.5331873 | 16.0975933 | -16.6888111 |
| H    | 59.4265763 | 14.2938080 | -14.0674632 |
| H    | 47.3749342 | 11.1448179 | -12.8534955 |
| H    | 49.3391837 | 12.7141516 | -11.4482991 |
| H    | 49.4349076 | 9.6529202 | -11.5885497 |
| H    | 49.0818103 | 10.5636629 | -10.0959402 |
| H    | 51.5539727 | 10.6847824 | -11.5042957 |
| H    | 51.2548844 | 12.7849663 | -12.672966 |
| H    | 51.1582027 | 11.4436265 | -15.3129992 |
| H    | 53.2400028 | 13.2636595 | -15.5016350 |
| H    | 52.2216288 | 14.0613465 | -14.2865312 |
| H    | 53.6581007 | 11.0858153 | -16.0389375 |
| H    | 54.8007309 | 9.2614982 | -14.1944409 |
| H    | 55.7296647 | 10.7606482 | -14.2142609 |
| H    | 57.1815932 | 8.8208650 | -15.0247028 |
| H | 57.7560200 | 9.5283928 | -17.7740118 |
| H | 58.9219293 | 7.6030690 | -15.7276872 |
| H | 60.7228126 | 9.1381554 | -15.4791944 |
| H | 59.2259517 | 10.0440563 | -18.5401960 |
| H | 60.7937908 | 11.3475017 | -16.6109494 |
| H | 59.5176439 | 10.8420735 | -17.7116764 |
| H | 55.1380231 | 3.3384632 | -18.8556165 |
| H | 58.0090423 | 3.4883952 | -19.3355081 |
| H | 58.2327369 | 1.5358790 | -17.8741878 |
| H | 56.4868429 | 1.4855867 | -17.6055122 |
| H | 59.5322082 | 3.5684656 | -17.0528922 |
| H | 55.4476759 | 2.9318881 | -16.0031962 |
| H | 56.853109 | 5.3538211 | -15.3576081 |
| H | 55.5990177 | 4.7183386 | -14.3292172 |
| H | 56.8863183 | 6.3156358 | -13.4242680 |
| H | 66.6061492 | 7.0423197 | -17.0723515 |
| H | 67.5508775 | 7.8109832 | -14.9175316 |
| H | 64.7776250 | 6.5078276 | -14.9138049 |
| H | 65.1519129 | 8.1178089 | -15.5222065 |
| H | 65.5074293 | 9.0105234 | -13.3771469 |
| H | 65.8756254 | 7.4452778 | -12.6425434 |
| H | 62.7411185 | 6.1168415 | -11.3352163 |
| H | 63.8573333 | 5.4327727 | -12.5360943 |
| H | 64.4973380 | 6.3692102 | -11.1506291 |
| H | 65.7204097 | 4.7206661 | -14.5929844 |
| H | 66.3951456 | 3.9970580 | -12.1133293 |
| H | 66.3279990 | 1.6281578 | -12.8273490 |
| H | 66.5598951 | 2.1077710 | -14.5231166 |
| H | 64.2247555 | 2.2513789 | -11.6423714 |
| H | 64.7342139 | 3.0355081 | -15.8122543 |
| H | 61.8142691 | 2.6770988 | -11.8608035 |
| H | 62.3328401 | 3.4968653 | -16.0178341 |
| H | 60.8591716 | 3.3131345 | -14.0443454 |
| H | 70.1241527 | 6.7973582 | -11.7745282 |
| H | 69.0267283 | 8.8888648 | -10.0546130 |
| H | 67.3883813 | 9.2115841 | -11.8386559 |
| H | 68.2673183 | 8.0482137 | -12.8669509 |
| H | 68.3504541 | 11.5046809 | -11.500741 |
| H | 70.8194104 | 9.0858183 | -13.8863000 |
| H | 70.2961826 | 12.9264252 | -12.4381701 |
| H | 69.6158705 | 6.4946179 | -9.3235567 |
| H | 67.5890997 | 5.7837959 | -7.5949080 |
| H | 67.6301010 | 3.9014202 | -9.9927855 |
| H | 66.2971060 | 4.9628937 | -9.5029908 |
| H | 65.2352499 | 4.5756104 | -7.2119423 |
| H | 67.8467216 | 1.7431642 | -9.0314972 |
| H | 64.4069915 | 2.8345812 | -5.6810250 |
| H | 67.0183193 | -0.0066396 | -7.5072036 |
| H | 65.2966723 | 0.5365379 | -5.8237557 |
| H | 63.3669462 | 7.0382112 | 3.0652601 |
| H | 61.9514571 | 8.4625655 | 0.9408673 |
| H | 64.6209920 | 6.9720744 | 0.8626247 |
H 64.4485183 8.7242801 1.0765431
H 63.5076889 10.1192441 -0.7489170
H 64.3445177 5.9710120 -1.3260427
H 63.3883976 10.4328561 -3.1900793
H 64.1845971 6.2803815 -3.7578122
H 63.7025937 8.5140535 -4.6938695
H 59.8536692 5.7716716 -1.4534651
H 58.5168372 5.6998115 -4.0479366
H 60.8477370 6.5785182 -4.8098933
H 61.1030034 6.9866217 -3.1016153
H 59.3410657 8.9597574 -2.0613705
H 57.7185119 10.5599081 -3.1527048
H 59.5246712 7.1377594 -6.8724467
H 56.8189453 11.1626295 -5.6946096
H 56.1894537 11.1626295 -5.6946096
H 58.2056340 8.3056665 -8.5757185
H 56.8767996 10.2856649 -8.0219050
H 57.3550161 3.3495653 -5.1539949
H 55.2108221 3.1394139 -7.1425309
H 57.1867855 5.4452325 -6.6905897
H 55.4483718 5.4947321 -6.3503687
H 53.8404716 5.1404122 -8.2872320
H 58.0112138 5.7454632 -8.9367158
H 53.3902069 5.7098087 -10.637227
H 57.5765593 6.2836142 -11.2692685
H 54.2841792 6.3840838 -12.5932578
H 58.7603869 3.5082900 -6.6034097
H 59.2387737 2.4489100 -9.2981247
H 61.6266074 3.1197275 -8.7422105
H 60.5025174 4.4849295 -8.7229246
H 61.0407928 3.7532720 -7.1990176
H 51.1834178 5.2539147 -6.9135538
H 53.1014782 7.4651455 -7.3913589
H 51.3927175 8.0671982 -9.0700974
H 51.6486384 6.3200395 -9.0596281
H 50.2123436 7.0016006 -8.2864278
H 50.1718264 7.2719703 -5.5900052
H 50.1564380 10.2081402 -5.1159930
H 47.8389460 9.6134811 -4.0153083
H 47.9501902 8.1141980 -4.9563281
H 47.9769708 11.8209041 -5.2051217
H 47.4318034 8.1456361 -7.3059885
H 47.1323082 13.0610135 -7.1544980
H 46.5825810 9.3798037 -9.2484191
H 46.4148103 11.8506749 -9.1725383
H 53.4642750 7.3568304 -2.2685649
H 55.5828137 8.5509258 -2.4559901
H 55.5314466 8.7794285 -4.9120200
H 54.7053951 7.2994380 -4.4217220
H 53.7643311 8.7240028 -4.9074159
H 52.6286908 10.3895987 -3.0279069
H 54.1921196 12.8763626 -3.3610817
H 51.9679978 13.9254191 -3.8048665
H 51.1976951 12.3384620 -3.6358136
H 52.3924402 11.4948837 -5.5921242
H 53.3488619 12.9692730 -5.7008918
H 51.6429188 14.1514713 -6.7392574
```
|    | X          | Y          | Z          |
|----|------------|------------|------------|
| H  | 61.5818048 | 4.3049313  | 1.1234565  |
| H  | 63.0983268 | 4.9103853  | 1.8233267  |
| H  | 61.5678841 | 5.3916322  | 2.5431174  |
| H  | 71.0586688 | 4.9182220  | -8.8231613 |
| H  | 69.978743  | 3.9230628  | -9.7900895 |
| H  | 70.439496  | 12.916322  | -4.0729026 |
| H  | 69.345009  | 12.325198  | -5.3465448 |
| H  | 68.775297  | 13.574761  | -4.2634163 |
| H  | 71.0586688 | 4.9182220  | -8.8231613 |
| H  | 70.873349  | 3.2132862  | -8.4117307 |
| H  | 69.978743  | 3.9230628  | -9.7900895 |
| H  | 68.775297  | 13.574761  | -4.2634163 |
| H  | 69.345009  | 12.325198  | -5.3465448 |
| H  | 68.775297  | 13.574761  | -4.2634163 |
| H  | 69.345009  | 12.325198  | -5.3465448 |
| H  | 68.775297  | 13.574761  | -4.2634163 |
| H  | 71.0586688 | 4.9182220  | -8.8231613 |
```

---

```
C     0.0000000     0.0000000     0.0000000
O     1.0565510     0.0000000     -0.6100000
H   -1.9431020     0.0000000     -0.5445000
```

---

```
O   -0.2729555     2.9865449     -0.6162852
H   -0.3982614     3.5661311     0.1376588
H   -0.9261729     3.2325585     -1.2741951
```

---

```
C     0.0000000     0.0000000     0.0000000
H     1.0699340     0.0000000     -0.4666620
H   -0.5133600     0.8891650     -0.3630000
C   -0.6835370     1.1839200     -0.4833330
```
H  -1.0257760  1.7766970  0.3636670
O   0.1964190  1.9459840 -1.2611110
H  -1.5391360  0.8875320  1.2611110
H  -0.2500020  2.7192060 -1.5767780
H   1.3199380  0.0000000  1.4136620

20
./polar/glyD/coord.xyz
C  -1.9360168  0.1840963  0.8155177
O  -1.5213268  1.5021942  0.5889724
H   0.7042312  1.5048147  0.0578110
C  -2.0891952 -0.6556391 -0.4586638
O  -0.8516877 -1.0601060 -1.0081941
H  -0.3079601 -1.4483131 -0.2981696
H  -2.6998058 -1.5394750 -0.2312247
H  -2.5867799 -0.0688264 -1.2336465
H  -2.9078930  0.2568050  1.3103234
H  -1.2415439 -0.3376591  1.4964232
C   2.0574989  0.6932737 -0.4577281
O   0.8386732  1.0960157 -1.0188717
H   0.3046035  0.3033905 -1.2451681
C   1.8986014 -0.1067099  0.8426369
O   1.3932639 -1.4128681  0.6313250
H   2.0180044 -1.9019491  0.0831643
H   2.8656972 -0.1536494  1.3578244
H   1.1774801  0.3900627  1.4949239
H   2.6097647  1.6104982 -0.2394724
H   2.6388034  0.0991094 -1.1802341

10
./polar/formD/coord.xyz
C  -0.3170973  0.0000011 -0.2685418
O  -0.4054799  0.0000040  1.0505503
O   0.6970437  0.0000040  1.0505503
H   0.4781235  0.0000040  1.0505503
H  -1.3276028  0.0000040  1.0505503
C   3.1256975 -0.1600099  1.4735726
C   3.2349918 -0.1208810  0.1566296
O   2.1059362 -0.0877971  2.0879945
H   2.3618961 -0.2370097 -0.2610452
H   4.1246523 -0.2701098  1.9223913

3
./polar/watM/coord.xyz
O   1.0369778  0.0406805 -0.0577372
H   2.0048877  0.0864158 -0.0659458
H   0.7581005  0.9540305 -0.2216657

17
./non-polar/AM5/coord.xyz
C   0.0000000  0.0000000  0.2890538
C   0.0000000  1.2759574 -0.5494194
C   0.0000000 -1.2759574 -0.5494194
C   0.0000000  2.5434137  0.3011658
C   0.0000000 -2.5434137  0.3011658
H   0.8787292  0.0000000  0.9485140
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| H | -0.8787292 | 0.0000000 | 0.9485140 |
| H | 0.8780102  | 1.2739334 | -1.2075176 |
| H | -0.8780102 | 1.2739334 | -1.2075176 |
| H | 0.8780102  | -1.2739334 | -1.2075176 |
| H | -0.8780102 | -1.2739334 | -1.2075176 |
| H | 0.8840252  | 2.5798987 | 0.9453810 |
| H | -0.8840252 | 2.5798987 | 0.9453810 |
| H | 0.0000000  | 3.4436170 | -0.3205143 |
| H | -0.8840252 | -2.5798987 | 0.9453810 |
| H | 0.0000000  | -3.4436170 | -0.3205143 |

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```
./non-polar/AD3/coord.xyz
C  0.4204721  1.8817695  0.0000000
C  -0.4204721  1.9972866  1.2682314
C  -0.4204721  1.9972866 -1.2682314
H  1.1909863  2.6612617  0.0000000
H  0.9522613  0.9233853  0.0000000
H  0.1959851  1.9126055  2.1678836
H  -1.1792913  1.2093343  1.3048524
H  -0.9387183  2.9606628  1.3048524
H  0.1959851  1.9126055 -2.1678836
H  -1.1792913  1.2093343 -1.3048524
H  -0.9387183  2.9606628 -1.3048524
C  -0.4204721 -1.8817695  0.0000000
C  0.4204721 -1.9972866 -1.2682314
C  0.4204721 -1.9972866  1.2682314
H  -0.9522613 -0.9233853  0.0000000
H  -1.1909863 -2.6612617  0.0000000
H  -0.1959851 -1.9126055 -2.1678836
H  0.9387183  2.9606628 -1.3048524
H  1.1792913 -1.2093343 -1.3048524
H  -0.1959851 -1.9126055  2.1678836
H  0.9387183 -2.9606628  1.3048524
H  1.1792913 -1.2093343  1.3048524
```

40

```
./non-polar/AD6/coord.xyz
C  0.6455512 -0.4075631  1.9460355
C  -0.6455512  0.4075631  1.9460355
C  1.9052445  0.4555481  1.9460345
C  -1.9052445 -0.4555481  1.9460345
C  3.1888719 -0.3704591  1.9460345
C  -3.1888719  0.3704591  1.9460345
H  0.6587912  1.0666783  2.8248308
H  0.6587912  1.0666773  1.0672393
H  -0.6587912  1.0666783  2.8248308
H  -0.6587912  1.0666773  1.0672393
H  1.8904095  1.1134623  1.0680263
H  1.8904085  1.1134633  2.8240438
H  -1.8904095 -1.1134623  1.0680263
H  -1.8904085 -1.1134633  2.8240438
H  4.0768971  0.2685301  1.9460345
H  3.2377869 -1.0138303  1.0619863
H  3.2377869 -1.0138303  2.8300818
```
|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| H   | 2.7887418 | -0.7496292 | 0.0000000 |
| H   | 1.0310143  | -0.7496292 | 0.0000000 |
| H   | 2.7886698  | 1.4087614  | -1.2756534 |
| H   | 1.0310863  | 1.4087614  | -1.2756534 |
| H   | 2.7886698  | 1.4087614  | 1.2756534  |
| H   | 1.0310863  | 1.4087614  | 1.2756534  |
| H   | 2.7879018  | -0.7471852  | -2.5492767 |
| H   | 1.0318543  | -0.7471852  | -2.5492767 |
| H   | 2.7879018  | -0.7471852  | 2.5492767  |
| H   | 1.0318543  | -0.7471852  | 2.5492767  |
| H   | 2.7939298  | 1.4057854  | -3.8552161 |
| H   | 1.0258263  | 1.4057854  | -3.8552161 |
| H   | 1.9098775  | 0.1399130  | -4.7190203 |
| H   | 1.9098775  | 0.1399130  | -4.7190203 |

C       
-3.7662738  -2.3264955  -0.1103441  
-2.4091733  -1.9832009  -0.7116737  
-1.7159935  -0.8595944  0.0546844  
-0.3588714  -0.5026170  -0.5458411  
 0.3352502   0.6151661   0.2281926  
 1.6888308   0.9797979  -0.3757822  
 2.3854876   2.0933863   0.4022359  
 3.7327114   2.4579087  -0.2090800  
 3.6070058   2.7997779  -1.2342996  
 4.2106228   3.2511454   0.3611748  
 4.3958170   1.5952647  -0.2166427  
 2.5321995   1.7738305   1.4361801  
 1.7435213   2.9773112   0.4173558  
 1.5483389   1.2974982  -1.4119594  
 2.3290245   0.0940800  -0.3888078  
-0.3058768  1.5001502   0.2361252  
 0.4761490   0.3014008  1.2648150  
 0.2792917  -1.3899883  -0.5490489  
-0.4937737  -0.1928989  -1.5852295  
-2.3559436   0.0262290   0.0513470  
-1.5805299  -1.1647659  1.0945991  
-2.5389547  -1.6830010  -1.7542008  
-1.7727606  -2.8714925  -0.7026782  
-3.6556128  -2.6345661  0.9266917  
-4.4266024  -1.4623275  -0.1412273  
-4.2370387  -3.1380195  -0.6607205  
-3.2871229  -5.5029610  2.7084948  
-1.9371947  -5.1597209  2.0908065  
-1.2292664  -4.0422012  2.8528490  
 0.1250792  -3.6954836  2.2400871  
 0.8326284  -2.5774593  3.0014955  
 2.1873714  -2.2332796  2.3882702  
 2.8958486  -1.1127602  3.1450718  
 4.2477192  -0.7777707  2.5275347  
 4.1264749  -0.4690474  1.4918604  
 4.7299059   0.0309629  3.0720804  
 4.9031363  -1.6459157  2.5505473  

52
/non-polar/AD8/coord.xyz
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| H       | 3.0360462  | -1.4124331 | 4.1863972  |
| H       | 2.2643868  | -0.2209290 | 3.1423170  |
| H       | 2.0453667  | -1.9302718 | 1.3485907  |
| H       | 2.8203260  | -3.1241210 | 2.3889108  |
| H       | 0.2003738  | -1.6858617 | 3.0038879  |
| H       | 0.9734610  | -2.8814164 | 4.0417926  |
| H       | 0.7580079  | -4.5863722 | 2.2372897  |
| H       | -0.0172925 | -3.3895111 | 1.2013358  |
| H       | -1.8625570 | -3.1514139 | 2.8571157  |
| H       | -1.0878471 | -4.3483003 | 3.8923855  |
| H       | -2.081755  | -4.8530652 | 1.0526727  |
| H       | -1.3036609 | -6.0498182 | 2.0872913  |
| H       | -3.1634749 | -5.8316210 | 3.7382689  |
| H       | -3.9420689 | -4.6340397 | 2.7048008  |
| H       | -3.7732161 | -6.2994801 | 2.1498716  |

16
/.non-polar/AD2/coord.xyz
| C       | 0.6841602  | 0.3377511  | -1.9114825 |
| C       | -0.6841602 | -0.3377511 | -1.9114825 |
| H       | 1.4896454  | -0.4014341 | -1.9114825 |
| H       | 0.8127732  | 0.9696603  | -2.7942918 |
| H       | 0.8127732  | 0.9696603  | -1.0286733 |
| H       | -1.4896454 | 0.4014341  | -1.9114825 |
| H       | -0.8127732 | -0.9696603 | -2.7942918 |
| C       | 0.6841602  | -0.3377511 | 1.9114825  |
| C       | -0.6841602 | 0.3377511  | 1.9114825  |
| H       | 1.4896454  | 0.4014341  | 1.9114825  |
| H       | 0.8127732  | -0.9696603 | 2.7942918  |
| H       | 0.8127732  | -0.9696603 | 1.0286733  |
| H       | -1.4896454 | -0.4014341 | 1.9114825  |
| H       | -0.8127732 | 0.9696603  | 2.7942918  |
| H       | -0.8127732 | 0.9696603  | 1.0286733  |

8
/.non-polar/AM2/coord.xyz
| C       | 0.0000000  | 0.0000000  | 0.7629882  |
| C       | 0.0000000  | 0.0000000  | -0.7629882 |
| H       | -0.8828090 | 0.5096900  | 1.1580401  |
| H       | 0.0000000  | -1.0193801 | 1.1580401  |
| H       | 0.8828090  | 0.5096900  | 1.1580401  |
| H       | 0.8828090  | -0.5096900 | -1.1580401 |
| H       | -0.8828090 | -0.5096900 | -1.1580401 |
| H       | 0.0000000  | 1.0193801  | -1.1580401 |

26
/.non-polar/AM8/coord.xyz
| C       | -4.0723487 | -0.7352776 | 0.0789607  |
| C       | -2.6813934 | -0.4192378 | -0.4569172 |
| C       | -2.0575181 | 0.7803448  | 0.2521823  |
| C       | -0.6635748 | 1.1033766  | -0.2799647 |
| C       | -0.0412253 | 2.3035421  | 0.4294783  |
| C       | 1.3525974  | 2.6267329  | -0.1028970 |
| C       | 1.9758331  | 3.8272975  | 0.6050956  |
| C       | 3.3665871  | 4.1436156  | 0.0688500  |
H  3.3227159  4.3708652 -0.9942001
H  3.7916779  5.0009149  0.5857992
H  4.0315299  3.2939709 -1.1742175
H  2.0381450  3.6213558  1.6762168
H  1.3295453  4.6983049  0.4737275
H  1.2907609  2.8329529 -1.1742175
H  1.9996825  1.7559624  0.0279281
H  0.0206707  2.0970974  1.5007848
H  0.0168789  0.2321678 -0.1498331
H  0.7253292  1.3098149 -1.3512855
H  2.7041718  0.1149902 -1.5278499
H  4.0286371 -0.9638140  1.1417403
H  4.7367070 -0.0600263 -0.0602635
H  4.4980163 -1.5916758 -0.4390090

14
./non-polar/AM4/coord.xyz
C  0.6232492  0.4407581  0.0000000
C -0.6232492 -0.4407581  0.0000000
C  1.9195875 -0.3647201  0.0000000
C -1.9195875  0.3647201  0.0000000
H  0.5976292  1.0985823  0.8779384
H  0.5976292  1.0985823 -0.8779384
H -0.5976292 -1.0985823  0.8779384
H -0.5976292 -1.0985823 -0.8779384
H  2.7973868  0.2880911  0.0000000
H  1.9787876 -1.0072833  0.8840144
H  1.9787876 -1.0072833 -0.8840144
H -2.7973868 -0.2880911  0.0000000
H -1.9787876  1.0072833  0.8840144
H -1.9787876  1.0072833 -0.8840144

34
./non-polar/AD5/coord.xyz
C -1.9517435  0.2128361  0.0000000
C -1.9517435 -0.6256372  1.2759574
C -1.9517435 -0.6256372 -1.2759574
C -1.9517435  0.2249481  2.5434137
C -1.9517435  0.2249481 -2.5434137
H -2.8304728  0.8722962  0.0000000
H -1.0730143  0.8722962  0.0000000
H -2.8297538 -1.2837354  1.2739334
H -1.0737333 -1.2837354  1.2739334
H -2.8297538 -1.2837354 -1.2739334
H -1.0737333 -1.2837354 -1.2739334
H -2.8357688  0.8691632  2.5798987
H -1.0677183  0.8691632  2.5798987
H -1.9517435 -0.3967321  3.4436170
H -2.8357688  0.8691632 -2.5798987
H -1.0677183  0.8691632 -2.5798987
H -1.9517435 -0.3967321 -3.4436170
C  1.9517435  0.2128361  0.0000000
