*SUPPORTING INFORMATION FOR*

# Direct detection of polar structure formation in helium nanodroplets by beam deflection measurements

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Contents

## I. $(DMSO)_n$ ion mass spectra

As described in the main text, deflection profiles of droplets doped with DMSO monomers, dimers, or trimers were acquired by setting the mass spectrometer to the masses of $(DMSO)^+$, $(DMSO)_2^+$ and $(DMSO)_3^+$ ions, respectively, and maintaining the pickup vapor pressure at a level such that the mass peak of interest would be dominant over the next higher one. This is illustrated in Fig. S1. The mass spectrometer is a Balzers QMG-511 crossed-beam quadrupole analyzer with its electron impact ionization source set to 90 eV impact energy.

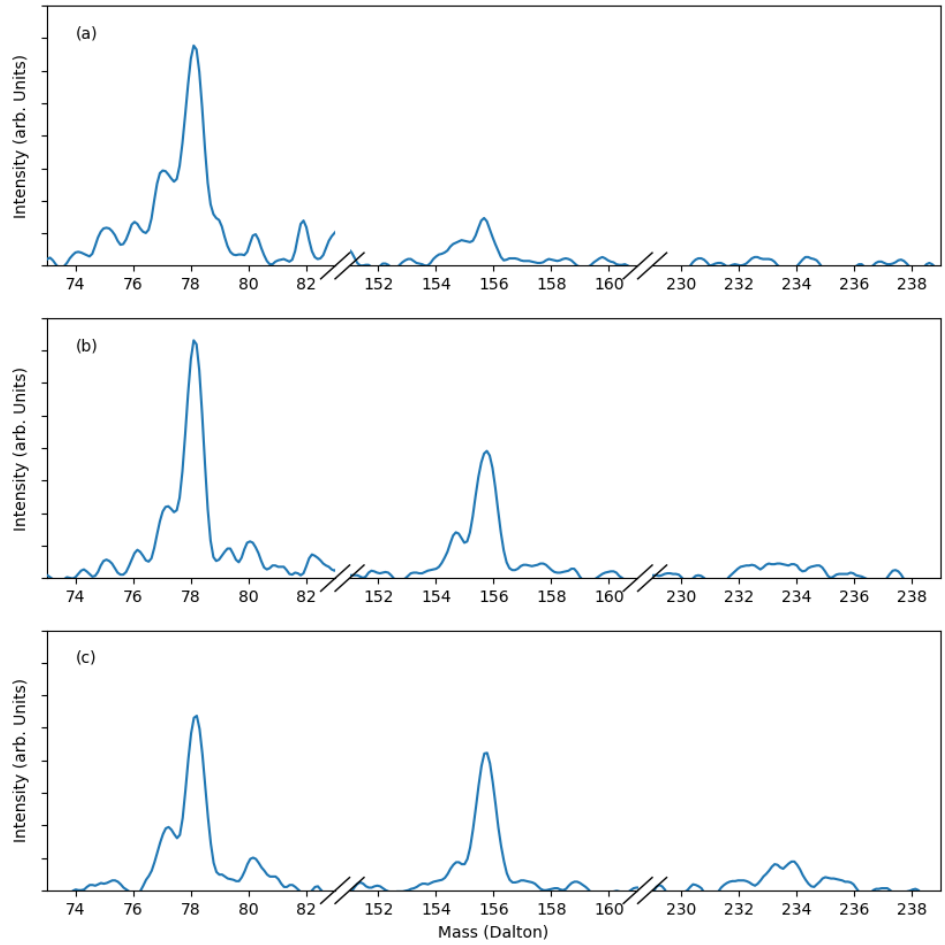


**Figure S1.** Representative mass spectra corresponding to deflection measurements on $(DMSO)_n$-doped nanodroplets. The mass spectrometer was set to the masses of intact ions: (a) 78 Da for the monomer, (b) 156 Da for the dimer, (c) 234 Da for the trimer.

## II. Ab initio calculations: Benchmarking

The potential energy surface was explored with the B3LYP(D2)/aug-cc-pVDZ method. The dipole moment of the isolated DMSO molecule in its equilibrium geometry calculated with this approach was 4.3 D, which is consistent with the tabulated value[S1] of 4.0 D within the expected accuracy of DFT.[S2] We validated this approach against the high-level CCSD(T)/aug-cc-pVTZ method. Basis set superposition error (BSSE) correction was used for all structures. The agreement is very good for all cluster structures, see Table S1. We also show the energetics of the respective minima at the DFTB/D3 level used for exploratory simulations. The DFT and CCSD(T) calculations were performed in the Gaussian 09, rev. D01 package,[S3] the DFTB results were calculated in the DFTB+ 18.2 program.[S4]

**Table S1.** Comparison of DMSO dimer binding energies at the CCSD(T), B3LYP(D2) and DFTB(D3) levels. The BSSE correction was accounted for in the CCSD(T) and B3LYP(D2) calculations.

| **Dimer complex** | Binding energy [eV] | | |
|---|---|---|---|
| | CCSD(T)/aug-cc-pVTZ | B3LYP/aug-cc-pVDZ D2 | DFTB |
| **D1** | 0.53 | 0.56 | 0.46 |
| **D2** | 0.46 | 0.47 | 0.41 |
| **D3** | 0.40 | 0.39 | 0.36 |
| **D4** | 0.33 | 0.33 | 0.28 |
| **D5** | 0.32 | 0.32 | 0.26 |

## III. Mapping of the $(DMSO)_2$ and $(DMSO)_3$ potential energy surfaces

The potential energy surfaces (PES) of DMSO complexes are rather rich and we mapped them in the following way. First, we performed accelerated molecular dynamics simulations with the molecular mechanics (MM) force field,[S5] using the so-called metadynamics method.[S6] Here, an additional potential is added along a preselected coordinate so that we can quickly overcome barriers along these coordinates. These simulations then also provide the free energy as a function of the selected coordinate [potential of mean force (PMF) or free energy surface (FES)]. We then selected different structures with distinct dipole moments from these metadynamical trajectories and performed further B3LYP optimization.

Metadynamics simulations were performed at 100 K to reveal the regions of interest in the dipole moment coordinate. This temperature is much higher than the experimental conditions, yet we opted for it to avoid ergodicity problems. Note that these simulations are only auxiliary, serving as a starting point for minimizations or MD simulations. The minimum on the PMF is found for a small yet non-zero dipole moment due to entropic reasons. The force field overestimates the dipole moment by 20% with respect to the *ab initio* value. The final PMFs for the dimer and trimer complexes are displayed in Fig. S2.

By clustering structures with similar dipoles together and performing 100 subsequent optimizations with Gaussian 09, for both the dimer and trimer structures, we were then able to map their PES landscapes.

The metadynamics parameters were as follows. The dimer simulation length was 100 ps, leap-frog stochastic integrator was utilized, the temperature was set to 100 K with a thermostat constant of $\tau$ =1.0 ps. For the trimer the simulation length was increased to 300 ps. The collective variable (CV) is the total dipole moment. An additional Gaussian potential was added every 100 steps. The Gaussian height was 0.015 kJ/mol and the CV gaussian width was 1.2 Debye.

MD simulations were performed with GROMACS 2018.4 code[S7] coupled with PLUMED 2.5 code[S8] for the FES simulations.

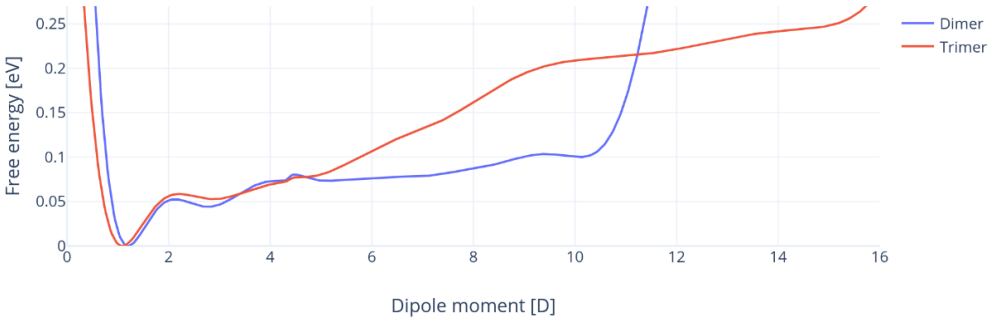


**Figure S2.** PMF for DMSO dimer and trimer complexes for the dipole moment coordinate at 100K.

## IV. Transition between two dimers at a distance and D5

Nudged elastic band (NEB) optimization[S9] was performed to find energy barriers between two DMSO molecules a distance apart (13.5 Å; in the minimal geometry at that separation the two DMSO molecules have aligned dipoles) and complex D5. Fig. S3 shows that the connection is barrierless.

The simulations were carried out in the TeraChem code[S10,S11] using the B3LYP(D2)/aug-cc-pVDZ method with 14 molecular images between the two structures. The images were generated by constrained minimization.

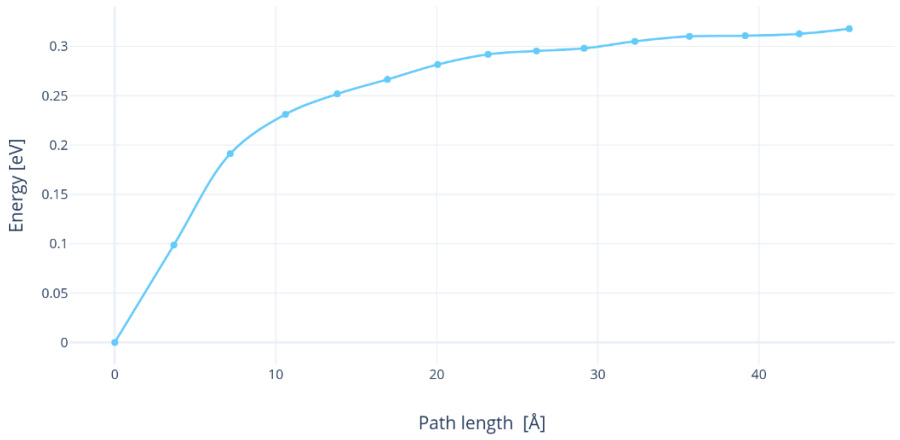


**Figure S3.** NEB calculations connecting the long-distance configuration to the D5 minimum.

## V. Transition between the D5 and D1 minima

We also performed NEB calculation connecting the D5 minimum with the global D1 minimum. The final energy curve is shown in Fig. S4.

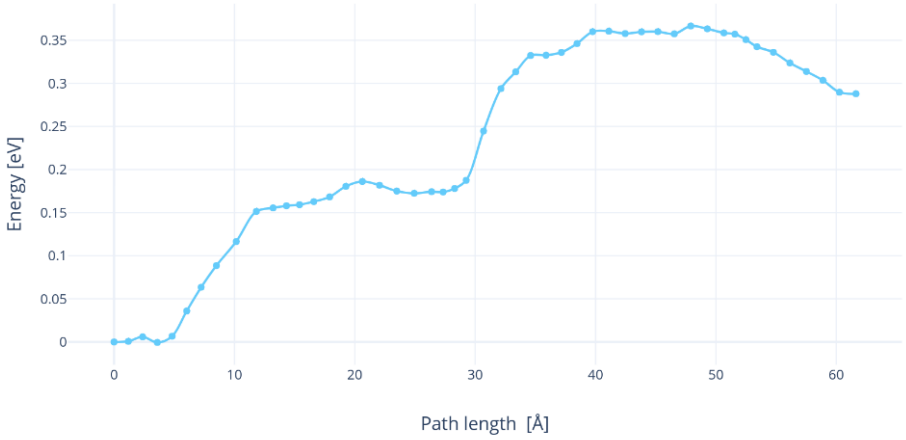


**Figure S4.** NEB calculations connecting the minima D1 and D5.

## VI. Two dimensional free energy surface

Additional insight into the topology of the multidimensional PES of DMSO aggregates can be brought about via modeling of free energy surfaces (FES). We evaluated the FES (i.e., the two dimensional version of the PMF in Fig. S2) as a function of two coordinates: the aggregate dipole moment and the interatomic S-S distance, see Figs. S5-S8. The graphs were once again generated using the metadynamics method and the temperature of 100 K to avoid convergence issues. It is clear that at large intermolecular distance the system prefers the high-dipole configuration, as mentioned above. At close distances one observes a number of minima separated by barriers.

The 2D metadynamics parameters were as follows. As before, for the dimer the simulation length was 100 ps, leap-frog stochastic integrator was utilized, the temperature was set to 100 K with thermostat constant $\tau$=1.0 ps. The first collective variable, CV1, was defined as the S-S interatomic distance between the DMSO monomers. An additional Gaussian potential was added at every 1000 steps. The Gaussian height was 0.015 kJ/mol and the CV1 Gaussian width was 0.1 nm. The second collective variable was the dipole moment with the same deposition parameters as CV1 and Gaussian width of 1.2 D. Upper energetic walls for CV1 were applied at 2 nm in order to keep the molecule in the area of interest.

For the trimer the simulation length was increased tenfold to 1000 ps, with the other parameters fixed. CV1 was redefined as the sum of S-S interatomic distances due to the presence of the third DMSO molecule, the other variables remained the same. The upper energetic walls for CV1 were shifted to 6.0 nm.

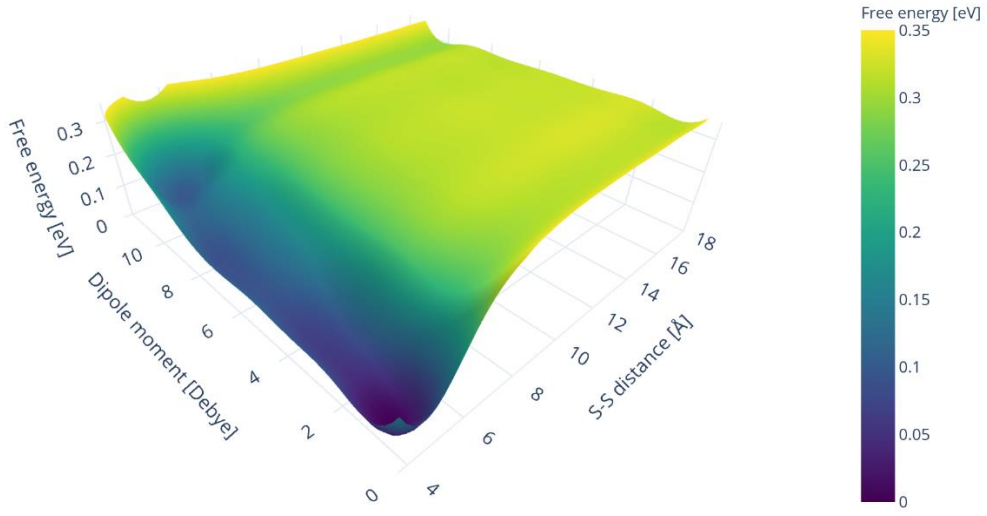


**Figure S5.** FES for the DMSO dimer at 100 K.

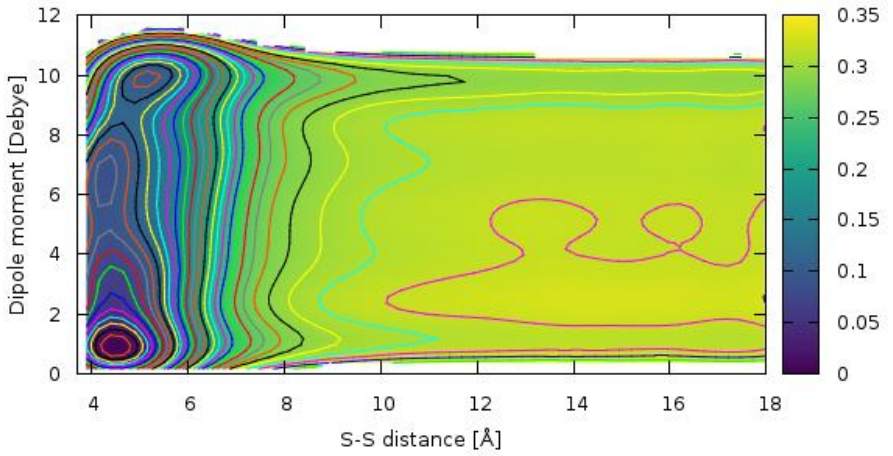


**Figure S6**. FES heatmap for the DMSO dimer at 100 K. Contour spacing 0.01 eV.

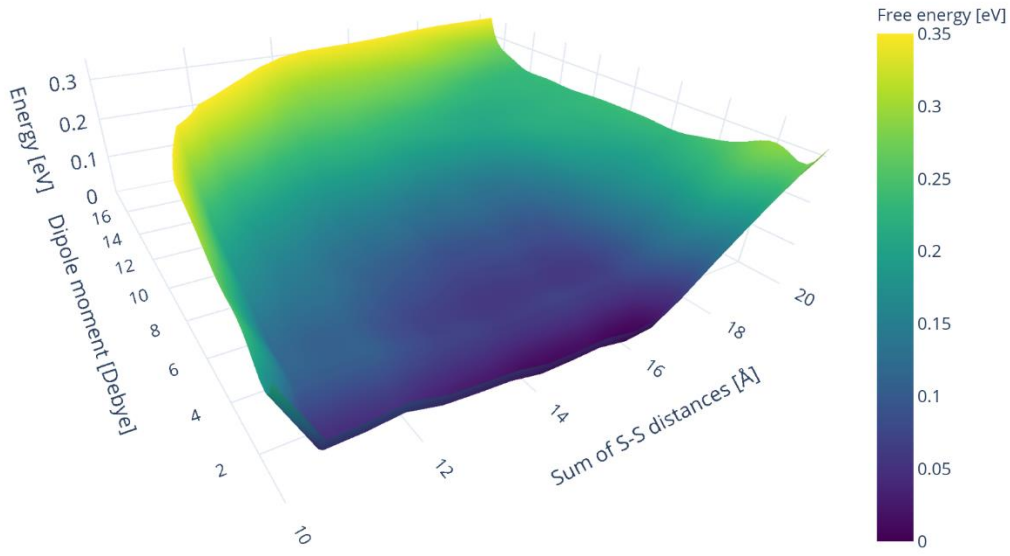


**Figure S7.** FES for the DMSO trimer at 100 K.

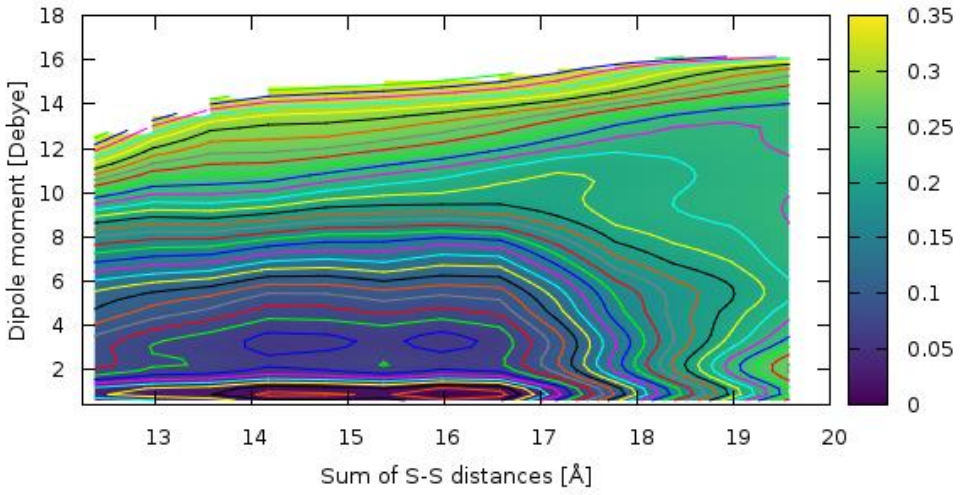


**Figure S8.** FES heatmap for the DMSO trimer at 100 K. Contour spacing 0.01 eV.

## VII. Force field parameters

The MM simulations were performed with parameters taken from ref S5. The parameters are summarized in Tables S2 and S3.

**Table S2.** Atomic type parameters for DMSO.

| Atom | Charge | $\varepsilon$ (kJ/mol) | $\sigma$ (nm) |
|---|---|---|---|
| O | -0.556 | 0.50242 | 0.30291 |
| S | 0.312 | 1.46537 | 0.35636 |
| C | -0.148 | 0.32657 | 0.36348 |
| H | 0.090 | 0.10048 | 0.23876 |

**Table S3.** Intermolecular parameters for DMSO.

| Bond | $b_0$ (nm) | $f_c$ (kJ mol$^{-1}$ nm$^{-2}$) |
|---|---|---|
| H-C | 0.111 | 134724.8 |
| C-S | 0.180 | 100416.0 |
| S-O | 0.153 | 225936.0 |

| Angles | $\theta_0$ (nm) | $f_c$ (kJ mol$^{-1}$ rad$^{-2}$) |
|---|---|---|
| H-C-H | 108.400 | 148.5320 |
| H-C-S | 111.300 | 192.8824 |
| C-S-O | 106.750 | 330.5360 |
| C-S-C | 95.000 | 142.2560 |

| Dihedrals | $\varphi_0$ (deg) | $f_c$ (kJ mol$^{-1}$) | $X$ |
|---|---|---|---|
| H-C-S-O | 0.0 | 0.8368 | 3 |
| H-C-S-C | 0.0 | 0.8368 | 3 |

## VIII. Cartesian coordinates of all structures

Geometries of the optimal structures presented in Figs. 2 and 4 of the main text are listed below, with all coordinates in Angstroms.

Monomer
10

| | | | |
|---|---|---|---|
| C | 1.390750 | 0.279323 | -0.278296 |
| S | 0.072728 | -0.679506 | 0.585004 |
| C | -1.342363 | 0.171624 | -0.236526 |
| O | 0.075720 | -0.189227 | 2.044957 |
| H | 1.346127 | 0.069130 | -1.356470 |
| H | 1.227420 | 1.344812 | -0.066434 |
| H | 2.347951 | -0.053762 | 0.141464 |
| H | -1.314193 | -0.035613 | -1.315827 |
| H | -2.257159 | -0.235280 | 0.211752 |
| H | -1.256995 | 1.246897 | -0.028367 |

D1
20

| | | | |
|---|---|---|---|
| C | 1.391830 | 0.296071 | -0.267191 |
| S | 0.073035 | -0.689518 | 0.555023 |
| C | -1.343411 | 0.188626 | -0.225497 |
| O | 0.078854 | -0.256270 | 2.047129 |
| H | 1.379923 | 0.056354 | -1.339642 |
| H | 1.179380 | 1.359143 | -0.087564 |
| H | 2.341205 | -0.018939 | 0.183566 |
| H | -1.345350 | -0.050790 | -1.298081 |
| H | -2.251051 | -0.199163 | 0.253587 |
| H | -1.209576 | 1.265306 | -0.051326 |
| S | -0.073081 | 3.587139 | 1.938615 |
| O | -0.078682 | 3.153903 | 0.446506 |
| C | -1.391839 | 2.601376 | 2.760682 |
| C | 1.343385 | 2.709142 | 2.719264 |
| H | -1.380080 | 2.841096 | 3.833135 |
| H | -2.341208 | 2.916257 | 2.309824 |
| H | -1.179218 | 1.538334 | 2.581077 |
| H | 1.345162 | 2.948483 | 3.791865 |
| H | 1.209699 | 1.632459 | 2.545001 |
| H | 2.251033 | 3.097074 | 2.240313 |

D2
20

| | | | |
|---|---|---|---|
| O | 8.826895 | 8.110270 | 10.400227 |
| S | 9.972464 | 7.608129 | 9.483674 |
| C | 11.539269 | 7.974326 | 10.379345 |
| H | 12.382316 | 7.730081 | 9.717863 |
| H | 11.525836 | 9.039717 | 10.646509 |
| H | 11.551024 | 7.328890 | 11.266521 |
| C | 10.186293 | 8.892506 | 8.183524 |
| H | 11.035534 | 8.602394 | 7.548535 |
| H | 9.256912 | 8.900193 | 7.600878 |
| H | 10.362717 | 9.852789 | 8.687985 |
| O | 10.697510 | 11.161246 | 10.536141 |
| S | 9.253455 | 11.346438 | 11.076378 |
| C | 9.145789 | 10.330797 | 12.600760 |
| H | 8.213528 | 10.584098 | 13.124409 |
| H | 9.133390 | 9.289859 | 12.256910 |
| H | 10.027135 | 10.559985 | 13.215271 |
| C | 9.274676 | 12.983721 | 11.916622 |
| H | 8.313117 | 13.137349 | 12.426572 |
| H | 10.112562 | 12.992963 | 12.626663 |
| H | 9.422581 | 13.740250 | 11.136213 |

D3
20

| | | | |
|---|---|---|---|
| C | -6.599507 | -9.935427 | -8.808258 |
| S | -6.050826 | -8.220930 | -8.418528 |
| C | -7.587463 | -7.381111 | -8.969174 |
| O | -4.975044 | -7.895873 | -9.486073 |
| H | -7.454125 | -10.195223 | -8.167596 |
| H | -6.867985 | -9.974321 | -9.872589 |
| H | -5.748550 | -10.596439 | -8.602335 |
| H | -8.424339 | -7.741197 | -8.354184 |
| H | -7.407231 | -6.311806 | -8.806702 |
| H | -7.734957 | -7.620273 | -10.031201 |
| S | -4.736135 | -4.653480 | -8.965041 |
| O | -5.810347 | -4.978975 | -7.896071 |
| C | -4.188088 | -2.938502 | -8.576590 |
| C | -3.198394 | -5.492320 | -8.416137 |
| H | -3.333958 | -2.678643 | -9.217880 |
| H | -5.039455 | -2.277959 | -8.782326 |
| H | -3.918996 | -2.898989 | -7.512438 |
| H | -2.362832 | -5.133640 | -9.033730 |
| H | -3.048402 | -5.251363 | -7.354870 |
| H | -3.379470 | -6.561814 | -8.576431 |

D4
20

| | | | |
|---|---|---|---|
| O | 10.770543 | 12.406453 | 7.172925 |
| S | 10.996603 | 12.217603 | 8.692035 |
| C | 12.663048 | 11.452412 | 8.865018 |
| H | 12.827871 | 11.198932 | 9.921240 |
| H | 12.692858 | 10.559951 | 8.226519 |
| H | 13.389878 | 12.202747 | 8.531247 |
| C | 10.042817 | 10.713973 | 9.163143 |
| H | 10.255542 | 10.475201 | 10.214216 |
| H | 8.982319 | 10.960304 | 9.031380 |
| H | 10.346341 | 9.897937 | 8.494552 |
| O | 11.783311 | 8.009573 | 5.181466 |
| S | 11.481115 | 9.357691 | 5.867285 |
| C | 12.445813 | 10.642888 | 4.970928 |
| H | 12.145669 | 11.622494 | 5.364081 |
| H | 13.505277 | 10.435700 | 5.167309 |
| H | 12.228607 | 10.534564 | 3.900118 |
| C | 9.828399 | 9.903572 | 5.270228 |
| H | 9.653478 | 10.918986 | 5.647899 |
| H | 9.840437 | 9.858877 | 4.173228 |
| H | 9.097072 | 9.191144 | 5.672183 |

D5
20

| | | | |
|---|---|---|---|
| C | 0.832083 | 0.053205 | 0.687160 |
| S | -0.018838 | 0.529481 | -0.873482 |
| S | 1.568387 | -2.573673 | -1.989863 |
| C | 0.721902 | -2.067199 | -3.541948 |
| C | -1.624708 | -0.272902 | -0.470355 |
| O | -0.252453 | 2.053432 | -0.806970 |
| O | 0.449839 | -2.770887 | -0.938584 |
| C | 2.024752 | -4.266109 | -2.547539 |
| H | 0.867295 | -1.043176 | 0.726962 |
| H | 1.838413 | 0.487869 | 0.644560 |
| H | 0.262499 | 0.486055 | 1.520395 |
| H | -1.455444 | -1.355871 | -0.418903 |
| H | -1.978107 | 0.143628 | 0.482340 |
| H | -2.317341 | -0.012725 | -1.280529 |
| H | 2.733390 | -4.189503 | -3.384114 |
| H | 2.491453 | -4.765940 | -1.690035 |
| H | 1.103863 | -4.786018 | -2.843846 |
| H | 1.450590 | -2.071775 | -4.364292 |
| H | -0.098565 | -2.774219 | -3.724319 |
| H | 0.340792 | -1.054444 | -3.366810 |

T1
30

| | | | |
|---|---|---|---|
| O | 18.325573 | 19.811653 | 21.617481 |
| S | 19.721884 | 20.312996 | 21.169378 |
| C | 20.228323 | 21.608815 | 22.376809 |
| H | 21.215482 | 21.985848 | 22.075579 |
| H | 19.485068 | 22.415686 | 22.369997 |
| H | 20.289383 | 21.113897 | 23.353709 |
| C | 19.440363 | 21.463757 | 19.758658 |
| H | 20.418372 | 21.838813 | 19.426676 |
| H | 18.968548 | 20.870817 | 18.965678 |
| H | 18.799604 | 22.289633 | 20.091628 |
| O | 18.271096 | 24.146530 | 21.392567 |
| S | 17.718310 | 25.601134 | 21.478337 |
| C | 16.938575 | 25.747636 | 23.136233 |
| H | 16.505635 | 26.754394 | 23.216988 |
| H | 16.166283 | 24.969074 | 23.217754 |
| H | 17.742714 | 25.618895 | 23.871189 |
| C | 16.151632 | 25.602873 | 20.517245 |
| H | 15.714781 | 26.608754 | 20.587075 |
| H | 16.422965 | 25.376776 | 19.478677 |
| H | 15.486136 | 24.843390 | 20.952583 |
| O | 14.642326 | 23.527870 | 22.517495 |
| S | 15.116812 | 22.043647 | 22.457649 |
| C | 16.675088 | 21.971241 | 23.424806 |
| H | 17.142014 | 20.993610 | 23.248081 |
| H | 17.321498 | 22.778503 | 23.058847 |
| H | 16.399735 | 22.113636 | 24.476868 |
| C | 15.887654 | 21.824953 | 20.806281 |
| H | 16.405169 | 20.856910 | 20.796220 |
| H | 15.074819 | 21.866766 | 20.071118 |
| H | 16.603161 | 22.645493 | 20.671394 |

T2
30

| | | | |
|---|---|---|---|
| C | 19.978371 | 22.960022 | 19.710536 |
| S | 19.735892 | 23.242403 | 21.510328 |
| C | 20.388685 | 21.613064 | 22.058900 |
| O | 18.198954 | 23.189838 | 21.745112 |
| C | 15.358815 | 23.917374 | 20.096399 |
| S | 14.121084 | 23.111607 | 21.194225 |
| C | 15.047600 | 23.377434 | 22.762579 |
| O | 14.190395 | 21.590951 | 20.897064 |
| S | 17.054341 | 20.556144 | 20.208772 |
| C | 15.942352 | 19.217124 | 19.628149 |

O 18.501515 20.064915 19.893824
C 16.827935 20.251673 22.004302
H 21.059208 22.936455 19.512556
H 19.496985 22.004570 19.454354
H 19.514939 23.811524 19.197357
H 21.467010 21.591478 21.848409
H 20.210845 21.552465 23.139753
H 19.850741 20.831749 21.503192
H 15.760191 20.345461 22.229074
H 17.216281 19.244890 22.206490
H 17.413863 21.021960 22.516917
H 14.919373 19.492859 19.911972
H 16.052332 19.168894 18.537795
H 16.267612 18.274891 20.088960
H 15.332881 24.997756 20.296283
H 16.349231 23.496971 20.310933
H 15.040118 23.707847 19.068112
H 15.045690 24.454363 22.980238
H 14.504377 22.828117 23.541197
H 16.073387 23.010200 22.639216

T3
30

C 19.318080 22.762136 22.418743
S 18.401131 21.379365 21.618767
C 18.852818 21.822207 19.888771
O 16.894078 21.701134 21.778298
O 19.025390 25.162225 20.116170
S 18.978878 26.478380 19.285963
C 18.218864 27.737277 20.375610
C 20.695828 27.130948 19.340978
C 16.290257 24.915699 22.126303
S 15.070039 25.136098 20.770491
C 15.850747 23.953991 19.603056
O 15.323351 26.555016 20.184537
H 20.393691 22.575593 22.293887
H 19.028486 23.706104 21.941314
H 19.045684 22.740531 23.480909
H 19.921248 21.605360 19.751253
H 18.245550 21.181412 19.238001
H 18.646287 22.887366 19.725303
H 20.713003 28.127033 18.877545
H 21.008893 27.173273 20.392785
H 21.324967 26.432136 18.776249
H 18.326517 28.718024 19.891996
H 17.157993 27.455148 20.467183

H 18.745592 27.706182 21.339379
H 16.277900 23.860237 22.428986
H 17.274927 25.192098 21.728825
H 15.980785 25.581780 22.940796
H 15.862931 22.963479 20.077728
H 15.245255 23.967205 18.688986
H 16.872837 24.307564 19.416185

T4
30

C 5.071517 -0.034670 -3.655985
S 4.287297 -0.194668 -1.997307
C 5.830416 -0.559251 -1.075361
O 3.893217 1.257561 -1.611793
S -0.020529 2.540318 0.295084
C 1.283159 3.066414 -0.885371
O 0.572434 2.732177 1.715202
C 3.644181 1.756288 1.598188
S 2.617946 0.269497 1.276626
C 1.964214 0.086045 2.982365
O 3.615924 -0.905124 1.078908
H 1.323627 0.953582 3.183548
H 1.388114 -0.847471 2.998202
H 2.818493 0.022048 3.669544
H 2.968760 2.565559 1.900207
H 4.362207 1.495270 2.386815
H 4.148555 1.979398 0.651252
H 0.822989 3.182558 -1.876460
H 1.688760 4.020594 -0.522132
H 2.057413 2.289562 -0.920766
H 5.497260 -1.005416 -3.946611
H 4.282043 0.264332 -4.356496
H 5.846821 0.740863 -3.594728
H 6.247662 -1.502562 -1.454190
H 6.520679 0.279922 -1.237121
H 5.523931 -0.655551 -0.027295
C -1.126902 3.988674 0.041019
H -1.509237 3.972861 -0.989222
H -1.948976 3.889460 0.760368
H -0.546405 4.899313 0.241051

T5
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| | | | |
|---|---|---|---|
| O | 16.634857 | 24.592189 | 18.933949 |
| S | 17.819686 | 24.188608 | 19.842340 |
| C | 18.546611 | 25.748060 | 20.487096 |
| H | 19.438384 | 25.480875 | 21.069767 |
| H | 18.776646 | 26.394312 | 19.630220 |
| H | 17.780785 | 26.213377 | 21.119207 |
| C | 19.237765 | 23.746631 | 18.763679 |
| H | 20.096423 | 23.565749 | 19.425082 |
| H | 18.955755 | 22.836787 | 18.219781 |
| H | 19.417204 | 24.574596 | 18.065138 |
| O | 20.209226 | 23.485765 | 22.163446 |
| S | 18.877554 | 23.104769 | 22.864853 |
| C | 19.254372 | 22.812446 | 24.636229 |
| H | 18.324234 | 22.468296 | 25.107880 |
| H | 20.058270 | 22.067975 | 24.708308 |
| H | 19.577739 | 23.772502 | 25.056335 |
| C | 18.574534 | 21.347602 | 22.430705 |
| H | 17.751416 | 20.981712 | 23.056223 |
| H | 18.299881 | 21.331231 | 21.369829 |
| H | 19.512448 | 20.803987 | 22.601658 |
| O | 15.856035 | 22.403783 | 23.805490 |
| S | 15.408064 | 22.687282 | 22.347855 |
| C | 15.384240 | 24.514743 | 22.152187 |
| H | 15.163099 | 24.748814 | 21.101020 |
| H | 14.647435 | 24.936357 | 22.847504 |
| H | 16.395863 | 24.844707 | 22.412702 |
| C | 13.585634 | 22.453003 | 22.322482 |
| H | 13.200021 | 22.813677 | 21.358789 |
| H | 13.395364 | 21.379488 | 22.440968 |
| H | 13.163459 | 23.017678 | 23.164279 |

T6
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| | | | |
|---|---|---|---|
| O | 18.248791 | 19.538962 | 25.445555 |
| S | 18.177691 | 19.442715 | 26.988687 |
| C | 18.433034 | 21.156221 | 27.613792 |
| H | 18.496857 | 21.127477 | 28.710183 |
| H | 19.356533 | 21.546423 | 27.166533 |
| H | 17.561677 | 21.740741 | 27.294830 |
| C | 19.813685 | 18.792657 | 27.529990 |
| H | 19.853766 | 18.804080 | 28.627823 |
| H | 19.884199 | 17.765020 | 27.153619 |
| H | 20.593531 | 19.428978 | 27.091708 |

| | | | |
|---|---|---|---|
| O | 22.122928 | 22.013981 | 19.259183 |
| S | 22.029013 | 21.907157 | 20.795300 |
| C | 22.263129 | 23.603652 | 21.467768 |
| H | 22.337954 | 23.520943 | 22.560161 |
| H | 23.173825 | 24.017982 | 21.015392 |
| H | 21.385740 | 24.187672 | 21.162752 |
| C | 23.639059 | 21.242274 | 21.387621 |
| H | 23.636418 | 21.292751 | 22.484521 |
| H | 23.704654 | 20.207811 | 21.027740 |
| H | 24.435317 | 21.852934 | 20.941810 |
| O | 22.288179 | 21.938705 | 24.307074 |
| S | 21.002813 | 21.173364 | 24.716842 |
| C | 20.992990 | 19.611911 | 23.748124 |
| H | 20.049272 | 19.097423 | 23.964572 |
| H | 21.091252 | 19.874277 | 22.687275 |
| H | 21.857084 | 19.027672 | 24.087681 |
| C | 19.609864 | 21.978664 | 23.829299 |
| H | 18.704772 | 21.397957 | 24.043202 |
| H | 19.535878 | 22.999435 | 24.224070 |
| H | 19.855097 | 21.990158 | 22.759892 |

T7
30

| | | | |
|---|---|---|---|
| C | 0.472180 | -0.265895 | 0.733682 |
| S | -0.136458 | 0.321670 | -0.898489 |
| O | -0.384447 | 1.846400 | -0.754727 |
| C | -1.785515 | -0.482541 | -0.798695 |
| O | 0.359320 | -2.893610 | -1.176365 |
| S | 1.641205 | -2.693731 | -2.021010 |
| C | 2.115524 | -4.372107 | -2.603230 |
| C | 1.077057 | -2.055772 | -3.650613 |
| H | 0.551026 | -1.358283 | 0.675742 |
| H | 1.451728 | 0.200982 | 0.892637 |
| H | -0.247228 | 0.058360 | 1.495983 |
| H | -1.625451 | -1.566818 | -0.828784 |
| H | -2.261186 | -0.155086 | 0.134675 |
| H | -2.355211 | -0.137931 | -1.670337 |
| H | 2.951015 | -4.283369 | -3.311612 |
| H | 2.420451 | -4.939134 | -1.715311 |
| H | 1.234961 | -4.831777 | -3.071533 |
| H | 1.927235 | -2.048859 | -4.346467 |
| H | 0.268384 | -2.708093 | -4.006330 |
| H | 0.713231 | -1.036965 | -3.472756 |
| S | -2.320128 | 1.993864 | 2.169713 |
| O | -3.154515 | 2.294445 | 3.432453 |
| C | -3.077491 | 2.942538 | 0.787412 |

C -0.788980 3.007148 2.285051
H -2.419933 2.841894 -0.086210
H -4.064898 2.499581 0.606587
H -3.180753 3.985061 1.116591
H -0.254575 2.912504 1.330540
H -1.090007 4.041603 2.496975
H -0.204794 2.601451 3.120616

T8
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O 22.134918 25.903523 23.940447
S 23.041269 24.808338 24.561304
C 22.070844 24.071469 25.935851
H 22.726180 23.402398 26.509576
H 21.686789 24.890733 26.558087
H 21.251172 23.507444 25.474200
C 24.246540 25.712157 25.614598
H 24.837479 24.984221 26.187314
H 24.891884 26.286350 24.938904
H 23.682050 26.382530 26.276309
O 18.026224 22.657810 23.136880
S 19.327282 23.413547 23.474273
C 18.847931 25.002640 24.270183
H 19.769957 25.568621 24.458552
H 18.190563 25.554032 23.588146
H 18.338681 24.736761 25.204821
C 19.960394 24.149959 21.912549
H 20.865655 24.718669 22.164650
H 20.186067 23.308764 21.246021
H 19.190316 24.810736 21.496604
O 18.606089 27.152941 21.810753
S 19.594310 28.340832 21.800217
C 21.206535 27.678398 21.199666
H 21.938315 28.498325 21.206754
H 21.524346 26.861633 21.859709
H 21.033168 27.327994 20.175000
C 20.127602 28.590982 23.547016
H 20.862715 29.407639 23.569519
H 19.226795 28.869318 24.107320
H 20.565929 27.657234 23.920780

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