

Supporting Information

Dyes for Guest-Host Liquid Crystal Applications: a General Approach to the Rapid Assessment of Useful Molecular Designs

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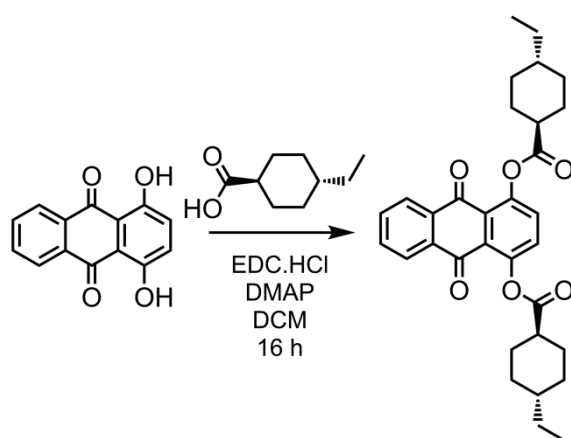
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1. Synthesis of dye 11

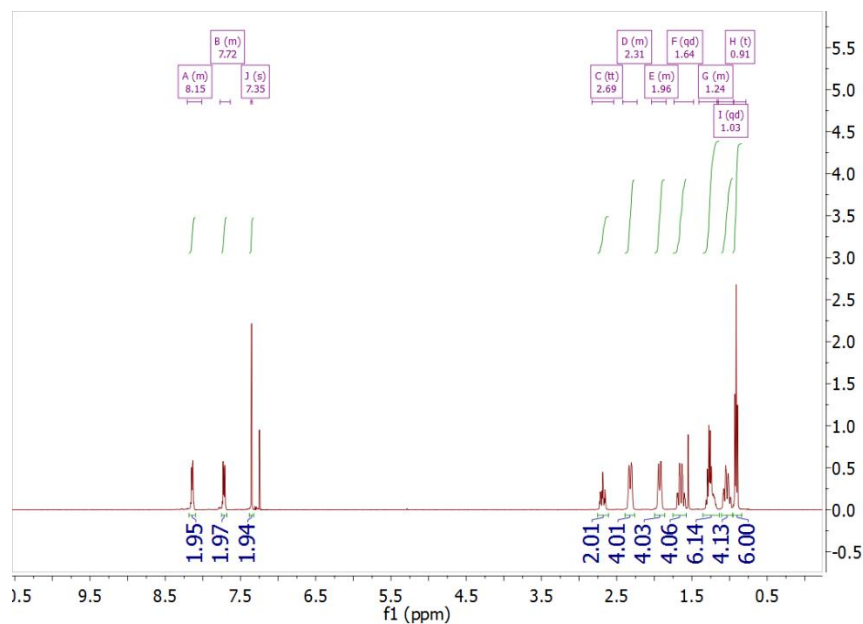
Miscellaneous solvents were purchased from Fisher Scientific and dried by sequential percolation through columns of activated alumina and copper Q5 catalyst prior to use. 1,4-Dihydroxyanthraquinone and DMAP were purchased from SigmaAldrich, *trans* 4-ethylcyclohexanecarboxylic acid was purchased from Synthon GMBH, EDC.HCl was purchased from Fluorochem. Reactions were monitored by thin layer chromatography (TLC) using an appropriate solvent system. Silica coated aluminium TLC plates used were purchased from Merck (Kieselgel 60 F-254) and visualised using, separately, visible and UV (254 nm) light. Column chromatography was performed using flash grade silica from Fluorochem (40 - 63 μ m particle size). Proton NMR spectra were recorded on a JEOL ECS spectrometer operating at 400 MHz (^1H) as solutions in deuterated chloroform. Mass spectra were recorded on a Bruker micrOTOF MS-Agilent series 1200LC spectrometer, and we thank Mr. Karl Heaton of the University of York for acquiring MS data. FTIR spectroscopy was performed using a Shimadzu IR Prestige-21 spectrometer with a Specac Golden Gate diamond ATR IR insert. The ATR stage was flushed with dry nitrogen during use to eliminate peaks resulting from atmospheric water and CO₂.



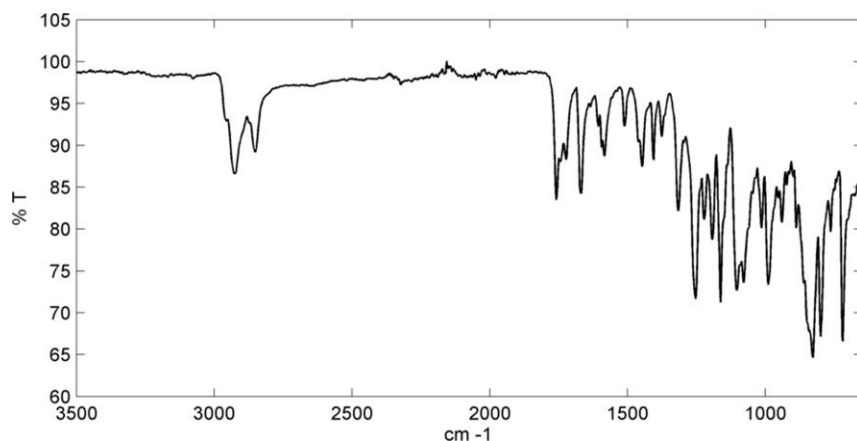
A suspension of 1,4-dihydroxyanthraquinone (1 g, 4.17 mmol), *trans* 4-ethylcyclohexanecarboxylic acid (1.56 g, 10 mmol), EDC.HCl (1.91 g, 10 mmol), and DMAP (50 mg) in DCM (25 ml) was stirred for 16 hours. The solvent was removed *in vacuo* and the crude material purified by flash chromatography over silica gel with DCM as the eluent. The chromatographed material was recrystallised from neat acetonitrile to afford the title compound as yellow needles. Yield: 1.42 g (66%). R_f (TLC): 0.66 (DCM). ^1H NMR (ppm): 0.91 (6H, t, $J = 7.2$ Hz, Cy-CH₂-CH₃), 1.03 (4H, qd, $J = 3.1$ Hz, $J = 13.3$ Hz, CyH), 1.16-1.33 (6H, m, Cy-CH₂-CH₃ + CyH), 1.64 (4H, qd, $J = 3.1$ Hz, $J = 13.3$ Hz, CyH), 1.88 – 1.98 (4H, m, CyH), 2.27 – 2.37 (4H, m, CyH), 2.69 (2H, tt, $J = 3.1$ Hz, $J = 13.3$ Hz, CyHCOOAr), 7.35 (2H, s, ArH), 7.68 – 7.76 (2H,

m, ArH), 8.10 – 8.17 (2H, m, ArH). FTIR (cm^{-1}): 653, 719, 763, 800, 829, 842, 860, 889, 898, 912, 923, 941, 954, 989, 1014, 1047, 1080, 1103, 1163, 1192, 1222, 1253, 1317, 1375, 1406, 1446, 1512, 1585, 1593, 1668, 1724, 1745, 1759, 2852, 2926. MS (APCI): 517.259104 (calcd. for $\text{C}_{32}\text{H}_{37}\text{O}_6$: 517.258465, M + H, mean error -1.0 ppm), 534.285386 (calcd. for $\text{C}_{32}\text{H}_{40}\text{NO}_6$: 534.285014, M + NH_4 , mean error -0.5 ppm).

^1H NMR spectrum (400 MHz, CDCl_3) of dye **11**:



FT-IR spectrum of dye **11**:



2. Polarized UV-visible absorption spectra of dyes in 5CB

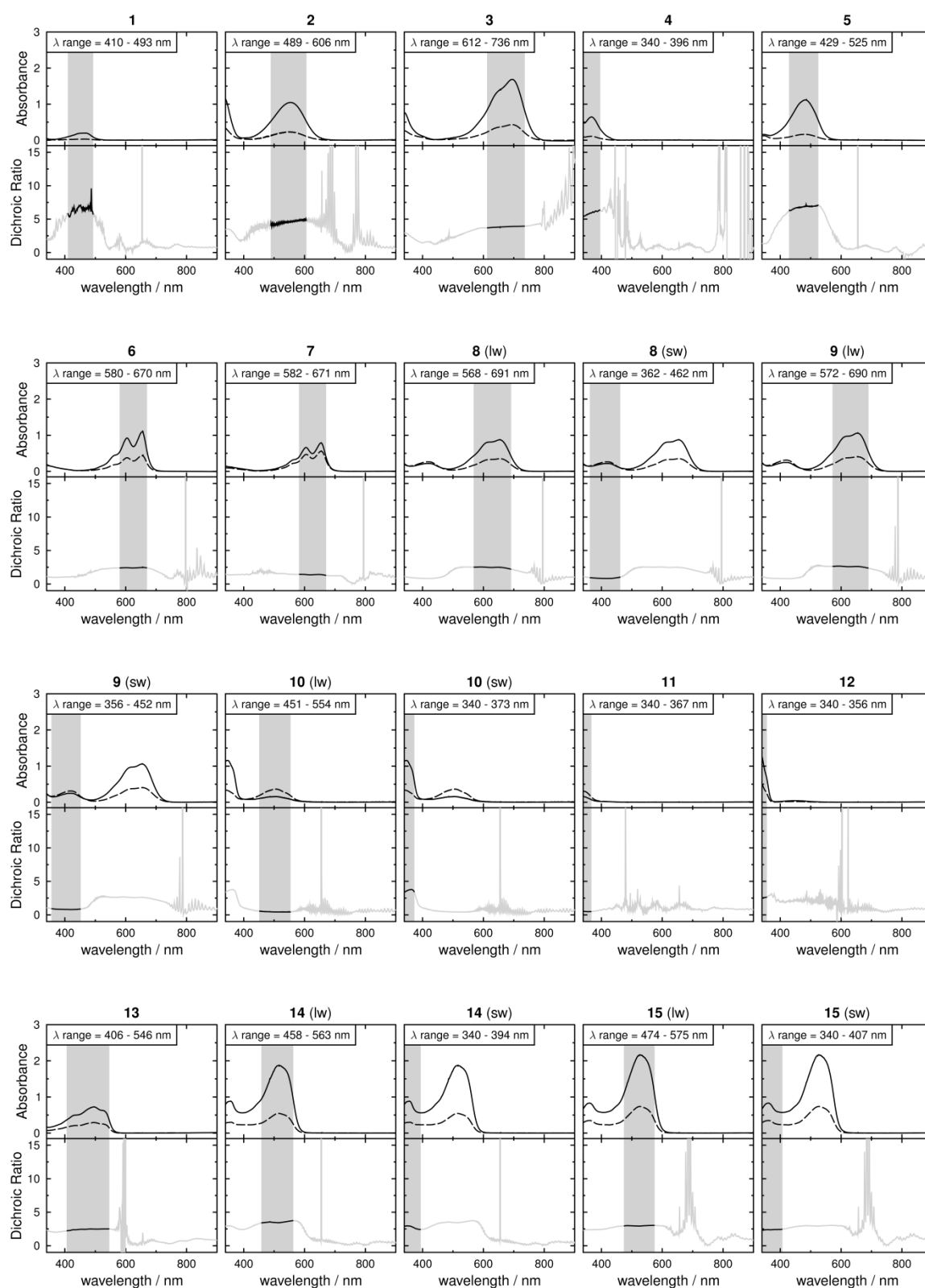


Figure S1. Polarized UV-visible absorption spectra of the dyes in 5CB at 298 K along with plots of dichroic ratio against wavelength. Shaded regions were used to determine the dichroic ratios and order

parameters given in Table 1 in the main text. Limits of the shaded regions are listed in the figure (sw = short-wavelength, lw = long-wavelength).

Table S1. Experimental absorption maxima, λ_{\max} , dichroic ratios, R_{exp} , and dichroic order parameters, S_{exp} , of the dyes at *ca.* 0.5 mol % in 5CB determined from the polarized UV-visible absorption spectra shown in Figure S1. The + and – values correspond to the differences between the mean dichroic order parameter, S_{exp} , and the dichroic order parameters calculated from the maximum and minimum experimental dichroic ratios, respectively, measured in the ranges over which the average dichroic ratios were determined (Figure S1).

| Dye | $\lambda_{\max} / \text{nm}^a$ | R_{exp} | S_{exp} | + | – |
|-----------|--------------------------------|------------------|------------------|------|------|
| 1 | 465 | 6.33 | 0.64 | 0.05 | 0.07 |
| 2 | 553 | 4.52 | 0.54 | 0.05 | 0.03 |
| 3 | 695 | 3.88 | 0.49 | 0.01 | 0.01 |
| 4 | 367 | 5.89 | 0.62 | 0.02 | 0.02 |
| 5 | 483 | 6.82 | 0.66 | 0.02 | 0.01 |
| 6 | 654 | 2.41 | 0.32 | 0.01 | 0.02 |
| 7 | 655 | 1.41 | 0.12 | 0.03 | 0.01 |
| 8 | 653 | 2.48 | 0.33 | 0.04 | 0.01 |
| | 419 | 0.88 | –0.04 | 0.02 | 0.06 |
| 9 | 655 | 2.62 | 0.35 | 0.04 | 0.01 |
| | 423 | 0.83 | –0.06 | 0.02 | 0.04 |
| 10 | 507 | 0.46 | –0.22 | 0.02 | 0.05 |
| | 345 | 3.66 | 0.47 | 0.03 | 0.01 |
| 11 | 345 | 0.48 | –0.21 | 0.01 | 0.02 |
| 12 | 340 ^b | 2.62 | 0.35 | 0.02 | 0.01 |
| 13 | 496 | 2.41 | 0.32 | 0.03 | 0.01 |
| 14 | 516 | 3.56 | 0.46 | 0.01 | 0.02 |
| | 357 | 2.76 | 0.37 | 0.04 | 0.03 |
| 15 | 530 | 3.00 | 0.40 | 0.01 | 0.01 |
| | 360 | 2.41 | 0.32 | 0.02 | 0.01 |

^a taken from spectrum with highest absorbance at the peak

^b short wavelength cut-off

3. Optimised dye structures

Conformers of each dye structure are denoted by different letters.

| | | | |
|----|------------|-----------|-----------|
| 1a | | | |
| C | -5.995752 | -1.010645 | 1.246397 |
| C | -5.425334 | -1.189483 | -0.013084 |
| C | -6.227339 | -1.080849 | -1.147738 |
| C | -7.577007 | -0.780017 | -1.019941 |
| C | -8.157703 | -0.587136 | 0.234083 |
| C | -7.345188 | -0.708049 | 1.362789 |
| S | -3.719508 | -1.699062 | -0.162868 |
| C | -2.882072 | -0.134420 | -0.189013 |
| C | -1.470090 | -0.073295 | -0.224286 |
| C | -0.826786 | 1.176980 | -0.234160 |
| C | -1.558402 | 2.355076 | -0.220005 |
| C | -2.943400 | 2.290900 | -0.190747 |
| C | -3.595526 | 1.069361 | -0.173412 |
| C | 0.658841 | 1.297350 | -0.256388 |
| C | 1.470090 | 0.073246 | -0.224337 |
| C | 0.826785 | -1.177032 | -0.233880 |
| C | -0.658842 | -1.297408 | -0.256042 |
| C | 1.558402 | -2.355124 | -0.219443 |
| C | 2.943400 | -2.290941 | -0.190228 |
| C | 3.595527 | -1.069398 | -0.173216 |
| C | 2.882073 | 0.134380 | -0.189110 |
| S | 3.719510 | 1.699028 | -0.163386 |
| C | 5.425340 | 1.189485 | -0.013520 |
| C | 6.227312 | 1.080560 | -1.148168 |
| C | 7.576984 | 0.779754 | -1.020331 |
| C | 8.157711 | 0.587190 | 0.233727 |
| C | 7.345227 | 0.708394 | 1.362425 |
| C | 5.995790 | 1.010965 | 1.245992 |
| C | 9.610655 | 0.224816 | 0.364555 |
| C | 9.849213 | -1.288241 | 0.341727 |
| C | 11.320452 | -1.652106 | 0.475904 |
| O | -1.180378 | -2.399183 | -0.293591 |
| O | 1.180376 | 2.399116 | -0.294230 |
| C | -9.610645 | -0.224735 | 0.364851 |
| C | -9.849236 | 1.288307 | 0.341401 |
| C | -11.320473 | 1.652198 | 0.475530 |
| H | 1.023441 | -3.296975 | -0.231058 |
| H | 3.530262 | -3.203657 | -0.179802 |
| H | 4.677561 | -1.045372 | -0.148082 |
| H | 5.789307 | 1.238277 | -2.128075 |
| H | 5.377320 | 1.116321 | 2.131029 |
| H | 7.780233 | 0.577047 | 2.349383 |
| H | 8.194122 | 0.703627 | -1.911311 |
| H | -1.023442 | 3.296923 | -0.231871 |
| H | -3.530262 | 3.203618 | -0.180543 |
| H | -4.677560 | 1.045341 | -0.148254 |
| H | -5.789360 | -1.238814 | -2.127617 |
| H | -8.194170 | -0.704121 | -1.910925 |
| H | -7.780167 | -0.576451 | 2.349725 |
| H | -5.377258 | -1.115773 | 2.131445 |
| H | 10.008528 | 0.636717 | 1.299290 |
| H | 11.466318 | -2.735420 | 0.454647 |
| H | 11.910809 | -1.221237 | -0.339169 |
| H | 11.736555 | -1.279240 | 1.417369 |
| H | 10.179663 | 0.689838 | -0.448846 |

| | | | |
|---|------------|-----------|-----------|
| H | 9.272830 | -1.751546 | 1.151084 |
| H | 9.445216 | -1.698074 | -0.591462 |
| H | -9.272805 | 1.751966 | 1.150522 |
| H | -9.445314 | 1.697755 | -0.591990 |
| H | -11.466362 | 2.735500 | 0.453836 |
| H | -11.910879 | 1.220980 | -0.339322 |
| H | -11.736501 | 1.279713 | 1.417179 |
| H | -10.179696 | -0.690111 | -0.448318 |
| H | -10.008450 | -0.636252 | 1.299784 |

1b

| | | | |
|---|------------|-----------|-----------|
| C | 6.138772 | 0.828370 | 1.255096 |
| C | 5.540858 | 1.076092 | 0.020271 |
| C | 6.299388 | 0.953651 | -1.142588 |
| C | 7.631758 | 0.569800 | -1.067312 |
| C | 8.238468 | 0.306047 | 0.161319 |
| C | 7.470583 | 0.443312 | 1.318986 |
| S | 3.862775 | 1.683831 | -0.059216 |
| C | 2.939362 | 0.169595 | -0.125155 |
| C | 1.525670 | 0.188237 | -0.139558 |
| C | 0.813144 | -1.023032 | -0.185451 |
| C | 1.477506 | -2.239758 | -0.223388 |
| C | 2.864150 | -2.253752 | -0.212968 |
| C | 3.584190 | -1.071842 | -0.163612 |
| C | -0.677165 | -1.060424 | -0.192821 |
| C | -1.418835 | 0.205276 | -0.121640 |
| C | -0.706404 | 1.416906 | -0.083795 |
| C | 0.783703 | 1.455525 | -0.110147 |
| C | -1.370790 | 2.632546 | -0.020200 |
| C | -2.757196 | 2.644828 | 0.010996 |
| C | -3.477103 | 1.462278 | -0.022979 |
| C | -2.832313 | 0.222182 | -0.091634 |
| S | -3.755303 | -1.292836 | -0.140508 |
| C | -5.435786 | -0.695935 | -0.035409 |
| C | -6.057836 | -0.570577 | 1.205683 |
| C | -7.393004 | -0.198239 | 1.280915 |
| C | -8.138857 | 0.049275 | 0.127516 |
| C | -7.505878 | -0.085887 | -1.108947 |
| C | -6.171020 | -0.457714 | -1.195441 |
| C | -9.598997 | 0.396021 | 0.212038 |
| C | -10.500088 | -0.842737 | 0.188785 |
| C | -11.978894 | -0.495262 | 0.275750 |
| O | 1.365372 | 2.527443 | -0.103182 |
| O | -1.259071 | -2.130651 | -0.251755 |
| C | 9.668910 | -0.150253 | 0.234462 |
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| C | 11.255671 | -2.135612 | 0.246426 |
| H | 0.890471 | -3.149376 | -0.260311 |
| H | 3.398959 | -3.197471 | -0.243625 |
| H | 4.666125 | -1.109504 | -0.155416 |
| H | 5.841145 | 1.164992 | -2.102926 |
| H | 5.555539 | 0.943905 | 2.162503 |
| H | 7.927266 | 0.257582 | 2.287230 |
| H | 8.215158 | 0.482975 | -1.979802 |
| H | -0.784003 | 3.542743 | 0.004424 |
| H | -3.291899 | 3.587683 | 0.062693 |
| H | -4.558815 | 1.498305 | 0.003284 |
| H | -5.690569 | -0.563363 | -2.162372 |
| H | -8.068584 | 0.101458 | -2.019384 |
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| H | -5.489272 | -0.765137 | 2.108903 |

| | | | |
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| H | 11.847519 | -1.725240 | -0.578120 |
| H | 11.723963 | -1.811738 | 1.181495 |
| H | 10.240525 | 0.298166 | -0.586354 |
| H | 9.227480 | -2.120371 | 0.984171 |
| H | 9.349506 | -2.033008 | -0.761191 |
| H | -10.300784 | -1.409859 | -0.727870 |
| H | -10.219739 | -1.501674 | 1.018715 |
| H | -12.600660 | -1.394334 | 0.256166 |
| H | -12.205485 | 0.045092 | 1.200566 |
| H | -12.286955 | 0.139790 | -0.561165 |
| H | -9.870112 | 1.052820 | -0.622744 |
| H | -9.790710 | 0.962119 | 1.130977 |

1c

| | | | |
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| C | -6.197907 | -0.381159 | 1.203197 |
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| C | -6.197756 | -0.381117 | -1.203195 |
| C | -7.510798 | 0.069400 | -1.197639 |
| C | -8.189093 | 0.301381 | -0.000111 |
| C | -7.510942 | 0.069366 | 1.197494 |
| S | -3.881214 | -1.290831 | 0.000125 |
| C | -2.880994 | 0.175258 | -0.000001 |
| C | -1.470062 | 0.084416 | 0.000034 |
| C | -0.696059 | 1.258312 | -0.000047 |
| C | -1.296936 | 2.508252 | -0.000153 |
| C | -2.681001 | 2.593216 | -0.000202 |
| C | -3.460959 | 1.448879 | -0.000130 |
| C | 0.794249 | 1.219641 | -0.000040 |
| C | 1.470061 | -0.084432 | 0.000014 |
| C | 0.696057 | -1.258328 | 0.000076 |
| C | -0.794250 | -1.219657 | 0.000166 |
| C | 1.296935 | -2.508267 | 0.000087 |
| C | 2.681001 | -2.593231 | 0.000044 |
| C | 3.460958 | -1.448894 | -0.000002 |
| C | 2.880993 | -0.175273 | -0.000013 |
| S | 3.881209 | 1.290818 | -0.000069 |
| C | 5.529550 | 0.602188 | -0.000151 |
| C | 6.197822 | 0.380975 | 1.203022 |
| C | 7.510863 | -0.069537 | 1.197341 |
| C | 8.189098 | -0.301368 | -0.000252 |
| C | 7.510883 | -0.069213 | -1.197792 |
| C | 6.197841 | 0.381301 | -1.203371 |
| C | 9.628462 | -0.734494 | -0.000286 |
| C | 10.600396 | 0.450004 | 0.000435 |
| C | 12.057560 | 0.012128 | 0.000416 |
| O | -1.430277 | -2.260307 | 0.000148 |
| O | 1.430277 | 2.260291 | 0.000088 |
| C | -9.628454 | 0.734518 | -0.000179 |
| C | -10.600398 | -0.449971 | 0.000306 |
| C | -12.057559 | -0.012083 | 0.000257 |
| H | -0.663707 | 3.387123 | -0.000209 |
| H | -3.166633 | 3.563630 | -0.000300 |
| H | -4.539498 | 1.542434 | -0.000167 |
| H | -5.681974 | -0.561482 | -2.140410 |
| H | -5.682241 | -0.561557 | 2.140469 |
| H | -8.020430 | 0.243036 | 2.141350 |
| H | -8.020175 | 0.243096 | -2.141549 |
| H | 0.663707 | -3.387139 | 0.000142 |
| H | 3.166633 | -3.563645 | 0.000052 |

| | | | |
|---|------------|-----------|-----------|
| H | 4.539497 | -1.542448 | -0.000030 |
| H | 5.682123 | 0.561808 | -2.140594 |
| H | 8.020327 | -0.242762 | -2.141694 |
| H | 8.020286 | -0.243348 | 2.141206 |
| H | 5.682089 | 0.561223 | 2.140286 |
| H | -9.825249 | 1.359669 | 0.878528 |
| H | -12.732087 | -0.872476 | 0.000604 |
| H | -12.289599 | 0.592404 | 0.883114 |
| H | -12.289727 | 0.591788 | -0.882987 |
| H | -9.825352 | 1.359037 | -0.879310 |
| H | -10.396312 | -1.077386 | -0.875027 |
| H | -10.396194 | -1.076769 | 0.876054 |
| H | 10.396361 | 1.077544 | -0.874820 |
| H | 10.396130 | 1.076672 | 0.876261 |
| H | 12.732082 | 0.872527 | 0.000933 |
| H | 12.289549 | -0.592487 | 0.883198 |
| H | 12.289791 | -0.591611 | -0.882903 |
| H | 9.825424 | -1.358885 | -0.879493 |
| H | 9.825203 | -1.359769 | 0.878344 |

2a

| | | | |
|---|------------|-----------|-----------|
| C | -5.909248 | -1.364014 | -0.638792 |
| C | -5.131206 | -0.444684 | 0.067900 |
| C | -5.769041 | 0.438694 | 0.942274 |
| C | -7.149806 | 0.415180 | 1.073751 |
| C | -7.937417 | -0.492736 | 0.365608 |
| C | -7.286536 | -1.387680 | -0.483360 |
| N | -3.737876 | -0.505453 | -0.071624 |
| C | -2.845459 | 0.520402 | -0.118576 |
| C | -1.445428 | 0.250535 | -0.062743 |
| C | -0.534008 | 1.326787 | -0.100850 |
| C | -0.974011 | 2.633283 | -0.212575 |
| C | -2.341017 | 2.885776 | -0.311438 |
| C | -3.259777 | 1.861035 | -0.266070 |
| C | 0.937980 | 1.114903 | -0.010191 |
| C | 1.445429 | -0.250534 | 0.062729 |
| C | 0.534009 | -1.326786 | 0.100837 |
| C | -0.937979 | -1.114902 | 0.010175 |
| C | 0.974012 | -2.633282 | 0.212568 |
| C | 2.341018 | -2.885774 | 0.311436 |
| C | 3.259777 | -1.861033 | 0.266068 |
| C | 2.845459 | -0.520400 | 0.118567 |
| N | 3.737875 | 0.505455 | 0.071610 |
| C | 5.131206 | 0.444685 | -0.067908 |
| C | 5.769045 | -0.438706 | -0.942267 |
| C | 7.149810 | -0.415194 | -1.073738 |
| C | 7.937418 | 0.492731 | -0.365604 |
| C | 7.286534 | 1.387687 | 0.483350 |
| C | 5.909245 | 1.364023 | 0.638777 |
| C | 9.435744 | 0.483326 | -0.487438 |
| C | 10.110211 | -0.473864 | 0.499708 |
| C | 11.626858 | -0.474260 | 0.375659 |
| O | -1.678129 | -2.100473 | -0.010391 |
| O | 1.678130 | 2.100474 | 0.010388 |
| C | -9.435742 | -0.483333 | 0.487449 |
| C | -10.110214 | 0.473869 | -0.499682 |
| C | -11.626861 | 0.474263 | -0.375627 |
| H | -0.240235 | 3.428747 | -0.234007 |
| H | -2.692785 | 3.904965 | -0.435917 |
| H | -4.315580 | 2.075688 | -0.371739 |
| H | -5.420561 | -2.059750 | -1.313567 |

| | | | |
|---|------------|-----------|-----------|
| H | -5.180000 | 1.121888 | 1.543724 |
| H | -7.625105 | 1.105905 | 1.765068 |
| H | -7.870006 | -2.116538 | -1.039044 |
| H | 0.240236 | -3.428746 | 0.234001 |
| H | 2.692785 | -3.904962 | 0.435920 |
| H | 4.315580 | -2.075684 | 0.371739 |
| H | 5.180006 | -1.121907 | -1.543710 |
| H | 7.625112 | -1.105928 | -1.765045 |
| H | 7.870002 | 2.116551 | 1.039027 |
| H | 5.420556 | 2.059767 | 1.313540 |
| H | -9.823168 | -1.496187 | 0.325318 |
| H | -12.085810 | 1.166398 | -1.086881 |
| H | -12.039878 | -0.521400 | -0.567570 |
| H | -11.941966 | 0.773177 | 0.629463 |
| H | -9.720269 | -0.202586 | 1.508669 |
| H | -9.720509 | 1.485592 | -0.336626 |
| H | -9.816888 | 0.197911 | -1.519346 |
| H | 9.816881 | -0.197894 | 1.519367 |
| H | 9.720507 | -1.485589 | 0.336663 |
| H | 12.085805 | -1.166387 | 1.086924 |
| H | 11.941967 | -0.773186 | -0.629425 |
| H | 12.039875 | 0.521405 | 0.567591 |
| H | 9.823170 | 1.496182 | -0.325318 |
| H | 9.720275 | 0.202567 | -1.508654 |
| H | -3.296382 | -1.424728 | -0.107489 |
| H | 3.296381 | 1.424730 | 0.107462 |

2b

| | | | |
|---|------------|-----------|-----------|
| C | 5.935555 | -0.938949 | -1.072404 |
| C | 5.150207 | -0.084345 | -0.295276 |
| C | 5.787130 | 0.788079 | 0.590225 |
| C | 7.172273 | 0.816797 | 0.666455 |
| C | 7.966067 | -0.027680 | -0.109374 |
| C | 7.317529 | -0.911930 | -0.971584 |
| N | 3.756329 | -0.194723 | -0.389432 |
| C | 2.820746 | 0.792391 | -0.354687 |
| C | 1.436110 | 0.458168 | -0.268816 |
| C | 0.478685 | 1.493264 | -0.220923 |
| C | 0.858324 | 2.822054 | -0.277627 |
| C | 2.209050 | 3.139694 | -0.407201 |
| C | 3.171924 | 2.155879 | -0.445287 |
| C | -0.978973 | 1.212095 | -0.093873 |
| C | -1.425242 | -0.176268 | -0.076986 |
| C | -0.468002 | -1.211405 | -0.127827 |
| C | 0.989809 | -0.930240 | -0.253494 |
| C | -0.847705 | -2.540231 | -0.072261 |
| C | -2.198201 | -2.857844 | 0.059691 |
| C | -3.160827 | -1.874008 | 0.103242 |
| C | -2.809652 | -0.510367 | 0.014716 |
| N | -3.744265 | 0.477185 | 0.056542 |
| C | -5.139786 | 0.365462 | -0.008162 |
| C | -5.909317 | 1.218011 | 0.786463 |
| C | -7.293065 | 1.192518 | 0.711979 |
| C | -7.958703 | 0.312424 | -0.141166 |
| C | -7.180465 | -0.527637 | -0.937649 |
| C | -5.794184 | -0.500364 | -0.887555 |
| C | -9.460172 | 0.246555 | -0.173983 |
| C | -10.035228 | -0.764775 | 0.822075 |
| C | -11.555425 | -0.823962 | 0.790204 |
| O | 1.769859 | -1.879967 | -0.349656 |
| O | -1.758767 | 2.162019 | 0.002927 |

| | | | |
|---|------------|-----------|-----------|
| C | 9.464101 | -0.024208 | 0.018391 |
| C | 9.974651 | -0.989827 | 1.091984 |
| C | 11.491452 | -0.986030 | 1.213871 |
| H | -0.080592 | -3.302478 | -0.118689 |
| H | -2.501619 | -3.896818 | 0.140143 |
| H | -4.201503 | -2.141396 | 0.234741 |
| H | -5.408463 | 1.900741 | 1.465612 |
| H | -5.216506 | -1.128743 | -1.556020 |
| H | -7.669152 | -1.204487 | -1.633311 |
| H | -7.869785 | 1.869704 | 1.335940 |
| H | 0.091025 | 3.584252 | -0.233513 |
| H | 2.512470 | 4.178499 | -0.489696 |
| H | 4.212982 | 2.422976 | -0.574490 |
| H | 5.196996 | 1.426966 | 1.237397 |
| H | 7.647382 | 1.506071 | 1.359273 |
| H | 7.907244 | -1.583874 | -1.589120 |
| H | 5.448492 | -1.618219 | -1.764895 |
| H | -9.875545 | 1.237928 | 0.042667 |
| H | -11.941943 | -1.552242 | 1.508382 |
| H | -11.994713 | 0.148696 | 1.034655 |
| H | -11.920190 | -1.109858 | -0.201783 |
| H | -9.795556 | -0.015854 | -1.184499 |
| H | -9.616818 | -1.754655 | 0.605057 |
| H | -9.690752 | -0.505716 | 1.830116 |
| H | 9.520232 | -0.724837 | 2.053842 |
| H | 9.619308 | -2.000333 | 0.858619 |
| H | 11.831805 | -1.682721 | 1.984782 |
| H | 11.965233 | -1.276961 | 0.270630 |
| H | 11.865563 | 0.008823 | 1.476926 |
| H | 9.914623 | -0.290168 | -0.945298 |
| H | 9.811502 | 0.988871 | 0.253404 |
| H | -3.338602 | 1.411144 | 0.124582 |
| H | 3.351715 | -1.128880 | -0.460353 |

2c

| | | | |
|---|-----------|-----------|-----------|
| C | 5.919114 | 0.839536 | 1.180608 |
| C | 5.139198 | 0.020553 | 0.361180 |
| C | 5.782804 | -0.879571 | -0.491141 |
| C | 7.167227 | -0.970320 | -0.493699 |
| C | 7.955485 | -0.161624 | 0.324977 |
| C | 7.302100 | 0.750799 | 1.153366 |
| N | 3.748009 | 0.190341 | 0.381044 |
| C | 2.776443 | -0.759357 | 0.311022 |
| C | 1.411358 | -0.372089 | 0.159967 |
| C | 0.416928 | -1.369624 | 0.078103 |
| C | 0.741114 | -2.711609 | 0.161852 |
| C | 2.071310 | -3.080560 | 0.353299 |
| C | 3.069396 | -2.134727 | 0.427010 |
| C | -1.021703 | -1.032735 | -0.113031 |
| C | -1.411357 | 0.371989 | -0.159624 |
| C | -0.416923 | 1.369521 | -0.077772 |
| C | 1.021684 | 1.032633 | 0.113541 |
| C | -0.741083 | 2.711501 | -0.161703 |
| C | -2.071254 | 3.080448 | -0.353325 |
| C | -3.069345 | 2.134619 | -0.427027 |
| C | -2.776422 | 0.759259 | -0.310848 |
| N | -3.748003 | -0.190427 | -0.380817 |
| C | -5.139189 | -0.020599 | -0.361112 |
| C | -5.919054 | -0.839715 | -1.180455 |
| C | -7.302040 | -0.750936 | -1.153353 |
| C | -7.955473 | 0.161662 | -0.325194 |

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|---|------------|-----------|-----------|
| C | -7.167266 | 0.970493 | 0.493397 |
| C | -5.782846 | 0.879706 | 0.490979 |
| C | -9.456482 | 0.231909 | -0.275666 |
| C | -10.063079 | -0.694282 | 0.782553 |
| C | -11.582195 | -0.619200 | 0.829312 |
| O | 1.834162 | 1.951747 | 0.235874 |
| O | -1.834123 | -1.951846 | -0.235775 |
| C | 9.456491 | -0.231822 | 0.275303 |
| C | 10.062970 | 0.694588 | -0.782793 |
| C | 11.582083 | 0.619549 | -0.829705 |
| H | 0.053158 | 3.443430 | -0.090032 |
| H | -2.329602 | 4.129514 | -0.456745 |
| H | -4.092635 | 2.440684 | -0.603343 |
| H | -5.426548 | -1.540243 | -1.847428 |
| H | -5.199420 | 1.491909 | 1.169338 |
| H | -7.647377 | 1.680787 | 1.161083 |
| H | -7.887275 | -1.396066 | -1.802918 |
| H | -0.053124 | -3.443541 | 0.090182 |
| H | 2.329682 | -4.129634 | 0.456576 |
| H | 4.092705 | -2.440798 | 0.603201 |
| H | 5.199337 | -1.491659 | -1.169567 |
| H | 7.647298 | -1.680472 | -1.161564 |
| H | 7.887375 | 1.395822 | 1.803003 |
| H | 5.426648 | 1.539923 | 1.847758 |
| H | -9.868379 | -0.028654 | -1.257907 |
| H | -11.991821 | -1.287679 | 1.591459 |
| H | -11.921588 | 0.395756 | 1.060686 |
| H | -12.022695 | -0.902352 | -0.132242 |
| H | -9.770790 | 1.262482 | -0.071781 |
| H | -9.743723 | -1.723096 | 0.579157 |
| H | -9.644686 | -0.436627 | 1.762595 |
| H | 9.644494 | 0.437112 | -1.762847 |
| H | 9.743609 | 1.723355 | -0.579169 |
| H | 11.991625 | 1.288185 | -1.591760 |
| H | 12.022665 | 0.902525 | 0.131864 |
| H | 11.921479 | -0.395354 | -1.061306 |
| H | 9.868468 | 0.028564 | 1.257557 |
| H | 9.770807 | -1.262347 | 0.071192 |
| H | -3.378596 | -1.140646 | -0.425638 |
| H | 3.378581 | 1.140542 | 0.426083 |

2d

| | | | |
|---|-----------|-----------|-----------|
| C | -5.996384 | -0.767992 | 1.153237 |
| C | -5.145684 | -0.047400 | 0.312463 |
| C | -5.704959 | 0.686881 | -0.735616 |
| C | -7.080669 | 0.713951 | -0.912843 |
| C | -7.940057 | 0.002113 | -0.076284 |
| C | -7.367915 | -0.745528 | 0.953267 |
| N | -3.761556 | -0.148183 | 0.513398 |
| C | -2.821978 | 0.830389 | 0.409314 |
| C | -1.435754 | 0.494561 | 0.428603 |
| C | -0.475504 | 1.522293 | 0.318552 |
| C | -0.855541 | 2.847938 | 0.212934 |
| C | -2.211107 | 3.171550 | 0.229254 |
| C | -3.175944 | 2.193556 | 0.323602 |
| C | 0.986298 | 1.235138 | 0.308071 |
| C | 1.426368 | -0.154544 | 0.362791 |
| C | 0.467781 | -1.178163 | 0.516569 |
| C | -0.991909 | -0.886252 | 0.581285 |
| C | 0.847107 | -2.504660 | 0.614524 |
| C | 2.201567 | -2.830270 | 0.577311 |

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|----|------------|-----------|-----------|
| C | 3.164086 | -1.858188 | 0.418292 |
| C | 2.808923 | -0.499110 | 0.286963 |
| N | 3.744478 | 0.477028 | 0.133347 |
| C | 5.110831 | 0.344372 | -0.146167 |
| C | 5.998080 | 1.248002 | 0.443028 |
| C | 7.351537 | 1.200866 | 0.148100 |
| C | 7.871754 | 0.248429 | -0.728469 |
| C | 6.975776 | -0.642543 | -1.318871 |
| C | 5.615913 | -0.595366 | -1.048174 |
| C | 9.347819 | 0.162205 | -0.999434 |
| C | 10.083130 | -0.751938 | -0.015024 |
| C | 11.576162 | -0.839773 | -0.295220 |
| O | -1.776507 | -1.820370 | 0.757918 |
| O | 1.775730 | 2.180075 | 0.249702 |
| C | -9.425556 | -0.003273 | -0.308319 |
| C | -9.884521 | -1.146820 | -1.217902 |
| C | -11.388960 | -1.148307 | -1.446733 |
| H | 0.078658 | -3.257725 | 0.733258 |
| H | 2.509842 | -3.865304 | 0.685274 |
| H | 4.212033 | -2.129564 | 0.422087 |
| H | 5.613213 | 1.988524 | 1.137192 |
| H | 4.939333 | -1.267446 | -1.563800 |
| H | 7.346347 | -1.377639 | -2.028229 |
| H | 8.020182 | 1.918895 | 0.614908 |
| H | -0.085708 | 3.604695 | 0.133146 |
| H | -2.517175 | 4.211518 | 0.176437 |
| H | -4.222831 | 2.467416 | 0.361125 |
| H | -5.059226 | 1.218782 | -1.425410 |
| H | -7.495574 | 1.293885 | -1.732775 |
| H | -8.010277 | -1.310684 | 1.623074 |
| H | -5.569657 | -1.337958 | 1.972465 |
| H | 9.789440 | 1.164888 | -0.955091 |
| H | 12.078876 | -1.496697 | 0.419812 |
| H | 11.768247 | -1.232544 | -1.299056 |
| H | 12.049993 | 0.145240 | -0.231166 |
| H | 9.513038 | -0.203869 | -2.019823 |
| H | 9.913296 | -0.385860 | 1.004342 |
| H | 9.634298 | -1.751433 | -0.055484 |
| H | -9.358745 | -1.071607 | -2.176917 |
| H | -9.571442 | -2.100050 | -0.776096 |
| H | -11.693564 | -1.974112 | -2.095404 |
| H | -11.932911 | -1.249696 | -0.501914 |
| H | -11.718876 | -0.216739 | -1.918096 |
| H | -9.947529 | -0.079948 | 0.653012 |
| H | -9.731628 | 0.951774 | -0.751483 |
| H | 3.356342 | 1.418460 | 0.199325 |
| H | -3.366379 | -1.067463 | 0.712476 |
| 2e | | | |
| C | 6.051103 | -0.756535 | -0.981680 |
| C | 5.136469 | -0.007332 | -0.238933 |
| C | 5.619756 | 0.832974 | 0.766552 |
| C | 6.984167 | 0.935090 | 0.995410 |
| C | 7.907150 | 0.196031 | 0.255723 |
| C | 7.410772 | -0.657854 | -0.729522 |
| N | 3.767293 | -0.181439 | -0.487137 |
| C | 2.789557 | 0.764707 | -0.508170 |
| C | 1.418337 | 0.375337 | -0.559135 |
| C | 0.419030 | 1.371240 | -0.579809 |
| C | 0.747506 | 2.714809 | -0.570753 |
| C | 2.090226 | 3.087741 | -0.554579 |

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|----|------------|-----------|-----------|
| C | 3.091486 | 2.142947 | -0.523458 |
| C | -1.030648 | 1.029596 | -0.611327 |
| C | -1.418360 | -0.375620 | -0.559123 |
| C | -0.419053 | -1.371525 | -0.579615 |
| C | 1.030629 | -1.029887 | -0.611112 |
| C | -0.747533 | -2.715092 | -0.570367 |
| C | -2.090254 | -3.088019 | -0.554155 |
| C | -3.091514 | -2.143217 | -0.523186 |
| C | -2.789579 | -0.764979 | -0.508122 |
| N | -3.767305 | 0.181182 | -0.487283 |
| C | -5.136471 | 0.007210 | -0.239004 |
| C | -6.051060 | 0.756524 | -0.981703 |
| C | -7.410728 | 0.657996 | -0.729487 |
| C | -7.907164 | -0.195835 | 0.255776 |
| C | -6.984229 | -0.935001 | 0.995416 |
| C | -5.619817 | -0.833048 | 0.766496 |
| C | -9.380174 | -0.275627 | 0.546203 |
| C | -9.841484 | 0.753987 | 1.581880 |
| C | -11.332622 | 0.668667 | 1.873086 |
| O | 1.854926 | -1.944064 | -0.674810 |
| O | -1.854947 | 1.943757 | -0.675230 |
| C | 9.380166 | 0.275997 | 0.546083 |
| C | 9.841588 | -0.753346 | 1.581976 |
| C | 11.332728 | -0.667839 | 1.873115 |
| H | 0.050991 | -3.445649 | -0.589664 |
| H | -2.357494 | -4.139735 | -0.576264 |
| H | -4.128764 | -2.453200 | -0.538625 |
| H | -5.683706 | 1.408973 | -1.767469 |
| H | -4.924055 | -1.390603 | 1.383564 |
| H | -7.339251 | -1.597728 | 1.779978 |
| H | -8.103784 | 1.247387 | -1.323588 |
| H | -0.051021 | 3.445360 | -0.590166 |
| H | 2.357465 | 4.139453 | -0.576846 |
| H | 4.128738 | 2.452922 | -0.538934 |
| H | 4.923951 | 1.390463 | 1.383631 |
| H | 7.339141 | 1.597857 | 1.779959 |
| H | 8.103879 | -1.247153 | -1.323654 |
| H | 5.683783 | -1.409019 | -1.767432 |
| H | -9.946138 | -0.128499 | -0.381425 |
| H | -11.637894 | 1.412612 | 2.613942 |
| H | -11.923750 | 0.839885 | 0.967496 |
| H | -11.604466 | -0.318134 | 2.261890 |
| H | -9.629939 | -1.281183 | 0.904963 |
| H | -9.269768 | 0.609152 | 2.506022 |
| H | -9.586027 | 1.757908 | 1.223085 |
| H | 9.269891 | -0.608348 | 2.506105 |
| H | 9.586199 | -1.757369 | 1.223416 |
| H | 11.638085 | -1.411596 | 2.614124 |
| H | 11.923841 | -0.839208 | 0.967544 |
| H | 11.604504 | 0.319070 | 2.261692 |
| H | 9.946104 | 0.128700 | -0.381534 |
| H | 9.629870 | 1.281654 | 0.904605 |
| H | -3.415648 | 1.128666 | -0.626181 |
| H | 3.415651 | -1.128961 | -0.625816 |
| 2f | | | |
| C | 5.929443 | -1.308944 | -0.674479 |
| C | 5.125629 | -0.435017 | 0.060871 |
| C | 5.730668 | 0.388697 | 1.013164 |
| C | 7.105968 | 0.353887 | 1.192948 |
| C | 7.919046 | -0.508298 | 0.457236 |

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|---|------------|-----------|-----------|
| C | 7.299873 | -1.345596 | -0.470781 |
| N | 3.739019 | -0.485582 | -0.135137 |
| C | 2.844305 | 0.539142 | -0.154196 |
| C | 1.445147 | 0.260520 | -0.191919 |
| C | 0.528671 | 1.332779 | -0.211612 |
| C | 0.963725 | 2.645630 | -0.211305 |
| C | 2.332045 | 2.909951 | -0.208869 |
| C | 3.255378 | 1.888535 | -0.181592 |
| C | -0.944293 | 1.109266 | -0.236866 |
| C | -1.445164 | -0.259793 | -0.192094 |
| C | -0.528680 | -1.332048 | -0.211778 |
| C | 0.944276 | -1.108527 | -0.237006 |
| C | -0.963717 | -2.644904 | -0.211566 |
| C | -2.332033 | -2.909242 | -0.209232 |
| C | -3.255381 | -1.887842 | -0.181992 |
| C | -2.844334 | -0.538442 | -0.154508 |
| N | -3.739085 | 0.486236 | -0.135465 |
| C | -5.125735 | 0.435487 | 0.060372 |
| C | -5.929575 | 1.309121 | -0.675283 |
| C | -7.300045 | 1.345602 | -0.471777 |
| C | -7.919197 | 0.508423 | 0.456351 |
| C | -7.106078 | -0.353459 | 1.192384 |
| C | -5.730753 | -0.388096 | 1.012781 |
| C | -9.412186 | 0.510674 | 0.632164 |
| C | -10.122896 | -0.495507 | -0.277787 |
| C | -11.634533 | -0.481538 | -0.103492 |
| O | 1.691056 | -2.087691 | -0.293756 |
| O | -1.691060 | 2.088455 | -0.293326 |
| C | 9.412015 | -0.510805 | 0.633201 |
| C | 10.123334 | 0.492510 | -0.279428 |
| C | 11.634952 | 0.478153 | -0.104985 |
| H | -0.226029 | -3.436826 | -0.228576 |
| H | -2.682014 | -3.936171 | -0.239811 |
| H | -4.313543 | -2.114471 | -0.210441 |
| H | -5.465949 | 1.959142 | -1.410644 |
| H | -5.119887 | -1.031284 | 1.636057 |
| H | -7.555859 | -0.997363 | 1.943341 |
| H | -7.903750 | 2.038263 | -1.051654 |
| H | 0.226054 | 3.437568 | -0.228327 |
| H | 2.682038 | 3.936876 | -0.239423 |
| H | 4.313544 | 2.115153 | -0.209964 |
| H | 5.119815 | 1.032085 | 1.636244 |
| H | 7.555786 | 0.997902 | 1.943785 |
| H | 7.903511 | -2.038535 | -1.050398 |
| H | 5.465830 | -1.959081 | -1.409748 |
| H | -9.803441 | 1.514759 | 0.429528 |
| H | -12.119208 | -1.208147 | -0.761281 |
| H | -11.917184 | -0.725006 | 0.925930 |
| H | -12.050369 | 0.504604 | -0.334459 |
| H | -9.660235 | 0.286331 | 1.676502 |
| H | -9.863276 | -0.276719 | -1.320234 |
| H | -9.731094 | -1.498799 | -0.073032 |
| H | 9.863676 | 0.271057 | -1.321303 |
| H | 9.732070 | 1.496566 | -0.077412 |
| H | 12.120092 | 1.202727 | -0.764674 |
| H | 11.917658 | 0.724216 | 0.923804 |
| H | 12.050239 | -0.508843 | -0.333278 |
| H | 9.802812 | -1.515638 | 0.433369 |
| H | 9.660037 | -0.283713 | 1.676946 |
| H | -3.304356 | 1.400862 | -0.261666 |
| H | 3.304288 | -1.400128 | -0.261843 |

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| 3a | | | |
| C | 5.922920 | 1.373130 | 0.712932 |
| C | 5.121612 | 0.474239 | 0.004950 |
| C | 5.733215 | -0.394596 | -0.903015 |
| C | 7.110688 | -0.378440 | -1.064769 |
| C | 7.921138 | 0.508302 | -0.355489 |
| C | 7.296209 | 1.390096 | 0.526439 |
| N | 3.733802 | 0.540320 | 0.181193 |
| C | 2.832001 | -0.481850 | 0.177744 |
| C | 1.437973 | -0.235789 | 0.096379 |
| C | 0.520447 | -1.328956 | 0.084244 |
| C | 0.993411 | -2.647329 | 0.167151 |
| C | 2.377641 | -2.865409 | 0.306074 |
| C | 3.262099 | -1.825612 | 0.313067 |
| C | -0.916705 | -1.113914 | -0.035622 |
| C | -1.437972 | 0.235775 | -0.096317 |
| C | -0.520446 | 1.328942 | -0.084180 |
| C | 0.916705 | 1.113900 | 0.035697 |
| C | -0.993408 | 2.647315 | -0.167104 |
| C | -2.377637 | 2.865394 | -0.306052 |
| C | -3.262094 | 1.825597 | -0.313050 |
| C | -2.831999 | 0.481836 | -0.177706 |
| N | -3.733802 | -0.540332 | -0.181155 |
| C | -5.121615 | -0.474241 | -0.004937 |
| C | -5.922915 | -1.373145 | -0.712912 |
| C | -7.296207 | -1.390099 | -0.526442 |
| C | -7.921146 | -0.508281 | 0.355454 |
| C | -7.110704 | 0.378475 | 1.064726 |
| C | -5.733228 | 0.394620 | 0.902995 |
| C | -9.416123 | -0.489710 | 0.511404 |
| C | -10.103630 | 0.498631 | -0.435341 |
| C | -11.616834 | 0.511237 | -0.275313 |
| O | 1.682921 | 2.112755 | 0.092345 |
| O | -1.682914 | -2.112770 | -0.092338 |
| C | 9.416111 | 0.489743 | -0.511466 |
| C | 10.103640 | -0.498619 | 0.435242 |
| C | 11.616841 | -0.511214 | 0.275187 |
| O | -0.208204 | 3.717710 | -0.143552 |
| H | -2.716697 | 3.888986 | -0.420588 |
| H | -4.317694 | 2.023205 | -0.451577 |
| H | -5.455476 | -2.056728 | -1.414643 |
| H | -5.125911 | 1.059194 | 1.507323 |
| H | -7.564932 | 1.057219 | 1.781521 |
| H | -7.897688 | -2.102492 | -1.084207 |
| O | 0.208205 | -3.717724 | 0.143606 |
| H | 2.716704 | -3.889002 | 0.420598 |
| H | 4.317700 | -2.023222 | 0.451580 |
| H | 5.125891 | -1.059157 | -1.507350 |
| H | 7.564906 | -1.057163 | -1.781590 |
| H | 7.897696 | 2.102478 | 1.084211 |
| H | 5.455490 | 2.056694 | 1.414688 |
| H | -9.816188 | -1.494693 | 0.332206 |
| H | -12.084730 | 1.225120 | -0.958660 |
| H | -12.045016 | -0.475146 | -0.481282 |
| H | -11.905074 | 0.788983 | 0.743805 |
| H | -9.674863 | -0.232950 | 1.545690 |
| H | -9.699656 | 1.502065 | -0.256506 |
| H | -9.837283 | 0.245316 | -1.468217 |
| H | 9.837310 | -0.245332 | 1.468130 |
| H | 9.699667 | -1.502051 | 0.256388 |

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| H | 12.084753 | -1.225113 | 0.958507 |
| H | 11.905064 | -0.788932 | -0.743943 |
| H | 12.045022 | 0.475165 | 0.481174 |
| H | 9.816174 | 1.494723 | -0.332248 |
| H | 9.674835 | 0.233011 | -1.545763 |
| H | -3.300104 | -1.460672 | -0.235506 |
| H | 3.300102 | 1.460658 | 0.235573 |
| H | 0.714101 | 3.363300 | -0.044679 |
| H | -0.714104 | -3.363311 | 0.044777 |

3b

| | | | |
|---|------------|-----------|-----------|
| C | -5.750304 | -0.490660 | -0.830633 |
| C | -5.127262 | 0.371779 | 0.075365 |
| C | -5.925899 | 1.212062 | 0.855122 |
| C | -7.306402 | 1.177883 | 0.739865 |
| C | -7.941059 | 0.300811 | -0.139977 |
| C | -7.134174 | -0.526948 | -0.920777 |
| N | -3.736288 | 0.492067 | 0.183602 |
| C | -2.791529 | -0.487009 | 0.105778 |
| C | -1.413931 | -0.172813 | -0.016275 |
| C | -0.448234 | -1.220097 | -0.102798 |
| C | -0.856892 | -2.561443 | -0.054979 |
| C | -2.223860 | -2.849496 | 0.122494 |
| C | -3.154412 | -1.853744 | 0.201979 |
| C | 0.972538 | -0.933216 | -0.262055 |
| C | 1.429184 | 0.440684 | -0.287468 |
| C | 0.463317 | 1.487960 | -0.202861 |
| C | -0.957374 | 1.201069 | -0.043021 |
| C | 0.871995 | 2.829304 | -0.251168 |
| C | 2.239156 | 3.117298 | -0.427385 |
| C | 3.169906 | 2.121483 | -0.503567 |
| C | 2.807015 | 0.754883 | -0.405742 |
| N | 3.752608 | -0.223966 | -0.478731 |
| C | 5.142005 | -0.105119 | -0.350793 |
| C | 5.950776 | -0.945591 | -1.120176 |
| C | 7.329703 | -0.909357 | -0.988994 |
| C | 7.953078 | -0.029399 | -0.103765 |
| C | 7.136418 | 0.800763 | 0.663806 |
| C | 5.753588 | 0.762384 | 0.557974 |
| C | 9.447874 | -0.016708 | 0.056116 |
| C | 9.942414 | -0.990222 | 1.130158 |
| C | 11.456449 | -0.979128 | 1.282139 |
| O | -1.765810 | 2.160406 | 0.077596 |
| O | 1.781011 | -1.892425 | -0.383064 |
| C | -9.440328 | 0.225594 | -0.217636 |
| C | -10.037717 | -0.798958 | 0.751492 |
| C | -11.555732 | -0.868715 | 0.672369 |
| O | -0.024962 | -3.592154 | -0.146910 |
| H | -2.511380 | -3.891561 | 0.207736 |
| H | -4.193788 | -2.106759 | 0.369691 |
| H | -5.449993 | 1.890892 | 1.555801 |
| H | -5.149534 | -1.107717 | -1.489398 |
| H | -7.597798 | -1.200148 | -1.636756 |
| H | -7.905820 | 1.845304 | 1.352802 |
| O | 0.039956 | 3.860018 | -0.160868 |
| H | 2.526663 | 4.159239 | -0.514118 |
| H | 4.209543 | 2.374194 | -0.670216 |
| H | 5.145231 | 1.388447 | 1.201013 |
| H | 7.591276 | 1.485449 | 1.374461 |
| H | 7.937765 | -1.569932 | -1.600906 |
| H | 5.484210 | -1.619732 | -1.831549 |

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|---|------------|-----------|-----------|
| H | -9.868588 | 1.212149 | -0.004195 |
| H | -11.958600 | -1.606469 | 1.371607 |
| H | -12.009603 | 0.098401 | 0.912036 |
| H | -11.887585 | -1.147982 | -0.332950 |
| H | -9.743934 | -0.029417 | -1.240022 |
| H | -9.605586 | -1.783807 | 0.538460 |
| H | -9.726080 | -0.546642 | 1.771871 |
| H | 9.467418 | -0.737412 | 2.085327 |
| H | 9.597711 | -2.000334 | 0.879729 |
| H | 11.785390 | -1.681228 | 2.053065 |
| H | 11.950362 | -1.258590 | 0.345797 |
| H | 11.819660 | 0.015199 | 1.561867 |
| H | 9.920685 | -0.269260 | -0.900495 |
| H | 9.782837 | 0.996243 | 0.308989 |
| H | -3.340414 | 1.428167 | 0.256774 |
| H | 3.357353 | -1.160115 | -0.554234 |
| H | -0.861107 | 3.459175 | -0.044878 |
| H | 0.876054 | -3.191230 | -0.262953 |

3c

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|---|------------|-----------|-----------|
| C | -5.741866 | 0.867971 | 0.454937 |
| C | -5.126553 | -0.023045 | -0.428178 |
| C | -5.933702 | -0.822454 | -1.241458 |
| C | -7.314473 | -0.723340 | -1.177874 |
| C | -7.939789 | 0.180725 | -0.318829 |
| C | -7.124892 | 0.969658 | 0.493049 |
| N | -3.738930 | -0.203183 | -0.487921 |
| C | -2.757434 | 0.735607 | -0.374656 |
| C | -1.400370 | 0.364937 | -0.195669 |
| C | -0.396413 | 1.371743 | -0.071468 |
| C | -0.746562 | 2.728637 | -0.139512 |
| C | -2.091776 | 3.072512 | -0.374411 |
| C | -3.058849 | 2.115849 | -0.489409 |
| C | 1.003054 | 1.026653 | 0.148427 |
| C | 1.400374 | -0.365043 | 0.196196 |
| C | 0.396412 | -1.371851 | 0.072047 |
| C | -1.003067 | -1.026762 | -0.147777 |
| C | 0.746583 | -2.728744 | 0.139969 |
| C | 2.091842 | -3.072622 | 0.374611 |
| C | 3.058924 | -2.115956 | 0.489523 |
| C | 2.757469 | -0.735707 | 0.374948 |
| N | 3.738959 | 0.203092 | 0.488182 |
| C | 5.126580 | 0.023004 | 0.428204 |
| C | 5.933823 | 0.822310 | 1.241492 |
| C | 7.314587 | 0.723248 | 1.177691 |
| C | 7.939806 | -0.180662 | 0.318413 |
| C | 7.124814 | -0.969493 | -0.493470 |
| C | 5.741790 | -0.867854 | -0.455141 |
| C | 9.438440 | -0.261160 | 0.230407 |
| C | 10.025839 | 0.678746 | -0.826654 |
| C | 11.542901 | 0.595246 | -0.910482 |
| O | -1.845135 | -1.951840 | -0.301270 |
| O | 1.845236 | 1.951741 | 0.301236 |
| C | -9.438434 | 0.261283 | -0.231054 |
| C | -10.026016 | -0.678441 | 0.826068 |
| C | -11.543088 | -0.594881 | 0.909661 |
| O | 0.123036 | 3.724356 | -0.015538 |
| H | -2.331850 | 4.125215 | -0.474408 |
| H | -4.079300 | 2.410750 | -0.699715 |
| H | -5.463864 | -1.514479 | -1.933222 |
| H | -5.137307 | 1.462624 | 1.130583 |

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|---|------------|-----------|-----------|
| H | -7.582462 | 1.671827 | 1.184659 |
| H | -7.921173 | -1.352803 | -1.823032 |
| O | -0.123040 | -3.724463 | 0.016166 |
| H | 2.331941 | -4.125328 | 0.474515 |
| H | 4.079408 | -2.410861 | 0.699656 |
| H | 5.137152 | -1.462419 | -1.130793 |
| H | 7.582305 | -1.671539 | -1.185258 |
| H | 7.921362 | 1.352629 | 1.822860 |
| H | 5.464064 | 1.514212 | 1.933433 |
| H | -9.876134 | 0.020289 | -1.207108 |
| H | -11.938949 | -1.273115 | 1.670434 |
| H | -11.870575 | 0.418188 | 1.165131 |
| H | -12.007689 | -0.859932 | -0.045680 |
| H | -9.739628 | 1.290518 | -0.002306 |
| H | -9.718260 | -1.705746 | 0.598527 |
| H | -9.583078 | -0.439437 | 1.800034 |
| H | 9.582766 | 0.439882 | -1.800593 |
| H | 9.718086 | 1.706007 | -0.598907 |
| H | 11.938630 | 1.273610 | -1.671208 |
| H | 12.007634 | 0.860161 | 0.044831 |
| H | 11.870381 | -0.417774 | -1.166159 |
| H | 9.876276 | -0.020306 | 1.206434 |
| H | 9.739633 | -1.290351 | 0.001454 |
| H | -3.380586 | -1.155423 | -0.543667 |
| H | 3.380595 | 1.155313 | 0.544141 |
| H | -1.001076 | -3.287294 | -0.138289 |
| H | 1.000979 | 3.287196 | 0.139471 |

3d

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|---|------------|-----------|-----------|
| C | 5.548559 | -0.570317 | -1.083481 |
| C | 5.094333 | 0.356629 | -0.141412 |
| C | 6.018542 | 1.234218 | 0.430940 |
| C | 7.357760 | 1.174473 | 0.079714 |
| C | 7.827681 | 0.234990 | -0.838438 |
| C | 6.895328 | -0.630458 | -1.410538 |
| N | 3.743615 | 0.501899 | 0.197359 |
| C | 2.796409 | -0.467699 | 0.341529 |
| C | 1.418442 | -0.144063 | 0.426373 |
| C | 0.449557 | -1.181244 | 0.575530 |
| C | 0.858221 | -2.520474 | 0.663133 |
| C | 2.234561 | -2.815244 | 0.620782 |
| C | 3.167056 | -1.829891 | 0.467238 |
| C | -0.977328 | -0.886264 | 0.633831 |
| C | -1.432544 | 0.482122 | 0.503390 |
| C | -0.461415 | 1.523511 | 0.407834 |
| C | 0.966846 | 1.231260 | 0.384718 |
| C | -0.870232 | 2.862858 | 0.322934 |
| C | -2.247324 | 3.156535 | 0.350979 |
| C | -3.182753 | 2.165306 | 0.429759 |
| C | -2.814524 | 0.797761 | 0.487515 |
| N | -3.765551 | -0.174479 | 0.579355 |
| C | -5.137307 | -0.070691 | 0.313966 |
| C | -6.025265 | -0.805751 | 1.103077 |
| C | -7.385746 | -0.781409 | 0.840278 |
| C | -7.911401 | -0.017488 | -0.202357 |
| C | -7.015614 | 0.709012 | -0.986461 |
| C | -5.649431 | 0.680355 | -0.746953 |
| C | -9.384265 | -0.022910 | -0.503824 |
| C | -9.794414 | -1.150782 | -1.455463 |
| C | -11.286055 | -1.153956 | -1.756296 |
| O | 1.786667 | 2.186363 | 0.323469 |

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| O | -1.793142 | -1.833414 | 0.792722 |
| C | 9.289712 | 0.135954 | -1.173047 |
| C | 10.049633 | -0.824044 | -0.252969 |
| C | 11.528929 | -0.920899 | -0.596031 |
| O | 0.021158 | -3.541824 | 0.801717 |
| H | 2.530559 | -3.852603 | 0.730777 |
| H | 4.219278 | -2.085582 | 0.471606 |
| H | 5.673877 | 1.963147 | 1.157707 |
| H | 4.841433 | -1.220514 | -1.586450 |
| H | 7.225310 | -1.354346 | -2.150758 |
| H | 8.055785 | 1.871861 | 0.534577 |
| O | -0.031344 | 3.887940 | 0.231237 |
| H | -2.539830 | 4.200333 | 0.323162 |
| H | -4.233067 | 2.424570 | 0.480019 |
| H | -4.974016 | 1.222148 | -1.399784 |
| H | -7.393138 | 1.301109 | -1.815645 |
| H | -8.057365 | -1.358182 | 1.470248 |
| H | -5.636158 | -1.387344 | 1.932808 |
| H | 9.749031 | 1.129684 | -1.111357 |
| H | 12.049686 | -1.611272 | 0.073054 |
| H | 11.675433 | -1.277419 | -1.620837 |
| H | 12.019350 | 0.054573 | -0.513825 |
| H | 9.407300 | -0.195435 | -2.211707 |
| H | 9.925898 | -0.494079 | 0.785208 |
| H | 9.585035 | -1.815375 | -0.312260 |
| H | -9.223890 | -1.055320 | -2.386722 |
| H | -9.498007 | -2.110977 | -1.017268 |
| H | -11.554241 | -1.966911 | -2.436478 |
| H | -11.874516 | -1.278514 | -0.841425 |
| H | -11.598081 | -0.213960 | -2.223048 |
| H | -9.950242 | -0.119597 | 0.430424 |
| H | -9.673351 | 0.939280 | -0.942812 |
| H | 3.368533 | 1.445786 | 0.278658 |
| H | -3.381385 | -1.097796 | 0.773890 |
| H | -0.884251 | -3.135490 | 0.834181 |
| H | 0.876174 | 3.485367 | 0.246401 |

3e

| | | | |
|---|-----------|-----------|-----------|
| C | -5.561456 | -0.848460 | 0.781708 |
| C | -5.123790 | 0.012940 | -0.227615 |
| C | -6.072293 | 0.777327 | -0.911432 |
| C | -7.418418 | 0.673176 | -0.598604 |
| C | -7.869917 | -0.201426 | 0.390332 |
| C | -6.914044 | -0.955777 | 1.070369 |
| N | -3.770118 | 0.195052 | -0.538264 |
| C | -2.779215 | -0.740749 | -0.568280 |
| C | -1.412519 | -0.367946 | -0.619826 |
| C | -0.399389 | -1.372854 | -0.648022 |
| C | -0.752703 | -2.730560 | -0.651175 |
| C | -2.117372 | -3.077808 | -0.645045 |
| C | -3.092084 | -2.122753 | -0.605398 |
| C | 1.016257 | -1.024409 | -0.664669 |
| C | 1.412480 | 0.367797 | -0.619860 |
| C | 0.399358 | 1.372716 | -0.648073 |
| C | -1.016302 | 1.024267 | -0.664658 |
| C | 0.752688 | 2.730418 | -0.651361 |
| C | 2.117352 | 3.077660 | -0.645135 |
| C | 3.092062 | 2.122606 | -0.605404 |
| C | 2.779187 | 0.740603 | -0.568251 |
| N | 3.770099 | -0.195179 | -0.538173 |
| C | 5.123782 | -0.013017 | -0.227594 |

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|---|------------|-----------|-----------|
| C | 6.072292 | -0.777372 | -0.911434 |
| C | 7.418424 | -0.673169 | -0.598651 |
| C | 7.869928 | 0.201470 | 0.390249 |
| C | 6.914046 | 0.955793 | 1.070309 |
| C | 5.561450 | 0.848409 | 0.781707 |
| C | 9.327788 | 0.287009 | 0.747192 |
| C | 9.737148 | -0.715267 | 1.830498 |
| C | 11.212921 | -0.624016 | 2.189958 |
| O | -1.874222 | 1.945871 | -0.713674 |
| O | 1.874155 | -1.946073 | -0.713352 |
| C | -9.327766 | -0.286839 | 0.747356 |
| C | -9.737060 | 0.715751 | 1.830392 |
| C | -11.212824 | 0.624624 | 2.189929 |
| O | 0.128065 | -3.723866 | -0.675897 |
| H | -2.368753 | -4.131712 | -0.688779 |
| H | -4.132830 | -2.420711 | -0.633368 |
| H | -5.742003 | 1.445456 | -1.700517 |
| H | -4.839416 | -1.416448 | 1.357868 |
| H | -7.232260 | -1.634676 | 1.856892 |
| H | -8.137502 | 1.274621 | -1.147945 |
| O | -0.128053 | 3.723747 | -0.676321 |
| H | 2.368745 | 4.131562 | -0.688881 |
| H | 4.132808 | 2.420566 | -0.633348 |
| H | 4.839408 | 1.416348 | 1.357912 |
| H | 7.232263 | 1.634729 | 1.856800 |
| H | 8.137497 | -1.274630 | -1.147989 |
| H | 5.742006 | -1.445500 | -1.700523 |
| H | -9.936017 | -0.114295 | -0.148599 |
| H | -11.480354 | 1.348911 | 2.964068 |
| H | -11.845983 | 0.820974 | 1.318519 |
| H | -11.468476 | -0.371832 | 2.564772 |
| H | -9.563147 | -1.301162 | 1.090806 |
| H | -9.122476 | 0.545976 | 2.722225 |
| H | -9.496545 | 1.728538 | 1.486446 |
| H | 9.122593 | -0.545261 | 2.722308 |
| H | 9.496637 | -1.728151 | 1.486836 |
| H | 11.480486 | -1.348092 | 2.964283 |
| H | 11.846054 | -0.820590 | 1.318579 |
| H | 11.468572 | 0.372544 | 2.564526 |
| H | 9.936003 | 0.114210 | -0.148737 |
| H | 9.563161 | 1.301437 | 1.090334 |
| H | -3.431729 | 1.145848 | -0.677288 |
| H | 3.431752 | -1.145980 | -0.677275 |
| H | 1.017939 | -3.283944 | -0.698653 |
| H | -1.017925 | 3.283855 | -0.699344 |

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|---|-----------|-----------|-----------|
| C | 5.584150 | -0.333716 | -1.039583 |
| C | 5.095156 | 0.474801 | -0.009886 |
| C | 5.985547 | 1.319439 | 0.656915 |
| C | 7.327246 | 1.342843 | 0.309514 |
| C | 7.831994 | 0.520868 | -0.698383 |
| C | 6.932609 | -0.312833 | -1.363163 |
| N | 3.737399 | 0.532935 | 0.329726 |
| C | 2.834044 | -0.488074 | 0.357735 |
| C | 1.439893 | -0.239554 | 0.419549 |
| C | 0.521097 | -1.331222 | 0.448304 |
| C | 0.994910 | -2.651740 | 0.442770 |
| C | 2.385126 | -2.875344 | 0.422642 |
| C | 3.269975 | -1.836576 | 0.381457 |
| C | -0.920112 | -1.111348 | 0.470163 |

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|----|------------|-----------|-----------|
| C | -1.439900 | 0.239516 | 0.419586 |
| C | -0.521102 | 1.331182 | 0.448332 |
| C | 0.920101 | 1.111302 | 0.470151 |
| C | -0.994917 | 2.651704 | 0.442818 |
| C | -2.385135 | 2.875305 | 0.422718 |
| C | -3.269982 | 1.836536 | 0.381541 |
| C | -2.834048 | 0.488034 | 0.357806 |
| N | -3.737410 | -0.532971 | 0.329819 |
| C | -5.095164 | -0.474820 | -0.009813 |
| C | -5.985583 | -1.319421 | 0.656995 |
| C | -7.327278 | -1.342803 | 0.309573 |
| C | -7.831988 | -0.520844 | -0.698355 |
| C | -6.932575 | 0.312824 | -1.363140 |
| C | -5.584123 | 0.333686 | -1.039536 |
| C | -9.297187 | -0.507948 | -1.033951 |
| C | -10.088615 | 0.518893 | -0.218461 |
| C | -11.569773 | 0.531730 | -0.567121 |
| O | 1.691601 | 2.105884 | 0.524518 |
| O | -1.691607 | -2.105921 | 0.524541 |
| C | 9.297199 | 0.507989 | -1.033943 |
| C | 10.088636 | -0.518770 | -0.218359 |
| C | 11.569802 | -0.531592 | -0.566989 |
| O | 0.207051 | -3.720161 | 0.469588 |
| H | 2.730021 | -3.902818 | 0.456752 |
| H | 4.333642 | -2.039548 | 0.397423 |
| H | 5.613110 | 1.955860 | 1.453428 |
| H | 4.900626 | -0.953734 | -1.609031 |
| H | 7.290437 | -0.943637 | -2.172431 |
| H | 7.999520 | 2.012832 | 0.838285 |
| O | -0.207054 | 3.720118 | 0.469630 |
| H | -2.730030 | 3.902779 | 0.456846 |
| H | -4.333650 | 2.039504 | 0.397523 |
| H | -4.900572 | 0.953684 | -1.608976 |
| H | -7.290379 | 0.943617 | -2.172427 |
| H | -7.999579 | -2.012757 | 0.838354 |
| H | -5.613172 | -1.955830 | 1.453529 |
| H | 9.722127 | 1.504427 | -0.864458 |
| H | 12.113535 | -1.270877 | 0.027414 |
| H | 11.725896 | -0.774638 | -1.623076 |
| H | 12.028796 | 0.445208 | -0.382683 |
| H | 9.426972 | 0.293258 | -2.101470 |
| H | 9.956136 | -0.304202 | 0.848572 |
| H | 9.656020 | -1.512679 | -0.382790 |
| H | -9.956143 | 0.304401 | 0.848489 |
| H | -9.655967 | 1.512777 | -0.382956 |
| H | -12.113495 | 1.271078 | 0.027214 |
| H | -11.725840 | 0.774698 | -1.623230 |
| H | -12.028801 | -0.445042 | -0.382747 |
| H | -9.722142 | -1.504363 | -0.864404 |
| H | -9.426928 | -0.293289 | -2.101497 |
| H | 3.316945 | 1.448914 | 0.477658 |
| H | -3.316962 | -1.448957 | 0.477714 |
| H | 0.718518 | 3.362171 | 0.501318 |
| H | -0.718514 | -3.362227 | 0.501289 |
| 4a | | | |
| C | 7.939158 | 0.240350 | 0.414392 |
| C | 7.384358 | -0.934176 | 0.923036 |
| C | 6.026495 | -1.193139 | 0.814100 |
| C | 5.169548 | -0.279660 | 0.193415 |
| C | 5.723197 | 0.899945 | -0.312669 |

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|----|------------|-----------|-----------|
| C | 7.082326 | 1.150817 | -0.204899 |
| C | 3.722708 | -0.548473 | 0.081691 |
| C | 3.246142 | -1.847295 | -0.153148 |
| C | 1.891063 | -2.103699 | -0.255765 |
| C | 0.966397 | -1.068740 | -0.130516 |
| C | 1.426579 | 0.233989 | 0.100147 |
| C | 2.790132 | 0.481861 | 0.206087 |
| C | 0.480176 | 1.372711 | 0.246782 |
| C | -0.966398 | 1.068719 | 0.130648 |
| C | -1.426580 | -0.234010 | -0.100015 |
| C | -0.480179 | -1.372740 | -0.246603 |
| C | -2.790131 | -0.481875 | -0.205996 |
| C | -3.722706 | 0.548466 | -0.081642 |
| C | -3.246139 | 1.847288 | 0.153197 |
| C | -1.891062 | 2.103686 | 0.255855 |
| O | 0.877373 | 2.503575 | 0.449943 |
| O | -0.877372 | -2.503590 | -0.449844 |
| C | -5.169542 | 0.279659 | -0.193409 |
| C | -5.723214 | -0.899936 | 0.312671 |
| C | -7.082341 | -1.150803 | 0.204861 |
| C | -7.939149 | -0.240339 | -0.414469 |
| C | -7.384326 | 0.934178 | -0.923109 |
| C | -6.026466 | 1.193135 | -0.814133 |
| C | -9.417935 | -0.497430 | -0.491883 |
| C | -10.178050 | 0.038049 | 0.725456 |
| C | -11.674424 | -0.226586 | 0.646249 |
| C | 9.417945 | 0.497447 | 0.491762 |
| C | 10.178025 | -0.038024 | -0.725603 |
| C | 11.674401 | 0.226617 | -0.646441 |
| H | 1.518167 | -3.104189 | -0.444846 |
| H | 3.955184 | -2.658655 | -0.280173 |
| H | 3.103805 | 1.499910 | 0.409399 |
| H | -1.518166 | 3.104175 | 0.444938 |
| H | -3.103803 | -1.499925 | -0.409305 |
| H | -3.955181 | 2.658653 | 0.280190 |
| H | -5.619826 | 2.101734 | -1.246764 |
| H | -8.026009 | 1.652470 | -1.425920 |
| H | -7.488178 | -2.073198 | 0.610990 |
| H | -5.084095 | -1.619527 | 0.814104 |
| H | 5.084057 | 1.619538 | -0.814072 |
| H | 7.488145 | 2.073219 | -0.611030 |
| H | 8.026060 | -1.652471 | 1.425817 |
| H | 5.619874 | -2.101745 | 1.246733 |
| H | 9.824024 | 0.035857 | 1.399516 |
| H | 9.599225 | 1.574960 | 0.581996 |
| H | 9.991418 | -1.114485 | -0.816102 |
| H | 9.763852 | 0.417967 | -1.632413 |
| H | 12.195225 | -0.163888 | -1.524880 |
| H | 11.884162 | 1.299405 | -0.585429 |
| H | 12.114121 | -0.245863 | 0.237915 |
| H | -9.823983 | -0.035842 | -1.399652 |
| H | -9.599216 | -1.574943 | -0.582119 |
| H | -9.763907 | -0.417940 | 1.632281 |
| H | -9.991441 | 1.114509 | 0.815956 |
| H | -12.195274 | 0.163925 | 1.524670 |
| H | -12.114116 | 0.245892 | -0.238123 |
| H | -11.884188 | -1.299373 | 0.585234 |
| 4b | | | |
| C | 6.048893 | 1.411675 | 0.453341 |
| C | 5.184617 | 0.534887 | -0.208781 |

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|---|------------|-----------|-----------|
| C | 5.742659 | -0.570044 | -0.858439 |
| C | 7.112159 | -0.785465 | -0.846075 |
| C | 7.975903 | 0.087292 | -0.183560 |
| C | 7.417214 | 1.188342 | 0.465812 |
| C | 3.727634 | 0.769508 | -0.224659 |
| C | 2.829320 | -0.296556 | -0.165546 |
| C | 1.456183 | -0.081295 | -0.179928 |
| C | 0.951501 | 1.223469 | -0.249661 |
| C | 1.841675 | 2.293923 | -0.309443 |
| C | 3.206323 | 2.070187 | -0.299250 |
| C | 0.547771 | -1.257688 | -0.110118 |
| C | -0.910251 | -0.987818 | -0.123186 |
| C | -1.414848 | 0.317049 | -0.191419 |
| C | -0.506458 | 1.493358 | -0.262416 |
| C | -2.787957 | 0.532635 | -0.203274 |
| C | -3.686265 | -0.533324 | -0.143532 |
| C | -3.165172 | -1.834275 | -0.072469 |
| C | -1.800527 | -2.058272 | -0.064185 |
| C | -5.143359 | -0.299077 | -0.153230 |
| C | -6.009179 | -1.169801 | -0.821403 |
| C | -7.377029 | -0.943492 | -0.832691 |
| C | -7.933705 | 0.154066 | -0.175429 |
| C | -7.068110 | 1.021975 | 0.490772 |
| C | -5.698994 | 0.803973 | 0.501438 |
| C | -9.420789 | 0.369529 | -0.149828 |
| C | -10.101645 | -0.333674 | 1.028600 |
| C | -11.607848 | -0.119076 | 1.050496 |
| O | -0.942169 | 2.626497 | -0.325042 |
| O | 0.983460 | -2.390859 | -0.047777 |
| C | 9.454724 | -0.175118 | -0.131280 |
| C | 9.862877 | -1.030263 | 1.072398 |
| C | 11.360925 | -1.292103 | 1.124747 |
| H | -1.393226 | -3.061245 | -0.001271 |
| H | -3.845842 | -2.675919 | 0.001751 |
| H | -3.137748 | 1.556226 | -0.281202 |
| H | 1.434298 | 3.296749 | -0.374140 |
| H | 3.179170 | -1.320015 | -0.086034 |
| H | 3.886670 | 2.911980 | -0.374242 |
| H | 5.642809 | 2.265451 | 0.986451 |
| H | 8.066313 | 1.881830 | 0.993371 |
| H | 7.521619 | -1.643595 | -1.371824 |
| H | 5.098514 | -1.252640 | -1.403382 |
| H | -5.052418 | 1.487769 | 1.041983 |
| H | -7.474537 | 1.884447 | 1.011686 |
| H | -8.026285 | -1.625774 | -1.374472 |
| H | -5.603630 | -2.015829 | -1.367174 |
| H | -9.860483 | 0.006530 | -1.086268 |
| H | -9.636141 | 1.443283 | -0.099828 |
| H | -9.875973 | -1.405447 | 0.981587 |
| H | -9.657486 | 0.027861 | 1.963356 |
| H | -12.070734 | -0.629442 | 1.899434 |
| H | -11.855747 | 0.944603 | 1.127168 |
| H | -12.075951 | -0.501407 | 0.137574 |
| H | 9.996191 | 0.777459 | -0.093911 |
| H | 9.771520 | -0.678143 | -1.052437 |
| H | 9.537077 | -0.529225 | 1.991425 |
| H | 9.316411 | -1.979817 | 1.035835 |
| H | 11.629024 | -1.901870 | 1.991752 |
| H | 11.702349 | -1.820425 | 0.228661 |
| H | 11.924450 | -0.355659 | 1.189900 |

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|----|------------|-----------|-----------|
| 4c | | | |
| C | -6.006232 | 1.486910 | -0.381771 |
| C | -5.138516 | 0.601829 | 0.264648 |
| C | -5.698773 | -0.463072 | 0.976396 |
| C | -7.073311 | -0.632356 | 1.038250 |
| C | -7.940626 | 0.248158 | 0.390808 |
| C | -7.379991 | 1.309635 | -0.319867 |
| C | -3.675602 | 0.785632 | 0.200133 |
| C | -2.818418 | -0.313357 | 0.133396 |
| C | -1.439883 | -0.147357 | 0.071992 |
| C | -0.887793 | 1.140039 | 0.070643 |
| C | -1.736671 | 2.243184 | 0.137038 |
| C | -3.106931 | 2.068522 | 0.203129 |
| C | -0.577270 | -1.357471 | -0.002007 |
| C | 0.887800 | -1.140090 | -0.070598 |
| C | 1.439890 | 0.147307 | -0.071943 |
| C | 0.577276 | 1.357421 | 0.002044 |
| C | 2.818425 | 0.313307 | -0.133343 |
| C | 3.675610 | -0.785681 | -0.200083 |
| C | 3.106940 | -2.068571 | -0.203089 |
| C | 1.736679 | -2.243234 | -0.136998 |
| C | 5.138522 | -0.601870 | -0.264611 |
| C | 6.006252 | -1.486969 | 0.381769 |
| C | 7.380008 | -1.309686 | 0.319849 |
| C | 7.940628 | -0.248179 | -0.390796 |
| C | 7.073300 | 0.632354 | -1.038191 |
| C | 5.698762 | 0.463057 | -0.976327 |
| C | 9.427788 | -0.033327 | -0.419200 |
| C | 9.922009 | 0.847833 | 0.732330 |
| C | 11.428261 | 1.061772 | 0.702498 |
| O | 1.054351 | 2.475553 | 0.003245 |
| O | -1.054345 | -2.475603 | -0.003224 |
| C | -9.427789 | 0.033319 | 0.419194 |
| C | -9.922033 | -0.847635 | -0.732483 |
| C | -11.428296 | -1.061511 | -0.702709 |
| H | 1.292434 | -3.232357 | -0.146125 |
| H | 3.753370 | -2.936249 | -0.282786 |
| H | 3.206567 | 1.325603 | -0.106383 |
| H | -1.292426 | 3.232308 | 0.146156 |
| H | -3.206560 | -1.325653 | 0.106431 |
| H | -3.753362 | 2.936201 | 0.282818 |
| H | -5.600071 | 2.310010 | -0.961117 |
| H | -8.032004 | 2.008307 | -0.836868 |
| H | -7.483350 | -1.459673 | 1.610842 |
| H | -5.050593 | -1.150125 | 1.510828 |
| H | 5.050574 | 1.150128 | -1.510727 |
| H | 7.483321 | 1.459697 | -1.610760 |
| H | 8.032036 | -2.008368 | 0.836816 |
| H | 5.600099 | -2.310088 | 0.961093 |
| H | 9.940337 | -1.001459 | -0.374810 |
| H | 9.714000 | 0.427894 | -1.371713 |
| H | 9.404510 | 1.813201 | 0.689164 |
| H | 9.627057 | 0.389030 | 1.683246 |
| H | 11.758082 | 1.690603 | 1.533867 |
| H | 11.964774 | 0.109931 | 0.772426 |
| H | 11.741046 | 1.548809 | -0.226820 |
| H | -9.940327 | 1.001466 | 0.374977 |
| H | -9.713996 | -0.428062 | 1.371630 |
| H | -9.627047 | -0.388697 | -1.683323 |
| H | -9.404577 | -1.813033 | -0.689459 |
| H | -11.758128 | -1.690210 | -1.534172 |

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|---|------------|-----------|-----------|
| H | -11.741121 | -1.548663 | 0.226534 |
| H | -11.964764 | -0.109636 | -0.772515 |

4d

| | | | |
|---|------------|-----------|-----------|
| C | -5.977604 | -1.181803 | -0.929917 |
| C | -5.139639 | -0.306380 | -0.233084 |
| C | -5.722195 | 0.798605 | 0.394557 |
| C | -7.090209 | 1.013759 | 0.330525 |
| C | -7.928181 | 0.140559 | -0.363535 |
| C | -7.344613 | -0.958680 | -0.994103 |
| C | -3.683661 | -0.537484 | -0.163851 |
| C | -2.786340 | 0.530810 | -0.185629 |
| C | -1.414613 | 0.319288 | -0.111969 |
| C | -0.909795 | -0.984099 | -0.020332 |
| C | -1.798821 | -2.057052 | -0.001480 |
| C | -3.162446 | -1.836983 | -0.070023 |
| C | -0.507636 | 1.498481 | -0.141364 |
| C | 0.948723 | 1.233417 | -0.056919 |
| C | 1.453143 | -0.069359 | 0.045224 |
| C | 0.546706 | -1.249236 | 0.062722 |
| C | 2.824640 | -0.280375 | 0.124219 |
| C | 3.721573 | 0.788474 | 0.111864 |
| C | 3.200307 | 2.087588 | 0.012551 |
| C | 1.837539 | 2.306545 | -0.073393 |
| C | 5.176455 | 0.558240 | 0.203566 |
| C | 6.080745 | 1.365494 | -0.492705 |
| C | 7.447075 | 1.148668 | -0.399051 |
| C | 7.963543 | 0.123418 | 0.393579 |
| C | 7.059738 | -0.680962 | 1.088405 |
| C | 5.692526 | -0.471629 | 0.995855 |
| C | 9.442376 | -0.135560 | 0.461300 |
| C | 9.921875 | -1.122857 | -0.607339 |
| C | 11.419368 | -1.383381 | -0.535549 |
| O | 0.982751 | -2.381036 | 0.144733 |
| O | -0.943518 | 2.630018 | -0.227711 |
| C | -9.415761 | 0.352117 | -0.392819 |
| C | -10.135301 | -0.340111 | 0.768989 |
| C | -11.641593 | -0.127468 | 0.737792 |
| H | 1.429987 | 3.309014 | -0.142463 |
| H | 3.877874 | 2.934799 | 0.028568 |
| H | 3.175205 | -1.305316 | 0.176399 |
| H | -1.391933 | -3.058874 | 0.079845 |
| H | -3.134904 | 1.553444 | -0.279622 |
| H | -3.843180 | -2.680664 | -0.025177 |
| H | -5.550068 | -2.029463 | -1.455993 |
| H | -7.971410 | -1.645164 | -1.556592 |
| H | -7.517849 | 1.877722 | 0.831629 |
| H | -5.098361 | 1.486066 | 0.956703 |
| H | 5.015878 | -1.096890 | 1.569392 |
| H | 7.435312 | -1.478288 | 1.723699 |
| H | 8.128204 | 1.786911 | -0.955166 |
| H | 5.709143 | 2.157799 | -1.134745 |
| H | 9.986902 | 0.809046 | 0.346899 |
| H | 9.701213 | -0.526711 | 1.452248 |
| H | 9.371343 | -2.064096 | -0.494997 |
| H | 9.655654 | -0.733156 | -1.596762 |
| H | 11.738525 | -2.089116 | -1.307198 |
| H | 11.989478 | -0.459012 | -0.674250 |
| H | 11.702409 | -1.802504 | 0.435499 |
| H | -9.821767 | -0.022132 | -1.339966 |
| H | -9.635437 | 1.425759 | -0.361965 |

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|---|------------|-----------|-----------|
| H | -9.906953 | -1.411965 | 0.740522 |
| H | -9.723151 | 0.031588 | 1.714362 |
| H | -12.132449 | -0.630213 | 1.575493 |
| H | -11.893043 | 0.936562 | 0.795665 |
| H | -12.078015 | -0.519289 | -0.186728 |

4e

| | | | |
|---|------------|-----------|-----------|
| C | -5.985993 | 1.476756 | 0.520008 |
| C | -5.145476 | 0.601675 | -0.174356 |
| C | -5.734808 | -0.453111 | -0.877642 |
| C | -7.110707 | -0.622496 | -0.884967 |
| C | -7.950686 | 0.248542 | -0.190634 |
| C | -7.361158 | 1.300073 | 0.511596 |
| C | -3.681183 | 0.785789 | -0.169741 |
| C | -2.821456 | -0.313336 | -0.165580 |
| C | -1.441629 | -0.147214 | -0.165776 |
| C | -0.890143 | 1.140434 | -0.162119 |
| C | -1.741383 | 2.243746 | -0.164008 |
| C | -3.113212 | 2.069026 | -0.170623 |
| C | -0.576485 | -1.357808 | -0.161250 |
| C | 0.890151 | -1.140489 | -0.162096 |
| C | 1.441636 | 0.147159 | -0.165737 |
| C | 0.576492 | 1.357754 | -0.161245 |
| C | 2.821465 | 0.313279 | -0.165505 |
| C | 3.681187 | -0.785849 | -0.169649 |
| C | 3.113217 | -2.069088 | -0.170538 |
| C | 1.741387 | -2.243804 | -0.163960 |
| C | 5.145483 | -0.601741 | -0.174236 |
| C | 5.985982 | -1.476810 | 0.520163 |
| C | 7.361151 | -1.300138 | 0.511760 |
| C | 7.950692 | -0.248638 | -0.190502 |
| C | 7.110731 | 0.622388 | -0.884872 |
| C | 5.734830 | 0.453016 | -0.877556 |
| C | 9.437900 | -0.034323 | -0.162234 |
| C | 9.888351 | 0.847009 | 1.006969 |
| C | 11.394413 | 1.062956 | 1.032002 |
| O | 1.053049 | 2.476122 | -0.159668 |
| O | -1.053040 | -2.476176 | -0.159721 |
| C | -9.437894 | 0.034232 | -0.162358 |
| C | -9.888390 | -0.846615 | 1.007204 |
| C | -11.394454 | -1.062531 | 1.032289 |
| H | 1.298270 | -3.233445 | -0.171926 |
| H | 3.762460 | -2.937774 | -0.201659 |
| H | 3.207404 | 1.326500 | -0.142542 |
| H | -1.298274 | 3.233390 | -0.171969 |
| H | -3.207386 | -1.326560 | -0.142623 |
| H | -3.762448 | 2.937717 | -0.201781 |
| H | -5.556536 | 2.291448 | 1.094375 |
| H | -7.991231 | 1.991385 | 1.064485 |
| H | -7.544002 | -1.441810 | -1.451897 |
| H | -5.109635 | -1.131682 | -1.448957 |
| H | 5.109664 | 1.131573 | -1.448894 |
| H | 7.544041 | 1.441674 | -1.451831 |
| H | 7.991216 | -1.991431 | 1.064680 |
| H | 5.556506 | -2.291489 | 1.094534 |
| H | 9.948375 | -1.002479 | -0.098213 |
| H | 9.760036 | 0.426618 | -1.103361 |
| H | 9.371359 | 1.811641 | 0.945256 |
| H | 9.559542 | 0.387339 | 1.946313 |
| H | 11.693201 | 1.691074 | 1.875550 |
| H | 11.929396 | 0.111731 | 1.119823 |

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|---|------------|-----------|-----------|
| H | 11.739738 | 1.551746 | 0.115213 |
| H | -9.948379 | 1.002411 | -0.098759 |
| H | -9.759983 | -0.427112 | -1.103300 |
| H | -9.371402 | -1.811274 | 0.945894 |
| H | -9.559597 | -0.386556 | 1.946363 |
| H | -11.693270 | -1.690300 | 1.876088 |
| H | -11.929425 | -0.111263 | 1.119711 |
| H | -11.739766 | -1.551689 | 0.115693 |

4f

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|---|------------|-----------|-----------|
| C | 6.065324 | 1.045650 | -0.886076 |
| C | 5.176284 | 0.234650 | -0.174535 |
| C | 5.700617 | -0.855616 | 0.525912 |
| C | 7.061982 | -1.117920 | 0.517922 |
| C | 7.950717 | -0.308537 | -0.190312 |
| C | 7.425168 | 0.775605 | -0.893665 |
| C | 3.728132 | 0.518967 | -0.167112 |
| C | 2.791939 | -0.515647 | -0.161919 |
| C | 1.427398 | -0.250535 | -0.154728 |
| C | 0.970154 | 1.073366 | -0.158174 |
| C | 1.898334 | 2.112769 | -0.162556 |
| C | 3.253936 | 1.839699 | -0.164771 |
| C | 0.477191 | -1.395590 | -0.154314 |
| C | -0.970146 | -1.073365 | -0.158186 |
| C | -1.427391 | 0.250537 | -0.154734 |
| C | -0.477182 | 1.395589 | -0.154312 |
| C | -2.791930 | 0.515649 | -0.161922 |
| C | -3.728122 | -0.518971 | -0.167107 |
| C | -3.253928 | -1.839700 | -0.164775 |
| C | -1.898324 | -2.112769 | -0.162570 |
| C | -5.176279 | -0.234651 | -0.174529 |
| C | -6.065318 | -1.045665 | -0.886050 |
| C | -7.425170 | -0.775633 | -0.893623 |
| C | -7.950715 | 0.308512 | -0.190284 |
| C | -7.061976 | 1.117925 | 0.517916 |
| C | -5.700611 | 0.855630 | 0.525903 |
| C | -9.430424 | 0.569533 | -0.161194 |
| C | -10.137124 | -0.152821 | 0.990122 |
| C | -11.635997 | 0.108000 | 1.015743 |
| O | -0.871953 | 2.545349 | -0.150548 |
| O | 0.871961 | -2.545349 | -0.150513 |
| C | 9.430426 | -0.569545 | -0.161233 |
| C | 10.137087 | 0.152804 | 0.990125 |
| C | 11.635963 | -0.107947 | 1.015804 |
| H | -1.527422 | -3.131674 | -0.153821 |
| H | -3.964442 | -2.659306 | -0.140744 |
| H | -3.104303 | 1.553970 | -0.184360 |
| H | 1.527434 | 3.131675 | -0.153776 |
| H | 3.104305 | -1.553972 | -0.184354 |
| H | 3.964450 | 2.659305 | -0.140743 |
| H | 5.683513 | 1.878729 | -1.467668 |
| H | 8.092451 | 1.411682 | -1.468700 |
| H | 7.444009 | -1.969111 | 1.074708 |
| H | 5.036365 | -1.493309 | 1.100310 |
| H | -5.036354 | 1.493330 | 1.100287 |
| H | -7.444003 | 1.969146 | 1.074655 |
| H | -8.092451 | -1.411734 | -1.468636 |
| H | -5.683507 | -1.878746 | -1.467638 |
| H | -9.877561 | 0.253284 | -1.110964 |
| H | -9.612293 | 1.647097 | -0.073992 |
| H | -9.944933 | -1.228837 | 0.906156 |

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|---|------------|-----------|-----------|
| H | -9.685250 | 0.161812 | 1.938034 |
| H | -12.117554 | -0.416491 | 1.845475 |
| H | -11.850758 | 1.175654 | 1.128322 |
| H | -12.112527 | -0.228059 | 0.089085 |
| H | 9.877563 | -0.253249 | -1.110984 |
| H | 9.612316 | -1.647104 | -0.074051 |
| H | 9.944846 | 1.228813 | 0.906170 |
| H | 9.685181 | -0.161871 | 1.938007 |
| H | 12.117448 | 0.416539 | 1.845582 |
| H | 11.850784 | -1.175592 | 1.128355 |
| H | 12.112529 | 0.228172 | 0.089185 |

5a

| | | | |
|---|------------|-----------|-----------|
| C | -6.009138 | 1.041135 | -0.942760 |
| C | -5.200131 | 0.175666 | -0.199507 |
| C | -5.813071 | -0.902110 | 0.447574 |
| C | -7.183919 | -1.088999 | 0.364134 |
| C | -7.993463 | -0.224224 | -0.373173 |
| C | -7.378597 | 0.842094 | -1.028711 |
| C | -3.751647 | 0.439048 | -0.089552 |
| C | -2.790570 | -0.600390 | -0.171246 |
| C | -1.414338 | -0.297855 | -0.084877 |
| C | -0.996649 | 1.037188 | 0.083944 |
| C | -1.935247 | 2.049548 | 0.165939 |
| C | -3.288799 | 1.739977 | 0.080471 |
| C | -0.436004 | -1.377392 | -0.181040 |
| C | 0.996649 | -1.037185 | -0.083967 |
| C | 1.414338 | 0.297857 | 0.084855 |
| C | 0.436004 | 1.377395 | 0.181010 |
| C | 2.790570 | 0.600392 | 0.171231 |
| C | 3.751647 | -0.439046 | 0.089542 |
| C | 3.288798 | -1.739976 | -0.080484 |
| C | 1.935247 | -2.049546 | -0.165958 |
| C | 5.200130 | -0.175665 | 0.199506 |
| C | 6.009131 | -1.041134 | 0.942763 |
| C | 7.378591 | -0.842095 | 1.028723 |
| C | 7.993462 | 0.224222 | 0.373189 |
| C | 7.183923 | 1.088998 | -0.364124 |
| C | 5.813075 | 0.902109 | -0.447572 |
| C | 9.483472 | 0.412589 | 0.426031 |
| C | 10.212227 | -0.311301 | -0.710400 |
| C | 11.721182 | -0.123677 | -0.654826 |
| O | 0.786432 | 2.553100 | 0.337572 |
| O | -0.786432 | -2.553097 | -0.337597 |
| C | -9.483474 | -0.412592 | -0.426006 |
| C | -10.212222 | 0.311296 | 0.710431 |
| C | -11.721177 | 0.123671 | 0.654866 |
| H | 1.596240 | -3.068621 | -0.306373 |
| H | 4.020326 | -2.536564 | -0.168437 |
| O | 3.207087 | 1.847158 | 0.342786 |
| H | -1.596240 | 3.068624 | 0.306352 |
| O | -3.207088 | -1.847157 | -0.342794 |
| H | -4.020327 | 2.536565 | 0.168428 |
| H | -5.554143 | 1.864185 | -1.485035 |
| H | -7.980700 | 1.520679 | -1.626618 |
| H | -7.636621 | -1.931516 | 0.879743 |
| H | -5.210344 | -1.595861 | 1.019524 |
| H | 5.210352 | 1.595861 | -1.019527 |
| H | 7.636629 | 1.931513 | -0.879731 |
| H | 7.980689 | -1.520680 | 1.626635 |
| H | 5.554132 | -1.864184 | 1.485036 |

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|---|------------|-----------|-----------|
| H | 9.866600 | 0.048751 | 1.386683 |
| H | 9.721137 | 1.481908 | 0.380335 |
| H | 9.965110 | -1.378546 | -0.668110 |
| H | 9.823654 | 0.051121 | -1.669269 |
| H | 12.218798 | -0.648377 | -1.474941 |
| H | 11.991868 | 0.934889 | -0.725001 |
| H | 12.133687 | -0.507492 | 0.283957 |
| H | -9.866609 | -0.048752 | -1.386655 |
| H | -9.721138 | -1.481911 | -0.380310 |
| H | -9.823643 | -0.051128 | 1.669297 |
| H | -9.965106 | 1.378541 | 0.668141 |
| H | -12.218788 | 0.648370 | 1.474986 |
| H | -12.133688 | 0.507487 | -0.283913 |
| H | -11.991862 | -0.934895 | 0.725041 |
| H | 2.389012 | 2.408912 | 0.388703 |
| H | -2.389014 | -2.408912 | -0.388705 |

5b

| | | | |
|---|------------|-----------|-----------|
| C | -5.802290 | 0.781741 | 0.598518 |
| C | -5.180477 | -0.231495 | -0.138354 |
| C | -5.989977 | -1.079925 | -0.900487 |
| C | -7.367938 | -0.926909 | -0.918994 |
| C | -7.990735 | 0.074602 | -0.174985 |
| C | -7.180978 | 0.922416 | 0.581773 |
| C | -3.720376 | -0.447214 | -0.104820 |
| C | -2.800009 | 0.630019 | -0.161144 |
| C | -1.411715 | 0.373750 | -0.153136 |
| C | -0.941578 | -0.952730 | -0.085909 |
| C | -1.840369 | -2.002146 | -0.027356 |
| C | -3.206145 | -1.738056 | -0.036158 |
| C | -0.476158 | 1.492442 | -0.224002 |
| C | 0.970235 | 1.199729 | -0.212752 |
| C | 1.440378 | -0.126719 | -0.145015 |
| C | 0.504853 | -1.245306 | -0.072491 |
| C | 1.869030 | 2.248909 | -0.274949 |
| C | 3.234781 | 1.984622 | -0.270566 |
| C | 3.749114 | 0.693813 | -0.201618 |
| C | 2.828646 | -0.383085 | -0.139838 |
| C | 5.209146 | 0.476887 | -0.174637 |
| C | 6.024735 | 1.331390 | 0.574250 |
| C | 7.403099 | 1.182210 | 0.578431 |
| C | 8.020516 | 0.178312 | -0.166968 |
| C | 7.205003 | -0.674675 | -0.911360 |
| C | 5.825789 | -0.537590 | -0.914090 |
| C | 9.510991 | -0.010668 | -0.130441 |
| C | 9.962234 | -0.964271 | 0.980242 |
| C | 11.471714 | -1.153928 | 1.012992 |
| O | 0.901933 | -2.414596 | -0.004313 |
| O | -0.873206 | 2.661847 | -0.290107 |
| C | -9.487045 | 0.213042 | -0.157624 |
| C | -10.142468 | -0.577743 | 0.978854 |
| C | -11.657565 | -0.437622 | 0.994928 |
| H | -1.460910 | -3.014751 | 0.034371 |
| H | -3.905463 | -2.564872 | 0.032398 |
| O | -3.266340 | 1.868775 | -0.235302 |
| H | 1.489562 | 3.261493 | -0.336978 |
| O | 3.294998 | -1.621794 | -0.064370 |
| H | 3.933735 | 2.811314 | -0.343698 |
| H | 5.570307 | 2.110565 | 1.178295 |
| H | 8.011816 | 1.857359 | 1.173608 |
| H | 7.661195 | -1.461114 | -1.506398 |

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|---|------------|-----------|-----------|
| H | 5.219897 | -1.215636 | -1.501364 |
| H | -5.200198 | 1.461514 | 1.187669 |
| H | -7.640323 | 1.714914 | 1.166247 |
| H | -7.971164 | -1.589738 | -1.533213 |
| H | -5.530170 | -1.851223 | -1.510548 |
| H | -9.898826 | -0.126798 | -1.115125 |
| H | -9.757243 | 1.271132 | -0.059944 |
| H | -9.864088 | -1.633817 | 0.883723 |
| H | -9.724292 | -0.239794 | 1.934222 |
| H | -12.102159 | -1.008468 | 1.814665 |
| H | -11.957365 | 0.608253 | 1.117336 |
| H | -12.098940 | -0.799467 | 0.060565 |
| H | 10.001580 | 0.959800 | 0.009606 |
| H | 9.855261 | -0.398094 | -1.096647 |
| H | 9.611335 | -0.578525 | 1.944489 |
| H | 9.464890 | -1.931375 | 0.842722 |
| H | 11.770804 | -1.835243 | 1.814119 |
| H | 11.839267 | -1.569463 | 0.069053 |
| H | 11.987128 | -0.201862 | 1.176554 |
| H | -2.471062 | 2.462389 | -0.280147 |
| H | 2.499700 | -2.215155 | -0.016594 |

5c

| | | | |
|---|------------|-----------|-----------|
| C | 5.792349 | 0.432809 | -1.026177 |
| C | 5.170689 | -0.552423 | -0.252148 |
| C | 5.985202 | -1.429757 | 0.471030 |
| C | 7.367053 | -1.329593 | 0.418565 |
| C | 7.988805 | -0.354079 | -0.360110 |
| C | 7.174467 | 0.520527 | -1.080394 |
| C | 3.703739 | -0.714309 | -0.214988 |
| C | 2.828977 | 0.397780 | -0.120995 |
| C | 1.433220 | 0.195334 | -0.061492 |
| C | 0.909728 | -1.112299 | -0.098275 |
| C | 1.763886 | -2.195792 | -0.193137 |
| C | 3.137651 | -1.984628 | -0.251456 |
| C | 0.545673 | 1.349605 | 0.045756 |
| C | -0.909880 | 1.112849 | 0.101762 |
| C | -1.433367 | -0.194786 | 0.065066 |
| C | -0.545806 | -1.349084 | -0.041755 |
| C | -1.764053 | 2.196400 | 0.195822 |
| C | -3.137871 | 1.985299 | 0.253076 |
| C | -3.703940 | 0.714978 | 0.216550 |
| C | -2.829156 | -0.397187 | 0.123873 |
| C | -5.170947 | 0.553206 | 0.251952 |
| C | -5.984287 | 1.429760 | -0.473441 |
| C | -7.366233 | 1.329710 | -0.422963 |
| C | -7.989204 | 0.355177 | 0.355915 |
| C | -7.176005 | -0.518657 | 1.078478 |
| C | -5.793810 | -0.431118 | 1.026190 |
| C | -9.485504 | 0.216614 | 0.376037 |
| C | -10.006950 | -0.743162 | -0.698068 |
| C | -11.521927 | -0.883639 | -0.674872 |
| O | -0.989972 | -2.502602 | -0.082141 |
| O | 0.989832 | 2.503112 | 0.086641 |
| C | 9.485061 | -0.215368 | -0.382309 |
| C | 10.008608 | 0.737746 | 0.696694 |
| C | 11.523442 | 0.879251 | 0.670691 |
| H | 1.343430 | -3.193265 | -0.230848 |
| H | 3.800466 | -2.838075 | -0.349404 |
| O | 3.345514 | 1.617931 | -0.076467 |
| H | -1.343584 | 3.193866 | 0.233545 |

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| O | -3.345717 | -1.617343 | 0.079679 |
| H | -3.800777 | 2.838785 | 0.350079 |
| H | -5.526327 | 2.186526 | -1.102812 |
| H | -7.973565 | 2.020172 | -1.001723 |
| H | -7.636127 | -1.282546 | 1.699316 |
| H | -5.189904 | -1.125084 | 1.596684 |
| H | 5.187586 | 1.127382 | -1.595009 |
| H | 7.633619 | 1.285189 | -1.700993 |
| H | 7.975267 | -2.020745 | 0.995581 |
| H | 5.528258 | -2.187294 | 1.100211 |
| H | 9.948075 | -1.199865 | -0.246242 |
| H | 9.805370 | 0.147299 | -1.366186 |
| H | 9.537467 | 1.718533 | 0.563792 |
| H | 9.682139 | 0.376558 | 1.678862 |
| H | 11.873443 | 1.561798 | 1.449862 |
| H | 12.014547 | -0.086342 | 0.829730 |
| H | 11.868490 | 1.269612 | -0.292297 |
| H | -9.948114 | 1.200285 | 0.232886 |
| H | -9.807875 | -0.139869 | 1.361510 |
| H | -9.677831 | -0.388497 | -1.681725 |
| H | -9.536720 | -1.723347 | -0.557687 |
| H | -11.870388 | -1.571264 | -1.450259 |
| H | -11.869624 | -1.267222 | 0.289888 |
| H | -12.012046 | 0.081136 | -0.841721 |
| H | 2.576751 | 2.242083 | 0.002149 |
| H | -2.576947 | -2.241563 | 0.001823 |

5d

| | | | |
|---|------------|-----------|-----------|
| C | 5.807067 | -0.428104 | 1.054739 |
| C | 5.206783 | 0.501025 | 0.198862 |
| C | 6.037572 | 1.271196 | -0.621234 |
| C | 7.415502 | 1.122819 | -0.583168 |
| C | 8.016697 | 0.205210 | 0.277564 |
| C | 7.185948 | -0.563312 | 1.094006 |
| C | 3.746699 | 0.717715 | 0.170018 |
| C | 2.827530 | -0.361636 | 0.191675 |
| C | 1.440100 | -0.108831 | 0.126901 |
| C | 0.969628 | 1.216953 | 0.048158 |
| C | 1.867156 | 2.268959 | 0.033789 |
| C | 3.232213 | 2.008090 | 0.094945 |
| C | 0.506358 | -1.231261 | 0.128795 |
| C | -0.938777 | -0.942383 | 0.049515 |
| C | -1.409902 | 0.384132 | -0.011176 |
| C | -0.476062 | 1.506427 | -0.015631 |
| C | -1.835368 | -1.995260 | 0.038741 |
| C | -3.199998 | -1.734668 | -0.033995 |
| C | -3.714583 | -0.443851 | -0.098526 |
| C | -2.797010 | 0.636902 | -0.082311 |
| C | -5.171456 | -0.230038 | -0.204930 |
| C | -5.934352 | -1.054150 | -1.038382 |
| C | -7.309381 | -0.901294 | -1.129892 |
| C | -7.975701 | 0.074951 | -0.389912 |
| C | -7.212143 | 0.898003 | 0.438735 |
| C | -5.836049 | 0.758222 | 0.528149 |
| C | -9.470935 | 0.211592 | -0.453349 |
| C | -10.189558 | -0.638231 | 0.599169 |
| C | -11.703390 | -0.499112 | 0.532593 |
| O | -0.873840 | 2.675904 | -0.075438 |
| O | 0.904062 | -2.400645 | 0.191003 |
| C | 9.507238 | 0.013509 | 0.288466 |
| C | 9.972751 | -1.075961 | -0.682564 |

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|---|------------|-----------|-----------|
| C | 11.482746 | -1.263898 | -0.674396 |
| H | 1.487048 | 3.281960 | -0.016377 |
| H | 3.930103 | 2.838899 | 0.103957 |
| O | 3.294993 | -1.600455 | 0.257096 |
| H | -1.455648 | -3.008025 | 0.096127 |
| O | -3.264327 | 1.875574 | -0.150763 |
| H | -3.899112 | -2.564446 | -0.021508 |
| H | -5.438756 | -1.805004 | -1.645951 |
| H | -7.875026 | -1.544046 | -1.798832 |
| H | -7.705719 | 1.670742 | 1.021704 |
| H | -5.269327 | 1.419578 | 1.171095 |
| H | 5.188383 | -1.040265 | 1.698492 |
| H | 7.629603 | -1.280846 | 1.778804 |
| H | 8.037102 | 1.729385 | -1.236019 |
| H | 5.595201 | 1.980776 | -1.313535 |
| H | 10.000800 | 0.958037 | 0.030762 |
| H | 9.837210 | -0.244849 | 1.301661 |
| H | 9.475598 | -2.018271 | -0.424776 |
| H | 9.631630 | -0.820928 | -1.692666 |
| H | 11.790894 | -2.045718 | -1.373875 |
| H | 11.998297 | -0.341034 | -0.959543 |
| H | 11.841695 | -1.547873 | 0.320249 |
| H | -9.824607 | -0.077603 | -1.450013 |
| H | -9.750267 | 1.262892 | -0.316479 |
| H | -9.902672 | -1.687767 | 0.464830 |
| H | -9.829775 | -0.351371 | 1.594183 |
| H | -12.194224 | -1.113300 | 1.292430 |
| H | -12.013211 | 0.538653 | 0.693170 |
| H | -12.087168 | -0.809826 | -0.444591 |
| H | 2.501173 | -2.197419 | 0.243479 |
| H | -2.470266 | 2.472350 | -0.144063 |

5e

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|---|-----------|-----------|-----------|
| C | 5.849529 | 0.360280 | -0.944284 |
| C | 5.173735 | -0.571426 | -0.149770 |
| C | 5.934222 | -1.399276 | 0.682103 |
| C | 7.316985 | -1.303190 | 0.714900 |
| C | 7.993501 | -0.382593 | -0.084399 |
| C | 7.232730 | 0.442993 | -0.913276 |
| C | 3.706663 | -0.729626 | -0.195797 |
| C | 2.833117 | 0.386928 | -0.218259 |
| C | 1.435389 | 0.189636 | -0.224149 |
| C | 0.909351 | -1.117518 | -0.215510 |
| C | 1.762793 | -2.205635 | -0.201259 |
| C | 3.138547 | -1.999489 | -0.192002 |
| C | 0.548143 | 1.349093 | -0.224291 |
| C | -0.909343 | 1.117476 | -0.215507 |
| C | -1.435391 | -0.189679 | -0.224138 |
| C | -0.548134 | -1.349142 | -0.224310 |
| C | -1.762773 | 2.205602 | -0.201269 |
| C | -3.138529 | 1.999473 | -0.192017 |
| C | -3.706655 | 0.729618 | -0.195784 |
| C | -2.833128 | -0.386949 | -0.218225 |
| C | -5.173727 | 0.571431 | -0.149749 |
| C | -5.934207 | 1.399334 | 0.682075 |
| C | -7.316973 | 1.303263 | 0.714872 |
| C | -7.993492 | 0.382625 | -0.084372 |
| C | -7.232725 | -0.443024 | -0.913194 |
| C | -5.849525 | -0.360322 | -0.944206 |
| C | -9.488873 | 0.248482 | -0.018051 |
| C | -9.947025 | -0.794429 | 1.006159 |

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|---|------------|-----------|-----------|
| C | -11.461546 | -0.925962 | 1.072765 |
| O | -0.994300 | -2.502543 | -0.226589 |
| O | 0.994337 | 2.502484 | -0.226635 |
| C | 9.488879 | -0.248423 | -0.018055 |
| C | 9.946995 | 0.794463 | 1.006193 |
| C | 11.461513 | 0.926010 | 1.072835 |
| H | 1.340883 | -3.203198 | -0.205551 |
| H | 3.802762 | -2.857483 | -0.200650 |
| O | 3.352249 | 1.606796 | -0.216676 |
| H | -1.340851 | 3.203160 | -0.205563 |
| O | -3.352306 | -1.606794 | -0.216626 |
| H | -3.802736 | 2.857473 | -0.200683 |
| H | -5.432922 | 2.113289 | 1.328248 |
| H | -7.882466 | 1.954514 | 1.375667 |
| H | -7.735274 | -1.164590 | -1.551570 |
| H | -5.286304 | -1.016807 | -1.595222 |
| H | 5.286308 | 1.016724 | -1.595339 |
| H | 7.735275 | 1.164512 | -1.551709 |
| H | 7.882482 | -1.954396 | 1.375736 |
| H | 5.432943 | -2.113203 | 1.328310 |
| H | 9.933665 | -1.218224 | 0.234379 |
| H | 9.877427 | 0.025404 | -1.006101 |
| H | 9.496783 | 1.761755 | 0.754751 |
| H | 9.549871 | 0.523428 | 1.991350 |
| H | 11.764614 | 1.674852 | 1.809605 |
| H | 11.929672 | -0.023492 | 1.352250 |
| H | 11.876347 | 1.225500 | 0.104832 |
| H | -9.933642 | 1.218282 | 0.234410 |
| H | -9.877414 | -0.025307 | -1.006110 |
| H | -9.496818 | -1.761718 | 0.754700 |
| H | -9.549920 | -0.523421 | 1.991331 |
| H | -11.764668 | -1.674815 | 1.809514 |
| H | -11.929702 | 0.023539 | 1.352187 |
| H | -11.876362 | -1.225431 | 0.104748 |
| H | 2.583410 | 2.235618 | -0.215804 |
| H | -2.583490 | -2.235642 | -0.215686 |

5f

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|---|-----------|-----------|-----------|
| C | -5.798329 | 0.847418 | 0.619335 |
| C | -5.205226 | -0.155792 | -0.154242 |
| C | -6.036931 | -0.941626 | -0.958739 |
| C | -7.408359 | -0.739664 | -0.981686 |
| C | -8.002810 | 0.251168 | -0.201174 |
| C | -7.171040 | 1.037801 | 0.596695 |
| C | -3.754451 | -0.427052 | -0.118967 |
| C | -2.792834 | 0.615142 | -0.108843 |
| C | -1.415393 | 0.305083 | -0.106269 |
| C | -0.997002 | -1.040208 | -0.111635 |
| C | -1.935870 | -2.055623 | -0.116224 |
| C | -3.290233 | -1.738706 | -0.117526 |
| C | -0.436919 | 1.388781 | -0.109147 |
| C | 0.997005 | 1.040214 | -0.111631 |
| C | 1.415386 | -0.305075 | -0.106272 |
| C | 0.436924 | -1.388771 | -0.109185 |
| C | 1.935885 | 2.055617 | -0.116236 |
| C | 3.290245 | 1.738682 | -0.117548 |
| C | 3.754449 | 0.427020 | -0.118972 |
| C | 2.792813 | -0.615159 | -0.108834 |
| C | 5.205226 | 0.155753 | -0.154242 |
| C | 6.036925 | 0.941553 | -0.958781 |
| C | 7.408354 | 0.739603 | -0.981722 |

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|---|------------|-----------|-----------|
| C | 8.002816 | -0.251178 | -0.201156 |
| C | 7.171057 | -1.037776 | 0.596759 |
| C | 5.798344 | -0.847406 | 0.619392 |
| C | 9.493615 | -0.440397 | -0.189534 |
| C | 10.183884 | 0.362547 | 0.917417 |
| C | 11.694109 | 0.176781 | 0.924453 |
| O | 0.788142 | -2.574597 | -0.112241 |
| O | -0.788104 | 2.574619 | -0.112237 |
| C | -9.493607 | 0.440397 | -0.189554 |
| C | -10.183881 | -0.362465 | 0.917453 |
| C | -11.694104 | -0.176690 | 0.924474 |
| H | -1.596035 | -3.084048 | -0.109470 |
| H | -4.020899 | -2.540596 | -0.098199 |
| O | -3.210146 | 1.873404 | -0.116736 |
| H | 1.596061 | 3.084046 | -0.109488 |
| O | 3.210070 | -1.873444 | -0.116701 |
| H | 4.020922 | 2.540562 | -0.098236 |
| H | 5.598660 | 1.701962 | -1.597614 |
| H | 8.028629 | 1.354352 | -1.628105 |
| H | 7.607836 | -1.821346 | 1.209886 |
| H | 5.178740 | -1.479961 | 1.241889 |
| H | -5.178715 | 1.480002 | 1.241793 |
| H | -7.607807 | 1.821411 | 1.209780 |
| H | -8.028641 | -1.354439 | -1.628037 |
| H | -5.598676 | -1.702071 | -1.597536 |
| H | -9.909017 | 0.144134 | -1.159910 |
| H | -9.728725 | 1.503529 | -0.060899 |
| H | -9.936859 | -1.423356 | 0.793676 |
| H | -9.764797 | -0.065512 | 1.885943 |
| H | -12.163436 | -0.756658 | 1.723774 |
| H | -11.963715 | 0.873896 | 1.073903 |
| H | -12.137186 | -0.498690 | -0.023544 |
| H | 9.909020 | -0.144198 | -1.159911 |
| H | 9.728743 | -1.503517 | -0.060806 |
| H | 9.936856 | 1.423429 | 0.793568 |
| H | 9.764802 | 0.065658 | 1.885928 |
| H | 12.163437 | 0.756807 | 1.723712 |
| H | 11.963724 | -0.873793 | 1.073955 |
| H | 12.137189 | 0.498718 | -0.023588 |
| H | -2.392011 | 2.436967 | -0.123214 |
| H | 2.391922 | -2.436981 | -0.123089 |

6a

| | | | |
|---|-----------|-----------|----------|
| C | -4.403832 | -0.697847 | 0.000000 |
| C | -4.403832 | 0.697847 | 0.000000 |
| C | -3.206563 | -1.392063 | 0.000000 |
| C | -1.995574 | -0.698125 | 0.000000 |
| C | -1.995574 | 0.698125 | 0.000000 |
| C | -3.206563 | 1.392064 | 0.000000 |
| H | -5.343869 | -1.239841 | 0.000000 |
| H | -3.174171 | -2.475369 | 0.000000 |
| H | -5.343869 | 1.239842 | 0.000000 |
| H | -3.174170 | 2.475370 | 0.000000 |
| C | -0.728814 | -1.459382 | 0.000000 |
| C | 0.526124 | -0.716770 | 0.000000 |
| C | 0.526124 | 0.716770 | 0.000000 |
| C | -0.728814 | 1.459382 | 0.000000 |
| O | -0.780210 | -2.696243 | 0.000000 |
| O | -0.780211 | 2.696243 | 0.000000 |
| C | 1.749900 | -1.432150 | 0.000000 |
| C | 2.954288 | -0.681556 | 0.000000 |

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|---|----------|-----------|-----------|
| C | 2.954289 | 0.681555 | 0.000000 |
| C | 1.749901 | 1.432150 | 0.000000 |
| H | 3.902606 | 1.205497 | 0.000000 |
| H | 3.902605 | -1.205498 | 0.000000 |
| N | 1.797110 | -2.783097 | 0.000000 |
| N | 1.797112 | 2.783096 | 0.000000 |
| C | 3.006313 | 3.557304 | 0.000000 |
| H | 0.884961 | 3.232255 | 0.000000 |
| H | 2.736269 | 4.613494 | 0.000000 |
| H | 3.622538 | 3.369691 | 0.888932 |
| H | 3.622538 | 3.369691 | -0.888932 |
| C | 3.006309 | -3.557306 | 0.000000 |
| H | 0.884958 | -3.232254 | 0.000000 |
| H | 2.736264 | -4.613495 | 0.000000 |
| H | 3.622535 | -3.369694 | -0.888932 |
| H | 3.622535 | -3.369694 | 0.888932 |

7a

| | | | |
|---|-----------|-----------|-----------|
| C | -1.392119 | 4.408357 | -0.000107 |
| C | -0.698058 | 3.197258 | -0.000043 |
| C | 0.698030 | 3.197273 | -0.000038 |
| C | 1.392049 | 4.408400 | -0.000077 |
| C | 0.697921 | 5.605680 | -0.000129 |
| C | -0.698028 | 5.605661 | -0.000157 |
| C | -1.459985 | 1.930256 | 0.000136 |
| C | -0.716976 | 0.675549 | 0.000268 |
| C | 0.716978 | 0.675565 | 0.000068 |
| C | 1.459987 | 1.930259 | -0.000079 |
| C | 1.433083 | -0.547777 | -0.000083 |
| C | 0.681401 | -1.752300 | -0.000340 |
| C | -0.681375 | -1.752311 | -0.000127 |
| C | -1.433066 | -0.547796 | 0.000371 |
| O | -2.696601 | 1.981989 | 0.000151 |
| O | 2.696606 | 1.981993 | -0.000279 |
| N | -2.783758 | -0.597948 | 0.001125 |
| C | -3.565860 | -1.807590 | -0.000571 |
| C | -5.049730 | -1.478228 | 0.000771 |
| C | -5.926078 | -2.722982 | -0.000335 |
| C | -7.417978 | -2.411660 | 0.000480 |
| C | -8.285660 | -3.662278 | -0.000564 |
| N | 2.783777 | -0.597920 | -0.000001 |
| C | 3.565880 | -1.807569 | -0.000606 |
| C | 5.049745 | -1.478214 | 0.000180 |
| C | 5.926098 | -2.722962 | -0.000204 |
| C | 7.417994 | -2.411623 | 0.000539 |
| C | 8.285695 | -3.662227 | 0.000155 |
| H | -1.205012 | -2.700688 | -0.000352 |
| H | 1.205060 | -2.700663 | -0.000713 |
| H | 2.475403 | 4.375543 | -0.000078 |
| H | 1.239825 | 6.545823 | -0.000147 |
| H | -1.239961 | 6.545788 | -0.000215 |
| H | -2.475471 | 4.375468 | -0.000091 |
| H | 3.238093 | 0.313014 | -0.000326 |
| H | -3.238059 | 0.313007 | 0.000233 |
| H | 3.331256 | -2.420872 | -0.883929 |
| H | 3.330608 | -2.422033 | 0.881718 |
| H | 5.278219 | -0.862879 | -0.878811 |
| H | 5.277488 | -0.863902 | 0.880070 |
| H | 5.686982 | -3.337956 | -0.878284 |
| H | 5.686314 | -3.338954 | 0.876992 |
| H | 7.657178 | -1.797148 | 0.877317 |

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|---|-----------|-----------|-----------|
| H | 7.657845 | -1.796153 | -0.875357 |
| H | -3.330471 | -2.422852 | 0.881156 |
| H | -3.331357 | -2.420099 | -0.884486 |
| H | -5.277246 | -0.864577 | 0.881180 |
| H | -5.278421 | -0.862238 | -0.877700 |
| H | -5.686354 | -3.339426 | 0.876559 |
| H | -5.686892 | -3.337519 | -0.878719 |
| H | -7.657787 | -1.795762 | -0.875128 |
| H | -7.657220 | -1.797621 | 0.877546 |
| H | 8.089127 | -4.279500 | 0.882753 |
| H | 9.350106 | -3.412246 | 0.000760 |
| H | 8.089876 | -4.278436 | -0.883351 |
| H | -8.089905 | -4.277971 | -0.884444 |
| H | -9.350075 | -3.412317 | 0.000279 |
| H | -8.089005 | -4.280062 | 0.881658 |

7b

| | | | |
|---|-----------|-----------|-----------|
| C | 4.881770 | -1.394770 | 0.517264 |
| C | 3.703737 | -0.699956 | 0.237267 |
| C | 3.704580 | 0.695859 | 0.237167 |
| C | 4.883452 | 1.389286 | 0.517082 |
| C | 6.047998 | 0.694587 | 0.793082 |
| C | 6.047156 | -0.701444 | 0.793165 |
| C | 2.471261 | -1.461100 | -0.056247 |
| C | 1.252636 | -0.718578 | -0.355431 |
| C | 1.253515 | 0.717351 | -0.355583 |
| C | 2.473047 | 1.458446 | -0.056548 |
| C | 0.067708 | 1.435400 | -0.651947 |
| C | -1.102972 | 0.681525 | -0.933487 |
| C | -1.103801 | -0.679999 | -0.933347 |
| C | 0.065954 | -1.435238 | -0.651647 |
| O | 2.522199 | -2.698350 | -0.038207 |
| O | 2.525499 | 2.695639 | -0.038802 |
| N | 0.029259 | -2.787501 | -0.679718 |
| C | -1.131248 | -3.593349 | -0.961078 |
| C | -2.065561 | -3.795086 | 0.232315 |
| C | -3.276700 | -4.649575 | -0.115339 |
| C | -4.210363 | -4.889188 | 1.065500 |
| C | -5.421210 | -5.738315 | 0.705425 |
| N | 0.032671 | 2.787703 | -0.680315 |
| C | -1.126987 | 3.594892 | -0.961334 |
| C | -2.060894 | 3.797431 | 0.232249 |
| C | -3.271258 | 4.653149 | -0.115094 |
| C | -4.204516 | 4.893488 | 1.065915 |
| C | -5.414671 | 5.743713 | 0.706098 |
| H | -2.029982 | -1.198648 | -1.148853 |
| H | -2.028521 | 1.201252 | -1.149101 |
| H | 4.851982 | 2.472618 | 0.509387 |
| H | 6.963234 | 1.235973 | 1.009344 |
| H | 6.961741 | -1.243909 | 1.009481 |
| H | 4.848989 | -2.478065 | 0.509717 |
| H | 0.920419 | 3.224838 | -0.441091 |
| H | 0.916500 | -3.225671 | -0.440511 |
| H | -0.762364 | 4.569174 | -1.301821 |
| H | -1.685613 | 3.174420 | -1.807644 |
| H | -2.389459 | 2.821001 | 0.608970 |
| H | -1.491820 | 4.261995 | 1.046064 |
| H | -3.835307 | 4.176990 | -0.929232 |
| H | -2.933219 | 5.621215 | -0.509840 |
| H | -3.642288 | 5.375516 | 1.875247 |
| H | -4.538524 | 3.927056 | 1.463852 |

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|---|-----------|-----------|-----------|
| H | -0.767650 | -4.567976 | -1.301684 |
| H | -1.689278 | -3.172103 | -1.807392 |
| H | -1.497099 | -4.260318 | 1.046176 |
| H | -2.393210 | -2.818368 | 0.609090 |
| H | -2.939520 | -5.617910 | -0.510164 |
| H | -3.840167 | -4.172771 | -0.929501 |
| H | -4.543581 | -3.922495 | 1.463463 |
| H | -3.648686 | -5.371779 | 1.874880 |
| H | -5.110100 | 6.727739 | 0.335137 |
| H | -6.065245 | 5.902163 | 1.570515 |
| H | -6.013304 | 5.267462 | -0.077168 |
| H | -6.019309 | -5.261483 | -0.077897 |
| H | -6.072056 | -5.896255 | 1.569732 |
| H | -5.117442 | -6.722578 | 0.334437 |

7c

| | | | |
|---|-----------|-----------|-----------|
| C | -1.353978 | -0.103831 | 0.476589 |
| C | -0.674255 | 1.117101 | 0.238252 |
| C | 0.679614 | 1.113667 | -0.239752 |
| C | 1.353042 | -0.110657 | -0.478441 |
| C | 0.639351 | -1.312499 | -0.224833 |
| C | -0.646245 | -1.309256 | 0.223239 |
| C | 1.382644 | 2.367207 | -0.485587 |
| C | 0.667210 | 3.635563 | -0.232619 |
| C | -0.648534 | 3.638891 | 0.232965 |
| C | -1.370738 | 2.374145 | 0.484742 |
| C | 1.324561 | 4.845179 | -0.464382 |
| C | 0.673514 | 6.044063 | -0.232310 |
| C | -0.641960 | 6.047390 | 0.234795 |
| C | -1.299420 | 4.851797 | 0.465775 |
| O | -2.537921 | 2.431563 | 0.894607 |
| O | 2.549992 | 2.418776 | -0.895730 |
| N | 2.622327 | -0.155716 | -0.945675 |
| C | 3.397679 | -1.350583 | -1.162321 |
| C | 4.011244 | -1.942378 | 0.106695 |
| C | 4.829367 | -3.196598 | -0.168538 |
| C | 5.453813 | -3.799712 | 1.084047 |
| C | 6.269146 | -5.053369 | 0.800695 |
| N | -2.623688 | -0.142481 | 0.943174 |
| C | -3.404530 | -1.333496 | 1.161271 |
| C | -4.021662 | -1.923212 | -0.106968 |
| C | -4.845280 | -3.173574 | 0.169495 |
| C | -5.473600 | -3.774149 | -1.082371 |
| C | -6.293758 | -5.024449 | -0.798113 |
| H | -1.139264 | -2.258678 | 0.393096 |
| H | 1.127643 | -2.264394 | -0.394493 |
| H | 2.345646 | 4.809790 | -0.826057 |
| H | 1.186728 | 6.982865 | -0.413389 |
| H | -1.150123 | 6.988774 | 0.416707 |
| H | -2.320704 | 4.821514 | 0.827350 |
| H | 3.044519 | 0.762183 | -1.070563 |
| H | -3.041044 | 0.777552 | 1.068691 |
| H | 4.197813 | -1.088099 | -1.861536 |
| H | 2.791834 | -2.108794 | -1.675378 |
| H | 4.640066 | -1.178376 | 0.578954 |
| H | 3.214570 | -2.168085 | 0.826191 |
| H | 5.623446 | -2.964057 | -0.891494 |
| H | 4.193389 | -3.950880 | -0.652738 |
| H | 4.660426 | -4.031975 | 1.805610 |
| H | 6.089844 | -3.047185 | 1.566326 |
| H | -4.202937 | -1.066819 | 1.860875 |

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|---|-----------|-----------|-----------|
| H | -2.801893 | -2.094255 | 1.674352 |
| H | -4.647333 | -1.156660 | -0.579278 |
| H | -3.226486 | -2.152937 | -0.826841 |
| H | -5.637600 | -2.937181 | 0.893117 |
| H | -4.212293 | -3.930614 | 0.653315 |
| H | -4.681952 | -4.009615 | -1.804804 |
| H | -6.107083 | -3.019019 | -1.563935 |
| H | 5.649993 | -5.833110 | 0.345105 |
| H | 6.701650 | -5.466266 | 1.716161 |
| H | 7.092697 | -4.842234 | 0.110879 |
| H | -5.677227 | -5.806853 | -0.343536 |
| H | -6.729263 | -5.435353 | -1.713053 |
| H | -7.115460 | -4.810013 | -0.107111 |

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|---|-----------|-----------|-----------|
| C | 5.465908 | -3.322329 | -0.159696 |
| C | 4.255454 | -3.311219 | -0.851210 |
| C | 3.354069 | -2.263573 | -0.726663 |
| C | 3.633174 | -1.191335 | 0.124505 |
| C | 4.849502 | -1.187417 | 0.812845 |
| C | 5.747821 | -2.231345 | 0.663552 |
| N | 2.789777 | -0.083741 | 0.261738 |
| C | 1.428098 | -0.053295 | 0.270188 |
| C | 0.717721 | 1.164980 | 0.163944 |
| C | -0.717796 | 1.165145 | 0.163882 |
| C | -1.428462 | -0.052961 | 0.270083 |
| C | -0.680646 | -1.241991 | 0.468093 |
| C | 0.679987 | -1.242149 | 0.468147 |
| C | 1.458797 | 2.419337 | 0.058764 |
| C | 0.698278 | 3.673126 | -0.117769 |
| C | -0.697782 | 3.673285 | -0.117830 |
| C | -1.458595 | 2.419663 | 0.058627 |
| C | 1.392866 | 4.873718 | -0.274040 |
| C | 0.698459 | 6.059970 | -0.435256 |
| C | -0.697396 | 6.060129 | -0.435318 |
| C | -1.392085 | 4.874032 | -0.274163 |
| N | -2.790140 | -0.083142 | 0.261533 |
| C | -3.633590 | -1.190753 | 0.124417 |
| C | -3.354710 | -2.262641 | -0.727328 |
| C | -4.255929 | -3.310378 | -0.851826 |
| C | -5.466065 | -3.321938 | -0.159655 |
| C | -5.747747 | -2.231348 | 0.664120 |
| C | -4.849505 | -1.187272 | 0.813360 |
| O | -2.693672 | 2.478254 | 0.107225 |
| O | 2.693886 | 2.477670 | 0.107502 |
| C | -6.424069 | -4.471041 | -0.282799 |
| C | 6.424241 | -4.471135 | -0.282882 |
| H | 1.240419 | 6.991558 | -0.560571 |
| H | 2.476142 | 4.842779 | -0.264438 |
| H | -1.239136 | 6.991838 | -0.560680 |
| H | -2.475370 | 4.843337 | -0.264657 |
| H | -1.211929 | -2.164492 | 0.668395 |
| H | 1.211026 | -2.164768 | 0.668537 |
| H | -3.207033 | 0.850664 | 0.280170 |
| H | 3.206801 | 0.850011 | 0.280430 |
| H | 5.080198 | -0.354785 | 1.469812 |
| H | 2.445313 | -2.260801 | -1.318143 |
| H | 6.688041 | -2.200824 | 1.206825 |
| H | 4.018655 | -4.131368 | -1.523172 |
| H | -2.446252 | -2.259365 | -1.319276 |
| H | -4.019362 | -4.130216 | -1.524254 |

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| H | -5.080022 | -0.354944 | 1.470770 |
| H | -6.687654 | -2.201255 | 1.207948 |
| H | 7.462004 | -4.132140 | -0.229410 |
| H | 6.276170 | -5.197287 | 0.524489 |
| H | 6.290102 | -5.001615 | -1.228665 |
| H | -7.461762 | -4.133392 | -0.220721 |
| H | -6.295572 | -4.996315 | -1.232285 |
| H | -6.269931 | -5.201412 | 0.519624 |

8b

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|---|-----------|-----------|-----------|
| C | 5.535602 | -3.274188 | -0.243552 |
| C | 4.433082 | -3.155405 | -1.089369 |
| C | 3.508304 | -2.131991 | -0.941217 |
| C | 3.650364 | -1.197098 | 0.087775 |
| C | 4.758073 | -1.300341 | 0.932330 |
| C | 5.684158 | -2.316989 | 0.760213 |
| N | 2.778790 | -0.115685 | 0.263321 |
| C | 1.424550 | -0.088430 | 0.118369 |
| C | 0.714225 | 1.133846 | 0.070593 |
| C | -0.714232 | 1.133847 | -0.070583 |
| C | -1.424556 | -0.088430 | -0.118373 |
| C | -0.678229 | -1.292873 | -0.055433 |
| C | 0.678226 | -1.292873 | 0.055394 |
| C | 1.445371 | 2.392568 | 0.196044 |
| C | 0.692009 | 3.658632 | 0.090983 |
| C | -0.692013 | 3.658633 | -0.090978 |
| C | -1.445379 | 2.392569 | -0.196023 |
| C | 1.380562 | 4.869354 | 0.182310 |
| C | 0.691988 | 6.066404 | 0.090973 |
| C | -0.691986 | 6.066405 | -0.090999 |
| C | -1.380563 | 4.869355 | -0.182320 |
| N | -2.778798 | -0.115683 | -0.263305 |
| C | -3.650370 | -1.197099 | -0.087774 |
| C | -3.508280 | -2.132032 | 0.941187 |
| C | -4.433053 | -3.155441 | 1.089337 |
| C | -5.535606 | -3.274192 | 0.243546 |
| C | -5.684196 | -2.316957 | -0.760170 |
| C | -4.758108 | -1.300304 | -0.932287 |
| O | -2.665327 | 2.445201 | -0.395951 |
| O | 2.665316 | 2.445198 | 0.395989 |
| C | -6.516562 | -4.399863 | 0.398585 |
| C | 6.516614 | -4.399811 | -0.398613 |
| H | 1.229261 | 7.006475 | 0.160933 |
| H | 2.454397 | 4.837504 | 0.325044 |
| H | -1.229257 | 7.006476 | -0.160972 |
| H | -2.454398 | 4.837506 | -0.325052 |
| H | -1.204088 | -2.237678 | -0.115078 |
| H | 1.204088 | -2.237679 | 0.115011 |
| H | -3.176911 | 0.809761 | -0.439310 |
| H | 3.176901 | 0.809757 | 0.439346 |
| H | 4.882930 | -0.573431 | 1.728601 |
| H | 2.691485 | -2.036167 | -1.648048 |
| H | 6.539268 | -2.371430 | 1.427910 |
| H | 4.304358 | -3.866785 | -1.900399 |
| H | -2.691441 | -2.036229 | 1.647997 |
| H | -4.304310 | -3.866844 | 1.900344 |
| H | -4.882998 | -0.573360 | -1.728522 |
| H | -6.539337 | -2.371364 | -1.427831 |
| H | 7.509549 | -4.114748 | -0.042623 |
| H | 6.202532 | -5.278837 | 0.175604 |
| H | 6.607432 | -4.708261 | -1.443177 |

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| H | -7.509227 | -4.115248 | 0.041498 |
| H | -6.201802 | -5.279267 | -0.174683 |
| H | -6.608252 | -4.707551 | 1.443301 |

9a

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|---|-----------|-----------|-----------|
| C | -3.469529 | -0.889701 | 1.079103 |
| C | -3.653621 | 0.052797 | 0.063373 |
| C | -4.797512 | -0.040008 | -0.733176 |
| C | -5.719151 | -1.054465 | -0.527842 |
| C | -5.531399 | -2.017649 | 0.463775 |
| C | -4.391449 | -1.910403 | 1.260451 |
| N | -2.787882 | 1.133163 | -0.143555 |
| C | -1.428707 | 1.159493 | -0.056843 |
| C | -0.716648 | 2.381723 | -0.039969 |
| C | 0.716443 | 2.381415 | 0.040328 |
| C | 1.427987 | 1.158943 | 0.057927 |
| C | 0.679370 | -0.045280 | 0.027536 |
| C | -0.680597 | -0.045023 | -0.025367 |
| C | -1.451995 | 3.640684 | -0.135464 |
| C | -0.694633 | 4.906581 | -0.062728 |
| C | 0.695696 | 4.906280 | 0.061787 |
| C | 1.452440 | 3.640049 | 0.135041 |
| C | 1.387739 | 6.116846 | 0.124334 |
| C | 0.696252 | 7.314037 | 0.061390 |
| C | -0.694041 | 7.314340 | -0.063359 |
| C | -1.386098 | 6.117451 | -0.125790 |
| N | 2.787190 | 1.132257 | 0.144716 |
| C | 3.652912 | 0.052023 | -0.062649 |
| C | 4.797740 | -0.039928 | 0.732690 |
| C | 5.719461 | -1.054230 | 0.527039 |
| C | 5.530973 | -2.018115 | -0.463760 |
| C | 4.390169 | -1.911670 | -1.259310 |
| C | 3.468092 | -0.891169 | -1.077627 |
| C | 6.503665 | -3.149638 | -0.647413 |
| C | 6.125321 | -4.397488 | 0.154414 |
| C | 7.108183 | -5.547498 | -0.025889 |
| C | 6.725763 | -6.787466 | 0.769902 |
| O | -2.679283 | 3.693764 | -0.283776 |
| O | 2.679701 | 3.692486 | 0.283722 |
| C | -6.503987 | -3.149316 | 0.647108 |
| C | -6.125270 | -4.397083 | -0.154669 |
| C | -7.108030 | -5.547222 | 0.025381 |
| C | -6.725422 | -6.787040 | -0.770550 |
| H | -1.233525 | 8.254525 | -0.111325 |
| H | 1.236182 | 8.253986 | 0.108947 |
| H | 2.466573 | 6.084802 | 0.222341 |
| H | -2.464948 | 6.085879 | -0.223784 |
| H | 1.206990 | -0.990175 | 0.065518 |
| H | -1.208631 | -0.989736 | -0.062270 |
| H | -3.192041 | 2.058975 | -0.303455 |
| H | 3.191506 | 2.058008 | 0.304504 |
| H | -4.953418 | 0.693544 | -1.517834 |
| H | -6.603890 | -1.101515 | -1.156799 |
| H | -4.232185 | -2.627706 | 2.061165 |
| H | -2.622290 | -0.800727 | 1.750091 |
| H | 2.620221 | -0.802888 | -1.747894 |
| H | 4.230298 | -2.629478 | -2.059451 |
| H | 6.604872 | -1.100599 | 1.155102 |
| H | 4.954280 | 0.694167 | 1.516718 |
| H | 7.506665 | -2.821635 | -0.350259 |
| H | 6.565265 | -3.411686 | -1.710459 |

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| H | -7.506950 | -2.821435 | 0.349688 |
| H | -6.565846 | -3.411408 | 1.710124 |
| H | -5.119367 | -4.721950 | 0.141102 |
| H | -6.056354 | -4.133152 | -1.217734 |
| H | -7.176134 | -5.800089 | 1.091157 |
| H | -8.110982 | -5.214427 | -0.270740 |
| H | -6.680735 | -6.569728 | -1.842588 |
| H | -7.446794 | -7.596047 | -0.625715 |
| H | -5.741667 | -7.161475 | -0.469485 |
| H | 6.056610 | -4.133590 | 1.217501 |
| H | 5.119393 | -4.722480 | -0.141135 |
| H | 7.176218 | -5.800213 | -1.091706 |
| H | 8.111129 | -5.214651 | 0.270191 |
| H | 6.681126 | -6.570305 | 1.841973 |
| H | 7.447209 | -7.596379 | 0.624908 |
| H | 5.742025 | -7.161956 | 0.468849 |

9b

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|---|-----------|-----------|-----------|
| C | -3.366929 | -0.950671 | 1.013840 |
| C | -3.634786 | 0.057259 | 0.082636 |
| C | -4.839424 | 0.009633 | -0.623246 |
| C | -5.737995 | -1.024982 | -0.415308 |
| C | -5.467632 | -2.052452 | 0.488556 |
| C | -4.267927 | -1.988931 | 1.197858 |
| N | -2.789845 | 1.153523 | -0.120864 |
| C | -1.428375 | 1.182530 | -0.132974 |
| C | -0.717844 | 2.405481 | -0.129522 |
| C | 0.717721 | 2.405532 | -0.129477 |
| C | 1.428339 | 1.182636 | -0.132900 |
| C | 0.680329 | -0.018550 | -0.232144 |
| C | -0.680274 | -0.018600 | -0.232167 |
| C | -1.458877 | 3.664101 | -0.135696 |
| C | -0.698172 | 4.928819 | -0.078537 |
| C | 0.697899 | 4.928862 | -0.078419 |
| C | 1.458685 | 3.664190 | -0.135501 |
| C | -1.392679 | 6.138899 | -0.037206 |
| C | -0.698150 | 7.335058 | 0.009593 |
| C | 0.697713 | 7.335100 | 0.009720 |
| C | 1.392324 | 6.138983 | -0.036963 |
| N | 2.789806 | 1.153702 | -0.120720 |
| C | 3.634735 | 0.057419 | 0.082881 |
| C | 4.839266 | 0.009569 | -0.623157 |
| C | 5.737813 | -1.025053 | -0.415110 |
| C | 5.467497 | -2.052302 | 0.489014 |
| C | 4.267876 | -1.988570 | 1.198448 |
| C | 3.366921 | -0.950296 | 1.014326 |
| C | 6.415296 | -3.205295 | 0.669530 |
| C | 6.060243 | -4.410765 | -0.204605 |
| C | 7.017201 | -5.583060 | -0.028824 |
| C | 6.652861 | -6.783067 | -0.891625 |
| O | 2.694039 | 3.718100 | -0.185216 |
| O | -2.694227 | 3.717946 | -0.185586 |
| C | -6.415495 | -3.205410 | 0.668977 |
| C | -6.059741 | -4.411335 | -0.204242 |
| C | -7.016809 | -5.583555 | -0.028570 |
| C | -6.651839 | -6.783984 | -0.890518 |
| H | 1.239520 | 8.274504 | 0.045196 |
| H | -1.240021 | 8.274429 | 0.044967 |
| H | -2.475960 | 6.107296 | -0.043612 |
| H | 2.475607 | 6.107447 | -0.043185 |
| H | -1.211489 | -0.954422 | -0.355911 |

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| H | 1.211627 | -0.954328 | -0.355874 |
| H | 3.206455 | 2.082856 | -0.217687 |
| H | -3.206517 | 2.082649 | -0.218029 |
| H | 2.467911 | -0.900680 | 1.618640 |
| H | 4.042622 | -2.757297 | 1.932877 |
| H | 6.669586 | -1.037269 | -0.973783 |
| H | 5.060239 | 0.792948 | -1.341211 |
| H | -2.467871 | -0.901247 | 1.618093 |
| H | -4.042615 | -2.757803 | 1.932119 |
| H | -6.669835 | -1.037041 | -0.973871 |
| H | -5.060462 | 0.793190 | -1.341085 |
| H | -7.435922 | -2.880165 | 0.435397 |
| H | -6.421627 | -3.514484 | 1.721272 |
| H | 6.420642 | -3.514928 | 1.721661 |
| H | 7.435888 | -2.879885 | 0.436888 |
| H | 6.046990 | -4.099079 | -1.256807 |
| H | 5.036827 | -4.732854 | 0.027189 |
| H | 8.037235 | -5.255001 | -0.265846 |
| H | 7.033320 | -5.880382 | 1.027509 |
| H | 5.651439 | -7.153559 | -0.649797 |
| H | 7.355476 | -7.608769 | -0.748848 |
| H | 6.659004 | -6.521673 | -1.954702 |
| H | -6.045689 | -4.100206 | -1.256597 |
| H | -5.036497 | -4.733288 | 0.028504 |
| H | -7.033690 | -5.880356 | 1.027898 |
| H | -8.036675 | -5.255622 | -0.266491 |
| H | -6.657283 | -6.523128 | -1.953730 |
| H | -7.354513 | -7.609645 | -0.747792 |
| H | -5.650562 | -7.154309 | -0.647831 |

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|---|-----------|-----------|-----------|
| C | -3.838099 | -0.709022 | 1.016060 |
| C | -3.864292 | 0.139225 | -0.094480 |
| C | -4.944982 | 0.051020 | -0.975455 |
| C | -5.959223 | -0.867851 | -0.756400 |
| C | -5.929483 | -1.738633 | 0.333252 |
| C | -4.850668 | -1.636748 | 1.211452 |
| N | -2.897599 | 1.126117 | -0.321728 |
| C | -1.555348 | 1.057361 | -0.096620 |
| C | -0.748604 | 2.218712 | -0.085960 |
| C | 0.663876 | 2.113929 | 0.146642 |
| C | 1.264088 | 0.845316 | 0.323114 |
| C | 0.424819 | -0.297481 | 0.286992 |
| C | -0.917870 | -0.195984 | 0.089081 |
| C | -1.362427 | 3.519979 | -0.341066 |
| C | -0.511638 | 4.725672 | -0.273577 |
| C | 0.854692 | 4.626941 | -0.005225 |
| C | 1.490134 | 3.315514 | 0.235194 |
| C | -1.088131 | 5.978288 | -0.490001 |
| C | -0.306429 | 7.119224 | -0.436870 |
| C | 1.059918 | 7.020406 | -0.169123 |
| C | 1.637557 | 5.781384 | 0.046474 |
| N | 2.598942 | 0.720275 | 0.563246 |
| C | 3.387411 | -0.435738 | 0.506965 |
| C | 4.417597 | -0.582495 | 1.439621 |
| C | 5.266836 | -1.675786 | 1.384616 |
| C | 5.115571 | -2.666380 | 0.413194 |
| C | 4.085176 | -2.510274 | -0.513098 |
| C | 3.237768 | -1.411590 | -0.481426 |
| C | 6.069338 | -3.826199 | 0.334380 |
| C | 7.336142 | -3.496958 | -0.459466 |

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| C | 8.316380 | -4.660455 | -0.540199 |
| C | 9.576710 | -4.321601 | -1.323794 |
| O | 2.695622 | 3.284520 | 0.512531 |
| O | -2.559782 | 3.655523 | -0.621157 |
| C | -7.005334 | -2.768159 | 0.539313 |
| C | -6.696059 | -4.103004 | -0.143354 |
| C | -7.781936 | -5.150261 | 0.069227 |
| C | -7.469862 | -6.477200 | -0.608192 |
| H | 1.670551 | 7.916444 | -0.129836 |
| H | -0.756883 | 8.092070 | -0.604110 |
| H | -2.150805 | 6.023047 | -0.697996 |
| H | 2.694867 | 5.673260 | 0.258482 |
| H | -1.517434 | -1.097188 | 0.054761 |
| H | 0.865509 | -1.274956 | 0.439554 |
| H | 3.061932 | 1.621393 | 0.703200 |
| H | -3.208521 | 2.063993 | -0.584545 |
| H | 2.475664 | -1.295065 | -1.244203 |
| H | 3.950738 | -3.257042 | -1.290985 |
| H | 6.058784 | -1.768416 | 2.122896 |
| H | 4.537010 | 0.168574 | 2.213994 |
| H | -3.041742 | -0.617099 | 1.746459 |
| H | -4.813604 | -2.280361 | 2.086318 |
| H | -6.792739 | -0.911551 | -1.452083 |
| H | -4.978551 | 0.711931 | -1.835777 |
| H | -7.958837 | -2.382948 | 0.159150 |
| H | -7.146603 | -2.939470 | 1.613119 |
| H | 5.567582 | -4.684659 | -0.126984 |
| H | 6.351830 | -4.138895 | 1.346889 |
| H | 7.830253 | -2.630285 | -0.002061 |
| H | 7.052483 | -3.181645 | -1.471650 |
| H | 8.587913 | -4.974695 | 0.475730 |
| H | 7.816954 | -5.522826 | -0.999884 |
| H | 9.337043 | -4.035895 | -2.353047 |
| H | 10.264044 | -5.171063 | -1.366385 |
| H | 10.111920 | -3.483458 | -0.866070 |
| H | -6.552952 | -3.932545 | -1.218103 |
| H | -5.737539 | -4.484129 | 0.231826 |
| H | -7.922700 | -5.310571 | 1.145747 |
| H | -8.737132 | -4.761083 | -0.305635 |
| H | -7.357202 | -6.351582 | -1.689908 |
| H | -8.263316 | -7.210738 | -0.440237 |
| H | -6.536416 | -6.904550 | -0.227856 |

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| C | -3.512742 | -0.964923 | 0.975335 |
| C | -3.808088 | 0.133580 | 0.162923 |
| C | -5.086406 | 0.227455 | -0.393193 |
| C | -6.033575 | -0.754929 | -0.151603 |
| C | -5.742101 | -1.868544 | 0.636582 |
| C | -4.465438 | -1.949231 | 1.192986 |
| N | -2.908991 | 1.183079 | -0.055861 |
| C | -1.556729 | 1.116461 | -0.206752 |
| C | -0.749741 | 2.276050 | -0.148065 |
| C | 0.673396 | 2.172540 | -0.303669 |
| C | 1.275139 | 0.910678 | -0.516884 |
| C | 0.423930 | -0.215424 | -0.656975 |
| C | -0.925216 | -0.117270 | -0.508949 |
| C | -1.378764 | 3.576237 | 0.070610 |
| C | -0.510387 | 4.762971 | 0.210153 |
| C | 0.873963 | 4.662016 | 0.060357 |
| C | 1.513665 | 3.365964 | -0.243727 |

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| C | -1.090676 | 6.002497 | 0.484059 |
| C | -0.294035 | 7.126719 | 0.614810 |
| C | 1.090108 | 7.025710 | 0.465387 |
| C | 1.670947 | 5.801045 | 0.185738 |
| N | 2.623543 | 0.783608 | -0.662133 |
| C | 3.396900 | -0.381411 | -0.626008 |
| C | 3.127789 | -1.451646 | 0.231443 |
| C | 3.962790 | -2.559600 | 0.249843 |
| C | 5.097188 | -2.635280 | -0.557621 |
| C | 5.368024 | -1.551158 | -1.393315 |
| C | 4.533625 | -0.445983 | -1.436703 |
| C | 6.027870 | -3.814116 | -0.485977 |
| C | 7.139954 | -3.629234 | 0.549578 |
| C | 8.089116 | -4.818110 | 0.633371 |
| C | 9.191805 | -4.626328 | 1.665032 |
| O | 2.736574 | 3.338415 | -0.430381 |
| O | -2.604300 | 3.726041 | 0.150183 |
| C | -6.757311 | -2.955100 | 0.857041 |
| C | -6.667741 | -4.081385 | -0.176219 |
| C | -7.701117 | -5.178414 | 0.045270 |
| C | -7.608956 | -6.299874 | -0.980090 |
| H | 1.711982 | 7.908977 | 0.567273 |
| H | -0.746798 | 8.088411 | 0.832610 |
| H | -2.168291 | 6.050696 | 0.588971 |
| H | 2.741719 | 5.692623 | 0.058221 |
| H | -1.542774 | -0.992625 | -0.669876 |
| H | 0.860271 | -1.167432 | -0.934049 |
| H | 3.103096 | 1.685941 | -0.706641 |
| H | -3.256807 | 2.143649 | -0.011731 |
| H | 4.748824 | 0.378965 | -2.108446 |
| H | 6.244518 | -1.578133 | -2.034985 |
| H | 3.733574 | -3.380534 | 0.923969 |
| H | 2.279650 | -1.403811 | 0.905278 |
| H | -2.547520 | -1.028730 | 1.465422 |
| H | -4.217313 | -2.789851 | 1.835488 |
| H | -7.023004 | -0.655468 | -0.589414 |
| H | -5.327110 | 1.081032 | -1.018947 |
| H | -7.765015 | -2.524087 | 0.830584 |
| H | -6.627923 | -3.378780 | 1.860221 |
| H | 6.478903 | -3.986273 | -1.470465 |
| H | 5.457221 | -4.718449 | -0.243722 |
| H | 6.687277 | -3.448440 | 1.532907 |
| H | 7.706936 | -2.721035 | 0.308151 |
| H | 7.514922 | -5.722512 | 0.871843 |
| H | 8.534976 | -4.994818 | -0.353793 |
| H | 9.802541 | -3.748304 | 1.431474 |
| H | 9.858082 | -5.492452 | 1.706875 |
| H | 8.774160 | -4.479392 | 2.666261 |
| H | -6.788526 | -3.657580 | -1.181364 |
| H | -5.659163 | -4.513560 | -0.150162 |
| H | -7.578229 | -5.591261 | 1.054676 |
| H | -8.705852 | -4.737787 | 0.019555 |
| H | -7.762040 | -5.920191 | -1.995466 |
| H | -8.360264 | -7.073475 | -0.798503 |
| H | -6.625197 | -6.779542 | -0.953289 |
| 9e | | | |
| C | -4.855567 | -0.172703 | 1.262435 |
| C | -3.630305 | -0.261576 | 0.595562 |
| C | -3.334554 | -1.435289 | -0.102736 |
| C | -4.234670 | -2.491277 | -0.108058 |

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| C | -5.459221 | -2.412886 | 0.554314 |
| C | -5.751613 | -1.228864 | 1.232810 |
| N | -2.789794 | 0.856961 | 0.600715 |
| C | -1.427822 | 0.889056 | 0.601251 |
| C | -0.717491 | 2.074596 | 0.302907 |
| C | 0.717800 | 2.074481 | 0.303115 |
| C | 1.427870 | 0.888846 | 0.601584 |
| C | 0.680244 | -0.254750 | 0.982919 |
| C | -0.680429 | -0.254647 | 0.982780 |
| C | -1.458379 | 3.294513 | -0.008554 |
| C | -0.697577 | 4.497261 | -0.404169 |
| C | 0.698482 | 4.497152 | -0.403953 |
| C | 1.458974 | 3.294292 | -0.008088 |
| C | -1.391919 | 5.651174 | -0.771040 |
| C | -0.697155 | 6.789380 | -1.141632 |
| C | 0.698650 | 6.789270 | -1.141419 |
| C | 1.393120 | 5.650956 | -0.770610 |
| N | 2.789849 | 0.856534 | 0.601363 |
| C | 3.630144 | -0.262118 | 0.596116 |
| C | 4.855463 | -0.173533 | 1.262926 |
| C | 5.751338 | -1.229840 | 1.233135 |
| C | 5.458731 | -2.413720 | 0.554493 |
| C | 4.234105 | -2.491841 | -0.107788 |
| C | 3.334145 | -1.435732 | -0.102262 |
| C | 6.455765 | -3.537272 | 0.488006 |
| C | 7.452314 | -3.374621 | -0.662573 |
| C | 8.471444 | -4.504359 | -0.742700 |
| C | 9.461533 | -4.330109 | -1.885715 |
| O | 2.693467 | 3.361953 | 0.038261 |
| O | -2.692885 | 3.362376 | 0.037282 |
| C | -6.456381 | -3.536349 | 0.488219 |
| C | -7.452885 | -3.374109 | -0.662459 |
| C | -8.472062 | -4.503839 | -0.742113 |
| C | -9.462220 | -4.329985 | -1.885128 |
| H | -1.238855 | 7.683738 | -1.431436 |
| H | 1.240579 | 7.683538 | -1.431069 |
| H | 2.476401 | 5.622466 | -0.754763 |
| H | -2.475210 | 5.622854 | -0.755528 |
| H | 1.212470 | -1.133625 | 1.326216 |
| H | -1.212851 | -1.133440 | 1.325956 |
| H | -3.207867 | 1.781563 | 0.473987 |
| H | 3.208114 | 1.781099 | 0.474974 |
| H | -5.091353 | 0.733160 | 1.811877 |
| H | -6.696762 | -1.136069 | 1.760859 |
| H | -3.983800 | -3.394312 | -0.658017 |
| H | -2.410877 | -1.510392 | -0.665767 |
| H | 5.091452 | 0.732233 | 1.812446 |
| H | 6.696535 | -1.137228 | 1.761134 |
| H | 3.983080 | -3.394765 | -0.657859 |
| H | 2.410427 | -1.510616 | -0.665264 |
| H | 5.927900 | -4.491469 | 0.375539 |
| H | 7.006588 | -3.596680 | 1.434364 |
| H | -7.007256 | -3.595312 | 1.434575 |
| H | -5.928606 | -4.490649 | 0.376180 |
| H | -6.900101 | -3.308314 | -1.608297 |
| H | -7.974199 | -2.414710 | -0.551642 |
| H | -7.944347 | -5.459584 | -0.854041 |
| H | -9.015378 | -4.568146 | 0.209311 |
| H | -10.027514 | -3.398521 | -1.779122 |
| H | -10.181678 | -5.152674 | -1.922142 |
| H | -8.947913 | -4.294293 | -2.850883 |

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| H | 6.899570 | -3.308367 | -1.608405 |
| H | 7.973673 | -2.415302 | -0.551309 |
| H | 9.014808 | -4.569046 | 0.208671 |
| H | 7.943685 | -5.460042 | -0.854960 |
| H | 8.947178 | -4.294144 | -2.851433 |
| H | 10.181031 | -5.152751 | -1.923017 |
| H | 10.026796 | -3.398653 | -1.779459 |

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|---|------------|-----------|-----------|
| C | 4.589087 | -0.506485 | -1.548762 |
| C | 3.602042 | -0.377349 | -0.568241 |
| C | 3.584968 | -1.294418 | 0.486045 |
| C | 4.510295 | -2.327149 | 0.530133 |
| C | 5.493620 | -2.470266 | -0.448279 |
| C | 5.519474 | -1.531483 | -1.480268 |
| N | 2.715343 | 0.703256 | -0.649958 |
| C | 1.394040 | 0.733540 | -0.317442 |
| C | 0.697202 | 1.955392 | -0.170671 |
| C | -0.697182 | 1.955304 | 0.170560 |
| C | -1.393922 | 0.733433 | 0.317352 |
| C | -0.663479 | -0.470758 | 0.150278 |
| C | 0.663675 | -0.470702 | -0.150326 |
| C | 1.402633 | 3.214144 | -0.400462 |
| C | 0.671444 | 4.480233 | -0.189581 |
| C | -0.671865 | 4.480117 | 0.189590 |
| C | -1.402838 | 3.213892 | 0.400387 |
| C | 1.339310 | 5.691007 | -0.379989 |
| C | 0.671043 | 6.888064 | -0.190182 |
| C | -0.671844 | 6.887946 | 0.190344 |
| C | -1.339923 | 5.690772 | 0.380075 |
| N | -2.715239 | 0.703180 | 0.649824 |
| C | -3.601933 | -0.377437 | 0.568184 |
| C | -3.584812 | -1.294591 | -0.486025 |
| C | -4.510116 | -2.327343 | -0.530050 |
| C | -5.493473 | -2.470388 | 0.448339 |
| C | -5.519379 | -1.531517 | 1.480247 |
| C | -4.589002 | -0.506505 | 1.548689 |
| C | -6.521544 | -3.564542 | 0.366293 |
| C | -7.778825 | -3.146416 | -0.400188 |
| C | -8.824760 | -4.250894 | -0.485266 |
| C | -10.072789 | -3.831428 | -1.249116 |
| O | -2.581263 | 3.265787 | 0.773373 |
| O | 2.581058 | 3.266365 | -0.773410 |
| C | 6.521716 | -3.564391 | -0.366171 |
| C | 7.779017 | -3.146167 | 0.400223 |
| C | 8.824994 | -4.250603 | 0.485340 |
| C | 10.073053 | -3.831025 | 1.249077 |
| H | 1.192424 | 7.828170 | -0.337353 |
| H | -1.193372 | 7.827961 | 0.337575 |
| H | -2.381843 | 5.658807 | 0.676593 |
| H | 2.381236 | 5.659226 | -0.676510 |
| H | -1.175428 | -1.415650 | 0.283397 |
| H | 1.175690 | -1.415558 | -0.283441 |
| H | 3.087402 | 1.626432 | -0.883590 |
| H | -3.087315 | 1.626374 | 0.883339 |
| H | 4.608845 | 0.200247 | -2.372285 |
| H | 6.274327 | -1.614030 | -2.257506 |
| H | 4.475127 | -3.031616 | 1.356789 |
| H | 2.861419 | -1.183300 | 1.286082 |
| H | -2.861228 | -1.183533 | -1.286040 |
| H | -4.474907 | -3.031885 | -1.356641 |

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| H | -6.274255 | -1.614011 | 2.257468 |
| H | -4.608793 | 0.200295 | 2.372154 |
| H | -6.805679 | -3.877051 | 1.378225 |
| H | -6.081517 | -4.444631 | -0.117397 |
| H | 6.805822 | -3.876980 | -1.378086 |
| H | 6.081728 | -4.444450 | 0.117610 |
| H | 7.493736 | -2.828963 | 1.411367 |
| H | 8.215004 | -2.261347 | -0.080997 |
| H | 8.380241 | -5.132888 | 0.963098 |
| H | 9.102367 | -4.564033 | -0.529201 |
| H | 10.556973 | -2.971807 | 0.773540 |
| H | 10.806420 | -4.640832 | 1.296002 |
| H | 9.829094 | -3.543445 | 2.276814 |
| H | -8.214863 | -2.261570 | 0.080941 |
| H | -7.493508 | -2.829284 | -1.411344 |
| H | -8.379949 | -5.133205 | -0.962919 |
| H | -9.102182 | -4.564243 | 0.529287 |
| H | -10.556771 | -2.972187 | -0.773686 |
| H | -10.806121 | -4.641268 | -1.296016 |
| H | -9.828776 | -3.543931 | -2.276864 |

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|---|-----------|-----------|-----------|
| C | 7.868248 | -1.025642 | -0.455047 |
| C | 7.391746 | -2.269633 | -0.036074 |
| C | 6.033084 | -2.518485 | 0.057015 |
| C | 5.106463 | -1.522966 | -0.254321 |
| C | 5.572880 | -0.279189 | -0.684379 |
| C | 6.935901 | -0.040520 | -0.781618 |
| C | 3.661736 | -1.888331 | -0.144209 |
| O | 3.309173 | -3.048342 | -0.050499 |
| C | 9.342743 | -0.743102 | -0.516218 |
| C | 9.888094 | -0.176251 | 0.797806 |
| C | 11.382725 | 0.114569 | 0.748371 |
| C | 11.919838 | 0.684121 | 2.053877 |
| N | 2.799688 | -0.812162 | -0.149891 |
| C | 1.419556 | -0.805131 | -0.140463 |
| C | 0.715401 | 0.421648 | -0.154641 |
| C | -0.715401 | 0.421647 | -0.154641 |
| C | -1.419555 | -0.805133 | -0.140463 |
| C | -0.683661 | -2.006956 | -0.127105 |
| C | 0.683664 | -2.006955 | -0.127105 |
| C | -1.455302 | 1.694319 | -0.180927 |
| C | -0.696759 | 2.961671 | -0.208013 |
| C | 0.696755 | 2.961672 | -0.208013 |
| C | 1.455300 | 1.694321 | -0.180926 |
| C | 1.392787 | 4.170206 | -0.229817 |
| C | 0.697400 | 5.367506 | -0.252436 |
| C | -0.697408 | 5.367505 | -0.252436 |
| C | -1.392793 | 4.170204 | -0.229817 |
| O | 2.686654 | 1.755818 | -0.178264 |
| O | -2.686656 | 1.755813 | -0.178262 |
| N | -2.799687 | -0.812165 | -0.149892 |
| C | -3.661735 | -1.888333 | -0.144208 |
| C | -5.106462 | -1.522967 | -0.254320 |
| C | -6.033084 | -2.518485 | 0.057018 |
| C | -7.391745 | -2.269632 | -0.036071 |
| C | -7.868246 | -1.025642 | -0.455048 |
| C | -6.935899 | -0.040521 | -0.781622 |
| C | -5.572878 | -0.279191 | -0.684381 |
| C | -9.342741 | -0.743101 | -0.516219 |
| C | -9.888093 | -0.176252 | 0.797806 |

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| C | -11.382724 | 0.114569 | 0.748371 |
| C | -11.919836 | 0.684120 | 2.053877 |
| O | -3.309172 | -3.048343 | -0.050495 |
| H | 1.229616 | -2.938897 | -0.109846 |
| H | -1.229612 | -2.938898 | -0.109846 |
| H | -2.475893 | 4.140659 | -0.227156 |
| H | 2.475887 | 4.140662 | -0.227155 |
| H | 1.239304 | 6.307133 | -0.269251 |
| H | -1.239313 | 6.307131 | -0.269251 |
| H | -3.193956 | 0.128021 | -0.124256 |
| H | 3.193957 | 0.128023 | -0.124253 |
| H | 4.886217 | 0.510577 | -0.971812 |
| H | 7.283412 | 0.928284 | -1.128878 |
| H | 5.657800 | -3.487743 | 0.365288 |
| H | 8.099441 | -3.055547 | 0.212306 |
| H | -4.886215 | 0.510573 | -0.971817 |
| H | -7.283409 | 0.928282 | -1.128883 |
| H | -5.657800 | -3.487743 | 0.365293 |
| H | -8.099441 | -3.055545 | 0.212311 |
| H | 9.547182 | -0.033376 | -1.326234 |
| H | 9.882688 | -1.664616 | -0.762514 |
| H | -9.882687 | -1.664615 | -0.762517 |
| H | -9.547180 | -0.033374 | -1.326233 |
| H | 9.341297 | 0.742062 | 1.046791 |
| H | 9.675862 | -0.883531 | 1.609486 |
| H | -9.675860 | -0.883533 | 1.609485 |
| H | -9.341295 | 0.742061 | 1.046792 |
| H | -11.587064 | 0.815430 | -0.071009 |
| H | -11.922192 | -0.807929 | 0.499051 |
| H | 11.922193 | -0.807928 | 0.499052 |
| H | 11.587066 | 0.815430 | -0.071009 |
| H | -12.993003 | 0.884822 | 1.992715 |
| H | -11.758619 | -0.010852 | 2.884179 |
| H | -11.419991 | 1.623878 | 2.309646 |
| H | 12.993005 | 0.884824 | 1.992715 |
| H | 11.419992 | 1.623880 | 2.309645 |
| H | 11.758620 | -0.010850 | 2.884179 |

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| C | 5.567230 | -0.036144 | 0.013181 |
| C | 5.105404 | -1.241473 | -0.518668 |
| C | 6.035399 | -2.210718 | -0.896853 |
| C | 7.392600 | -1.973975 | -0.763182 |
| C | 7.864547 | -0.769867 | -0.235749 |
| C | 6.929227 | 0.190167 | 0.150226 |
| C | 3.662020 | -1.593541 | -0.678671 |
| O | 3.310593 | -2.740988 | -0.875030 |
| C | 9.336238 | -0.540055 | -0.037439 |
| C | 9.834791 | -1.071950 | 1.309406 |
| C | 11.327857 | -0.857847 | 1.522895 |
| C | 11.817507 | -1.390542 | 2.862160 |
| N | 2.799587 | -0.521454 | -0.589336 |
| C | 1.419538 | -0.513560 | -0.601129 |
| C | 0.715410 | 0.707347 | -0.480020 |
| C | -0.715411 | 0.707340 | -0.480015 |
| C | -1.419529 | -0.513573 | -0.601119 |
| C | -0.683648 | -1.709541 | -0.720869 |
| C | 0.683667 | -1.709535 | -0.720874 |
| C | 1.455221 | 1.972706 | -0.340814 |
| C | 0.696727 | 3.232644 | -0.201192 |
| C | -0.696758 | 3.232636 | -0.201185 |

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| C | -1.455237 | 1.972688 | -0.340805 |
| C | -1.392773 | 4.434425 | -0.071759 |
| C | -0.697433 | 5.624980 | 0.057388 |
| C | 0.697375 | 5.624989 | 0.057381 |
| C | 1.392729 | 4.434443 | -0.071773 |
| N | -2.799578 | -0.521473 | -0.589318 |
| C | -3.662009 | -1.593562 | -0.678644 |
| O | -3.310581 | -2.741010 | -0.874998 |
| O | 2.686606 | 2.034278 | -0.337643 |
| O | -2.686622 | 2.034239 | -0.337606 |
| C | -5.105393 | -1.241494 | -0.518643 |
| C | -6.035388 | -2.210744 | -0.896816 |
| C | -7.392589 | -1.974001 | -0.763149 |
| C | -7.864537 | -0.769886 | -0.235731 |
| C | -6.929218 | 0.190153 | 0.150233 |
| C | -5.567221 | -0.036159 | 0.013191 |
| C | -9.336228 | -0.540072 | -0.037426 |
| C | -9.834782 | -1.071949 | 1.309427 |
| C | -11.327848 | -0.857841 | 1.522913 |
| C | -11.817499 | -1.390518 | 2.862184 |
| H | -1.229568 | -2.636382 | -0.820089 |
| H | 1.229594 | -2.636371 | -0.820098 |
| H | 2.475825 | 4.405215 | -0.076952 |
| H | -2.475870 | 4.405184 | -0.076927 |
| H | -1.239375 | 6.559340 | 0.157912 |
| H | 1.239306 | 6.559355 | 0.157899 |
| H | 3.193655 | 0.417355 | -0.531462 |
| H | -3.193648 | 0.417335 | -0.531448 |
| H | -4.878217 | 0.734590 | 0.343550 |
| H | -7.273121 | 1.131822 | 0.568341 |
| H | -5.663638 | -3.147909 | -1.295394 |
| H | -8.103259 | -2.734961 | -1.073262 |
| H | 4.878226 | 0.734600 | 0.343549 |
| H | 7.273130 | 1.131831 | 0.568347 |
| H | 5.663650 | -3.147878 | -1.295442 |
| H | 8.103270 | -2.734931 | -1.073304 |
| H | -9.554235 | 0.531841 | -0.105551 |
| H | -9.895082 | -1.026407 | -0.845435 |
| H | 9.895093 | -1.026379 | -0.845455 |
| H | 9.554245 | 0.531859 | -0.105550 |
| H | -9.601539 | -2.141889 | 1.381081 |
| H | -9.272559 | -0.586133 | 2.116976 |
| H | 9.272568 | -0.586145 | 2.116962 |
| H | 9.601547 | -2.141891 | 1.381046 |
| H | 11.881899 | -1.342403 | 0.708928 |
| H | 11.554182 | 0.213371 | 1.447221 |
| H | -11.554171 | 0.213376 | 1.447224 |
| H | -11.881890 | -1.342407 | 0.708951 |
| H | 12.890583 | -1.224848 | 2.991696 |
| H | 11.302692 | -0.900207 | 3.694607 |
| H | 11.634473 | -2.466218 | 2.950056 |
| H | -12.890575 | -1.224821 | 2.991718 |
| H | -11.634467 | -2.466193 | 2.950095 |
| H | -11.302684 | -0.900173 | 3.694625 |
| 10c | | | |
| C | -5.507372 | -0.398483 | 0.885607 |
| C | -5.037511 | -1.620630 | 0.400476 |
| C | -5.953925 | -2.641353 | 0.146819 |
| C | -7.308638 | -2.437248 | 0.348224 |
| C | -7.789368 | -1.215097 | 0.822317 |

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|---|------------|-----------|-----------|
| C | -6.865170 | -0.205228 | 1.092373 |
| C | -3.595098 | -1.934853 | 0.168798 |
| O | -3.211159 | -3.080841 | 0.035488 |
| C | -9.262293 | -0.978404 | 1.001549 |
| C | -9.913833 | -0.362173 | -0.239927 |
| C | -11.406825 | -0.111156 | -0.069170 |
| C | -12.048451 | 0.508423 | -1.302737 |
| N | -2.774562 | -0.828185 | 0.111243 |
| C | -1.402507 | -0.769126 | -0.024168 |
| C | -0.747420 | 0.483830 | -0.070166 |
| C | 0.675681 | 0.538977 | -0.207155 |
| C | 1.421526 | -0.659910 | -0.293720 |
| C | 0.734553 | -1.889287 | -0.238740 |
| C | -0.625661 | -1.941935 | -0.108950 |
| C | -1.529491 | 1.726961 | 0.034069 |
| C | -0.820668 | 3.022449 | -0.000576 |
| C | 0.565210 | 3.076402 | -0.135688 |
| C | 1.365198 | 1.839385 | -0.246832 |
| C | -1.556991 | 4.202890 | 0.098909 |
| C | -0.909007 | 5.426199 | 0.064741 |
| C | 0.478145 | 5.480268 | -0.070754 |
| C | 1.213299 | 4.310997 | -0.171265 |
| N | 2.795124 | -0.613647 | -0.419915 |
| C | 3.694071 | -1.655169 | -0.510402 |
| O | 3.379787 | -2.828620 | -0.564654 |
| O | 2.586839 | 1.948597 | -0.371896 |
| O | -2.757119 | 1.741080 | 0.147541 |
| C | 5.127287 | -1.233480 | -0.547948 |
| C | 5.584492 | 0.035806 | -0.188014 |
| C | 6.939153 | 0.329730 | -0.237458 |
| C | 7.872463 | -0.624464 | -0.643254 |
| C | 7.406375 | -1.893110 | -0.994214 |
| C | 6.056660 | -2.196798 | -0.941799 |
| C | 9.342041 | -0.310715 | -0.651359 |
| C | 10.015181 | -0.614086 | 0.690366 |
| C | 11.504892 | -0.294787 | 0.697458 |
| C | 12.168776 | -0.592232 | 2.034552 |
| H | -1.134516 | -2.894287 | -0.076214 |
| H | 1.311833 | -2.799622 | -0.309205 |
| H | 2.291310 | 4.323686 | -0.279476 |
| H | -2.633355 | 4.131202 | 0.200412 |
| H | -1.482129 | 6.343987 | 0.142307 |
| H | 0.982936 | 6.440090 | -0.098514 |
| H | 3.148071 | 0.341006 | -0.482156 |
| H | -3.203739 | 0.096952 | 0.127654 |
| H | -4.825013 | 0.408841 | 1.131321 |
| H | -7.214215 | 0.746951 | 1.481616 |
| H | -5.574022 | -3.593801 | -0.205162 |
| H | -8.009075 | -3.241596 | 0.142038 |
| H | 4.899515 | 0.806999 | 0.149573 |
| H | 7.279420 | 1.321595 | 0.045972 |
| H | 5.690610 | -3.182711 | -1.205048 |
| H | 8.115183 | -2.651220 | -1.315248 |
| H | -9.425633 | -0.315313 | 1.859148 |
| H | -9.760351 | -1.925692 | 1.237488 |
| H | 9.836128 | -0.888681 | -1.440828 |
| H | 9.490285 | 0.747175 | -0.897086 |
| H | -9.406558 | 0.580586 | -0.480989 |
| H | -9.746341 | -1.023521 | -1.099432 |
| H | 9.511976 | -0.043615 | 1.481325 |
| H | 9.862972 | -1.672201 | 0.938027 |

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| H | 12.001026 | -0.868127 | -0.095888 |
| H | 11.648451 | 0.762708 | 0.441512 |
| H | -11.907275 | -1.057716 | 0.171083 |
| H | -11.565936 | 0.543629 | 0.797042 |
| H | 13.235971 | -0.354724 | 2.014280 |
| H | 11.713393 | -0.007477 | 2.840225 |
| H | 12.068811 | -1.649832 | 2.298628 |
| H | -13.118360 | 0.679767 | -1.155621 |
| H | -11.587776 | 1.471418 | -1.545257 |
| H | -11.932933 | -0.140937 | -2.176436 |

11a

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|---|------------|-----------|-----------|
| C | 5.431474 | -1.961221 | -0.721108 |
| C | 4.926897 | -0.708328 | 0.009634 |
| C | 5.757590 | -0.432678 | 1.256440 |
| C | 7.240361 | -0.319428 | 0.917882 |
| C | 7.769014 | -1.558382 | 0.192474 |
| C | 6.915918 | -1.836264 | -1.045338 |
| C | 3.467263 | -0.820304 | 0.343915 |
| O | 2.969398 | -0.864023 | 1.427237 |
| C | 9.247300 | -1.442837 | -0.179884 |
| C | 10.197717 | -1.329698 | 1.005142 |
| O | 2.724508 | -0.914167 | -0.813453 |
| C | 1.362053 | -0.825087 | -0.710956 |
| C | 0.701558 | 0.391008 | -0.492845 |
| C | -0.714860 | 0.410930 | -0.483059 |
| C | -1.411443 | -0.787983 | -0.685834 |
| C | -0.731789 | -1.976621 | -0.907506 |
| C | 0.647052 | -1.994861 | -0.921505 |
| C | 1.481730 | 1.650415 | -0.322570 |
| C | 0.729185 | 2.927194 | -0.266938 |
| C | -0.665411 | 2.947942 | -0.265334 |
| C | -1.456336 | 1.694281 | -0.318368 |
| C | -1.342104 | 4.164817 | -0.192657 |
| C | -0.629019 | 5.350541 | -0.131426 |
| C | 0.765380 | 5.329685 | -0.132628 |
| C | 1.442352 | 4.123075 | -0.195262 |
| O | -2.669095 | 1.745054 | -0.245383 |
| O | 2.694968 | 1.662996 | -0.244148 |
| O | -2.777200 | -0.843298 | -0.759505 |
| C | -3.493263 | -0.684427 | 0.407986 |
| C | -4.956085 | -0.548358 | 0.099357 |
| C | -5.536324 | -1.887665 | -0.378983 |
| C | -7.029141 | -1.765884 | -0.668328 |
| C | -7.815366 | -1.239016 | 0.533427 |
| C | -7.212509 | 0.084649 | 1.005496 |
| C | -5.722782 | -0.024299 | 1.308160 |
| C | -9.308334 | -1.088354 | 0.241109 |
| C | -10.033807 | -2.390787 | -0.072058 |
| O | -2.976217 | -0.710068 | 1.482892 |
| H | -1.309853 | -2.879642 | -1.064681 |
| H | 1.197651 | -2.912662 | -1.091238 |
| H | 2.525076 | 4.075735 | -0.187975 |
| H | 1.321456 | 6.259724 | -0.080752 |
| H | -1.156944 | 6.296793 | -0.078541 |
| H | -2.425736 | 4.150172 | -0.183397 |
| H | -5.028372 | 0.170868 | -0.725678 |
| H | 5.004926 | 0.142087 | -0.680494 |
| H | -5.375436 | -2.642454 | 0.402215 |
| H | -5.001148 | -2.228141 | -1.270281 |
| H | -7.414393 | -2.741011 | -0.983004 |

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|---|------------|-----------|-----------|
| H | -7.179540 | -1.081027 | -1.515609 |
| H | -7.703190 | -1.968013 | 1.352130 |
| H | -7.746686 | 0.437260 | 1.895003 |
| H | -7.373877 | 0.844035 | 0.226640 |
| H | -5.557981 | -0.703599 | 2.152469 |
| H | -5.316026 | 0.945803 | 1.608127 |
| H | 5.400998 | 0.480169 | 1.741750 |
| H | 5.598075 | -1.244912 | 1.975571 |
| H | 7.807447 | -0.142540 | 1.837016 |
| H | 7.404231 | 0.559500 | 0.276864 |
| H | 7.658452 | -2.417276 | 0.874054 |
| H | 7.264784 | -2.750400 | -1.539393 |
| H | 7.060088 | -1.018527 | -1.766054 |
| H | 4.850966 | -2.120361 | -1.633898 |
| H | 5.270028 | -2.837129 | -0.078350 |
| H | 9.522920 | -2.321351 | -0.776844 |
| H | 9.378152 | -0.575685 | -0.841645 |
| H | -9.782780 | -0.614570 | 1.109502 |
| H | -9.435816 | -0.384888 | -0.593040 |
| H | -9.666909 | -2.854119 | -0.992142 |
| H | -11.106701 | -2.221781 | -0.199510 |
| H | -9.907593 | -3.116533 | 0.738368 |
| H | 10.033220 | -0.412044 | 1.576373 |
| H | 11.239731 | -1.323558 | 0.673298 |
| H | 10.074252 | -2.174197 | 1.691427 |

11b

| | | | |
|---|------------|-----------|-----------|
| C | -5.917642 | 0.304867 | 1.154825 |
| C | -5.044453 | -0.388903 | 0.116262 |
| C | -5.642568 | -1.744786 | -0.287281 |
| C | -7.079601 | -1.587478 | -0.774085 |
| C | -7.970846 | -0.892216 | 0.256200 |
| C | -7.350685 | 0.447274 | 0.656071 |
| C | -3.636981 | -0.548464 | 0.613383 |
| O | -3.238081 | -0.397917 | 1.728467 |
| C | -9.407196 | -0.706717 | -0.233422 |
| C | -10.168376 | -2.000816 | -0.490746 |
| O | -2.816925 | -0.959185 | -0.413600 |
| C | -1.466555 | -0.975764 | -0.187300 |
| C | -0.697259 | 0.192851 | -0.106765 |
| C | 0.705660 | 0.082636 | 0.060303 |
| C | 1.281226 | -1.192792 | 0.134288 |
| C | 0.494468 | -2.332200 | 0.046362 |
| C | -0.871611 | -2.225317 | -0.106360 |
| C | -1.344471 | 1.530251 | -0.246103 |
| C | -0.470989 | 2.728231 | -0.233649 |
| C | 0.901364 | 2.621859 | -0.011064 |
| C | 1.547521 | 1.305453 | 0.205852 |
| C | -1.048762 | 3.982208 | -0.427561 |
| C | -0.257733 | 5.118861 | -0.406223 |
| C | 1.114797 | 5.012465 | -0.183128 |
| C | 1.692140 | 3.769707 | 0.017434 |
| O | 2.617505 | -1.417967 | 0.345242 |
| C | 3.507361 | -1.100489 | -0.652740 |
| O | 3.158814 | -0.695873 | -1.720704 |
| O | 2.726337 | 1.252467 | 0.494309 |
| O | -2.545949 | 1.664243 | -0.376625 |
| C | 4.912968 | -1.399690 | -0.207705 |
| C | 5.314258 | -0.585011 | 1.029616 |
| C | 6.739680 | -0.920555 | 1.452362 |
| C | 7.754532 | -0.715131 | 0.326948 |

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|---|------------|-----------|-----------|
| C | 7.328493 | -1.515917 | -0.904921 |
| C | 5.905296 | -1.190392 | -1.345874 |
| C | 9.169131 | -1.055830 | 0.795392 |
| C | 10.271086 | -0.708444 | -0.197275 |
| H | -1.502709 | -3.103652 | -0.173232 |
| H | 0.981163 | -3.298507 | 0.108072 |
| H | 2.754909 | 3.657263 | 0.197238 |
| H | 1.731850 | 5.904569 | -0.165964 |
| H | -0.707731 | 6.093718 | -0.561361 |
| H | -2.118928 | 4.035157 | -0.590287 |
| H | -4.974061 | 0.234587 | -0.784186 |
| H | 4.914836 | -2.460858 | 0.083905 |
| H | -5.624038 | -2.414075 | 0.583372 |
| H | -5.025233 | -2.207985 | -1.062117 |
| H | -7.482233 | -2.573201 | -1.028151 |
| H | -7.086043 | -0.997560 | -1.702261 |
| H | -8.000251 | -1.528077 | 1.155900 |
| H | -7.966148 | 0.923891 | 1.427403 |
| H | -7.370169 | 1.119393 | -0.214143 |
| H | -5.897368 | -0.279657 | 2.082120 |
| H | -5.492763 | 1.282936 | 1.398183 |
| H | 5.619915 | -1.798568 | -2.209289 |
| H | 5.844574 | -0.146522 | -1.675528 |
| H | 8.014309 | -1.332486 | -1.737976 |
| H | 7.404771 | -2.588136 | -0.670000 |
| H | 7.736183 | 0.352001 | 0.053374 |
| H | 7.018649 | -0.309962 | 2.318829 |
| H | 6.786298 | -1.968334 | 1.783971 |
| H | 4.611562 | -0.775708 | 1.844138 |
| H | 5.232047 | 0.481149 | 0.792321 |
| H | 9.357703 | -0.526583 | 1.737894 |
| H | 9.213426 | -2.126581 | 1.037374 |
| H | -9.950966 | -0.114559 | 0.513123 |
| H | -9.393440 | -0.098657 | -1.148284 |
| H | -9.724592 | -2.583873 | -1.302484 |
| H | -11.206432 | -1.796972 | -0.767860 |
| H | -10.183250 | -2.633622 | 0.403029 |
| H | 10.186248 | -1.284319 | -1.123014 |
| H | 11.259031 | -0.914247 | 0.224130 |
| H | 10.239751 | 0.353390 | -0.463523 |

12a

| | | | |
|---|-----------|-----------|-----------|
| C | 2.619125 | -1.281472 | 0.000779 |
| C | 1.757549 | -0.185575 | -0.000055 |
| C | 2.278184 | 1.112505 | -0.000935 |
| C | 3.649279 | 1.298562 | -0.000903 |
| C | 4.510330 | 0.201303 | 0.000023 |
| C | 3.993690 | -1.088556 | 0.000875 |
| N | 0.379803 | -0.494340 | -0.000097 |
| N | -0.379779 | 0.494244 | 0.000320 |
| C | -1.757542 | 0.185530 | 0.000138 |
| C | -2.619074 | 1.281462 | 0.000891 |
| C | -3.993648 | 1.088607 | 0.000766 |
| C | -4.510343 | -0.201229 | -0.000123 |
| C | -3.649338 | -1.298525 | -0.000879 |
| C | -2.278235 | -1.112528 | -0.000751 |
| H | -4.056564 | -2.304368 | -0.001578 |
| H | -5.584291 | -0.355998 | -0.000234 |
| H | -4.661278 | 1.943528 | 0.001355 |
| H | -2.183740 | 2.274767 | 0.001572 |
| H | -1.589553 | -1.948552 | -0.001336 |

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|---|----------|-----------|-----------|
| H | 1.589466 | 1.948501 | -0.001636 |
| H | 4.056462 | 2.304423 | -0.001634 |
| H | 5.584271 | 0.356116 | 0.000038 |
| H | 4.661356 | -1.943450 | 0.001573 |
| H | 2.183833 | -2.274796 | 0.001367 |

13a

| | | | |
|---|-----------|-----------|-----------|
| C | -2.329199 | -1.326111 | 0.000138 |
| C | -2.109376 | 0.055822 | 0.000094 |
| C | -3.198494 | 0.942866 | 0.000034 |
| C | -4.482960 | 0.403672 | -0.000053 |
| C | -4.718820 | -0.968100 | -0.000048 |
| C | -3.614343 | -1.827574 | 0.000067 |
| N | -0.831699 | 0.630916 | 0.000082 |
| N | 0.155040 | -0.161353 | 0.000056 |
| C | 1.405279 | 0.415617 | 0.000023 |
| C | 2.533005 | -0.476080 | 0.000002 |
| C | 3.845558 | 0.066321 | -0.000013 |
| C | 4.007428 | 1.477179 | -0.000018 |
| C | 2.936950 | 2.321686 | -0.000018 |
| C | 1.619228 | 1.808579 | -0.000002 |
| C | 2.385653 | -1.878633 | -0.000004 |
| C | 3.488017 | -2.699760 | -0.000027 |
| C | 4.787755 | -2.163103 | -0.000042 |
| C | 4.958352 | -0.801608 | -0.000034 |
| O | 0.616906 | 2.670611 | -0.000039 |
| C | -2.993691 | 2.428845 | 0.000006 |
| C | -6.114682 | -1.517218 | -0.000136 |
| H | -5.330666 | 1.083945 | -0.000097 |
| H | -1.469704 | -1.985079 | 0.000225 |
| H | -3.771411 | -2.902448 | 0.000118 |
| H | 5.015052 | 1.882469 | -0.000023 |
| H | 3.054596 | 3.399341 | -0.000030 |
| H | 1.385961 | -2.293859 | 0.000008 |
| H | 3.353180 | -3.776637 | -0.000037 |
| H | 5.647958 | -2.823772 | -0.000060 |
| H | 5.954881 | -0.369960 | -0.000045 |
| H | -0.215761 | 2.101767 | -0.000024 |
| H | -3.953284 | 2.949172 | 0.000646 |
| H | -2.431263 | 2.756307 | -0.879856 |
| H | -2.430123 | 2.756219 | 0.879156 |
| H | -6.858546 | -0.718084 | -0.000448 |
| H | -6.291878 | -2.142583 | 0.880790 |
| H | -6.291589 | -2.143029 | -0.880801 |

13b

| | | | |
|---|-----------|-----------|-----------|
| C | -4.888571 | -0.744666 | -0.010235 |
| C | -3.801454 | 0.155235 | -0.004755 |
| C | -2.473136 | -0.348209 | -0.004629 |
| C | -2.286515 | -1.746726 | -0.009916 |
| C | -3.364662 | -2.599447 | -0.015192 |
| C | -4.679323 | -2.100792 | -0.015401 |
| C | -4.004029 | 1.560488 | 0.000767 |
| C | -2.957495 | 2.434190 | 0.006165 |
| C | -1.625232 | 1.959186 | 0.006274 |
| C | -1.371477 | 0.574148 | 0.000943 |
| N | -0.104347 | 0.025196 | 0.000431 |
| N | 0.860832 | 0.843012 | 0.004638 |
| C | 2.170485 | 0.347999 | 0.003691 |
| C | 2.580435 | -1.005420 | 0.020367 |
| C | 3.950648 | -1.255749 | 0.018766 |

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|---|-----------|-----------|-----------|
| C | 4.921312 | -0.255252 | -0.000062 |
| C | 4.491035 | 1.070683 | -0.011047 |
| C | 3.140691 | 1.358563 | -0.009374 |
| C | 6.380841 | -0.598352 | -0.034653 |
| C | 1.642965 | -2.173926 | 0.044084 |
| O | -0.650480 | 2.852822 | 0.011575 |
| H | 4.275258 | -2.293318 | 0.035334 |
| H | 2.797672 | 2.387894 | -0.015745 |
| H | 5.216634 | 1.878145 | -0.018639 |
| H | -5.022681 | 1.937185 | 0.000670 |
| H | -3.104961 | 3.508185 | 0.010418 |
| H | -1.276455 | -2.135182 | -0.009730 |
| H | -3.198515 | -3.671969 | -0.019256 |
| H | -5.520201 | -2.785856 | -0.019600 |
| H | -5.897070 | -0.341653 | -0.010291 |
| H | 0.198121 | 2.313168 | 0.010267 |
| H | 2.212108 | -3.106305 | 0.069773 |
| H | 0.991359 | -2.180637 | -0.833640 |
| H | 0.980599 | -2.138244 | 0.912917 |
| H | 6.576005 | -1.565591 | 0.434196 |
| H | 6.979735 | 0.158048 | 0.478405 |
| H | 6.741735 | -0.655630 | -1.067916 |

13c

| | | | |
|---|-----------|-----------|-----------|
| C | 4.665908 | -1.227347 | 0.005479 |
| C | 3.736854 | -0.166350 | -0.004132 |
| C | 2.337108 | -0.447092 | 0.000785 |
| C | 1.938313 | -1.802665 | 0.016163 |
| C | 2.872505 | -2.813984 | 0.025460 |
| C | 4.247560 | -2.534260 | 0.019971 |
| C | 4.190983 | 1.178536 | -0.018295 |
| C | 3.321451 | 2.228342 | -0.027068 |
| C | 1.936613 | 1.973705 | -0.022255 |
| C | 1.427425 | 0.665690 | -0.009439 |
| N | 0.040780 | 0.689240 | -0.008342 |
| N | -0.602737 | -0.389946 | 0.000192 |
| C | -2.003227 | -0.309688 | 0.001282 |
| C | -2.828386 | 0.840994 | 0.033247 |
| C | -4.206661 | 0.642443 | 0.032545 |
| C | -4.808509 | -0.614999 | -0.001189 |
| C | -3.977958 | -1.733776 | -0.027015 |
| C | -2.606351 | -1.574485 | -0.024696 |
| C | -6.301629 | -0.751664 | -0.035268 |
| C | -2.325683 | 2.253388 | 0.073437 |
| O | 1.108263 | 3.020323 | -0.030274 |
| H | -4.845571 | 1.521896 | 0.061951 |
| H | -1.946663 | -2.435013 | -0.041353 |
| H | -4.408403 | -2.730298 | -0.045992 |
| H | 5.261500 | 1.360844 | -0.021887 |
| H | 3.656777 | 3.258607 | -0.037531 |
| H | 0.882800 | -2.026962 | 0.020640 |
| H | 2.535565 | -3.845712 | 0.037407 |
| H | 4.970189 | -3.343129 | 0.027329 |
| H | 5.725043 | -0.986941 | 0.001307 |
| H | 0.217438 | 2.622241 | -0.027338 |
| H | -3.167688 | 2.947500 | 0.127712 |
| H | -1.743358 | 2.495436 | -0.821248 |
| H | -1.682420 | 2.426835 | 0.941315 |
| H | -6.791323 | 0.075880 | 0.483585 |
| H | -6.626529 | -1.686501 | 0.427590 |
| H | -6.667661 | -0.753048 | -1.068312 |

13d

| | | | |
|---|-----------|-----------|-----------|
| C | 4.640614 | 1.094151 | -0.159780 |
| C | 3.721359 | 0.031157 | -0.045156 |
| C | 2.320027 | 0.300060 | -0.058936 |
| C | 1.907336 | 1.644311 | -0.194082 |
| C | 2.832469 | 2.658315 | -0.305539 |
| C | 4.209761 | 2.391216 | -0.287283 |
| C | 4.185144 | -1.304761 | 0.083463 |
| C | 3.324492 | -2.356115 | 0.195584 |
| C | 1.937119 | -2.113677 | 0.185975 |
| C | 1.420226 | -0.813662 | 0.058984 |
| N | 0.037269 | -0.841937 | 0.054582 |
| N | -0.622562 | 0.225773 | 0.021136 |
| C | -2.016519 | 0.061124 | -0.031959 |
| C | -2.792992 | 1.185990 | 0.295004 |
| C | -4.179247 | 1.065070 | 0.247100 |
| C | -4.815856 | -0.114992 | -0.130484 |
| C | -4.020511 | -1.213236 | -0.471084 |
| C | -2.643319 | -1.127146 | -0.422883 |
| C | -6.311851 | -0.201096 | -0.203037 |
| C | -2.150980 | 2.479760 | 0.699243 |
| O | 1.117368 | -3.157378 | 0.308034 |
| H | -4.784859 | 1.927936 | 0.512263 |
| H | -2.027129 | -1.971221 | -0.709101 |
| H | -4.491323 | -2.140329 | -0.785623 |
| H | 5.257007 | -1.478962 | 0.092426 |
| H | 3.668842 | -3.378502 | 0.295887 |
| H | 0.849489 | 1.859182 | -0.205934 |
| H | 2.486500 | 3.681909 | -0.408781 |
| H | 4.924908 | 3.202074 | -0.374106 |
| H | 5.701952 | 0.864065 | -0.145781 |
| H | 0.223299 | -2.764165 | 0.283405 |
| H | -2.909787 | 3.228860 | 0.934850 |
| H | -1.519162 | 2.871170 | -0.103481 |
| H | -1.507158 | 2.352390 | 1.573333 |
| H | -6.785479 | 0.654446 | 0.282831 |
| H | -6.680451 | -1.112289 | 0.276884 |
| H | -6.652167 | -0.223191 | -1.244141 |

13e

| | | | |
|---|-----------|-----------|-----------|
| C | -4.977029 | -0.768787 | 0.000029 |
| C | -3.854468 | 0.073081 | 0.000050 |
| C | -2.557791 | -0.487639 | 0.000023 |
| C | -2.430238 | -1.883611 | -0.000027 |
| C | -3.548140 | -2.694977 | -0.000046 |
| C | -4.831791 | -2.140463 | -0.000018 |
| C | -4.003878 | 1.503121 | 0.000087 |
| C | -2.948845 | 2.346443 | 0.000106 |
| C | -1.588257 | 1.854099 | 0.000118 |
| C | -1.404374 | 0.401281 | 0.000052 |
| N | -0.207948 | -0.167938 | 0.000014 |
| N | 0.844761 | 0.583000 | 0.000014 |
| C | 2.133184 | 0.048459 | -0.000018 |
| C | 2.352690 | -1.329536 | 0.000017 |
| C | 3.643838 | -1.821792 | -0.000003 |
| C | 4.744523 | -0.961031 | -0.000060 |
| C | 4.498649 | 0.409325 | -0.000092 |
| C | 3.213250 | 0.944110 | -0.000074 |
| C | 2.991883 | 2.428124 | -0.000098 |
| C | 6.144328 | -1.502128 | -0.000105 |

| | | | |
|---|-----------|-----------|-----------|
| O | -0.618287 | 2.639945 | 0.000090 |
| H | 5.340743 | 1.096595 | -0.000135 |
| H | 1.498468 | -1.994856 | 0.000065 |
| H | 3.802346 | -2.896303 | 0.000028 |
| H | -5.014816 | 1.902892 | 0.000097 |
| H | -3.069213 | 3.423998 | 0.000123 |
| H | -1.436902 | -2.315246 | -0.000049 |
| H | -3.426607 | -3.773350 | -0.000084 |
| H | -5.704912 | -2.783807 | -0.000034 |
| H | -5.966556 | -0.321249 | 0.000048 |
| H | 0.665026 | 1.606066 | 0.000041 |
| H | 3.945206 | 2.958517 | -0.000271 |
| H | 2.426447 | 2.755695 | 0.879422 |
| H | 2.426160 | 2.755636 | -0.879453 |
| H | 6.882218 | -0.697250 | 0.000076 |
| H | 6.327939 | -2.125232 | -0.881311 |
| H | 6.327870 | -2.125572 | 0.880873 |

13f

| | | | |
|---|-----------|-----------|-----------|
| C | 3.153589 | 1.357743 | -0.002137 |
| C | 2.195485 | 0.336100 | 0.001877 |
| C | 2.605171 | -1.009750 | 0.007911 |
| C | 3.979108 | -1.252401 | 0.007368 |
| C | 4.945051 | -0.250817 | 0.000980 |
| C | 4.503712 | 1.072592 | -0.002086 |
| N | 0.873617 | 0.783293 | 0.002786 |
| N | -0.161847 | 0.010647 | 0.000563 |
| C | -1.371552 | 0.556648 | 0.000542 |
| C | -2.502618 | -0.359075 | -0.001724 |
| C | -3.812908 | 0.169850 | -0.002363 |
| C | -3.996272 | 1.595831 | -0.000683 |
| C | -2.961317 | 2.463497 | 0.001528 |
| C | -1.588728 | 2.003683 | 0.002331 |
| C | -2.342511 | -1.752301 | -0.003204 |
| C | -3.440871 | -2.590146 | -0.005339 |
| C | -4.737372 | -2.066686 | -0.006031 |
| C | -4.914850 | -0.698701 | -0.004531 |
| O | -0.638417 | 2.812854 | 0.004366 |
| C | 1.666447 | -2.179540 | 0.017225 |
| C | 6.409066 | -0.578653 | -0.016986 |
| H | 4.305484 | -2.289261 | 0.013685 |
| H | 2.815953 | 2.390036 | -0.003502 |
| H | 5.222316 | 1.886459 | -0.003439 |
| H | -5.016399 | 1.971606 | -0.001220 |
| H | -3.106825 | 3.537972 | 0.002820 |
| H | -1.340010 | -2.161816 | -0.002610 |
| H | -3.293521 | -3.665345 | -0.006467 |
| H | -5.594905 | -2.730647 | -0.007699 |
| H | -5.914737 | -0.274697 | -0.004997 |
| H | 0.665999 | 1.803166 | 0.003830 |
| H | 2.237674 | -3.110435 | 0.026928 |
| H | 1.012985 | -2.178711 | -0.859124 |
| H | 1.009368 | -2.162442 | 0.890666 |
| H | 6.581918 | -1.640356 | 0.170772 |
| H | 6.953055 | -0.008040 | 0.741419 |
| H | 6.854815 | -0.335143 | -0.987490 |

13g

| | | | |
|---|-----------|-----------|-----------|
| C | -2.731079 | -1.537676 | 0.580346 |
| C | -2.017013 | -0.459350 | 0.037718 |
| C | -2.726234 | 0.623059 | -0.532043 |

| | | | |
|---|-----------|-----------|-----------|
| C | -4.117862 | 0.586881 | -0.462106 |
| C | -4.832766 | -0.452890 | 0.126537 |
| C | -4.109308 | -1.531377 | 0.639491 |
| N | -0.631963 | -0.622838 | 0.063293 |
| N | 0.063029 | 0.443087 | 0.169971 |
| C | 1.396722 | 0.600063 | 0.176741 |
| C | 2.382727 | -0.425378 | 0.003564 |
| C | 3.743627 | -0.019103 | 0.034656 |
| C | 4.074135 | 1.367938 | 0.235434 |
| C | 3.142168 | 2.331765 | 0.397087 |
| C | 1.729649 | 2.012744 | 0.376668 |
| C | 2.089370 | -1.785976 | -0.195347 |
| C | 3.110914 | -2.706128 | -0.359327 |
| C | 4.446909 | -2.307512 | -0.327559 |
| C | 4.752793 | -0.973078 | -0.131432 |
| O | 0.835199 | 2.859211 | 0.513503 |
| C | -2.076232 | 1.753642 | -1.286545 |
| C | -6.330332 | -0.419600 | 0.202234 |
| H | -4.670025 | 1.408359 | -0.911958 |
| H | -2.158588 | -2.371440 | 0.971487 |
| H | -4.632970 | -2.374009 | 1.080871 |
| H | 5.129145 | 1.629504 | 0.253834 |
| H | 3.405652 | 3.372469 | 0.546434 |
| H | 1.055995 | -2.102156 | -0.216541 |
| H | 2.863147 | -3.751334 | -0.513354 |
| H | 5.239488 | -3.036749 | -0.455079 |
| H | 5.788441 | -0.646948 | -0.104478 |
| H | -0.373373 | 1.374303 | 0.316232 |
| H | -2.798565 | 2.197109 | -1.974520 |
| H | -1.224178 | 1.409146 | -1.879738 |
| H | -1.716026 | 2.560685 | -0.639063 |
| H | -6.750781 | 0.299683 | -0.503898 |
| H | -6.663789 | -0.131305 | 1.205443 |
| H | -6.761767 | -1.400892 | -0.013239 |

13h

| | | | |
|---|-----------|-----------|-----------|
| C | -2.594363 | -1.082505 | 0.434438 |
| C | -2.016475 | 0.134531 | 0.043012 |
| C | -2.853138 | 1.230202 | -0.261567 |
| C | -4.227825 | 1.049232 | -0.201727 |
| C | -4.814146 | -0.165846 | 0.157391 |
| C | -3.969717 | -1.226479 | 0.483675 |
| N | -0.650152 | 0.372233 | -0.032544 |
| N | 0.091607 | -0.666931 | -0.102571 |
| C | 1.428522 | -0.769665 | -0.094590 |
| C | 2.371927 | 0.300633 | 0.038985 |
| C | 3.747730 | -0.053006 | 0.055098 |
| C | 4.136001 | -1.435356 | -0.059576 |
| C | 3.245678 | -2.442128 | -0.187133 |
| C | 1.821713 | -2.177696 | -0.220235 |
| C | 2.022743 | 1.657942 | 0.148879 |
| C | 3.004676 | 2.626388 | 0.273842 |
| C | 4.354931 | 2.279160 | 0.290559 |
| C | 4.715591 | 0.948072 | 0.181405 |
| O | 0.964174 | -3.062073 | -0.339096 |
| C | -2.263562 | 2.552060 | -0.648844 |
| C | -6.305480 | -0.323142 | 0.182528 |
| H | -4.870566 | 1.892030 | -0.443680 |
| H | -1.975140 | -1.917236 | 0.750168 |
| H | -4.394179 | -2.174137 | 0.800916 |
| H | 5.200433 | -1.655250 | -0.041532 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.551707 | -3.478264 | -0.273945 |
| H | 0.977387 | 1.932566 | 0.133688 |
| H | 2.714275 | 3.668542 | 0.358401 |
| H | 5.116478 | 3.045266 | 0.387164 |
| H | 5.763360 | 0.662391 | 0.192279 |
| H | -0.307883 | -1.622317 | -0.205487 |
| H | -3.050220 | 3.280712 | -0.853922 |
| H | -1.632726 | 2.461636 | -1.537482 |
| H | -1.626848 | 2.945396 | 0.149390 |
| H | -6.797957 | 0.589914 | 0.526851 |
| H | -6.609051 | -1.142376 | 0.838205 |
| H | -6.691481 | -0.543782 | -0.819272 |

14a

| | | | |
|---|-----------|-----------|-----------|
| C | 7.039800 | 1.219696 | 0.000050 |
| C | 6.057007 | 0.207477 | 0.000027 |
| C | 4.682847 | 0.563199 | 0.000005 |
| C | 4.343298 | 1.930967 | -0.000004 |
| C | 5.322249 | 2.896686 | 0.000012 |
| C | 6.683029 | 2.545059 | 0.000045 |
| C | 6.411558 | -1.168287 | 0.000018 |
| C | 5.469667 | -2.154118 | 0.000007 |
| C | 4.093458 | -1.829363 | 0.000006 |
| C | 3.688412 | -0.477260 | -0.000003 |
| N | 2.375042 | -0.080021 | -0.000031 |
| N | 1.499676 | -0.996251 | -0.000019 |
| C | 0.163700 | -0.577232 | -0.000045 |
| C | -0.803025 | -1.591903 | 0.000010 |
| C | -2.147157 | -1.282145 | 0.000011 |
| C | -2.548377 | 0.058343 | -0.000051 |
| C | -1.582827 | 1.070328 | -0.000122 |
| C | -0.237003 | 0.763400 | -0.000116 |
| N | -3.886289 | 0.492327 | -0.000063 |
| N | -4.735561 | -0.423527 | 0.000058 |
| C | -6.076443 | 0.010640 | 0.000041 |
| C | -7.037181 | -1.000477 | 0.000016 |
| C | -8.387532 | -0.680100 | -0.000005 |
| C | -8.781147 | 0.652533 | 0.000013 |
| C | -7.821456 | 1.664906 | 0.000055 |
| C | -6.473915 | 1.352163 | 0.000068 |
| O | 3.223028 | -2.820881 | 0.000011 |
| H | -9.132049 | -1.468885 | -0.000032 |
| H | -6.696706 | -2.030154 | 0.000012 |
| H | -5.710782 | 2.120733 | 0.000104 |
| H | -8.133488 | 2.704194 | 0.000079 |
| H | -9.835907 | 0.907030 | 0.000001 |
| H | -2.906792 | -2.053875 | 0.000065 |
| H | -0.471308 | -2.625002 | 0.000046 |
| H | 0.518355 | 1.538588 | -0.000170 |
| H | -1.924847 | 2.099554 | -0.000179 |
| H | 7.465538 | -1.430600 | 0.000023 |
| H | 5.736604 | -3.204685 | -0.000004 |
| H | 3.296239 | 2.205723 | -0.000026 |
| H | 5.039607 | 3.944462 | -0.000002 |
| H | 7.443800 | 3.317989 | 0.000070 |
| H | 8.086208 | 0.929439 | 0.000076 |
| H | 2.317463 | -2.382231 | 0.000010 |

14b

| | | | |
|---|----------|----------|-----------|
| C | 6.763520 | 1.688988 | -0.000112 |
| C | 5.926155 | 0.553512 | -0.000006 |

| | | | |
|---|-----------|-----------|-----------|
| C | 4.516622 | 0.721030 | -0.000101 |
| C | 3.995515 | 2.030496 | -0.000331 |
| C | 4.835309 | 3.119299 | -0.000424 |
| C | 6.231080 | 2.954051 | -0.000307 |
| C | 6.462816 | -0.761908 | 0.000133 |
| C | 5.662276 | -1.865618 | 0.000222 |
| C | 4.255009 | -1.729038 | 0.000168 |
| C | 3.671486 | -0.443856 | 0.000008 |
| N | 2.316477 | -0.226395 | -0.000126 |
| N | 1.571890 | -1.251691 | 0.000074 |
| C | 0.192035 | -1.015607 | 0.000092 |
| C | -0.629208 | -2.144810 | -0.000163 |
| C | -2.005309 | -2.001039 | -0.000099 |
| C | -2.579082 | -0.729913 | 0.000135 |
| C | -1.753468 | 0.405283 | 0.000592 |
| C | -0.384496 | 0.265451 | 0.000590 |
| N | -3.984865 | -0.693448 | -0.000006 |
| N | -4.480273 | 0.453269 | -0.000507 |
| C | -5.889181 | 0.491516 | -0.000219 |
| C | -6.456802 | 1.765582 | 0.000524 |
| C | -7.836469 | 1.914888 | 0.000793 |
| C | -8.652902 | 0.790411 | 0.000186 |
| C | -8.086700 | -0.484496 | -0.000685 |
| C | -6.712153 | -0.640057 | -0.000881 |
| O | 3.525998 | -2.828938 | 0.000336 |
| H | -8.274559 | 2.907148 | 0.001458 |
| H | -5.791719 | 2.622215 | 0.000888 |
| H | -6.249701 | -1.619458 | -0.001558 |
| H | -8.728065 | -1.359790 | -0.001236 |
| H | -9.732057 | 0.903056 | 0.000311 |
| H | -2.663931 | -2.862201 | -0.000249 |
| H | -0.170417 | -3.127545 | -0.000382 |
| H | 0.267625 | 1.129763 | 0.001054 |
| H | -2.220118 | 1.382777 | 0.000975 |
| H | 7.542513 | -0.879758 | 0.000180 |
| H | 6.068125 | -2.870707 | 0.000315 |
| H | 2.920953 | 2.161070 | -0.000462 |
| H | 4.414255 | 4.119480 | -0.000603 |
| H | 6.880827 | 3.822431 | -0.000383 |
| H | 7.839532 | 1.542510 | -0.000023 |
| H | 2.569844 | -2.516625 | 0.000297 |

14c

| | | | |
|---|-----------|-----------|-----------|
| C | -6.490280 | 1.350821 | 0.000030 |
| C | -6.093339 | 0.009218 | -0.000021 |
| C | -7.055451 | -1.000510 | -0.000040 |
| C | -8.405596 | -0.678929 | -0.000009 |
| C | -8.798564 | 0.653879 | 0.000042 |
| C | -7.837666 | 1.664930 | 0.000062 |
| N | -4.752376 | -0.425963 | -0.000055 |
| N | -3.902948 | 0.490289 | -0.000045 |
| C | -2.566232 | 0.060360 | -0.000033 |
| C | -2.159700 | -1.279608 | -0.000038 |
| C | -0.817816 | -1.592783 | -0.000029 |
| C | 0.144670 | -0.572684 | -0.000014 |
| C | -0.252185 | 0.766127 | -0.000009 |
| C | -1.600018 | 1.069294 | -0.000018 |
| N | 1.480733 | -0.948331 | -0.000006 |
| N | 2.433121 | -0.066708 | 0.000007 |
| C | 3.690137 | -0.466218 | 0.000020 |
| C | 4.713172 | 0.573430 | 0.000004 |

| | | | |
|---|-----------|-----------|-----------|
| C | 6.073303 | 0.195416 | 0.000015 |
| C | 6.418449 | -1.202249 | 0.000045 |
| C | 5.491996 | -2.184017 | 0.000063 |
| C | 4.075046 | -1.885291 | 0.000049 |
| C | 4.394598 | 1.937209 | -0.000025 |
| C | 5.390779 | 2.895281 | -0.000043 |
| C | 6.737152 | 2.522026 | -0.000031 |
| C | 7.069532 | 1.182297 | -0.000003 |
| O | 3.224274 | -2.792773 | 0.000075 |
| H | -9.150620 | -1.467304 | -0.000025 |
| H | -6.716238 | -2.030631 | -0.000079 |
| H | -5.726688 | 2.118949 | 0.000045 |
| H | -8.148413 | 2.704662 | 0.000102 |
| H | -9.853103 | 0.909293 | 0.000067 |
| H | -2.917468 | -2.053292 | -0.000051 |
| H | -0.495857 | -2.629781 | -0.000033 |
| H | 0.500965 | 1.542977 | 0.000001 |
| H | -1.939311 | 2.099283 | -0.000015 |
| H | 7.475021 | -1.458116 | 0.000055 |
| H | 5.760941 | -3.234290 | 0.000088 |
| H | 3.351537 | 2.228894 | -0.000034 |
| H | 5.122047 | 3.946570 | -0.000065 |
| H | 7.514071 | 3.278629 | -0.000045 |
| H | 8.111101 | 0.875027 | 0.000006 |
| H | 1.776179 | -1.941691 | -0.000017 |

14d

| | | | |
|---|-----------|-----------|-----------|
| C | -6.729389 | -0.638459 | -0.000813 |
| C | -5.909050 | 0.494938 | 0.000146 |
| C | -6.480820 | 1.767099 | 0.001252 |
| C | -7.860956 | 1.912607 | 0.001541 |
| C | -8.674675 | 0.786183 | 0.000626 |
| C | -8.104526 | -0.486829 | -0.000576 |
| N | -4.499704 | 0.460416 | 0.000024 |
| N | -4.001873 | -0.685601 | 0.000037 |
| C | -2.598129 | -0.722582 | -0.000261 |
| C | -2.020793 | -1.992894 | -0.000182 |
| C | -0.646663 | -2.141670 | -0.000341 |
| C | 0.171120 | -1.008766 | -0.000587 |
| C | -0.399714 | 0.271704 | -0.000709 |
| C | -1.770015 | 0.408813 | -0.000546 |
| N | 1.545294 | -1.202538 | -0.000662 |
| N | 2.373146 | -0.203113 | -0.000570 |
| C | 3.671898 | -0.434451 | -0.000294 |
| C | 4.549843 | 0.730320 | -0.000286 |
| C | 5.947789 | 0.533269 | 0.000759 |
| C | 6.473088 | -0.807046 | 0.001641 |
| C | 5.683253 | -1.901671 | 0.001409 |
| C | 4.239571 | -1.790893 | 0.000234 |
| C | 4.055489 | 2.040716 | -0.001299 |
| C | 4.917952 | 3.120703 | -0.001200 |
| C | 6.301616 | 2.926472 | -0.000098 |
| C | 6.806499 | 1.641833 | 0.000856 |
| O | 3.515180 | -2.802268 | -0.000149 |
| H | -8.301583 | 2.903799 | 0.002452 |
| H | -5.818289 | 2.625747 | 0.001906 |
| H | -6.264445 | -1.616694 | -0.001723 |
| H | -8.743216 | -1.364139 | -0.001345 |
| H | -9.754141 | 0.895844 | 0.000815 |
| H | -2.677520 | -2.855516 | 0.000060 |
| H | -0.198433 | -3.130021 | -0.000250 |

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|---|-----------|-----------|-----------|
| H | 0.251230 | 1.136545 | -0.000890 |
| H | -2.233842 | 1.387634 | -0.000612 |
| H | 7.554081 | -0.922075 | 0.002483 |
| H | 6.087101 | -2.907795 | 0.002019 |
| H | 2.983214 | 2.193093 | -0.002187 |
| H | 4.514385 | 4.127929 | -0.001999 |
| H | 6.972942 | 3.778192 | -0.000023 |
| H | 7.879308 | 1.473389 | 0.001680 |
| H | 1.969407 | -2.148299 | -0.000615 |

15a

| | | | |
|---|-----------|-----------|-----------|
| C | -6.125196 | 1.760472 | 0.000031 |
| C | -5.788776 | 0.402190 | 0.000000 |
| C | -6.791086 | -0.584534 | -0.000036 |
| C | -8.120013 | -0.165299 | -0.000040 |
| C | -8.453289 | 1.182350 | -0.000011 |
| C | -7.451156 | 2.149965 | 0.000025 |
| N | -4.461194 | -0.066502 | 0.000003 |
| N | -3.582583 | 0.822747 | 0.000016 |
| C | -2.258043 | 0.350899 | 0.000018 |
| C | -1.894646 | -0.999339 | 0.000026 |
| C | -0.564763 | -1.384650 | 0.000027 |
| C | 0.426229 | -0.377481 | 0.000018 |
| C | 0.065644 | 0.974255 | 0.000010 |
| C | -1.265489 | 1.334426 | 0.000011 |
| N | 1.754451 | -0.814212 | 0.000018 |
| N | 2.651387 | 0.082792 | 0.000016 |
| C | 3.953127 | -0.350399 | 0.000015 |
| C | 4.976684 | 0.661292 | -0.000011 |
| C | 6.340173 | 0.266870 | -0.000022 |
| C | 6.655940 | -1.118455 | -0.000006 |
| C | 5.686473 | -2.077371 | 0.000021 |
| C | 4.320194 | -1.713581 | 0.000033 |
| C | 4.675311 | 2.037989 | -0.000029 |
| C | 5.680813 | 2.975944 | -0.000055 |
| C | 7.031137 | 2.586152 | -0.000065 |
| C | 7.350878 | 1.251309 | -0.000049 |
| O | 3.419062 | -2.677938 | 0.000065 |
| H | -8.906415 | -0.913960 | -0.000068 |
| C | -6.449852 | -2.045180 | -0.000069 |
| H | -5.320311 | 2.485466 | 0.000058 |
| H | -7.708737 | 3.203829 | 0.000050 |
| H | -9.496956 | 1.479741 | -0.000015 |
| H | -2.682119 | -1.743992 | 0.000033 |
| C | -0.189219 | -2.837176 | 0.000036 |
| H | 0.850505 | 1.719773 | 0.000004 |
| H | -1.571541 | 2.374667 | 0.000005 |
| H | 7.702101 | -1.410401 | -0.000014 |
| H | 5.923696 | -3.135073 | 0.000035 |
| H | 3.636286 | 2.341765 | -0.000021 |
| H | 5.427750 | 4.031236 | -0.000068 |
| H | 7.813360 | 3.337387 | -0.000086 |
| H | 8.388804 | 0.931964 | -0.000056 |
| H | 2.527481 | -2.203906 | 0.000080 |
| H | -1.083157 | -3.462968 | 0.000049 |
| H | 0.407665 | -3.096453 | -0.879806 |
| H | 0.407679 | -3.096437 | 0.879873 |
| H | -7.359042 | -2.650105 | -0.000090 |
| H | -5.855212 | -2.313334 | -0.877019 |
| H | -5.855224 | -2.313376 | 0.876876 |

15b

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|---|-----------|-----------|-----------|
| C | 6.661831 | -1.164213 | 0.000168 |
| C | 5.831182 | -0.036090 | 0.000086 |
| C | 6.400577 | 1.260862 | -0.000008 |
| C | 7.792114 | 1.340608 | -0.000012 |
| C | 8.607770 | 0.215406 | 0.000071 |
| C | 8.039833 | -1.052040 | 0.000161 |
| N | 4.470508 | -0.381129 | 0.000104 |
| N | 3.637733 | 0.552511 | 0.000031 |
| C | 2.292830 | 0.130248 | 0.000051 |
| C | 1.882406 | -1.205711 | 0.000141 |
| C | 0.539723 | -1.544907 | 0.000144 |
| C | -0.415424 | -0.504186 | 0.000055 |
| C | -0.007766 | 0.834010 | -0.000031 |
| C | 1.335312 | 1.147785 | -0.000033 |
| N | -1.757913 | -0.894785 | 0.000056 |
| N | -2.625123 | 0.030756 | -0.000014 |
| C | -3.940236 | -0.361885 | 0.000007 |
| C | -4.932480 | 0.680433 | -0.000139 |
| C | -6.307494 | 0.327567 | -0.000161 |
| C | -6.665580 | -1.047327 | -0.000034 |
| C | -5.725717 | -2.035115 | 0.000111 |
| C | -4.348893 | -1.713108 | 0.000140 |
| C | -4.589727 | 2.047476 | -0.000270 |
| C | -5.566414 | 3.015436 | -0.000411 |
| C | -6.928014 | 2.666726 | -0.000431 |
| C | -7.287841 | 1.342201 | -0.000308 |
| O | -3.478237 | -2.705065 | 0.000302 |
| H | 8.248740 | 2.326024 | -0.000083 |
| C | 5.610723 | 2.533656 | -0.000102 |
| H | 6.173408 | -2.132290 | 0.000237 |
| H | 8.662976 | -1.939453 | 0.000226 |
| H | 9.686461 | 0.333373 | 0.000063 |
| H | 2.644466 | -1.976237 | 0.000205 |
| C | 0.114349 | -2.983565 | 0.000239 |
| H | -0.766236 | 1.606438 | -0.000099 |
| H | 1.674684 | 2.177733 | -0.000103 |
| H | -7.720193 | -1.307048 | -0.000052 |
| H | -5.994844 | -3.085163 | 0.000215 |
| H | -3.541927 | 2.319519 | -0.000255 |
| H | -5.281484 | 4.062595 | -0.000509 |
| H | -7.687110 | 3.441329 | -0.000543 |
| H | -8.334948 | 1.054417 | -0.000322 |
| H | -2.572430 | -2.258198 | 0.000329 |
| H | 0.986224 | -3.639655 | 0.000303 |
| H | -0.491239 | -3.221942 | 0.880075 |
| H | -0.491205 | -3.222069 | -0.879585 |
| H | 6.288840 | 3.390744 | -0.000163 |
| H | 4.953450 | 2.596595 | -0.870469 |
| H | 4.953446 | 2.596722 | 0.870254 |

15c

| | | | |
|---|-----------|-----------|-----------|
| C | -6.191620 | 1.869718 | 0.000027 |
| C | -5.726526 | 0.548273 | -0.000087 |
| C | -6.649406 | -0.526337 | -0.000216 |
| C | -8.003681 | -0.196373 | -0.000223 |
| C | -8.455368 | 1.117889 | -0.000108 |
| C | -7.542478 | 2.164480 | 0.000019 |
| N | -4.324228 | 0.481170 | -0.000056 |
| N | -3.801541 | -0.655279 | -0.000133 |
| C | -2.391910 | -0.647904 | -0.000102 |

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|---|-----------|-----------|-----------|
| C | -1.603702 | 0.506695 | -0.000002 |
| C | -0.217858 | 0.464656 | 0.000026 |
| C | 0.398201 | -0.815679 | -0.000051 |
| C | -0.398393 | -1.969631 | -0.000151 |
| C | -1.775193 | -1.897376 | -0.000177 |
| N | 1.765512 | -1.101299 | -0.000043 |
| N | 2.596422 | -0.143830 | 0.000041 |
| C | 3.928168 | -0.493740 | 0.000060 |
| C | 4.880727 | 0.583796 | 0.000151 |
| C | 6.268760 | 0.283424 | 0.000172 |
| C | 6.678815 | -1.076359 | 0.000102 |
| C | 5.775811 | -2.097488 | 0.000015 |
| C | 4.387521 | -1.827366 | -0.000006 |
| C | 4.488104 | 1.938039 | 0.000220 |
| C | 5.428013 | 2.941856 | 0.000306 |
| C | 6.801781 | 2.644421 | 0.000328 |
| C | 7.210223 | 1.334177 | 0.000261 |
| O | 3.558456 | -2.855015 | -0.000089 |
| H | -8.728125 | -1.005509 | -0.000322 |
| C | -6.265918 | -1.974312 | -0.000348 |
| H | -5.442032 | 2.653179 | 0.000122 |
| H | -7.879612 | 3.195060 | 0.000109 |
| H | -9.521565 | 1.319641 | -0.000118 |
| H | -2.111849 | 1.464235 | 0.000054 |
| C | 0.532358 | 1.762332 | 0.000136 |
| H | 0.103788 | -2.930884 | -0.000208 |
| H | -2.391796 | -2.788827 | -0.000254 |
| H | 7.742401 | -1.296280 | 0.000118 |
| H | 6.082794 | -3.137130 | -0.000038 |
| H | 3.431528 | 2.172522 | 0.000203 |
| H | 5.103991 | 3.977629 | 0.000359 |
| H | 7.531471 | 3.446788 | 0.000396 |
| H | 8.267310 | 1.085437 | 0.000276 |
| H | 2.637302 | -2.447031 | -0.000087 |
| H | -0.174369 | 2.595110 | 0.000179 |
| H | 1.182717 | 1.848316 | 0.874364 |
| H | 1.182757 | 1.848441 | -0.874051 |
| H | -7.164676 | -2.596096 | -0.000438 |
| H | -5.655684 | -2.226398 | -0.870743 |
| H | -5.655739 | -2.226571 | 0.870036 |

15d

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|---|-----------|-----------|-----------|
| C | -6.495383 | -1.085446 | -0.000099 |
| C | -5.772419 | 0.112652 | -0.000006 |
| C | -6.437845 | 1.351721 | 0.000081 |
| C | -7.831448 | 1.343605 | 0.000073 |
| C | -8.548273 | 0.154804 | -0.000019 |
| C | -7.877140 | -1.065869 | -0.000106 |
| N | -4.365532 | 0.166778 | 0.000007 |
| N | -3.790106 | -0.942813 | -0.000077 |
| C | -2.384919 | -0.885065 | -0.000067 |
| C | -1.636837 | 0.296556 | 0.000025 |
| C | -0.250716 | 0.302366 | 0.000030 |
| C | 0.409203 | -0.956437 | -0.000063 |
| C | -0.346987 | -2.137256 | -0.000155 |
| C | -1.725461 | -2.112582 | -0.000158 |
| N | 1.785568 | -1.194142 | -0.000075 |
| N | 2.581760 | -0.207379 | 0.000011 |
| C | 3.925041 | -0.508210 | -0.000018 |
| C | 4.837442 | 0.603729 | 0.000058 |
| C | 6.235493 | 0.354397 | 0.000027 |

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|---|-----------|-----------|-----------|
| C | 6.695204 | -0.989464 | -0.000078 |
| C | 5.830476 | -2.043183 | -0.000150 |
| C | 4.433252 | -1.824210 | -0.000121 |
| C | 4.395244 | 1.942527 | 0.000161 |
| C | 5.297618 | 2.980217 | 0.000231 |
| C | 6.681323 | 2.733314 | 0.000202 |
| C | 7.137760 | 1.438963 | 0.000101 |
| O | 3.642390 | -2.881365 | -0.000189 |
| H | -8.361732 | 2.291110 | 0.000139 |
| C | -5.680368 | 2.646334 | 0.000182 |
| H | -5.940736 | -2.015907 | -0.000164 |
| H | -8.434574 | -1.996553 | -0.000177 |
| H | -9.633174 | 0.179504 | -0.000024 |
| H | -2.176784 | 1.236597 | 0.000094 |
| C | 0.454182 | 1.625192 | 0.000131 |
| H | 0.188131 | -3.080540 | -0.000224 |
| H | -2.312982 | -3.023360 | -0.000228 |
| H | 7.766168 | -1.169989 | -0.000100 |
| H | 6.175423 | -3.070832 | -0.000229 |
| H | 3.330771 | 2.137684 | 0.000184 |
| H | 4.935929 | 4.003431 | 0.000311 |
| H | 7.381084 | 3.561920 | 0.000258 |
| H | 8.203279 | 1.229269 | 0.000077 |
| H | 2.706803 | -2.508019 | -0.000143 |
| H | -0.280700 | 2.433310 | 0.000184 |
| H | 1.101146 | 1.733623 | 0.874357 |
| H | 1.101161 | 1.733751 | -0.874068 |
| H | -6.370436 | 3.492676 | 0.000239 |
| H | -5.033198 | 2.727034 | 0.877206 |
| H | -5.033186 | 2.727163 | -0.876822 |

15e

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|---|-----------|-----------|-----------|
| C | 7.430651 | -0.772192 | -0.000144 |
| C | 6.345036 | 0.128881 | -0.000113 |
| C | 5.016397 | -0.372102 | -0.000125 |
| C | 4.826634 | -1.769253 | -0.000168 |
| C | 5.903666 | -2.624259 | -0.000198 |
| C | 7.218735 | -2.128267 | -0.000186 |
| C | 6.550677 | 1.534307 | -0.000070 |
| C | 5.507597 | 2.411989 | -0.000041 |
| C | 4.174158 | 1.940847 | -0.000052 |
| C | 3.915879 | 0.554008 | -0.000093 |
| N | 2.650908 | 0.011845 | -0.000100 |
| N | 1.685893 | 0.834526 | -0.000072 |
| C | 0.378752 | 0.342422 | -0.000054 |
| C | -0.030385 | -1.012367 | -0.000057 |
| C | -1.399103 | -1.256707 | -0.000027 |
| C | -2.354160 | -0.241130 | 0.000005 |
| C | -1.937741 | 1.093633 | 0.000004 |
| C | -0.589767 | 1.363649 | -0.000025 |
| N | -3.693987 | -0.667990 | 0.000040 |
| N | -4.537410 | 0.254669 | 0.000090 |
| C | -5.882327 | -0.161116 | 0.000137 |
| C | -6.271279 | -1.505200 | 0.000096 |
| C | -7.611351 | -1.842676 | 0.000151 |
| C | -8.574830 | -0.836512 | 0.000248 |
| C | -8.189428 | 0.497130 | 0.000287 |
| C | -6.845092 | 0.864386 | 0.000232 |
| C | -6.446246 | 2.310287 | 0.000279 |
| C | 0.902910 | -2.184395 | -0.000087 |
| O | 3.202298 | 2.834507 | -0.000023 |

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|---|-----------|-----------|-----------|
| H | -8.946155 | 1.275747 | 0.000362 |
| H | -5.495486 | -2.261195 | 0.000022 |
| H | -7.910040 | -2.885613 | 0.000119 |
| H | -9.629322 | -1.092848 | 0.000292 |
| H | -1.761537 | -2.279844 | -0.000025 |
| H | -0.235524 | 2.389183 | -0.000026 |
| H | -2.678082 | 1.883282 | 0.000027 |
| H | 7.570441 | 1.907974 | -0.000062 |
| H | 5.658714 | 3.485391 | -0.000009 |
| H | 3.816055 | -2.156281 | -0.000176 |
| H | 5.735394 | -3.696387 | -0.000231 |
| H | 8.058309 | -2.814841 | -0.000210 |
| H | 8.439823 | -0.371053 | -0.000135 |
| H | 2.351141 | 2.295945 | -0.000039 |
| H | 0.328559 | -3.113583 | -0.000083 |
| H | 1.559094 | -2.172790 | -0.874197 |
| H | 1.559132 | -2.172806 | 0.873994 |
| H | -7.330446 | 2.951119 | 0.000351 |
| H | -5.841249 | 2.554470 | 0.877121 |
| H | -5.841333 | 2.554550 | -0.876599 |

15f

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|---|-----------|-----------|-----------|
| C | -7.380138 | 0.883655 | -0.000150 |
| C | -6.328652 | -0.057159 | -0.000141 |
| C | -4.982395 | 0.394126 | -0.000118 |
| C | -4.741139 | 1.783416 | -0.000104 |
| C | -5.785592 | 2.677772 | -0.000113 |
| C | -7.118141 | 2.230976 | -0.000136 |
| C | -6.585648 | -1.454133 | -0.000155 |
| C | -5.575300 | -2.369437 | -0.000147 |
| C | -4.225407 | -1.947669 | -0.000125 |
| C | -3.916709 | -0.571567 | -0.000108 |
| N | -2.632725 | -0.075207 | -0.000074 |
| N | -1.697741 | -0.931511 | -0.000059 |
| C | -0.373890 | -0.485078 | -0.000027 |
| C | 0.081820 | 0.854840 | 0.000002 |
| C | 1.458085 | 1.052285 | 0.000041 |
| C | 2.377799 | 0.004808 | 0.000050 |
| C | 1.915811 | -1.314288 | 0.000019 |
| C | 0.559044 | -1.538313 | -0.000018 |
| N | 3.735177 | 0.384718 | 0.000094 |
| N | 4.534932 | -0.577299 | 0.000097 |
| C | 5.906572 | -0.278590 | 0.000140 |
| C | 6.698588 | -1.434155 | 0.000149 |
| C | 8.079627 | -1.368378 | 0.000191 |
| C | 8.689685 | -0.120730 | 0.000225 |
| C | 7.912457 | 1.031375 | 0.000215 |
| C | 6.519050 | 0.998600 | 0.000174 |
| C | 5.773118 | 2.297639 | 0.000167 |
| C | -0.810303 | 2.058518 | -0.000004 |
| O | -3.286801 | -2.876516 | -0.000122 |
| H | 8.402390 | 2.000666 | 0.000242 |
| H | 6.177628 | -2.385101 | 0.000121 |
| H | 8.672537 | -2.276233 | 0.000198 |
| H | 9.771722 | -0.038994 | 0.000258 |
| H | 1.852534 | 2.063555 | 0.000065 |
| H | 0.170389 | -2.551313 | -0.000040 |
| H | 2.629884 | -2.127686 | 0.000026 |
| H | -7.618318 | -1.790580 | -0.000172 |
| H | -5.765779 | -3.436575 | -0.000159 |
| H | -3.717044 | 2.133109 | -0.000087 |

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|---|-----------|-----------|-----------|
| H | -5.577583 | 3.742911 | -0.000102 |
| H | -7.931760 | 2.948109 | -0.000142 |
| H | -8.403471 | 0.520101 | -0.000167 |
| H | -2.416593 | -2.370171 | -0.000110 |
| H | -0.204092 | 2.967343 | 0.000028 |
| H | -1.466483 | 2.069803 | -0.874099 |
| H | -1.466534 | 2.069774 | 0.874052 |
| H | 6.480199 | 3.130956 | 0.000198 |
| H | 5.118633 | 2.383247 | -0.870354 |
| H | 5.118580 | 2.383226 | 0.870650 |

15g

| | | | |
|---|-----------|-----------|-----------|
| C | 7.018419 | 1.833625 | 0.000051 |
| C | 6.173960 | 0.703316 | 0.000051 |
| C | 4.765510 | 0.880181 | 0.000030 |
| C | 4.252586 | 2.192971 | 0.000013 |
| C | 5.099213 | 3.276394 | 0.000013 |
| C | 6.493956 | 3.102012 | 0.000031 |
| C | 6.702430 | -0.615473 | 0.000071 |
| C | 5.894459 | -1.713864 | 0.000071 |
| C | 4.488212 | -1.567666 | 0.000049 |
| C | 3.912664 | -0.278880 | 0.000029 |
| N | 2.558688 | -0.053946 | 0.000012 |
| N | 1.812941 | -1.079873 | 0.000022 |
| C | 0.433043 | -0.856209 | 0.000007 |
| C | -0.387244 | -1.999457 | 0.000008 |
| C | -1.763422 | -1.810390 | -0.000015 |
| C | -2.330248 | -0.537125 | -0.000036 |
| C | -1.499597 | 0.591927 | -0.000033 |
| C | -0.134385 | 0.428179 | -0.000013 |
| N | -3.738862 | -0.495747 | -0.000064 |
| N | -4.217496 | 0.660284 | -0.000060 |
| C | -5.615974 | 0.783042 | -0.000054 |
| C | -6.027617 | 2.122104 | -0.000050 |
| C | -7.365576 | 2.470853 | -0.000043 |
| C | -8.319942 | 1.461894 | -0.000038 |
| C | -7.921440 | 0.130520 | -0.000039 |
| C | -6.581481 | -0.253304 | -0.000046 |
| C | -6.256081 | -1.715566 | -0.000044 |
| C | 0.197998 | -3.380420 | 0.000031 |
| O | 3.748927 | -2.661535 | 0.000043 |
| H | -8.677667 | -0.648975 | -0.000033 |
| H | -5.246916 | 2.874544 | -0.000053 |
| H | -7.661026 | 3.514180 | -0.000042 |
| H | -9.377121 | 1.706608 | -0.000033 |
| H | -2.433370 | -2.664193 | -0.000017 |
| H | 0.531415 | 1.282224 | -0.000012 |
| H | -1.953477 | 1.574960 | -0.000049 |
| H | 7.781357 | -0.740074 | 0.000087 |
| H | 6.293585 | -2.721679 | 0.000086 |
| H | 3.178792 | 2.329952 | -0.000002 |
| H | 4.684683 | 4.279304 | -0.000002 |
| H | 7.149254 | 3.966247 | 0.000031 |
| H | 8.093514 | 1.680485 | 0.000066 |
| H | 2.794531 | -2.333054 | 0.000015 |
| H | -0.593403 | -4.131885 | 0.000030 |
| H | 0.826490 | -3.549280 | -0.879803 |
| H | 0.826468 | -3.549260 | 0.879885 |
| H | -7.179023 | -2.300932 | -0.000035 |
| H | -5.656544 | -1.991951 | -0.870492 |
| H | -5.656530 | -1.991948 | 0.870395 |

15h

| | | | |
|---|-----------|-----------|-----------|
| C | -6.926483 | 1.931729 | -0.000029 |
| C | -6.121991 | 0.772688 | -0.000069 |
| C | -4.708333 | 0.900077 | -0.000047 |
| C | -4.149941 | 2.194124 | 0.000019 |
| C | -4.958230 | 3.306529 | 0.000058 |
| C | -6.358114 | 3.181114 | 0.000033 |
| C | -6.696271 | -0.526925 | -0.000130 |
| C | -5.927336 | -1.652974 | -0.000170 |
| C | -4.516789 | -1.556247 | -0.000153 |
| C | -3.896434 | -0.288167 | -0.000086 |
| N | -2.535716 | -0.111095 | -0.000044 |
| N | -1.826614 | -1.163008 | -0.000022 |
| C | -0.439966 | -0.988953 | 0.000002 |
| C | 0.338743 | -2.161009 | 0.000031 |
| C | 1.720628 | -2.021367 | 0.000052 |
| C | 2.332598 | -0.769012 | 0.000044 |
| C | 1.542797 | 0.389689 | 0.000017 |
| C | 0.172899 | 0.274856 | -0.000004 |
| N | 3.738339 | -0.780968 | 0.000066 |
| N | 4.273749 | 0.348824 | 0.000054 |
| C | 5.681602 | 0.346135 | 0.000074 |
| C | 6.448836 | -0.824016 | 0.000111 |
| C | 7.828957 | -0.752985 | 0.000130 |
| C | 8.454176 | 0.491836 | 0.000111 |
| C | 7.693432 | 1.653052 | 0.000074 |
| C | 6.300566 | 1.609123 | 0.000055 |
| C | 5.495199 | 2.874517 | 0.000015 |
| C | -0.295957 | -3.519855 | 0.000038 |
| O | -3.816375 | -2.675066 | -0.000210 |
| H | 8.187852 | 2.619774 | 0.000060 |
| H | 5.929198 | -1.774492 | 0.000125 |
| H | 8.420757 | -1.662229 | 0.000159 |
| H | 9.537413 | 0.557020 | 0.000126 |
| H | 2.361633 | -2.896981 | 0.000074 |
| H | -0.462216 | 1.151947 | -0.000027 |
| H | 2.030603 | 1.356438 | 0.000011 |
| H | -7.778894 | -0.613795 | -0.000147 |
| H | -6.361648 | -2.646128 | -0.000221 |
| H | -3.072039 | 2.293858 | 0.000039 |
| H | -4.508801 | 4.294295 | 0.000108 |
| H | -6.982823 | 4.067699 | 0.000064 |
| H | -8.006254 | 1.816189 | -0.000048 |
| H | -2.850830 | -2.380070 | -0.000219 |
| H | 0.467739 | -4.299412 | 0.000060 |
| H | -0.930111 | -3.665826 | 0.879895 |
| H | -0.930085 | -3.665848 | -0.879834 |
| H | 6.153178 | 3.746090 | 0.000006 |
| H | 4.845263 | 2.930973 | -0.876862 |
| H | 4.845236 | 2.931012 | 0.876870 |

15i

| | | | |
|---|----------|-----------|-----------|
| C | 7.379795 | 1.213829 | 0.000024 |
| C | 6.356568 | 0.254539 | -0.000003 |
| C | 5.007211 | 0.669931 | -0.000004 |
| C | 4.726290 | 2.042326 | 0.000023 |
| C | 5.748429 | 2.972231 | 0.000050 |
| C | 7.084267 | 2.561929 | 0.000050 |
| C | 6.662297 | -1.151673 | -0.000029 |
| C | 5.707833 | -2.106848 | -0.000057 |

| | | | |
|---|-----------|-----------|-----------|
| C | 4.300858 | -1.768051 | -0.000062 |
| C | 3.956099 | -0.340343 | -0.000032 |
| N | 2.709229 | 0.094876 | -0.000024 |
| N | 1.738004 | -0.765957 | 0.000002 |
| C | 0.407486 | -0.367361 | 0.000000 |
| C | -0.577000 | -1.380125 | 0.000045 |
| C | -1.905234 | -0.995306 | 0.000044 |
| C | -2.274905 | 0.354301 | 0.000000 |
| C | -1.282858 | 1.336220 | -0.000043 |
| C | 0.051400 | 0.982362 | -0.000044 |
| N | -3.599038 | 0.820969 | 0.000000 |
| N | -4.477015 | -0.069340 | 0.000021 |
| C | -5.805228 | 0.399527 | 0.000008 |
| C | -6.142335 | 1.757432 | -0.000012 |
| C | -7.468531 | 2.146965 | -0.000025 |
| C | -8.470864 | 1.179795 | -0.000018 |
| C | -8.136884 | -0.167690 | 0.000003 |
| C | -6.807837 | -0.586624 | 0.000016 |
| C | -6.466469 | -2.047356 | 0.000037 |
| C | -0.189711 | -2.830185 | 0.000094 |
| O | 3.423858 | -2.653038 | -0.000098 |
| H | -8.922965 | -0.916779 | 0.000009 |
| H | -5.337740 | 2.482763 | -0.000017 |
| H | -7.725830 | 3.200958 | -0.000041 |
| H | -9.514562 | 1.477065 | -0.000028 |
| H | -2.689896 | -1.743069 | 0.000078 |
| H | 0.832881 | 1.730907 | -0.000077 |
| H | -1.588117 | 2.376553 | -0.000075 |
| H | 7.711099 | -1.437687 | -0.000029 |
| H | 5.946945 | -3.164330 | -0.000081 |
| H | 3.691695 | 2.362670 | 0.000022 |
| H | 5.508972 | 4.030564 | 0.000071 |
| H | 7.881665 | 3.296933 | 0.000071 |
| H | 8.412497 | 0.877873 | 0.000025 |
| H | 2.021239 | -1.763505 | 0.000038 |
| H | -1.078576 | -3.462013 | 0.000127 |
| H | 0.408242 | -3.091871 | -0.879949 |
| H | 0.408262 | -3.091806 | 0.880142 |
| H | -7.375555 | -2.652549 | 0.000045 |
| H | -5.871717 | -2.315587 | -0.876876 |
| H | -5.871719 | -2.315562 | 0.876960 |

15j

| | | | |
|---|-----------|-----------|-----------|
| C | -7.315837 | 1.308437 | -0.000266 |
| C | -6.323449 | 0.317218 | -0.000151 |
| C | -4.961447 | 0.689700 | -0.000149 |
| C | -4.637582 | 2.052679 | -0.000263 |
| C | -5.629880 | 3.014336 | -0.000375 |
| C | -6.978128 | 2.646474 | -0.000377 |
| C | -6.673699 | -1.078381 | -0.000035 |
| C | -5.749766 | -2.063084 | 0.000078 |
| C | -4.332792 | -1.768827 | 0.000091 |
| C | -3.942970 | -0.353261 | -0.000027 |
| N | -2.682203 | 0.041736 | -0.000034 |
| N | -1.740361 | -0.850524 | 0.000049 |
| C | -0.396623 | -0.497693 | 0.000047 |
| C | 0.552496 | -1.543051 | 0.000147 |
| C | 1.893320 | -1.203277 | 0.000146 |
| C | 2.309014 | 0.132133 | 0.000051 |
| C | 1.351314 | 1.147293 | -0.000048 |
| C | 0.005526 | 0.838852 | -0.000050 |

| | | | |
|---|-----------|-----------|-----------|
| N | 3.653080 | 0.550373 | 0.000046 |
| N | 4.485811 | -0.383601 | 0.000134 |
| C | 5.846946 | -0.037746 | 0.000109 |
| C | 6.678705 | -1.164831 | 0.000228 |
| C | 8.056797 | -1.051913 | 0.000228 |
| C | 8.624499 | 0.215553 | 0.000107 |
| C | 7.807735 | 1.339851 | -0.000012 |
| C | 6.416135 | 1.259098 | -0.000015 |
| C | 5.625941 | 2.532018 | -0.000149 |
| C | 0.116682 | -2.979323 | 0.000251 |
| O | -3.484605 | -2.681776 | 0.000195 |
| H | 8.263360 | 2.325797 | -0.000107 |
| H | 6.191150 | -2.133375 | 0.000321 |
| H | 8.680178 | -1.939223 | 0.000322 |
| H | 9.703114 | 0.334166 | 0.000104 |
| H | 2.653082 | -1.976226 | 0.000222 |
| H | -0.749989 | 1.613676 | -0.000127 |
| H | 1.689027 | 2.177638 | -0.000123 |
| H | -7.731039 | -1.330985 | -0.000041 |
| H | -6.021988 | -3.112538 | 0.000164 |
| H | -3.593368 | 2.340191 | -0.000260 |
| H | -5.357074 | 4.064591 | -0.000462 |
| H | -7.751900 | 3.406310 | -0.000465 |
| H | -8.358604 | 1.005191 | -0.000266 |
| H | -2.057084 | -1.838272 | 0.000118 |
| H | 0.984025 | -3.640318 | 0.000317 |
| H | -0.489760 | -3.220660 | 0.880288 |
| H | -0.489731 | -3.220797 | -0.879768 |
| H | 6.304038 | 3.389211 | -0.000230 |
| H | 4.968749 | 2.595116 | -0.870562 |
| H | 4.968736 | 2.595291 | 0.870241 |

15k

| | | | |
|---|-----------|-----------|-----------|
| C | 7.251717 | 1.282105 | 0.000214 |
| C | 6.289993 | 0.261178 | 0.000157 |
| C | 4.916589 | 0.591541 | 0.000139 |
| C | 4.552449 | 1.944971 | 0.000176 |
| C | 5.515495 | 2.936117 | 0.000231 |
| C | 6.874347 | 2.609414 | 0.000251 |
| C | 6.682735 | -1.122613 | 0.000117 |
| C | 5.788617 | -2.134264 | 0.000062 |
| C | 4.363079 | -1.883010 | 0.000041 |
| C | 3.931129 | -0.481265 | 0.000080 |
| N | 2.656988 | -0.120430 | 0.000064 |
| N | 1.745822 | -1.041841 | -0.000030 |
| C | 0.376822 | -0.802540 | -0.000044 |
| C | -0.234049 | 0.474207 | 0.000056 |
| C | -1.620127 | 0.512765 | 0.000024 |
| C | -2.408887 | -0.640638 | -0.000100 |
| C | -1.786343 | -1.887574 | -0.000198 |
| C | -0.410245 | -1.962452 | -0.000169 |
| N | -3.816504 | -0.649860 | -0.000135 |
| N | -4.342747 | 0.485295 | -0.000031 |
| C | -5.745673 | 0.548116 | -0.000080 |
| C | -6.215456 | 1.867809 | 0.000065 |
| C | -7.567302 | 2.158540 | 0.000047 |
| C | -8.477348 | 1.109561 | -0.000120 |
| C | -8.021095 | -0.203054 | -0.000266 |
| C | -6.665659 | -0.528752 | -0.000251 |
| C | -6.278084 | -1.975831 | -0.000417 |
| C | 0.522789 | 1.769943 | 0.000193 |

| | | | |
|---|-----------|-----------|-----------|
| O | 3.544534 | -2.823159 | -0.000002 |
| H | -8.742792 | -1.014710 | -0.000396 |
| H | -5.468478 | 2.653796 | 0.000193 |
| H | -7.907268 | 3.188244 | 0.000162 |
| H | -9.544155 | 1.308039 | -0.000139 |
| H | -2.127753 | 1.470551 | 0.000099 |
| H | 0.083484 | -2.929343 | -0.000244 |
| H | -2.399123 | -2.781654 | -0.000296 |
| H | 7.747262 | -1.342933 | 0.000133 |
| H | 6.091715 | -3.175254 | 0.000033 |
| H | 3.500541 | 2.202453 | 0.000161 |
| H | 5.210957 | 3.977671 | 0.000260 |
| H | 7.624814 | 3.392265 | 0.000294 |
| H | 8.303131 | 1.010275 | 0.000228 |
| H | 2.103790 | -2.018511 | -0.000110 |
| H | -0.182398 | 2.603451 | 0.000252 |
| H | 1.170941 | 1.858051 | 0.875815 |
| H | 1.170986 | 1.858211 | -0.875380 |
| H | -7.175150 | -2.600133 | -0.000534 |
| H | -5.667285 | -2.226385 | -0.870868 |
| H | -5.667358 | -2.226605 | 0.870022 |

151

| | | | |
|---|-----------|-----------|-----------|
| C | 7.187492 | 1.378826 | 0.000188 |
| C | 6.260641 | 0.326260 | 0.000062 |
| C | 4.876878 | 0.610344 | 0.000073 |
| C | 4.467363 | 1.950673 | 0.000211 |
| C | 5.396614 | 2.973654 | 0.000334 |
| C | 6.765634 | 2.692687 | 0.000323 |
| C | 6.700179 | -1.043432 | -0.000078 |
| C | 5.841091 | -2.084851 | -0.000203 |
| C | 4.407950 | -1.882053 | -0.000203 |
| C | 3.928158 | -0.495394 | -0.000058 |
| N | 2.642719 | -0.178281 | -0.000033 |
| N | 1.763157 | -1.130499 | -0.000086 |
| C | 0.387188 | -0.938391 | -0.000076 |
| C | -0.267316 | 0.317042 | -0.000025 |
| C | -1.653590 | 0.307934 | -0.000018 |
| C | -2.402240 | -0.872606 | -0.000058 |
| C | -1.736980 | -2.097488 | -0.000108 |
| C | -0.359335 | -2.124914 | -0.000117 |
| N | -3.805061 | -0.933107 | -0.000048 |
| N | -4.385582 | 0.174251 | 0.000001 |
| C | -5.792695 | 0.112638 | 0.000007 |
| C | -6.509811 | -1.088787 | -0.000031 |
| C | -7.891867 | -1.076552 | -0.000021 |
| C | -8.569860 | 0.140134 | 0.000027 |
| C | -7.858821 | 1.332426 | 0.000065 |
| C | -6.465259 | 1.347712 | 0.000057 |
| C | -5.714553 | 2.646323 | 0.000099 |
| C | 0.445292 | 1.637650 | 0.000022 |
| O | 3.621889 | -2.849251 | -0.000326 |
| H | -8.393780 | 2.277365 | 0.000104 |
| H | -5.950635 | -2.016534 | -0.000068 |
| H | -8.444067 | -2.010414 | -0.000050 |
| H | -9.654873 | 0.159120 | 0.000036 |
| H | -2.192936 | 1.248297 | 0.000021 |
| H | 0.167568 | -3.074123 | -0.000155 |
| H | -2.320751 | -3.010665 | -0.000139 |
| H | 7.771598 | -1.227224 | -0.000083 |
| H | 6.179215 | -3.114973 | -0.000310 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.407369 | 2.172363 | 0.000220 |
| H | 5.057377 | 4.004417 | 0.000440 |
| H | 7.489371 | 3.500319 | 0.000421 |
| H | 8.247455 | 1.142571 | 0.000178 |
| H | 2.153709 | -2.094484 | -0.000119 |
| H | -0.287313 | 2.447213 | 0.000054 |
| H | 1.090171 | 1.747492 | 0.875588 |
| H | 1.090166 | 1.747556 | -0.875541 |
| H | -6.408914 | 3.489217 | 0.000134 |
| H | -5.067697 | 2.730435 | 0.877089 |
| H | -5.067707 | 2.730498 | -0.876891 |

15m

| | | | |
|---|-----------|-----------|-----------|
| C | -6.859204 | 0.871773 | 0.000216 |
| C | -5.898783 | -0.155777 | 0.000125 |
| C | -6.291877 | -1.498476 | 0.000073 |
| C | -7.633041 | -1.832463 | 0.000113 |
| C | -8.594101 | -0.824211 | 0.000205 |
| C | -8.204588 | 0.508256 | 0.000255 |
| N | -4.552356 | 0.256566 | 0.000090 |
| N | -3.711845 | -0.669270 | 0.000054 |
| C | -2.371726 | -0.250831 | 0.000027 |
| C | -1.418356 | -1.266949 | 0.000018 |
| C | -0.048367 | -1.028230 | -0.000005 |
| C | 0.358677 | 0.321413 | -0.000022 |
| C | -0.599378 | 1.352000 | -0.000015 |
| C | -1.946475 | 1.081779 | 0.000009 |
| N | 1.674346 | 0.767839 | -0.000047 |
| N | 2.713578 | -0.007132 | -0.000059 |
| C | 3.919887 | 0.537611 | -0.000069 |
| C | 5.052727 | -0.378529 | -0.000131 |
| C | 6.362197 | 0.150978 | -0.000155 |
| C | 6.546620 | 1.577729 | -0.000117 |
| C | 5.513457 | 2.446837 | -0.000057 |
| C | 4.140519 | 1.988334 | -0.000024 |
| C | 4.891855 | -1.770782 | -0.000168 |
| C | 5.990605 | -2.609058 | -0.000227 |
| C | 7.286248 | -2.085274 | -0.000251 |
| C | 7.464000 | -0.716767 | -0.000215 |
| O | 3.191807 | 2.796403 | 0.000041 |
| C | 0.889779 | -2.198830 | -0.000008 |
| C | -6.456485 | 2.316690 | 0.000273 |
| H | -8.958986 | 1.289204 | 0.000327 |
| H | -5.518370 | -2.256823 | 0.000002 |
| H | -7.934192 | -2.874748 | 0.000072 |
| H | -9.649283 | -1.077680 | 0.000237 |
| H | -1.781335 | -2.289764 | 0.000032 |
| H | -0.252221 | 2.381202 | -0.000030 |
| H | -2.682840 | 1.875239 | 0.000015 |
| H | 7.567154 | 1.952201 | -0.000137 |
| H | 5.660027 | 3.521066 | -0.000025 |
| H | 3.889419 | -2.180322 | -0.000149 |
| H | 5.843311 | -3.684157 | -0.000255 |
| H | 8.143983 | -2.748902 | -0.000298 |
| H | 8.463914 | -0.293061 | -0.000233 |
| H | 1.880545 | 1.786886 | -0.000073 |
| H | 0.315733 | -3.127682 | 0.000008 |
| H | 1.543971 | -2.191005 | -0.875589 |
| H | 1.543995 | -2.190990 | 0.875554 |
| H | -7.338904 | 2.960048 | 0.000338 |
| H | -5.850754 | 2.559299 | 0.877096 |

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| C | 8.092318 | -1.379692 | 0.000208 |
| C | 8.706988 | -0.134387 | 0.000239 |
| C | 7.933168 | 1.019927 | 0.000224 |
| N | 4.549249 | -0.577289 | 0.000097 |
| N | 3.752514 | 0.387655 | 0.000091 |
| C | 2.395035 | 0.015809 | 0.000048 |
| C | 1.476547 | 1.063247 | 0.000048 |
| C | 0.099178 | 0.870645 | 0.000009 |
| C | -0.353464 | -0.464366 | -0.000032 |
| C | 0.569189 | -1.526042 | -0.000034 |
| C | 1.924970 | -1.301059 | 0.000005 |
| N | -1.684280 | -0.865475 | -0.000072 |
| N | -2.695345 | -0.054698 | -0.000078 |
| C | -3.920555 | -0.555896 | -0.000109 |
| C | -5.019205 | 0.400684 | -0.000119 |
| C | -6.347084 | -0.080534 | -0.000147 |
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| C | -7.416517 | 0.826930 | -0.000156 |
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| C | -0.798560 | 2.072393 | 0.000015 |
| C | 5.798166 | 2.293493 | 0.000164 |
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| 15o | | | |
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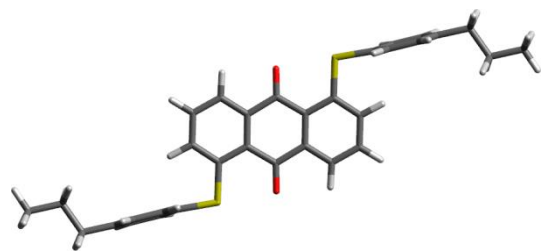
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| C | 3.915008 | -0.271539 | 0.000050 |
| C | 4.798524 | 0.887971 | 0.000032 |
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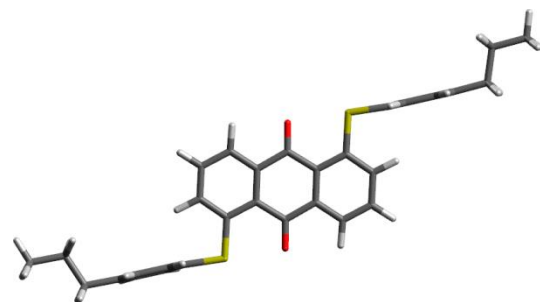
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| H | 0.468846 | -4.296314 | -0.000047 |
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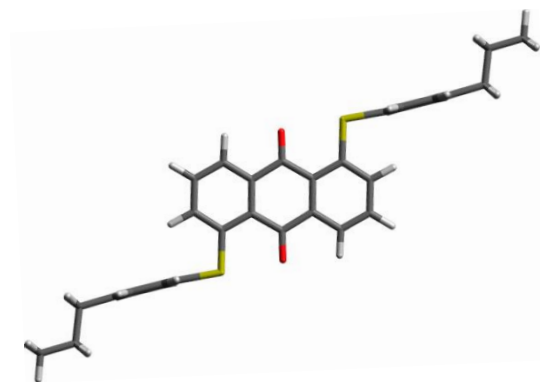
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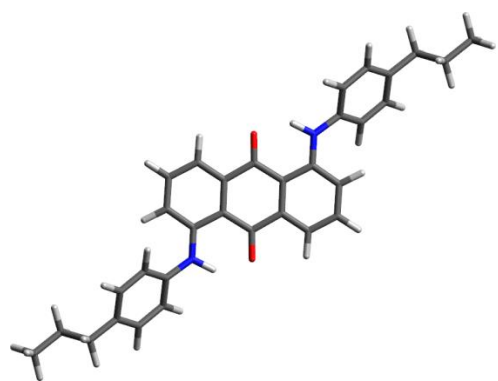
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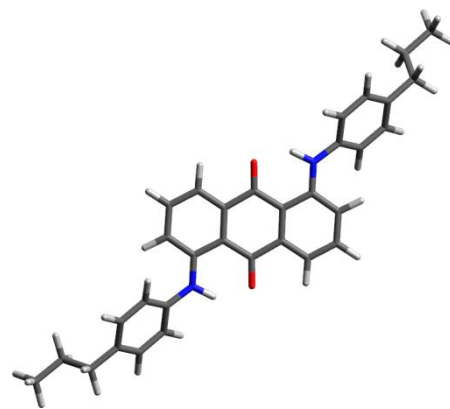
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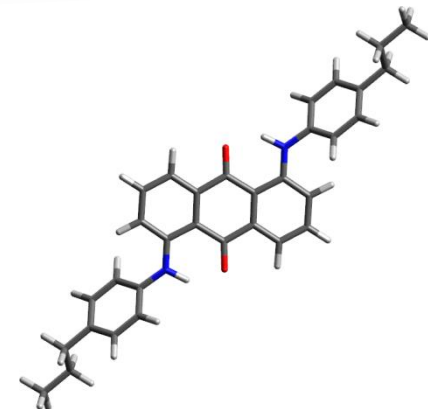
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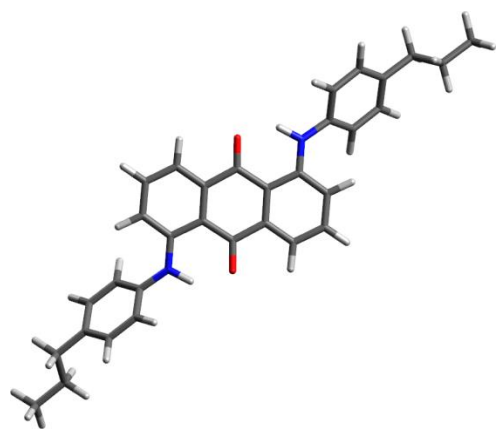
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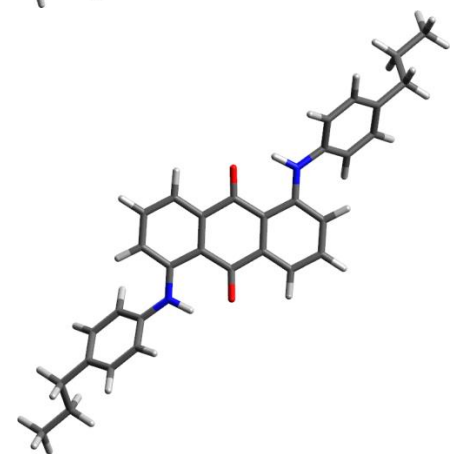
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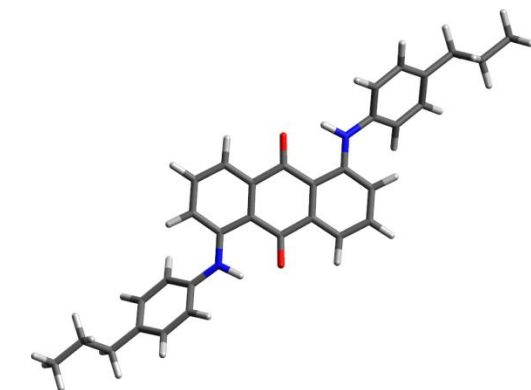
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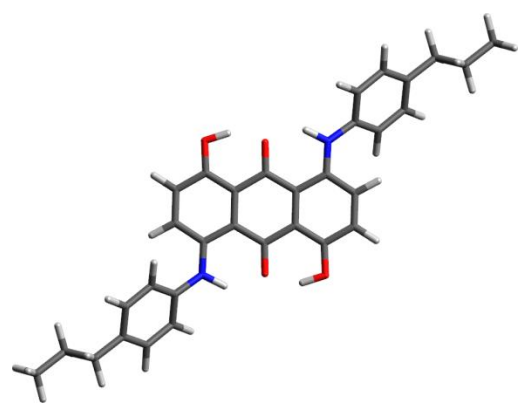
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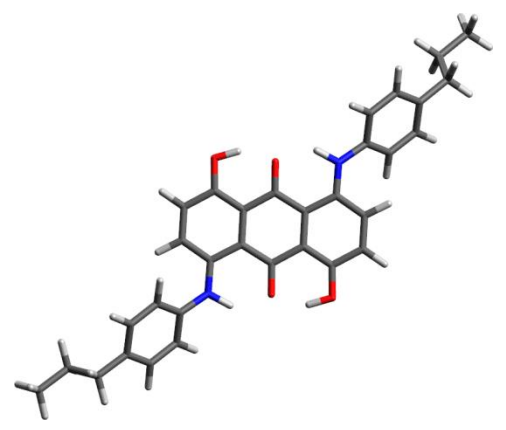
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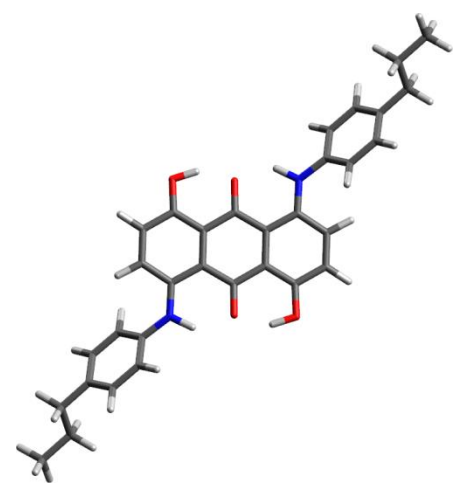
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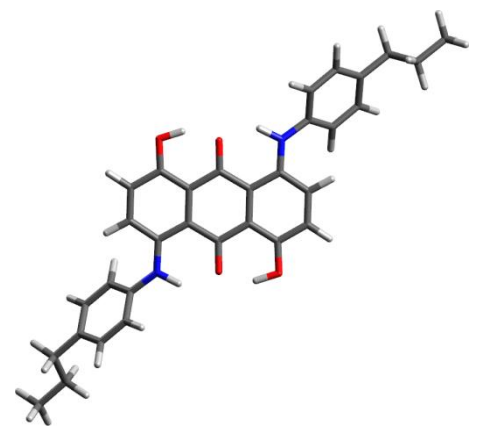
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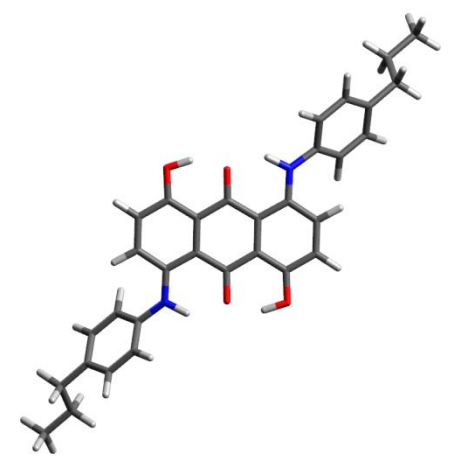
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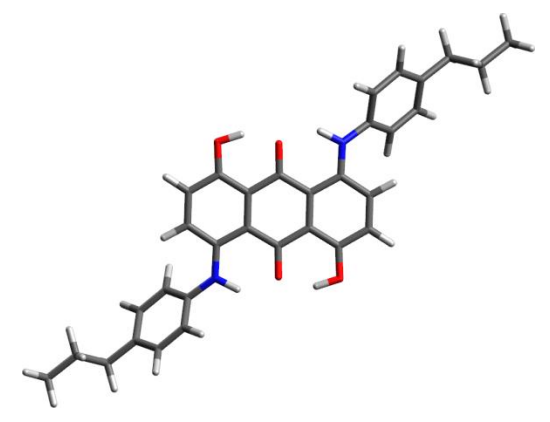
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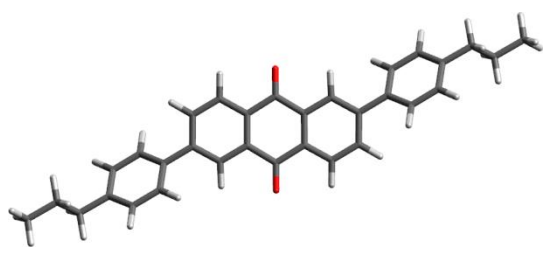
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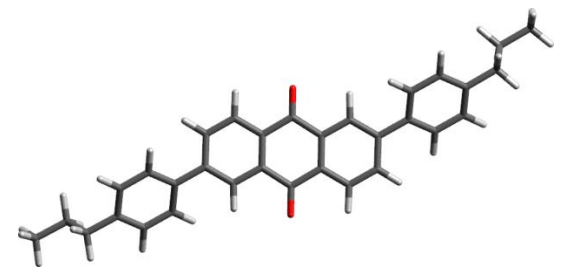
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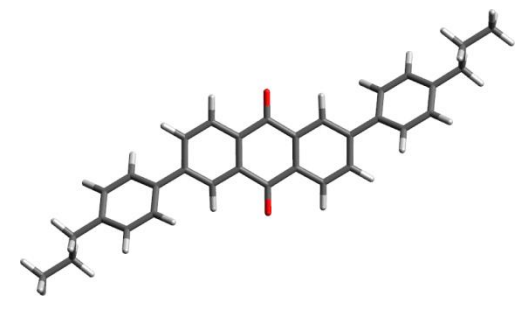
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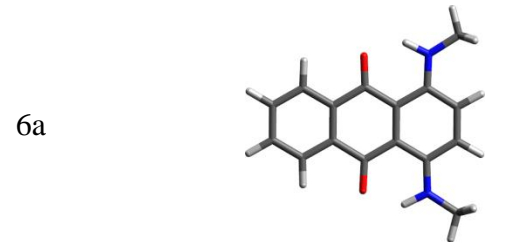
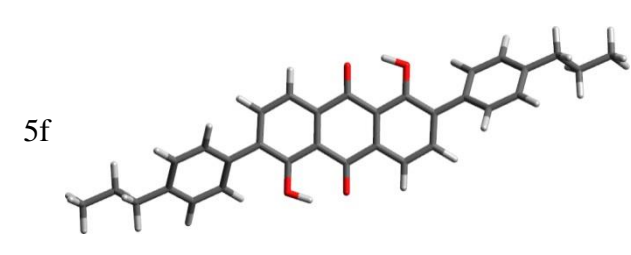
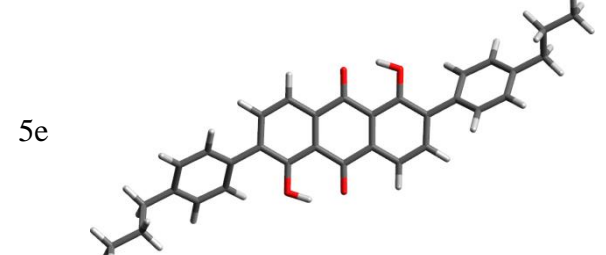
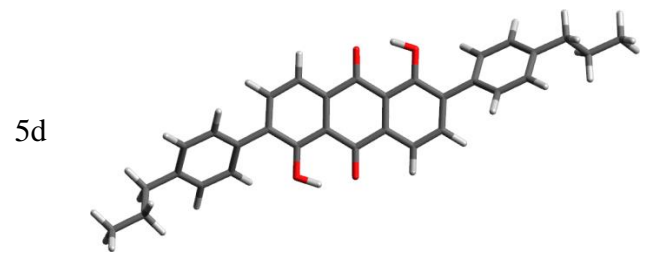
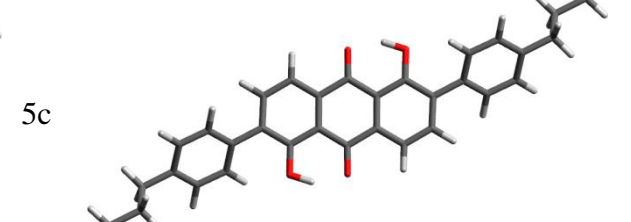
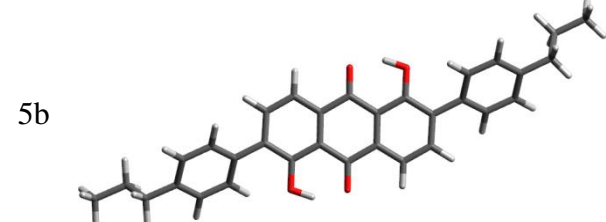
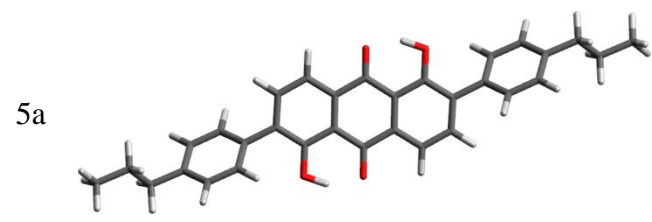
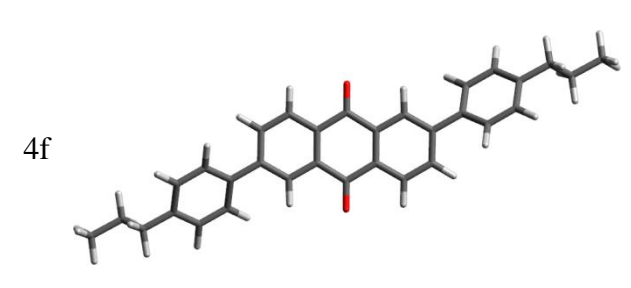
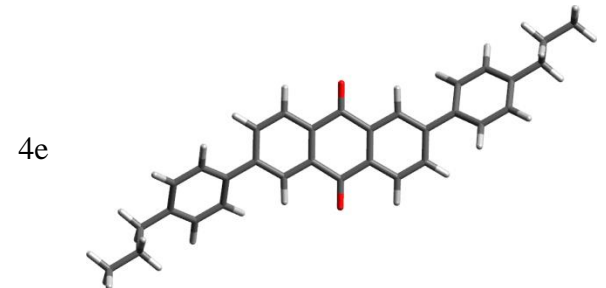
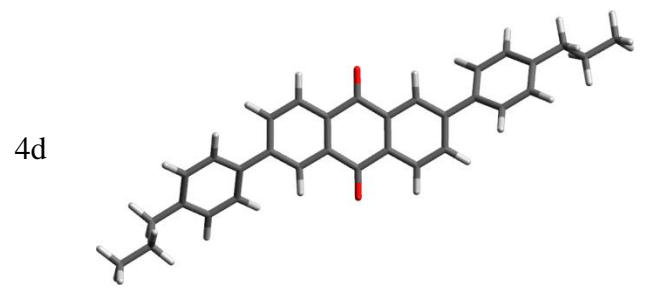


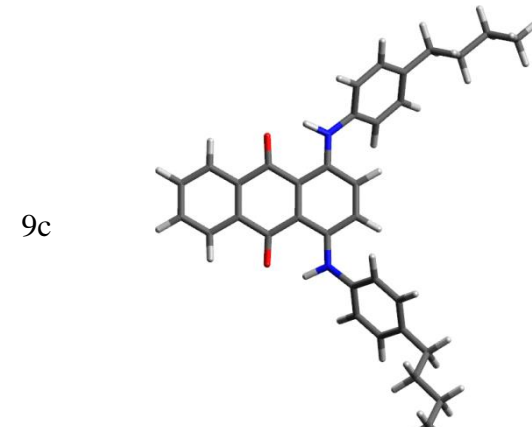
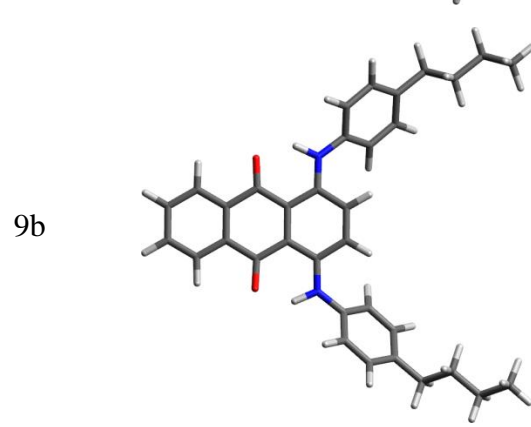
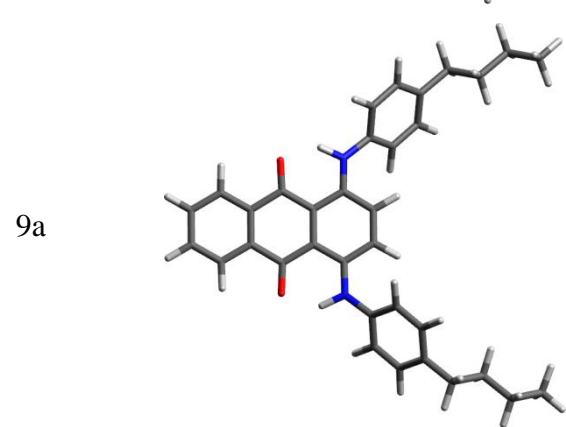
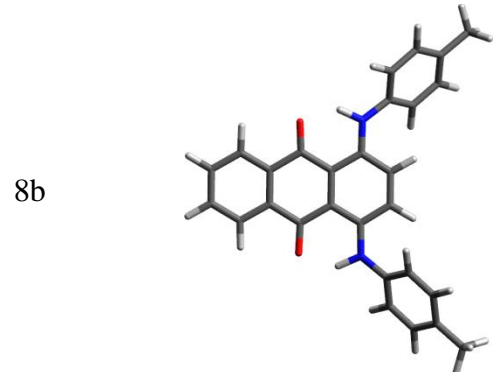
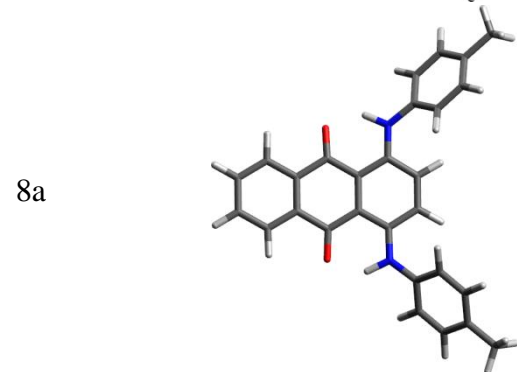
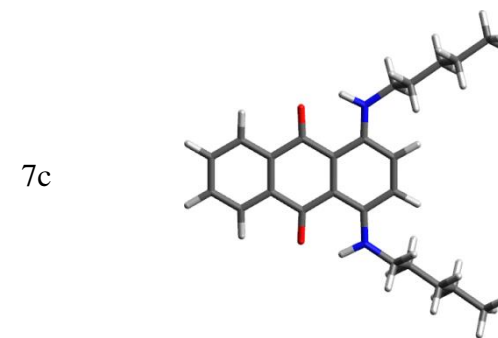
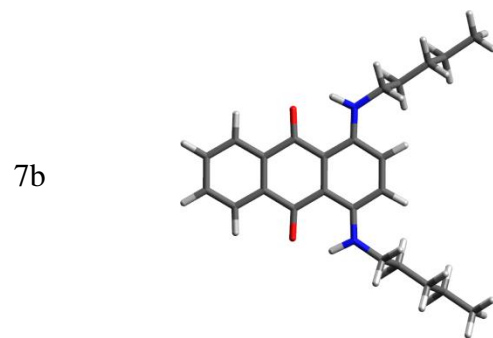
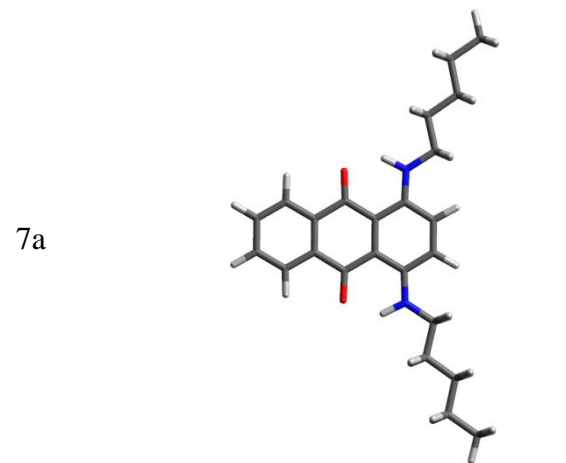
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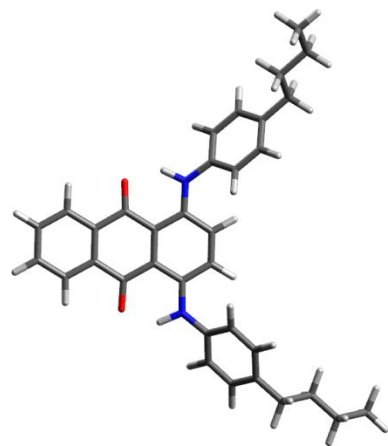
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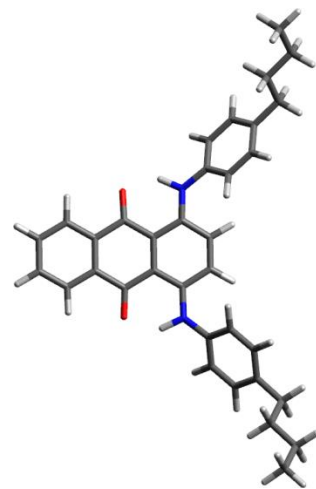




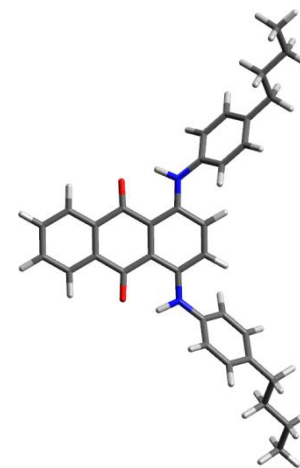
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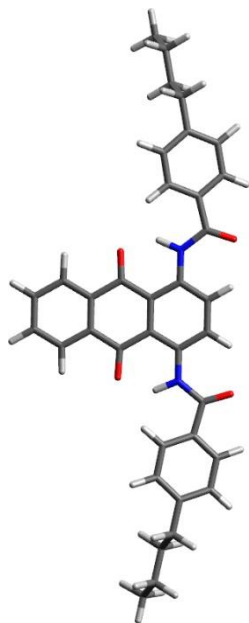
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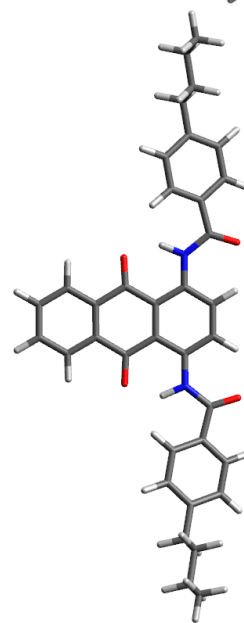
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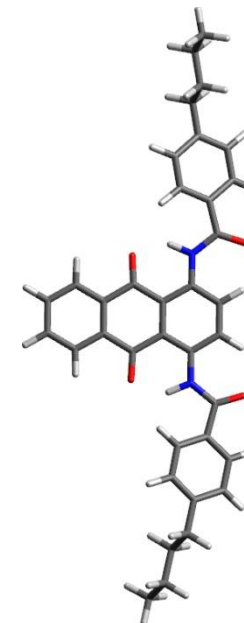
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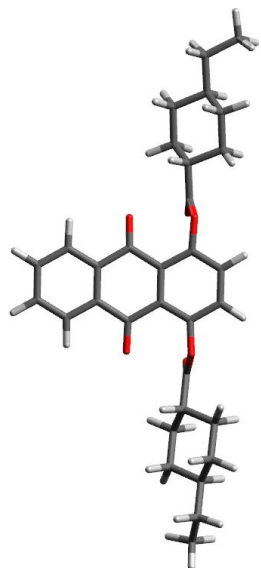
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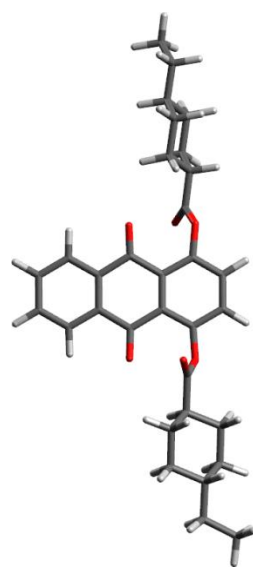
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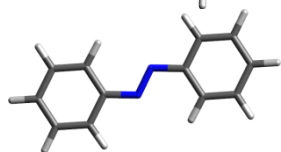
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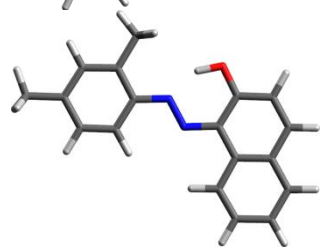
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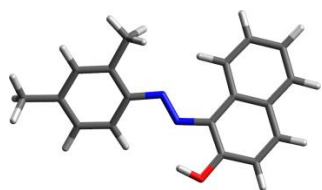
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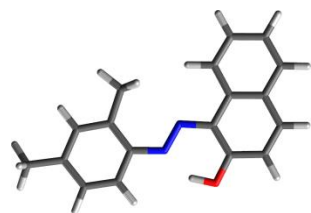
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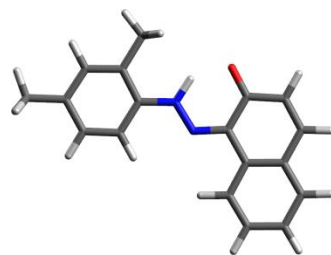
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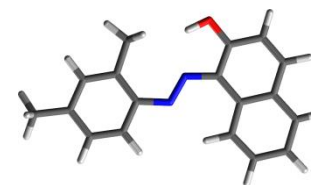
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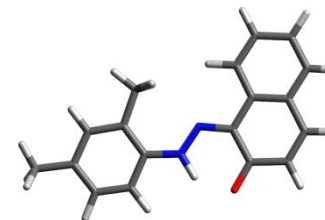
13e

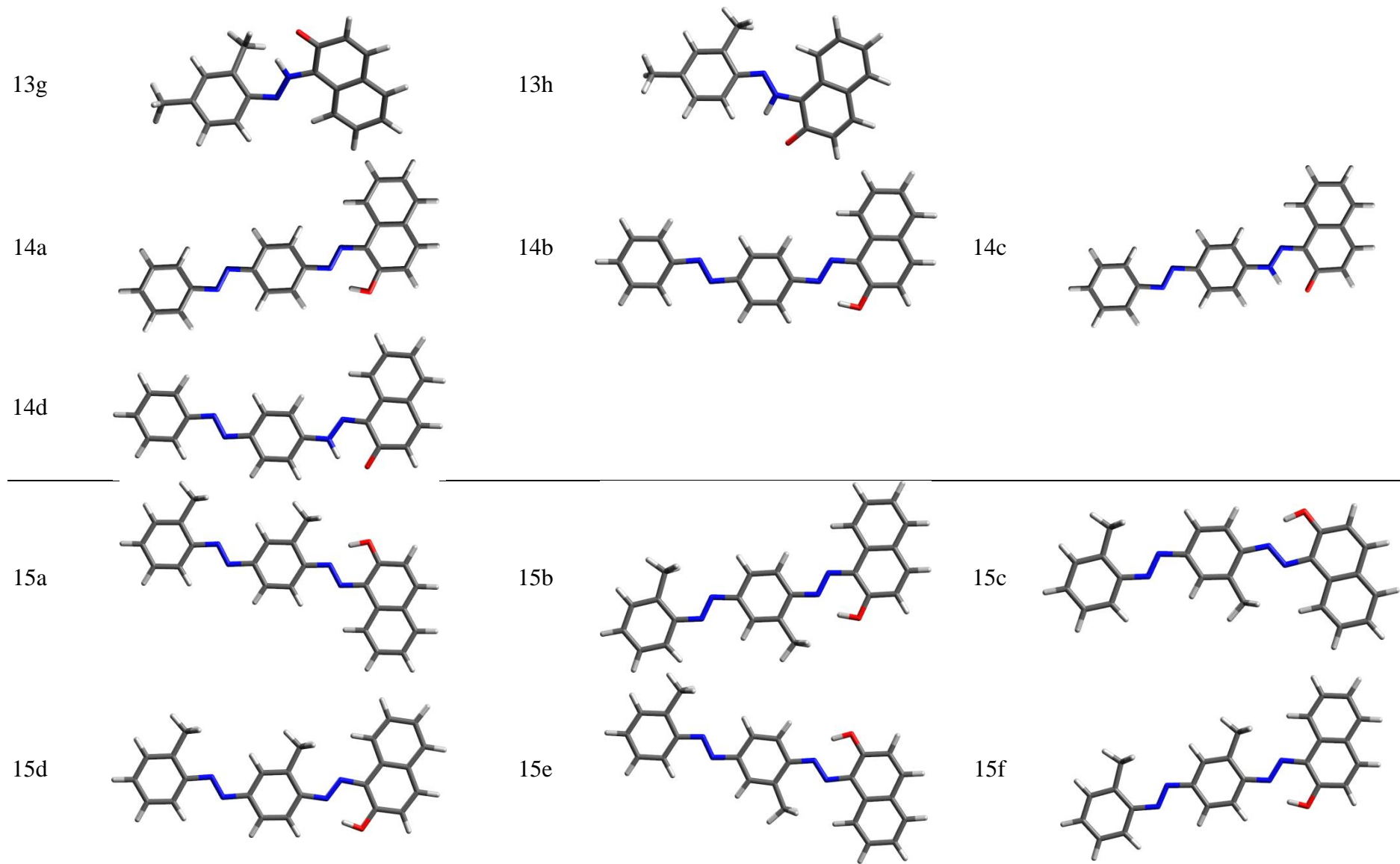


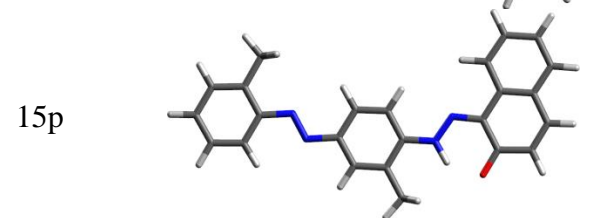
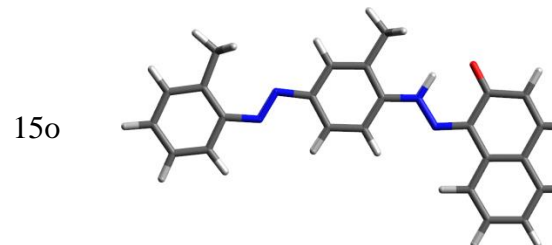
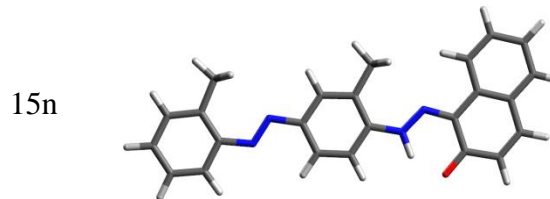
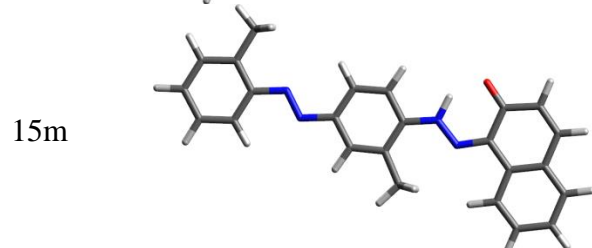
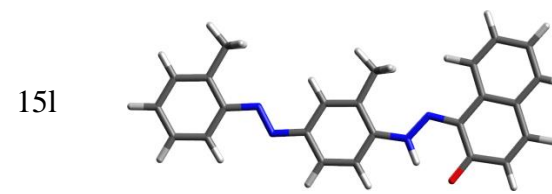
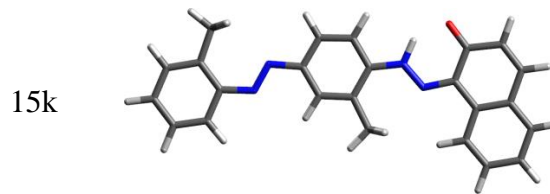
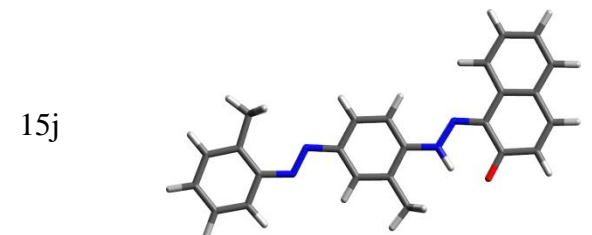
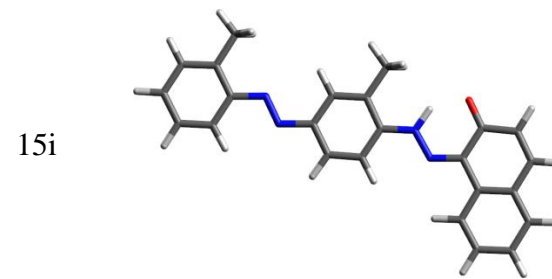
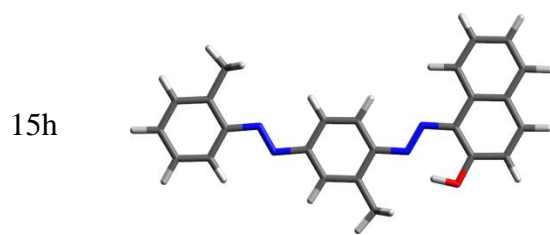
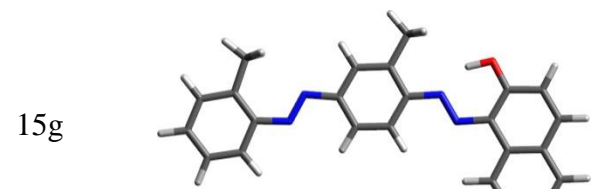
13c



13f







4. Conformation energies, quadrupole tensors, surface tensors and visible transitions (allocation to bands) of dyes

Table S2. Calculated values of the energies, E , degeneracies, g , surface tensor components, T^{20} and T^{22} , quadrupole tensor components, Q_{xx} , Q_{yy} , Q_{zz} , Euler angles, α' , β' and γ' , between the surface tensor and quadrupole frames, angles, α_{TDM} and β_{TDM} , between the surface tensor frames and the calculated TDM vectors, transition wavelengths, λ , oscillator strengths, f , and the allocations of the calculated transitions to either the short wavelength (sw) or long wavelength (lw) experimental absorption bands where applicable.

| Structure | $E / \text{kJ mol}^{-1}$ ^a | g | $T^{20} / \text{\AA}^2$ | $T^{22} / \text{\AA}^2$ | $Q_{xx} / \text{D \AA}$ | $Q_{yy} / \text{D \AA}$ | $Q_{zz} / \text{D \AA}$ | $\alpha' / ^\circ$ | $\beta' / ^\circ$ | $\gamma' / ^\circ$ | λ / nm | f | $\alpha_{\text{TDM}} / ^\circ$ | $\beta_{\text{TDM}} / ^\circ$ | band ^b | |
|-----------|---------------------------------------|-------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--------------------|-------------------|--------------------|-----------------------|-----|--------------------------------|-------------------------------|-------------------|---|
| 1 | a | 0.265 | 1 | 155.0 | 41.3 | -39.3 | -17.6 | 56.9 | 180 | 1 | -180 | 434 | 0.292 | 0 | 9 | - |
| | b | 0.217 | 2 | 153.0 | 36.7 | -38.2 | -18.1 | 56.3 | -178 | 7 | 180 | 433 | 0.297 | -7 | 1 | - |
| | c | 0.000 | 1 | 158.2 | 28.8 | -37.3 | -18.7 | 55.9 | -180 | 12 | -180 | 433 | 0.302 | 180 | 5 | - |
| 2 | a | 0.225 | 1 | 151.5 | 61.9 | -23.1 | -8.1 | 31.1 | 0 | 170 | 70 | 519 | 0.376 | 169 | 11 | - |
| | b | 0.185 | 2 | 146.3 | 60.2 | -22.4 | -7.6 | 30.0 | 174 | 166 | -115 | 519 | 0.372 | -18 | 17 | - |
| | c | 0.382 | 1 | 148.0 | 58.5 | -21.8 | -7.5 | 29.3 | -12 | 162 | 62 | 518 | 0.370 | 156 | 23 | - |
| | d | 0.000 | 2 | 144.8 | 53.3 | -18.3 | -11.1 | 29.5 | 4 | 166 | 91 | 521 | 0.364 | 189 | 19 | - |
| | | | | | | | | | | | | 487 | 0.001 | 107 | 41 | - |
| | e | 0.208 | 1 | 140.8 | 46.6 | -17.7 | -10.9 | 28.6 | 180 | 162 | -90 | 518 | 0.362 | 0 | 25 | - |
| 3 | f | 0.255 | 1 | 151.3 | 56.5 | -18.8 | -12.1 | 30.9 | -180 | 171 | -90 | 521 | 0.368 | 0 | 12 | - |
| | a | 0.206 | 1 | 151.3 | 67.7 | -27.0 | -11.8 | 38.8 | -176 | 3 | 131 | 610 | 0.582 | 169 | 14 | - |
| | b | 0.268 | 2 | 146.1 | 65.1 | -26.2 | -11.7 | 37.9 | -10 | 8 | -35 | 610 | 0.576 | -17 | 20 | - |
| | c | 0.372 | 1 | 147.4 | 62.3 | -25.6 | -11.9 | 37.4 | 165 | 13 | 150 | 610 | 0.571 | 158 | 27 | - |
| | d | 0.000 | 2 | 143.1 | 58.1 | -21.7 | -15.8 | 37.5 | -174 | 9 | 168 | 611 | 0.568 | 186 | 22 | - |
| | e | 0.034 | 1 | 138.9 | 51.4 | -21.2 | -15.3 | 36.5 | 0 | 15 | 0 | 610 | 0.562 | 0 | 29 | - |
| 4 | f | 0.199 | 1 | 148.8 | 60.5 | -22.3 | -16.0 | 38.3 | 180 | 4 | -180 | 611 | 0.573 | 180 | 15 | - |
| | a | 0.369 | 1 | 152.7 | 59.8 | -28.6 | -13.1 | 41.8 | -3 | 171 | 117 | 369 | 0.072 | 38 | 7 | - |
| | | | | | | | | | | | | 364 | 0.338 | 35 | 7 | - |
| | b | 0.130 | 2 | 147.6 | 59.8 | -27.7 | -13.1 | 40.8 | 175 | 168 | -125 | 369 | 0.073 | 163 | 3 | - |
| | | | | | | | | | | | | 364 | 0.336 | 169 | 3 | - |
| | c | 0.109 | 1 | 147.8 | 61.0 | -26.9 | -13.1 | 40.0 | 10 | 164 | 129 | 369 | 0.077 | 243 | 3 | - |
| 5 | d | 0.191 | 2 | 149.4 | 55.3 | -21.3 | -19.6 | 41.0 | -174 | 168 | -101 | 404 | 0.007 | 138 | 5 | - |
| | | | | | | | | | | | | 364 | 0.405 | 131 | 4 | - |
| | e | 0.181 | 1 | 146.8 | 55.3 | -21.1 | -18.8 | 39.9 | 0 | 164 | 90 | 404 | 0.006 | 180 | 2 | - |
| | | | | | | | | | | | | 365 | 0.406 | 180 | 2 | - |
| | f | 0.000 | 1 | 152.0 | 53.0 | -21.3 | -20.6 | 41.9 | -180 | 172 | -90 | 404 | 0.006 | 180 | 9 | - |
| | | | | | | | | | | | | 365 | 0.407 | 180 | 7 | - |
| 6 | a | 0.176 | 1 | 156.5 | 57.2 | -24.4 | -8.0 | 32.4 | 1 | 167 | 125 | 466 | 0.616 | 92 | 3 | - |
| | b | 0.215 | 2 | 151.8 | 57.5 | -23.0 | -8.0 | 31.1 | 177 | 163 | -128 | 466 | 0.615 | -12 | 4 | - |
| | c | 0.189 | 1 | 152.2 | 58.4 | -21.9 | -8.0 | 29.9 | 5 | 160 | 129 | 466 | 0.612 | 207 | 10 | - |
| | d | 0.214 | 2 | 152.7 | 52.8 | -16.2 | -14.7 | 30.9 | 2 | 16 | -32 | 465 | 0.614 | 33 | 6 | - |
| | e | 0.000 | 1 | 150.4 | 52.3 | -14.7 | -14.6 | 29.3 | 0 | 160 | 90 | 465 | 0.611 | 180 | 10 | - |
| | f | 0.156 | 1 | 156.0 | 51.5 | -16.8 | -15.7 | 32.5 | 0 | 12 | 0 | 466 | 0.621 | 180 | 1 | - |
| 6 | a | 0.000 | 1 | 54.5 | 64.7 | -14.5 | -1.6 | 16.1 | 0 | 180 | 90 | 548 | 0.210 | 180 | 0 | - |

| Structure | $E / \text{kJ mol}^{-1 \text{ a}}$ | g | $T^{20} / \text{\AA}^2$ | $T^{22} / \text{\AA}^2$ | $Q_{xx} / \text{D \AA}$ | $Q_{yy} / \text{D \AA}$ | $Q_{zz} / \text{D \AA}$ | $\alpha' / ^\circ$ | $\beta' / ^\circ$ | $\gamma' / ^\circ$ | λ / nm | f | $\alpha_{\text{TDM}} / ^\circ$ | $\beta_{\text{TDM}} / ^\circ$ | band ^b | | | | | | | | | | | |
|-----------|------------------------------------|-------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--------------------|-------------------|--------------------|-----------------------|-------|--------------------------------|-------------------------------|-------------------|------|-----|-------|-----|-----|----|-----|-------|-------|-----|----|
| 7 | a | 0.000 | 1 | 102.5 | 78.9 | 7.3 | 5.3 | -12.6 | -90 | 90 | 550 | 0.212 | 180 | 90 | - | | | | | | | | | | | |
| | b | 3.228 | 2 | 78.8 | 62.7 | 8.2 | 3.0 | -11.2 | 90 | 104 | 550 | 0.233 | 90 | 9 | - | | | | | | | | | | | |
| | c | 3.044 | 2 | 69.9 | 62.1 | 8.1 | 3.1 | -11.2 | -89 | 90 | 550 | 0.231 | -7 | 0 | - | | | | | | | | | | | |
| 8 | a | 0.000 | 1 | 69.7 | 85.0 | 13.5 | 2.4 | -16.0 | -93 | 90 | 91 | 580 | 0.255 | -10 | 89 | lw | | | | | | | | | | |
| | | | | | | | | | | | | 408 | 0.107 | 180 | 1 | sw | | | | | | | | | | |
| | | | | | | | | | | | | 388 | 0.005 | -13 | 89 | sw | | | | | | | | | | |
| | b | 0.929 | 1 | 67.8 | 74.9 | 12.3 | 2.2 | -14.5 | -90 | 86 | 90 | 575 | 0.254 | 180 | 90 | lw | | | | | | | | | | |
| | | | | | | | | | | | | 423 | 0.076 | -90 | 11 | sw | | | | | | | | | | |
| | | | | | | | | | | | | 381 | 0.117 | -90 | 14 | sw | | | | | | | | | | |
| | | | | | | | | | | | | 367 | 0.067 | -90 | 12 | sw | | | | | | | | | | |
| | | | | | | | | | | | | 360 | 0.002 | 180 | 90 | sw | | | | | | | | | | |
| | | | | | | | | | | | | 360 | 0.002 | 180 | 90 | sw | | | | | | | | | | |
| | a | 1.035 | 1 | 105.8 | 78.8 | 8.5 | 4.7 | -13.2 | -83 | 90 | 0 | 576 | 0.271 | -2 | 0 | lw | | | | | | | | | | |
| | | | | | | | | | | | | 423 | 0.083 | 170 | 90 | sw | | | | | | | | | | |
| | | | | | | | | | | | | 382 | 0.129 | -13 | 90 | sw | | | | | | | | | | |
| 368 | | | | | | | | | | | | 0.067 | 168 | 90 | sw | | | | | | | | | | | |
| 360 | | | | | | | | | | | | 0.001 | -11 | 1 | sw | | | | | | | | | | | |
| b | | | | | | | | | | | | 0.044 | 1 | 108.0 | 79.8 | 10.2 | 4.0 | -14.3 | -90 | 81 | 0 | 580 | 0.273 | 269 | 2 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 408 | 0.114 | 0 | 90 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 388 | 0.005 | 269 | 3 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 384 | 0.150 | 0 | 90 | sw |
| | c | 0.913 | 2 | 71.1 | 83.0 | 8.0 | 4.6 | -12.7 | -80 | 91 | -22 | | | | | | | | | | | 575 | 0.264 | 5 | 37 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 424 | 0.087 | 173 | 53 | sw |
| 382 | | | | | | | | | | | | 0.133 | 168 | 53 | sw | | | | | | | | | | | |
| 366 | | | | | | | | | | | | 0.073 | 171 | 52 | sw | | | | | | | | | | | |
| 360 | | | | | | | | | | | | 0.002 | 9 | 35 | sw | | | | | | | | | | | |
| d | | | | | | | | | | | | 0.000 | 2 | 74.7 | 87.9 | 9.6 | 5.0 | -14.6 | -92 | 88 | 22 | 581 | 0.265 | 212 | 12 | lw |
| | 410 | 0.123 | -4 | 81 | sw | | | | | | | | | | | | | | | | | | | | | |
| | 387 | 0.005 | 220 | 14 | sw | | | | | | | | | | | | | | | | | | | | | |
| | 385 | 0.156 | -4 | 81 | sw | | | | | | | | | | | | | | | | | | | | | |
| | e | 0.039 | 1 | 92.4 | 75.8 | 8.9 | 6.1 | -15.0 | -95 | 90 | 90 | | | | | | | | | | | 581 | 0.258 | -12 | 90 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 410 | 0.129 | 243 | 0 | sw |
| 387 | | | | | | | | | | | | 0.006 | -16 | 90 | sw | | | | | | | | | | | |
| 385 | | | | | | | | | | | | 0.162 | 183 | 0 | sw | | | | | | | | | | | |
| f | | | | | | | | | | | | 0.972 | 1 | 91.3 | 65.7 | 7.6 | 5.1 | -12.7 | -90 | 100 | 90 | 575 | 0.259 | 180 | 90 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 424 | 0.091 | 90 | 2 | sw |
| | 382 | 0.140 | 90 | 6 | sw | | | | | | | | | | | | | | | | | | | | | |
| | 367 | 0.075 | 90 | 3 | sw | | | | | | | | | | | | | | | | | | | | | |
| | 360 | 0.002 | 0 | 90 | sw | | | | | | | | | | | | | | | | | | | | | |
| | 10 | a | 0.019 | 1 | 154.0 | 98.4 | -28.3 | -8.2 | 36.5 | 0 | 180 | | | | | | | | | | | 76 | 493 | 0.164 | 183 | 90 |
| 368 | | | | | | | | | | | | 0.039 | -16 | 0 | sw | | | | | | | | | | | |
| 356 | | | | | | | | | | | | 0.090 | -16 | 0 | sw | | | | | | | | | | | |

| Structure | $E / \text{kJ mol}^{-1}$ ^a | g | $T^{20} / \text{\AA}^2$ | $T^{22} / \text{\AA}^2$ | $Q_{xx} / \text{D \AA}$ | $Q_{yy} / \text{D \AA}$ | $Q_{zz} / \text{D \AA}$ | $\alpha' / ^\circ$ | $\beta' / ^\circ$ | $\gamma' / ^\circ$ | λ / nm | f | $\alpha_{\text{TDM}} / ^\circ$ | $\beta_{\text{TDM}} / ^\circ$ | band ^b |
|-----------|---------------------------------------|-----|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--------------------|-------------------|--------------------|-----------------------|-------|--------------------------------|-------------------------------|-------------------|
| | | | | | | | | | | | 355 | 0.003 | 4 | 90 | sw |
| | | | | | | | | | | | 346 | 0.173 | -16 | 0 | sw |
| | | | | | | | | | | | 336 | 0.016 | -16 | 0 | sw |
| | | | | | | | | | | | 333 | 0.150 | -16 | 0 | sw |
| | | | | | | | | | | | 332 | 0.005 | 173 | 90 | sw |
| b | 0.264 | 1 | 150.6 | 91.3 | -28.0 | -7.4 | 35.4 | 0 | 180 | 88 | 493 | 0.168 | 173 | 90 | lw |
| | | | | | | | | | | | 367 | 0.038 | -1 | 0 | sw |
| | | | | | | | | | | | 356 | 0.095 | -1 | 0 | sw |
| | | | | | | | | | | | 355 | 0.002 | 12 | 90 | sw |
| | | | | | | | | | | | 346 | 0.171 | -1 | 0 | sw |
| | | | | | | | | | | | 336 | 0.017 | -1 | 0 | sw |
| | | | | | | | | | | | 333 | 0.148 | -1 | 0 | sw |
| | | | | | | | | | | | 332 | 0.004 | 187 | 90 | sw |
| c | 0.000 | 1 | 158.1 | 96.9 | -27.9 | -8.3 | 36.2 | 141 | 175 | -136 | 493 | 0.165 | 175 | 84 | lw |
| | | | | | | | | | | | 368 | 0.040 | -45 | 6 | sw |
| | | | | | | | | | | | 356 | 0.091 | -44 | 6 | sw |
| | | | | | | | | | | | 355 | 0.003 | -1 | 74 | sw |
| | | | | | | | | | | | 346 | 0.175 | -45 | 7 | sw |
| | | | | | | | | | | | 336 | 0.017 | -46 | 6 | sw |
| | | | | | | | | | | | 333 | 0.147 | -45 | 6 | sw |
| | | | | | | | | | | | 332 | 0.005 | 186 | 89 | sw |
| 11 a | 0.000 | 1 | 143.2 | 60.4 | 16.5 | 5.7 | -22.2 | -97 | 93 | 92 | 419 | 0.003 | -14 | 87 | - |
| | | | | | | | | | | | 344 | 0.090 | -11 | 87 | - |
| b | 0.299 | 1 | 143.0 | 52.4 | 18.0 | 6.4 | -24.4 | -98 | 79 | 99 | 377 | 0.004 | -6 | 81 | - |
| | | | | | | | | | | | 343 | 0.084 | -6 | 84 | - |
| 12 a | 0.000 | 1 | 56.6 | 41.5 | 11.6 | 1.4 | -13.0 | 90 | 90 | 179 | 320 | 0.792 | 0 | 2 | - |
| 13 a | 3.772 | 1 | 77.4 | 67.0 | -15.6 | -1.1 | 16.7 | -180 | 176 | -90 | 418 | 0.584 | 0 | 7 | - |
| b | 14.808 | 1 | 81.8 | 66.5 | -15.4 | -2.2 | 17.6 | 7 | 174 | 97 | 409 | 0.568 | 182 | 11 | - |
| c | 39.506 | 1 | 78.9 | 68.0 | -15.7 | -1.8 | 17.5 | -12 | 176 | 77 | 401 | 0.629 | 4 | 4 | - |
| d | 28.669 | 1 | 78.0 | 63.5 | -14.7 | -2.0 | 16.7 | -19 | 178 | 67 | 478 | 0.050 | 175 | 9 | - |
| | | | | | | | | | | | 404 | 0.573 | 173 | 11 | - |
| e | 0.000 | 1 | 77.7 | 67.1 | -14.9 | -2.5 | 17.4 | 180 | 179 | -90 | 432 | 0.573 | 180 | 8 | - |
| f | 12.886 | 1 | 81.7 | 66.6 | -14.4 | -3.9 | 18.4 | 11 | 178 | 101 | 425 | 0.568 | 181 | 11 | - |
| g | 65.001 | 1 | 74.2 | 51.7 | -14.5 | -5.8 | 20.3 | 87 | 179 | -156 | 471 | 0.521 | 12 | 13 | - |
| h | 51.653 | 1 | 77.8 | 63.9 | -14.3 | -6.4 | 20.7 | -28 | 178 | 82 | 481 | 0.577 | 187 | 14 | - |
| 14 a | 5.476 | 1 | 107.3 | 85.4 | -23.7 | -2.8 | 26.5 | -180 | 178 | -90 | 468 | 1.154 | 180 | 4 | lw |
| | | | | | | | | | | | 372 | 0.170 | 0 | 16 | sw |
| | | | | | | | | | | | 356 | 0.148 | 180 | 20 | sw |
| | | | | | | | | | | | 337 | 0.140 | 180 | 7 | sw |
| b | 5.533 | 1 | 104.2 | 86.6 | -23.3 | -1.8 | 25.1 | 180 | 176 | -90 | 464 | 1.132 | 180 | 1 | lw |
| | | | | | | | | | | | 370 | 0.154 | 0 | 19 | sw |
| | | | | | | | | | | | 355 | 0.130 | 180 | 19 | sw |

| Structure | $E / \text{kJ mol}^{-1 \text{ a}}$ | g | $T^{20} / \text{\AA}^2$ | $T^{22} / \text{\AA}^2$ | $Q_{xx} / \text{D \AA}$ | $Q_{yy} / \text{D \AA}$ | $Q_{zz} / \text{D \AA}$ | $\alpha' / ^\circ$ | $\beta' / ^\circ$ | $\gamma' / ^\circ$ | λ / nm | f | $\alpha_{\text{TDM}} / ^\circ$ | $\beta_{\text{TDM}} / ^\circ$ | band ^b | | | | | | | | | | | |
|-----------|------------------------------------|-----|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--------------------|-------------------|--------------------|-----------------------|--------|--------------------------------|-------------------------------|-------------------|-------|------|------|------|-----|-----|-----|-------|-----|----|----|
| c | 0.000 | 1 | 107.5 | 85.5 | -22.3 | -4.4 | 26.7 | 180 | 173 | -90 | 339 | 0.203 | 180 | 14 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 468 | 1.231 | 180 | 4 | lw | | | | | | | | | | | |
| | | | | | | | | | | | 381 | 0.080 | 0 | 32 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 357 | 0.098 | 0 | 14 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 337 | 0.180 | 180 | 13 | sw | | | | | | | | | | | |
| d | 0.355 | 1 | 104.5 | 86.7 | -21.8 | -3.4 | 25.2 | -180 | 169 | -90 | 465 | 1.208 | 180 | 1 | lw | | | | | | | | | | | |
| | | | | | | | | | | | 380 | 0.072 | 0 | 37 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 360 | 0.097 | 0 | 10 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 336 | 0.188 | 180 | 19 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 337 | 0.180 | 180 | 13 | sw | | | | | | | | | | | |
| 15 a | 6.505 | 1 | 114.1 | 96.1 | -22.3 | -1.3 | 23.6 | 180 | 173 | -90 | 477 | 1.221 | 180 | 4 | lw | | | | | | | | | | | |
| | | | | | | | | | | | 376 | 0.196 | 0 | 9 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 363 | 0.046 | 180 | 41 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 343 | 0.072 | 180 | 7 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 338 | 0.023 | 0 | 52 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 337 | 0.047 | 180 | 29 | sw | | | | | | | | | | | |
| | | | | | | | | | | | b | 15.443 | 1 | 114.2 | 94.5 | -22.6 | -1.0 | 23.6 | -180 | 180 | -90 | 471 | 1.194 | 0 | 5 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 371 | 0.174 | 180 | 11 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 357 | 0.080 | 0 | 33 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 337 | 0.093 | 0 | 24 | sw |
| 335 | 0.033 | 180 | 20 | sw | | | | | | | | | | | | | | | | | | | | | | |
| 328 | 0.065 | 180 | 14 | sw | | | | | | | | | | | | | | | | | | | | | | |
| c | 27.420 | 1 | 115.8 | 95.5 | -22.1 | -1.7 | 23.8 | 180 | 175 | -90 | | | | | | | | | | | | 462 | 1.161 | 180 | 3 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 366 | 0.192 | 0 | 14 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 352 | 0.122 | 180 | 20 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 337 | 0.128 | 180 | 9 | sw |
| | | | | | | | | | | | 329 | 0.022 | 0 | 62 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 324 | 0.069 | 180 | 26 | sw | | | | | | | | | | | |
| | | | | | | | | | | | d | 18.730 | 1 | 116.4 | 96.8 | -21.2 | -0.6 | 21.8 | 0 | 178 | 90 | 468 | 1.179 | 180 | 5 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 370 | 0.224 | 0 | 6 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 357 | 0.095 | 180 | 34 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 343 | 0.090 | 180 | 23 | sw |
| 333 | 0.030 | 0 | 8 | sw | | | | | | | | | | | | | | | | | | | | | | |
| 331 | 0.027 | 0 | 52 | sw | | | | | | | | | | | | | | | | | | | | | | |
| e | 18.181 | 1 | 116.6 | 94.0 | -22.0 | -1.8 | 23.8 | 0 | 175 | 90 | | | | | | | | | | | | 470 | 1.194 | 0 | 7 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 371 | 0.245 | 180 | 9 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 358 | 0.073 | 0 | 27 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 342 | 0.066 | 180 | 8 | sw |
| | | | | | | | | | | | 334 | 0.027 | 0 | 70 | sw | | | | | | | | | | | |
| | | | | | | | | | | | 330 | 0.062 | 180 | 13 | sw | | | | | | | | | | | |
| | | | | | | | | | | | f | 27.210 | 1 | 118.7 | 93.6 | -22.2 | -2.0 | 24.2 | -180 | 179 | -90 | 463 | 1.172 | 0 | 7 | lw |
| | | | | | | | | | | | | | | | | | | | | | | 366 | 0.205 | 180 | 10 | sw |
| | | | | | | | | | | | | | | | | | | | | | | 352 | 0.115 | 0 | 26 | sw |

| Structure | $E / \text{kJ mol}^{-1 \text{ a}}$ | g | $T^{20} / \text{\AA}^2$ | $T^{22} / \text{\AA}^2$ | $Q_{xx} / \text{D \AA}$ | $Q_{yy} / \text{D \AA}$ | $Q_{zz} / \text{D \AA}$ | $\alpha' / ^\circ$ | $\beta' / ^\circ$ | $\gamma' / ^\circ$ | λ / nm | f | $\alpha_{\text{TDM}} / ^\circ$ | $\beta_{\text{TDM}} / ^\circ$ | band ^b |
|-----------|------------------------------------|-----|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--------------------|-------------------|--------------------|-----------------------|-------|--------------------------------|-------------------------------|-------------------|
| g | 15.496 | 1 | 109.6 | 95.9 | -22.6 | -0.2 | 22.7 | 180 | 172 | -90 | 336 | 0.093 | 0 | 7 | sw |
| | | | | | | | | | | | 330 | 0.012 | 180 | 30 | sw |
| | | | | | | | | | | | 324 | 0.117 | 180 | 21 | sw |
| | | | | | | | | | | | 468 | 1.161 | 0 | 0 | lw |
| | | | | | | | | | | | 370 | 0.156 | 0 | 16 | sw |
| | | | | | | | | | | | 356 | 0.066 | 180 | 29 | sw |
| | | | | | | | | | | | 339 | 0.158 | 180 | 18 | sw |
| | | | | | | | | | | | 333 | 0.010 | 0 | 59 | sw |
| | | | | | | | | | | | 326 | 0.061 | 180 | 41 | sw |
| h | 6.390 | 1 | 107.8 | 96.2 | 20.3 | 1.4 | -21.8 | 90 | 90 | 179 | 473 | 1.180 | 0 | 2 | lw |
| | | | | | | | | | | | 374 | 0.164 | 180 | 7 | sw |
| | | | | | | | | | | | 361 | 0.050 | 0 | 50 | sw |
| | | | | | | | | | | | 345 | 0.135 | 0 | 32 | sw |
| | | | | | | | | | | | 336 | 0.032 | 180 | 40 | sw |
| | | | | | | | | | | | 334 | 0.021 | 0 | 32 | sw |
| | | | | | | | | | | | 479 | 1.241 | 180 | 5 | lw |
| | | | | | | | | | | | 383 | 0.051 | 0 | 38 | sw |
| | | | | | | | | | | | 363 | 0.123 | 0 | 11 | sw |
| i | 0.000 | 1 | 114.3 | 96.2 | -21.2 | -3.4 | 24.6 | -180 | 167 | -90 | 345 | 0.119 | 180 | 12 | sw |
| | | | | | | | | | | | 333 | 0.029 | 180 | 46 | sw |
| | | | | | | | | | | | 327 | 0.011 | 0 | 44 | sw |
| | | | | | | | | | | | 474 | 1.209 | 0 | 6 | lw |
| | | | | | | | | | | | 380 | 0.059 | 180 | 35 | sw |
| | | | | | | | | | | | 357 | 0.116 | 180 | 10 | sw |
| | | | | | | | | | | | 339 | 0.162 | 0 | 20 | sw |
| | | | | | | | | | | | 326 | 0.006 | 180 | 62 | sw |
| | | | | | | | | | | | 325 | 0.043 | 180 | 17 | sw |
| j | 9.073 | 1 | 114.3 | 94.6 | -21.5 | -2.5 | 24.0 | 0 | 174 | 90 | 467 | 1.244 | 180 | 4 | lw |
| | | | | | | | | | | | 377 | 0.081 | 0 | 30 | sw |
| | | | | | | | | | | | 359 | 0.093 | 0 | 13 | sw |
| | | | | | | | | | | | 336 | 0.150 | 180 | 10 | sw |
| | | | | | | | | | | | 322 | 0.044 | 180 | 45 | sw |
| | | | | | | | | | | | 320 | 0.019 | 0 | 15 | sw |
| | | | | | | | | | | | 472 | 1.274 | 180 | 5 | lw |
| | | | | | | | | | | | 380 | 0.067 | 0 | 27 | sw |
| | | | | | | | | | | | 365 | 0.090 | 0 | 13 | sw |
| k | 23.071 | 1 | 115.9 | 95.5 | -20.7 | -3.7 | 24.4 | -180 | 169 | -90 | 342 | 0.126 | 180 | 28 | sw |
| | | | | | | | | | | | 330 | 0.031 | 0 | 16 | sw |
| | | | | | | | | | | | 322 | 0.011 | 0 | 67 | sw |
| | | | | | | | | | | | 474 | 1.280 | 0 | 7 | lw |
| | | | | | | | | | | | 380 | 0.078 | 180 | 25 | sw |
| | | | | | | | | | | | 364 | 0.105 | 180 | 18 | sw |
| | | | | | | | | | | | 472 | 1.274 | 180 | 5 | lw |
| | | | | | | | | | | | 380 | 0.067 | 0 | 27 | sw |
| | | | | | | | | | | | 365 | 0.090 | 0 | 13 | sw |
| l | 14.228 | 1 | 116.6 | 96.7 | -19.7 | -2.2 | 21.9 | -180 | 174 | -90 | 330 | 0.031 | 0 | 16 | sw |
| | | | | | | | | | | | 322 | 0.011 | 0 | 67 | sw |
| | | | | | | | | | | | 474 | 1.280 | 0 | 7 | lw |
| | | | | | | | | | | | 380 | 0.078 | 180 | 25 | sw |
| | | | | | | | | | | | 364 | 0.105 | 180 | 18 | sw |
| | | | | | | | | | | | 472 | 1.274 | 180 | 5 | lw |
| | | | | | | | | | | | 380 | 0.067 | 0 | 27 | sw |
| | | | | | | | | | | | 365 | 0.090 | 0 | 13 | sw |
| | | | | | | | | | | | 342 | 0.126 | 180 | 28 | sw |
| m | 13.662 | 1 | 116.7 | 94.0 | -20.8 | -4.0 | 24.7 | 0 | 170 | 90 | 330 | 0.031 | 0 | 16 | sw |
| | | | | | | | | | | | 322 | 0.011 | 0 | 67 | sw |
| | | | | | | | | | | | 474 | 1.280 | 0 | 7 | lw |
| | | | | | | | | | | | 380 | 0.078 | 180 | 25 | sw |
| | | | | | | | | | | | 364 | 0.105 | 180 | 18 | sw |
| | | | | | | | | | | | 472 | 1.274 | 180 | 5 | lw |
| | | | | | | | | | | | 380 | 0.067 | 0 | 27 | sw |
| | | | | | | | | | | | 365 | 0.090 | 0 | 13 | sw |
| | | | | | | | | | | | 342 | 0.126 | 180 | 28 | sw |

| Structure | $E / \text{kJ mol}^{-1}$ ^a | g | $T^{20} / \text{\AA}^2$ | $T^{22} / \text{\AA}^2$ | $Q_{xx} / \text{D \AA}$ | $Q_{yy} / \text{D \AA}$ | $Q_{zz} / \text{D \AA}$ | $\alpha' / ^\circ$ | $\beta' / ^\circ$ | $\gamma' / ^\circ$ | λ / nm | f | $\alpha_{\text{TDM}} / ^\circ$ | $\beta_{\text{TDM}} / ^\circ$ | band ^b |
|-----------|---------------------------------------|-----|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--------------------|-------------------|--------------------|-----------------------|-------|--------------------------------|-------------------------------|-------------------|
| n | 22.914 | 1 | 118.8 | 93.6 | -21.0 | -3.8 | 24.7 | 0 | 176 | 90 | 343 | 0.112 | 0 | 1 | sw |
| | | | | | | | | | | | 330 | 0.030 | 0 | 45 | sw |
| | | | | | | | | | | | 321 | 0.020 | 180 | 32 | sw |
| | | | | | | | | | | | 468 | 1.248 | 0 | 8 | lw |
| | | | | | | | | | | | 377 | 0.086 | 180 | 25 | sw |
| | | | | | | | | | | | 358 | 0.106 | 180 | 15 | sw |
| | | | | | | | | | | | 336 | 0.145 | 0 | 13 | sw |
| | | | | | | | | | | | 323 | 0.014 | 180 | 9 | sw |
| | | | | | | | | | | | 319 | 0.057 | 180 | 28 | sw |
| o | 9.524 | 1 | 110.0 | 96.0 | -21.3 | -2.1 | 23.4 | 180 | 164 | -90 | 472 | 1.174 | 180 | 0 | lw |
| | | | | | | | | | | | 379 | 0.051 | 0 | 45 | sw |
| | | | | | | | | | | | 359 | 0.119 | 0 | 8 | sw |
| | | | | | | | | | | | 338 | 0.157 | 180 | 19 | sw |
| | | | | | | | | | | | 324 | 0.013 | 180 | 5 | sw |
| | | | | | | | | | | | 322 | 0.037 | 180 | 58 | sw |
| | | | | | | | | | | | 476 | 1.199 | 0 | 2 | lw |
| | | | | | | | | | | | 382 | 0.036 | 180 | 46 | sw |
| | | | | | | | | | | | 365 | 0.119 | 180 | 6 | sw |
| p | 0.269 | 1 | 108.1 | 96.4 | -20.4 | 0.0 | 20.4 | 0 | 169 | 90 | 344 | 0.141 | 0 | 37 | sw |
| | | | | | | | | | | | 331 | 0.024 | 180 | 17 | sw |
| | | | | | | | | | | | 325 | 0.008 | 0 | 88 | sw |

^a relative to lowest energy conformer as calculated for the isolated molecules by DFT; ^b only listed where multiple bands are present in experimental spectra.

The influence of the choice of origin on the calculated quadrupoles in the molecules exhibiting permanent dipoles was tested for dye **10**, which has the largest calculated quadrupole moment, and for dye **11**. Molecular quadrupoles were calculated from the centre of mass and after translation by $\pm 1 \text{ \AA}$ and $\pm 2 \text{ \AA}$ in the x , y and z axes defined as the principal moment of inertia axes. The dichroic order parameters that were calculated using these different quadrupole origins varied from those calculated using the centre-of-mass origin by less than the range of experimental values given in Table S1 for each of these dyes.

5. Calculated structure, quadrupole tensor and surface tensor of 5CB

5cb

| | | | |
|---|-----------|-----------|-----------|
| C | -1.822298 | 0.624005 | 0.642108 |
| C | -1.107737 | 1.402525 | -0.268583 |
| C | 0.256660 | 1.230615 | -0.446203 |
| C | 0.958658 | 0.265165 | 0.280926 |
| C | 0.244117 | -0.517206 | 1.192648 |
| C | -1.119331 | -0.337081 | 1.369334 |
| C | 2.411256 | 0.081981 | 0.095305 |
| C | 2.983102 | -1.195548 | 0.110116 |
| C | 4.344082 | -1.372886 | -0.065066 |
| C | 5.172501 | -0.264426 | -0.262326 |
| C | 4.616250 | 1.017833 | -0.279475 |
| C | 3.254082 | 1.182039 | -0.101697 |
| C | 6.576170 | -0.440642 | -0.444590 |
| N | 7.712502 | -0.583360 | -0.592213 |
| C | -3.307704 | 0.786140 | 0.803679 |
| C | -4.108407 | -0.122228 | -0.133913 |
| C | -5.614764 | 0.038698 | 0.021597 |
| C | -6.419447 | -0.862658 | -0.907079 |
| C | -7.923866 | -0.694751 | -0.747053 |
| H | 4.773782 | -2.368005 | -0.060725 |
| H | 5.259723 | 1.878297 | -0.422467 |
| H | 2.836252 | 2.182844 | -0.090244 |
| H | 2.345265 | -2.063769 | 0.235640 |
| H | 0.768735 | -1.252573 | 1.794509 |
| H | 0.781612 | 1.837878 | -1.176867 |
| H | -1.647649 | -0.946286 | 2.097503 |
| H | -1.630660 | 2.156119 | -0.850892 |
| H | -3.584790 | 1.830033 | 0.616456 |
| H | -3.589209 | 0.569993 | 1.840852 |
| H | -3.818683 | 0.088785 | -1.171075 |
| H | -3.826392 | -1.166363 | 0.051812 |
| H | -5.897979 | -0.168880 | 1.062569 |
| H | -5.890197 | 1.086132 | -0.162667 |
| H | -6.134481 | -0.655166 | -1.946169 |
| H | -6.144024 | -1.908443 | -0.721483 |
| H | -8.475786 | -1.352690 | -1.423955 |
| H | -8.241288 | -0.927979 | 0.274516 |
| H | -8.231686 | 0.334130 | -0.960194 |

$$Q_{xx} = 23.729 \text{ D } \text{\AA}$$

$$Q_{yy} = 10.080 \text{ D } \text{\AA}$$

$$Q_{zz} = -33.809 \text{ D } \text{\AA}$$

$$\alpha = -132.317^\circ$$

$$\beta = 7.238^\circ$$

$$\gamma = 127.500^\circ$$

$$T^{20} = 89.7 \text{ \AA}^2$$

$$T^{22} = 22.6 \text{ \AA}^2$$

6. Calculated dichroic order parameters using a range of scaling factors for F_{ZZ}

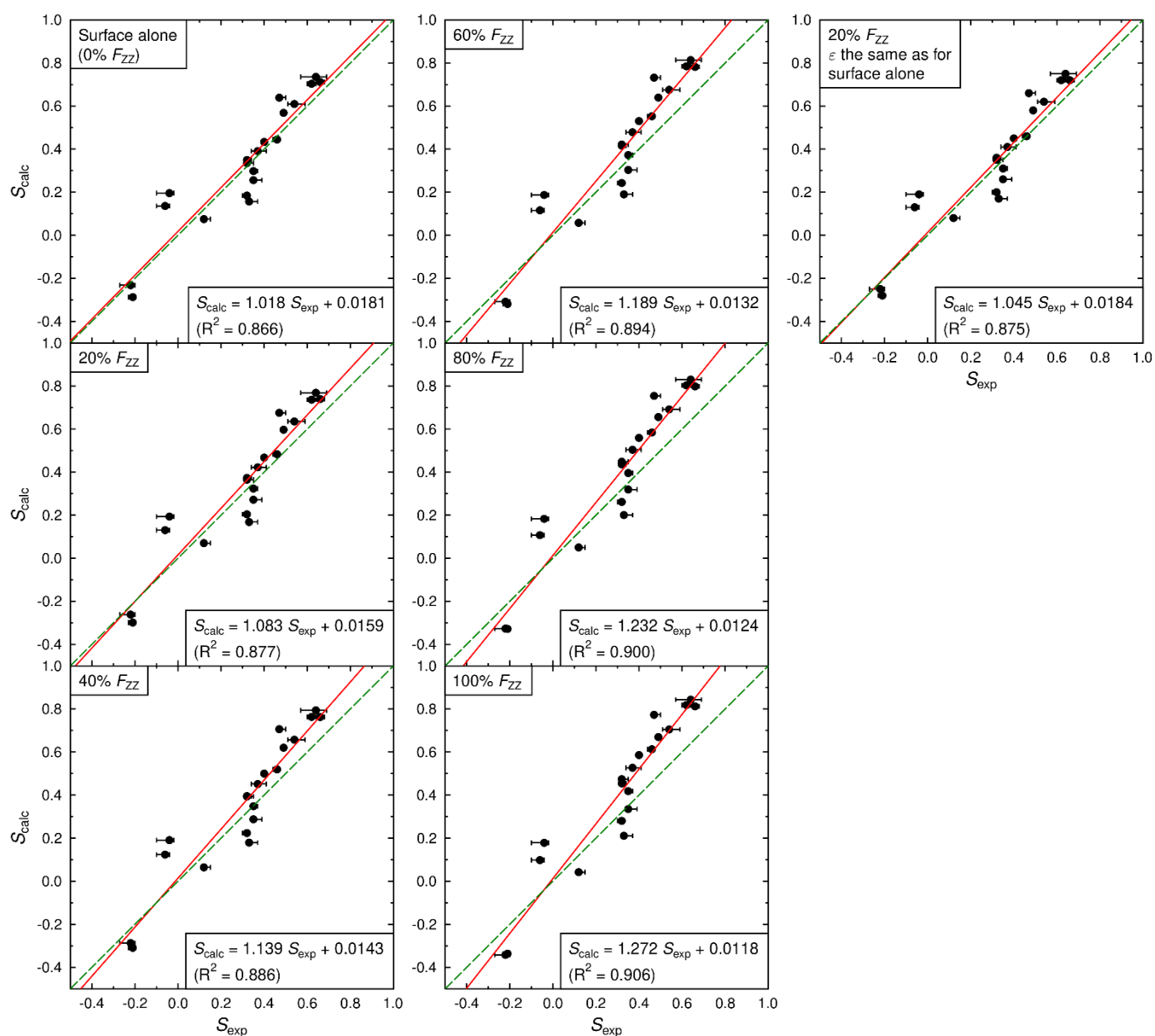


Figure S2. Plots of dichroic order parameters calculated using the surface tensor alone and the combined surface tensor and quadrupole model against experimental values for a range of F_{ZZ} scaling factors, along with linear fits to the data; bars correspond to the maximum and minimum experimental values given in Table S1. The dashed green line corresponds to $S_{\text{calc}} = S_{\text{exp}}$. Also shown (top right) is an equivalent plot for an F_{ZZ} scaling factor of 20% but where the orienting strength for the surface tensor component (ϵ) was not refitted for the combined surface and quadrupole model.