# Neighbouring group participation vs. addition to oxacarbenium ions: studies on the synthesis of mycobacterial oligosaccharides

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## Supporting information

**Crystal Structure Determination of compound 8**

Measurements were carried out at 150 K on a Bruker-Nonius Apex X8 diffractometer equipped with an Apex II CCD detector and using graphite monochromated Mo-Kα radiation from a FR591 rotating anode generator. The structure was solved by direct methods and refined using SHELXL-97. Compound **8** crystallises in the chiral space group $P2_12_12_1$ and the configuration was established on the basis of the refined Flack parameter and of the known stereochemistry of the D-xylofuranose starting material from which **8** was prepared. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms could be located in a difference Fourier map but, in the final stages of the refinement, they were placed in calculated positions and refined using a riding model.

The structure has been deposited at the Cambridge Crystallographic Data Centre and information on the structure can be obtained by quoting the CCDC code 735329 at:
http://www.ccdc.cam.ac.uk/deposit

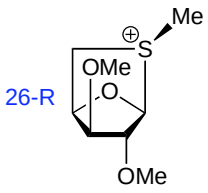
Telephone: (44) 01223 762910
Facsimile: (44) 01223 336033
Postal Address: CCDC, 12 Union Road, CAMBRIDGE CB2 1EZ, UK

**Table S1. Crystal data and structure refinement for compound 8.**

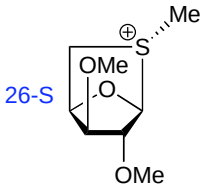
| | | |
|---|---|---|
| CCDC code | 735329 | |
| Formula | $C_{19}H_{20}O_3S$ | |
| Formula weight | 328.41 | |
| Size | 0.24 x 0.17 x 0.05 mm | |
| Crystal morphology | Colourless fragment | |
| Temperature | 150K | |
| Wavelength | 0.71073 Å [Mo-$K_\alpha$] | |
| Crystal system | Orthorhombic | |
| Space group | $P2_12_12_1$ | |
| Unit cell dimensions | $a$ = 5.6114(4) Å | α = 90° |
| | $b$ = 11.6946(9) Å | β = 90° |
| | $c$ = 25.505(2) Å | γ = 90° |
| Volume | 1673.7(2) Å$^3$ | |
| $Z$ | 4 | |
| Density (calculated) | 1.303 Mg/m$^3$ | |
| Absorption coefficient | 0.206 mm$^{-1}$ | |
| $F$(000) | 696 | |
| Data collection range | 2.96 ≤ θ ≤ 29.39° | |
| Index ranges | $-7 \le h \le 4$, $-16 \le k \le 16$, $-31 \le l \le 34$ | |
| Reflections collected | 12065 | |
| Independent reflections | 4551 [$R$(int) = 0.0414] | |
| Observed reflections | 3551 [$I > 2\sigma(I)$] | |
| Absorption correction | none | |
| Refinement method | Full | |
| Data / restraints / parameters | 4551 / 0 / 208 | |
| Goodness of fit | 1.045 | |
| Final $R$ indices [$I > 2\sigma(I)$] | $R_1$ = 0.0437, $wR_2$ = 0.0972 | |
| $R$ indices (all data) | $R_1$ = 0.0626, $wR_2$ = 0.1051 | |
| Largest diff. peak and hole | 0.331 and -0.281e.Å$^{-3}$ | |
| Absolute structure parameter | -0.03(8) | |

**Density Functional Theory Structures and Energies for MTX Derivatives**

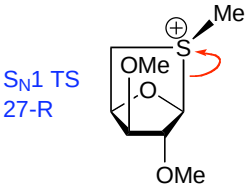
Structures of intermediates and transition states are labeled according to Figure S1



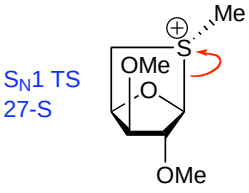

REACTANT_ENDO_ME_X



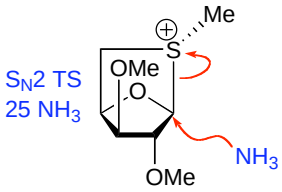

REACTANT_EXO_ME_X



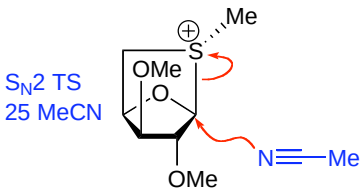

REACTANT_ENDO_ME_X_SN1



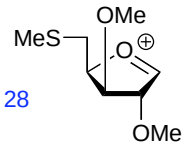

REACTANT_EXO_ME_X_SN1



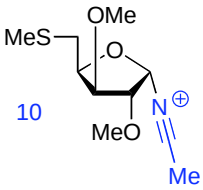

REACTANT_EXO_ME_X_NH3_SN2



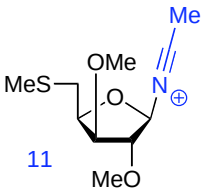

REACTANT_EXO_ME_X_MeCN_SN2



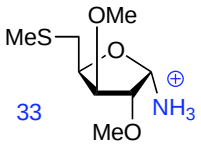

OXACARBENIUMX



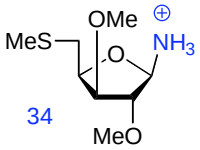

MeCN_ADDUCT_1_X




MeCN_ADDUCT_2_X




AMMONIA_ADDUCT_1_CONF_X




AMMONIA_ADDUCT_2_CONF_X

**Figure S1.** Structures and file names for structures from DFT calculations. X represents the conformation number for that structure.

ammonia

| | | | |
|---|---|---|---|
| Sum of electronic and zero-point Energies= | | | -56.513437 |
| Sum of electronic and thermal Energies= | | | -56.510579 |
| Sum of electronic and thermal Enthalpies= | | | -56.509635 |
| Sum of electronic and thermal Free Energies= | | | -56.532517 |
| Zero-point correction= | | 0.034510 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | | = | -2.55 |

Coordinates:

| | | | |
|---|---|---|---|
| N | -0.000004 | -0.000338 | -0.119192 |
| H | 0.001371 | 0.939270 | 0.277447 |
| H | 0.813202 | -0.469631 | 0.278443 |
| H | -0.814547 | -0.467275 | 0.278454 |

MeCN

| | | | |
|---|---|---|---|
| Sum of electronic and zero-point Energies= | | | -132.709286 |
| Sum of electronic and thermal Energies= | | | -132.705692 |
| Sum of electronic and thermal Enthalpies= | | | -132.704748 |
| Sum of electronic and thermal Free Energies= | | | -132.733302 |
| Zero-point correction= | | 0.045641 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | | = | -2.94 |

Coordinates:

| | | | |
|---|---|---|---|
| C | -1.181408 | 0.000003 | -0.000029 |
| C | 0.280611 | -0.000019 | 0.000119 |
| N | 1.441004 | 0.000006 | -0.000050 |
| H | -1.560882 | -0.217751 | 1.003207 |
| H | -1.560665 | 0.977775 | -0.313109 |
| H | -1.560697 | -0.759971 | -0.690289 |

REACTANT_ENDO_ME_1

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.207997 |
| Sum of electronic and thermal Energies= | | -937.195024 |
| Sum of electronic and thermal Enthalpies= | | -937.194080 |
| Sum of electronic and thermal Free Energies= | | -937.247075 |
| Zero-point correction= | 0.230848 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.22 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.586626 | -1.361204 | -1.360556 |
| C | 0.541750 | 0.063434 | -1.574360 |
| C | 1.865020 | 0.575699 | -0.962666 |
| S | 2.074372 | -0.471730 | 0.552844 |
| C | 1.701180 | 0.659936 | 1.941121 |
| C | -0.700985 | 0.522024 | -0.759370 |
| O | -0.474513 | 1.811634 | -0.242459 |
| C | -1.659860 | 2.575144 | 0.010047 |
| C | -0.822260 | -0.608176 | 0.329705 |
| O | -1.896380 | -1.484549 | 0.131444 |
| C | -3.132276 | -1.060767 | 0.708923 |
| C | 0.417429 | -1.445359 | -0.003585 |
| H | 0.485884 | 0.252919 | -2.645860 |
| H | -1.590824 | 0.493444 | -1.399947 |
| H | -0.824266 | -0.184941 | 1.343332 |
| H | 0.477269 | -2.465005 | 0.370707 |
| H | 2.714872 | 0.362792 | -1.612279 |
| H | 1.837815 | 1.630258 | -0.686892 |
| H | 2.626227 | 1.198578 | 2.161077 |
| H | 0.901751 | 1.349037 | 1.665974 |
| H | 1.431275 | 0.045576 | 2.803352 |
| H | -2.249638 | 2.688834 | -0.907651 |
| H | -2.280844 | 2.110469 | 0.786863 |
| H | -1.327301 | 3.556120 | 0.351921 |
| H | -3.846885 | -1.861773 | 0.516885 |
| H | -3.031130 | -0.913106 | 1.792918 |
| H | -3.500003 | -0.134174 | 0.247776 |

REACTANT_ENDO_ME_1_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.183200 |
| Sum of electronic and thermal Energies= | | -937.169469 |
| Sum of electronic and thermal Enthalpies= | | -937.168525 |
| Sum of electronic and thermal Free Energies= | | -937.224766 |
| Zero-point correction= | 0.228229 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.57 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.381104 | -1.022729 | -1.393281 |
| C | 0.457647 | 0.478534 | -1.129951 |
| C | 1.571973 | 0.795865 | -0.121738 |
| S | 2.758517 | -0.601152 | 0.073974 |
| C | 3.959163 | 0.216703 | 1.181526 |
| C | -0.981750 | 0.743715 | -0.616632 |
| O | -1.003173 | 1.889029 | 0.157104 |
| C | -2.287673 | 2.521232 | 0.282622 |
| C | -1.307840 | -0.590822 | 0.150984 |
| O | -2.653146 | -0.942949 | 0.053534 |
| C | -3.177687 | -1.699877 | 1.158604 |
| C | -0.476838 | -1.553820 | -0.637984 |
| H | 0.665302 | 0.877857 | -2.120478 |
| H | -1.678191 | 0.801702 | -1.466819 |
| H | -0.943667 | -0.508883 | 1.188208 |
| H | -0.624492 | -2.629764 | -0.737548 |
| H | 2.104031 | 1.675222 | -0.496039 |
| H | 1.144087 | 1.060697 | 0.848301 |
| H | 4.435706 | 1.064800 | 0.683803 |
| H | 3.484038 | 0.537466 | 2.112485 |
| H | 4.719289 | -0.533967 | 1.410256 |
| H | -2.693211 | 2.771958 | -0.704945 |
| H | -2.995105 | 1.877321 | 0.816900 |
| H | -2.116034 | 3.434116 | 0.852872 |
| H | -4.239500 | -1.832845 | 0.952236 |
| H | -2.696106 | -2.682685 | 1.235375 |
| H | -3.042657 | -1.150540 | 2.098354 |

REACTANT_ENDO_ME_1_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.175120 |
| Sum of electronic and thermal Energies= | | -937.161527 |
| Sum of electronic and thermal Enthalpies= | | -937.160582 |
| Sum of electronic and thermal Free Energies= | | -937.215839 |
| Zero-point correction= | 0.228007 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.86 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.558237 | -2.042853 | -0.997857 |
| C | 0.508175 | -0.940568 | -1.006150 |
| C | 1.579400 | -1.379672 | 0.026388 |
| S | 2.328904 | -0.166533 | 1.166361 |
| C | 3.398401 | 0.799805 | 0.044647 |
| C | -0.433159 | 0.282715 | -0.797267 |
| O | 0.225112 | 1.435662 | -0.442933 |
| C | -0.427728 | 2.655407 | -0.839282 |
| C | -1.466253 | -0.287948 | 0.241635 |
| O | -2.718486 | 0.309322 | 0.133972 |
| C | -3.467774 | 0.404168 | 1.358942 |
| C | -1.525964 | -1.695157 | -0.262739 |
| H | 0.897739 | -0.984210 | -2.022300 |
| H | -0.994958 | 0.416373 | -1.736756 |
| H | -1.024407 | -0.231077 | 1.249439 |
| H | -2.364091 | -2.389453 | -0.187229 |
| H | 1.130983 | -2.118165 | 0.699308 |
| H | 2.367789 | -1.905053 | -0.520923 |
| H | 4.067919 | 0.142523 | -0.517310 |
| H | 2.805423 | 1.422563 | -0.627658 |
| H | 4.003837 | 1.443450 | 0.687786 |
| H | -0.576163 | 2.679422 | -1.926121 |
| H | -1.391871 | 2.765541 | -0.332946 |
| H | 0.241993 | 3.461322 | -0.539875 |
| H | -4.380433 | 0.945098 | 1.109857 |
| H | -3.726764 | -0.589545 | 1.745056 |
| H | -2.897151 | 0.956191 | 2.115389 |

REACTANT_ENDO_ME_2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.207250 |
| Sum of electronic and thermal Energies= | | -937.194192 |
| Sum of electronic and thermal Enthalpies= | | -937.193247 |
| Sum of electronic and thermal Free Energies= | | -937.246537 |
| Zero-point correction= | 0.230762 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.43 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.357322 | -0.953200 | -1.687557 |
| C | 0.419170 | 0.467327 | -1.443712 |
| C | 1.800320 | 0.676347 | -0.781207 |
| S | 1.994832 | -0.812313 | 0.304598 |
| C | 1.776002 | -0.167283 | 2.004684 |
| C | -0.753763 | 0.717343 | -0.438014 |
| O | -0.486855 | 1.711383 | 0.520706 |
| C | -0.842690 | 3.042992 | 0.125211 |
| C | -0.897019 | -0.679576 | 0.254964 |
| O | -2.059477 | -1.375234 | -0.094291 |
| C | -3.220182 | -0.995169 | 0.650240 |
| C | 0.240559 | -1.451432 | -0.417126 |
| H | 0.341502 | 0.980185 | -2.402260 |
| H | -1.673195 | 0.931804 | -0.996011 |

| | | | |
|---|---|---|---|
| H | -0.799847 | -0.579286 | 1.343657 |
| H | 0.230666 | -2.538636 | -0.383807 |
| H | 2.608730 | 0.642506 | -1.512553 |
| H | 1.863742 | 1.579136 | -0.172757 |
| H | 2.751327 | 0.211005 | 2.320738 |
| H | 1.022688 | 0.621342 | 2.025324 |
| H | 1.496921 | -1.010646 | 2.640806 |
| H | -0.661853 | 3.680728 | 0.991416 |
| H | -0.233577 | 3.394786 | -0.717952 |
| H | -1.903225 | 3.093366 | -0.149628 |
| H | -4.025800 | -1.644418 | 0.306159 |
| H | -3.062061 | -1.143167 | 1.726994 |
| H | -3.495644 | 0.051420 | 0.465201 |

REACTANT_ENDO_ME_2_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.182618 | |
| Sum of electronic and thermal Energies= | -937.168918 | |
| Sum of electronic and thermal Enthalpies= | -937.167974 | |
| Sum of electronic and thermal Free Energies= | -937.224248 | |
| Zero-point correction= | 0.228212 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.28 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.363670 | -1.113061 | -1.416758 |
| C | 0.375745 | 0.393009 | -1.116696 |
| C | 1.494621 | 0.736075 | -0.125393 |
| S | 2.716774 | -0.629531 | 0.081513 |
| C | 3.840961 | 0.192889 | 1.263270 |
| C | -1.076534 | 0.580426 | -0.559787 |
| O | -1.230161 | 1.590731 | 0.379133 |
| C | -1.479329 | 2.897444 | -0.164743 |
| C | -1.348652 | -0.798043 | 0.118017 |
| O | -2.662640 | -1.231239 | 0.122670 |
| C | -3.379218 | -1.015028 | 1.355673 |
| C | -0.505861 | -1.695862 | -0.721313 |
| H | 0.551070 | 0.808953 | -2.107024 |
| H | -1.778465 | 0.689796 | -1.399674 |
| H | -0.891576 | -0.774671 | 1.126993 |
| H | -0.605240 | -2.776215 | -0.833299 |
| H | 2.008083 | 1.623190 | -0.509175 |
| H | 1.061151 | 0.996568 | 0.844226 |
| H | 4.309691 | 1.071356 | 0.812980 |
| H | 3.317922 | 0.467162 | 2.183315 |
| H | 4.616315 | -0.539571 | 1.500199 |
| H | -1.666477 | 3.547594 | 0.689935 |
| H | -0.611910 | 3.271899 | -0.722266 |
| H | -2.360296 | 2.883167 | -0.817591 |
| H | -4.394132 | -1.365756 | 1.170241 |
| H | -2.931465 | -1.596650 | 2.170072 |
| H | -3.390398 | 0.048773 | 1.612317 |

REACTANT_ENDO_ME_2_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.175120 | |
| Sum of electronic and thermal Energies= | -937.161527 | |
| Sum of electronic and thermal Enthalpies= | -937.160583 | |
| Sum of electronic and thermal Free Energies= | -937.215841 | |
| Zero-point correction= | 0.228006 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.86 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.558681 | -2.042737 | -0.997736 |
| C | 0.507882 | -0.940666 | -1.006149 |
| C | 1.579207 | -1.379907 | 0.026219 |
| S | 2.328622 | -0.166776 | 1.166266 |
| C | 3.398762 | 0.799176 | 0.044821 |
| C | -0.433085 | 0.282835 | -0.797042 |
| O | 0.225652 | 1.435466 | -0.442497 |
| C | -0.426348 | 2.655533 | -0.839199 |
| C | -1.466400 | -0.287615 | 0.241727 |
| O | -2.718538 | 0.309824 | 0.133699 |
| C | -3.468355 | 0.404381 | 1.358369 |
| C | -1.526290 | -1.694856 | -0.262543 |
| H | 0.897325 | -0.984239 | -2.022350 |
| H | -0.994887 | 0.416880 | -1.736471 |
| H | -1.024786 | -0.230685 | 1.249613 |
| H | -2.364504 | -2.389036 | -0.186935 |
| H | 1.130746 | -2.118364 | 0.699156 |
| H | 2.367537 | -1.905348 | -0.521109 |
| H | 4.068161 | 0.141634 | -0.516979 |
| H | 2.806190 | 1.422159 | -0.627631 |
| H | 4.004292 | 1.442582 | 0.688109 |
| H | 0.243771 | 3.461098 | -0.539736 |
| H | -0.574481 | 2.679475 | -1.926082 |
| H | -1.390566 | 2.766347 | -0.333147 |
| H | -4.380722 | 0.945721 | 1.109109 |
| H | -3.727843 | -0.589415 | 1.743934 |
| H | -2.897884 | 0.955888 | 2.115309 |

REACTANT_ENDO_ME_3

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.209536 | |
| Sum of electronic and thermal Energies= | -937.196524 | |
| Sum of electronic and thermal Enthalpies= | -937.195580 | |
| Sum of electronic and thermal Free Energies= | -937.248484 | |
| Zero-point correction= | 0.230878 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.20 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.273070 | -1.120657 | -1.587644 |
| C | 0.612077 | 0.280781 | -1.556141 |
| C | 1.980228 | 0.321121 | -0.839383 |
| S | 1.829235 | -0.971392 | 0.478786 |
| C | 1.672974 | -0.011587 | 2.029960 |
| C | -0.522831 | 0.911245 | -0.705374 |
| O | -0.023399 | 2.004814 | 0.022702 |
| C | -1.019531 | 2.961153 | 0.410602 |
| C | -0.996828 | -0.288419 | 0.179205 |
| O | -2.287647 | -0.661660 | -0.213801 |
| C | -3.005976 | -1.466672 | 0.724739 |
| C | -0.002196 | -1.373459 | -0.271605 |
| H | 0.676606 | 0.647167 | -2.580075 |
| H | -1.358542 | 1.200926 | -1.353643 |
| H | -0.949572 | -0.051695 | 1.249560 |
| H | -0.209616 | -2.424948 | -0.083287 |
| H | 2.787506 | 0.003715 | -1.500550 |
| H | 2.203240 | 1.288597 | -0.388289 |
| H | 2.689428 | 0.219630 | 2.357778 |
| H | 1.100612 | 0.900783 | 1.857429 |
| H | 1.196687 | -0.656506 | 2.772144 |
| H | -0.489738 | 3.766150 | 0.921419 |
| H | -1.533836 | 3.361008 | -0.471377 |
| H | -1.757918 | 2.518041 | 1.090738 |
| H | -4.000802 | -1.609602 | 0.301798 |
| H | -2.536521 | -2.448795 | 0.869434 |
| H | -3.088982 | -0.957145 | 1.694258 |

REACTANT_ENDO_ME_3_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.183200 | |
| Sum of electronic and thermal Energies= | -937.169469 | |
| Sum of electronic and thermal Enthalpies= | -937.168525 | |
| Sum of electronic and thermal Free Energies= | -937.224766 | |
| Zero-point correction= | 0.228229 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.57 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.381104 | -1.022728 | -1.393281 |
| C | 0.457647 | 0.478535 | -1.129950 |
| C | 1.571973 | 0.795866 | -0.121739 |
| S | 2.758516 | -0.601152 | 0.073974 |
| C | 3.959163 | 0.216701 | 1.181526 |
| C | -0.981750 | 0.743715 | -0.616631 |
| O | -1.003173 | 1.889028 | 0.157107 |
| C | -2.287673 | 2.521233 | 0.282622 |
| C | -1.307840 | -0.590823 | 0.150984 |
| O | -2.653146 | -0.942949 | 0.053535 |
| C | -3.177687 | -1.699879 | 1.158603 |
| C | -0.476838 | -1.553820 | -0.637985 |
| H | 0.665301 | 0.877859 | -2.120477 |
| H | -1.678191 | 0.801703 | -1.466818 |
| H | -0.943667 | -0.508885 | 1.188208 |
| H | -0.624493 | -2.629764 | -0.737552 |
| H | 2.104033 | 1.675221 | -0.496041 |
| H | 1.144088 | 1.060700 | 0.848301 |
| H | 4.435707 | 1.064799 | 0.683803 |
| H | 3.484038 | 0.537464 | 2.112485 |
| H | 4.719289 | -0.533969 | 1.410256 |
| H | -2.116034 | 3.434116 | 0.852874 |
| H | -2.693207 | 2.771962 | -0.704946 |
| H | -2.995107 | 1.877322 | 0.816897 |
| H | -4.239499 | -1.832847 | 0.952236 |
| H | -2.696105 | -2.682687 | 1.235373 |
| H | -3.042656 | -1.150543 | 2.098355 |

REACTANT_ENDO_ME_3_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.175120 |
| Sum of electronic and thermal Energies= | | -937.161527 |
| Sum of electronic and thermal Enthalpies= | | -937.160582 |
| Sum of electronic and thermal Free Energies= | | -937.215839 |
| Zero-point correction= | 0.228007 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.86 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.558244 | -2.042843 | -0.997868 |
| C | 0.508173 | -0.940561 | -1.006157 |
| C | 1.579397 | -1.379676 | 0.026378 |
| S | 2.328903 | -0.166550 | 1.166362 |
| C | 3.398398 | 0.799801 | 0.044657 |
| C | -0.433157 | 0.282724 | -0.797266 |
| O | 0.225118 | 1.435667 | -0.442927 |
| C | -0.427716 | 2.655416 | -0.839273 |
| C | -1.466251 | -0.287941 | 0.241635 |
| O | -2.718482 | 0.309334 | 0.133977 |
| C | -3.467780 | 0.404148 | 1.358944 |
| C | -1.525968 | -1.695148 | -0.262748 |
| H | 0.897735 | -0.984199 | -2.022308 |
| H | -0.994956 | 0.416389 | -1.736754 |
| H | -1.024404 | -0.231078 | 1.249439 |
| H | -2.364098 | -2.389441 | -0.187239 |
| H | 1.130977 | -2.118174 | 0.699291 |
| H | 2.367783 | -1.905055 | -0.520938 |
| H | 4.067918 | 0.142527 | -0.517306 |
| H | 2.805419 | 1.422565 | -0.627642 |
| H | 4.003832 | 1.443441 | 0.687803 |
| H | 0.242008 | 3.461327 | -0.539861 |
| H | -0.576148 | 2.679435 | -1.926113 |
| H | -1.391861 | 2.765552 | -0.332940 |
| H | -4.380438 | 0.945081 | 1.109866 |
| H | -3.726768 | -0.589575 | 1.745031 |
| H | -2.897163 | 0.956154 | 2.115409 |

REACTANT_ENDO_ME_4

| | | | |
|---|---|---|---|
| Sum of electronic and zero-point Energies= | | | -937.204356 |
| Sum of electronic and thermal Energies= | | | -937.191535 |
| Sum of electronic and thermal Enthalpies= | | | -937.190591 |
| Sum of electronic and thermal Free Energies= | | | -937.242805 |
| Zero-point correction= | | 0.231325 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | | = | -35.64 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.130246 | -1.503109 | 1.072841 |
| C | -0.147782 | -0.160187 | 1.527377 |
| C | -1.663346 | 0.012574 | 1.281199 |
| S | -1.950322 | -0.870493 | -0.322423 |
| C | -2.223704 | 0.472139 | -1.535304 |
| C | 0.711317 | 0.729860 | 0.588301 |
| O | 0.051884 | 1.950734 | 0.351830 |
| C | 0.918988 | 3.014252 | -0.068303 |
| C | 0.850352 | -0.160503 | -0.699647 |
| O | 2.142675 | -0.530164 | -1.089659 |
| C | 2.963560 | -1.279341 | -0.184046 |
| C | -0.010741 | -1.368047 | -0.287683 |
| H | 0.104280 | -0.094559 | 2.585550 |
| H | 1.697396 | 0.901727 | 1.035897 |
| H | 0.448540 | 0.375447 | -1.561935 |
| H | 0.095952 | -2.311646 | -0.819863 |
| H | -2.253123 | -0.508035 | 2.036642 |
| H | -1.971400 | 1.055027 | 1.194827 |
| H | -3.284646 | 0.728528 | -1.481618 |
| H | -1.598778 | 1.332712 | -1.293828 |
| H | -2.001072 | 0.071966 | -2.527351 |
| H | 0.287468 | 3.895138 | -0.189840 |
| H | 1.681549 | 3.212294 | 0.694775 |
| H | 1.410437 | 2.778768 | -1.020428 |
| H | 3.929334 | -1.366860 | -0.682677 |
| H | 3.103602 | -0.763993 | 0.773666 |
| H | 2.565314 | -2.282786 | 0.003488 |

REACTANT_ENDO_ME_4_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.176813 |
| Sum of electronic and thermal Energies= | | -937.163187 |
| Sum of electronic and thermal Enthalpies= | | -937.162242 |
| Sum of electronic and thermal Free Energies= | | -937.217885 |
| Zero-point correction= | 0.228207 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.03 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.305321 | -1.380090 | 0.954352 |
| C | -0.360558 | 0.145213 | 1.129210 |
| C | -1.584184 | 0.718983 | 0.397471 |
| S | -2.790596 | -0.585347 | -0.097263 |
| C | -4.070567 | 0.497619 | -0.822700 |
| C | 1.014753 | 0.559619 | 0.541496 |
| O | 0.945567 | 1.857412 | 0.064495 |
| C | 2.212398 | 2.500131 | -0.152256 |
| C | 1.228995 | -0.538785 | -0.573759 |
| O | 2.493352 | -0.822930 | -1.063862 |
| C | 3.486208 | -1.245019 | -0.114023 |
| C | 0.494552 | -1.691337 | 0.036344 |
| H | -0.438524 | 0.243097 | 2.209953 |
| H | 1.791947 | 0.449803 | 1.312798 |
| H | 0.624970 | -0.218972 | -1.441482 |
| H | 0.598182 | -2.752527 | -0.197756 |
| H | -2.068915 | 1.420354 | 1.082655 |
| H | -1.265974 | 1.283827 | -0.481563 |
| H | -4.501705 | 1.156474 | -0.065026 |
| H | -3.667766 | 1.082007 | -1.654179 |
| H | -4.850307 | -0.168175 | -1.199953 |
| H | 1.979945 | 3.520070 | -0.458341 |

| | | | |
|---|---|---|---|
| H | 2.798568 | 2.521394 | 0.775329 |
| H | 2.779523 | 1.997520 | -0.943492 |
| H | 4.335795 | -1.579209 | -0.709318 |
| H | 3.802581 | -0.420171 | 0.533277 |
| H | 3.132839 | -2.083607 | 0.502731 |

REACTANT_ENDO_ME_4_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.167785 | |
| Sum of electronic and thermal Energies= | -937.154296 | |
| Sum of electronic and thermal Enthalpies= | -937.153352 | |
| Sum of electronic and thermal Free Energies= | -937.208082 | |
| Zero-point correction= | 0.227882 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -40.07 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.641354 | -2.073616 | 0.708104 |
| C | -0.369635 | -0.929554 | 0.931949 |
| C | -1.636099 | -1.351918 | 0.134969 |
| S | -2.550148 | -0.161939 | -0.902981 |
| C | -3.384334 | 0.870174 | 0.351300 |
| C | 0.535859 | 0.281774 | 0.557788 |
| O | -0.189093 | 1.414793 | 0.262795 |
| C | 0.548952 | 2.645716 | 0.327411 |
| C | 1.402682 | -0.317552 | -0.615636 |
| O | 2.596334 | 0.273077 | -0.998374 |
| C | 3.608783 | 0.429772 | 0.009852 |
| C | 1.511976 | -1.731113 | -0.134952 |
| H | -0.550577 | -0.983527 | 2.004520 |
| H | 1.204927 | 0.453942 | 1.418413 |
| H | 0.756856 | -0.325410 | -1.511100 |
| H | 2.267686 | -2.473122 | -0.400625 |
| H | -1.350512 | -2.140010 | -0.569617 |
| H | -2.323381 | -1.818257 | 0.847167 |
| H | -3.969641 | 0.252311 | 1.038324 |
| H | -2.667336 | 1.488336 | 0.894695 |
| H | -4.069256 | 1.518354 | -0.201285 |
| H | -0.178104 | 3.438130 | 0.150812 |
| H | 1.000316 | 2.776347 | 1.319985 |
| H | 1.322616 | 2.679793 | -0.446893 |
| H | 4.510374 | 0.726111 | -0.526084 |
| H | 3.344181 | 1.211304 | 0.729863 |
| H | 3.806350 | -0.511099 | 0.543229 |

REACTANT_ENDO_ME_5

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.208329 | |
| Sum of electronic and thermal Energies= | -937.195202 | |
| Sum of electronic and thermal Enthalpies= | -937.194258 | |
| Sum of electronic and thermal Free Energies= | -937.247716 | |
| Zero-point correction= | 0.230721 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.39 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.175505 | -0.747251 | -1.757341 |
| C | 0.645357 | 0.389438 | -1.416279 |
| C | 1.911316 | -0.234911 | -0.785914 |
| S | 1.263104 | -1.664730 | 0.195530 |
| C | 1.402881 | -1.117527 | 1.938710 |
| C | -0.217556 | 1.158036 | -0.361997 |
| O | 0.533785 | 1.768440 | 0.657684 |
| C | 0.903559 | 3.130910 | 0.402617 |
| C | -1.109921 | 0.028778 | 0.230478 |
| O | -2.436815 | 0.246594 | -0.159457 |
| C | -3.421935 | -0.420009 | 0.634967 |
| C | -0.564756 | -1.194706 | -0.524964 |
| H | 0.869145 | 0.935339 | -2.332557 |
| H | -0.873932 | 1.874819 | -0.868094 |
| H | -1.010522 | -0.027168 | 1.320424 |
| H | -1.143803 | -2.114336 | -0.577163 |
| H | 2.578012 | -0.647926 | -1.543838 |
| H | 2.448685 | 0.445293 | -0.124300 |
| H | 2.425556 | -1.339110 | 2.253525 |
| H | 1.186459 | -0.052221 | 2.027376 |
| H | 0.709711 | -1.721933 | 2.528538 |
| H | 1.406417 | 3.486056 | 1.303015 |
| H | 1.588025 | 3.213361 | -0.451817 |
| H | 0.013583 | 3.743202 | 0.215834 |
| H | -4.389502 | -0.099801 | 0.247421 |
| H | -3.348665 | -1.512648 | 0.550095 |
| H | -3.334220 | -0.129558 | 1.690259 |

REACTANT_ENDO_ME_5_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.182618 | |
| Sum of electronic and thermal Energies= | -937.168918 | |
| Sum of electronic and thermal Enthalpies= | -937.167974 | |
| Sum of electronic and thermal Free Energies= | -937.224249 | |
| Zero-point correction= | 0.228212 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.28 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.363660 | -1.113061 | -1.416755 |
| C | 0.375747 | 0.393011 | -1.116695 |
| C | 1.494623 | 0.736068 | -0.125390 |
| S | 2.716751 | -0.629557 | 0.081530 |
| C | 3.840984 | 0.192871 | 1.263237 |
| C | -1.076529 | 0.580441 | -0.559784 |
| O | -1.230140 | 1.590743 | 0.379142 |
| C | -1.479281 | 2.897463 | -0.164729 |
| C | -1.348663 | -0.798027 | 0.118015 |
| O | -2.662655 | -1.231210 | 0.122652 |
| C | -3.379235 | -1.015044 | 1.355662 |
| C | -0.505877 | -1.695855 | -0.721310 |
| H | 0.551078 | 0.808948 | -2.107025 |
| H | -1.778462 | 0.689824 | -1.399668 |
| H | -0.891597 | -0.774660 | 1.126996 |
| H | -0.605263 | -2.776207 | -0.833292 |
| H | 2.008098 | 1.623178 | -0.509169 |
| H | 1.061152 | 0.996567 | 0.844226 |
| H | 4.309718 | 1.071318 | 0.812913 |
| H | 3.317973 | 0.467176 | 2.183289 |
| H | 4.616331 | -0.539597 | 1.500164 |
| H | -1.666418 | 3.547613 | 0.689952 |
| H | -0.611855 | 3.271903 | -0.722250 |
| H | -2.360248 | 2.883207 | -0.817578 |
| H | -4.394149 | -1.365764 | 1.170216 |
| H | -2.931484 | -1.596694 | 2.170042 |
| H | -3.390414 | 0.048748 | 1.612344 |

REACTANT_ENDO_ME_5_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.175120 | |
| Sum of electronic and thermal Energies= | -937.161527 | |
| Sum of electronic and thermal Enthalpies= | -937.160582 | |
| Sum of electronic and thermal Free Energies= | -937.215839 | |
| Zero-point correction= | 0.228007 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.86 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.558238 | -2.042852 | -0.997859 |
| C | 0.508175 | -0.940567 | -1.006151 |
| C | 1.579400 | -1.379673 | 0.026387 |
| S | 2.328902 | -0.166535 | 1.166362 |
| C | 3.398400 | 0.799805 | 0.044650 |
| C | -0.433158 | 0.282716 | -0.797268 |
| O | 0.225113 | 1.435663 | -0.442933 |
| C | -0.427725 | 2.655408 | -0.839283 |

| | | | |
|---|---|---|---|
| C | -1.466253 | -0.287947 | 0.241635 |
| O | -2.718486 | 0.309323 | 0.133973 |
| C | -3.467773 | 0.404167 | 1.358944 |
| C | -1.525964 | -1.695156 | -0.262741 |
| H | 0.897739 | -0.984209 | -2.022301 |
| H | -0.994957 | 0.416375 | -1.736756 |
| H | -1.024406 | -0.231077 | 1.249438 |
| H | -2.364092 | -2.389451 | -0.187231 |
| H | 1.130982 | -2.118167 | 0.699305 |
| H | 2.367788 | -1.905053 | -0.520925 |
| H | 4.067919 | 0.142524 | -0.517308 |
| H | 2.805422 | 1.422563 | -0.627655 |
| H | 4.003835 | 1.443449 | 0.687790 |
| H | 0.241996 | 3.461322 | -0.539874 |
| H | -0.576158 | 2.679423 | -1.926122 |
| H | -1.391870 | 2.765543 | -0.332949 |
| H | -4.380432 | 0.945097 | 1.109860 |
| H | -3.726762 | -0.589547 | 1.745055 |
| H | -2.897150 | 0.956188 | 2.115392 |

REACTANT_ENDO_ME_6

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.202973 | |
| Sum of electronic and thermal Energies= | -937.190011 | |
| Sum of electronic and thermal Enthalpies= | -937.189066 | |
| Sum of electronic and thermal Free Energies= | -937.241949 | |
| Zero-point correction= | 0.231121 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.87 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.432140 | -1.085026 | 1.379736 |
| C | -0.070042 | 0.270006 | 1.418572 |
| C | -1.593391 | 0.110540 | 1.211971 |
| S | -1.729026 | -1.259466 | -0.027711 |
| C | -2.224327 | -0.427839 | -1.582732 |
| C | 0.619827 | 0.952537 | 0.191306 |
| O | -0.194759 | 1.886393 | -0.474746 |
| C | -0.052839 | 3.242949 | -0.030836 |
| C | 0.899013 | -0.262173 | -0.757629 |
| O | 2.233801 | -0.517803 | -1.087445 |
| C | 3.178536 | -0.785135 | -0.043984 |
| C | 0.265191 | -1.404018 | 0.053478 |
| H | 0.170202 | 0.691439 | 2.394830 |
| H | 1.564797 | 1.411118 | 0.503285 |
| H | 0.410472 | -0.088009 | -1.717311 |
| H | 0.530728 | -2.435482 | -0.170850 |
| H | -2.090170 | -0.234886 | 2.119397 |
| H | -2.077458 | 1.005439 | 0.819640 |
| H | -3.312521 | -0.333260 | -1.550092 |
| H | -1.745856 | 0.548508 | -1.668112 |
| H | -1.947202 | -1.088107 | -2.408156 |
| H | -0.689981 | 3.846070 | -0.678908 |
| H | -0.374657 | 3.366045 | 1.011641 |
| H | 0.987210 | 3.574626 | -0.132676 |
| H | 4.140755 | -0.876052 | -0.548780 |
| H | 3.235804 | 0.033971 | 0.683095 |
| H | 2.961029 | -1.719674 | 0.485145 |

REACTANT_ENDO_ME_6_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.176314 | |
| Sum of electronic and thermal Energies= | -937.162645 | |
| Sum of electronic and thermal Enthalpies= | -937.161700 | |
| Sum of electronic and thermal Free Energies= | -937.217830 | |
| Zero-point correction= | 0.228051 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.27 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.158744 | -1.268624 | 1.120875 |
| C | -0.263098 | 0.265768 | 1.039207 |
| C | -1.528180 | 0.672969 | 0.273870 |
| S | -2.704913 | -0.725990 | 0.029108 |
| C | -4.010334 | 0.177616 | -0.874398 |
| C | 1.084347 | 0.615085 | 0.319112 |
| O | 1.046657 | 1.734901 | -0.495105 |
| C | 1.315222 | 2.983094 | 0.161412 |
| C | 1.303907 | -0.649672 | -0.575650 |
| O | 2.554935 | -0.965079 | -1.066622 |
| C | 3.621111 | -1.092495 | -0.113977 |
| C | 0.639537 | -1.703185 | 0.254835 |
| H | -0.306568 | 0.531782 | 2.093640 |
| H | 1.880269 | 0.688112 | 1.074714 |
| H | 0.651872 | -0.517971 | -1.459868 |
| H | 0.775487 | -2.784640 | 0.195520 |
| H | -2.020160 | 1.460286 | 0.853535 |
| H | -1.250323 | 1.096915 | -0.694985 |
| H | -4.451965 | 0.958034 | -0.249732 |
| H | -3.625939 | 0.602953 | -1.805262 |
| H | -4.778294 | -0.562429 | -1.111770 |
| H | 1.343717 | 3.735717 | -0.626483 |
| H | 0.526788 | 3.238450 | 0.880434 |
| H | 2.285094 | 2.951388 | 0.672993 |
| H | 4.460502 | -1.508995 | -0.670532 |
| H | 3.911048 | -0.119784 | 0.297570 |
| H | 3.359222 | -1.778652 | 0.704852 |

REACTANT_ENDO_ME_6_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.167785 | |
| Sum of electronic and thermal Energies= | -937.154296 | |
| Sum of electronic and thermal Enthalpies= | -937.153352 | |
| Sum of electronic and thermal Free Energies= | -937.208082 | |
| Zero-point correction= | 0.227882 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -40.07 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.641355 | -2.073616 | 0.708103 |
| C | -0.369634 | -0.929554 | 0.931950 |
| C | -1.636099 | -1.351918 | 0.134971 |
| S | -2.550148 | -0.161940 | -0.902981 |
| C | -3.384333 | 0.870175 | 0.351299 |
| C | 0.535859 | 0.281774 | 0.557788 |
| O | -0.189094 | 1.414793 | 0.262795 |
| C | 0.548951 | 2.645716 | 0.327410 |
| C | 1.402682 | -0.317552 | -0.615636 |
| O | 2.596335 | 0.273076 | -0.998374 |
| C | 3.608783 | 0.429773 | 0.009853 |
| C | 1.511976 | -1.731113 | -0.134953 |
| H | -0.550574 | -0.983528 | 2.004521 |
| H | 1.204927 | 0.453943 | 1.418413 |
| H | 0.756857 | -0.325409 | -1.511101 |
| H | 2.267685 | -2.473123 | -0.400628 |
| H | -1.350514 | -2.140012 | -0.569613 |
| H | -2.323382 | -1.818255 | 0.847171 |
| H | -3.969640 | 0.252314 | 1.038323 |
| H | -2.667335 | 1.488338 | 0.894692 |
| H | -4.069256 | 1.518354 | -0.201288 |
| H | -0.178106 | 3.438130 | 0.150814 |
| H | 1.000316 | 2.776347 | 1.319984 |
| H | 1.322613 | 2.679795 | -0.446895 |
| H | 4.510376 | 0.726105 | -0.526083 |
| H | 3.344183 | 1.211309 | 0.729860 |
| H | 3.806345 | -0.511097 | 0.543235 |

REACTANT_EXO_ME_1

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.211961 | |

Sum of electronic and thermal Energies= -937.198936
Sum of electronic and thermal Enthalpies= -937.197992
Sum of electronic and thermal Free Energies= -937.251331
Zero-point correction= 0.230640 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -35.42
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.813165 | -0.743116 | 1.372433 |
| C | -0.403746 | 0.636731 | 1.319161 |
| C | -1.481229 | 1.326720 | 0.448173 |
| S | -1.784778 | 0.100641 | -0.909602 |
| C | -3.407306 | -0.596426 | -0.435994 |
| C | 0.965514 | 0.595675 | 0.582522 |
| O | 1.103520 | 1.774801 | -0.164948 |
| C | 2.442164 | 2.094734 | -0.550952 |
| C | 0.836693 | -0.715631 | -0.279392 |
| O | 1.638415 | -1.778485 | 0.153673 |
| C | 2.979115 | -1.756471 | -0.338938 |
| C | -0.595087 | -1.136612 | 0.075640 |
| H | -0.376384 | 1.037376 | 2.331977 |
| H | 1.777290 | 0.467632 | 1.310347 |
| H | 0.976122 | -0.496741 | -1.348490 |
| H | -0.893490 | -2.165352 | -0.120232 |
| H | -2.418180 | 1.472543 | 0.988310 |
| H | -1.130167 | 2.257406 | 0.004002 |
| H | -4.157957 | 0.186890 | -0.562975 |
| H | -3.622476 | -1.421541 | -1.118702 |
| H | -3.367903 | -0.939332 | 0.600011 |
| H | 2.390709 | 3.050342 | -1.074191 |
| H | 3.088078 | 2.194689 | 0.330612 |
| H | 2.860704 | 1.336051 | -1.225029 |
| H | 3.455151 | -2.662594 | 0.037333 |
| H | 2.994903 | -1.763590 | -1.437323 |
| H | 3.533172 | -0.881959 | 0.027398 |

REACTANT_EXO_ME_1_MeCN_SN2
Sum of electronic and zero-point Energies= -1069.921917
Sum of electronic and thermal Energies= -1069.903414
Sum of electronic and thermal Enthalpies= -1069.902469
Sum of electronic and thermal Free Energies= -1069.971687
Zero-point correction= 0.276513 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -32.81
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.124657 | -1.501823 | -0.220026 |
| C | 0.706931 | -0.563380 | -1.221281 |
| C | 2.227294 | -0.668381 | -1.175819 |
| S | 2.991797 | -0.332955 | 0.461731 |
| C | 3.418577 | -2.033882 | 0.990352 |
| C | 0.102892 | 0.817322 | -0.858348 |
| O | 1.077440 | 1.803816 | -1.025143 |
| C | 0.583613 | 3.145463 | -1.048147 |
| C | -0.404235 | 0.631724 | 0.593179 |
| O | -1.509201 | 1.433900 | 0.871431 |
| C | -1.738502 | 1.687375 | 2.261736 |
| C | -0.635240 | -0.877181 | 0.631263 |
| H | 0.344759 | -0.926552 | -2.186753 |
| H | -0.776407 | 1.024948 | -1.488504 |
| H | 0.435414 | 0.813322 | 1.283386 |
| H | -0.834662 | -1.432175 | 1.543846 |
| H | 2.532910 | -1.663311 | -1.511292 |
| H | 2.620933 | 0.062484 | -1.886404 |
| H | 4.142190 | -2.483754 | 0.305579 |
| H | 3.883377 | -1.941584 | 1.975333 |
| H | 2.533733 | -2.670027 | 1.072017 |
| H | 1.442287 | 3.778094 | -1.276158 |
| H | -0.180070 | 3.266515 | -1.828443 |
| H | 0.158277 | 3.437077 | -0.081552 |
| H | -2.565531 | 2.396973 | 2.310377 |
| H | -2.017741 | 0.772960 | 2.802464 |
| H | -0.851177 | 2.129027 | 2.732133 |
| C | -3.460560 | -1.225026 | -0.330393 |
| C | -4.818286 | -1.481456 | -0.784935 |
| H | -4.793121 | -2.008944 | -1.743921 |
| H | -5.342568 | -2.099270 | -0.048702 |
| H | -5.351161 | -0.532953 | -0.906662 |
| N | -2.384038 | -1.011166 | 0.027117 |

REACTANT_EXO_ME_1_SN1_A
Sum of electronic and zero-point Energies= -937.183200
Sum of electronic and thermal Energies= -937.169469
Sum of electronic and thermal Enthalpies= -937.168525
Sum of electronic and thermal Free Energies= -937.224766
Zero-point correction= 0.228229 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -37.57
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.381104 | -1.022731 | -1.393278 |
| C | 0.457648 | 0.478533 | -1.129950 |
| C | 1.571973 | 0.795865 | -0.121738 |
| S | 2.758515 | -0.601154 | 0.073976 |
| C | 3.959166 | 0.216704 | 1.181521 |
| C | -0.981750 | 0.743715 | -0.616632 |
| O | -1.003171 | 1.889029 | 0.157103 |
| C | -2.287671 | 2.521233 | 0.282622 |
| C | -1.307841 | -0.590821 | 0.150985 |
| O | -2.653147 | -0.942949 | 0.053532 |
| C | -3.177691 | -1.699875 | 1.158602 |
| C | -0.476837 | -1.553821 | -0.637980 |
| H | 0.665303 | 0.877854 | -2.120478 |
| H | -1.678191 | 0.801702 | -1.466819 |
| H | -0.943671 | -0.508881 | 1.188210 |
| H | -0.624492 | -2.629765 | -0.737542 |
| H | 2.104032 | 1.675220 | -0.496040 |
| H | 1.144087 | 1.060699 | 0.848301 |
| H | 3.484045 | 0.537470 | 2.112481 |
| H | 4.719293 | -0.533966 | 1.410250 |
| H | 4.435708 | 1.064800 | 0.683794 |
| H | -2.116031 | 3.434118 | 0.852870 |
| H | -2.693211 | 2.771957 | -0.704945 |
| H | -2.995102 | 1.877323 | 0.816902 |
| H | -4.239502 | -1.832846 | 0.952230 |
| H | -2.696107 | -2.682681 | 1.235378 |
| H | -3.042665 | -1.150534 | 2.098351 |

REACTANT_EXO_ME_1_SN1_B
Sum of electronic and zero-point Energies= -937.176047
Sum of electronic and thermal Energies= -937.162338
Sum of electronic and thermal Enthalpies= -937.161394
Sum of electronic and thermal Free Energies= -937.217436
Zero-point correction= 0.227940 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -37.83
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.369766 | -1.985769 | -1.138382 |
| C | 0.428088 | -0.686865 | -1.313530 |
| C | 1.725806 | -0.852868 | -0.498235 |
| S | 2.242586 | 0.584304 | 0.542842 |
| C | 3.777591 | -0.173702 | 1.184654 |
| C | -0.679005 | 0.323560 | -0.897538 |
| O | -0.166620 | 1.562758 | -0.615510 |
| C | -1.060968 | 2.672900 | -0.806349 |
| C | -1.357546 | -0.443161 | 0.301004 |
| O | -2.690102 | -0.095671 | 0.484475 |

| | | | |
|---|---|---|---|
| C | -3.158808 | -0.127429 | 1.844774 |
| C | -1.240735 | -1.830206 | -0.234776 |
| H | 0.626983 | -0.662306 | -2.383370 |
| H | -1.425783 | 0.363123 | -1.706951 |
| H | -0.720507 | -0.299764 | 1.191444 |
| H | -1.905641 | -2.672958 | -0.039228 |
| H | 1.616049 | -1.722748 | 0.159324 |
| H | 2.533014 | -1.089146 | -1.197637 |
| H | 4.482370 | -0.387366 | 0.376065 |
| H | 4.224579 | 0.569283 | 1.849873 |
| H | 3.573768 | -1.082891 | 1.757993 |
| H | -0.464982 | 3.566335 | -0.622820 |
| H | -1.443914 | 2.684740 | -1.833997 |
| H | -1.895871 | 2.627276 | -0.099707 |
| H | -4.185676 | 0.236239 | 1.815621 |
| H | -3.144705 | -1.148398 | 2.246051 |
| H | -2.545698 | 0.525799 | 2.477187 |

REACTANT_EXO_ME_1_NH3_SN2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.730269 |
| Sum of electronic and thermal Energies= | | -993.713700 |
| Sum of electronic and thermal Enthalpies= | | -993.712756 |
| Sum of electronic and thermal Free Energies= | | -993.774393 |
| Zero-point correction= | 0.266744 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.98 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.496935 | -1.030826 | -1.155280 |
| C | 0.695632 | 0.401804 | -1.387295 |
| C | 2.029240 | 0.762236 | -0.704342 |
| S | 2.108143 | 0.043991 | 0.981971 |
| C | 3.275661 | -1.340381 | 0.717140 |
| C | -0.537631 | 1.055741 | -0.723408 |
| O | -0.189160 | 2.330091 | -0.271363 |
| C | -1.301242 | 3.166138 | 0.064547 |
| C | -0.940777 | 0.046456 | 0.390331 |
| O | -2.326908 | -0.179635 | 0.345341 |
| C | -2.882983 | -0.724881 | 1.545459 |
| C | -0.095664 | -1.168214 | -0.005403 |
| H | 0.746601 | 0.543891 | -2.466741 |
| H | -1.368690 | 1.092424 | -1.443501 |
| H | -0.640818 | 0.413057 | 1.378674 |
| H | -0.017711 | -2.125025 | 0.486465 |
| H | 2.874154 | 0.391737 | -1.288397 |
| H | 2.094664 | 1.848504 | -0.619746 |
| H | 4.263861 | -0.945391 | 0.470486 |
| H | 3.337728 | -1.888889 | 1.659838 |
| H | 2.925048 | -2.003916 | -0.077117 |
| H | -0.880816 | 4.132708 | 0.344008 |
| H | -1.969911 | 3.288950 | -0.797038 |
| H | -1.870709 | 2.757127 | 0.908183 |
| H | -3.965494 | -0.721062 | 1.409140 |
| H | -2.542694 | -1.754070 | 1.716967 |
| H | -2.622897 | -0.105533 | 2.413746 |
| N | -1.857897 | -2.729498 | -0.990842 |
| H | -1.502283 | -3.043618 | -1.893597 |
| H | -2.263418 | -3.547840 | -0.536511 |
| H | -2.621964 | -2.080856 | -1.172261 |

REACTANT_EXO_ME_2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.210928 |
| Sum of electronic and thermal Energies= | | -937.197809 |
| Sum of electronic and thermal Enthalpies= | | -937.196865 |
| Sum of electronic and thermal Free Energies= | | -937.250548 |
| Zero-point correction= | 0.230551 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.83 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.761362 | -0.451639 | 1.462514 |
| C | -0.262601 | 0.847825 | 1.090032 |
| C | -1.300855 | 1.410998 | 0.085336 |
| S | -1.834356 | -0.072724 | -0.889534 |
| C | -3.448979 | -0.465335 | -0.128047 |
| C | 1.083488 | 0.514452 | 0.368271 |
| O | 1.446683 | 1.429727 | -0.627787 |
| C | 2.192101 | 2.561312 | -0.163105 |
| C | 0.769844 | -0.881595 | -0.264840 |
| O | 1.553365 | -1.932988 | 0.218600 |
| C | 2.861394 | -2.001258 | -0.357488 |
| C | -0.645795 | -1.132809 | 0.275173 |
| H | -0.186009 | 1.459660 | 1.988637 |
| H | 1.869899 | 0.390084 | 1.123830 |
| H | 0.813125 | -0.809595 | -1.362085 |
| H | -0.999848 | -2.161041 | 0.328223 |
| H | -2.181633 | 1.830511 | 0.573969 |
| H | -0.859546 | 2.127395 | -0.608563 |
| H | -4.145407 | 0.335146 | -0.387527 |
| H | -3.795277 | -1.405440 | -0.563449 |
| H | -3.329463 | -0.549854 | 0.953881 |
| H | 2.465711 | 3.133399 | -1.050504 |
| H | 1.597932 | 3.196720 | 0.507667 |
| H | 3.102137 | 2.239644 | 0.358645 |
| H | 3.334624 | -2.885146 | 0.071190 |
| H | 2.802769 | -2.105607 | -1.449037 |
| H | 3.459619 | -1.114637 | -0.110937 |

REACTANT_EXO_ME_2_MeCN_SN2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.922143 |
| Sum of electronic and thermal Energies= | | -1069.903602 |
| Sum of electronic and thermal Enthalpies= | | -1069.902658 |
| Sum of electronic and thermal Free Energies= | | -1069.972273 |
| Zero-point correction= | 0.276457 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -32.13 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.040555 | -1.501907 | -0.333613 |
| C | 0.662587 | -0.440231 | -1.180378 |
| C | 2.177389 | -0.598088 | -1.117237 |
| S | 2.914883 | -0.486284 | 0.563976 |
| C | 3.361264 | -2.239291 | 0.852345 |
| C | 0.071520 | 0.891251 | -0.621319 |
| O | 1.003185 | 1.927805 | -0.466615 |
| C | 1.179749 | 2.756511 | -1.617610 |
| C | -0.486150 | 0.488311 | 0.763469 |
| O | -1.623180 | 1.156396 | 1.206045 |
| C | -1.355148 | 2.384127 | 1.900882 |
| C | -0.726474 | -0.990819 | 0.578079 |
| H | 0.310892 | -0.662004 | -2.191917 |
| H | -0.772647 | 1.214951 | -1.247317 |
| H | 0.344673 | 0.550147 | 1.487596 |
| H | -0.978764 | -1.655305 | 1.398772 |
| H | 2.455995 | -1.559327 | -1.558242 |
| H | 2.622372 | 0.183479 | -1.738948 |
| H | 4.108540 | -2.575789 | 0.129127 |
| H | 3.801104 | -2.281098 | 1.852123 |
| H | 2.485961 | -2.892887 | 0.821350 |
| H | 1.876379 | 3.542546 | -1.323529 |
| H | 1.604061 | 2.200888 | -2.464582 |
| H | 0.227132 | 3.207709 | -1.926009 |
| H | -2.327803 | 2.778580 | 2.197481 |
| H | -0.746297 | 2.199281 | 2.794981 |
| H | -0.842064 | 3.104100 | 1.255702 |
| C | -3.617061 | -1.143119 | -0.346243 |

| | | | |
|---|---|---|---|
| C | -5.024136 | -1.294363 | -0.683175 |
| H | -5.494804 | -1.998230 | 0.010803 |
| H | -5.526807 | -0.324802 | -0.609296 |
| H | -5.121725 | -1.677082 | -1.704078 |
| N | -2.498578 | -1.016955 | -0.089578 |

REACTANT_EXO_ME_2_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.183605 | |
| Sum of electronic and thermal Energies= | -937.169928 | |
| Sum of electronic and thermal Enthalpies= | -937.168983 | |
| Sum of electronic and thermal Free Energies= | -937.224806 | |
| Zero-point correction= | 0.227991 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.75 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.665816 | -1.055747 | -1.058161 |
| C | 0.512434 | 0.451428 | -0.823140 |
| C | 1.418848 | 0.918501 | 0.333248 |
| S | 2.653576 | -0.261573 | 0.989035 |
| C | 3.899621 | -0.279744 | -0.350803 |
| C | -1.028005 | 0.550132 | -0.544196 |
| O | -1.407339 | 1.535550 | 0.358788 |
| C | -1.596417 | 2.842360 | -0.207887 |
| C | -1.352362 | -0.848258 | 0.063799 |
| O | -2.610478 | -1.363377 | -0.189930 |
| C | -3.590149 | -1.125337 | 0.842312 |
| C | -0.301342 | -1.689450 | -0.571652 |
| H | 0.825096 | 0.851311 | -1.786571 |
| H | -1.568720 | 0.639364 | -1.497972 |
| H | -1.107776 | -0.808598 | 1.145539 |
| H | -0.306053 | -2.774641 | -0.681635 |
| H | 1.923474 | 1.834966 | 0.011735 |
| H | 0.790383 | 1.183913 | 1.187573 |
| H | 4.272818 | 0.729267 | -0.545556 |
| H | 4.726961 | -0.891036 | 0.018238 |
| H | 3.515185 | -0.730108 | -1.269577 |
| H | -1.974941 | 3.468311 | 0.600224 |
| H | -0.651436 | 3.259847 | -0.577215 |
| H | -2.329253 | 2.808480 | -1.023032 |
| H | -4.516658 | -1.564719 | 0.473734 |
| H | -3.293564 | -1.618341 | 1.775708 |
| H | -3.722495 | -0.052060 | 1.008584 |

REACTANT_EXO_ME_2_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.176781 | |
| Sum of electronic and thermal Energies= | -937.163165 | |
| Sum of electronic and thermal Enthalpies= | -937.162220 | |
| Sum of electronic and thermal Free Energies= | -937.217845 | |
| Zero-point correction= | 0.228067 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.86 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.478337 | -2.116617 | -0.924274 |
| C | 0.317902 | -0.818868 | -1.183133 |
| C | 1.632169 | -0.953867 | -0.393023 |
| S | 2.135790 | 0.510860 | 0.615579 |
| C | 3.756489 | -0.152288 | 1.141885 |
| C | -0.788523 | 0.226990 | -0.799406 |
| O | -0.377113 | 1.480878 | -0.401413 |
| C | -0.111301 | 2.412796 | -1.464209 |
| C | -1.521882 | -0.494849 | 0.370589 |
| O | -2.848690 | -0.163904 | 0.565366 |
| C | -3.095337 | 0.794467 | 1.616406 |
| C | -1.391286 | -1.906353 | -0.082267 |
| H | 0.493828 | -0.872297 | -2.256292 |
| H | -1.492912 | 0.282297 | -1.645473 |
| H | -0.894218 | -0.374174 | 1.277477 |
| H | -2.030020 | -2.746918 | 0.193369 |
| H | 1.556380 | -1.820707 | 0.273141 |
| H | 2.431101 | -1.178412 | -1.105789 |
| H | 4.412771 | -0.324587 | 0.284091 |
| H | 4.204121 | 0.615493 | 1.777749 |
| H | 3.646433 | -1.071480 | 1.724515 |
| H | 0.064855 | 3.372994 | -0.980350 |
| H | 0.782663 | 2.123915 | -2.027824 |
| H | -0.976525 | 2.486908 | -2.134343 |
| H | -4.169491 | 0.976852 | 1.599669 |
| H | -2.806179 | 0.381636 | 2.589951 |
| H | -2.551715 | 1.723690 | 1.422370 |

REACTANT_EXO_ME_2_NH3_SN2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -993.728370 | |
| Sum of electronic and thermal Energies= | -993.711718 | |
| Sum of electronic and thermal Enthalpies= | -993.710774 | |
| Sum of electronic and thermal Free Energies= | -993.772888 | |
| Zero-point correction= | 0.266577 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.24 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.662844 | -0.848439 | 1.187544 |
| C | -0.531025 | 0.604927 | 1.225707 |
| C | -1.745737 | 1.167972 | 0.453631 |
| S | -2.074300 | 0.157634 | -1.043742 |
| C | -3.476858 | -0.867758 | -0.470785 |
| C | 0.825511 | 0.853204 | 0.498913 |
| O | 0.917162 | 2.076919 | -0.172448 |
| C | 1.302631 | 3.185189 | 0.648809 |
| C | 0.893722 | -0.321018 | -0.516843 |
| O | 2.129624 | -0.984706 | -0.565261 |
| C | 3.068809 | -0.374715 | -1.463329 |
| C | -0.194242 | -1.239882 | 0.031414 |
| H | -0.548464 | 0.893424 | 2.276824 |
| H | 1.642101 | 0.723416 | 1.223843 |
| H | 0.623024 | 0.043023 | -1.514761 |
| H | -0.459530 | -2.223020 | -0.321119 |
| H | -2.641568 | 1.173465 | 1.077317 |
| H | -1.528015 | 2.186253 | 0.125130 |
| H | -4.348540 | -0.231618 | -0.300684 |
| H | -3.702341 | -1.575911 | -1.271371 |
| H | -3.214221 | -1.405209 | 0.443539 |
| H | 1.408805 | 4.039175 | -0.021176 |
| H | 0.543185 | 3.415456 | 1.408165 |
| H | 2.261120 | 2.987981 | 1.145642 |
| H | 3.969329 | -0.988441 | -1.419956 |
| H | 2.678363 | -0.367814 | -2.489021 |
| H | 3.306818 | 0.650768 | -1.158745 |
| N | 1.245074 | -3.119975 | 1.102056 |
| H | 1.166599 | -3.191840 | 2.115899 |
| H | 1.225475 | -4.072237 | 0.737564 |
| H | 2.162731 | -2.736896 | 0.884617 |

REACTANT_EXO_ME_3

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.213415 | |
| Sum of electronic and thermal Energies= | -937.200322 | |
| Sum of electronic and thermal Enthalpies= | -937.199378 | |
| Sum of electronic and thermal Free Energies= | -937.252888 | |
| Zero-point correction= | 0.230638 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.48 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.748071 | 0.518070 | 1.458363 |
| C | 0.379877 | -0.860829 | 1.256081 |
| C | 1.448045 | -1.416607 | 0.282424 |
| S | 1.711911 | -0.033194 | -0.921402 |

| | | | |
|---|---|---|---|
| C | 3.323351 | 0.637582 | -0.376555 |
| C | -1.009188 | -0.772366 | 0.571791 |
| O | -1.174702 | -1.876498 | -0.272884 |
| C | -2.526760 | -2.113603 | -0.679209 |
| C | -0.936686 | 0.604971 | -0.166726 |
| O | -1.877644 | 1.476673 | 0.389845 |
| C | -2.193753 | 2.620906 | -0.407189 |
| C | 0.488008 | 1.050679 | 0.222600 |
| H | 0.392453 | -1.375199 | 2.216269 |
| H | -1.800240 | -0.705505 | 1.330065 |
| H | -1.068735 | 0.486520 | -1.251768 |
| H | 0.770875 | 2.099736 | 0.145484 |
| H | 2.398299 | -1.619415 | 0.779052 |
| H | 1.094894 | -2.290544 | -0.264547 |
| H | 4.089537 | -0.109386 | -0.596116 |
| H | 3.517801 | 1.540466 | -0.959718 |
| H | 3.283972 | 0.857318 | 0.692325 |
| H | -2.508535 | -3.013872 | -1.294439 |
| H | -3.171346 | -2.275525 | 0.193557 |
| H | -2.920938 | -1.276443 | -1.269623 |
| H | -2.981118 | 3.154180 | 0.126398 |
| H | -1.330718 | 3.289484 | -0.528917 |
| H | -2.559933 | 2.318919 | -1.397492 |

REACTANT_EXO_ME_3_MeCN_SN2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -1069.921917 | |
| Sum of electronic and thermal Energies= | -1069.903413 | |
| Sum of electronic and thermal Enthalpies= | -1069.902469 | |
| Sum of electronic and thermal Free Energies= | -1069.971688 | |
| Zero-point correction= | 0.276513 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -32.81 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.124695 | -1.501842 | -0.220188 |
| C | 0.707007 | -0.563321 | -1.221344 |
| C | 2.227368 | -0.668302 | -1.175807 |
| S | 2.991780 | -0.332938 | 0.461798 |
| C | 3.418597 | -2.033878 | 0.990350 |
| C | 0.102931 | 0.817347 | -0.858346 |
| O | 1.077474 | 1.803865 | -1.025032 |
| C | 0.583634 | 3.145509 | -1.047957 |
| C | -0.404257 | 0.631642 | 0.593145 |
| O | -1.509238 | 1.433793 | 0.871414 |
| C | -1.738574 | 1.687189 | 2.261727 |
| C | -0.635265 | -0.877268 | 0.631103 |
| H | 0.344894 | -0.926428 | -2.186863 |
| H | -0.776342 | 1.025003 | -1.488529 |
| H | 0.435363 | 0.813187 | 1.283399 |
| H | 2.533015 | -1.663213 | -1.511308 |
| H | 2.621035 | 0.062601 | -1.886338 |
| H | 4.142251 | -2.483690 | 0.305581 |
| H | 3.883359 | -1.941613 | 1.975352 |
| H | 2.533773 | -2.670057 | 1.071952 |
| H | 1.442311 | 3.778165 | -1.275882 |
| H | -0.180015 | 3.266612 | -1.828278 |
| H | 0.158251 | 3.437045 | -0.081359 |
| H | -2.565606 | 2.396781 | 2.310388 |
| H | -2.017823 | 0.772742 | 2.802398 |
| H | -0.851262 | 2.128816 | 2.732171 |
| H | -0.834698 | -1.432333 | 1.543634 |
| C | -3.460586 | -1.224963 | -0.330452 |
| C | -4.818402 | -1.481291 | -0.784780 |
| H | -4.793426 | -2.008710 | -1.743808 |
| H | -5.342591 | -2.099129 | -0.048501 |
| H | -5.351249 | -0.532752 | -0.906352 |
| N | -2.383984 | -1.011220 | 0.026885 |

REACTANT_EXO_ME_3_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.183811 | |
| Sum of electronic and thermal Energies= | -937.170123 | |
| Sum of electronic and thermal Enthalpies= | -937.169179 | |
| Sum of electronic and thermal Free Energies= | -937.224947 | |
| Zero-point correction= | 0.228107 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.97 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.659925 | -0.953247 | 1.059928 |
| C | -0.592957 | 0.549444 | 0.831423 |
| C | -1.511968 | 0.976999 | -0.336539 |
| S | -2.726609 | -0.238429 | -0.959739 |
| C | -3.946241 | -0.280555 | 0.403628 |
| C | 0.928288 | 0.734152 | 0.576253 |
| O | 1.142645 | 1.863067 | -0.193522 |
| C | 2.462410 | 2.424542 | -0.106952 |
| C | 1.325082 | -0.624924 | -0.108413 |
| O | 2.605219 | -1.044980 | 0.249671 |
| C | 3.296839 | -1.834979 | -0.734022 |
| C | 0.303529 | -1.533831 | 0.497896 |
| H | -0.930714 | 0.943402 | 1.788315 |
| H | 1.468217 | 0.776591 | 1.534323 |
| H | 1.173483 | -0.538634 | -1.197457 |
| H | 0.364433 | -2.616797 | 0.612752 |
| H | -2.025537 | 1.892371 | -0.028532 |
| H | -0.898514 | 1.240822 | -1.200866 |
| H | -4.337684 | 0.720647 | 0.602704 |
| H | -4.766744 | -0.911751 | 0.053508 |
| H | -3.533537 | -0.718624 | 1.316239 |
| H | 2.436714 | 3.338823 | -0.699759 |
| H | 2.713345 | 2.663954 | 0.933498 |
| H | 3.212486 | 1.738424 | -0.516139 |
| H | 4.289373 | -2.020206 | -0.323836 |
| H | 2.790128 | -2.792539 | -0.907305 |
| H | 3.376890 | -1.285433 | -1.679880 |

REACTANT_EXO_ME_3_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.176047 | |
| Sum of electronic and thermal Energies= | -937.162338 | |
| Sum of electronic and thermal Enthalpies= | -937.161394 | |
| Sum of electronic and thermal Free Energies= | -937.217436 | |
| Zero-point correction= | 0.227940 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -37.83 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.369756 | -1.985757 | -1.138397 |
| C | 0.428088 | -0.686844 | -1.313534 |
| C | 1.725812 | -0.852852 | -0.498248 |
| S | 2.242593 | 0.584303 | 0.542853 |
| C | 3.777603 | -0.173713 | 1.184642 |
| C | -0.679010 | 0.323568 | -0.897526 |
| O | -0.166637 | 1.562766 | -0.615476 |
| C | -1.060979 | 2.672907 | -0.806348 |
| C | -1.357548 | -0.443172 | 0.301005 |
| O | -2.690111 | -0.095699 | 0.484470 |
| C | -3.158816 | -0.127443 | 1.844770 |
| C | -1.240723 | -1.830211 | -0.234786 |
| H | 0.626976 | -0.662275 | -2.383375 |
| H | -1.425788 | 0.363141 | -1.706939 |
| H | -0.720518 | -0.299775 | 1.191451 |
| H | -1.905618 | -2.672972 | -0.039239 |
| H | 1.616066 | -1.722746 | 0.159293 |
| H | 2.533016 | -1.089110 | -1.197661 |
| H | 4.482378 | -0.387360 | 0.376044 |
| H | 4.224594 | 0.569259 | 1.849874 |

| | | | |
|---|---|---|---|
| H | 3.573785 | -1.082914 | 1.757964 |
| H | -0.465011 | 3.566342 | -0.622756 |
| H | -1.443854 | 2.684772 | -1.834022 |
| H | -1.895930 | 2.627261 | -0.099764 |
| H | -4.185684 | 0.236226 | 1.815613 |
| H | -3.144715 | -1.148408 | 2.246056 |
| H | -2.545706 | 0.525791 | 2.477176 |

REACTANT_EXO_ME_3_NH3_SN2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.730265 |
| Sum of electronic and thermal Energies= | | -993.713698 |
| Sum of electronic and thermal Enthalpies= | | -993.712754 |
| Sum of electronic and thermal Free Energies= | | -993.774382 |
| Zero-point correction= | 0.266749 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.97 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.497680 | -1.030303 | -1.155950 |
| C | 0.695735 | 0.402540 | -1.387344 |
| C | 2.028961 | 0.763355 | -0.703846 |
| S | 2.107734 | 0.044490 | 0.982263 |
| C | 3.275802 | -1.339376 | 0.717187 |
| C | -0.538016 | 1.055603 | -0.723495 |
| O | -0.190344 | 2.330045 | -0.271085 |
| C | -1.302958 | 3.165377 | 0.064851 |
| C | -0.940733 | 0.045820 | 0.389941 |
| O | -2.326819 | -0.180575 | 0.345225 |
| C | -2.882419 | -0.726097 | 1.545441 |
| C | -0.095146 | -1.168414 | -0.006215 |
| H | 0.746890 | 0.545099 | -2.466719 |
| H | -1.368982 | 1.092005 | -1.443713 |
| H | -0.640746 | 0.412211 | 1.378345 |
| H | 2.874236 | 0.393458 | -1.287762 |
| H | 2.093869 | 1.849619 | -0.618831 |
| H | 4.263894 | -0.943956 | 0.470784 |
| H | 3.337945 | -1.888136 | 1.659733 |
| H | 2.925563 | -2.002820 | -0.077314 |
| H | -0.883124 | 4.132110 | 0.344642 |
| H | -1.971541 | 3.288043 | -0.796822 |
| H | -1.872347 | 2.755817 | 0.908269 |
| H | -3.964971 | -0.722558 | 1.409435 |
| H | -2.541789 | -1.755208 | 1.716762 |
| H | -2.622259 | -0.106774 | 2.413724 |
| H | -0.016302 | -2.125052 | 0.485785 |
| N | -1.856194 | -2.729759 | -0.990771 |
| H | -1.501043 | -3.041774 | -1.894430 |
| H | -2.259523 | -3.549602 | -0.537194 |
| H | -2.621655 | -2.082198 | -1.170140 |

REACTANT_EXO_ME_4

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.207830 |
| Sum of electronic and thermal Energies= | | -937.194847 |
| Sum of electronic and thermal Enthalpies= | | -937.193902 |
| Sum of electronic and thermal Free Energies= | | -937.246976 |
| Zero-point correction= | 0.230964 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -36.02 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.595702 | 0.973102 | 1.123816 |
| C | 0.178506 | -0.390754 | 1.350754 |
| C | 1.329897 | -1.251290 | 0.777547 |
| S | 1.803634 | -0.364542 | -0.779602 |
| C | 3.375873 | 0.434137 | -0.296232 |
| C | -1.107490 | -0.533401 | 0.491821 |
| O | -1.198865 | -1.852773 | 0.024937 |
| C | -2.489836 | -2.211688 | -0.481564 |
| C | -0.870138 | 0.517542 | -0.653233 |
| O | -1.819836 | 1.532324 | -0.807820 |
| C | -2.078252 | 2.417884 | 0.287506 |
| C | 0.520972 | 1.047338 | -0.248383 |
| H | 0.045381 | -0.543997 | 2.421322 |
| H | -1.989308 | -0.258469 | 1.084480 |
| H | -0.846408 | 0.002779 | -1.618298 |
| H | 0.862546 | 2.001875 | -0.647460 |
| H | 2.200798 | -1.270698 | 1.434636 |
| H | 1.006134 | -2.259014 | 0.518599 |
| H | 4.120517 | -0.352304 | -0.153073 |
| H | 3.682973 | 1.080557 | -1.121454 |
| H | 3.227593 | 1.006291 | 0.621978 |
| H | -2.419334 | -3.256490 | -0.785934 |
| H | -3.254164 | -2.106150 | 0.298764 |
| H | -2.767720 | -1.596308 | -1.346438 |
| H | -2.882500 | 3.069579 | -0.055422 |
| H | -2.412684 | 1.883971 | 1.185037 |
| H | -1.205183 | 3.031221 | 0.540138 |

REACTANT_EXO_ME_4_MeCN_SN2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.910796 |
| Sum of electronic and thermal Energies= | | -1069.892590 |
| Sum of electronic and thermal Enthalpies= | | -1069.891646 |
| Sum of electronic and thermal Free Energies= | | -1069.959789 |
| Zero-point correction= | 0.276925 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -34.94 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.023002 | -1.382849 | 0.288193 |
| C | -0.667327 | -0.385270 | 1.177690 |
| C | -2.169293 | -0.651602 | 1.188722 |
| S | -2.970119 | -0.606143 | -0.466144 |
| C | -3.285509 | -2.389997 | -0.734945 |
| C | -0.225555 | 1.005779 | 0.639221 |
| O | -1.351866 | 1.837692 | 0.592754 |
| C | -1.091606 | 3.217510 | 0.343690 |
| C | 0.390574 | 0.683244 | -0.753944 |
| O | 1.431224 | 1.443685 | -1.305117 |
| C | 2.270378 | 2.228394 | -0.457328 |
| C | 0.707426 | -0.804926 | -0.630905 |
| H | -0.253503 | -0.578992 | 2.171543 |
| H | 0.539750 | 1.430691 | 1.305287 |
| H | -0.441476 | 0.713948 | -1.471956 |
| H | -2.357148 | -1.627479 | 1.644865 |
| H | -2.635277 | 0.110638 | 1.817163 |
| H | -3.978317 | -2.781514 | 0.014524 |
| H | -3.754373 | -2.473301 | -1.718853 |
| H | -2.360239 | -2.971818 | -0.731581 |
| H | -2.060202 | 3.717917 | 0.375413 |
| H | -0.440481 | 3.642419 | 1.120489 |
| H | -0.638553 | 3.373574 | -0.643769 |
| H | 3.059448 | 2.606923 | -1.109537 |
| H | 1.731375 | 3.079736 | -0.028061 |
| H | 2.727304 | 1.645384 | 0.351960 |
| H | 0.862482 | -1.405367 | -1.524520 |
| C | 3.450175 | -1.336652 | 0.146043 |
| C | 4.768943 | -1.848623 | 0.480551 |
| H | 4.701491 | -2.918475 | 0.704589 |
| H | 5.446166 | -1.698107 | -0.366665 |
| H | 5.160257 | -1.320192 | 1.356047 |
| N | 2.410447 | -0.906154 | -0.115435 |

REACTANT_EXO_ME_4_SN1_A

| | |
|---|---|
| Sum of electronic and zero-point Energies= | -937.176813 |
| Sum of electronic and thermal Energies= | -937.163186 |
| Sum of electronic and thermal Enthalpies= | -937.162242 |

Sum of electronic and thermal Free Energies= -937.217883
Zero-point correction= 0.228208 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -39.03
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.305319 | -1.379884 | 0.954699 |
| C | -0.360522 | 0.145423 | 1.129285 |
| C | -1.584053 | 0.719101 | 0.397303 |
| S | -2.790553 | -0.585267 | -0.097113 |
| C | -4.070417 | 0.497545 | -0.822969 |
| C | 1.014810 | 0.559653 | 0.541529 |
| O | 0.945769 | 1.857458 | 0.064554 |
| C | 2.212673 | 2.500005 | -0.152289 |
| C | 1.228786 | -0.538797 | -0.573741 |
| O | 2.493056 | -0.823116 | -1.063974 |
| C | 3.485954 | -1.245355 | -0.114247 |
| C | 0.494293 | -1.691244 | 0.036518 |
| H | -0.438572 | 0.243548 | 2.209999 |
| H | 1.792034 | 0.449705 | 1.312783 |
| H | 0.624725 | -0.218915 | -1.441405 |
| H | 0.597804 | -2.752455 | -0.197528 |
| H | -2.068743 | 1.420722 | 1.082256 |
| H | -1.265755 | 1.283658 | -0.481886 |
| H | -3.667425 | 1.081918 | -1.654367 |
| H | -4.849985 | -0.168339 | -1.200417 |
| H | -4.501834 | 1.156410 | -0.065465 |
| H | 1.980339 | 3.520003 | -0.458268 |
| H | 2.798951 | 2.521103 | 0.775230 |
| H | 2.779632 | 1.997370 | -0.943629 |
| H | 4.335426 | -1.579669 | -0.709639 |
| H | 3.802523 | -0.420557 | 0.533021 |
| H | 3.132539 | -2.083893 | 0.502547 |

REACTANT_EXO_ME_4_SN1_B
Sum of electronic and zero-point Energies= -937.169177
Sum of electronic and thermal Energies= -937.155591
Sum of electronic and thermal Enthalpies= -937.154647
Sum of electronic and thermal Free Energies= -937.210000
Zero-point correction= 0.227868 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -39.72
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.445375 | -2.066681 | 0.756301 |
| C | -0.307896 | -0.776634 | 1.146384 |
| C | -1.703336 | -0.895661 | 0.499856 |
| S | -2.375801 | 0.608507 | -0.339290 |
| C | -3.987976 | -0.125014 | -0.792335 |
| C | 0.733097 | 0.276736 | 0.674909 |
| O | 0.152026 | 1.511218 | 0.525203 |
| C | 1.048927 | 2.632663 | 0.491373 |
| C | 1.273903 | -0.407973 | -0.645169 |
| O | 2.451209 | 0.002227 | -1.243902 |
| C | 3.640790 | -0.018128 | -0.437322 |
| C | 1.228214 | -1.832960 | -0.204206 |
| H | -0.362095 | -0.849110 | 2.230906 |
| H | 1.549012 | 0.300061 | 1.416371 |
| H | 0.469811 | -0.273944 | -1.394057 |
| H | 1.815710 | -2.671927 | -0.582647 |
| H | -1.678480 | -1.706835 | -0.236421 |
| H | -2.404844 | -1.204477 | 1.280361 |
| H | -4.559760 | -0.408277 | 0.096107 |
| H | -4.534465 | 0.657817 | -1.324279 |
| H | -3.871241 | -0.986252 | -1.456872 |
| H | 0.413797 | 3.517661 | 0.467408 |
| H | 1.673855 | 2.652415 | 1.393549 |
| H | 1.676821 | 2.604055 | -0.405565 |
| H | 4.465533 | 0.155968 | -1.128189 |
| H | 3.628541 | 0.775561 | 0.317178 |
| H | 3.787412 | -0.991119 | 0.053028 |

REACTANT_EXO_ME_4_NH3_SN2
Sum of electronic and zero-point Energies= -993.728370
Sum of electronic and thermal Energies= -993.711718
Sum of electronic and thermal Enthalpies= -993.710774
Sum of electronic and thermal Free Energies= -993.772885
Zero-point correction= 0.266577 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -33.24
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.662790 | -0.848454 | 1.187375 |
| C | -0.530826 | 0.604868 | 1.225575 |
| C | -1.745493 | 1.168238 | 0.453619 |
| S | -2.074488 | 0.157824 | -1.043586 |
| C | -3.477267 | -0.867112 | -0.470373 |
| C | 0.825692 | 0.852926 | 0.498675 |
| O | 0.917651 | 2.076754 | -0.172421 |
| C | 1.303309 | 3.184759 | 0.649108 |
| C | 0.893429 | -0.321145 | -0.517287 |
| O | 2.129097 | -0.985283 | -0.565950 |
| C | 3.068853 | -0.374585 | -1.462942 |
| C | -0.194684 | -1.239827 | 0.031030 |
| H | -0.548134 | 0.893370 | 2.276692 |
| H | 1.642304 | 0.722706 | 1.223508 |
| H | 0.622737 | 0.043110 | -1.515141 |
| H | -2.641269 | 1.174051 | 1.077381 |
| H | -1.527476 | 2.186415 | 0.124993 |
| H | -4.348799 | -0.230717 | -0.300459 |
| H | -3.702895 | -1.575427 | -1.270775 |
| H | -3.214726 | -1.404376 | 0.444085 |
| H | 1.409589 | 4.038900 | -0.020661 |
| H | 0.543922 | 3.414943 | 1.408548 |
| H | 2.261784 | 2.987280 | 1.145861 |
| H | 3.969197 | -0.988583 | -1.419799 |
| H | 2.678865 | -0.366510 | -2.488800 |
| H | 3.306978 | 0.650522 | -1.157189 |
| H | -0.459420 | -2.223273 | -0.321074 |
| N | 1.244937 | -3.120029 | 1.102174 |
| H | 1.166857 | -3.191036 | 2.116089 |
| H | 1.225730 | -4.072619 | 0.738524 |
| H | 2.162265 | -2.736599 | 0.883929 |

REACTANT_EXO_ME_5
Sum of electronic and zero-point Energies= -937.211635
Sum of electronic and thermal Energies= -937.198455
Sum of electronic and thermal Enthalpies= -937.197511
Sum of electronic and thermal Free Energies= -937.251432
Zero-point correction= 0.230489 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -35.98
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.666177 | 0.326747 | 1.488636 |
| C | 0.166187 | -0.963321 | 1.082033 |
| C | 1.214541 | -1.508777 | 0.079374 |
| S | 1.756553 | -0.014930 | -0.872253 |
| C | 3.371464 | 0.356652 | -0.099570 |
| C | -1.169813 | -0.611464 | 0.352440 |
| O | -1.508238 | -1.495540 | -0.679426 |
| C | -2.340825 | -2.593211 | -0.284941 |
| C | -0.866950 | 0.800277 | -0.224696 |
| O | -1.752346 | 1.725598 | 0.335984 |
| C | -1.904299 | 2.941912 | -0.400726 |
| C | 0.556784 | 1.038427 | 0.321842 |
| H | 0.074975 | -1.593723 | 1.966138 |
| H | -1.973720 | -0.506154 | 1.090785 |

| | | | |
|---|---|---|---|
| H | -0.915739 | 0.789420 | -1.322001 |
| H | 0.941505 | 2.053816 | 0.405917 |
| H | 2.090863 | -1.934247 | 0.570829 |
| H | 0.778559 | -2.216695 | -0.626439 |
| H | 4.063931 | -0.445194 | -0.365385 |
| H | 3.727183 | 1.299287 | -0.521559 |
| H | 3.249336 | 0.428668 | 0.983046 |
| H | -2.572235 | -3.143465 | -1.197785 |
| H | -1.829807 | -3.262042 | 0.420760 |
| H | -3.271071 | -2.230385 | 0.168533 |
| H | -2.658293 | 3.524576 | 0.129381 |
| H | -0.970054 | 3.518976 | -0.438909 |
| H | -2.247544 | 2.738632 | -1.423354 |

REACTANT_EXO_ME_5_MeCN_SN2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -1069.922143 | |
| Sum of electronic and thermal Energies= | -1069.903602 | |
| Sum of electronic and thermal Enthalpies= | -1069.902658 | |
| Sum of electronic and thermal Free Energies= | -1069.972275 | |
| Zero-point correction= | 0.276458 | (Hartree/Particle) |
| DCM DeltaG (solv) (kcal/mol) = -32.13 | | |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.040488 | -1.501766 | -0.333737 |
| C | 0.662629 | -0.440092 | -1.180418 |
| C | 2.177425 | -0.598042 | -1.117195 |
| S | 2.914810 | -0.486616 | 0.564094 |
| C | 3.360688 | -2.239777 | 0.852281 |
| C | 0.071622 | 0.891398 | -0.621315 |
| O | 1.003334 | 1.927905 | -0.466591 |
| C | 1.179979 | 2.756574 | -1.617601 |
| C | -0.486062 | 0.488435 | 0.763460 |
| O | -1.623059 | 1.156556 | 1.206066 |
| C | -1.354978 | 2.384262 | 1.900927 |
| C | -0.726472 | -0.990671 | 0.578006 |
| H | 0.310972 | -0.661789 | -2.191986 |
| H | -0.772536 | 1.215152 | -1.247299 |
| H | 0.344763 | 0.550201 | 1.487589 |
| H | 2.456032 | -1.559198 | -1.558380 |
| H | 2.622500 | 0.183642 | -1.738693 |
| H | 4.107993 | -2.576359 | 0.129132 |
| H | 3.800349 | -2.281858 | 1.852126 |
| H | 2.485216 | -2.893133 | 0.821030 |
| H | 1.876611 | 3.542602 | -1.323508 |
| H | 1.604322 | 2.200914 | -2.464534 |
| H | 0.227389 | 3.207784 | -1.926064 |
| H | -2.327616 | 2.778722 | 2.197574 |
| H | -0.746096 | 2.199381 | 2.794998 |
| H | -0.841908 | 3.104246 | 1.255748 |
| H | -0.978799 | -1.655180 | 1.398669 |
| C | -3.617100 | -1.143054 | -0.346255 |
| C | -5.024141 | -1.294551 | -0.683216 |
| H | -5.121587 | -1.680589 | -1.702881 |
| H | -5.495488 | -1.995829 | 0.012921 |
| H | -5.526260 | -0.324451 | -0.612720 |
| N | -2.498636 | -1.016693 | -0.089597 |

REACTANT_EXO_ME_5_SN1_A

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.183605 | |
| Sum of electronic and thermal Energies= | -937.169928 | |
| Sum of electronic and thermal Enthalpies= | -937.168983 | |
| Sum of electronic and thermal Free Energies= | -937.224806 | |
| Zero-point correction= | 0.227991 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) = | -37.75 | |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.665816 | -1.055746 | -1.058160 |
| C | 0.512435 | 0.451429 | -0.823138 |
| C | 1.418847 | 0.918500 | 0.333251 |
| S | 2.653576 | -0.261575 | 0.989034 |
| C | 3.899620 | -0.279743 | -0.350805 |
| C | -1.028005 | 0.550133 | -0.544196 |
| O | -1.407339 | 1.535551 | 0.358788 |
| C | -1.596416 | 2.842362 | -0.207886 |
| C | -1.352362 | -0.848257 | 0.063799 |
| O | -2.610478 | -1.363374 | -0.189932 |
| C | -3.590149 | -1.125341 | 0.842312 |
| C | -0.301342 | -1.689449 | -0.571652 |
| H | 0.825098 | 0.851313 | -1.786569 |
| H | -1.568719 | 0.639366 | -1.497973 |
| H | -1.107778 | -0.808598 | 1.145538 |
| H | -0.306054 | -2.774640 | -0.681637 |
| H | 1.923473 | 1.834966 | 0.011741 |
| H | 0.790382 | 1.183909 | 1.187577 |
| H | 4.272815 | 0.729269 | -0.545557 |
| H | 4.726962 | -0.891034 | 0.018235 |
| H | 3.515184 | -0.730106 | -1.269579 |
| H | -1.974940 | 3.468312 | 0.600225 |
| H | -0.651434 | 3.259848 | -0.577213 |
| H | -2.329252 | 2.808482 | -1.023031 |
| H | -4.516659 | -1.564719 | 0.473730 |
| H | -3.293565 | -1.618352 | 1.775703 |
| H | -3.722493 | -0.052064 | 1.008592 |

REACTANT_EXO_ME_5_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.176781 | |
| Sum of electronic and thermal Energies= | -937.163165 | |
| Sum of electronic and thermal Enthalpies= | -937.162220 | |
| Sum of electronic and thermal Free Energies= | -937.217845 | |
| Zero-point correction= | 0.228067 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) = | -37.86 | |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.478337 | -2.116617 | -0.924272 |
| C | 0.317903 | -0.818869 | -1.183132 |
| C | 1.632169 | -0.953867 | -0.393023 |
| S | 2.135792 | 0.510860 | 0.615578 |
| C | 3.756490 | -0.152288 | 1.141884 |
| C | -0.788522 | 0.226990 | -0.799405 |
| O | -0.377111 | 1.480877 | -0.401411 |
| C | -0.111302 | 2.412797 | -1.464207 |
| C | -1.521883 | -0.494848 | 0.370588 |
| O | -2.848691 | -0.163904 | 0.565363 |
| C | -3.095340 | 0.794467 | 1.616404 |
| C | -1.391286 | -1.906353 | -0.082266 |
| H | 0.493828 | -0.872299 | -2.256291 |
| H | -1.492910 | 0.282299 | -1.645473 |
| H | -0.894221 | -0.374173 | 1.277477 |
| H | -2.030021 | -2.746918 | 0.193369 |
| H | 1.556380 | -1.820707 | 0.273143 |
| H | 2.431101 | -1.178414 | -1.105788 |
| H | 4.412772 | -0.324588 | 0.284089 |
| H | 4.204124 | 0.615494 | 1.777747 |
| H | 3.646435 | -1.071479 | 1.724514 |
| H | 0.064855 | 3.372994 | -0.980346 |
| H | 0.782661 | 2.123917 | -2.027824 |
| H | -0.976527 | 2.486910 | -2.134338 |
| H | -4.169495 | 0.976851 | 1.599665 |
| H | -2.806184 | 0.381634 | 2.589949 |
| H | -2.551718 | 1.723689 | 1.422370 |

REACTANT_EXO_ME_5_NH3_SN2

Sum of electronic and zero-point Energies= -993.728679
Sum of electronic and thermal Energies= -993.712035
Sum of electronic and thermal Enthalpies= -993.711091
Sum of electronic and thermal Free Energies= -993.773196
Zero-point correction= 0.266651 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -34.11
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.324914 | -0.863061 | 1.267042 |
| C | -0.696356 | 0.552169 | 1.208371 |
| C | -2.042552 | 0.617006 | 0.457089 |
| S | -2.035877 | -0.492413 | -1.005191 |
| C | -3.011740 | -1.905219 | -0.371984 |
| C | 0.482483 | 1.198235 | 0.421394 |
| O | 0.123617 | 2.307416 | -0.348280 |
| C | 0.213950 | 3.566611 | 0.327396 |
| C | 0.971451 | 0.052690 | -0.493980 |
| O | 2.372783 | -0.009240 | -0.472234 |
| C | 2.965657 | -0.598744 | -1.633770 |
| C | 0.283217 | -1.154090 | 0.152330 |
| H | -0.794202 | 0.889830 | 2.240380 |
| H | 1.295711 | 1.433651 | 1.121767 |
| H | 0.607122 | 0.204508 | -1.515477 |
| H | -2.869637 | 0.334218 | 1.111343 |
| H | -2.199691 | 1.636348 | 0.098598 |
| H | -4.041377 | -1.588407 | -0.190577 |
| H | -3.007549 | -2.669562 | -1.152493 |
| H | -2.571859 | -2.305684 | 0.544541 |
| H | -0.025269 | 4.327893 | -0.416002 |
| H | -0.500311 | 3.637692 | 1.158915 |
| H | 1.230082 | 3.732489 | 0.706348 |
| H | 4.043031 | -0.465488 | -1.525388 |
| H | 2.738748 | -1.670517 | -1.705635 |
| H | 2.625366 | -0.091167 | -2.545100 |
| H | 0.339897 | -2.192656 | -0.131531 |
| N | 2.242718 | -2.254530 | 1.367535 |
| H | 1.992016 | -2.397417 | 2.345644 |
| H | 2.714844 | -3.104909 | 1.060125 |
| H | 2.929529 | -1.503393 | 1.331541 |

REACTANT_EXO_ME_6
Sum of electronic and zero-point Energies= -937.205701
Sum of electronic and thermal Energies= -937.192619
Sum of electronic and thermal Enthalpies= -937.191675
Sum of electronic and thermal Free Energies= -937.245300
Zero-point correction= 0.230730 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -36.56
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.523782 | 0.759361 | 1.239776 |
| C | 0.007302 | -0.587558 | 1.162439 |
| C | 1.142186 | -1.413497 | 0.507249 |
| S | 1.848849 | -0.271126 | -0.769133 |
| C | 3.389359 | 0.289994 | 0.039756 |
| C | -1.213193 | -0.453181 | 0.192176 |
| O | -1.436094 | -1.585138 | -0.603114 |
| C | -2.325865 | -2.556948 | -0.040899 |
| C | -0.775848 | 0.739546 | -0.721267 |
| O | -1.639207 | 1.835149 | -0.802030 |
| C | -1.980180 | 2.541952 | 0.394431 |
| C | 0.588857 | 1.093884 | -0.093970 |
| H | -0.218196 | -0.927687 | 2.173152 |
| H | -2.107861 | -0.185655 | 0.766357 |
| H | -0.680915 | 0.376808 | -1.748573 |
| H | 1.010560 | 2.082730 | -0.270424 |
| H | 1.937117 | -1.670274 | 1.209184 |
| H | 0.768485 | -2.300183 | -0.005533 |
| H | 4.070379 | -0.562587 | 0.091815 |
| H | 3.826227 | 1.066671 | -0.592097 |
| H | 3.160114 | 0.672222 | 1.036613 |
| H | -2.457301 | -3.326700 | -0.802363 |
| H | -1.912683 | -3.014098 | 0.868651 |
| H | -3.297927 | -2.104399 | 0.190365 |
| H | -2.677952 | 3.318279 | 0.079020 |
| H | -2.477127 | 1.898457 | 1.130730 |
| H | -1.108062 | 3.014298 | 0.862682 |

REACTANT_EXO_ME_6_MeCN_SN2
Sum of electronic and zero-point Energies= -1069.922143
Sum of electronic and thermal Energies= -1069.903602
Sum of electronic and thermal Enthalpies= -1069.902658
Sum of electronic and thermal Free Energies= -1069.972268
Zero-point correction= 0.276458 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -32.13
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.040476 | -1.501888 | -0.333557 |
| C | 0.662537 | -0.440261 | -1.180357 |
| C | 2.177335 | -0.598183 | -1.117232 |
| S | 2.914865 | -0.486354 | 0.563964 |
| C | 3.361142 | -2.239376 | 0.852394 |
| C | 0.071540 | 0.891261 | -0.621323 |
| O | 1.003256 | 1.927775 | -0.466663 |
| C | 1.179915 | 2.756374 | -1.617720 |
| C | -0.486124 | 0.488378 | 0.763484 |
| O | -1.623116 | 1.156520 | 1.206069 |
| C | -1.355022 | 2.384279 | 1.900833 |
| C | -0.726516 | -0.990744 | 0.578133 |
| H | 0.310819 | -0.662044 | -2.191886 |
| H | -0.772623 | 1.214985 | -1.247315 |
| H | 0.344717 | 0.550194 | 1.487592 |
| H | 2.455893 | -1.559448 | -1.558210 |
| H | 2.622346 | 0.183343 | -1.738976 |
| H | 4.108421 | -2.575935 | 0.129208 |
| H | 3.800948 | -2.281182 | 1.852187 |
| H | 2.485804 | -2.892924 | 0.821388 |
| H | 1.876542 | 3.542421 | -1.323663 |
| H | 1.604275 | 2.200666 | -2.464613 |
| H | 0.227330 | 3.207564 | -1.926226 |
| H | -2.327653 | 2.778765 | 2.197465 |
| H | -0.746127 | 2.199462 | 2.794908 |
| H | -0.841957 | 3.104210 | 1.255591 |
| H | -0.978839 | -1.655168 | 1.398865 |
| C | -3.617111 | -1.143050 | -0.346211 |
| C | -5.024155 | -1.294417 | -0.683221 |
| H | -5.494299 | -2.000010 | 0.009357 |
| H | -5.527379 | -0.325304 | -0.607233 |
| H | -5.121690 | -1.675048 | -1.704909 |
| N | -2.498649 | -1.016817 | -0.089488 |

REACTANT_EXO_ME_6_SN1_A
Sum of electronic and zero-point Energies= -937.176968
Sum of electronic and thermal Energies= -937.163436
Sum of electronic and thermal Enthalpies= -937.162491
Sum of electronic and thermal Free Energies= -937.217791
Zero-point correction= 0.228088 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -39.66
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.484756 | -1.192126 | 0.778888 |
| C | -0.397067 | 0.343869 | 0.793526 |
| C | -1.483708 | 0.953105 | -0.113789 |
| S | -2.743783 | -0.170807 | -0.819448 |
| C | -3.801566 | -0.509706 | 0.634716 |

| | | | |
|---|---|---|---|
| C | 1.079966 | 0.574247 | 0.316060 |
| O | 1.275855 | 1.696811 | -0.474388 |
| C | 1.529210 | 2.916291 | 0.239119 |
| C | 1.349848 | -0.694959 | -0.554440 |
| O | 2.637363 | -1.125129 | -0.804651 |
| C | 3.474877 | -1.378873 | 0.332846 |
| C | 0.432943 | -1.688974 | 0.084773 |
| H | -0.567052 | 0.553546 | 1.848586 |
| H | 1.740881 | 0.579404 | 1.194816 |
| H | 0.897621 | -0.488814 | -1.544476 |
| H | 0.464618 | -2.776650 | -0.002359 |
| H | -1.979883 | 1.752420 | 0.445224 |
| H | -0.997129 | 1.418197 | -0.975274 |
| H | -4.191981 | 0.421355 | 1.054191 |
| H | -4.641225 | -1.101527 | 0.261690 |
| H | -3.280591 | -1.087235 | 1.402661 |
| H | 1.760202 | 3.664403 | -0.519163 |
| H | 0.650641 | 3.238789 | 0.812028 |
| H | 2.387098 | 2.800178 | 0.912943 |
| H | 4.367254 | -1.862361 | -0.064230 |
| H | 3.764050 | -0.449779 | 0.835781 |
| H | 2.991311 | -2.055467 | 1.053077 |

REACTANT_EXO_ME_6_SN1_B

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.169732 | |
| Sum of electronic and thermal Energies= | -937.156213 | |
| Sum of electronic and thermal Enthalpies= | -937.155269 | |
| Sum of electronic and thermal Free Energies= | -937.210410 | |
| Zero-point correction= | 0.228059 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.70 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.643393 | -1.876955 | 1.029773 |
| C | -0.192204 | -0.580124 | 1.174675 |
| C | -1.581420 | -0.904649 | 0.596132 |
| S | -2.301724 | 0.344555 | -0.560380 |
| C | -3.934036 | -0.460035 | -0.737098 |
| C | 0.789708 | 0.435769 | 0.487599 |
| O | 0.250486 | 1.574624 | -0.064456 |
| C | 0.003353 | 2.655599 | 0.849475 |
| C | 1.413920 | -0.450460 | -0.637253 |
| O | 2.575860 | -0.080199 | -1.281303 |
| C | 3.693816 | 0.282655 | -0.457010 |
| C | 1.446470 | -1.768911 | 0.067285 |
| H | -0.231235 | -0.460973 | 2.256168 |
| H | 1.562224 | 0.678415 | 1.235905 |
| H | 0.634591 | -0.539332 | -1.420247 |
| H | 2.081294 | -2.629117 | -0.154880 |
| H | -1.530542 | -1.867467 | 0.075216 |
| H | -2.269552 | -1.041733 | 1.435541 |
| H | -4.458043 | -0.513024 | 0.221524 |
| H | -4.508981 | 0.173725 | -1.416829 |
| H | -3.846080 | -1.457781 | -1.176457 |
| H | -0.272557 | 3.508975 | 0.230897 |
| H | -0.823737 | 2.418923 | 1.527801 |
| H | 0.909694 | 2.890515 | 1.422071 |
| H | 4.537102 | 0.385458 | -1.139613 |
| H | 3.522104 | 1.238093 | 0.049797 |
| H | 3.925744 | -0.496373 | 0.284248 |

REACTANT_EXO_ME_6_NH3_SN2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -993.728371 | |
| Sum of electronic and thermal Energies= | -993.711719 | |
| Sum of electronic and thermal Enthalpies= | -993.710775 | |
| Sum of electronic and thermal Free Energies= | -993.772890 | |
| Zero-point correction= | 0.266576 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.24 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.662717 | -0.848540 | 1.187264 |
| C | -0.530959 | 0.604805 | 1.225627 |
| C | -1.745693 | 1.168042 | 0.453693 |
| S | -2.074355 | 0.157791 | -1.043688 |
| C | -3.476716 | -0.867804 | -0.470622 |
| C | 0.825526 | 0.853205 | 0.498769 |
| O | 0.917113 | 2.077015 | -0.172427 |
| C | 1.302584 | 3.185182 | 0.648969 |
| C | 0.893702 | -0.320912 | -0.517115 |
| O | 2.129507 | -0.984826 | -0.565342 |
| C | 3.069088 | -0.374709 | -1.462906 |
| C | -0.194397 | -1.239746 | 0.030945 |
| H | -0.548327 | 0.893175 | 2.276779 |
| H | 1.642165 | 0.723324 | 1.223624 |
| H | 0.623231 | 0.043237 | -1.515061 |
| H | -2.641516 | 1.173579 | 1.077392 |
| H | -1.527853 | 2.186310 | 0.125239 |
| H | -4.348481 | -0.231775 | -0.300532 |
| H | -3.702123 | -1.576036 | -1.271160 |
| H | -3.213945 | -1.405151 | 0.443722 |
| H | 1.408784 | 4.039246 | -0.020912 |
| H | 0.543129 | 3.415371 | 1.408341 |
| H | 2.261061 | 2.987899 | 1.145795 |
| H | 3.969570 | -0.988471 | -1.419262 |
| H | 2.679069 | -0.367618 | -2.488759 |
| H | 3.307010 | 0.650715 | -1.158050 |
| H | -0.459097 | -2.223115 | -0.321388 |
| N | 1.244743 | -3.120240 | 1.102042 |
| H | 1.165695 | -3.191494 | 2.115867 |
| H | 1.225687 | -4.072733 | 0.738119 |
| H | 2.162396 | -2.737001 | 0.884840 |

OXACARBENIUM1

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.186871 | |
| Sum of electronic and thermal Energies= | -937.172413 | |
| Sum of electronic and thermal Enthalpies= | -937.171469 | |
| Sum of electronic and thermal Free Energies= | -937.229615 | |
| Zero-point correction= | 0.227964 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.65 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.520724 | -1.218469 | 0.751117 |
| C | -0.597354 | 0.303847 | 0.703902 |
| C | -1.552446 | 0.730846 | -0.404839 |
| S | -3.325700 | 0.492226 | -0.057093 |
| C | -3.559777 | -1.280122 | -0.441719 |
| C | 0.898125 | 0.684957 | 0.507037 |
| O | 0.983326 | 1.857150 | -0.227634 |
| C | 2.224678 | 2.567080 | -0.099089 |
| C | 1.516761 | -0.575846 | -0.189837 |
| O | 2.776592 | -0.900206 | 0.321288 |
| C | 3.681481 | -1.528117 | -0.603878 |
| C | 0.545029 | -1.635134 | 0.223935 |
| H | -0.994586 | 0.557726 | 1.685866 |
| H | 1.387241 | 0.775345 | 1.489079 |
| H | 1.507462 | -0.430010 | -1.282475 |
| H | 0.706892 | -2.713696 | 0.222734 |
| H | -1.408798 | 1.811127 | -0.510731 |
| H | -1.268478 | 0.282393 | -1.364726 |
| H | -4.635438 | -1.458652 | -0.368829 |
| H | -3.242051 | -1.506888 | -1.463879 |
| H | -3.051259 | -1.931883 | 0.273184 |
| H | 3.057891 | 1.988731 | -0.515793 |
| H | 2.101206 | 3.490673 | -0.664582 |

| | | | |
|---|---|---|---|
| H | 2.430972 | 2.799818 | 0.952691 |
| H | 4.622542 | -1.645332 | -0.066819 |
| H | 3.316629 | -2.514264 | -0.917022 |
| H | 3.828435 | -0.893556 | -1.486450 |

OXACARBENIUM2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.187671 |
| Sum of electronic and thermal Energies= | | -937.173114 |
| Sum of electronic and thermal Enthalpies= | | -937.172170 |
| Sum of electronic and thermal Free Energies= | | -937.230963 |
| Zero-point correction= | 0.227975 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.10 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.274149 | -1.502829 | 0.584719 |
| C | -0.621640 | -0.015386 | 0.553927 |
| C | -1.550252 | 0.243637 | -0.624096 |
| S | -3.152310 | -0.635768 | -0.529167 |
| C | -4.116947 | 0.525236 | 0.506214 |
| C | 0.787933 | 0.633900 | 0.481191 |
| O | 0.706668 | 1.820949 | -0.231527 |
| C | 1.809650 | 2.718700 | -0.038532 |
| C | 1.676129 | -0.475680 | -0.181106 |
| O | 2.934192 | -0.574656 | 0.418704 |
| C | 3.997390 | -1.027163 | -0.438262 |
| C | 0.886117 | -1.704384 | 0.146613 |
| H | -1.126388 | 0.128983 | 1.508512 |
| H | 1.182783 | 0.787328 | 1.497416 |
| H | 1.717346 | -0.311476 | -1.270702 |
| H | 1.242648 | -2.735564 | 0.149146 |
| H | -1.704910 | 1.325936 | -0.676291 |
| H | -1.070105 | -0.048298 | -1.564114 |
| H | -5.113957 | 0.087040 | 0.596109 |
| H | -3.698248 | 0.634006 | 1.510763 |
| H | -4.203816 | 1.501212 | 0.021543 |
| H | 1.936116 | 2.955204 | 1.025072 |
| H | 2.741641 | 2.294264 | -0.430880 |
| H | 1.559602 | 3.624146 | -0.591521 |
| H | 4.904188 | -0.985222 | 0.164803 |
| H | 3.832116 | -2.058315 | -0.774498 |
| H | 4.093972 | -0.367828 | -1.309552 |

OXACARBENIUM3

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.185873 |
| Sum of electronic and thermal Energies= | | -937.171368 |
| Sum of electronic and thermal Enthalpies= | | -937.170424 |
| Sum of electronic and thermal Free Energies= | | -937.228881 |
| Zero-point correction= | 0.227785 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -38.92 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.526400 | -1.282081 | -0.833736 |
| C | 0.520428 | 0.242779 | -0.677713 |
| C | 1.433859 | 0.627889 | 0.480164 |
| S | 3.224487 | 0.517846 | 0.147308 |
| C | 3.554436 | -1.262421 | 0.403962 |
| C | -1.007617 | 0.522016 | -0.473145 |
| O | -1.299705 | 1.577669 | 0.383138 |
| C | -1.426810 | 2.862168 | -0.250904 |
| C | -1.530562 | -0.809056 | 0.143110 |
| O | -2.812979 | -1.195514 | -0.207511 |
| C | -3.838058 | -0.867266 | 0.753239 |
| C | -0.533984 | -1.785450 | -0.379928 |
| H | 0.925769 | 0.577444 | -1.632101 |
| H | -1.485128 | 0.646205 | -1.456508 |
| H | -1.380731 | -0.750118 | 1.239808 |
| H | -0.647940 | -2.868573 | -0.439781 |
| H | 1.232759 | 1.684739 | 0.684310 |
| H | 1.164455 | 0.085440 | 1.394353 |
| H | 4.639036 | -1.374497 | 0.330757 |
| H | 3.242222 | -1.580138 | 1.403110 |
| H | 3.088825 | -1.886399 | -0.362817 |
| H | -0.476347 | 3.192969 | -0.687425 |
| H | -2.199002 | 2.834247 | -1.028872 |
| H | -1.723138 | 3.556036 | 0.535871 |
| H | -4.776263 | -1.190797 | 0.303304 |
| H | -3.674099 | -1.407773 | 1.692981 |
| H | -3.862096 | 0.211142 | 0.938235 |

OXACARBENIUM4

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.188299 |
| Sum of electronic and thermal Energies= | | -937.173709 |
| Sum of electronic and thermal Enthalpies= | | -937.172765 |
| Sum of electronic and thermal Free Energies= | | -937.231611 |
| Zero-point correction= | 0.228035 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -38.82 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.237865 | -1.491182 | -0.687083 |
| C | 0.515827 | 0.009297 | -0.823427 |
| C | 1.587756 | 0.390227 | 0.176158 |
| S | 3.110306 | -0.585314 | -0.128408 |
| C | 4.304774 | 0.408566 | 0.834567 |
| C | -0.892300 | 0.617099 | -0.588645 |
| O | -0.758937 | 1.851225 | 0.030989 |
| C | -1.907082 | 2.705910 | -0.071818 |
| C | -1.635493 | -0.470340 | 0.262603 |
| O | -2.951138 | -0.666688 | -0.168406 |
| C | -3.880779 | -1.087825 | 0.844987 |
| C | -0.839257 | -1.693960 | -0.071144 |
| H | 0.875369 | 0.088889 | -1.849125 |
| H | -1.430654 | 0.689505 | -1.545867 |
| H | -1.555097 | -0.220004 | 1.332790 |
| H | -1.144707 | -2.732901 | 0.060135 |
| H | 1.779389 | 1.458199 | 0.025942 |
| H | 1.223537 | 0.263824 | 1.202610 |
| H | 5.271345 | -0.087111 | 0.717551 |
| H | 4.377501 | 1.425644 | 0.440640 |
| H | 4.043357 | 0.426094 | 1.895552 |
| H | -2.177178 | 2.868750 | -1.122326 |
| H | -2.766395 | 2.285786 | 0.464882 |
| H | -1.618384 | 3.652110 | 0.386001 |
| H | -4.854437 | -1.129277 | 0.357071 |
| H | -3.628088 | -2.081243 | 1.236107 |
| H | -3.903444 | -0.363924 | 1.668881 |

OXACARBENIUM6

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.185920 |
| Sum of electronic and thermal Energies= | | -937.171369 |
| Sum of electronic and thermal Enthalpies= | | -937.170425 |
| Sum of electronic and thermal Free Energies= | | -937.229195 |
| Zero-point correction= | 0.227801 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.25 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.411439 | -1.229904 | -0.834022 |
| C | 0.527123 | 0.282717 | -0.659619 |
| C | 1.488074 | 0.584767 | 0.484163 |
| S | 3.259504 | 0.351790 | 0.121084 |
| C | 3.462590 | -1.453744 | 0.328054 |
| C | -0.968684 | 0.680372 | -0.414205 |
| O | -1.144112 | 1.739909 | 0.466491 |
| C | -1.299285 | 3.031310 | -0.145786 |
| C | -1.595220 | -0.610625 | 0.183388 |

| | | | |
|---|---|---|---|
| O | -2.875760 | -0.860032 | -0.307846 |
| C | -3.831167 | -1.349447 | 0.650405 |
| C | -0.660115 | -1.659428 | -0.328808 |
| H | 0.934663 | 0.602608 | -1.618067 |
| H | -1.454498 | 0.863452 | -1.383382 |
| H | -1.548322 | -0.550032 | 1.283445 |
| H | -0.848772 | -2.731174 | -0.398940 |
| H | 1.366935 | 1.650564 | 0.703822 |
| H | 1.191790 | 0.051259 | 1.395888 |
| H | 4.535322 | -1.641896 | 0.238274 |
| H | 3.139013 | -1.774122 | 1.322807 |
| H | 2.944660 | -2.022810 | -0.448029 |
| H | -1.500519 | 3.725601 | 0.670205 |
| H | -0.387336 | 3.341849 | -0.670464 |
| H | -2.144725 | 3.028313 | -0.843712 |
| H | -4.780964 | -1.405758 | 0.118938 |
| H | -3.557974 | -2.347285 | 1.014895 |
| H | -3.913764 | -0.654531 | 1.494443 |

OXACARBENIUM7

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.190793 | |
| Sum of electronic and thermal Energies= | -937.176275 | |
| Sum of electronic and thermal Enthalpies= | -937.175331 | |
| Sum of electronic and thermal Free Energies= | -937.233376 | |
| Zero-point correction= | 0.228255 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -38.40 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.289601 | -1.010751 | 0.611102 |
| C | 0.374458 | -0.011206 | -0.571939 |
| C | 1.681098 | 0.750070 | -0.483467 |
| S | 3.174553 | -0.283281 | -0.717472 |
| C | 3.593333 | -0.718882 | 1.009978 |
| C | -0.941390 | 0.768081 | -0.422062 |
| O | -0.715557 | 1.867967 | 0.417816 |
| C | -1.669257 | 2.930227 | 0.291986 |
| C | -1.875553 | -0.242626 | 0.290263 |
| O | -2.359793 | -1.235568 | -0.593954 |
| C | -3.701540 | -1.705792 | -0.344411 |
| C | -0.879617 | -1.061547 | 1.063447 |
| H | 0.354853 | -0.690407 | -1.425810 |
| H | -1.342990 | 1.045472 | -1.405466 |
| H | -2.655081 | 0.237092 | 0.888558 |
| H | -1.076371 | -1.778888 | 1.860303 |
| H | 1.666652 | 1.471714 | -1.308871 |
| H | 1.734942 | 1.329806 | 0.440454 |
| H | 4.540336 | -1.261709 | 0.956060 |
| H | 3.742190 | 0.180212 | 1.613889 |
| H | 2.843174 | -1.368162 | 1.467462 |
| H | -2.680201 | 2.607806 | 0.574957 |
| H | -1.340599 | 3.714389 | 0.974420 |
| H | -1.685210 | 3.316934 | -0.734442 |
| H | -3.908363 | -2.428643 | -1.133436 |
| H | -3.781440 | -2.195793 | 0.632120 |
| H | -4.407948 | -0.870466 | -0.403139 |

OXACARBENIUM9

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.186351 | |
| Sum of electronic and thermal Energies= | -937.171742 | |
| Sum of electronic and thermal Enthalpies= | -937.170797 | |
| Sum of electronic and thermal Free Energies= | -937.229825 | |
| Zero-point correction= | 0.227757 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -38.42 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.271710 | -1.568764 | -0.670640 |
| C | 0.534697 | -0.059167 | -0.552900 |
| C | 1.430478 | 0.177502 | 0.654041 |
| S | 3.057559 | -0.657581 | 0.575707 |
| C | 4.003721 | 0.527758 | -0.448208 |
| C | -0.922797 | 0.502680 | -0.453102 |
| O | -1.065737 | 1.603928 | 0.386498 |
| C | -0.881584 | 2.880850 | -0.244318 |
| C | -1.726380 | -0.695908 | 0.133046 |
| O | -3.030286 | -0.849685 | -0.304925 |
| C | -4.038636 | -0.282921 | 0.557311 |
| C | -0.892786 | -1.853150 | -0.299998 |
| H | 1.045271 | 0.154434 | -1.491658 |
| H | -1.308894 | 0.703724 | -1.463304 |
| H | -1.644325 | -0.644501 | 1.238156 |
| H | -1.200413 | -2.898874 | -0.350061 |
| H | 1.562138 | 1.259944 | 0.756818 |
| H | 0.937040 | -0.158639 | 1.571758 |
| H | 4.056418 | 1.507505 | 0.034314 |
| H | 5.014404 | 0.118325 | -0.519643 |
| H | 3.600756 | 0.620773 | -1.460851 |
| H | -1.565038 | 2.995923 | -1.094293 |
| H | -1.112942 | 3.627384 | 0.515703 |
| H | 0.152725 | 3.019049 | -0.583959 |
| H | -4.988279 | -0.459053 | 0.052839 |
| H | -4.039569 | -0.785657 | 1.531719 |
| H | -3.876008 | 0.791264 | 0.688446 |

OXACARBENIUM11

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -937.187252 | |
| Sum of electronic and thermal Energies= | -937.172643 | |
| Sum of electronic and thermal Enthalpies= | -937.171699 | |
| Sum of electronic and thermal Free Energies= | -937.230614 | |
| Zero-point correction= | 0.227888 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -38.40 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.235553 | -1.545335 | -0.800681 |
| C | 0.429407 | -0.016180 | -0.823659 |
| C | 1.478208 | 0.342904 | 0.207285 |
| S | 3.037584 | -0.562919 | -0.127379 |
| C | 4.163954 | 0.360505 | 0.977189 |
| C | -1.020685 | 0.487827 | -0.531850 |
| O | -1.088466 | 1.635579 | 0.252527 |
| C | -1.073234 | 2.874198 | -0.475112 |
| C | -1.665801 | -0.701659 | 0.241271 |
| O | -3.008002 | -0.942592 | -0.002022 |
| C | -3.917378 | -0.395897 | 0.974924 |
| C | -0.842366 | -1.851047 | -0.234254 |
| H | 0.785780 | 0.148572 | -1.840609 |
| H | -1.564784 | 0.604511 | -1.480371 |
| H | -1.439617 | -0.565577 | 1.317263 |
| H | -1.099070 | -2.909390 | -0.169096 |
| H | 1.643812 | 1.423096 | 0.120136 |
| H | 1.108682 | 0.153132 | 1.221466 |
| H | 5.145940 | -0.104135 | 0.861146 |
| H | 4.232227 | 1.410915 | 0.682068 |
| H | 3.854539 | 0.275047 | 2.021921 |
| H | -0.116941 | 3.029425 | -0.990149 |
| H | -1.891758 | 2.905349 | -1.204307 |
| H | -1.214042 | 3.659954 | 0.267352 |
| H | -4.916551 | -0.636964 | 0.613043 |
| H | -3.757817 | -0.861710 | 1.954621 |
| H | -3.797069 | 0.689363 | 1.050224 |

OXACARBENIUM12

| | |
|---|---|
| Sum of electronic and zero-point Energies= | -937.186380 |
| Sum of electronic and thermal Energies= | -937.171739 |

Sum of electronic and thermal Enthalpies= -937.170795
Sum of electronic and thermal Free Energies= -937.230276
Zero-point correction= 0.227825 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -38.65
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.147542 | -1.489606 | 0.654100 |
| C | -0.531299 | -0.011683 | 0.530518 |
| C | -1.472046 | 0.144757 | -0.654892 |
| S | -3.022184 | -0.821404 | -0.537669 |
| C | -4.031636 | 0.275907 | 0.523489 |
| C | 0.871475 | 0.668542 | 0.387531 |
| O | 0.895331 | 1.752314 | -0.484283 |
| C | 0.708703 | 3.037045 | 0.128342 |
| C | 1.776107 | -0.462889 | -0.174094 |
| O | 3.033273 | -0.486359 | 0.429524 |
| C | 4.136625 | -0.805420 | -0.437379 |
| C | 1.017631 | -1.688397 | 0.229860 |
| H | -1.032652 | 0.173167 | 1.480350 |
| H | 1.253959 | 0.931542 | 1.383979 |
| H | 1.815413 | -0.375765 | -1.272730 |
| H | 1.397184 | -2.709949 | 0.280090 |
| H | -1.694628 | 1.212087 | -0.757240 |
| H | -0.972299 | -0.153969 | -1.582318 |
| H | -5.004194 | -0.213342 | 0.617854 |
| H | -3.609365 | 0.392721 | 1.525730 |
| H | -4.175199 | 1.252333 | 0.052852 |
| H | 0.837121 | 3.769863 | -0.668545 |
| H | -0.296686 | 3.139994 | 0.556258 |
| H | 1.459922 | 3.206933 | 0.908944 |
| H | 5.032315 | -0.707089 | 0.175651 |
| H | 4.065623 | -1.832485 | -0.816064 |
| H | 4.176568 | -0.101544 | -1.277099 |

OXACARBENIUM13
Sum of electronic and zero-point Energies= -937.187337
Sum of electronic and thermal Energies= -937.172741
Sum of electronic and thermal Enthalpies= -937.171797
Sum of electronic and thermal Free Energies= -937.230754
Zero-point correction= 0.228031 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -38.59
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.108151 | -1.447280 | -0.824560 |
| C | 0.423748 | 0.055018 | -0.801527 |
| C | 1.516941 | 0.293557 | 0.218341 |
| S | 2.996889 | -0.710392 | -0.185717 |
| C | 4.209768 | 0.080903 | 0.929768 |
| C | -0.971756 | 0.670719 | -0.459704 |
| O | -0.915771 | 1.778341 | 0.379842 |
| C | -0.884626 | 3.050004 | -0.286516 |
| C | -1.722369 | -0.485302 | 0.258738 |
| O | -3.049048 | -0.594496 | -0.160586 |
| C | -4.000778 | -0.937213 | 0.862487 |
| C | -0.966490 | -1.686664 | -0.218025 |
| H | 0.771153 | 0.230082 | -1.819832 |
| H | -1.513575 | 0.885423 | -1.391476 |
| H | -1.614276 | -0.359803 | 1.348322 |
| H | -1.294741 | -2.726114 | -0.180338 |
| H | 1.760469 | 1.361245 | 0.173665 |
| H | 1.150912 | 0.087223 | 1.231079 |
| H | 5.152621 | -0.448393 | 0.773303 |
| H | 4.348977 | 1.135092 | 0.675913 |
| H | 3.915000 | -0.025260 | 1.976843 |
| H | -1.755111 | 3.164179 | -0.943542 |
| H | -0.920828 | 3.801875 | 0.502105 |
| H | 0.036037 | 3.179882 | -0.869373 |
| H | -4.977250 | -0.910472 | 0.379195 |
| H | -3.818761 | -1.943371 | 1.259817 |
| H | -3.964140 | -0.203965 | 1.676851 |

OXACARBENIUM14
Sum of electronic and zero-point Energies= -937.191525
Sum of electronic and thermal Energies= -937.176872
Sum of electronic and thermal Enthalpies= -937.175928
Sum of electronic and thermal Free Energies= -937.235764
Zero-point correction= 0.228455 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -36.81
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.706161 | -1.465981 | 1.132614 |
| C | 0.187333 | -0.825411 | 0.032508 |
| C | 1.614078 | -0.824032 | 0.523688 |
| S | 2.659556 | -0.289878 | -0.896854 |
| C | 4.273651 | -0.184866 | -0.045231 |
| C | -0.514474 | 0.520670 | -0.194017 |
| O | -0.015037 | 1.449778 | 0.728499 |
| C | -0.085728 | 2.817350 | 0.303564 |
| C | -1.987233 | 0.211909 | 0.172035 |
| O | -2.642200 | -0.550748 | -0.825612 |
| C | -4.042490 | -0.262044 | -1.024588 |
| C | -1.804693 | -0.863370 | 1.207485 |
| H | 0.031458 | -1.513751 | -0.801351 |
| H | -0.418374 | 0.839798 | -1.238411 |
| H | -2.545714 | 1.093890 | 0.496055 |
| H | -2.546061 | -1.261920 | 1.900300 |
| H | 1.723128 | -0.124884 | 1.355597 |
| H | 1.893738 | -1.833356 | 0.841229 |
| H | 4.994022 | 0.127615 | -0.804924 |
| H | 4.250608 | 0.561168 | 0.753067 |
| H | 4.573256 | -1.159440 | 0.347986 |
| H | -1.122602 | 3.134850 | 0.129457 |
| H | 0.337336 | 3.408573 | 1.116129 |
| H | 0.504025 | 2.966419 | -0.608239 |
| H | -4.361707 | -0.913692 | -1.837802 |
| H | -4.630497 | -0.480720 | -0.126487 |
| H | -4.170993 | 0.787871 | -1.309608 |

OXACARBENIUM15
Sum of electronic and zero-point Energies= -937.186380
Sum of electronic and thermal Energies= -937.171739
Sum of electronic and thermal Enthalpies= -937.170795
Sum of electronic and thermal Free Energies= -937.230276
Zero-point correction= 0.227825 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -38.65
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.147462 | -1.489661 | 0.653981 |
| C | -0.531229 | -0.011714 | 0.530481 |
| C | -1.472052 | 0.144715 | -0.654889 |
| S | -3.022137 | -0.821585 | -0.537431 |
| C | -4.031694 | 0.276053 | 0.523277 |
| C | 0.871492 | 0.668496 | 0.387470 |
| O | 0.895227 | 1.752334 | -0.484327 |
| C | 0.708425 | 3.036984 | 0.128354 |
| C | 1.776167 | -0.462828 | -0.174074 |
| O | 3.033343 | -0.486230 | 0.429563 |
| C | 4.136710 | -0.805228 | -0.437297 |
| C | 1.017687 | -1.688403 | 0.229726 |
| H | -1.032597 | 0.173124 | 1.480308 |
| H | 1.253990 | 0.931541 | 1.383903 |
| H | 1.815554 | -0.375867 | -1.272739 |
| H | 1.397301 | -2.709936 | 0.279925 |
| H | -1.694738 | 1.212016 | -0.757203 |

| | | | |
|---|---|---|---|
| H | -0.972379 | -0.154029 | -1.582345 |
| H | -5.004622 | -0.212614 | 0.616866 |
| H | -3.610070 | 0.392347 | 1.525857 |
| H | -4.174314 | 1.252695 | 0.052799 |
| H | 1.459786 | 3.207074 | 0.908779 |
| H | 0.836444 | 3.769879 | -0.668533 |
| H | -0.296884 | 3.139688 | 0.556538 |
| H | 5.032346 | -0.707583 | 0.175928 |
| H | 4.065408 | -1.832058 | -0.816575 |
| H | 4.177075 | -0.100907 | -1.276629 |

OXACARBENIUM16

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.181128 |
| Sum of electronic and thermal Energies= | | -937.166742 |
| Sum of electronic and thermal Enthalpies= | | -937.165798 |
| Sum of electronic and thermal Free Energies= | | -937.223573 |
| Zero-point correction= | 0.227867 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -40.57 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.485226 | -1.341013 | 0.362894 |
| C | -0.490415 | 0.167853 | 0.657789 |
| C | -1.560894 | 0.835283 | -0.197536 |
| S | -3.281514 | 0.502780 | 0.307979 |
| C | -3.630924 | -1.081538 | -0.536582 |
| C | 0.984170 | 0.570672 | 0.368757 |
| O | 1.007023 | 1.831494 | -0.214404 |
| C | 2.286995 | 2.483643 | -0.195489 |
| C | 1.500522 | -0.572604 | -0.581263 |
| O | 2.841356 | -0.925751 | -0.613421 |
| C | 3.422084 | -1.399444 | 0.613039 |
| C | 0.547607 | -1.682898 | -0.264583 |
| H | -0.761824 | 0.193610 | 1.712446 |
| H | 1.557266 | 0.551173 | 1.307728 |
| H | 1.246266 | -0.251535 | -1.608463 |
| H | 0.648405 | -2.738195 | -0.525891 |
| H | -1.403860 | 1.910928 | -0.066315 |
| H | -1.408400 | 0.628342 | -1.262683 |
| H | -4.691731 | -1.280010 | -0.364688 |
| H | -3.466608 | -0.996750 | -1.614763 |
| H | -3.051349 | -1.910293 | -0.122382 |
| H | 3.022865 | 1.930283 | -0.789871 |
| H | 2.126358 | 3.468657 | -0.633647 |
| H | 2.648153 | 2.594339 | 0.835048 |
| H | 4.417951 | -1.752915 | 0.346425 |
| H | 3.511532 | -0.599713 | 1.355922 |
| H | 2.849099 | -2.236042 | 1.038123 |

OXACARBENIUM17

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.190792 |
| Sum of electronic and thermal Energies= | | -937.176275 |
| Sum of electronic and thermal Enthalpies= | | -937.175331 |
| Sum of electronic and thermal Free Energies= | | -937.233373 |
| Zero-point correction= | 0.228256 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -38.40 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.289742 | -1.010960 | 0.610923 |
| C | 0.374606 | -0.011088 | -0.571860 |
| C | 1.681086 | 0.750362 | -0.483126 |
| S | 3.174790 | -0.282485 | -0.717454 |
| C | 3.593001 | -0.719623 | 1.009733 |
| C | -0.941431 | 0.768005 | -0.421903 |
| O | -0.715710 | 1.867964 | 0.417897 |
| C | -1.669739 | 2.929949 | 0.292234 |
| C | -1.875411 | -0.242852 | 0.290393 |
| O | -2.359424 | -1.236074 | -0.593716 |
| C | -3.701672 | -1.705300 | -0.344997 |
| C | -0.879458 | -1.061901 | 1.063332 |
| H | 0.355172 | -0.690110 | -1.425882 |
| H | -1.343072 | 1.045288 | -1.405325 |
| H | -2.655001 | 0.236644 | 0.888757 |
| H | -1.076138 | -1.779494 | 1.859985 |
| H | 1.666537 | 1.472158 | -1.308413 |
| H | 1.734782 | 1.329968 | 0.440884 |
| H | 3.742068 | 0.178932 | 1.614404 |
| H | 2.842553 | -1.369032 | 1.466554 |
| H | 4.539856 | -1.262685 | 0.955526 |
| H | -1.341310 | 3.714064 | 0.974824 |
| H | -1.685796 | 3.316831 | -0.734129 |
| H | -2.680603 | 2.607182 | 0.575120 |
| H | -3.907822 | -2.429507 | -1.132950 |
| H | -3.782986 | -2.193472 | 0.632339 |
| H | -4.407635 | -0.869767 | -0.406102 |

OXACARBENIUM18

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.181964 |
| Sum of electronic and thermal Energies= | | -937.167576 |
| Sum of electronic and thermal Enthalpies= | | -937.166632 |
| Sum of electronic and thermal Free Energies= | | -937.224023 |
| Zero-point correction= | 0.228347 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.07 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.286214 | -0.965002 | 0.753136 |
| C | 0.250920 | -0.050857 | -0.501264 |
| C | 1.496377 | 0.816569 | -0.500913 |
| S | 3.056293 | -0.111948 | -0.733476 |
| C | 3.573883 | -0.400712 | 0.997767 |
| C | -1.121322 | 0.635948 | -0.373952 |
| O | -0.932041 | 1.876927 | 0.252242 |
| C | -1.996364 | 2.817441 | 0.055214 |
| C | -1.938986 | -0.290908 | 0.581648 |
| O | -2.766121 | -1.317115 | 0.081028 |
| C | -2.323537 | -2.097399 | -1.045329 |
| C | -0.833175 | -0.997492 | 1.317562 |
| H | 0.285103 | -0.786527 | -1.305821 |
| H | -1.599601 | 0.731914 | -1.357897 |
| H | -2.562632 | 0.306481 | 1.250892 |
| H | -0.933349 | -1.628023 | 2.202009 |
| H | 1.395474 | 1.488158 | -1.361376 |
| H | 1.532015 | 1.450470 | 0.387553 |
| H | 4.553146 | -0.882005 | 0.936721 |
| H | 3.684285 | 0.545328 | 1.534277 |
| H | 2.889465 | -1.066043 | 1.529461 |
| H | -2.135528 | 3.025282 | -1.012977 |
| H | -2.942316 | 2.459430 | 0.482374 |
| H | -1.692592 | 3.728734 | 0.570710 |
| H | -3.133108 | -2.803381 | -1.230696 |
| H | -2.185234 | -1.471062 | -1.933218 |
| H | -1.407009 | -2.661617 | -0.832042 |

OXACARBENIUM20

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.194027 |
| Sum of electronic and thermal Energies= | | -937.179452 |
| Sum of electronic and thermal Enthalpies= | | -937.178508 |
| Sum of electronic and thermal Free Energies= | | -937.236694 |
| Zero-point correction= | 0.228307 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -36.32 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.577998 | -1.181107 | 1.461793 |
| C | 0.374382 | -0.610890 | 0.335583 |
| C | 1.707952 | -0.284938 | 0.960807 |

| | | | |
|---|---|---|---|
| S | 2.852362 | 0.246372 | -0.374187 |
| C | 3.533110 | -1.364762 | -0.916861 |
| C | -0.473355 | 0.539837 | -0.225128 |
| O | -0.183062 | 1.703148 | 0.500943 |
| C | -0.440870 | 2.928978 | -0.196557 |
| C | -1.927830 | 0.103637 | 0.080331 |
| O | -2.381224 | -0.902900 | -0.807326 |
| C | -3.776047 | -0.840435 | -1.171683 |
| C | -1.737466 | -0.730188 | 1.317396 |
| H | 0.414706 | -1.463604 | -0.343567 |
| H | -0.312361 | 0.647126 | -1.303762 |
| H | -2.616406 | 0.946768 | 0.181216 |
| H | -2.505527 | -1.087695 | 2.004631 |
| H | 1.613377 | 0.550516 | 1.655060 |
| H | 2.114752 | -1.151846 | 1.488413 |
| H | 4.255156 | -1.132177 | -1.703688 |
| H | 4.056417 | -1.861536 | -0.095941 |
| H | 2.768465 | -2.024718 | -1.335698 |
| H | 0.154242 | 2.981351 | -1.115753 |
| H | -1.505750 | 3.041186 | -0.440761 |
| H | -0.143071 | 3.729986 | 0.480469 |
| H | -3.932520 | -1.661971 | -1.870665 |
| H | -4.426488 | -0.971938 | -0.299941 |
| H | -3.993761 | 0.116023 | -1.659619 |

OXACARBENIUM21

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -937.194026 |
| Sum of electronic and thermal Energies= | | -937.179452 |
| Sum of electronic and thermal Enthalpies= | | -937.178507 |
| Sum of electronic and thermal Free Energies= | | -937.236693 |
| Zero-point correction= | 0.228308 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -36.32 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.577974 | -1.181244 | 1.461600 |
| C | 0.374314 | -0.610976 | 0.335533 |
| C | 1.707921 | -0.285065 | 0.960734 |
| S | 2.852246 | 0.246447 | -0.374247 |
| C | 3.533475 | -1.364554 | -0.916715 |
| C | -0.473383 | 0.539845 | -0.225118 |
| O | -0.183008 | 1.703106 | 0.500994 |
| C | -0.440978 | 2.928986 | -0.196355 |
| C | -1.927848 | 0.103656 | 0.080374 |
| O | -2.381262 | -0.902944 | -0.807225 |
| C | -3.776035 | -0.840354 | -1.171766 |
| C | -1.737462 | -0.730283 | 1.317342 |
| H | 0.414664 | -1.463599 | -0.343736 |
| H | -0.312419 | 0.647166 | -1.303753 |
| H | -2.616444 | 0.946760 | 0.181289 |
| H | -2.505468 | -1.087853 | 2.004600 |
| H | 1.613374 | 0.550260 | 1.655145 |
| H | 2.114763 | -1.152057 | 1.488167 |
| H | 4.253923 | -1.132045 | -1.705027 |
| H | 4.058614 | -1.860185 | -0.096277 |
| H | 2.768645 | -2.025512 | -1.333635 |
| H | -0.142590 | 3.729928 | 0.480490 |
| H | 0.153585 | 2.981235 | -1.115913 |
| H | -1.505984 | 3.041428 | -0.439906 |
| H | -3.932441 | -1.661763 | -1.870914 |
| H | -4.426597 | -0.971984 | -0.300135 |
| H | -3.993635 | 0.116199 | -1.659562 |

MeCN_ADDUCT_1_1

| | |
|---|---|
| Sum of electronic and zero-point Energies= | -1069.923230 |
| Sum of electronic and thermal Energies= | -1069.905503 |
| Sum of electronic and thermal Enthalpies= | -1069.904559 |
| Sum of electronic and thermal Free Energies= | -1069.970459 |
| Zero-point correction= 0.277823 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) = | -33.83 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.018992 | -1.449801 | -0.530087 |
| C | 0.681110 | -0.333919 | -1.225463 |
| C | 2.195083 | -0.476952 | -1.078253 |
| S | 2.825671 | -0.541438 | 0.646579 |
| C | 3.142533 | -2.336797 | 0.822866 |
| C | 0.054154 | 0.953008 | -0.613068 |
| O | 0.951518 | 2.009512 | -0.391141 |
| C | 1.151662 | 2.872555 | -1.510723 |
| C | -0.519233 | 0.480318 | 0.738379 |
| O | -1.689001 | 1.119601 | 1.165697 |
| C | -1.463883 | 2.320116 | 1.919036 |
| C | -0.800237 | -1.006768 | 0.462602 |
| N | -2.255613 | -1.129156 | 0.009604 |
| C | -3.349384 | -1.220762 | -0.330833 |
| C | -4.726898 | -1.344557 | -0.766326 |
| H | 0.417892 | -0.445187 | -2.282938 |
| H | -0.786506 | 1.289967 | -1.240221 |
| H | 0.280734 | 0.522499 | 1.488449 |
| H | -0.769635 | -1.661797 | 1.335749 |
| H | 2.519917 | -1.382693 | -1.598332 |
| H | 2.673603 | 0.370902 | -1.575514 |
| H | 3.497604 | -2.488818 | 1.845434 |
| H | 2.234760 | -2.924775 | 0.666894 |
| H | 3.923853 | -2.662855 | 0.131022 |
| H | 0.200108 | 3.306233 | -1.848095 |
| H | 1.812462 | 3.670248 | -1.168533 |
| H | 1.626017 | 2.352278 | -2.353675 |
| H | -0.940143 | 3.072702 | 1.321658 |
| H | -2.450711 | 2.690399 | 2.200881 |
| H | -0.880554 | 2.105575 | 2.823469 |
| H | -4.819859 | -0.981107 | -1.795266 |
| H | -5.035682 | -2.394362 | -0.718194 |
| H | -5.366820 | -0.744073 | -0.110335 |

MeCN_ADDUCT_1_7

| | |
|---|---|
| Sum of electronic and zero-point Energies= | -1069.920472 |
| Sum of electronic and thermal Energies= | -1069.901697 |
| Sum of electronic and thermal Enthalpies= | -1069.900753 |
| Sum of electronic and thermal Free Energies= | -1069.970218 |
| Zero-point correction= 0.277548 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) = | -35.61 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.218417 | -1.190581 | -0.573011 |
| C | -0.894194 | -0.163776 | 0.246945 |
| C | -2.167376 | 0.264226 | -0.476747 |
| S | -3.376278 | -1.091951 | -0.726786 |
| C | -4.263144 | -1.044931 | 0.872023 |
| C | 0.172528 | 0.961285 | 0.418434 |
| O | -0.320101 | 2.274895 | 0.377569 |
| C | -0.810690 | 2.767868 | 1.624694 |
| C | 1.120233 | 0.739428 | -0.777355 |
| O | 2.456264 | 1.099536 | -0.589872 |
| C | 2.745680 | 2.481856 | -0.848659 |
| C | 1.004530 | -0.776142 | -0.986180 |
| N | 2.095820 | -1.448491 | -0.135859 |
| C | 2.896986 | -2.017263 | 0.461106 |
| C | 3.905395 | -2.732763 | 1.218662 |
| H | -1.135890 | -0.653755 | 1.193466 |
| H | 0.746570 | 0.793803 | 1.344075 |
| H | 0.685026 | 1.224809 | -1.664604 |
| H | 1.242650 | -1.142372 | -1.987189 |

| | | | |
|---|---|---|---|
| H | -2.647653 | 1.081548 | 0.069218 |
| H | -1.920596 | 0.649537 | -1.470722 |
| H | -5.037385 | -1.814173 | 0.814804 |
| H | -3.609170 | -1.279854 | 1.717358 |
| H | -4.745106 | -0.075369 | 1.028236 |
| H | -1.096845 | 3.806618 | 1.453527 |
| H | -1.689093 | 2.207091 | 1.970901 |
| H | -0.031203 | 2.726961 | 2.397817 |
| H | 3.816706 | 2.602205 | -0.680353 |
| H | 2.508325 | 2.737226 | -1.889386 |
| H | 2.184479 | 3.137908 | -0.177018 |
| H | 3.417060 | -3.400802 | 1.936507 |
| H | 4.522925 | -3.324328 | 0.533944 |
| H | 4.537248 | -2.015924 | 1.753966 |

MeCN_ADDUCT_1_8

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.920440 |
| Sum of electronic and thermal Energies= | | -1069.901633 |
| Sum of electronic and thermal Enthalpies= | | -1069.900688 |
| Sum of electronic and thermal Free Energies= | | -1069.970505 |
| Zero-point correction= | 0.277512 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.63 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.238610 | -1.202727 | -0.575149 |
| C | -0.898288 | -0.168233 | 0.247112 |
| C | -2.168547 | 0.276586 | -0.471839 |
| S | -3.395562 | -1.063922 | -0.718478 |
| C | -4.277272 | -1.005524 | 0.882753 |
| C | 0.182811 | 0.943135 | 0.415291 |
| O | -0.293182 | 2.262998 | 0.380349 |
| C | -0.772363 | 2.758300 | 1.630999 |
| C | 1.120516 | 0.712905 | -0.786514 |
| O | 2.460652 | 1.062003 | -0.607318 |
| C | 2.761235 | 2.439981 | -0.877231 |
| C | 0.986624 | -0.802323 | -0.997762 |
| N | 2.076074 | -1.485687 | -0.158710 |
| C | 2.894228 | -1.999096 | 0.464521 |
| C | 3.914333 | -2.657434 | 1.257288 |
| H | -1.143215 | -0.655150 | 1.194395 |
| H | 0.759921 | 0.766512 | 1.337373 |
| H | 0.684275 | 1.202654 | -1.670785 |
| H | 1.210250 | -1.167023 | -2.002597 |
| H | -2.636628 | 1.099623 | 0.076113 |
| H | -1.920410 | 0.659213 | -1.466536 |
| H | -5.061264 | -1.764995 | 0.827795 |
| H | -3.623981 | -1.248645 | 1.726287 |
| H | -4.746595 | -0.029985 | 1.040231 |
| H | -1.045251 | 3.801358 | 1.464450 |
| H | -1.656815 | 2.208090 | 1.978672 |
| H | 0.009472 | 2.704350 | 2.400980 |
| H | 3.834189 | 2.551792 | -0.715335 |
| H | 2.520904 | 2.690255 | -1.918481 |
| H | 2.209525 | 3.105594 | -0.207184 |
| H | 3.473861 | -3.013033 | 2.195080 |
| H | 4.318762 | -3.508900 | 0.699298 |
| H | 4.718936 | -1.947119 | 1.476086 |

MeCN_ADDUCT_1_10

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.922643 |
| Sum of electronic and thermal Energies= | | -1069.903978 |
| Sum of electronic and thermal Enthalpies= | | -1069.903034 |
| Sum of electronic and thermal Free Energies= | | -1069.972182 |
| Zero-point correction= | 0.277850 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -34.10 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.287984 | -1.720214 | -0.149977 |
| C | 0.573057 | -1.010958 | -1.109769 |
| C | 2.023429 | -1.416555 | -0.852139 |
| S | 2.592639 | -1.211056 | 0.887159 |
| C | 3.843531 | 0.114288 | 0.703186 |
| C | 0.207758 | 0.482116 | -0.947264 |
| O | 1.325100 | 1.291697 | -1.185507 |
| C | 1.024867 | 2.642356 | -1.546126 |
| C | -0.369118 | 0.573933 | 0.481404 |
| O | -1.315089 | 1.601269 | 0.597249 |
| C | -1.465073 | 2.133463 | 1.918085 |
| C | -0.952112 | -0.854833 | 0.662819 |
| N | -2.422495 | -0.806942 | 0.234846 |
| C | -3.515823 | -0.829841 | -0.120687 |
| C | -4.894493 | -0.862247 | -0.569495 |
| H | 0.283218 | -1.375425 | -2.100352 |
| H | -0.603458 | 0.739574 | -1.647966 |
| H | 0.456602 | 0.673130 | 1.195925 |
| H | -1.012170 | -1.232194 | 1.686088 |
| H | 2.126598 | -2.474794 | -1.108054 |
| H | 2.673742 | -0.843149 | -1.517258 |
| H | 4.208233 | 0.334744 | 1.709685 |
| H | 4.683116 | -0.229240 | 0.093968 |
| H | 3.397711 | 1.010185 | 0.267516 |
| H | 1.980639 | 3.114019 | -1.779307 |
| H | 0.378032 | 2.674294 | -2.433618 |
| H | 0.537423 | 3.183135 | -0.727459 |
| H | -2.169310 | 2.962964 | 1.837403 |
| H | -1.866097 | 1.386633 | 2.617241 |
| H | -0.507619 | 2.505392 | 2.302333 |
| H | -5.214310 | 0.148961 | -0.843013 |
| H | -4.977255 | -1.521043 | -1.441002 |
| H | -5.532204 | -1.244049 | 0.235199 |

MeCN_ADDUCT_1_12

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.923323 |
| Sum of electronic and thermal Energies= | | -1069.904659 |
| Sum of electronic and thermal Enthalpies= | | -1069.903715 |
| Sum of electronic and thermal Free Energies= | | -1069.973252 |
| Zero-point correction= | 0.277796 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.14 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.193663 | -0.560925 | -0.910167 |
| C | -0.729583 | 0.144839 | 0.260151 |
| C | -2.239633 | 0.190808 | 0.148432 |
| S | -2.935021 | -1.506422 | 0.264977 |
| C | -4.700724 | -1.088859 | 0.478603 |
| C | 0.011805 | 1.485439 | 0.213128 |
| O | -0.562805 | 2.298347 | -0.780395 |
| C | -0.289031 | 3.690071 | -0.641720 |
| C | 1.444475 | 1.040402 | -0.198545 |
| O | 2.231098 | 0.613846 | 0.887602 |
| C | 2.928436 | 1.668745 | 1.555644 |
| C | 1.112631 | -0.201366 | -1.093667 |
| N | 1.988328 | -1.349101 | -0.685522 |
| C | 2.535401 | -2.311550 | -0.377898 |
| C | 3.229917 | -3.522542 | 0.011367 |
| H | -0.424568 | -0.402407 | 1.161185 |
| H | 0.020357 | 1.975564 | 1.196340 |
| H | 1.955036 | 1.810483 | -0.790507 |
| H | 1.335725 | -0.068120 | -2.155135 |
| H | -2.622278 | 0.794134 | 0.980108 |
| H | -2.524954 | 0.671522 | -0.790076 |
| H | -5.235238 | -2.037568 | 0.568989 |
| H | -4.863345 | -0.503488 | 1.388218 |

| | | | |
|---|---|---|---|
| H | -5.087216 | -0.549264 | -0.390241 |
| H | 0.786186 | 3.909177 | -0.710202 |
| H | -0.804401 | 4.189386 | -1.463591 |
| H | -0.671021 | 4.074212 | 0.313963 |
| H | 2.237504 | 2.399299 | 1.993724 |
| H | 3.503353 | 1.198746 | 2.354905 |
| H | 3.610656 | 2.183471 | 0.866146 |
| H | 3.968386 | -3.783977 | -0.754275 |
| H | 3.734251 | -3.362829 | 0.970350 |
| H | 2.504408 | -4.337938 | 0.109839 |

MeCN_ADDUCT_1_15

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.923321 |
| Sum of electronic and thermal Energies= | | -1069.904659 |
| Sum of electronic and thermal Enthalpies= | | -1069.903714 |
| Sum of electronic and thermal Free Energies= | | -1069.973228 |
| Zero-point correction= | 0.277799 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.14 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.193705 | -0.560795 | -0.910323 |
| C | -0.729516 | 0.144875 | 0.260120 |
| C | -2.239564 | 0.190943 | 0.148486 |
| S | -2.935047 | -1.506260 | 0.264925 |
| C | -4.700712 | -1.088611 | 0.478665 |
| C | 0.011961 | 1.485428 | 0.213185 |
| O | -0.562629 | 2.298453 | -0.780257 |
| C | -0.288775 | 3.690147 | -0.641479 |
| C | 1.444581 | 1.040318 | -0.198549 |
| O | 2.231098 | 0.613501 | 0.887586 |
| C | 2.928682 | 1.668195 | 1.555689 |
| C | 1.112604 | -0.201276 | -1.093874 |
| N | 1.988234 | -1.349116 | -0.686011 |
| C | 2.535057 | -2.311589 | -0.378014 |
| C | 3.229305 | -3.522611 | 0.011616 |
| H | -0.424475 | -0.402485 | 1.161075 |
| H | 0.020597 | 1.975483 | 1.196432 |
| H | 1.955264 | 1.810432 | -0.790355 |
| H | 1.335597 | -0.067815 | -2.155337 |
| H | -2.622130 | 0.794218 | 0.980237 |
| H | -2.524908 | 0.671752 | -0.789966 |
| H | -5.235270 | -2.037298 | 0.569029 |
| H | -4.863259 | -0.503278 | 1.388318 |
| H | -5.087224 | -0.548952 | -0.390132 |
| H | -0.804218 | 4.189564 | -1.463243 |
| H | -0.670636 | 4.074219 | 0.314285 |
| H | 0.786445 | 3.909216 | -0.710065 |
| H | 3.503486 | 1.198013 | 2.354924 |
| H | 3.611025 | 2.182807 | 0.866225 |
| H | 2.237921 | 2.398888 | 1.993814 |
| H | 2.504019 | -4.338512 | 0.107521 |
| H | 3.969726 | -3.782829 | -0.752557 |
| H | 3.731297 | -3.363622 | 0.971948 |

MeCN_ADDUCT_1_16

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.923153 |
| Sum of electronic and thermal Energies= | | -1069.904579 |
| Sum of electronic and thermal Enthalpies= | | -1069.903635 |
| Sum of electronic and thermal Free Energies= | | -1069.972285 |
| Zero-point correction= | 0.278011 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.55 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.381147 | -1.668432 | 0.391495 |
| C | -0.537042 | -0.827217 | 1.172362 |
| C | -1.967122 | -1.304532 | 0.911560 |
| S | -2.457589 | -1.410091 | -0.859967 |
| C | -3.661954 | -0.036609 | -0.998494 |
| C | -0.175465 | 0.627624 | 0.767520 |
| O | -1.250225 | 1.531753 | 0.718535 |
| C | -1.590258 | 2.117213 | 1.976476 |
| C | 0.448957 | 0.478926 | -0.633393 |
| O | 1.458753 | 1.395583 | -0.952433 |
| C | 0.983559 | 2.622443 | -1.523852 |
| C | 1.030738 | -0.948264 | -0.569219 |
| N | 2.498837 | -0.839276 | -0.190151 |
| C | 3.608727 | -0.755852 | 0.095018 |
| C | 5.008479 | -0.653111 | 0.458464 |
| H | -0.292358 | -1.021981 | 2.221787 |
| H | 0.606813 | 1.007586 | 1.444128 |
| H | -0.354145 | 0.464482 | -1.380431 |
| H | 1.063920 | -1.479348 | -1.523305 |
| H | -2.060525 | -2.312481 | 1.325998 |
| H | -2.675299 | -0.664983 | 1.445248 |
| H | -3.988860 | -0.023258 | -2.041445 |
| H | -4.532272 | -0.221279 | -0.363575 |
| H | -3.200275 | 0.919703 | -0.745841 |
| H | -2.386903 | 2.835456 | 1.777301 |
| H | -1.953315 | 1.368665 | 2.693150 |
| H | -0.728203 | 2.641221 | 2.411099 |
| H | 1.870112 | 3.222516 | -1.734432 |
| H | 0.442205 | 2.429744 | -2.458972 |
| H | 0.328533 | 3.157298 | -0.829324 |
| H | 5.611955 | -1.244870 | -0.238343 |
| H | 5.318671 | 0.396364 | 0.412115 |
| H | 5.150400 | -1.033407 | 1.475948 |

MeCN_ADDUCT_1_18

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.922348 |
| Sum of electronic and thermal Energies= | | -1069.903494 |
| Sum of electronic and thermal Enthalpies= | | -1069.902550 |
| Sum of electronic and thermal Free Energies= | | -1069.975141 |
| Zero-point correction= | 0.277614 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -34.97 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.062602 | -0.592366 | -0.846705 |
| C | -0.685662 | 0.119526 | 0.275616 |
| C | -2.188284 | -0.028462 | 0.149517 |
| S | -2.670521 | -1.796168 | 0.299067 |
| C | -4.472366 | -1.593739 | 0.523853 |
| C | -0.094463 | 1.534979 | 0.137856 |
| O | -0.637802 | 2.249624 | -0.947016 |
| C | -1.560195 | 3.284227 | -0.605160 |
| C | 1.379212 | 1.214498 | -0.221714 |
| O | 2.165568 | 0.883236 | 0.896412 |
| C | 2.718470 | 2.012141 | 1.579499 |
| C | 1.184378 | -0.074763 | -1.082910 |
| N | 2.205621 | -1.093619 | -0.689132 |
| C | 2.885421 | -1.970103 | -0.389990 |
| C | 3.745310 | -3.074884 | -0.015475 |
| H | -0.329959 | -0.331113 | 1.210916 |
| H | -0.153492 | 2.097016 | 1.078419 |
| H | 1.822467 | 2.022750 | -0.815618 |
| H | 1.353848 | 0.070210 | -2.153124 |
| H | -2.658378 | 0.536376 | 0.963123 |
| H | -2.516857 | 0.384669 | -0.808229 |
| H | -4.886578 | -2.599737 | 0.625808 |
| H | -4.699511 | -1.025050 | 1.430314 |
| H | -4.928423 | -1.113640 | -0.346263 |
| H | -1.834062 | 3.771857 | -1.542160 |
| H | -2.465401 | 2.886527 | -0.130006 |
| H | -1.095865 | 4.021832 | 0.063637 |

| | | | |
|---|---|---|---|
| H | 3.328923 | 1.610826 | 2.389782 |
| H | 3.346896 | 2.607330 | 0.904173 |
| H | 1.936490 | 2.653162 | 2.004119 |
| H | 4.391576 | -3.339216 | -0.859456 |
| H | 4.360124 | -2.786309 | 0.843725 |
| H | 3.124954 | -3.937925 | 0.251608 |

MeCN_ADDUCT_1_19

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.922275 |
| Sum of electronic and thermal Energies= | | -1069.903495 |
| Sum of electronic and thermal Enthalpies= | | -1069.902551 |
| Sum of electronic and thermal Free Energies= | | -1069.972653 |
| Zero-point correction= | 0.277691 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.00 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.063871 | -0.592865 | -0.847896 |
| C | -0.685560 | 0.118635 | 0.275692 |
| C | -2.188431 | -0.027147 | 0.150187 |
| S | -2.673021 | -1.794429 | 0.297418 |
| C | -4.474402 | -1.589917 | 0.524279 |
| C | -0.093229 | 1.533537 | 0.138854 |
| O | -0.637470 | 2.248824 | -0.945252 |
| C | -1.552090 | 3.289638 | -0.601303 |
| C | 1.379990 | 1.212270 | -0.221798 |
| O | 2.166252 | 0.877729 | 0.895436 |
| C | 2.720466 | 2.004678 | 1.580705 |
| C | 1.182714 | -0.074748 | -1.086026 |
| N | 2.204408 | -1.094618 | -0.697333 |
| C | 2.883494 | -1.969922 | -0.393180 |
| C | 3.743080 | -3.071797 | -0.009638 |
| H | -0.329865 | -0.333563 | 1.210195 |
| H | -0.151442 | 2.094920 | 1.079801 |
| H | 1.824174 | 2.021171 | -0.814134 |
| H | 1.349289 | 0.073800 | -2.156189 |
| H | -2.657257 | 0.537073 | 0.964974 |
| H | -2.516948 | 0.388016 | -0.806665 |
| H | -4.889828 | -2.595548 | 0.624888 |
| H | -4.699937 | -1.022462 | 1.431913 |
| H | -4.930631 | -1.107762 | -0.344601 |
| H | -1.829909 | 3.774913 | -1.538358 |
| H | -2.456006 | 2.898347 | -0.118380 |
| H | -1.079515 | 4.027546 | 0.061331 |
| H | 3.331331 | 1.601134 | 2.389571 |
| H | 3.348746 | 2.601023 | 0.906271 |
| H | 1.939273 | 2.645225 | 2.007474 |
| H | 3.129018 | -3.962271 | 0.166372 |
| H | 4.458072 | -3.276780 | -0.813768 |
| H | 4.283428 | -2.812459 | 0.907015 |

MeCN_ADDUCT_1_21

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.920477 |
| Sum of electronic and thermal Energies= | | -1069.901660 |
| Sum of electronic and thermal Enthalpies= | | -1069.900716 |
| Sum of electronic and thermal Free Energies= | | -1069.970677 |
| Zero-point correction= | 0.277499 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -35.62 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.217591 | -1.188493 | -0.574774 |
| C | -0.893532 | -0.163121 | 0.246680 |
| C | -2.167242 | 0.265008 | -0.475995 |
| S | -3.375047 | -1.091786 | -0.728211 |
| C | -4.260838 | -1.049302 | 0.871304 |
| C | 0.172637 | 0.962471 | 0.419008 |
| O | -0.320741 | 2.275770 | 0.378875 |
| C | -0.811172 | 2.768085 | 1.626324 |
| C | 1.120588 | 0.741741 | -0.776819 |
| O | 2.456374 | 1.102339 | -0.589299 |
| C | 2.745066 | 2.485078 | -0.846606 |
| C | 1.005420 | -0.773556 | -0.986628 |
| N | 2.096569 | -1.447150 | -0.135549 |
| C | 2.895068 | -2.019633 | 0.461497 |
| C | 3.900455 | -2.742212 | 1.216524 |
| H | -1.134537 | -0.654276 | 1.192777 |
| H | 0.746691 | 0.794745 | 1.344611 |
| H | 0.685008 | 1.227367 | -1.663789 |
| H | 1.244696 | -1.139362 | -1.987486 |
| H | -2.648138 | 1.080958 | 0.071461 |
| H | -1.921016 | 0.652178 | -1.469383 |
| H | -5.034604 | -1.818917 | 0.812722 |
| H | -3.606166 | -1.285866 | 1.715635 |
| H | -4.743351 | -0.080455 | 1.030215 |
| H | -1.097570 | 3.806852 | 1.455680 |
| H | -1.689395 | 2.206985 | 1.972457 |
| H | -0.031505 | 2.726987 | 2.399243 |
| H | 3.816014 | 2.605764 | -0.678079 |
| H | 2.507560 | 2.741476 | -1.887051 |
| H | 2.183542 | 3.140111 | -0.174244 |
| H | 4.877311 | -2.606381 | 0.739459 |
| H | 3.939234 | -2.355827 | 2.240579 |
| H | 3.647965 | -3.807991 | 1.235258 |

MeCN_ADDUCT_2_1

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.926626 |
| Sum of electronic and thermal Energies= | | -1069.908272 |
| Sum of electronic and thermal Enthalpies= | | -1069.907328 |
| Sum of electronic and thermal Free Energies= | | -1069.973908 |
| Zero-point correction= | 0.278039 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.34 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.335159 | 0.044623 | -1.653700 |
| C | 0.359708 | -1.162322 | -0.821261 |
| C | -1.049085 | -1.729670 | -0.701915 |
| S | -2.302649 | -0.630633 | 0.091953 |
| C | -3.766484 | -1.086500 | -0.908350 |
| C | 1.123598 | -0.770627 | 0.465371 |
| O | 0.283425 | -0.303355 | 1.503136 |
| C | 0.140453 | -1.192316 | 2.615363 |
| C | 1.995377 | 0.414707 | -0.024789 |
| O | 3.113360 | 0.001398 | -0.761388 |
| C | 4.268469 | -0.295302 | 0.026173 |
| C | 1.054947 | 1.049720 | -1.069862 |
| N | 0.093014 | 1.972096 | -0.363735 |
| C | -0.875363 | 2.356949 | 0.130421 |
| C | -2.025379 | 2.953336 | 0.776448 |
| H | 0.967340 | -1.883831 | -1.379084 |
| H | 1.755096 | -1.597750 | 0.808085 |
| H | 2.251954 | 1.093609 | 0.798935 |
| H | 1.564509 | 1.668800 | -1.808702 |
| H | -1.405641 | -1.941964 | -1.714007 |
| H | -1.000193 | -2.682256 | -0.163360 |
| H | -4.607503 | -0.504641 | -0.522314 |
| H | -3.618893 | -0.845645 | -1.964670 |
| H | -4.000330 | -2.147939 | -0.794479 |
| H | 1.118118 | -1.421525 | 3.058849 |
| H | -0.476129 | -0.672777 | 3.350179 |
| H | -0.359892 | -2.124442 | 2.327585 |
| H | 5.056132 | -0.560793 | -0.679860 |
| H | 4.579395 | 0.581004 | 0.610233 |
| H | 4.094679 | -1.140124 | 0.705417 |
| H | -1.777991 | 3.972461 | 1.094707 |

| | | | |
|---|---|---|---|
| H | -2.863646 | 2.978959 | 0.073019 |
| H | -2.298725 | 2.345140 | 1.644393 |

MeCN_ADDUCT_2_2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.927149 |
| Sum of electronic and thermal Energies= | | -1069.908906 |
| Sum of electronic and thermal Enthalpies= | | -1069.907962 |
| Sum of electronic and thermal Free Energies= | | -1069.974512 |
| Zero-point correction= | 0.278177 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.28 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.143029 | -0.496318 | -1.569293 |
| C | 0.295460 | -1.406936 | -0.435167 |
| C | -1.063771 | -1.926636 | 0.023434 |
| S | -2.341134 | -0.653239 | 0.415322 |
| C | -3.681624 | -1.191076 | -0.711563 |
| C | 1.159764 | -0.663176 | 0.602559 |
| O | 0.341839 | -0.028687 | 1.564906 |
| C | 0.972698 | 0.180327 | 2.828917 |
| C | 1.913914 | 0.373947 | -0.274453 |
| O | 2.998028 | -0.185036 | -0.965296 |
| C | 4.230766 | -0.179163 | -0.243158 |
| C | 0.853610 | 0.655407 | -1.360663 |
| N | -0.089217 | 1.713287 | -0.853970 |
| C | -1.058874 | 2.137920 | -0.389364 |
| C | -2.178739 | 2.867021 | 0.170263 |
| H | 0.873871 | -2.253909 | -0.820266 |
| H | 1.862774 | -1.356329 | 1.080838 |
| H | 2.192671 | 1.274667 | 0.289833 |
| H | 1.267378 | 1.049261 | -2.289221 |
| H | -1.478203 | -2.556365 | -0.767641 |
| H | -0.915450 | -2.555852 | 0.906063 |
| H | -4.011320 | -2.202869 | -0.463203 |
| H | -4.521658 | -0.508891 | -0.555129 |
| H | -3.368105 | -1.143133 | -1.757623 |
| H | 0.223882 | 0.635145 | 3.479365 |
| H | 1.299137 | -0.772172 | 3.266184 |
| H | 1.837566 | 0.852958 | 2.747754 |
| H | 4.972898 | -0.625615 | -0.905952 |
| H | 4.533404 | 0.846747 | 0.006275 |
| H | 4.168349 | -0.772557 | 0.678453 |
| H | -3.074147 | 2.678704 | -0.430018 |
| H | -2.352475 | 2.524184 | 1.194698 |
| H | -1.950294 | 3.939350 | 0.164867 |

MeCN_ADDUCT_2_3

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.927145 |
| Sum of electronic and thermal Energies= | | -1069.908823 |
| Sum of electronic and thermal Enthalpies= | | -1069.907879 |
| Sum of electronic and thermal Free Energies= | | -1069.974671 |
| Zero-point correction= | 0.278116 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.23 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.452419 | -0.091083 | -1.564454 |
| C | 0.274227 | -1.284383 | -0.731200 |
| C | -1.195145 | -1.685600 | -0.710289 |
| S | -2.369476 | -0.430229 | -0.037496 |
| C | -3.759796 | -0.666691 | -1.205117 |
| C | 0.972585 | -0.968310 | 0.610303 |
| O | 0.094156 | -0.410867 | 1.570390 |
| C | -0.113802 | -1.217184 | 2.734582 |
| C | 2.009111 | 0.099579 | 0.197259 |
| O | 3.104777 | -0.554928 | -0.373520 |
| C | 4.292240 | 0.232034 | -0.486591 |
| C | 1.226058 | 0.838072 | -0.924563 |
| N | 0.319793 | 1.864947 | -0.294577 |
| C | -0.642663 | 2.318011 | 0.154451 |
| C | -1.762496 | 3.015563 | 0.750762 |
| H | 0.836098 | -2.077292 | -1.237462 |
| H | 1.492457 | -1.848822 | 1.000040 |
| H | 2.285239 | 0.752333 | 1.035069 |
| H | 1.841587 | 1.397153 | -1.630152 |
| H | -1.499901 | -1.888634 | -1.740718 |
| H | -1.295150 | -2.619208 | -0.146464 |
| H | -4.553709 | 0.018241 | -0.895886 |
| H | -3.463922 | -0.433349 | -2.231513 |
| H | -4.144911 | -1.687814 | -1.148084 |
| H | 0.833922 | -1.408134 | 3.253771 |
| H | -0.776854 | -0.650555 | 3.389933 |
| H | -0.591923 | -2.171403 | 2.482621 |
| H | 5.057768 | -0.428959 | -0.894256 |
| H | 4.157874 | 1.083598 | -1.167573 |
| H | 4.610760 | 0.601525 | 0.496936 |
| H | -2.561760 | 3.120148 | 0.010578 |
| H | -2.130400 | 2.432250 | 1.600632 |
| H | -1.436858 | 4.006437 | 1.087598 |

MeCN_ADDUCT_2_5

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.926625 |
| Sum of electronic and thermal Energies= | | -1069.908271 |
| Sum of electronic and thermal Enthalpies= | | -1069.907327 |
| Sum of electronic and thermal Free Energies= | | -1069.973902 |
| Zero-point correction= | 0.278040 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.33 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.334901 | 0.044613 | -1.653625 |
| C | 0.359791 | -1.162355 | -0.821226 |
| C | -1.048873 | -1.729969 | -0.701849 |
| S | -2.302543 | -0.631111 | 0.092161 |
| C | -3.766343 | -1.087300 | -0.908076 |
| C | 1.123724 | -0.770480 | 0.465308 |
| O | 0.283520 | -0.303113 | 1.503052 |
| C | 0.141043 | -1.191966 | 2.615498 |
| C | 1.995324 | 0.414933 | -0.024950 |
| O | 3.113484 | 0.002153 | -0.761535 |
| C | 4.268135 | -0.295883 | 0.026167 |
| C | 1.054732 | 1.049685 | -1.070029 |
| N | 0.092768 | 1.972248 | -0.363631 |
| C | -0.875527 | 2.357406 | 0.130430 |
| C | -2.025733 | 2.954024 | 0.775955 |
| H | 0.967600 | -1.883703 | -1.379074 |
| H | 1.755209 | -1.597580 | 0.808075 |
| H | 2.251631 | 1.093977 | 0.798757 |
| H | 1.564086 | 1.668927 | -1.808873 |
| H | -1.405454 | -1.942256 | -1.713933 |
| H | -0.999872 | -2.682555 | -0.163318 |
| H | -4.000213 | -2.148683 | -0.793741 |
| H | -4.607395 | -0.505280 | -0.522364 |
| H | -3.618619 | -0.846931 | -1.964484 |
| H | -0.477573 | -0.673465 | 3.349322 |
| H | -0.356937 | -2.125257 | 2.327443 |
| H | 1.118659 | -1.418898 | 3.060238 |
| H | 5.055992 | -0.560890 | -0.679827 |
| H | 4.579162 | 0.579654 | 0.611330 |
| H | 4.093770 | -1.141380 | 0.704408 |
| H | -1.778096 | 3.972829 | 1.094962 |
| H | -2.863539 | 2.980245 | 0.072011 |
| H | -2.299976 | 2.345477 | 1.643398 |

MeCN_ADDUCT_2_6

Sum of electronic and zero-point Energies= -1069.922875
Sum of electronic and thermal Energies= -1069.904446
Sum of electronic and thermal Enthalpies= -1069.903502
Sum of electronic and thermal Free Energies= -1069.970727
Zero-point correction= 0.278238 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -32.66
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.515543 | 0.217294 | 1.896938 |
| C | -0.690132 | -0.527900 | 1.539903 |
| C | -0.356261 | -1.929463 | 1.024616 |
| S | 0.740049 | -2.057185 | -0.450760 |
| C | -0.437836 | -2.505024 | -1.780937 |
| C | -1.452489 | 0.445566 | 0.601736 |
| O | -2.283116 | -0.158103 | -0.356914 |
| C | -3.593433 | -0.481454 | 0.114754 |
| C | -0.333604 | 1.251392 | -0.095059 |
| O | -0.607346 | 2.599093 | -0.350027 |
| C | -1.429584 | 2.833128 | -1.497127 |
| C | 0.781045 | 1.205913 | 0.972228 |
| N | 2.100821 | 0.925067 | 0.345845 |
| C | 3.137785 | 0.634347 | -0.055215 |
| C | 4.432003 | 0.247247 | -0.577959 |
| H | -1.219573 | -0.651514 | 2.490300 |
| H | -2.025450 | 1.151512 | 1.221992 |
| H | -0.032446 | 0.711402 | -1.003213 |
| H | 0.917005 | 2.183371 | 1.445503 |
| H | 0.152413 | -2.465721 | 1.831069 |
| H | -1.284088 | -2.469128 | 0.813650 |
| H | -1.211818 | -1.743769 | -1.886867 |
| H | 0.147662 | -2.572882 | -2.701366 |
| H | -0.884244 | -3.481507 | -1.577634 |
| H | -4.142845 | -0.871328 | -0.743429 |
| H | -3.568062 | -1.246083 | 0.902560 |
| H | -4.103561 | 0.411784 | 0.498574 |
| H | -1.490567 | 3.916528 | -1.608428 |
| H | -0.977424 | 2.395834 | -2.398003 |
| H | -2.434653 | 2.418753 | -1.365609 |
| H | 5.170643 | 0.247574 | 0.230955 |
| H | 4.353752 | -0.758836 | -1.005293 |
| H | 4.741112 | 0.954718 | -1.355149 |

MeCN_ADDUCT_2_7
Sum of electronic and zero-point Energies= -1069.922885
Sum of electronic and thermal Energies= -1069.904447
Sum of electronic and thermal Enthalpies= -1069.903503
Sum of electronic and thermal Free Energies= -1069.970802
Zero-point correction= 0.278227 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -32.66
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.515548 | 0.218172 | 1.896795 |
| C | -0.689415 | -0.528228 | 1.539933 |
| C | -0.354260 | -1.929467 | 1.024605 |
| S | 0.742446 | -2.056066 | -0.450565 |
| C | -0.434674 | -2.505457 | -1.780880 |
| C | -1.452910 | 0.444442 | 0.601857 |
| O | -2.282976 | -0.160083 | -0.356737 |
| C | -3.592877 | -0.484937 | 0.115047 |
| C | -0.334957 | 1.251464 | -0.095043 |
| O | -0.610308 | 2.598793 | -0.350232 |
| C | -1.431883 | 2.831714 | -1.498031 |
| C | 0.779729 | 1.207370 | 0.972277 |
| N | 2.099850 | 0.928288 | 0.345923 |
| C | 3.136401 | 0.636053 | -0.055116 |
| C | 4.430523 | 0.248627 | -0.577814 |
| H | -1.218601 | -0.652392 | 2.490405 |
| H | -2.026542 | 1.149804 | 1.222158 |
| H | -0.033169 | 0.711669 | -1.003097 |
| H | 0.914289 | 2.184911 | 1.445762 |
| H | 0.154559 | -2.465477 | 1.831130 |
| H | -1.281641 | -2.469746 | 0.813260 |
| H | -1.209241 | -1.744877 | -1.887428 |
| H | 0.151185 | -2.573304 | -2.701079 |
| H | -0.880374 | -3.482190 | -1.577239 |
| H | -4.141940 | -0.875354 | -0.743113 |
| H | -3.566584 | -1.249604 | 0.902790 |
| H | -4.103962 | 0.407699 | 0.498996 |
| H | -1.494492 | 3.915035 | -1.609206 |
| H | -0.978203 | 2.395304 | -2.398577 |
| H | -2.436401 | 2.415692 | -1.367489 |
| H | 5.173898 | 0.270156 | 0.226448 |
| H | 4.357359 | -0.766035 | -0.985333 |
| H | 4.729589 | 0.943207 | -1.370418 |

MeCN_ADDUCT_2_8
Sum of electronic and zero-point Energies= -1069.927151
Sum of electronic and thermal Energies= -1069.908907
Sum of electronic and thermal Enthalpies= -1069.907963
Sum of electronic and thermal Free Energies= -1069.974511
Zero-point correction= 0.278176 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -33.28
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.143038 | -0.493467 | -1.569888 |
| C | 0.295835 | -1.406134 | -0.437443 |
| C | -1.063218 | -1.926691 | 0.020690 |
| S | -2.340642 | -0.653948 | 0.414419 |
| C | -3.681268 | -1.190470 | -0.712919 |
| C | 1.160293 | -0.664118 | 0.601389 |
| O | 0.342402 | -0.031522 | 1.565000 |
| C | 0.973311 | 0.175088 | 2.829373 |
| C | 1.914000 | 0.374774 | -0.273915 |
| O | 2.998145 | -0.182701 | -0.965953 |
| C | 4.231046 | -0.177565 | -0.244096 |
| C | 0.853350 | 0.658023 | -1.359247 |
| N | -0.089608 | 1.714848 | -0.850083 |
| C | -1.060144 | 2.137911 | -0.385769 |
| C | -2.181244 | 2.865700 | 0.173260 |
| H | 0.874217 | -2.252326 | -0.824260 |
| H | 1.863550 | -1.358001 | 1.078236 |
| H | 2.192645 | 1.274510 | 0.291983 |
| H | 1.266539 | 1.053935 | -2.287187 |
| H | -1.477673 | -2.555486 | -0.771115 |
| H | -0.914728 | -2.556989 | 0.902518 |
| H | -4.521537 | -0.508880 | -0.555178 |
| H | -3.368088 | -1.140898 | -1.759001 |
| H | -4.010509 | -2.202759 | -0.465968 |
| H | 0.224471 | 0.628453 | 3.480806 |
| H | 1.299980 | -0.778210 | 3.264710 |
| H | 1.838013 | 0.848071 | 2.749476 |
| H | 4.973084 | -0.623160 | -0.907569 |
| H | 4.533657 | 0.848070 | 0.006466 |
| H | 4.168911 | -0.772048 | 0.676825 |
| H | -3.076443 | 2.674671 | -0.426458 |
| H | -2.354139 | 2.524229 | 1.198287 |
| H | -1.954883 | 3.938454 | 0.166091 |

MeCN_ADDUCT_2_9
Sum of electronic and zero-point Energies= -1069.922713
Sum of electronic and thermal Energies= -1069.904267
Sum of electronic and thermal Enthalpies= -1069.903322
Sum of electronic and thermal Free Energies= -1069.970797

Zero-point correction= 0.278223 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -32.67
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.476368 | 0.159738 | 1.931544 |
| C | -0.754353 | -0.520454 | 1.535569 |
| C | -0.477142 | -1.933202 | 1.017685 |
| S | 0.651063 | -2.103449 | -0.429006 |
| C | -0.512938 | -2.488616 | -1.790958 |
| C | -1.440374 | 0.496354 | 0.584785 |
| O | -2.271346 | -0.057847 | -0.403281 |
| C | -3.608556 | -0.321840 | 0.028421 |
| C | -0.263824 | 1.251000 | -0.073747 |
| O | -0.461342 | 2.613406 | -0.321743 |
| C | -1.248622 | 2.899366 | -1.481508 |
| C | 0.818028 | 1.139397 | 1.022697 |
| N | 2.136617 | 0.801790 | 0.423691 |
| C | 3.155280 | 0.540712 | -0.039231 |
| C | 4.425281 | 0.184152 | -0.638089 |
| H | -1.316248 | -0.623672 | 2.469550 |
| H | -1.995646 | 1.225149 | 1.194512 |
| H | 0.033185 | 0.705467 | -0.980001 |
| H | 0.990875 | 2.104828 | 1.508947 |
| H | -0.017409 | -2.499803 | 1.832655 |
| H | -1.424634 | -2.424079 | 0.776906 |
| H | -1.245220 | -1.689666 | -1.914307 |
| H | 0.091841 | -2.584175 | -2.696358 |
| H | -1.012696 | -3.441973 | -1.602481 |
| H | -4.150682 | -0.679881 | -0.848059 |
| H | -3.641896 | -1.091818 | 0.810644 |
| H | -4.086881 | 0.592115 | 0.404380 |
| H | -1.245736 | 3.984977 | -1.587847 |
| H | -0.806861 | 2.440660 | -2.376902 |
| H | -2.277933 | 2.542829 | -1.369630 |
| H | 4.338431 | -0.813123 | -1.083601 |
| H | 4.680726 | 0.913123 | -1.414647 |
| H | 5.207335 | 0.178108 | 0.128593 |

MeCN_ADDUCT_2_10
Sum of electronic and zero-point Energies= -1069.919640
Sum of electronic and thermal Energies= -1069.901411
Sum of electronic and thermal Enthalpies= -1069.900466
Sum of electronic and thermal Free Energies= -1069.966579
Zero-point correction= 0.278327 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -34.13
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.608405 | 0.037864 | -1.516345 |
| C | 0.547524 | -1.141485 | -0.646000 |
| C | -0.854706 | -1.742461 | -0.666581 |
| S | -2.228462 | -0.678720 | -0.045329 |
| C | -3.530949 | -1.143940 | -1.245319 |
| C | 1.153217 | -0.702825 | 0.709272 |
| O | 0.161279 | -0.331641 | 1.649944 |
| C | -0.001018 | -1.234446 | 2.749013 |
| C | 1.964754 | 0.579140 | 0.360536 |
| O | 3.321180 | 0.433963 | 0.062116 |
| C | 3.725582 | -0.506505 | -0.936575 |
| C | 1.151305 | 1.111321 | -0.854664 |
| N | 0.037507 | 1.971602 | -0.341943 |
| C | -0.999135 | 2.296695 | 0.046807 |
| C | -2.231342 | 2.856095 | 0.562297 |
| H | 1.212376 | -1.875605 | -1.115483 |
| H | 1.816074 | -1.473752 | 1.117467 |
| H | 1.923190 | 1.269289 | 1.205231 |
| H | 1.723500 | 1.750101 | -1.528901 |
| H | -1.088922 | -1.992228 | -1.705383 |
| H | -0.836854 | -2.679651 | -0.099713 |
| H | -4.428845 | -0.584331 | -0.970030 |
| H | -3.245084 | -0.883899 | -2.268166 |
| H | -3.757259 | -2.210953 | -1.178375 |
| H | 0.937660 | -1.341692 | 3.307174 |
| H | -0.760309 | -0.796566 | 3.398298 |
| H | -0.344295 | -2.221302 | 2.415297 |
| H | 4.802885 | -0.373081 | -1.041673 |
| H | 3.530587 | -1.540346 | -0.623911 |
| H | 3.245882 | -0.319710 | -1.905331 |
| H | -2.067355 | 3.906468 | 0.829462 |
| H | -3.011199 | 2.786010 | -0.202177 |
| H | -2.537493 | 2.288537 | 1.446645 |

MeCN_ADDUCT_2_11
Sum of electronic and zero-point Energies= -1069.920932
Sum of electronic and thermal Energies= -1069.902778
Sum of electronic and thermal Enthalpies= -1069.901834
Sum of electronic and thermal Free Energies= -1069.968058
Zero-point correction= 0.278371 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -34.14
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.438526 | -0.498462 | -1.451574 |
| C | 0.502486 | -1.342969 | -0.258360 |
| C | -0.869175 | -1.924778 | 0.077195 |
| S | -2.250655 | -0.727466 | 0.324577 |
| C | -3.495384 | -1.441313 | -0.814012 |
| C | 1.212197 | -0.509071 | 0.827803 |
| O | 0.248794 | 0.029455 | 1.710794 |
| C | 0.755849 | 0.371817 | 3.002068 |
| C | 1.918194 | 0.632716 | 0.034857 |
| O | 3.256006 | 0.449893 | -0.323264 |
| C | 3.630827 | -0.736206 | -1.029386 |
| C | 0.983303 | 0.739750 | -1.205775 |
| N | -0.120633 | 1.698199 | -0.893895 |
| C | -1.173791 | 2.052861 | -0.573863 |
| C | -2.408584 | 2.722513 | -0.216472 |
| H | 1.147616 | -2.183622 | -0.537187 |
| H | 1.947567 | -1.113529 | 1.374340 |
| H | 1.901672 | 1.556573 | 0.617899 |
| H | 1.473078 | 1.142464 | -2.093591 |
| H | -1.165730 | -2.586212 | -0.741028 |
| H | -0.769252 | -2.533544 | 0.980852 |
| H | -4.390204 | -0.817557 | -0.738106 |
| H | -3.141825 | -1.440991 | -1.848387 |
| H | -3.759749 | -2.456189 | -0.507065 |
| H | -0.097280 | 0.719629 | 3.586562 |
| H | 1.199137 | -0.504568 | 3.492301 |
| H | 1.508510 | 1.169832 | 2.947329 |
| H | 4.690051 | -0.615352 | -1.259294 |
| H | 3.507215 | -1.634458 | -0.411200 |
| H | 3.073370 | -0.857437 | -1.966708 |
| H | -2.279633 | 3.803796 | -0.345023 |
| H | -3.216234 | 2.369114 | -0.864572 |
| H | -2.655540 | 2.495099 | 0.824944 |

MeCN_ADDUCT_2_14
Sum of electronic and zero-point Energies= -1069.920862
Sum of electronic and thermal Energies= -1069.903748
Sum of electronic and thermal Enthalpies= -1069.902804
Sum of electronic and thermal Free Energies= -1069.965442
Zero-point correction= 0.278576 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -34.09
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.371136 | -0.992623 | -1.137767 |

| | | | |
|---|---|---|---|
| C | 0.506334 | -1.330180 | 0.278141 |
| C | -0.839297 | -1.739420 | 0.877548 |
| S | -2.266758 | -0.614819 | 0.575202 |
| C | -3.276921 | -1.662288 | -0.538415 |
| C | 1.238717 | -0.145377 | 0.941459 |
| O | 0.299840 | 0.682306 | 1.600326 |
| C | 0.855541 | 1.488335 | 2.641647 |
| C | 1.892265 | 0.614297 | -0.252848 |
| O | 3.215615 | 0.304844 | -0.574941 |
| C | 3.573610 | -1.058820 | -0.815312 |
| C | 0.898369 | 0.254598 | -1.395801 |
| N | -0.203546 | 1.258176 | -1.393804 |
| C | -1.253195 | 1.659540 | -1.105082 |
| C | -2.461843 | 2.440826 | -0.916382 |
| H | 1.159799 | -2.209336 | 0.305670 |
| H | 2.006604 | -0.497098 | 1.642500 |
| H | 1.889059 | 1.689328 | -0.058026 |
| H | 1.336869 | 0.298646 | -2.393559 |
| H | -1.122560 | -2.717402 | 0.480789 |
| H | -0.721206 | -1.841280 | 1.959711 |
| H | -4.176973 | -1.093173 | -0.786480 |
| H | -2.734809 | -1.904759 | -1.455593 |
| H | -3.581773 | -2.578403 | -0.026527 |
| H | 1.586731 | 2.210518 | 2.254298 |
| H | 0.021798 | 2.027681 | 3.094080 |
| H | 1.339648 | 0.863482 | 3.403259 |
| H | 4.622252 | -1.035961 | -1.113951 |
| H | 3.480992 | -1.670131 | 0.091233 |
| H | 2.981718 | -1.508891 | -1.622092 |
| H | -2.645800 | 2.574078 | 0.153568 |
| H | -2.330780 | 3.416434 | -1.400149 |
| H | -3.312830 | 1.920845 | -1.366008 |

MeCN_ADDUCT_2_15

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.920941 |
| Sum of electronic and thermal Energies= | | -1069.902789 |
| Sum of electronic and thermal Enthalpies= | | -1069.901844 |
| Sum of electronic and thermal Free Energies= | | -1069.967998 |
| Zero-point correction= | 0.278369 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -34.00 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.443910 | -0.501233 | -1.453636 |
| C | 0.501426 | -1.343716 | -0.258577 |
| C | -0.872605 | -1.923216 | 0.070615 |
| S | -2.251288 | -0.723343 | 0.321393 |
| C | -3.503360 | -1.441606 | -0.806265 |
| C | 1.208315 | -0.509108 | 0.828942 |
| O | 0.242925 | 0.032075 | 1.708137 |
| C | 0.745931 | 0.372959 | 3.001417 |
| C | 1.918573 | 0.630815 | 0.036993 |
| O | 3.257631 | 0.446278 | -0.315408 |
| C | 3.634201 | -0.740995 | -1.018704 |
| C | 0.988809 | 0.736861 | -1.207650 |
| N | -0.115472 | 1.696763 | -0.901453 |
| C | -1.167162 | 2.053599 | -0.578982 |
| C | -2.399228 | 2.726616 | -0.218445 |
| H | 1.146267 | -2.186004 | -0.533203 |
| H | 1.941133 | -1.113784 | 1.378594 |
| H | 1.900349 | 1.555450 | 0.618760 |
| H | 1.482640 | 1.137603 | -2.094079 |
| H | -1.168518 | -2.578466 | -0.752851 |
| H | -0.776569 | -2.538172 | 0.970553 |
| H | -4.397719 | -0.817634 | -0.726941 |
| H | -3.156694 | -1.445315 | -1.842985 |
| H | -3.765564 | -2.455321 | -0.493662 |
| H | -0.108304 | 0.724076 | 3.582313 |
| H | 1.183894 | -0.504935 | 3.493703 |
| H | 1.501718 | 1.168190 | 2.949420 |
| H | 4.694805 | -0.622045 | -1.243195 |
| H | 3.505911 | -1.638550 | -0.400471 |
| H | 3.081475 | -0.862048 | -1.958833 |
| H | -3.208004 | 2.381085 | -0.869376 |
| H | -2.647955 | 2.493718 | 0.821316 |
| H | -2.265074 | 3.808080 | -0.339979 |

MeCN_ADDUCT_2_16

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.922670 |
| Sum of electronic and thermal Energies= | | -1069.904258 |
| Sum of electronic and thermal Enthalpies= | | -1069.903314 |
| Sum of electronic and thermal Free Energies= | | -1069.970533 |
| Zero-point correction= | 0.278252 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -32.67 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.480168 | 0.152280 | 1.930642 |
| C | -0.758219 | -0.515042 | 1.535913 |
| C | -0.496050 | -1.930668 | 1.017130 |
| S | 0.624595 | -2.112136 | -0.433922 |
| C | -0.548268 | -2.490081 | -1.790248 |
| C | -1.434615 | 0.509264 | 0.586344 |
| O | -2.273074 | -0.035083 | -0.400850 |
| C | -3.611765 | -0.287851 | 0.033014 |
| C | -0.251448 | 1.251598 | -0.073760 |
| O | -0.435839 | 2.616046 | -0.320529 |
| C | -1.219192 | 2.910429 | -1.481037 |
| C | 0.830856 | 1.128177 | 1.021211 |
| N | 2.145825 | 0.778385 | 0.420349 |
| C | 3.161693 | 0.508157 | -0.043842 |
| C | 4.440164 | 0.166545 | -0.633319 |
| H | -1.320274 | -0.612618 | 2.470446 |
| H | -1.981103 | 1.243993 | 1.196986 |
| H | 0.038674 | 0.703836 | -0.980990 |
| H | 1.014569 | 2.091737 | 1.507380 |
| H | -0.038850 | -2.501100 | 1.830849 |
| H | -1.448803 | -2.413152 | 0.780129 |
| H | 0.051885 | -2.593669 | -2.697881 |
| H | -1.056625 | -3.438067 | -1.597383 |
| H | -1.272821 | -1.683997 | -1.912952 |
| H | -4.160476 | -0.633125 | -0.844498 |
| H | -3.651347 | -1.063324 | 0.809543 |
| H | -4.078857 | 0.628451 | 0.417347 |
| H | -1.209650 | 3.996393 | -1.584037 |
| H | -0.777820 | 2.452332 | -2.376867 |
| H | -2.250923 | 2.559484 | -1.372751 |
| H | 5.215536 | 0.170993 | 0.140400 |
| H | 4.371921 | -0.831494 | -1.080577 |
| H | 4.691699 | 0.899696 | -1.407368 |

MeCN_ADDUCT_2_17

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.920935 |
| Sum of electronic and thermal Energies= | | -1069.902786 |
| Sum of electronic and thermal Enthalpies= | | -1069.901841 |
| Sum of electronic and thermal Free Energies= | | -1069.967979 |
| Zero-point correction= | 0.278375 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -34.00 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.443155 | -0.509816 | -1.450737 |
| C | 0.500858 | -1.345376 | -0.250828 |
| C | -0.873118 | -1.922940 | 0.082067 |
| S | -2.252095 | -0.721626 | 0.323990 |
| C | -3.502651 | -1.445924 | -0.801455 |

| | | | |
|---|---|---|---|
| C | 1.207772 | -0.504509 | 0.831760 |
| O | 0.242438 | 0.042009 | 1.707766 |
| C | 0.745739 | 0.390769 | 2.998831 |
| C | 1.918316 | 0.630557 | 0.033149 |
| O | 3.257341 | 0.443711 | -0.318118 |
| C | 3.633914 | -0.747860 | -1.014121 |
| C | 0.988667 | 0.729454 | -1.212223 |
| N | -0.115133 | 1.691752 | -0.911725 |
| C | -1.165769 | 2.051238 | -0.588803 |
| C | -2.396543 | 2.726771 | -0.228624 |
| H | 1.145746 | -2.189185 | -0.520598 |
| H | 1.940434 | -1.106045 | 1.385051 |
| H | 1.900243 | 1.558654 | 0.609381 |
| H | 1.482771 | 1.124593 | -2.101004 |
| H | -1.168702 | -2.584198 | -0.736690 |
| H | -0.777140 | -2.531427 | 0.986396 |
| H | -3.154354 | -1.455645 | -1.837583 |
| H | -3.765702 | -2.457734 | -0.483443 |
| H | -4.396876 | -0.821149 | -0.727108 |
| H | -0.108405 | 0.745102 | 3.577908 |
| H | 1.184122 | -0.484019 | 3.496244 |
| H | 1.501287 | 1.185890 | 2.941847 |
| H | 4.694464 | -0.630162 | -1.239527 |
| H | 3.505869 | -1.641591 | -0.390324 |
| H | 3.081088 | -0.874834 | -1.953426 |
| H | -2.260467 | 3.807898 | -0.351013 |
| H | -3.206119 | 2.382191 | -0.879077 |
| H | -2.645383 | 2.495112 | 0.811385 |

MeCN_ADDUCT_2_18

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.920943 |
| Sum of electronic and thermal Energies= | | -1069.902576 |
| Sum of electronic and thermal Enthalpies= | | -1069.901631 |
| Sum of electronic and thermal Free Energies= | | -1069.968774 |
| Zero-point correction= | 0.278158 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.79 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.342333 | 0.038992 | 1.418816 |
| C | -0.102001 | -1.092940 | 0.617019 |
| C | 0.755690 | -1.357754 | -0.632116 |
| S | 2.556448 | -1.053073 | -0.486073 |
| C | 3.020008 | -2.111947 | 0.930214 |
| C | -1.566680 | -0.695242 | 0.275606 |
| O | -2.094149 | -1.262578 | -0.892162 |
| C | -2.607320 | -2.586041 | -0.730780 |
| C | -1.475349 | 0.843990 | 0.096740 |
| O | -2.551520 | 1.587133 | 0.587530 |
| C | -3.727048 | 1.541456 | -0.228069 |
| C | -0.248464 | 1.193693 | 0.969796 |
| N | 0.775566 | 1.960289 | 0.175108 |
| C | 1.740933 | 2.337544 | -0.327545 |
| C | 2.933741 | 2.842242 | -0.975320 |
| H | -0.040743 | -1.938832 | 1.303731 |
| H | -2.206555 | -0.896221 | 1.147946 |
| H | -1.294297 | 1.057554 | -0.968520 |
| H | -0.505044 | 1.863687 | 1.792796 |
| H | 0.586700 | -2.393750 | -0.944220 |
| H | 0.434762 | -0.736913 | -1.474517 |
| H | 4.107603 | -2.051993 | 1.016202 |
| H | 2.569533 | -1.759190 | 1.860960 |
| H | 2.744035 | -3.152521 | 0.739166 |
| H | -3.046217 | -2.865010 | -1.689780 |
| H | -1.815157 | -3.303609 | -0.477148 |
| H | -3.381376 | -2.615940 | 0.047511 |
| H | -4.444182 | 2.215735 | 0.241508 |
| H | -3.507876 | 1.887663 | -1.247301 |
| H | -4.146843 | 0.531120 | -0.276196 |
| H | 3.596391 | 1.993859 | -1.180073 |
| H | 2.664747 | 3.338626 | -1.914145 |
| H | 3.438016 | 3.554495 | -0.313253 |

MeCN_ADDUCT_2_19

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.924633 |
| Sum of electronic and thermal Energies= | | -1069.905975 |
| Sum of electronic and thermal Enthalpies= | | -1069.905031 |
| Sum of electronic and thermal Free Energies= | | -1069.973976 |
| Zero-point correction= | 0.277887 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.68 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.478914 | -0.094952 | -1.676958 |
| C | 0.636886 | 0.423513 | -0.857684 |
| C | 1.756464 | -0.601716 | -0.848801 |
| S | 3.200098 | 0.112250 | 0.037018 |
| C | 4.436334 | -1.190434 | -0.298205 |
| C | -0.007925 | 0.761760 | 0.494306 |
| O | -0.129270 | -0.399513 | 1.296786 |
| C | 0.223912 | -0.211830 | 2.670497 |
| C | -1.427260 | 1.209137 | 0.060939 |
| O | -1.465086 | 2.469548 | -0.547962 |
| C | -1.544317 | 3.570692 | 0.360557 |
| C | -1.676252 | 0.212868 | -1.095884 |
| N | -2.274819 | -1.058820 | -0.536039 |
| C | -2.627566 | -2.098283 | -0.194019 |
| C | -3.076894 | -3.402370 | 0.251332 |
| H | 0.959975 | 1.348089 | -1.344857 |
| H | 0.539139 | 1.558974 | 1.006729 |
| H | -2.156718 | 1.111252 | 0.877287 |
| H | -2.417011 | 0.560666 | -1.819412 |
| H | 1.420119 | -1.516254 | -0.353609 |
| H | 2.037259 | -0.830711 | -1.881737 |
| H | 5.361030 | -0.871841 | 0.188744 |
| H | 4.126269 | -2.150373 | 0.123492 |
| H | 4.618139 | -1.290239 | -1.371660 |
| H | -0.423098 | 0.532475 | 3.154453 |
| H | 0.086066 | -1.177209 | 3.161659 |
| H | 1.272390 | 0.093639 | 2.762550 |
| H | -1.613819 | 4.467079 | -0.256586 |
| H | -2.438759 | 3.491079 | 0.992963 |
| H | -0.653644 | 3.640548 | 0.997461 |
| H | -4.147053 | -3.362519 | 0.482140 |
| H | -2.903470 | -4.138548 | -0.541288 |
| H | -2.518770 | -3.691069 | 1.148499 |

MeCN_ADDUCT_2_20

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.924384 |
| Sum of electronic and thermal Energies= | | -1069.906566 |
| Sum of electronic and thermal Enthalpies= | | -1069.905622 |
| Sum of electronic and thermal Free Energies= | | -1069.971977 |
| Zero-point correction= | 0.277746 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -33.82 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.437679 | -0.030611 | -1.677159 |
| C | 0.660725 | 0.444877 | -0.810425 |
| C | 1.769933 | -0.591819 | -0.832446 |
| S | 3.239119 | 0.080728 | 0.044171 |
| C | 4.459849 | -1.213012 | -0.374024 |
| C | -0.018787 | 0.725867 | 0.540671 |
| O | -0.200887 | -0.460946 | 1.293057 |
| C | 0.413229 | -0.458463 | 2.588239 |
| C | -1.418858 | 1.209128 | 0.086202 |

| | | | |
|---|---|---|---|
| O | -1.420968 | 2.491657 | -0.475339 |
| C | -1.516556 | 3.559170 | 0.471310 |
| C | -1.648593 | 0.263171 | -1.116582 |
| N | -2.280963 | -1.016830 | -0.622372 |
| C | -2.761920 | -1.990483 | -0.246244 |
| C | -3.358583 | -3.220419 | 0.236730 |
| H | 1.001619 | 1.387845 | -1.247791 |
| H | 0.514520 | 1.495283 | 1.107063 |
| H | -2.168872 | 1.092082 | 0.880395 |
| H | -2.364706 | 0.649739 | -1.845622 |
| H | 1.426177 | -1.514781 | -0.357610 |
| H | 2.034952 | -0.800556 | -1.873747 |
| H | 5.399353 | -0.916119 | 0.098015 |
| H | 4.157638 | -2.187158 | 0.019644 |
| H | 4.610309 | -1.272576 | -1.455282 |
| H | 0.180329 | -1.424101 | 3.041725 |
| H | 1.499581 | -0.345689 | 2.506358 |
| H | 0.002826 | 0.341586 | 3.218562 |
| H | -1.552856 | 4.478922 | -0.113405 |
| H | -2.432837 | 3.468783 | 1.069873 |
| H | -0.647290 | 3.591521 | 1.139768 |
| H | -3.071162 | -3.374204 | 1.283017 |
| H | -4.449773 | -3.150789 | 0.163103 |
| H | -3.005336 | -4.062516 | -0.369259 |

MeCN_ADDUCT_2_21

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1069.922730 |
| Sum of electronic and thermal Energies= | | -1069.903986 |
| Sum of electronic and thermal Enthalpies= | | -1069.903042 |
| Sum of electronic and thermal Free Energies= | | -1069.972388 |
| Zero-point correction= | 0.277425 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -34.67 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.268577 | -0.190252 | -1.178793 |
| C | 0.840389 | 0.486330 | 0.000114 |
| C | 1.807733 | -0.448798 | 0.710233 |
| S | 3.176833 | -1.093816 | -0.320800 |
| C | 4.266867 | 0.371478 | -0.406617 |
| C | -0.389965 | 0.939125 | 0.814856 |
| O | -0.908235 | -0.093799 | 1.636460 |
| C | -0.721802 | 0.096093 | 3.040924 |
| C | -1.429143 | 1.202119 | -0.301912 |
| O | -1.186358 | 2.380604 | -1.018712 |
| C | -1.751440 | 3.558927 | -0.438903 |
| C | -1.064002 | 0.068070 | -1.284214 |
| N | -1.828017 | -1.187901 | -0.900627 |
| C | -2.263929 | -2.219150 | -0.638281 |
| C | -2.823000 | -3.513391 | -0.301799 |
| H | 1.355848 | 1.369508 | -0.389209 |
| H | -0.180960 | 1.848388 | 1.388845 |
| H | -2.458200 | 1.136668 | 0.076167 |
| H | -1.375111 | 0.259392 | -2.313638 |
| H | 2.225937 | 0.069251 | 1.581806 |
| H | 1.265068 | -1.324311 | 1.075785 |
| H | 5.159905 | 0.054181 | -0.950863 |
| H | 3.807051 | 1.198535 | -0.954962 |
| H | 4.566161 | 0.700755 | 0.592955 |
| H | -1.209932 | -0.745230 | 3.536638 |
| H | 0.340893 | 0.103185 | 3.311921 |
| H | -1.188173 | 1.031157 | 3.377720 |
| H | -1.513658 | 4.375670 | -1.121296 |
| H | -2.841476 | 3.464451 | -0.345818 |
| H | -1.321004 | 3.776296 | 0.546983 |
| H | -3.802641 | -3.625271 | -0.779058 |
| H | -2.152035 | -4.302189 | -0.659956 |
| H | -2.933012 | -3.591329 | 0.785108 |

AMMONIA_ADDUCT_1_CONF_1

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758120 |
| Sum of electronic and thermal Energies= | | -993.742147 |
| Sum of electronic and thermal Enthalpies= | | -993.741202 |
| Sum of electronic and thermal Free Energies= | | -993.802666 |
| Zero-point correction= | 0.271792 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.49 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.180655 | -0.946955 | -0.829900 |
| C | -0.438165 | -0.046901 | 0.303595 |
| C | -1.825805 | 0.544659 | 0.158017 |
| S | -3.089536 | -0.785006 | 0.267416 |
| C | -4.590405 | 0.244255 | 0.428950 |
| C | 0.737996 | 0.937633 | 0.244306 |
| O | 0.508537 | 1.885101 | -0.769739 |
| C | 1.241771 | 3.101663 | -0.631133 |
| C | 1.903480 | 0.003480 | -0.173458 |
| O | 2.384427 | -0.794082 | 0.896879 |
| C | 3.396601 | -0.183159 | 1.712832 |
| C | 1.155868 | -0.949608 | -1.150253 |
| N | 1.671093 | -2.392488 | -0.932688 |
| H | -0.367684 | -0.636819 | 1.225158 |
| H | 0.919843 | 1.408037 | 1.219823 |
| H | 2.720848 | 0.543578 | -0.665860 |
| H | 1.315181 | -0.725230 | -2.208134 |
| H | 2.069394 | -2.414154 | 0.026050 |
| H | 0.872803 | -3.033663 | -1.007743 |
| H | 2.394284 | -2.672304 | -1.603850 |
| H | -1.978650 | 1.255487 | 0.978961 |
| H | -1.900900 | 1.084663 | -0.788613 |
| H | -4.555697 | 0.857753 | 1.333766 |
| H | -4.732164 | 0.877533 | -0.450968 |
| H | -5.433035 | -0.447337 | 0.503443 |
| H | 0.953186 | 3.732056 | -1.473377 |
| H | 0.986433 | 3.609789 | 0.308139 |
| H | 2.327837 | 2.935664 | -0.665242 |
| H | 3.013520 | 0.716753 | 2.204865 |
| H | 3.666653 | -0.920852 | 2.468988 |
| H | 4.276537 | 0.071903 | 1.109690 |

AMMONIA_ADDUCT_1_CONF_2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.757719 |
| Sum of electronic and thermal Energies= | | -993.741758 |
| Sum of electronic and thermal Enthalpies= | | -993.740814 |
| Sum of electronic and thermal Free Energies= | | -993.802117 |
| Zero-point correction= | 0.271623 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.23 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.242934 | -0.756276 | -1.062217 |
| C | -0.537730 | 0.072061 | 0.114923 |
| C | -1.827876 | 0.832159 | -0.142161 |
| S | -3.302831 | -0.246932 | -0.290944 |
| C | -3.754424 | -0.442049 | 1.470984 |
| C | 0.736202 | 0.914908 | 0.276735 |
| O | 0.726213 | 1.962113 | -0.662965 |
| C | 1.552415 | 3.076418 | -0.327288 |
| C | 1.838859 | -0.106774 | -0.101150 |
| O | 2.102109 | -1.044447 | 0.931097 |
| C | 3.073961 | -0.629830 | 1.904106 |
| C | 1.114112 | -0.878006 | -1.241768 |
| N | 1.451036 | -2.383500 | -1.121177 |
| H | -0.637744 | -0.593800 | 0.980128 |
| H | 0.851201 | 1.280699 | 1.305937 |

| | | | |
|---|---|---|---|
| H | 2.762068 | 0.373741 | -0.446737 |
| H | 1.415725 | -0.577998 | -2.248831 |
| H | 0.604655 | -2.919573 | -1.345308 |
| H | 2.214467 | -2.681283 | -1.737838 |
| H | 1.730658 | -2.537426 | -0.133278 |
| H | -1.988070 | 1.560497 | 0.660610 |
| H | -1.736094 | 1.387995 | -1.077241 |
| H | -3.994167 | 0.523863 | 1.924819 |
| H | -4.649625 | -1.068679 | 1.491093 |
| H | -2.971646 | -0.942519 | 2.049490 |
| H | 1.236072 | 3.527499 | 0.622463 |
| H | 2.613048 | 2.796903 | -0.256236 |
| H | 1.430080 | 3.803402 | -1.131345 |
| H | 2.734930 | 0.261546 | 2.442117 |
| H | 3.177425 | -1.457868 | 2.606018 |
| H | 4.038835 | -0.426018 | 1.423882 |

AMMONIA_ADDUCT_1_CONF_3

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.757713 |
| Sum of electronic and thermal Energies= | | -993.741804 |
| Sum of electronic and thermal Enthalpies= | | -993.740860 |
| Sum of electronic and thermal Free Energies= | | -993.801879 |
| Zero-point correction= | 0.271785 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.58 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.479615 | -0.796350 | -0.626277 |
| C | -0.439732 | 0.137523 | 0.510906 |
| C | -1.734704 | 0.927901 | 0.564579 |
| S | -3.216477 | -0.088066 | 0.937655 |
| C | -3.786305 | -0.524747 | -0.745531 |
| C | 0.844322 | 0.937596 | 0.250993 |
| O | 0.607384 | 1.885954 | -0.761279 |
| C | 1.509524 | 2.992014 | -0.768516 |
| C | 1.795585 | -0.163813 | -0.282432 |
| O | 2.314075 | -0.990985 | 0.747330 |
| C | 3.512461 | -0.511619 | 1.378562 |
| C | 0.788998 | -1.027604 | -1.100988 |
| N | 1.109096 | -2.524676 | -0.855567 |
| H | -0.318020 | -0.453147 | 1.426092 |
| H | 1.227374 | 1.397563 | 1.171774 |
| H | 2.598974 | 0.238396 | -0.910913 |
| H | 0.842862 | -0.879350 | -2.182302 |
| H | 1.644166 | -2.561190 | 0.034458 |
| H | 0.222926 | -3.034551 | -0.765991 |
| H | 1.669648 | -2.948674 | -1.602306 |
| H | -1.649929 | 1.655436 | 1.379186 |
| H | -1.879015 | 1.487029 | -0.362423 |
| H | -3.051415 | -1.131549 | -1.278396 |
| H | -4.704113 | -1.103587 | -0.613984 |
| H | -4.020544 | 0.374247 | -1.322320 |
| H | 1.457731 | 3.547229 | 0.177251 |
| H | 2.547872 | 2.676507 | -0.943379 |
| H | 1.193949 | 3.641183 | -1.586470 |
| H | 4.319802 | -0.406166 | 0.643713 |
| H | 3.336875 | 0.448555 | 1.874284 |
| H | 3.785159 | -1.258590 | 2.124591 |

AMMONIA_ADDUCT_1_CONF_4

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.757254 |
| Sum of electronic and thermal Energies= | | -993.741237 |
| Sum of electronic and thermal Enthalpies= | | -993.740293 |
| Sum of electronic and thermal Free Energies= | | -993.801923 |
| Zero-point correction= | 0.271779 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.20 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.054448 | -0.983361 | -0.783235 |
| C | -0.347346 | -0.049384 | 0.313444 |
| C | -1.778161 | 0.428257 | 0.164407 |
| S | -2.936517 | -0.992688 | 0.300957 |
| C | -4.510520 | -0.080168 | 0.467771 |
| C | 0.768032 | 1.006185 | 0.174672 |
| O | 0.561604 | 1.884419 | -0.906036 |
| C | 0.136081 | 3.204589 | -0.560776 |
| C | 1.974355 | 0.120492 | -0.218131 |
| O | 2.504907 | -0.609383 | 0.875183 |
| C | 3.478336 | 0.090410 | 1.666734 |
| C | 1.270951 | -0.909155 | -1.144955 |
| N | 1.883139 | -2.307201 | -0.897894 |
| H | -0.220797 | -0.588704 | 1.260058 |
| H | 0.947620 | 1.539019 | 1.117009 |
| H | 2.747892 | 0.698433 | -0.736166 |
| H | 1.387298 | -0.706792 | -2.212902 |
| H | 2.617011 | -2.554422 | -1.570335 |
| H | 2.291262 | -2.275885 | 0.056329 |
| H | 1.130065 | -3.003162 | -0.946206 |
| H | -1.990646 | 1.137777 | 0.972981 |
| H | -1.897635 | 0.935945 | -0.796881 |
| H | -5.295751 | -0.834453 | 0.559266 |
| H | -4.515458 | 0.544744 | 1.365472 |
| H | -4.711208 | 0.529133 | -0.417679 |
| H | 0.080677 | 3.761703 | -1.497212 |
| H | 0.861092 | 3.689318 | 0.106660 |
| H | -0.851281 | 3.203284 | -0.083939 |
| H | 3.034833 | 0.967804 | 2.148575 |
| H | 4.328340 | 0.400301 | 1.046995 |
| H | 3.812100 | -0.611382 | 2.431624 |

AMMONIA_ADDUCT_1_CONF_5

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.756818 |
| Sum of electronic and thermal Energies= | | -993.740856 |
| Sum of electronic and thermal Enthalpies= | | -993.739912 |
| Sum of electronic and thermal Free Energies= | | -993.801218 |
| Zero-point correction= | 0.271715 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -42.98 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.122339 | -0.808208 | -1.015049 |
| C | -0.458457 | 0.035838 | 0.139684 |
| C | -1.809442 | 0.678569 | -0.125346 |
| S | -3.190023 | -0.519172 | -0.279867 |
| C | -3.626401 | -0.756538 | 1.480463 |
| C | 0.757972 | 0.979907 | 0.241792 |
| O | 0.749976 | 1.981351 | -0.748834 |
| C | 0.443513 | 3.302212 | -0.295766 |
| C | 1.918039 | 0.025542 | -0.125241 |
| O | 2.246990 | -0.875895 | 0.918736 |
| C | 3.171112 | -0.370448 | 1.895539 |
| C | 1.235121 | -0.811799 | -1.239711 |
| N | 1.701126 | -2.280647 | -1.123176 |
| H | -0.494241 | -0.605790 | 1.028346 |
| H | 0.875945 | 1.392590 | 1.251531 |
| H | 2.797778 | 0.572514 | -0.482886 |
| H | 1.480336 | -0.490527 | -2.255656 |
| H | 0.904214 | -2.889770 | -1.341704 |
| H | 2.484561 | -2.509791 | -1.744210 |
| H | 1.998166 | -2.408927 | -0.136938 |
| H | -2.041613 | 1.390752 | 0.674473 |
| H | -1.761490 | 1.230756 | -1.067043 |
| H | -4.463097 | -1.459514 | 1.496428 |
| H | -2.803726 | -1.188084 | 2.058846 |
| H | -3.951687 | 0.183008 | 1.936451 |

| | | | |
|---|---|---|---|
| H | -0.577947 | 3.371686 | 0.096892 |
| H | 0.536872 | 3.952594 | -1.166732 |
| H | 1.153029 | 3.627375 | 0.476810 |
| H | 3.352148 | -1.185864 | 2.596515 |
| H | 2.745152 | 0.482794 | 2.433414 |
| H | 4.112347 | -0.072198 | 1.418262 |

AMMONIA_ADDUCT_1_CONF_6

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.756900 |
| Sum of electronic and thermal Energies= | | -993.740934 |
| Sum of electronic and thermal Enthalpies= | | -993.739990 |
| Sum of electronic and thermal Free Energies= | | -993.801182 |
| Zero-point correction= | 0.271744 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.31 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.362854 | -0.882278 | -0.569201 |
| C | -0.361728 | 0.127524 | 0.501857 |
| C | -1.713600 | 0.817353 | 0.534833 |
| S | -3.114882 | -0.283874 | 0.975801 |
| C | -3.667020 | -0.844028 | -0.676235 |
| C | 0.859666 | 0.997264 | 0.143779 |
| O | 0.617638 | 1.841147 | -0.957840 |
| C | 0.483047 | 3.232075 | -0.654942 |
| C | 1.865311 | -0.072831 | -0.340403 |
| O | 2.449212 | -0.802757 | 0.725706 |
| C | 3.610802 | -0.199402 | 1.318567 |
| C | 0.903263 | -1.045250 | -1.081486 |
| N | 1.337748 | -2.501020 | -0.778744 |
| H | -0.177249 | -0.390044 | 1.450585 |
| H | 1.242975 | 1.544757 | 1.013840 |
| H | 2.625077 | 0.354331 | -1.004537 |
| H | 0.911510 | -0.943746 | -2.169621 |
| H | 0.494993 | -3.071970 | -0.648595 |
| H | 1.916348 | -2.914288 | -1.517764 |
| H | 1.888703 | -2.457501 | 0.100973 |
| H | -1.682426 | 1.588400 | 1.312391 |
| H | -1.911142 | 1.308755 | -0.421599 |
| H | -3.973190 | 0.005393 | -1.293082 |
| H | -2.893971 | -1.420824 | -1.187691 |
| H | -4.538102 | -1.481381 | -0.503836 |
| H | 1.383064 | 3.615036 | -0.155684 |
| H | -0.392864 | 3.428774 | -0.025086 |
| H | 0.358234 | 3.741876 | -1.611441 |
| H | 3.953912 | -0.889408 | 2.089968 |
| H | 3.360903 | 0.762775 | 1.777215 |
| H | 4.396694 | -0.056941 | 0.567205 |

AMMONIA_ADDUCT_1_CONF_7

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.753644 |
| Sum of electronic and thermal Energies= | | -993.737483 |
| Sum of electronic and thermal Enthalpies= | | -993.736539 |
| Sum of electronic and thermal Free Energies= | | -993.798549 |
| Zero-point correction= | 0.271465 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.89 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.266243 | -1.487738 | 0.376925 |
| C | -0.647389 | -0.068933 | 0.455869 |
| C | -1.603706 | 0.278875 | -0.683492 |
| S | -3.170977 | -0.671027 | -0.658038 |
| C | -4.157163 | 0.339153 | 0.504848 |
| C | 0.717166 | 0.677070 | 0.407555 |
| O | 0.699342 | 1.957909 | -0.159310 |
| C | 0.264356 | 2.995441 | 0.722833 |
| C | 1.581439 | -0.252155 | -0.464808 |
| O | 2.957826 | -0.278135 | -0.162037 |
| C | 3.746086 | 0.762285 | -0.771915 |
| C | 0.986107 | -1.641261 | -0.160855 |
| N | 1.902487 | -2.321515 | 0.904327 |
| H | -1.148776 | 0.037073 | 1.420290 |
| H | 1.153851 | 0.707321 | 1.420963 |
| H | 1.414969 | -0.008069 | -1.522483 |
| H | 0.995677 | -2.337183 | -1.004247 |
| H | 2.859729 | -1.951158 | 0.756016 |
| H | 1.886418 | -3.343666 | 0.835546 |
| H | 1.580453 | -2.061301 | 1.843223 |
| H | -1.823689 | 1.350630 | -0.664975 |
| H | -1.134331 | 0.072798 | -1.651236 |
| H | -4.284718 | 1.359169 | 0.130998 |
| H | -5.139372 | -0.136422 | 0.563450 |
| H | -3.725282 | 0.356895 | 1.509944 |
| H | 0.365622 | 3.930195 | 0.169945 |
| H | 0.891882 | 3.033812 | 1.623594 |
| H | -0.784645 | 2.866156 | 1.019552 |
| H | 4.771797 | 0.597380 | -0.441079 |
| H | 3.398503 | 1.747549 | -0.451838 |
| H | 3.691357 | 0.686720 | -1.864180 |

AMMONIA_ADDUCT_1_CONF_8

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758897 |
| Sum of electronic and thermal Energies= | | -993.742923 |
| Sum of electronic and thermal Enthalpies= | | -993.741979 |
| Sum of electronic and thermal Free Energies= | | -993.803616 |
| Zero-point correction= | 0.271947 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -42.07 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.586004 | -1.569885 | -0.686724 |
| C | -0.276425 | -0.732060 | 0.163864 |
| C | -1.720123 | -0.973029 | -0.236119 |
| S | -2.807469 | -0.066635 | 0.936351 |
| C | -4.430324 | -0.431562 | 0.180177 |
| C | 0.268287 | 0.684834 | -0.067264 |
| O | -0.182596 | 1.166210 | -1.310659 |
| C | -0.347193 | 2.583824 | -1.380142 |
| C | 1.789762 | 0.420906 | -0.169962 |
| O | 2.400818 | 0.153879 | 1.082986 |
| C | 2.796538 | 1.313119 | 1.833607 |
| C | 1.774256 | -0.922521 | -0.951731 |
| N | 2.905360 | -1.823375 | -0.410604 |
| H | -0.104173 | -1.024953 | 1.205926 |
| H | 0.012762 | 1.356963 | 0.759845 |
| H | 2.317834 | 1.214854 | -0.711849 |
| H | 1.948179 | -0.818447 | -2.025946 |
| H | 3.096943 | -1.486996 | 0.553941 |
| H | 2.572904 | -2.793997 | -0.395651 |
| H | 3.767340 | -1.769039 | -0.963784 |
| H | -1.933757 | -2.045802 | -0.191791 |
| H | -1.877469 | -0.612685 | -1.255244 |
| H | -5.179775 | 0.061645 | 0.803590 |
| H | -4.491409 | -0.030303 | -0.834888 |
| H | -4.627189 | -1.506894 | 0.174310 |
| H | -1.089896 | 2.924567 | -0.648527 |
| H | -0.702527 | 2.802394 | -2.388267 |
| H | 0.601360 | 3.113620 | -1.213004 |
| H | 3.275733 | 0.941879 | 2.739965 |
| H | 3.505965 | 1.920839 | 1.258758 |
| H | 1.926690 | 1.919446 | 2.105827 |

AMMONIA_ADDUCT_1_CONF_9

| | |
|---|---|
| Sum of electronic and zero-point Energies= | -993.759572 |
| Sum of electronic and thermal Energies= | -993.743601 |

Sum of electronic and thermal Enthalpies= -993.742657
Sum of electronic and thermal Free Energies= -993.804209
Zero-point correction= 0.271776 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -42.14
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.536177 | -1.274164 | -1.159040 |
| C | -0.415682 | -0.632395 | -0.228873 |
| C | -1.784672 | -0.605342 | -0.887894 |
| S | -3.055424 | 0.141205 | 0.202371 |
| C | -3.561705 | -1.305094 | 1.204257 |
| C | 0.226191 | 0.733796 | 0.056249 |
| O | -0.031196 | 1.607545 | -1.017730 |
| C | -0.059918 | 2.992795 | -0.668020 |
| C | 1.733301 | 0.384928 | 0.055452 |
| O | 2.153563 | -0.295686 | 1.228852 |
| C | 2.502923 | 0.550639 | 2.335623 |
| C | 1.766392 | -0.655836 | -1.095472 |
| N | 2.796232 | -1.749968 | -0.744761 |
| H | -0.427485 | -1.227714 | 0.690628 |
| H | -0.111820 | 1.142239 | 1.014758 |
| H | 2.366901 | 1.256540 | -0.149229 |
| H | 2.069351 | -0.243720 | -2.062188 |
| H | 3.723113 | -1.579352 | -1.149642 |
| H | 2.869831 | -1.745003 | 0.291688 |
| H | 2.442131 | -2.653640 | -1.077542 |
| H | -2.086824 | -1.617082 | -1.174466 |
| H | -1.742315 | 0.010182 | -1.788035 |
| H | -3.962773 | -2.097653 | 0.566607 |
| H | -2.746327 | -1.694844 | 1.820111 |
| H | -4.356971 | -0.952959 | 1.866022 |
| H | 0.905238 | 3.332962 | -0.266740 |
| H | -0.849666 | 3.192087 | 0.066739 |
| H | -0.274068 | 3.537606 | -1.588587 |
| H | 2.825208 | -0.112746 | 3.138821 |
| H | 1.639189 | 1.133567 | 2.670984 |
| H | 3.321125 | 1.227535 | 2.060867 |

AMMONIA_ADDUCT_1_CONF_10
Sum of electronic and zero-point Energies= -993.754673
Sum of electronic and thermal Energies= -993.738511
Sum of electronic and thermal Enthalpies= -993.737567
Sum of electronic and thermal Free Energies= -993.799677
Zero-point correction= 0.271546 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -43.74
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.233024 | -1.442242 | -0.594203 |
| C | 0.552103 | -0.013347 | -0.743053 |
| C | 1.652966 | 0.394721 | 0.227367 |
| S | 3.114820 | -0.696437 | 0.015480 |
| C | 4.384745 | 0.347402 | 0.815231 |
| C | -0.813396 | 0.686009 | -0.496373 |
| O | -0.753624 | 1.980582 | 0.033957 |
| C | -0.500445 | 3.008574 | -0.927685 |
| C | -1.494326 | -0.247941 | 0.522828 |
| O | -2.898427 | -0.339347 | 0.428638 |
| C | -3.632639 | 0.688890 | 1.120989 |
| C | -0.889226 | -1.625574 | 0.176416 |
| N | -1.935850 | -2.403038 | -0.672758 |
| H | 0.906695 | 0.085837 | -1.770951 |
| H | -1.402921 | 0.672005 | -1.429094 |
| H | -1.186376 | 0.041738 | 1.536078 |
| H | -0.705295 | -2.271133 | 1.039811 |
| H | -1.864339 | -3.417590 | -0.548743 |
| H | -2.870575 | -2.054838 | -0.387138 |
| H | -1.784725 | -2.192097 | -1.665808 |
| H | 1.297442 | 0.370919 | 1.264079 |
| H | 1.937217 | 1.428548 | 0.004392 |
| H | 5.321788 | -0.211720 | 0.757115 |
| H | 4.508189 | 1.297939 | 0.288677 |
| H | 4.149054 | 0.527243 | 1.867682 |
| H | -1.267716 | 3.008119 | -1.713627 |
| H | 0.489174 | 2.900709 | -1.390025 |
| H | -0.539233 | 3.952955 | -0.383290 |
| H | -3.423467 | 0.644072 | 2.196182 |
| H | -3.370003 | 1.676520 | 0.734181 |
| H | -4.687563 | 0.480696 | 0.940635 |

AMMONIA_ADDUCT_1_CONF_11
Sum of electronic and zero-point Energies= -993.754675
Sum of electronic and thermal Energies= -993.738512
Sum of electronic and thermal Enthalpies= -993.737568
Sum of electronic and thermal Free Energies= -993.799690
Zero-point correction= 0.271544 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -43.73
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.232995 | -1.441288 | -0.596302 |
| C | 0.551986 | -0.012325 | -0.743569 |
| C | 1.652704 | 0.395055 | 0.227349 |
| S | 3.114433 | -0.696179 | 0.015104 |
| C | 4.384337 | 0.346910 | 0.815880 |
| C | -0.813662 | 0.686494 | -0.496245 |
| O | -0.754151 | 1.980863 | 0.034580 |
| C | -0.501029 | 3.009213 | -0.926708 |
| C | -1.493940 | -0.248093 | 0.522817 |
| O | -2.898012 | -0.340402 | 0.428629 |
| C | -3.632942 | 0.687992 | 1.119984 |
| C | -0.888005 | -1.625445 | 0.176183 |
| N | -1.934692 | -2.404299 | -0.671304 |
| H | 0.906623 | 0.087911 | -1.771342 |
| H | -1.403411 | 0.672555 | -1.428809 |
| H | -1.186270 | 0.041658 | 1.536127 |
| H | -0.702091 | -2.270212 | 1.039747 |
| H | -1.782593 | -2.196052 | -1.664781 |
| H | -1.864361 | -3.418579 | -0.544558 |
| H | -2.869255 | -2.054377 | -0.386927 |
| H | 1.937107 | 1.428990 | 0.005054 |
| H | 1.297002 | 0.370713 | 1.263992 |
| H | 4.508122 | 1.297736 | 0.289929 |
| H | 4.148366 | 0.526176 | 1.868364 |
| H | 5.321282 | -0.212366 | 0.757686 |
| H | 0.488334 | 2.901183 | -1.389552 |
| H | -1.268664 | 3.009398 | -1.712290 |
| H | -0.539204 | 3.953353 | -0.381856 |
| H | -4.687717 | 0.478910 | 0.939800 |
| H | -3.423745 | 0.644318 | 2.195214 |
| H | -3.370960 | 1.675435 | 0.732264 |

AMMONIA_ADDUCT_1_CONF_12
Sum of electronic and zero-point Energies= -993.758896
Sum of electronic and thermal Energies= -993.742924
Sum of electronic and thermal Enthalpies= -993.741979
Sum of electronic and thermal Free Energies= -993.803610
Zero-point correction= 0.271948 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -42.07
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.586060 | -1.569928 | -0.686811 |
| C | -0.276345 | -0.732231 | 0.163883 |
| C | -1.720072 | -0.973408 | -0.235893 |
| S | -2.807379 | -0.067238 | 0.936765 |
| C | -4.430149 | -0.430758 | 0.179738 |

| | | | |
|---|---|---|---|
| C | 0.268181 | 0.684736 | -0.067295 |
| O | -0.182983 | 1.166114 | -1.310570 |
| C | -0.347690 | 2.583716 | -1.379994 |
| C | 1.789690 | 0.420970 | -0.170183 |
| O | 2.400932 | 0.154245 | 1.082768 |
| C | 2.796708 | 1.313671 | 1.833079 |
| C | 1.774310 | -0.922602 | -0.951740 |
| N | 2.905496 | -1.823309 | -0.410297 |
| H | -0.103895 | -1.025069 | 1.205936 |
| H | 0.012727 | 1.356790 | 0.759887 |
| H | 2.317616 | 1.214892 | -0.712242 |
| H | 1.948422 | -0.818706 | -2.025939 |
| H | 3.767172 | -1.769832 | -0.964019 |
| H | 3.097618 | -1.486021 | 0.553842 |
| H | 2.572705 | -2.793796 | -0.394200 |
| H | -1.877633 | -0.612936 | -1.254946 |
| H | -1.933485 | -2.046232 | -0.191736 |
| H | -4.490635 | -0.028806 | -0.835092 |
| H | -4.627613 | -1.505972 | 0.173093 |
| H | -5.179569 | 0.062445 | 0.803192 |
| H | -0.703932 | 2.802185 | -2.387819 |
| H | -1.089756 | 2.924503 | -0.647754 |
| H | 0.600997 | 3.113553 | -1.213755 |
| H | 3.505560 | 1.921615 | 1.257759 |
| H | 1.926812 | 1.919694 | 2.105820 |
| H | 3.276606 | 0.942638 | 2.739148 |

AMMONIA_ADDUCT_1_CONF_13

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.753544 |
| Sum of electronic and thermal Energies= | | -993.737423 |
| Sum of electronic and thermal Enthalpies= | | -993.736479 |
| Sum of electronic and thermal Free Energies= | | -993.798162 |
| Zero-point correction= | 0.271474 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -44.42 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.566753 | -1.223622 | -0.539130 |
| C | 0.629173 | 0.251055 | -0.623270 |
| C | 1.604668 | 0.802123 | 0.412541 |
| S | 3.371718 | 0.484136 | 0.056289 |
| C | 3.589196 | -1.227233 | 0.665675 |
| C | -0.851678 | 0.688856 | -0.422289 |
| O | -1.048523 | 1.934928 | 0.184892 |
| C | -0.942285 | 3.054474 | -0.700516 |
| C | -1.416278 | -0.418112 | 0.485768 |
| O | -2.783239 | -0.716513 | 0.319312 |
| C | -3.695370 | 0.129069 | 1.047565 |
| C | -0.592668 | -1.645422 | 0.055918 |
| N | -1.449381 | -2.429248 | -0.995027 |
| H | 0.999151 | 0.464068 | -1.628125 |
| H | -1.378351 | 0.644223 | -1.391830 |
| H | -1.187091 | -0.176491 | 1.532550 |
| H | -0.410769 | -2.377611 | 0.846901 |
| H | -1.233825 | -3.430794 | -1.005777 |
| H | -2.443381 | -2.264291 | -0.749032 |
| H | -1.267139 | -2.055313 | -1.932909 |
| H | 1.506795 | 1.891550 | 0.429291 |
| H | 1.352132 | 0.449983 | 1.419557 |
| H | 3.022576 | -1.947681 | 0.073180 |
| H | 4.655827 | -1.445054 | 0.569029 |
| H | 3.315492 | -1.302947 | 1.722495 |
| H | -1.660058 | 2.968497 | -1.527369 |
| H | -1.177359 | 3.937642 | -0.105349 |
| H | 0.070586 | 3.156266 | -1.110637 |
| H | -3.524343 | 0.027853 | 2.125597 |
| H | -3.573579 | 1.173254 | 0.750045 |
| H | -4.696981 | -0.221798 | 0.798007 |

AMMONIA_ADDUCT_1_CONF_14

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.753545 |
| Sum of electronic and thermal Energies= | | -993.737423 |
| Sum of electronic and thermal Enthalpies= | | -993.736479 |
| Sum of electronic and thermal Free Energies= | | -993.798167 |
| Zero-point correction= | 0.271473 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -44.42 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.566840 | -1.223646 | -0.538934 |
| C | 0.629158 | 0.251012 | -0.623307 |
| C | 1.604696 | 0.802271 | 0.412360 |
| S | 3.371727 | 0.484091 | 0.056134 |
| C | 3.589165 | -1.227119 | 0.665994 |
| C | -0.851699 | 0.688816 | -0.422282 |
| O | -1.048512 | 1.934873 | 0.184922 |
| C | -0.942454 | 3.054448 | -0.700460 |
| C | -1.416260 | -0.418189 | 0.485789 |
| O | -2.783225 | -0.716636 | 0.319478 |
| C | -3.695310 | 0.129056 | 1.047630 |
| C | -0.592671 | -1.645450 | 0.055883 |
| N | -1.449343 | -2.429106 | -0.995296 |
| H | 0.999069 | 0.463928 | -1.628210 |
| H | -1.378408 | 0.644216 | -1.391807 |
| H | -1.186970 | -0.176565 | 1.532551 |
| H | -0.410942 | -2.377799 | 0.846756 |
| H | -1.233006 | -3.430473 | -1.006891 |
| H | -1.267847 | -2.054343 | -1.932990 |
| H | -2.443337 | -2.265060 | -0.748786 |
| H | 1.352173 | 0.450379 | 1.419462 |
| H | 1.506896 | 1.891708 | 0.428847 |
| H | 4.655801 | -1.444966 | 0.569465 |
| H | 3.315405 | -1.302545 | 1.722817 |
| H | 3.022576 | -1.947720 | 0.073660 |
| H | 0.070452 | 3.156532 | -1.110426 |
| H | -1.177870 | 3.937551 | -0.105332 |
| H | -1.660067 | 2.968279 | -1.527432 |
| H | -3.574258 | 1.173081 | 0.749240 |
| H | -3.523567 | 0.028798 | 2.125637 |
| H | -4.696902 | -0.222516 | 0.798987 |

AMMONIA_ADDUCT_1_CONF_15

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758895 |
| Sum of electronic and thermal Energies= | | -993.742923 |
| Sum of electronic and thermal Enthalpies= | | -993.741979 |
| Sum of electronic and thermal Free Energies= | | -993.803604 |
| Zero-point correction= | 0.271948 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -42.07 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.585980 | -1.569680 | -0.687221 |
| C | -0.276453 | -0.732152 | 0.163560 |
| C | -1.720163 | -0.973153 | -0.236406 |
| S | -2.807444 | -0.067707 | 0.936876 |
| C | -4.430287 | -0.430306 | 0.179507 |
| C | 0.268128 | 0.684847 | -0.067201 |
| O | -0.182842 | 1.166452 | -1.310425 |
| C | -0.346408 | 2.584189 | -1.379898 |
| C | 1.789676 | 0.420991 | -0.169857 |
| O | 2.400544 | 0.153659 | 1.083118 |
| C | 2.796270 | 1.312700 | 1.834067 |
| C | 1.774291 | -0.922268 | -0.951918 |
| N | 2.905358 | -1.823199 | -0.410863 |
| H | -0.104098 | -1.025192 | 1.205575 |
| H | 0.012516 | 1.356723 | 0.760084 |

| | | | |
|---|---|---|---|
| H | 2.317866 | 1.215040 | -0.711484 |
| H | 1.948317 | -0.817952 | -2.026088 |
| H | 2.572784 | -2.793775 | -0.395715 |
| H | 3.767241 | -1.769083 | -0.964216 |
| H | 3.097099 | -1.486659 | 0.553623 |
| H | -1.877738 | -0.611957 | -1.255197 |
| H | -1.933553 | -2.046007 | -0.192990 |
| H | -5.179555 | 0.062824 | 0.803202 |
| H | -4.490575 | -0.027820 | -0.835121 |
| H | -4.628104 | -1.505450 | 0.172322 |
| H | -0.701685 | 2.803001 | -2.387988 |
| H | -1.088777 | 2.925472 | -0.648192 |
| H | 0.602538 | 3.113306 | -1.212853 |
| H | 3.274830 | 0.941190 | 2.740647 |
| H | 3.506223 | 1.920213 | 1.259650 |
| H | 1.926479 | 1.919293 | 2.105859 |

AMMONIA_ADDUCT_1_CONF_16

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.754430 |
| Sum of electronic and thermal Energies= | | -993.738729 |
| Sum of electronic and thermal Enthalpies= | | -993.737785 |
| Sum of electronic and thermal Free Energies= | | -993.798533 |
| Zero-point correction= | 0.272127 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -42.02 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.201514 | -1.362017 | 0.626751 |
| C | -0.345104 | -0.036878 | 1.220117 |
| C | -1.804369 | 0.415484 | 1.168284 |
| S | -2.569407 | 0.331218 | -0.507255 |
| C | -3.868897 | -0.923423 | -0.207047 |
| C | 0.665890 | 0.885653 | 0.476453 |
| O | -0.026826 | 1.827302 | -0.299006 |
| C | 0.707006 | 3.007546 | -0.616771 |
| C | 1.494576 | -0.090053 | -0.406477 |
| O | 2.637429 | -0.609877 | 0.258206 |
| C | 3.808297 | 0.216484 | 0.199238 |
| C | 0.515088 | -1.274009 | -0.555303 |
| N | 1.301012 | -2.579385 | -0.623958 |
| H | -0.041547 | -0.153676 | 2.265205 |
| H | 1.330149 | 1.381690 | 1.197502 |
| H | 1.762426 | 0.360906 | -1.369974 |
| H | -0.125007 | -1.211929 | -1.441741 |
| H | 2.186938 | -2.392386 | -0.112916 |
| H | 0.766325 | -3.318080 | -0.152980 |
| H | 1.512894 | -2.872201 | -1.583593 |
| H | -2.390373 | -0.219637 | 1.837788 |
| H | -1.867406 | 1.442117 | 1.538909 |
| H | -4.592051 | -0.572718 | 0.533813 |
| H | -4.389055 | -1.063956 | -1.158336 |
| H | -3.441967 | -1.879103 | 0.109301 |
| H | 1.038805 | 3.521260 | 0.295767 |
| H | 1.581954 | 2.790907 | -1.246160 |
| H | 0.023887 | 3.653261 | -1.169771 |
| H | 3.632585 | 1.182042 | 0.685478 |
| H | 4.590181 | -0.320066 | 0.737809 |
| H | 4.117047 | 0.379685 | -0.840900 |

AMMONIA_ADDUCT_1_CONF_17

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.754428 |
| Sum of electronic and thermal Energies= | | -993.738728 |
| Sum of electronic and thermal Enthalpies= | | -993.737784 |
| Sum of electronic and thermal Free Energies= | | -993.798528 |
| Zero-point correction= | 0.272129 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -42.02 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.202098 | -1.361587 | 0.627050 |
| C | -0.345257 | -0.036290 | 1.220188 |
| C | -1.804321 | 0.416695 | 1.168129 |
| S | -2.569487 | 0.331802 | -0.507303 |
| C | -3.867700 | -0.924164 | -0.207090 |
| C | 0.666144 | 0.885757 | 0.476441 |
| O | -0.026180 | 1.827789 | -0.298896 |
| C | 0.708377 | 3.007475 | -0.617042 |
| C | 1.494333 | -0.090386 | -0.406480 |
| O | 2.636916 | -0.610645 | 0.258356 |
| C | 3.808224 | 0.215065 | 0.199086 |
| C | 0.514339 | -1.273908 | -0.555139 |
| N | 1.299662 | -2.579608 | -0.623848 |
| H | -0.041854 | -0.153058 | 2.265322 |
| H | 1.330729 | 1.381428 | 1.197444 |
| H | 1.762425 | 0.360324 | -1.370025 |
| H | -0.125901 | -1.211617 | -1.441458 |
| H | 0.764050 | -3.318512 | -0.154257 |
| H | 1.512681 | -2.871631 | -1.583480 |
| H | 2.185063 | -2.393463 | -0.111643 |
| H | -2.390665 | -0.217588 | 1.838128 |
| H | -1.866812 | 1.443643 | 1.537959 |
| H | -3.439789 | -1.879482 | 0.109016 |
| H | -4.591064 | -0.574300 | 0.533964 |
| H | -4.387889 | -1.065026 | -1.158314 |
| H | 1.582986 | 2.790152 | -1.246665 |
| H | 0.025544 | 3.653594 | -1.169925 |
| H | 1.040808 | 3.521086 | 0.295327 |
| H | 4.117746 | 0.376756 | -0.841060 |
| H | 3.632674 | 1.181354 | 0.683932 |
| H | 4.589482 | -0.321160 | 0.738886 |

AMMONIA_ADDUCT_1_CONF_18

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.754230 |
| Sum of electronic and thermal Energies= | | -993.738434 |
| Sum of electronic and thermal Enthalpies= | | -993.737490 |
| Sum of electronic and thermal Free Energies= | | -993.797960 |
| Zero-point correction= | 0.272028 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.16 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.168604 | -1.421184 | 0.035195 |
| C | -0.144343 | -0.281739 | 0.903768 |
| C | -1.644764 | -0.244267 | 1.160753 |
| S | -2.695858 | -0.120972 | -0.346338 |
| C | -4.234788 | -0.821872 | 0.348487 |
| C | 0.541680 | 0.920347 | 0.217966 |
| O | -0.187588 | 1.453334 | -0.858523 |
| C | -0.786994 | 2.734084 | -0.633553 |
| C | 1.786887 | 0.249112 | -0.407664 |
| O | 2.787976 | -0.081544 | 0.541560 |
| C | 3.705128 | 0.978245 | 0.855349 |
| C | 1.163651 | -1.091868 | -0.862684 |
| N | 2.221053 | -2.200366 | -0.748513 |
| H | 0.361003 | -0.459984 | 1.861929 |
| H | 0.821633 | 1.688666 | 0.949764 |
| H | 2.189390 | 0.841876 | -1.236900 |
| H | 0.808895 | -1.092428 | -1.897957 |
| H | 1.756698 | -3.075161 | -0.479919 |
| H | 2.747581 | -2.348296 | -1.616413 |
| H | 2.870703 | -1.889568 | -0.000359 |
| H | -1.913307 | -1.171063 | 1.678888 |
| H | -1.850027 | 0.583614 | 1.850660 |
| H | -4.086953 | -1.852352 | 0.685419 |
| H | -4.621328 | -0.211890 | 1.169644 |
| H | -4.967777 | -0.818913 | -0.462194 |

| | | | |
|---|---|---|---|
| H | -1.565255 | 2.685166 | 0.135329 |
| H | -0.024701 | 3.473035 | -0.352453 |
| H | -1.244443 | 3.024160 | -1.579770 |
| H | 4.223995 | 1.320504 | -0.048292 |
| H | 3.185334 | 1.821585 | 1.321645 |
| H | 4.424249 | 0.562064 | 1.561585 |

AMMONIA_ADDUCT_1_CONF_19

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.757556 |
| Sum of electronic and thermal Energies= | | -993.741743 |
| Sum of electronic and thermal Enthalpies= | | -993.740798 |
| Sum of electronic and thermal Free Energies= | | -993.801010 |
| Zero-point correction= | 0.272069 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -41.09 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.333839 | -1.687165 | -1.037240 |
| C | 0.449660 | -0.498793 | -1.377997 |
| C | 1.897914 | -0.674551 | -0.918061 |
| S | 2.116962 | -1.104406 | 0.858763 |
| C | 2.842317 | 0.436915 | 1.534582 |
| C | -0.364363 | 0.669260 | -0.759375 |
| O | 0.377143 | 1.789649 | -0.353099 |
| C | 0.697003 | 2.703904 | -1.404934 |
| C | -1.063934 | 0.034240 | 0.457675 |
| O | -2.391322 | 0.477711 | 0.673560 |
| C | -2.514594 | 1.688682 | 1.440262 |
| C | -1.102921 | -1.469951 | 0.090336 |
| N | -2.563597 | -1.842239 | -0.276450 |
| H | 0.438127 | -0.458891 | -2.471693 |
| H | -1.147930 | 0.968618 | -1.474769 |
| H | -0.447819 | 0.170964 | 1.351965 |
| H | -0.829044 | -2.131265 | 0.915289 |
| H | -2.660906 | -1.819964 | -1.298051 |
| H | -2.830354 | -2.774516 | 0.053161 |
| H | -3.167820 | -1.109323 | 0.147534 |
| H | 2.334774 | -1.491965 | -1.498734 |
| H | 2.470827 | 0.229589 | -1.141853 |
| H | 3.822624 | 0.623615 | 1.089230 |
| H | 2.181144 | 1.290333 | 1.373379 |
| H | 2.972951 | 0.268356 | 2.606537 |
| H | -0.213584 | 3.059048 | -1.905914 |
| H | 1.204561 | 3.547663 | -0.935561 |
| H | 1.364442 | 2.253255 | -2.151069 |
| H | -3.582754 | 1.894530 | 1.515746 |
| H | -2.090307 | 1.549662 | 2.441569 |
| H | -2.007495 | 2.516662 | 0.937488 |

AMMONIA_ADDUCT_1_CONF_20

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.755516 |
| Sum of electronic and thermal Energies= | | -993.739659 |
| Sum of electronic and thermal Enthalpies= | | -993.738715 |
| Sum of electronic and thermal Free Energies= | | -993.799859 |
| Zero-point correction= | 0.271786 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -41.20 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.122634 | -1.865311 | -0.808301 |
| C | 0.575452 | -0.707214 | -1.364732 |
| C | 2.027539 | -0.689469 | -0.889444 |
| S | 2.244704 | -0.767148 | 0.937713 |
| C | 2.958810 | 0.882507 | 1.292327 |
| C | -0.313558 | 0.494685 | -0.979873 |
| O | 0.458009 | 1.659101 | -0.884392 |
| C | -0.253200 | 2.881492 | -1.079032 |
| C | -1.011442 | 0.051508 | 0.330940 |
| O | -2.366386 | 0.483255 | 0.409423 |
| C | -2.711558 | 1.265760 | 1.567274 |
| C | -0.946060 | -1.502740 | 0.237950 |
| N | -2.370861 | -2.014916 | -0.106353 |
| H | 0.571308 | -0.859386 | -2.448237 |
| H | -1.101150 | 0.615978 | -1.741170 |
| H | -0.432566 | 0.382007 | 1.195750 |
| H | -0.668579 | -1.996490 | 1.172104 |
| H | -2.384972 | -2.299368 | -1.092594 |
| H | -2.664318 | -2.811843 | 0.466116 |
| H | -3.004325 | -1.199334 | 0.044331 |
| H | 2.531665 | -1.560763 | -1.316636 |
| H | 2.518358 | 0.207510 | -1.274648 |
| H | 3.070269 | 0.944099 | 2.377782 |
| H | 3.945455 | 0.977625 | 0.832839 |
| H | 2.298047 | 1.677379 | 0.942031 |
| H | -0.801012 | 2.870865 | -2.030588 |
| H | -0.958437 | 3.080439 | -0.261593 |
| H | 0.497868 | 3.672405 | -1.102576 |
| H | -2.536662 | 0.706308 | 2.493902 |
| H | -2.135407 | 2.196190 | 1.586643 |
| H | -3.772587 | 1.499620 | 1.471306 |

AMMONIA_ADDUCT_1_CONF_21

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.754231 |
| Sum of electronic and thermal Energies= | | -993.738435 |
| Sum of electronic and thermal Enthalpies= | | -993.737491 |
| Sum of electronic and thermal Free Energies= | | -993.797959 |
| Zero-point correction= | 0.272027 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.16 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.168520 | -1.421088 | 0.033996 |
| C | -0.144289 | -0.282138 | 0.903299 |
| C | -1.644646 | -0.245011 | 1.160594 |
| S | -2.696061 | -0.121104 | -0.346221 |
| C | -4.235054 | -0.821462 | 0.348998 |
| C | 0.541555 | 0.920267 | 0.217837 |
| O | -0.187618 | 1.453213 | -0.858694 |
| C | -0.787511 | 2.733686 | -0.633581 |
| C | 1.787035 | 0.249392 | -0.407554 |
| O | 2.787854 | -0.081192 | 0.541989 |
| C | 3.705030 | 0.978598 | 0.855802 |
| C | 1.164196 | -1.091676 | -0.863055 |
| N | 2.221772 | -2.200087 | -0.748164 |
| H | 0.361265 | -0.460737 | 1.861279 |
| H | 0.821195 | 1.688536 | 0.949823 |
| H | 2.189694 | 0.842349 | -1.236571 |
| H | 0.810238 | -1.092365 | -1.898598 |
| H | 2.871471 | -1.888682 | -0.000282 |
| H | 1.757419 | -3.074688 | -0.478898 |
| H | 2.748270 | -2.348620 | -1.615974 |
| H | -1.912976 | -1.172078 | 1.678364 |
| H | -1.849832 | 0.582532 | 1.850933 |
| H | -4.968363 | -0.817981 | -0.461391 |
| H | -4.087567 | -1.852090 | 0.685633 |
| H | -4.621002 | -0.211496 | 1.170449 |
| H | -1.564536 | 2.684814 | 0.136553 |
| H | -0.025243 | 3.473290 | -0.354101 |
| H | -1.246658 | 3.022871 | -1.579238 |
| H | 4.423734 | 0.562583 | 1.562555 |
| H | 4.224373 | 1.320418 | -0.047727 |
| H | 3.185131 | 1.822204 | 1.321507 |

AMMONIA_ADDUCT_1_CONF_23

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.751651 |
| Sum of electronic and thermal Energies= | | -993.735454 |

Sum of electronic and thermal Enthalpies= -993.734510
Sum of electronic and thermal Free Energies= -993.797173
Zero-point correction= 0.271319 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -44.54
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.367712 | -1.458618 | -0.462630 |
| C | 0.669730 | -0.048281 | -0.761899 |
| C | 1.745643 | 0.474967 | 0.179034 |
| S | 3.247629 | -0.575420 | 0.063303 |
| C | 4.485370 | 0.598353 | 0.721199 |
| C | -0.696792 | 0.662842 | -0.637520 |
| O | -0.517397 | 2.003976 | -0.290840 |
| C | -1.582637 | 2.883102 | -0.653100 |
| C | -1.437332 | -0.186791 | 0.425754 |
| O | -2.843257 | -0.228875 | 0.248127 |
| C | -3.638476 | 0.182786 | 1.376126 |
| C | -0.819304 | -1.591950 | 0.205977 |
| N | -1.813635 | -2.390656 | -0.699064 |
| H | 1.045545 | -0.045768 | -1.786978 |
| H | -1.250131 | 0.573037 | -1.587517 |
| H | -1.171619 | 0.172780 | 1.425423 |
| H | -0.719729 | -2.203511 | 1.107036 |
| H | -1.850264 | -3.387671 | -0.466422 |
| H | -2.743579 | -1.944129 | -0.569301 |
| H | -1.518560 | -2.303521 | -1.678323 |
| H | 1.984695 | 1.497120 | -0.129662 |
| H | 1.381134 | 0.517754 | 1.212227 |
| H | 4.558285 | 1.491811 | 0.094920 |
| H | 4.259442 | 0.878915 | 1.753533 |
| H | 5.444321 | 0.074800 | 0.702614 |
| H | -2.498509 | 2.675718 | -0.085166 |
| H | -1.802658 | 2.813405 | -1.726765 |
| H | -1.236873 | 3.891016 | -0.419648 |
| H | -4.679226 | 0.080927 | 1.066523 |
| H | -3.448316 | -0.451700 | 2.249777 |
| H | -3.434251 | 1.228291 | 1.627646 |

AMMONIA_ADDUCT_1_CONF_24
Sum of electronic and zero-point Energies= -993.755512
Sum of electronic and thermal Energies= -993.739656
Sum of electronic and thermal Enthalpies= -993.738712
Sum of electronic and thermal Free Energies= -993.799822
Zero-point correction= 0.271790 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -41.21
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.121740 | -1.868092 | -0.802775 |
| C | 0.574646 | -0.710515 | -1.362945 |
| C | 2.027109 | -0.690627 | -0.888938 |
| S | 2.245673 | -0.765148 | 0.938162 |
| C | 2.960377 | 0.885079 | 1.288992 |
| C | -0.314908 | 0.491751 | -0.980204 |
| O | 0.455910 | 1.656896 | -0.887749 |
| C | -0.255833 | 2.878364 | -1.086297 |
| C | -1.011091 | 0.050716 | 0.332102 |
| O | -2.364997 | 0.484663 | 0.414134 |
| C | -2.705124 | 1.270072 | 1.571494 |
| C | -0.948556 | -1.503412 | 0.239629 |
| N | -2.373963 | -2.012095 | -0.109323 |
| H | 0.569684 | -0.865269 | -2.446086 |
| H | -1.103105 | 0.610942 | -1.741258 |
| H | -0.429156 | 0.380186 | 1.195279 |
| H | -0.676297 | -1.997803 | 1.174993 |
| H | -2.666971 | -2.814859 | 0.455157 |
| H | -3.007285 | -1.198022 | 0.049079 |
| H | -2.388804 | -2.286811 | -1.098289 |
| H | 2.531752 | -1.562056 | -1.315239 |
| H | 2.516629 | 0.206278 | -1.275952 |
| H | 2.299241 | 1.679458 | 0.938231 |
| H | 3.073235 | 0.948556 | 2.374194 |
| H | 3.946442 | 0.979390 | 0.828093 |
| H | -0.803017 | 2.864757 | -2.038179 |
| H | -0.961692 | 3.079263 | -0.269897 |
| H | 0.494866 | 3.669569 | -1.111642 |
| H | -2.127568 | 2.199704 | 1.587092 |
| H | -3.766130 | 1.505267 | 1.478590 |
| H | -2.527959 | 0.712175 | 2.498616 |

AMMONIA_ADDUCT_1_CONF_25
Sum of electronic and zero-point Energies= -993.749804
Sum of electronic and thermal Energies= -993.734000
Sum of electronic and thermal Enthalpies= -993.733056
Sum of electronic and thermal Free Energies= -993.793866
Zero-point correction= 0.272001 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -44.38
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.110021 | -0.610980 | -0.991739 |
| C | -0.388543 | -0.049043 | 0.341911 |
| C | -1.802885 | 0.490974 | 0.385439 |
| S | -3.002193 | -0.866138 | 0.070964 |
| C | -4.531477 | -0.065016 | 0.670767 |
| C | 0.768218 | 0.945980 | 0.557880 |
| O | 0.575442 | 2.251294 | 0.079094 |
| C | 0.468904 | 2.471647 | -1.327631 |
| C | 1.957205 | 0.172376 | -0.087374 |
| O | 2.535198 | -0.745062 | 0.828144 |
| C | 3.550458 | -0.198318 | 1.687040 |
| C | 1.245451 | -0.664095 | -1.198466 |
| N | 1.697016 | -2.151654 | -1.080594 |
| H | -0.288930 | -0.863410 | 1.071646 |
| H | 0.958481 | 1.066290 | 1.628004 |
| H | 2.718908 | 0.842640 | -0.502236 |
| H | 1.489657 | -0.365177 | -2.220034 |
| H | 2.149552 | -2.248279 | -0.150402 |
| H | 0.863334 | -2.746941 | -1.149513 |
| H | 2.365282 | -2.427727 | -1.807249 |
| H | -1.969640 | 0.895664 | 1.390257 |
| H | -1.937698 | 1.303427 | -0.332439 |
| H | -4.763937 | 0.829686 | 0.087183 |
| H | -5.334848 | -0.792558 | 0.532545 |
| H | -4.458374 | 0.184775 | 1.732915 |
| H | 0.304537 | 3.543791 | -1.444810 |
| H | 1.398173 | 2.210318 | -1.855002 |
| H | -0.368126 | 1.928720 | -1.779629 |
| H | 3.898313 | -1.022264 | 2.310673 |
| H | 4.381794 | 0.198882 | 1.092596 |
| H | 3.140560 | 0.592907 | 2.322843 |

AMMONIA_ADDUCT_2_CONF_1
Sum of electronic and zero-point Energies= -993.758937
Sum of electronic and thermal Energies= -993.743081
Sum of electronic and thermal Enthalpies= -993.742137
Sum of electronic and thermal Free Energies= -993.803235
Zero-point correction= 0.271631 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -43.72
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.164178 | -0.934223 | 0.954148 |
| C | 0.383823 | -0.352388 | -0.382725 |
| C | 1.718512 | 0.369276 | -0.425836 |
| S | 3.082170 | -0.784204 | 0.007643 |
| C | 4.500304 | 0.210454 | -0.574461 |

| | | | |
|---|---|---|---|
| C | -0.872101 | 0.498138 | -0.624295 |
| O | -0.750082 | 1.763388 | 0.039676 |
| C | -1.389128 | 2.862343 | -0.628704 |
| C | -1.957852 | -0.333137 | 0.110959 |
| O | -2.312836 | -1.511036 | -0.550915 |
| C | -3.309747 | -1.358093 | -1.565570 |
| C | -1.140674 | -0.777926 | 1.339923 |
| N | -1.140096 | 0.385322 | 2.385437 |
| H | 0.382171 | -1.193329 | -1.082549 |
| H | -1.076802 | 0.633209 | -1.690081 |
| H | -2.836050 | 0.279398 | 0.372169 |
| H | -1.529285 | -1.660980 | 1.850766 |
| H | -0.373111 | 0.226384 | 3.049091 |
| H | -0.951289 | 1.253956 | 1.841492 |
| H | -2.020426 | 0.479149 | 2.904110 |
| H | 1.867886 | 0.732224 | -1.450045 |
| H | 1.710232 | 1.234347 | 0.243241 |
| H | 5.395223 | -0.380326 | -0.364352 |
| H | 4.443730 | 0.392552 | -1.651462 |
| H | 4.572545 | 1.159066 | -0.035073 |
| H | -1.210646 | 3.746499 | -0.015047 |
| H | -0.945658 | 3.012821 | -1.618998 |
| H | -2.469078 | 2.697892 | -0.731845 |
| H | -4.231143 | -0.932567 | -1.146041 |
| H | -2.959569 | -0.726446 | -2.391771 |
| H | -3.511679 | -2.360865 | -1.942959 |

AMMONIA_ADDUCT_2_CONF_2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758946 |
| Sum of electronic and thermal Energies= | | -993.743090 |
| Sum of electronic and thermal Enthalpies= | | -993.742146 |
| Sum of electronic and thermal Free Energies= | | -993.803256 |
| Zero-point correction= | 0.271621 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.72 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.166717 | -0.920839 | 0.963287 |
| C | 0.386380 | -0.351923 | -0.379314 |
| C | 1.720358 | 0.370437 | -0.428451 |
| S | 3.084003 | -0.775516 | 0.025171 |
| C | 4.501298 | 0.201115 | -0.588752 |
| C | -0.870585 | 0.494224 | -0.629088 |
| O | -0.752058 | 1.763861 | 0.027273 |
| C | -1.404471 | 2.854299 | -0.642151 |
| C | -1.955563 | -0.335493 | 0.108990 |
| O | -2.303661 | -1.519271 | -0.546367 |
| C | -3.303623 | -1.377982 | -1.559791 |
| C | -1.140274 | -0.768690 | 1.343513 |
| N | -1.148047 | 0.401109 | 2.381666 |
| H | 0.385624 | -1.199740 | -1.070765 |
| H | -1.073091 | 0.622712 | -1.696147 |
| H | -2.837225 | 0.274879 | 0.363226 |
| H | -1.526784 | -1.650079 | 1.858851 |
| H | -0.957145 | 1.266116 | 1.832663 |
| H | -2.031911 | 0.497132 | 2.893866 |
| H | -0.385167 | 0.247893 | 3.051360 |
| H | 1.709016 | 1.244813 | 0.228321 |
| H | 1.872747 | 0.718976 | -1.457179 |
| H | 4.576104 | 1.164248 | -0.076155 |
| H | 4.441357 | 0.353195 | -1.670218 |
| H | 5.396365 | -0.384468 | -0.365149 |
| H | -2.484292 | 2.682471 | -0.734331 |
| H | -1.225905 | 3.743575 | -0.035939 |
| H | -0.971208 | 3.001160 | -1.637502 |
| H | -2.964481 | -0.736575 | -2.383084 |
| H | -3.489280 | -2.382098 | -1.941916 |
| H | -4.231544 | -0.969646 | -1.137588 |

AMMONIA_ADDUCT_2_CONF_3

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758480 |
| Sum of electronic and thermal Energies= | | -993.742814 |
| Sum of electronic and thermal Enthalpies= | | -993.741870 |
| Sum of electronic and thermal Free Energies= | | -993.802115 |
| Zero-point correction= | 0.271856 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.47 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.301027 | 0.267710 | 1.267133 |
| C | -0.520882 | 0.229603 | -0.188106 |
| C | -1.708990 | -0.661581 | -0.521700 |
| S | -3.285356 | -0.187939 | 0.278995 |
| C | -3.766539 | 1.264438 | -0.722381 |
| C | 0.839768 | -0.209766 | -0.753015 |
| O | 0.979010 | -1.633326 | -0.642538 |
| C | 1.756393 | -2.248767 | -1.681458 |
| C | 1.823146 | 0.453162 | 0.246933 |
| O | 1.922442 | 1.839971 | 0.103426 |
| C | 2.862241 | 2.278667 | -0.882090 |
| C | 1.037870 | 0.223843 | 1.553607 |
| N | 1.319488 | -1.230284 | 2.055506 |
| H | -0.706118 | 1.262999 | -0.495449 |
| H | 0.982789 | 0.118247 | -1.786569 |
| H | 2.810100 | -0.037352 | 0.241619 |
| H | 1.307916 | 0.895452 | 2.370996 |
| H | 1.227562 | -1.840447 | 1.215941 |
| H | 0.599618 | -1.484424 | 2.741835 |
| H | 2.246074 | -1.351914 | 2.479076 |
| H | -1.838897 | -0.678228 | -1.610629 |
| H | -1.505319 | -1.687470 | -0.205717 |
| H | -4.744335 | 1.578363 | -0.348619 |
| H | -3.070596 | 2.099983 | -0.604372 |
| H | -3.865655 | 1.000269 | -1.779379 |
| H | 2.785839 | -1.869101 | -1.692538 |
| H | 1.763263 | -3.319469 | -1.472388 |
| H | 1.290911 | -2.073220 | -2.657415 |
| H | 2.850888 | 3.368337 | -0.845843 |
| H | 3.871700 | 1.915579 | -0.647358 |
| H | 2.582086 | 1.948970 | -1.890556 |

AMMONIA_ADDUCT_2_CONF_4

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758475 |
| Sum of electronic and thermal Energies= | | -993.742812 |
| Sum of electronic and thermal Enthalpies= | | -993.741867 |
| Sum of electronic and thermal Free Energies= | | -993.802103 |
| Zero-point correction= | 0.271861 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.47 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.302053 | 0.269991 | 1.265783 |
| C | -0.520813 | 0.229757 | -0.189570 |
| C | -1.708831 | -0.661659 | -0.522944 |
| S | -3.285234 | -0.188475 | 0.277943 |
| C | -3.765968 | 1.265017 | -0.722027 |
| C | 0.840197 | -0.210625 | -0.752897 |
| O | 0.978918 | -1.634122 | -0.640871 |
| C | 1.757650 | -2.250670 | -1.678114 |
| C | 1.822971 | 0.453118 | 0.247090 |
| O | 1.922728 | 1.839743 | 0.101970 |
| C | 2.864095 | 2.276989 | -0.882686 |
| C | 1.036553 | 0.225615 | 1.553386 |
| N | 1.316956 | -1.228167 | 2.057037 |
| H | -0.705627 | 1.262733 | -0.498556 |
| H | 0.984090 | 0.116274 | -1.786688 |

| | | | |
|---|---|---|---|
| H | 2.809798 | -0.037647 | 0.243160 |
| H | 1.306309 | 0.897901 | 2.370310 |
| H | 0.596302 | -1.481233 | 2.742943 |
| H | 1.225547 | -1.839139 | 1.218010 |
| H | 2.243076 | -1.349824 | 2.481618 |
| H | -1.838892 | -0.678206 | -1.611862 |
| H | -1.504936 | -1.687544 | -0.207106 |
| H | -4.744388 | 1.577903 | -0.349028 |
| H | -3.070616 | 2.100773 | -0.602068 |
| H | -3.863701 | 1.002211 | -1.779496 |
| H | 1.293329 | -2.076333 | -2.654844 |
| H | 2.787059 | -1.870873 | -1.688416 |
| H | 1.764422 | -3.321126 | -1.467782 |
| H | 3.873267 | 1.914679 | -0.645529 |
| H | 2.585833 | 1.945352 | -1.891046 |
| H | 2.852304 | 3.366720 | -0.848456 |

AMMONIA_ADDUCT_2_CONF_5

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.759916 |
| Sum of electronic and thermal Energies= | | -993.744466 |
| Sum of electronic and thermal Enthalpies= | | -993.743522 |
| Sum of electronic and thermal Free Energies= | | -993.802810 |
| Zero-point correction= | 0.272023 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -40.17 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.268895 | -0.985675 | 1.651270 |
| C | -0.281656 | 0.443552 | 1.378319 |
| C | -1.605014 | 0.902594 | 0.758144 |
| S | -2.015246 | 0.197291 | -0.901617 |
| C | -3.838352 | 0.075678 | -0.769080 |
| C | 1.017035 | 0.682613 | 0.554896 |
| O | 0.938379 | 1.717641 | -0.387185 |
| C | 1.242977 | 3.018306 | 0.120938 |
| C | 1.249937 | -0.663890 | -0.170900 |
| O | 2.574556 | -1.107474 | -0.263294 |
| C | 3.380050 | -0.385778 | -1.201261 |
| C | 0.498366 | -1.664876 | 0.721979 |
| N | -0.472770 | -2.510667 | -0.122155 |
| H | -0.218612 | 0.918044 | 2.361952 |
| H | 1.854271 | 0.836018 | 1.252139 |
| H | 0.793241 | -0.583406 | -1.172429 |
| H | 1.177564 | -2.371862 | 1.204430 |
| H | -0.987586 | -3.164616 | 0.477634 |
| H | -1.162427 | -1.830634 | -0.550115 |
| H | 0.010300 | -3.043181 | -0.854989 |
| H | -1.592467 | 1.992561 | 0.671730 |
| H | -2.411526 | 0.622548 | 1.442273 |
| H | -4.140590 | -0.559761 | 0.066936 |
| H | -4.269898 | 1.072941 | -0.660376 |
| H | -4.193107 | -0.359007 | -1.706623 |
| H | 1.202166 | 3.697601 | -0.731584 |
| H | 0.515776 | 3.346135 | 0.875975 |
| H | 2.249338 | 3.042600 | 0.559712 |
| H | 2.924707 | -0.399105 | -2.200793 |
| H | 3.527452 | 0.654412 | -0.890861 |
| H | 4.342332 | -0.898405 | -1.228599 |

AMMONIA_ADDUCT_2_CONF_6

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.757982 |
| Sum of electronic and thermal Energies= | | -993.742288 |
| Sum of electronic and thermal Enthalpies= | | -993.741344 |
| Sum of electronic and thermal Free Energies= | | -993.801736 |
| Zero-point correction= | 0.271717 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -44.04 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.447605 | -0.792403 | 0.803862 |
| C | 0.426887 | -0.189717 | -0.545709 |
| C | 1.647634 | 0.694583 | -0.754294 |
| S | 3.235031 | -0.200177 | -0.940372 |
| C | 3.679356 | -0.559848 | 0.796916 |
| C | -0.944019 | 0.498295 | -0.612408 |
| O | -0.891733 | 1.763900 | 0.062616 |
| C | -1.734109 | 2.785607 | -0.494702 |
| C | -1.821002 | -0.468508 | 0.226873 |
| O | -2.098819 | -1.678661 | -0.413108 |
| C | -3.220158 | -1.650120 | -1.301857 |
| C | -0.813500 | -0.809245 | 1.342228 |
| N | -0.846795 | 0.342248 | 2.399241 |
| H | 0.439419 | -1.024410 | -1.251919 |
| H | -1.292634 | 0.617979 | -1.642076 |
| H | -2.732893 | 0.023121 | 0.603255 |
| H | -1.022633 | -1.736769 | 1.878770 |
| H | -0.821178 | 1.227173 | 1.846895 |
| H | -1.678097 | 0.327335 | 3.000546 |
| H | -0.007443 | 0.280110 | 2.986119 |
| H | 1.720251 | 1.451289 | 0.032295 |
| H | 1.515184 | 1.228158 | -1.702386 |
| H | 3.739111 | 0.361479 | 1.384656 |
| H | 4.674155 | -1.011190 | 0.762094 |
| H | 2.985402 | -1.264652 | 1.258792 |
| H | -1.579298 | 3.680442 | 0.109793 |
| H | -1.442765 | 2.992969 | -1.529969 |
| H | -2.792181 | 2.497103 | -0.461738 |
| H | -3.328908 | -2.666211 | -1.681860 |
| H | -4.134053 | -1.359352 | -0.766901 |
| H | -3.057341 | -0.966439 | -2.144349 |

AMMONIA_ADDUCT_2_CONF_7

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.760610 |
| Sum of electronic and thermal Energies= | | -993.745212 |
| Sum of electronic and thermal Enthalpies= | | -993.744267 |
| Sum of electronic and thermal Free Energies= | | -993.802914 |
| Zero-point correction= | 0.272230 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.87 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.248395 | -1.306981 | -1.590982 |
| C | 0.439668 | 0.134392 | -1.508817 |
| C | 1.835381 | 0.491819 | -0.978354 |
| S | 2.392788 | -0.251201 | 0.616847 |
| C | 2.061720 | 1.072711 | 1.842069 |
| C | -0.803977 | 0.626599 | -0.716164 |
| O | -0.610104 | 1.784194 | 0.055592 |
| C | -0.803189 | 3.013940 | -0.650281 |
| C | -1.163056 | -0.568332 | 0.195001 |
| O | -2.524688 | -0.823512 | 0.396066 |
| C | -3.181766 | 0.093759 | 1.276539 |
| C | -0.585486 | -1.760606 | -0.584348 |
| N | 0.270394 | -2.637327 | 0.344208 |
| H | 0.401107 | 0.482128 | -2.545882 |
| H | -1.635355 | 0.762498 | -1.423864 |
| H | -0.644067 | -0.426469 | 1.158013 |
| H | -1.371721 | -2.410531 | -0.976894 |
| H | 1.041819 | -2.014230 | 0.707840 |
| H | -0.275834 | -3.030553 | 1.119417 |
| H | 0.697310 | -3.406493 | -0.184493 |
| H | 2.568994 | 0.151691 | -1.714605 |
| H | 1.934293 | 1.577903 | -0.898219 |
| H | 1.026254 | 1.411007 | 1.795184 |
| H | 2.283533 | 0.648176 | 2.824197 |
| H | 2.741373 | 1.907955 | 1.658697 |

| | | | |
|---|---|---|---|
| H | -0.058929 | 3.150957 | -1.445825 |
| H | -1.808821 | 3.059295 | -1.087825 |
| H | -0.691993 | 3.812036 | 0.085087 |
| H | -2.678205 | 0.128762 | 2.252585 |
| H | -3.214398 | 1.104595 | 0.856282 |
| H | -4.197326 | -0.283528 | 1.402025 |

AMMONIA_ADDUCT_2_CONF_8

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.760614 |
| Sum of electronic and thermal Energies= | | -993.745213 |
| Sum of electronic and thermal Enthalpies= | | -993.744268 |
| Sum of electronic and thermal Free Energies= | | -993.802923 |
| Zero-point correction= | 0.272226 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -39.87 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.250120 | -1.305658 | -1.591425 |
| C | 0.439999 | 0.135883 | -1.508797 |
| C | 1.835053 | 0.494546 | -0.977425 |
| S | 2.392796 | -0.250853 | 0.616561 |
| C | 2.061337 | 1.071374 | 1.843502 |
| C | -0.804363 | 0.626800 | -0.716408 |
| O | -0.611625 | 1.784249 | 0.055890 |
| C | -0.805675 | 3.014102 | -0.649539 |
| C | -1.162552 | -0.568745 | 0.194268 |
| O | -2.523927 | -0.824841 | 0.395812 |
| C | -3.180949 | 0.090954 | 1.277876 |
| C | -0.584478 | -1.760249 | -0.585818 |
| N | 0.270886 | -2.637719 | 0.342461 |
| H | 0.401549 | 0.483824 | -2.545793 |
| H | -1.635648 | 0.762304 | -1.424288 |
| H | -0.643165 | -0.427034 | 1.157087 |
| H | -1.370448 | -2.409829 | -0.979493 |
| H | 0.697536 | -3.406918 | -0.186404 |
| H | 1.042460 | -2.014987 | 0.706338 |
| H | -0.275604 | -3.030913 | 1.117498 |
| H | 2.569559 | 0.157473 | -1.714169 |
| H | 1.931863 | 1.580610 | -0.894654 |
| H | 1.026205 | 1.410623 | 1.795685 |
| H | 2.281356 | 0.645140 | 2.825294 |
| H | 2.741943 | 1.906346 | 1.662423 |
| H | -0.062025 | 3.151615 | -1.445568 |
| H | -1.811629 | 3.059163 | -1.086372 |
| H | -0.694281 | 3.812054 | 0.085954 |
| H | -2.677595 | 0.123909 | 2.254106 |
| H | -3.213152 | 1.102598 | 0.859560 |
| H | -4.196644 | -0.286278 | 1.402420 |

AMMONIA_ADDUCT_2_CONF_9

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758594 |
| Sum of electronic and thermal Energies= | | -993.742837 |
| Sum of electronic and thermal Enthalpies= | | -993.741893 |
| Sum of electronic and thermal Free Energies= | | -993.802261 |
| Zero-point correction= | 0.271963 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.54 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.055357 | -0.975279 | 0.901695 |
| C | 0.303438 | -0.336198 | -0.404215 |
| C | 1.676567 | 0.311020 | -0.398228 |
| S | 2.969234 | -0.930280 | 0.013444 |
| C | 4.446963 | -0.006059 | -0.535708 |
| C | -0.914346 | 0.587276 | -0.589678 |
| O | -0.808947 | 1.792546 | 0.175872 |
| C | -0.523720 | 2.989425 | -0.564610 |
| C | -2.033609 | -0.249213 | 0.083970 |
| O | -2.415624 | -1.370471 | -0.656326 |
| C | -3.402095 | -1.121749 | -1.662749 |
| C | -1.246983 | -0.796999 | 1.289209 |
| N | -1.218230 | 0.294378 | 2.407958 |
| H | 0.261699 | -1.136782 | -1.148908 |
| H | -1.122394 | 0.805622 | -1.641101 |
| H | -2.890104 | 0.381627 | 0.367132 |
| H | -1.670801 | -1.696333 | 1.740389 |
| H | -0.473738 | 0.058246 | 3.073927 |
| H | -0.982842 | 1.190192 | 1.932515 |
| H | -2.105332 | 0.390150 | 2.914596 |
| H | 1.870819 | 0.704358 | -1.403362 |
| H | 1.702988 | 1.143536 | 0.312410 |
| H | 5.304258 | -0.652874 | -0.333806 |
| H | 4.570819 | 0.923634 | 0.026804 |
| H | 4.410063 | 0.203757 | -1.608546 |
| H | -1.302565 | 3.168334 | -1.314745 |
| H | -0.519629 | 3.807759 | 0.156798 |
| H | 0.454438 | 2.929200 | -1.052810 |
| H | -3.032108 | -0.439529 | -2.438421 |
| H | -3.622997 | -2.089754 | -2.113233 |
| H | -4.316287 | -0.706696 | -1.218327 |

AMMONIA_ADDUCT_2_CONF_10

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758403 |
| Sum of electronic and thermal Energies= | | -993.742663 |
| Sum of electronic and thermal Enthalpies= | | -993.741719 |
| Sum of electronic and thermal Free Energies= | | -993.802274 |
| Zero-point correction= | 0.271889 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.20 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.195430 | -0.374597 | 1.246082 |
| C | 0.449892 | -0.240295 | -0.197908 |
| C | 1.689140 | 0.612909 | -0.427273 |
| S | 3.215404 | 0.011022 | 0.385710 |
| C | 3.659925 | -1.391202 | -0.700617 |
| C | -0.880834 | 0.307706 | -0.747675 |
| O | -1.032236 | 1.709375 | -0.494061 |
| C | -0.912252 | 2.578593 | -1.631272 |
| C | -1.905647 | -0.405602 | 0.170821 |
| O | -2.035392 | -1.771872 | -0.092991 |
| C | -2.961400 | -2.098299 | -1.134057 |
| C | -1.148623 | -0.310602 | 1.508920 |
| N | -1.400962 | 1.102145 | 2.127618 |
| H | 0.594755 | -1.255087 | -0.581032 |
| H | -1.028327 | 0.080538 | -1.807388 |
| H | -2.875264 | 0.115571 | 0.174476 |
| H | -1.457792 | -1.040103 | 2.260246 |
| H | -0.693456 | 1.272926 | 2.851323 |
| H | -1.271663 | 1.783687 | 1.351212 |
| H | -2.334990 | 1.212329 | 2.537785 |
| H | 1.863742 | 0.700644 | -1.506568 |
| H | 1.521801 | 1.620147 | -0.035337 |
| H | 4.610177 | -1.776399 | -0.322539 |
| H | 2.922561 | -2.197934 | -0.659764 |
| H | 3.804079 | -1.061077 | -1.733668 |
| H | -1.095771 | 3.591058 | -1.268797 |
| H | 0.090855 | 2.524207 | -2.066485 |
| H | -1.661053 | 2.321292 | -2.389123 |
| H | -2.988109 | -3.187189 | -1.183424 |
| H | -3.963700 | -1.717255 | -0.897826 |
| H | -2.641197 | -1.701218 | -2.105649 |

AMMONIA_ADDUCT_2_CONF_11

| | |
|---|---|
| Sum of electronic and zero-point Energies= | -993.743707 |
| Sum of electronic and thermal Energies= | -993.727601 |

Sum of electronic and thermal Enthalpies= -993.726656
Sum of electronic and thermal Free Energies= -993.788690
Zero-point correction= 0.271544 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -45.65
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.585967 | -1.034198 | 0.900483 |
| C | -0.565380 | 0.427128 | 0.667150 |
| C | -1.439067 | 0.801412 | -0.526617 |
| S | -3.243919 | 0.757913 | -0.231331 |
| C | -3.604653 | -1.034115 | -0.252081 |
| C | 0.956375 | 0.747338 | 0.492056 |
| O | 1.250235 | 1.826951 | -0.348264 |
| C | 1.217229 | 3.107484 | 0.292078 |
| C | 1.494432 | -0.557680 | -0.124115 |
| O | 2.833300 | -0.905494 | 0.067916 |
| C | 3.778167 | -0.157143 | -0.713660 |
| C | 0.645011 | -1.579449 | 0.623946 |
| N | 0.415953 | -2.839287 | -0.239963 |
| H | -0.976669 | 0.865515 | 1.578220 |
| H | 1.415823 | 0.879230 | 1.484545 |
| H | 1.237235 | -0.540226 | -1.199903 |
| H | 1.167136 | -1.961386 | 1.509968 |
| H | -0.127113 | -3.541096 | 0.277993 |
| H | -0.111951 | -2.600318 | -1.088352 |
| H | 1.320900 | -3.249509 | -0.507868 |
| H | -1.224780 | 1.841028 | -0.791753 |
| H | -1.182385 | 0.201916 | -1.409630 |
| H | -3.285143 | -1.488941 | -1.196533 |
| H | -3.156590 | -1.555135 | 0.596546 |
| H | -4.692090 | -1.120700 | -0.185193 |
| H | 1.524136 | 3.833636 | -0.461697 |
| H | 0.209664 | 3.360699 | 0.646364 |
| H | 1.916137 | 3.139878 | 1.138036 |
| H | 3.785550 | 0.897060 | -0.424838 |
| H | 3.545909 | -0.235673 | -1.784132 |
| H | 4.752032 | -0.605510 | -0.514346 |

AMMONIA_ADDUCT_2_CONF_12
Sum of electronic and zero-point Energies= -993.757738
Sum of electronic and thermal Energies= -993.742021
Sum of electronic and thermal Enthalpies= -993.741077
Sum of electronic and thermal Free Energies= -993.801314
Zero-point correction= 0.271844 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -43.88
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.352620 | -0.889669 | 0.713276 |
| C | 0.352992 | -0.147506 | -0.564902 |
| C | 1.626027 | 0.675742 | -0.689801 |
| S | 3.161976 | -0.290923 | -0.944765 |
| C | 3.576319 | -0.815593 | 0.757176 |
| C | -0.981770 | 0.615615 | -0.528896 |
| O | -0.928856 | 1.762378 | 0.329234 |
| C | -0.920249 | 3.044160 | -0.319202 |
| C | -1.898262 | -0.411122 | 0.184275 |
| O | -2.217784 | -1.519895 | -0.602348 |
| C | -3.337846 | -1.339040 | -1.474910 |
| C | -0.910855 | -0.927820 | 1.248318 |
| N | -0.906806 | 0.075134 | 2.446222 |
| H | 0.310067 | -0.899518 | -1.358016 |
| H | -1.340424 | 0.885927 | -1.526206 |
| H | -2.789623 | 0.073786 | 0.611571 |
| H | -1.157564 | -1.908243 | 1.660674 |
| H | -0.077163 | -0.100073 | 3.023650 |
| H | -0.840572 | 1.025228 | 2.022876 |
| H | -1.744412 | 0.012937 | 3.035593 |
| H | 1.736887 | 1.351549 | 0.164386 |
| H | 1.540848 | 1.293243 | -1.591178 |
| H | 4.545307 | -1.316131 | 0.685606 |
| H | 3.683116 | 0.049413 | 1.419182 |
| H | 2.841904 | -1.516854 | 1.157283 |
| H | -0.935230 | 3.793182 | 0.473813 |
| H | -0.018208 | 3.174775 | -0.925550 |
| H | -1.810829 | 3.160372 | -0.947322 |
| H | -3.148637 | -0.563922 | -2.228101 |
| H | -3.486544 | -2.295964 | -1.975784 |
| H | -4.238867 | -1.080007 | -0.903420 |

AMMONIA_ADDUCT_2_CONF_13
Sum of electronic and zero-point Energies= -993.758720
Sum of electronic and thermal Energies= -993.743029
Sum of electronic and thermal Enthalpies= -993.742085
Sum of electronic and thermal Free Energies= -993.802373
Zero-point correction= 0.271873 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -43.86
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.061535 | -0.960801 | 0.774842 |
| C | 0.415224 | -0.270056 | -0.481792 |
| C | 1.789753 | 0.362443 | -0.360625 |
| S | 3.043263 | -0.911754 | 0.068442 |
| C | 4.558599 | 0.013131 | -0.365618 |
| C | -0.767539 | 0.679946 | -0.721799 |
| O | -0.611780 | 1.869555 | 0.062513 |
| C | -1.200436 | 3.048296 | -0.511213 |
| C | -1.948217 | -0.138679 | -0.152858 |
| O | -2.269142 | -1.142457 | -1.067500 |
| C | -3.532331 | -1.780804 | -0.863222 |
| C | -1.252300 | -0.745417 | 1.092938 |
| N | -1.245734 | 0.326680 | 2.237027 |
| H | 0.414422 | -1.038674 | -1.259676 |
| H | -0.904505 | 0.915044 | -1.780685 |
| H | -2.814975 | 0.493078 | 0.098053 |
| H | -1.716789 | -1.638431 | 1.516644 |
| H | -0.539009 | 0.059484 | 2.931887 |
| H | -0.959509 | 1.218943 | 1.778797 |
| H | -2.150529 | 0.446357 | 2.705472 |
| H | 1.781026 | 1.167425 | 0.379425 |
| H | 2.041935 | 0.798518 | -1.334780 |
| H | 5.397152 | -0.652385 | -0.146663 |
| H | 4.578558 | 0.266213 | -1.429481 |
| H | 4.662897 | 0.918315 | 0.239149 |
| H | -0.738047 | 3.268096 | -1.479333 |
| H | -0.996518 | 3.865909 | 0.181681 |
| H | -2.284126 | 2.935499 | -0.640762 |
| H | -3.649433 | -2.490128 | -1.682878 |
| H | -3.566803 | -2.327871 | 0.088505 |
| H | -4.349229 | -1.047606 | -0.893319 |

AMMONIA_ADDUCT_2_CONF_14
Sum of electronic and zero-point Energies= -993.758562
Sum of electronic and thermal Energies= -993.742915
Sum of electronic and thermal Enthalpies= -993.741971
Sum of electronic and thermal Free Energies= -993.802174
Zero-point correction= 0.271767 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -43.38
Coordinates:

| | | | |
|---|---|---|---|
| O | 0.180058 | -0.629112 | 1.042510 |
| C | 0.548523 | -0.140515 | -0.299459 |
| C | 1.789709 | 0.737171 | -0.220223 |
| S | 3.268648 | -0.077494 | 0.487875 |
| C | 3.797989 | -1.118989 | -0.918446 |

| | | | |
|---|---|---|---|
| C | -0.734873 | 0.537290 | -0.806247 |
| O | -0.831546 | 1.862157 | -0.266859 |
| C | -1.508101 | 2.808905 | -1.109916 |
| C | -1.830664 | -0.340443 | -0.163504 |
| O | -1.906590 | -1.540157 | -0.873454 |
| C | -3.079780 | -2.322238 | -0.634997 |
| C | -1.176179 | -0.576399 | 1.221813 |
| N | -1.443150 | 0.678814 | 2.123736 |
| H | 0.734343 | -1.030613 | -0.907172 |
| H | -0.801816 | 0.544403 | -1.897437 |
| H | -2.802832 | 0.173892 | -0.104797 |
| H | -1.542460 | -1.437067 | 1.785699 |
| H | -0.781857 | 0.666562 | 2.908607 |
| H | -1.244846 | 1.503137 | 1.516019 |
| H | -2.399535 | 0.735564 | 2.490713 |
| H | 2.020777 | 1.107743 | -1.226222 |
| H | 1.592616 | 1.610071 | 0.406591 |
| H | 4.726015 | -1.603265 | -0.604489 |
| H | 3.068216 | -1.898258 | -1.156249 |
| H | 4.004062 | -0.510810 | -1.804124 |
| H | -2.547545 | 2.511176 | -1.296256 |
| H | -1.488063 | 3.763780 | -0.582705 |
| H | -0.979992 | 2.909727 | -2.064002 |
| H | -3.005199 | -3.189262 | -1.291862 |
| H | -3.138058 | -2.668088 | 0.405825 |
| H | -3.985257 | -1.752278 | -0.881982 |

AMMONIA_ADDUCT_2_CONF_15

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.757742 |
| Sum of electronic and thermal Energies= | | -993.742149 |
| Sum of electronic and thermal Enthalpies= | | -993.741205 |
| Sum of electronic and thermal Free Energies= | | -993.800956 |
| Zero-point correction= | 0.271822 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.86 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.326480 | -0.861542 | 0.615648 |
| C | 0.465722 | -0.063913 | -0.623665 |
| C | 1.758604 | 0.737834 | -0.600283 |
| S | 3.288682 | -0.251185 | -0.791192 |
| C | 3.558735 | -0.868825 | 0.908731 |
| C | -0.843531 | 0.734427 | -0.684690 |
| O | -0.760348 | 1.878474 | 0.177058 |
| C | -1.521885 | 3.017129 | -0.258629 |
| C | -1.852239 | -0.270556 | -0.085769 |
| O | -2.120261 | -1.248022 | -1.044259 |
| C | -3.270271 | -2.060288 | -0.792940 |
| C | -0.973271 | -0.852395 | 1.051507 |
| N | -1.016841 | 0.139674 | 2.263660 |
| H | 0.478689 | -0.781847 | -1.447785 |
| H | -1.108554 | 1.021788 | -1.705632 |
| H | -2.768043 | 0.218593 | 0.282300 |
| H | -1.276122 | -1.825808 | 1.443216 |
| H | -1.894735 | 0.111284 | 2.793763 |
| H | -0.236623 | -0.069955 | 2.896007 |
| H | -0.882055 | 1.087340 | 1.845714 |
| H | 1.814345 | 1.365947 | 0.293423 |
| H | 1.748698 | 1.410089 | -1.465727 |
| H | 4.517581 | -1.392900 | 0.886476 |
| H | 3.635310 | -0.039849 | 1.619296 |
| H | 2.779033 | -1.567517 | 1.218025 |
| H | -1.355742 | 3.802778 | 0.479830 |
| H | -1.165795 | 3.357007 | -1.236794 |
| H | -2.592655 | 2.785772 | -0.318529 |
| H | -3.366043 | -2.723716 | -1.652783 |
| H | -3.153371 | -2.668038 | 0.114515 |
| H | -4.173093 | -1.441485 | -0.705022 |

AMMONIA_ADDUCT_2_CONF_16

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758397 |
| Sum of electronic and thermal Energies= | | -993.742620 |
| Sum of electronic and thermal Enthalpies= | | -993.741676 |
| Sum of electronic and thermal Free Energies= | | -993.802191 |
| Zero-point correction= | 0.271895 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.42 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.054950 | -0.962856 | 0.754638 |
| C | 0.333851 | -0.272480 | -0.492023 |
| C | 1.744514 | 0.270665 | -0.354176 |
| S | 2.913578 | -1.077709 | 0.088997 |
| C | 4.486816 | -0.250349 | -0.335699 |
| C | -0.797745 | 0.750346 | -0.700771 |
| O | -0.648888 | 1.900486 | 0.139127 |
| C | -0.272148 | 3.117980 | -0.523139 |
| C | -2.015882 | -0.027152 | -0.161170 |
| O | -2.368596 | -0.997053 | -1.101616 |
| C | -3.671457 | -1.562838 | -0.937197 |
| C | -1.360537 | -0.696897 | 1.072579 |
| N | -1.318316 | 0.337128 | 2.249969 |
| H | 0.288111 | -1.024776 | -1.284619 |
| H | -0.932946 | 1.031990 | -1.748163 |
| H | -2.850809 | 0.642873 | 0.091297 |
| H | -1.868756 | -1.580101 | 1.465695 |
| H | -2.223814 | 0.480200 | 2.710474 |
| H | -0.634707 | 0.014591 | 2.944268 |
| H | -0.988125 | 1.232811 | 1.832952 |
| H | 1.776209 | 1.068820 | 0.394335 |
| H | 2.040318 | 0.690405 | -1.323154 |
| H | 4.640956 | 0.650739 | 0.264570 |
| H | 4.533605 | -0.006893 | -1.401015 |
| H | 5.280545 | -0.964593 | -0.103594 |
| H | -1.017110 | 3.386948 | -1.280465 |
| H | -0.238288 | 3.891489 | 0.245385 |
| H | 0.714136 | 3.024608 | -0.989462 |
| H | -4.443636 | -0.783678 | -0.982372 |
| H | -3.806512 | -2.258286 | -1.765943 |
| H | -3.763225 | -2.113976 | 0.008470 |

AMMONIA_ADDUCT_2_CONF_17

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758429 |
| Sum of electronic and thermal Energies= | | -993.742615 |
| Sum of electronic and thermal Enthalpies= | | -993.741671 |
| Sum of electronic and thermal Free Energies= | | -993.802599 |
| Zero-point correction= | 0.271618 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.16 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.073947 | -0.645431 | 1.022654 |
| C | 0.478702 | -0.166060 | -0.312199 |
| C | 1.772424 | 0.628478 | -0.204913 |
| S | 3.181908 | -0.271186 | 0.542350 |
| C | 3.665562 | -1.367641 | -0.838233 |
| C | -0.764115 | 0.598025 | -0.808593 |
| O | -0.859840 | 1.901120 | -0.221457 |
| C | -0.615803 | 3.009020 | -1.102924 |
| C | -1.904413 | -0.240499 | -0.196949 |
| O | -2.018945 | -1.424565 | -0.929243 |
| C | -3.237309 | -2.147641 | -0.735735 |
| C | -1.281046 | -0.533670 | 1.190308 |
| N | -1.504554 | 0.708648 | 2.120607 |
| H | 0.613192 | -1.057375 | -0.931958 |
| H | -0.835739 | 0.641746 | -1.898341 |

| | | | |
|---|---|---|---|
| H | -2.849120 | 0.320770 | -0.148559 |
| H | -1.692593 | -1.389514 | 1.729868 |
| H | -2.463585 | 0.795474 | 2.474579 |
| H | -0.857751 | 0.644227 | 2.914750 |
| H | -1.263264 | 1.543473 | 1.545867 |
| H | 2.055722 | 0.979219 | -1.204785 |
| H | 1.614928 | 1.509994 | 0.422822 |
| H | 4.552067 | -1.908670 | -0.498011 |
| H | 2.888749 | -2.098944 | -1.078748 |
| H | 3.930135 | -0.789520 | -1.728471 |
| H | -1.324957 | 2.995852 | -1.938264 |
| H | -0.765161 | 3.913966 | -0.512320 |
| H | 0.409787 | 2.989539 | -1.485660 |
| H | -4.104753 | -1.527487 | -0.997111 |
| H | -3.189364 | -3.007139 | -1.404900 |
| H | -3.342257 | -2.506232 | 0.297175 |

AMMONIA_ADDUCT_2_CONF_18

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -993.761191 | |
| Sum of electronic and thermal Energies= | -993.745536 | |
| Sum of electronic and thermal Enthalpies= | -993.744592 | |
| Sum of electronic and thermal Free Energies= | -993.804823 | |
| Zero-point correction= | 0.272255 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -41.56 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.640877 | -0.876121 | -1.532611 |
| C | 0.217291 | 0.101086 | -0.832388 |
| C | 1.640144 | -0.429545 | -0.810545 |
| S | 2.737801 | 0.837707 | -0.056694 |
| C | 4.365414 | 0.088554 | -0.417589 |
| C | -0.490578 | 0.299138 | 0.516255 |
| O | -0.234937 | -0.800470 | 1.397782 |
| C | 0.363728 | -0.468596 | 2.665203 |
| C | -1.979214 | 0.198918 | 0.090743 |
| O | -2.432948 | 1.297759 | -0.643363 |
| C | -2.856892 | 2.415257 | 0.143899 |
| C | -1.869106 | -0.957857 | -0.921241 |
| N | -1.873404 | -2.303706 | -0.131340 |
| H | 0.160765 | 1.031271 | -1.404998 |
| H | -0.239700 | 1.252439 | 0.986970 |
| H | -2.630783 | -0.030585 | 0.948574 |
| H | -2.685551 | -1.011783 | -1.644000 |
| H | -1.216324 | -2.162717 | 0.667610 |
| H | -2.799866 | -2.569818 | 0.219911 |
| H | -1.518812 | -3.048800 | -0.741045 |
| H | 1.685706 | -1.364280 | -0.243866 |
| H | 1.959245 | -0.622586 | -1.839635 |
| H | 4.522625 | -0.000330 | -1.495680 |
| H | 5.115006 | 0.767963 | -0.005192 |
| H | 4.468579 | -0.887964 | 0.062697 |
| H | -0.301548 | 0.179794 | 3.247375 |
| H | 0.506816 | -1.412151 | 3.193939 |
| H | 1.329594 | 0.020281 | 2.508276 |
| H | -3.222820 | 3.160237 | -0.563105 |
| H | -3.668488 | 2.126204 | 0.824787 |
| H | -2.030053 | 2.844376 | 0.723388 |

AMMONIA_ADDUCT_2_CONF_19

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -993.762088 | |
| Sum of electronic and thermal Energies= | -993.746399 | |
| Sum of electronic and thermal Enthalpies= | -993.745455 | |
| Sum of electronic and thermal Free Energies= | -993.806056 | |
| Zero-point correction= | 0.272068 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -41.60 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.560926 | -0.238999 | -1.767635 |
| C | 0.393673 | 0.188171 | -0.719021 |
| C | 1.677880 | -0.613202 | -0.858543 |
| S | 2.952017 | -0.102378 | 0.357121 |
| C | 3.678757 | 1.358562 | -0.473451 |
| C | -0.398105 | 0.018099 | 0.583963 |
| O | -0.399045 | -1.359027 | 0.985483 |
| C | -0.167295 | -1.593251 | 2.386024 |
| C | -1.834463 | 0.378439 | 0.123521 |
| O | -2.019459 | 1.740801 | -0.130977 |
| C | -2.321635 | 2.532018 | 1.022388 |
| C | -1.833132 | -0.306799 | -1.256673 |
| N | -2.139872 | -1.824544 | -1.047498 |
| H | 0.572092 | 1.253751 | -0.888042 |
| H | -0.020209 | 0.660381 | 1.380921 |
| H | -2.597261 | -0.024981 | 0.808658 |
| H | -2.579411 | 0.072524 | -1.957635 |
| H | -3.127272 | -2.021012 | -0.849926 |
| H | -1.857044 | -2.339676 | -1.888641 |
| H | -1.548799 | -2.121892 | -0.239768 |
| H | 1.482562 | -1.671289 | -0.669926 |
| H | 2.070915 | -0.514867 | -1.874911 |
| H | 4.101792 | 1.080468 | -1.442410 |
| H | 2.958071 | 2.171344 | -0.595627 |
| H | 4.486853 | 1.704848 | 0.175588 |
| H | 0.807821 | -1.190738 | 2.677109 |
| H | -0.957068 | -1.140885 | 2.997985 |
| H | -0.172279 | -2.675447 | 2.523984 |
| H | -2.479013 | 3.547789 | 0.658619 |
| H | -3.236542 | 2.173009 | 1.512259 |
| H | -1.497023 | 2.532105 | 1.746093 |

AMMONIA_ADDUCT_2_CONF_20

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -993.759918 | |
| Sum of electronic and thermal Energies= | -993.744467 | |
| Sum of electronic and thermal Enthalpies= | -993.743523 | |
| Sum of electronic and thermal Free Energies= | -993.802813 | |
| Zero-point correction= | 0.272022 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -40.18 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.267882 | -0.986396 | 1.651350 |
| C | -0.281636 | 0.442887 | 1.378595 |
| C | -1.605530 | 0.901081 | 0.758955 |
| S | -2.015132 | 0.196756 | -0.901361 |
| C | -3.838308 | 0.075456 | -0.769638 |
| C | 1.016672 | 0.682848 | 0.554862 |
| O | 0.937129 | 1.717964 | -0.387058 |
| C | 1.240759 | 3.018773 | 0.121274 |
| C | 1.250360 | -0.663436 | -0.171123 |
| O | 2.575269 | -1.106199 | -0.263378 |
| C | 3.380306 | -0.384150 | -1.201469 |
| C | 0.499310 | -1.664997 | 0.721570 |
| N | -0.471764 | -2.510839 | -0.122635 |
| H | -0.218600 | 0.917263 | 2.362282 |
| H | 1.853996 | 0.836702 | 1.251902 |
| H | 0.793753 | -0.583115 | -1.172708 |
| H | 1.178843 | -2.371966 | 1.203574 |
| H | 0.011348 | -3.043072 | -0.855652 |
| H | -0.986316 | -3.165062 | 0.477086 |
| H | -1.161708 | -1.830946 | -0.550389 |
| H | -2.411609 | 0.619462 | 1.442953 |
| H | -1.594256 | 1.991150 | 0.673580 |
| H | -4.141022 | -0.560027 | 0.066176 |
| H | -4.269714 | 1.072788 | -0.660991 |
| H | -4.192756 | -0.359055 | -1.707375 |

| | | | |
|---|---|---|---|
| H | 0.513534 | 3.345780 | 0.876645 |
| H | 2.247255 | 3.043848 | 0.559699 |
| H | 1.199047 | 3.698237 | -0.731070 |
| H | 3.525771 | 0.656601 | -0.892057 |
| H | 2.925728 | -0.399276 | -2.201330 |
| H | 4.343429 | -0.895258 | -1.227560 |

AMMONIA_ADDUCT_2_CONF_21

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.761188 |
| Sum of electronic and thermal Energies= | | -993.745535 |
| Sum of electronic and thermal Enthalpies= | | -993.744591 |
| Sum of electronic and thermal Free Energies= | | -993.804809 |
| Zero-point correction= | 0.272258 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -41.56 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -0.641060 | -0.876297 | -1.532488 |
| C | 0.217050 | 0.101169 | -0.832573 |
| C | 1.640004 | -0.429205 | -0.810993 |
| S | 2.737753 | 0.838659 | -0.058330 |
| C | 4.365174 | 0.087533 | -0.415978 |
| C | -0.490576 | 0.299298 | 0.516196 |
| O | -0.234475 | -0.800039 | 1.397922 |
| C | 0.364775 | -0.467742 | 2.664954 |
| C | -1.979269 | 0.198610 | 0.091022 |
| O | -2.433390 | 1.297231 | -0.643183 |
| C | -2.857821 | 2.414594 | 0.144009 |
| C | -1.869092 | -0.958319 | -0.920767 |
| N | -1.872773 | -2.304037 | -0.130626 |
| H | 0.160216 | 1.031273 | -1.405292 |
| H | -0.239858 | 1.252769 | 0.986651 |
| H | -2.630614 | -0.030890 | 0.949019 |
| H | -2.685714 | -1.012623 | -1.643297 |
| H | -1.518071 | -3.049114 | -0.740287 |
| H | -1.215568 | -2.162715 | 0.668164 |
| H | -2.799072 | -2.570400 | 0.220867 |
| H | 1.685971 | -1.363566 | -0.243721 |
| H | 1.958675 | -0.622875 | -1.840100 |
| H | 5.114834 | 0.767185 | -0.004104 |
| H | 4.467077 | -0.888128 | 0.066322 |
| H | 4.523506 | -0.003585 | -1.493719 |
| H | 1.330515 | 0.021189 | 2.507420 |
| H | -0.300269 | 0.180799 | 3.247225 |
| H | 0.508165 | -1.411117 | 3.193931 |
| H | -3.223569 | 3.159587 | -0.563074 |
| H | -3.669651 | 2.125352 | 0.824538 |
| H | -2.031281 | 2.843779 | 0.723879 |

AMMONIA_ADDUCT_2_CONF_22

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.757403 |
| Sum of electronic and thermal Energies= | | -993.741663 |
| Sum of electronic and thermal Enthalpies= | | -993.740719 |
| Sum of electronic and thermal Free Energies= | | -993.801161 |
| Zero-point correction= | 0.271754 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.85 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.213960 | -0.900240 | 0.578047 |
| C | 0.389728 | -0.074498 | -0.638377 |
| C | 1.741048 | 0.622921 | -0.607331 |
| S | 3.194324 | -0.478010 | -0.792493 |
| C | 3.426238 | -1.094698 | 0.913276 |
| C | -0.862645 | 0.818304 | -0.637619 |
| O | -0.753252 | 1.893151 | 0.304659 |
| C | -0.605777 | 3.209139 | -0.253173 |
| C | -1.925936 | -0.149082 | -0.078983 |
| O | -2.251096 | -1.067231 | -1.078883 |
| C | -3.461441 | -1.799717 | -0.870043 |
| C | -1.081960 | -0.835746 | 1.023857 |
| N | -1.065151 | 0.090300 | 2.287285 |
| H | 0.336885 | -0.762381 | -1.486582 |
| H | -1.131436 | 1.181219 | -1.632899 |
| H | -2.805889 | 0.384620 | 0.309412 |
| H | -1.441429 | -1.808337 | 1.367271 |
| H | -0.304974 | -0.204976 | 2.909564 |
| H | -0.868552 | 1.050412 | 1.930602 |
| H | -1.946853 | 0.088295 | 2.811880 |
| H | 1.791665 | 1.292577 | -1.473439 |
| H | 1.841594 | 1.238645 | 0.292191 |
| H | 2.598373 | -1.730544 | 1.232294 |
| H | 4.343927 | -1.688021 | 0.893176 |
| H | 3.566942 | -0.265797 | 1.614119 |
| H | -1.460320 | 3.450273 | -0.895287 |
| H | -0.576020 | 3.901408 | 0.589388 |
| H | 0.324091 | 3.292467 | -0.824866 |
| H | -3.402526 | -2.446399 | 0.015977 |
| H | -4.317054 | -1.119126 | -0.769758 |
| H | -3.593971 | -2.423469 | -1.754393 |

AMMONIA_ADDUCT_2_CONF_23

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -993.758721 |
| Sum of electronic and thermal Energies= | | -993.743030 |
| Sum of electronic and thermal Enthalpies= | | -993.742086 |
| Sum of electronic and thermal Free Energies= | | -993.802375 |
| Zero-point correction= | 0.271872 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -43.86 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.061452 | -0.960860 | 0.774814 |
| C | 0.415170 | -0.270095 | -0.481816 |
| C | 1.789729 | 0.362328 | -0.360649 |
| S | 3.043230 | -0.911999 | 0.068077 |
| C | 4.558582 | 0.013275 | -0.365114 |
| C | -0.767545 | 0.679976 | -0.721789 |
| O | -0.611725 | 1.869573 | 0.062477 |
| C | -1.200163 | 3.048391 | -0.511320 |
| C | -1.948269 | -0.138601 | -0.152831 |
| O | -2.269276 | -1.142289 | -1.067511 |
| C | -3.532310 | -1.780883 | -0.863036 |
| C | -1.252339 | -0.745366 | 1.092960 |
| N | -1.245707 | 0.326806 | 2.237033 |
| H | 0.414306 | -1.038700 | -1.259711 |
| H | -0.904543 | 0.915021 | -1.780686 |
| H | -2.814971 | 0.493214 | 0.098157 |
| H | -1.716856 | -1.638334 | 1.516736 |
| H | -0.538873 | 0.059663 | 2.931798 |
| H | -0.959599 | 1.219089 | 1.778778 |
| H | -2.150444 | 0.446420 | 2.705603 |
| H | 2.041839 | 0.798573 | -1.334746 |
| H | 1.781118 | 1.167165 | 0.379561 |
| H | 5.397218 | -0.651661 | -0.144723 |
| H | 4.579558 | 0.265528 | -1.429154 |
| H | 4.661784 | 0.918985 | 0.239053 |
| H | -0.996105 | 3.866006 | 0.181530 |
| H | -0.737720 | 3.268052 | -1.479446 |
| H | -2.283869 | 2.935772 | -0.640869 |
| H | -4.349297 | -1.047748 | -0.892329 |
| H | -3.649725 | -2.489730 | -1.683059 |
| H | -3.566286 | -2.328516 | 0.088381 |

AMMONIA_ADDUCT_2_CONF_24

| | |
|---|---|
| Sum of electronic and zero-point Energies= | -993.762088 |
| Sum of electronic and thermal Energies= | -993.746399 |

Sum of electronic and thermal Enthalpies= -993.745455
Sum of electronic and thermal Free Energies= -993.806059
Zero-point correction= 0.272067 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -41.59
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.560994 | -0.239003 | -1.767608 |
| C | 0.393631 | 0.188173 | -0.719022 |
| C | 1.677844 | -0.613183 | -0.858599 |
| S | 2.952025 | -0.102389 | 0.357036 |
| C | 3.678675 | 1.358629 | -0.473480 |
| C | -0.398114 | 0.018078 | 0.583982 |
| O | -0.399098 | -1.359057 | 0.985476 |
| C | -0.166995 | -1.593359 | 2.385945 |
| C | -1.834478 | 0.378447 | 0.123582 |
| O | -2.019468 | 1.740810 | -0.130908 |
| C | -2.321537 | 2.532040 | 1.022476 |
| C | -1.833194 | -0.306778 | -1.256618 |
| N | -2.139975 | -1.824511 | -1.047462 |
| H | 0.572029 | 1.253756 | -0.888047 |
| H | -0.020197 | 0.660331 | 1.380952 |
| H | -2.597260 | -0.024969 | 0.808740 |
| H | -2.579478 | 0.072582 | -1.957555 |
| H | -1.857154 | -2.339638 | -1.888609 |
| H | -1.548915 | -2.121886 | -0.239732 |
| H | -3.127382 | -2.020956 | -0.849900 |
| H | 1.482539 | -1.671276 | -0.670000 |
| H | 2.070852 | -0.514818 | -1.874974 |
| H | 2.958062 | 2.171538 | -0.595239 |
| H | 4.487051 | 1.704662 | 0.175344 |
| H | 4.101335 | 1.080671 | -1.442643 |
| H | 0.808206 | -1.190887 | 2.676804 |
| H | -0.956602 | -1.141001 | 2.998126 |
| H | -0.171976 | -2.675562 | 2.523853 |
| H | -2.478977 | 3.547800 | 0.658704 |
| H | -3.236382 | 2.173020 | 1.512453 |
| H | -1.496847 | 2.532158 | 1.746092 |

AMMONIA_ADDUCT_2_CONF_25
Sum of electronic and zero-point Energies= -993.761190
Sum of electronic and thermal Energies= -993.745536
Sum of electronic and thermal Enthalpies= -993.744592
Sum of electronic and thermal Free Energies= -993.804819
Zero-point correction= 0.272255 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -41.56
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.640866 | -0.875831 | -1.532689 |
| C | 0.217253 | 0.101238 | -0.832228 |
| C | 1.640098 | -0.429416 | -0.810436 |
| S | 2.737871 | 0.837947 | -0.056937 |
| C | 4.365419 | 0.088459 | -0.417439 |
| C | -0.490690 | 0.299048 | 0.516419 |
| O | -0.235141 | -0.800679 | 1.397815 |
| C | 0.364222 | -0.469098 | 2.664987 |
| C | -1.979301 | 0.198868 | 0.090798 |
| O | -2.432990 | 1.297851 | -0.643122 |
| C | -2.857113 | 2.415137 | 0.144347 |
| C | -1.869119 | -0.957727 | -0.921384 |
| N | -1.873386 | -2.303715 | -0.131744 |
| H | 0.160771 | 1.031544 | -1.404650 |
| H | -0.239891 | 1.252288 | 0.987303 |
| H | -2.630910 | -0.030800 | 0.948553 |
| H | -2.685529 | -1.011544 | -1.644193 |
| H | -1.518781 | -3.048695 | -0.741581 |
| H | -1.216316 | -2.162869 | 0.667239 |
| H | -2.799845 | -2.569910 | 0.219456 |
| H | 1.685699 | -1.364052 | -0.243593 |
| H | 1.959069 | -0.622663 | -1.839528 |
| H | 5.115072 | 0.768160 | -0.005634 |
| H | 4.468614 | -0.887710 | 0.063547 |
| H | 4.522511 | -0.001218 | -1.495483 |
| H | -0.300551 | 0.179533 | 3.247467 |
| H | 0.507156 | -1.412730 | 3.193628 |
| H | 1.330201 | 0.019432 | 2.507681 |
| H | -2.030434 | 2.844017 | 0.724241 |
| H | -3.222756 | 3.160363 | -0.562545 |
| H | -3.668951 | 2.125926 | 0.824879 |

AMMONIA_ADDUCT_2_CONF_26
Sum of electronic and zero-point Energies= -993.761189
Sum of electronic and thermal Energies= -993.745536
Sum of electronic and thermal Enthalpies= -993.744591
Sum of electronic and thermal Free Energies= -993.804811
Zero-point correction= 0.272257 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -41.56
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.640964 | -0.875402 | -1.532787 |
| C | 0.217092 | 0.101572 | -0.832104 |
| C | 1.639980 | -0.428984 | -0.810611 |
| S | 2.737911 | 0.838457 | -0.057504 |
| C | 4.365294 | 0.088105 | -0.416945 |
| C | -0.490826 | 0.298941 | 0.516630 |
| O | -0.235274 | -0.800964 | 1.397780 |
| C | 0.365427 | -0.469872 | 2.664455 |
| C | -1.979441 | 0.198724 | 0.091019 |
| O | -2.433257 | 1.297864 | -0.642589 |
| C | -2.857482 | 2.414888 | 0.145207 |
| C | -1.869181 | -0.957581 | -0.921463 |
| N | -1.873299 | -2.303781 | -0.132164 |
| H | 0.160465 | 1.032021 | -1.404279 |
| H | -0.240164 | 1.252093 | 0.987769 |
| H | -2.630980 | -0.031228 | 0.948747 |
| H | -2.685602 | -1.011320 | -1.644263 |
| H | -1.518702 | -3.048571 | -0.742240 |
| H | -1.216175 | -2.163115 | 0.666796 |
| H | -2.799708 | -2.570125 | 0.219050 |
| H | 1.685772 | -1.363575 | -0.243699 |
| H | 1.958675 | -0.622322 | -1.839772 |
| H | 4.467882 | -0.887861 | 0.064589 |
| H | 4.522800 | -0.002204 | -1.494876 |
| H | 5.115064 | 0.767703 | -0.005184 |
| H | -0.298608 | 0.178849 | 3.247673 |
| H | 0.508505 | -1.413674 | 3.192755 |
| H | 1.331414 | 0.018388 | 2.506376 |
| H | -3.223334 | 3.160222 | -0.561462 |
| H | -3.669190 | 2.125371 | 0.825762 |
| H | -2.030803 | 2.843761 | 0.725108 |

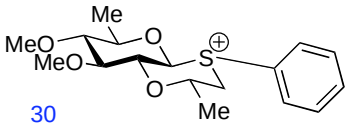
AMMONIA_ADDUCT_2_CONF_27
Sum of electronic and zero-point Energies= -993.761190
Sum of electronic and thermal Energies= -993.745536
Sum of electronic and thermal Enthalpies= -993.744592
Sum of electronic and thermal Free Energies= -993.804821
Zero-point correction= 0.272255 (Hartree/Particle)
DCMDeltaG(solv)(kcal/mol) = -41.56
Coordinates:

| | | | |
|---|---|---|---|
| O | -0.640885 | -0.876047 | -1.532607 |
| C | 0.217254 | 0.101151 | -0.832338 |
| C | 1.640115 | -0.429462 | -0.810542 |
| S | 2.737829 | 0.837893 | -0.056967 |
| C | 4.365387 | 0.088381 | -0.417356 |

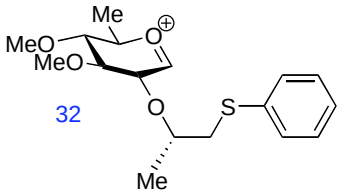
| | | | |
|---|---|---|---|
| C | -0.490627 | 0.299122 | 0.516309 |
| O | -0.234989 | -0.800509 | 1.397799 |
| C | 0.364054 | -0.468727 | 2.665067 |
| C | -1.979259 | 0.198873 | 0.090789 |
| O | -2.433055 | 1.297742 | -0.643239 |
| C | -2.856980 | 2.415192 | 0.144101 |
| C | -1.869115 | -0.957836 | -0.921259 |
| N | -1.873401 | -2.303727 | -0.131418 |
| H | 0.160707 | 1.031366 | -1.404899 |
| H | -0.239792 | 1.252416 | 0.987064 |
| H | -2.630801 | -0.030715 | 0.948617 |
| H | -2.685545 | -1.011755 | -1.644036 |
| H | -1.519039 | -3.048848 | -0.741223 |
| H | -1.216150 | -2.162842 | 0.667404 |
| H | -2.799822 | -2.569728 | 0.220027 |
| H | 1.685733 | -1.364121 | -0.243737 |
| H | 1.959115 | -0.622655 | -1.839636 |
| H | 4.468544 | -0.887777 | 0.063664 |
| H | 4.522540 | -0.001332 | -1.495388 |
| H | 5.115027 | 0.768082 | -0.005530 |
| H | 0.507310 | -1.412320 | 3.193691 |
| H | 1.329859 | 0.020192 | 2.507906 |
| H | -0.301068 | 0.179607 | 3.247478 |
| H | -2.030087 | 2.844387 | 0.723458 |
| H | -3.223099 | 3.160142 | -0.562836 |
| H | -3.668436 | 2.126053 | 0.825121 |

**Density Functional Theory Structures and Energies for Boons-type Sugar Derivatives**

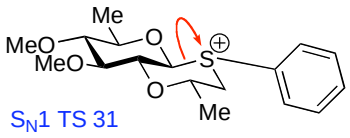
Structures of intermediates and transition states are labeled according to Figure S2



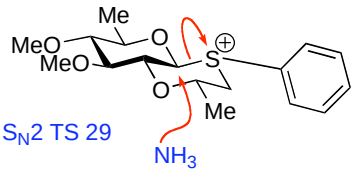

H_Ph_eq_REACTANT




H_Ph_OXACARBENIUM_CONF_X




H_Ph_eq_SN1_TS1




H_Ph_eq_NH3_SN2

**Figure S2.** Structures and file names for structures from DFT calculations. X represents the conformation number for that structure.

H_Ph_eq_REACTANT

| | | | |
|---|---|---|---|
| Sum of electronic and zero-point Energies= | | | -1361.257870 |
| Sum of electronic and thermal Energies= | | | -1361.235189 |
| Sum of electronic and thermal Enthalpies= | | | -1361.234245 |
| Sum of electronic and thermal Free Energies= | | | -1361.310133 |
| Zero-point correction= | | 0.401944 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | | = | -30.89 |
| Coordinates: | | | |
| O | 0.095727 | -1.391394 | -0.529960 |
| C | 1.204459 | -2.099340 | 0.105916 |
| C | 1.216543 | -3.502610 | -0.468465 |
| C | 2.516970 | -1.324693 | -0.129191 |
| O | 3.507893 | -1.964342 | 0.645625 |
| C | 4.778254 | -2.124745 | 0.012502 |
| C | 2.402050 | 0.157093 | 0.289714 |
| O | 3.553734 | 0.835268 | -0.155224 |
| C | 4.094757 | 1.794791 | 0.753813 |
| C | 1.139600 | 0.799129 | -0.319898 |
| C | -0.056628 | -0.115145 | -0.023025 |
| S | -1.541342 | 0.590283 | -0.919409 |
| C | -1.442312 | 2.317779 | -0.264948 |
| C | -0.022096 | 2.881951 | -0.467883 |
| O | 0.932595 | 2.089054 | 0.235207 |
| C | 0.063445 | 4.303620 | 0.075222 |
| C | -2.986925 | -0.149980 | -0.164149 |
| C | -3.232456 | -0.087469 | 1.212965 |
| C | -4.377915 | -0.700543 | 1.714809 |
| C | -5.257762 | -1.363188 | 0.852157 |
| C | -4.998691 | -1.419287 | -0.517865 |
| C | -3.856035 | -0.811157 | -1.039261 |
| H | 1.009492 | -2.133110 | 1.188469 |
| H | 2.761997 | -1.362188 | -1.201092 |
| H | 2.322928 | 0.195139 | 1.386789 |
| H | 0.220597 | 2.877763 | -1.541655 |
| H | 1.355064 | -3.474845 | -1.554282 |
| H | 2.038995 | -4.065247 | -0.020286 |
| H | 0.276915 | -4.017106 | -0.248544 |
| H | 5.418432 | -2.627156 | 0.740623 |
| H | 4.696175 | -2.752762 | -0.885635 |
| H | 5.214110 | -1.158483 | -0.259407 |
| H | 4.991749 | 2.193597 | 0.275707 |
| H | 3.389437 | 2.610512 | 0.945717 |
| H | 4.374092 | 1.320788 | 1.704234 |
| H | 1.288122 | 0.866739 | -1.408497 |
| H | -0.299494 | -0.096983 | 1.051417 |
| H | -2.194746 | 2.884978 | -0.819635 |
| H | -1.703289 | 2.300359 | 0.795948 |
| H | -0.155961 | 4.322932 | 1.147410 |
| H | 1.075760 | 4.686736 | -0.077090 |
| H | -0.638392 | 4.963744 | -0.443499 |
| H | -2.552432 | 0.421509 | 1.889280 |
| H | -4.583290 | -0.661512 | 2.779925 |
| H | -6.148176 | -1.837600 | 1.253026 |
| H | -5.682052 | -1.935373 | -1.184557 |
| H | -3.645681 | -0.852864 | -2.103491 |

H_Ph_eq_NH3_SN2

| | | | |
|---|---|---|---|
| Sum of electronic and zero-point Energies= | | | -1417.768685 |
| Sum of electronic and thermal Energies= | | | -1417.741959 |
| Sum of electronic and thermal Enthalpies= | | | -1417.741015 |
| Sum of electronic and thermal Free Energies= | | | -1417.828282 |
| Zero-point correction= | | 0.437553 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | | = | -25.49 |
| Coordinates: | | | |
| O | 0.543243 | -1.590972 | 0.899694 |
| C | 1.724737 | -2.262312 | 0.274669 |
| C | 1.205258 | -3.277846 | -0.725492 |
| C | 2.798668 | -1.290396 | -0.282221 |
| O | 4.021409 | -1.833042 | 0.162469 |
| C | 5.120932 | -1.720640 | -0.746042 |
| C | 2.609059 | 0.178731 | 0.150070 |
| O | 3.464101 | 0.968622 | -0.633521 |

| | | | |
|---|---|---|---|
| C | 3.992610 | 2.127168 | 0.015860 |
| C | 1.125747 | 0.526250 | -0.148570 |
| C | 0.264329 | -0.357458 | 0.709559 |
| S | -1.727539 | 0.085980 | -0.954808 |
| C | -1.568518 | 1.906904 | -0.635249 |
| C | -0.144901 | 2.431699 | -0.875951 |
| O | 0.800638 | 1.875868 | 0.062532 |
| C | -0.091367 | 3.945153 | -0.701666 |
| C | -3.376632 | -0.275729 | -0.346848 |
| C | -3.756001 | -0.006290 | 0.974677 |
| C | -5.041478 | -0.335509 | 1.401249 |
| C | -5.939294 | -0.946438 | 0.521681 |
| C | -5.553113 | -1.225204 | -0.789899 |
| C | -4.272512 | -0.888543 | -1.231393 |
| H | 2.164519 | -2.756792 | 1.142005 |
| H | 2.756509 | -1.297913 | -1.382726 |
| H | 2.818619 | 0.287272 | 1.220708 |
| H | 0.181126 | 2.165706 | -1.892173 |
| H | 0.714204 | -2.791823 | -1.575359 |
| H | 2.053958 | -3.857224 | -1.102892 |
| H | 0.500808 | -3.967946 | -0.253589 |
| H | 5.946493 | -2.265147 | -0.284025 |
| H | 4.879017 | -2.184451 | -1.712432 |
| H | 5.405936 | -0.677729 | -0.908731 |
| H | 4.642031 | 2.613704 | -0.714323 |
| H | 3.196475 | 2.816143 | 0.315384 |
| H | 4.587679 | 1.845420 | 0.895091 |
| H | 0.986590 | 0.262562 | -1.208244 |
| H | -2.273015 | 2.411970 | -1.302179 |
| H | -1.862671 | 2.110364 | 0.398789 |
| H | -0.396658 | 4.231551 | 0.310031 |
| H | 0.928053 | 4.302322 | -0.870772 |
| H | -0.753270 | 4.439437 | -1.418877 |
| H | -3.061295 | 0.457747 | 1.669434 |
| H | -5.339741 | -0.121628 | 2.423332 |
| H | -6.938056 | -1.204654 | 0.860389 |
| H | -6.249347 | -1.697586 | -1.476253 |
| H | -3.973454 | -1.092172 | -2.254980 |
| H | -0.412581 | 0.066934 | 1.436297 |
| N | 1.167220 | 0.743471 | 3.261303 |
| H | 1.267796 | 1.752461 | 3.151720 |
| H | 0.447092 | 0.609153 | 3.971885 |
| H | 2.032996 | 0.421281 | 3.694302 |

H_Ph_eq_SN1_TS1

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1361.226466 |
| Sum of electronic and thermal Energies= | | -1361.203295 |
| Sum of electronic and thermal Enthalpies= | | -1361.202351 |
| Sum of electronic and thermal Free Energies= | | -1361.282504 |
| Zero-point correction= | 0.399283 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -31.17 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -2.419152 | -1.816252 | -1.678724 |
| C | -3.673364 | -1.679540 | -0.807580 |
| C | -4.041767 | -3.085912 | -0.394178 |
| C | -3.448680 | -0.673365 | 0.332483 |
| O | -4.742934 | -0.331361 | 0.766677 |
| C | -4.938287 | -0.344728 | 2.188426 |
| C | -2.684155 | 0.573517 | -0.150631 |
| O | -2.464781 | 1.466379 | 0.905972 |
| C | -3.210650 | 2.690324 | 0.839938 |
| C | -1.303462 | 0.129627 | -0.692887 |
| C | -1.437112 | -1.032246 | -1.614999 |
| S | 2.454438 | 0.667615 | 0.957933 |
| C | 1.726576 | 0.782208 | -0.734072 |
| C | 0.506045 | 1.728182 | -0.693423 |
| O | -0.633193 | 1.134081 | -1.395345 |
| C | 0.768462 | 3.067091 | -1.359744 |
| C | 4.003814 | -0.176595 | 0.614708 |
| C | 4.109253 | -1.556929 | 0.826854 |
| C | 5.322829 | -2.205692 | 0.593243 |
| C | 6.429402 | -1.481485 | 0.146165 |
| C | 6.326530 | -0.103780 | -0.059943 |
| C | 5.119122 | 0.552283 | 0.180185 |
| H | -4.389328 | -1.267550 | -1.523243 |
| H | -2.873084 | -1.151072 | 1.139891 |
| H | -3.241694 | 1.049756 | -0.969242 |
| H | 0.179130 | 1.884797 | 0.342237 |
| H | -3.281714 | -3.525963 | 0.258875 |
| H | -4.986833 | -3.033989 | 0.154560 |
| H | -4.186739 | -3.729079 | -1.265878 |
| H | -5.974665 | -0.044976 | 2.350230 |
| H | -4.784125 | -1.352120 | 2.596149 |
| H | -4.264599 | 0.360168 | 2.685492 |
| H | -2.927613 | 3.262529 | 1.724625 |
| H | -2.948022 | 3.258277 | -0.060987 |
| H | -4.288512 | 2.497268 | 0.853511 |
| H | -0.718580 | -0.235941 | 0.176011 |
| H | -0.652534 | -1.227993 | -2.349915 |
| H | 2.482651 | 1.151060 | -1.432839 |
| H | 1.436637 | -0.219384 | -1.073343 |
| H | 1.006951 | 2.931035 | -2.419808 |
| H | -0.101925 | 3.724045 | -1.277577 |
| H | 1.619004 | 3.554683 | -0.872939 |
| H | 3.248508 | -2.114732 | 1.183864 |
| H | 5.404065 | -3.275429 | 0.764102 |
| H | 7.373340 | -1.987945 | -0.033267 |
| H | 7.189775 | 0.463327 | -0.396221 |
| H | 5.042043 | 1.626838 | 0.042850 |

H_Ph_eq_SN1_TS2

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1361.220043 |
| Sum of electronic and thermal Energies= | | -1361.196729 |
| Sum of electronic and thermal Enthalpies= | | -1361.195785 |
| Sum of electronic and thermal Free Energies= | | -1361.276910 |
| Zero-point correction= | 0.399036 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -34.08 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 2.385184 | 2.004953 | -1.359154 |
| C | 3.752862 | 1.737804 | -0.718054 |
| C | 4.265484 | 3.087631 | -0.271473 |
| C | 3.643949 | 0.656881 | 0.369106 |
| O | 4.967832 | 0.234050 | 0.590784 |
| C | 5.366264 | 0.152513 | 1.966975 |
| C | 2.763889 | -0.520861 | -0.090995 |
| O | 2.654412 | -1.491411 | 0.914737 |
| C | 3.367042 | -2.712840 | 0.667216 |
| C | 1.341273 | 0.002895 | -0.398599 |
| C | 1.386721 | 1.257081 | -1.206553 |
| S | -3.301135 | -1.312801 | -0.694415 |
| C | -1.672174 | -0.708618 | -0.047633 |
| C | -0.466939 | -1.634417 | -0.370375 |
| O | 0.557784 | -0.896968 | -1.122892 |
| C | -0.755383 | -2.865222 | -1.215354 |
| C | -4.370485 | -0.059152 | 0.024229 |
| C | -4.856865 | -0.213255 | 1.329592 |
| C | -5.714738 | 0.745101 | 1.870318 |
| C | -6.098205 | 1.851727 | 1.109187 |
| C | -5.623976 | 2.000559 | -0.195613 |
| C | -4.760693 | 1.048225 | -0.740027 |

| | | | |
|---|---|---|---|
| H | 4.320333 | 1.350042 | -1.567844 |
| H | 3.209340 | 1.093289 | 1.281354 |
| H | 3.180899 | -0.946675 | -1.014319 |
| H | 0.006925 | -1.941977 | 0.568534 |
| H | 3.645177 | 3.511129 | 0.524511 |
| H | 5.280086 | 2.946831 | 0.112771 |
| H | 4.310333 | 3.789671 | -1.107915 |
| H | 6.397120 | -0.204332 | 1.958948 |
| H | 5.328064 | 1.139061 | 2.446615 |
| H | 4.733713 | -0.549971 | 2.518895 |
| H | 3.186007 | -3.347597 | 1.535854 |
| H | 2.985214 | -3.209715 | -0.233058 |
| H | 4.440974 | -2.529152 | 0.560001 |
| H | 0.881198 | 0.286611 | 0.568305 |
| H | 0.502828 | 1.558832 | -1.773930 |
| H | -1.493814 | 0.282928 | -0.478196 |
| H | -1.773241 | -0.584642 | 1.034542 |
| H | -1.158915 | -2.587534 | -2.193285 |
| H | 0.165346 | -3.436013 | -1.365252 |
| H | -1.483913 | -3.506321 | -0.711390 |
| H | -4.574789 | -1.087289 | 1.909467 |
| H | -6.093763 | 0.620400 | 2.880741 |
| H | -6.774196 | 2.591216 | 1.528911 |
| H | -5.931955 | 2.853774 | -0.793543 |
| H | -4.400678 | 1.150945 | -1.759537 |

H_Ph_OXACARBENIUM_CONF_3

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -1361.226769 | |
| Sum of electronic and thermal Energies= | -1361.202649 | |
| Sum of electronic and thermal Enthalpies= | -1361.201704 | |
| Sum of electronic and thermal Free Energies= | -1361.285991 | |
| Zero-point correction= | 0.399390 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -31.60 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -1.979205 | -1.622044 | 1.498974 |
| C | -2.561482 | -1.862130 | 0.116176 |
| C | -3.150112 | -3.252516 | 0.151441 |
| C | -3.554832 | -0.731282 | -0.188432 |
| O | -4.049102 | -0.993623 | -1.474813 |
| C | -5.436984 | -0.698441 | -1.681750 |
| C | -2.892194 | 0.661596 | -0.122027 |
| O | -3.934720 | 1.589488 | 0.063076 |
| C | -3.674007 | 2.905629 | -0.425112 |
| C | -1.851394 | 0.757503 | 1.021875 |
| C | -1.725876 | -0.447996 | 1.887849 |
| S | 2.211371 | -0.094320 | -0.566894 |
| C | 1.848688 | 0.724141 | 1.053842 |
| C | 0.540900 | 1.510502 | 1.025210 |
| O | -0.499728 | 0.565111 | 0.573934 |
| C | 0.530869 | 2.728103 | 0.110820 |
| C | 3.997864 | -0.267315 | -0.445846 |
| C | 4.836122 | 0.782376 | -0.844723 |
| C | 6.221025 | 0.629818 | -0.774564 |
| C | 6.771894 | -0.570398 | -0.319481 |
| C | 5.937194 | -1.621041 | 0.065436 |
| C | 4.550564 | -1.473051 | 0.003368 |
| H | -1.684807 | -1.804948 | -0.535683 |
| H | -4.355899 | -0.760759 | 0.567877 |
| H | -2.352421 | 0.828259 | -1.065510 |
| H | 0.293873 | 1.808657 | 2.053770 |
| H | -3.988347 | -3.313074 | 0.852647 |
| H | -3.514065 | -3.491798 | -0.850541 |
| H | -2.391839 | -3.987914 | 0.432637 |
| H | -5.650821 | -0.981030 | -2.713513 |
| H | -6.067570 | -1.289430 | -1.004624 |
| H | -5.642061 | 0.366116 | -1.536104 |
| H | -4.594461 | 3.473632 | -0.282720 |
| H | -2.866156 | 3.398745 | 0.134320 |
| H | -3.413720 | 2.886284 | -1.491131 |
| H | -1.980828 | 1.675798 | 1.600613 |
| H | -1.271540 | -0.389947 | 2.877643 |
| H | 1.811676 | -0.029581 | 1.847508 |
| H | 2.662622 | 1.417451 | 1.284952 |
| H | 0.764394 | 2.443209 | -0.917418 |
| H | -0.438475 | 3.236811 | 0.133578 |
| H | 1.286029 | 3.443219 | 0.454403 |
| H | 3.897247 | -2.289669 | 0.295316 |
| H | 7.850548 | -0.688634 | -0.272076 |
| H | 6.363937 | -2.557683 | 0.412627 |
| H | 6.869211 | 1.444266 | -1.085217 |
| H | 4.404136 | 1.706697 | -1.216918 |

H_Ph_OXACARBENIUM_CONF_4

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -1361.223075 | |
| Sum of electronic and thermal Energies= | -1361.199254 | |
| Sum of electronic and thermal Enthalpies= | -1361.198310 | |
| Sum of electronic and thermal Free Energies= | -1361.279804 | |
| Zero-point correction= | 0.399355 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -34.23 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 3.613754 | -2.005581 | -0.081449 |
| C | 4.359240 | -0.793260 | 0.479659 |
| C | 5.821623 | -1.046734 | 0.193208 |
| C | 3.783382 | 0.513310 | -0.083646 |
| O | 4.321162 | 1.503426 | 0.755650 |
| C | 4.776767 | 2.698879 | 0.103483 |
| C | 2.239534 | 0.559823 | -0.057809 |
| O | 1.856887 | 1.740012 | -0.702667 |
| C | 0.747487 | 2.456881 | -0.141264 |
| C | 1.677910 | -0.675515 | -0.820952 |
| C | 2.462796 | -1.926410 | -0.579057 |
| S | -2.473216 | 0.214855 | -0.768723 |
| C | -1.845665 | -1.255911 | 0.158311 |
| C | -0.365435 | -1.111659 | 0.500588 |
| O | 0.304791 | -0.952139 | -0.782918 |
| C | 0.154885 | -2.317144 | 1.279987 |
| C | -4.188088 | 0.246695 | -0.226171 |
| C | -4.537025 | 0.827361 | 1.000852 |
| C | -5.874548 | 0.871668 | 1.394258 |
| C | -6.867839 | 0.352728 | 0.560270 |
| C | -6.522821 | -0.212534 | -0.668419 |
| C | -5.185057 | -0.268242 | -1.063899 |
| H | 4.137970 | -0.867145 | 1.547934 |
| H | 4.116884 | 0.643510 | -1.124829 |
| H | 1.916294 | 0.546286 | 0.992506 |
| H | -0.223694 | -0.195655 | 1.086108 |
| H | 6.024414 | -1.051377 | -0.882263 |
| H | 6.395944 | -0.238688 | 0.654503 |
| H | 6.149507 | -1.994731 | 0.627147 |
| H | 3.955351 | 3.197856 | -0.416522 |
| H | 5.163016 | 3.339827 | 0.897324 |
| H | 5.583610 | 2.472924 | -0.605884 |
| H | 0.692400 | 3.395822 | -0.694229 |
| H | -0.192863 | 1.910514 | -0.266040 |
| H | 0.923834 | 2.673749 | 0.920371 |
| H | 1.882504 | -0.462485 | -1.889289 |
| H | 2.039281 | -2.883479 | -0.893413 |
| H | -2.414979 | -1.342357 | 1.087682 |
| H | -2.001273 | -2.165929 | -0.430567 |
| H | 0.005952 | -3.247911 | 0.722366 |

| | | | |
|---|---|---|---|
| H | 1.219931 | -2.219661 | 1.540370 |
| H | -0.375758 | -2.406523 | 2.233657 |
| H | -4.911955 | -0.704872 | -2.019639 |
| H | -7.909428 | 0.395483 | 0.865335 |
| H | -7.293993 | -0.611354 | -1.321244 |
| H | -6.142162 | 1.322421 | 2.345803 |
| H | -3.764958 | 1.250728 | 1.637059 |

H_Ph_OXACARBENIUM_CONF_8

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -1361.229255 | |
| Sum of electronic and thermal Energies= | -1361.205387 | |
| Sum of electronic and thermal Enthalpies= | -1361.204443 | |
| Sum of electronic and thermal Free Energies= | -1361.285992 | |
| Zero-point correction= | 0.399935 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -28.86 |

Coordinates:

| | | | |
|---|---|---|---|
| O | -1.189285 | -1.772954 | -0.610107 |
| C | -2.615361 | -1.467859 | -1.022608 |
| C | -3.266388 | -2.807236 | -1.279306 |
| C | -3.277932 | -0.608798 | 0.064088 |
| O | -4.564753 | -0.323012 | -0.417570 |
| C | -5.614491 | -0.332706 | 0.559683 |
| C | -2.492372 | 0.690341 | 0.330107 |
| O | -2.962721 | 1.201515 | 1.553232 |
| C | -2.835953 | 2.615497 | 1.707872 |
| C | -0.964334 | 0.443132 | 0.376499 |
| C | -0.515645 | -0.941343 | 0.063306 |
| S | 3.715454 | 1.154565 | -1.334412 |
| C | 1.926136 | 1.113228 | -1.759700 |
| C | 1.045273 | 1.555756 | -0.589167 |
| O | -0.285015 | 0.933801 | -0.794695 |
| C | 0.863455 | 3.061174 | -0.476152 |
| C | 3.753190 | -0.150790 | -0.095483 |
| C | 3.427901 | -1.475327 | -0.431673 |
| C | 3.472244 | -2.474943 | 0.542549 |
| C | 3.867470 | -2.167378 | 1.848828 |
| C | 4.215918 | -0.857169 | 2.177783 |
| C | 4.150916 | 0.152508 | 1.213149 |
| H | -2.490598 | -0.893623 | -1.945736 |
| H | -3.314180 | -1.189492 | 1.000025 |
| H | -2.685192 | 1.381209 | -0.503660 |
| H | 1.451123 | 1.143663 | 0.341479 |
| H | -3.331647 | -3.400265 | -0.361674 |
| H | -4.277098 | -2.627772 | -1.653249 |
| H | -2.710279 | -3.371682 | -2.032349 |
| H | -5.446608 | 0.427712 | 1.327498 |
| H | -6.532302 | -0.113540 | 0.012137 |
| H | -5.700495 | -1.320344 | 1.031596 |
| H | -3.301636 | 2.862987 | 2.662823 |
| H | -1.783413 | 2.931624 | 1.735358 |
| H | -3.350371 | 3.148106 | 0.897714 |
| H | -0.533940 | 0.824227 | 1.306253 |
| H | 0.505543 | -1.262953 | 0.281595 |
| H | 1.801204 | 1.774966 | -2.622296 |
| H | 1.651706 | 0.103422 | -2.076511 |
| H | 0.363856 | 3.456310 | -1.366141 |
| H | 0.278678 | 3.334607 | 0.408085 |
| H | 1.846607 | 3.534924 | -0.388536 |
| H | 4.416567 | 1.173585 | 1.470304 |
| H | 3.920143 | -2.950415 | 2.599584 |
| H | 4.537343 | -0.615154 | 3.186767 |
| H | 3.234869 | -3.500642 | 0.272721 |
| H | 3.176866 | -1.727832 | -1.458732 |

H_Ph_OXACARBENIUM_CONF_9

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -1361.228945 | |
| Sum of electronic and thermal Energies= | -1361.205042 | |
| Sum of electronic and thermal Enthalpies= | -1361.204098 | |
| Sum of electronic and thermal Free Energies= | -1361.286141 | |
| Zero-point correction= | 0.399652 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -29.13 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 2.648264 | -1.575799 | -1.347651 |
| C | 3.648222 | -1.006927 | -0.350415 |
| C | 5.013753 | -1.334326 | -0.905297 |
| C | 3.344025 | 0.488707 | -0.172651 |
| O | 4.285607 | 0.958411 | 0.754680 |
| C | 4.774053 | 2.287716 | 0.527089 |
| C | 1.901656 | 0.730105 | 0.321976 |
| O | 1.578787 | 2.059768 | -0.006507 |
| C | 0.566909 | 2.653787 | 0.808189 |
| C | 0.893202 | -0.265174 | -0.307547 |
| C | 1.450606 | -1.182376 | -1.341034 |
| S | -3.500147 | -1.900766 | 0.051390 |
| C | -1.684667 | -2.054848 | -0.216790 |
| C | -0.859147 | -1.499269 | 0.946824 |
| O | 0.561474 | -1.357272 | 0.563085 |
| C | -0.849704 | -2.389025 | 2.177128 |
| C | -3.702652 | -0.128064 | -0.192179 |
| C | -3.865619 | 0.718926 | 0.912848 |
| C | -4.060253 | 2.089047 | 0.719354 |
| C | -4.090865 | 2.617242 | -0.572772 |
| C | -3.936958 | 1.773347 | -1.676025 |
| C | -3.751666 | 0.402877 | -1.489616 |
| H | 3.432666 | -1.564928 | 0.565178 |
| H | 3.455885 | 0.984156 | -1.150869 |
| H | 1.884550 | 0.559261 | 1.408664 |
| H | -1.208637 | -0.489164 | 1.192658 |
| H | 5.192220 | -0.819430 | -1.854453 |
| H | 5.761563 | -1.001902 | -0.181422 |
| H | 5.125358 | -2.411514 | -1.053999 |
| H | 3.965138 | 3.021964 | 0.581127 |
| H | 5.502291 | 2.476523 | 1.317078 |
| H | 5.270026 | 2.359485 | -0.449743 |
| H | 0.478125 | 3.689931 | 0.478681 |
| H | -0.407736 | 2.159949 | 0.683325 |
| H | 0.851220 | 2.628322 | 1.868258 |
| H | 0.007941 | 0.259817 | -0.678904 |
| H | 0.810921 | -1.671319 | -2.076313 |
| H | -1.482633 | -3.122700 | -0.352949 |
| H | -1.445050 | -1.539927 | -1.154617 |
| H | -0.418616 | -3.367835 | 1.942044 |
| H | -0.270211 | -1.933735 | 2.984604 |
| H | -1.876868 | -2.537077 | 2.522928 |
| H | -3.669368 | -0.260137 | -2.346480 |
| H | -4.251476 | 3.681171 | -0.721429 |
| H | -3.983573 | 2.178984 | -2.682774 |
| H | -4.199935 | 2.739337 | 1.578344 |
| H | -3.859871 | 0.301694 | 1.915486 |

H_Ph_OXACARBENIUM_CONF_14

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | -1361.211367 | |
| Sum of electronic and thermal Energies= | -1361.187704 | |
| Sum of electronic and thermal Enthalpies= | -1361.186760 | |
| Sum of electronic and thermal Free Energies= | -1361.266921 | |
| Zero-point correction= | 0.399271 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -31.54 |

Coordinates:

| | | | |
|---|---|---|---|
| O | 0.769959 | -1.014457 | -2.287181 |

| | | | |
|---|---|---|---|
| C | 0.419818 | -2.108883 | -1.272073 |
| C | 0.350937 | -3.390048 | -2.069443 |
| C | 1.447915 | -2.102712 | -0.125230 |
| O | 1.091755 | -3.109207 | 0.786302 |
| C | 0.142659 | -2.797624 | 1.810077 |
| C | 1.634232 | -0.691602 | 0.471267 |
| O | 2.629255 | -0.796935 | 1.445226 |
| C | 2.645234 | 0.205097 | 2.471278 |
| C | 2.083580 | 0.271149 | -0.670912 |
| C | 1.410955 | 0.024040 | -1.974871 |
| S | -0.921490 | 2.168038 | 0.763042 |
| C | -0.150617 | 2.327912 | -0.897713 |
| C | 1.349018 | 2.655447 | -0.857141 |
| O | 2.157663 | 1.613109 | -0.261291 |
| C | 1.689275 | 3.919803 | -0.078892 |
| C | -2.258529 | 1.020546 | 0.432232 |
| C | -2.997453 | 1.024245 | -0.759568 |
| C | -4.050290 | 0.122074 | -0.929257 |
| C | -4.393398 | -0.766313 | 0.091176 |
| C | -3.673328 | -0.753974 | 1.287977 |
| C | -2.603339 | 0.126119 | 1.458003 |
| H | -0.568034 | -1.781940 | -0.933194 |
| H | 2.417076 | -2.423182 | -0.531512 |
| H | 0.693494 | -0.305411 | 0.888028 |
| H | 1.672360 | 2.799932 | -1.899885 |
| H | 1.325692 | -3.643660 | -2.497732 |
| H | 0.060750 | -4.193578 | -1.387505 |
| H | -0.391191 | -3.319988 | -2.868645 |
| H | -0.793394 | -2.383736 | 1.411645 |
| H | -0.072339 | -3.748415 | 2.300001 |
| H | 0.569003 | -2.106588 | 2.544451 |
| H | 3.332521 | -0.164884 | 3.233572 |
| H | 2.997685 | 1.166620 | 2.088095 |
| H | 1.646918 | 0.332850 | 2.909151 |
| H | 3.125588 | -0.039218 | -0.911054 |
| H | 1.529782 | 0.726333 | -2.802454 |
| H | -0.349849 | 1.390704 | -1.440260 |
| H | -0.641698 | 3.117313 | -1.477394 |
| H | 1.402308 | 3.824678 | 0.972360 |
| H | 2.764677 | 4.108348 | -0.128914 |
| H | 1.164411 | 4.778123 | -0.509223 |
| H | -2.045923 | 0.132191 | 2.390760 |
| H | -5.223948 | -1.453248 | -0.039665 |
| H | -3.942808 | -1.430610 | 2.094006 |
| H | -4.618546 | 0.134503 | -1.855056 |
| H | -2.779773 | 1.742519 | -1.544146 |

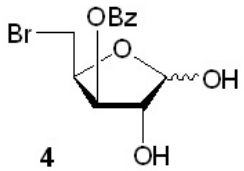
H_Ph_OXACARBENIUM_CONF_15

| | | |
|---|---|---|
| Sum of electronic and zero-point Energies= | | -1361.230385 |
| Sum of electronic and thermal Energies= | | -1361.206453 |
| Sum of electronic and thermal Enthalpies= | | -1361.205509 |
| Sum of electronic and thermal Free Energies= | | -1361.287784 |
| Zero-point correction= | 0.399899 | (Hartree/Particle) |
| DCMDeltaG(solv)(kcal/mol) | = | -30.62 |

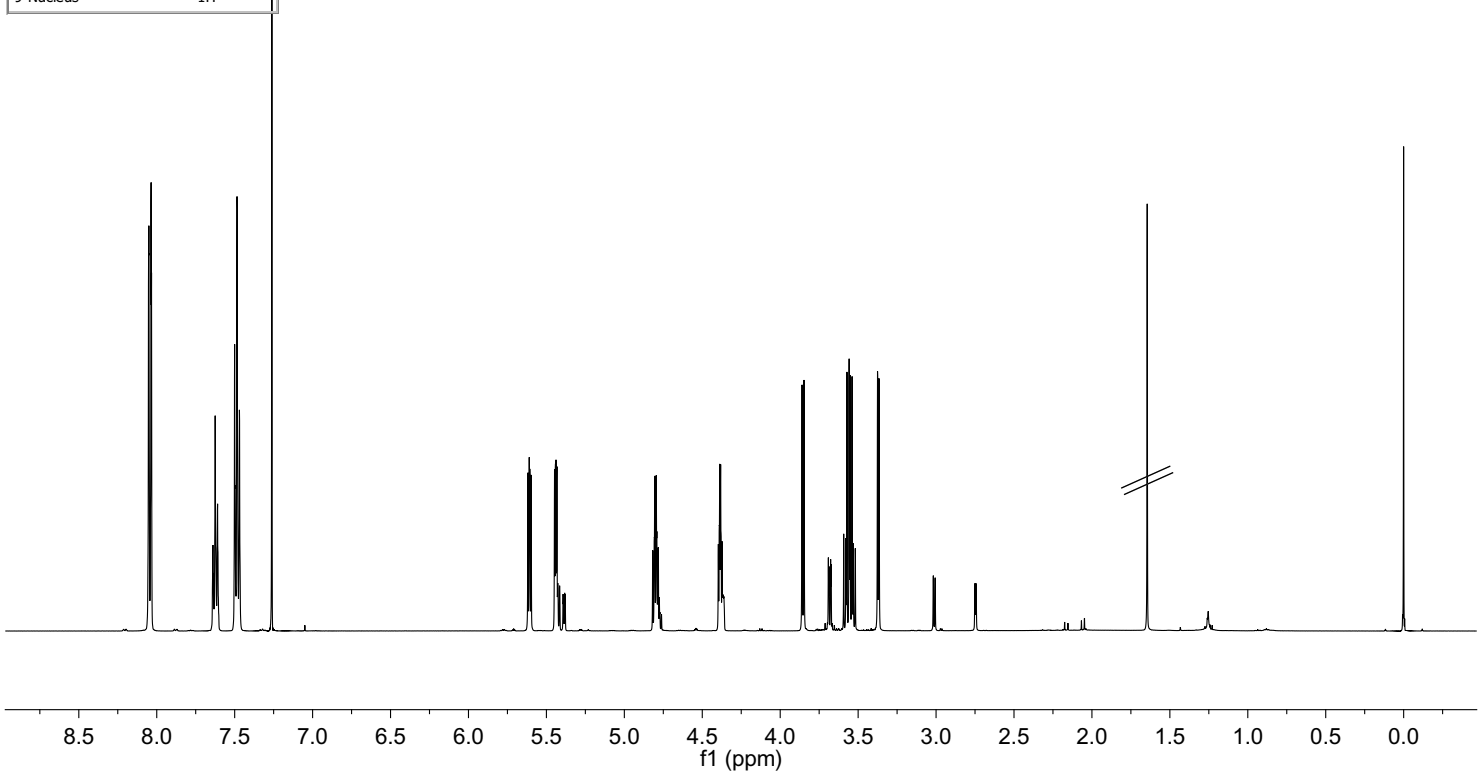
Coordinates:

| | | | |
|---|---|---|---|
| O | 1.210089 | 1.910807 | -0.734490 |
| C | 2.737195 | 1.834749 | -0.699912 |
| C | 3.204231 | 3.204268 | -0.261464 |
| C | 3.203486 | 0.651808 | 0.162757 |
| O | 4.560569 | 0.485783 | -0.165721 |
| C | 5.441579 | 0.262347 | 0.944421 |
| C | 2.403945 | -0.622900 | -0.161910 |
| O | 2.837966 | -1.690728 | 0.638011 |
| C | 3.367695 | -2.814352 | -0.077542 |
| C | 0.911578 | -0.375728 | 0.120905 |
| C | 0.462517 | 0.984430 | -0.327314 |
| S | -3.883385 | -1.646011 | -0.423269 |
| C | -2.173838 | -1.914302 | -1.049135 |
| C | -1.113861 | -1.723419 | 0.041291 |
| O | 0.098766 | -1.242975 | -0.634638 |
| C | -0.789786 | -2.981858 | 0.833850 |
| C | -3.771059 | 0.099275 | 0.000867 |
| C | -3.475430 | 1.066142 | -0.974576 |
| C | -3.394384 | 2.415322 | -0.621958 |
| C | -3.635587 | 2.813975 | 0.697499 |
| C | -3.956465 | 1.858075 | 1.661795 |
| C | -4.014509 | 0.503739 | 1.319997 |
| H | 2.977012 | 1.643044 | -1.748984 |
| H | 3.077174 | 0.899814 | 1.228370 |
| H | 2.521773 | -0.846307 | -1.230998 |
| H | -1.446393 | -0.925328 | 0.717195 |
| H | 2.892893 | 3.425835 | 0.764106 |
| H | 4.297077 | 3.211719 | -0.305084 |
| H | 2.827550 | 3.982546 | -0.929998 |
| H | 5.156606 | -0.637639 | 1.497170 |
| H | 6.436284 | 0.135634 | 0.514650 |
| H | 5.446587 | 1.126811 | 1.621216 |
| H | 3.653701 | -3.546275 | 0.679440 |
| H | 2.609443 | -3.250782 | -0.738597 |
| H | 4.249585 | -2.528495 | -0.662166 |
| H | 0.752796 | -0.474314 | 1.206139 |
| H | -0.607077 | 1.200215 | -0.420867 |
| H | -2.156699 | -2.932428 | -1.449731 |
| H | -1.975597 | -1.230617 | -1.878612 |
| H | -0.433241 | -3.771806 | 0.165239 |
| H | -0.021179 | -2.796210 | 1.592044 |
| H | -1.691840 | -3.335526 | 1.343633 |
| H | -4.253989 | -0.240958 | 2.073198 |
| H | -3.593482 | 3.865965 | 0.964611 |
| H | -4.159818 | 2.162055 | 2.684712 |
| H | -3.183352 | 3.159365 | -1.385832 |
| H | -3.344610 | 0.767331 | -2.011268 |

| Parameter | Value |
|---|---|
| 1 Title | Sam43295 |
| 2 Spectrometer | avance500 |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg30 |
| 6 Number of Scans | 512 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |

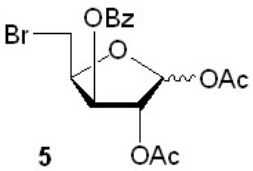



**4**



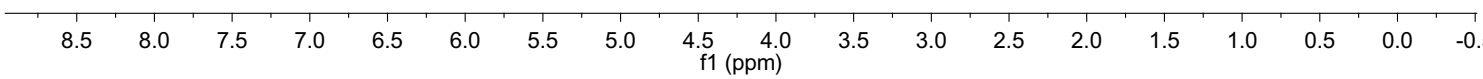



| Parameter | Value |
|---|---|
| 1 Title | Sam43296 |
| 2 Spectrometer | avance500 |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg30 |
| 6 Number of Scans | 512 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |

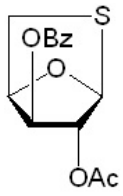



**5**





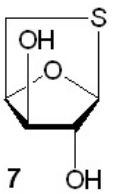
| Parameter | Value |
|---|---|
| 1 Title | Sam44713 |
| 2 Spectrometer | avance500 |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg30 |
| 6 Number of Scans | 32 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |




**6**

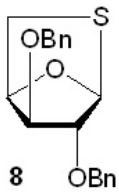



| Parameter | Value |
|---|---|
| 1 Title | Sam45613 |
| 2 Spectrometer | avance500 |
| 3 Solvent | D2O |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg0f2pr |
| 6 Number of Scans | 64 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |

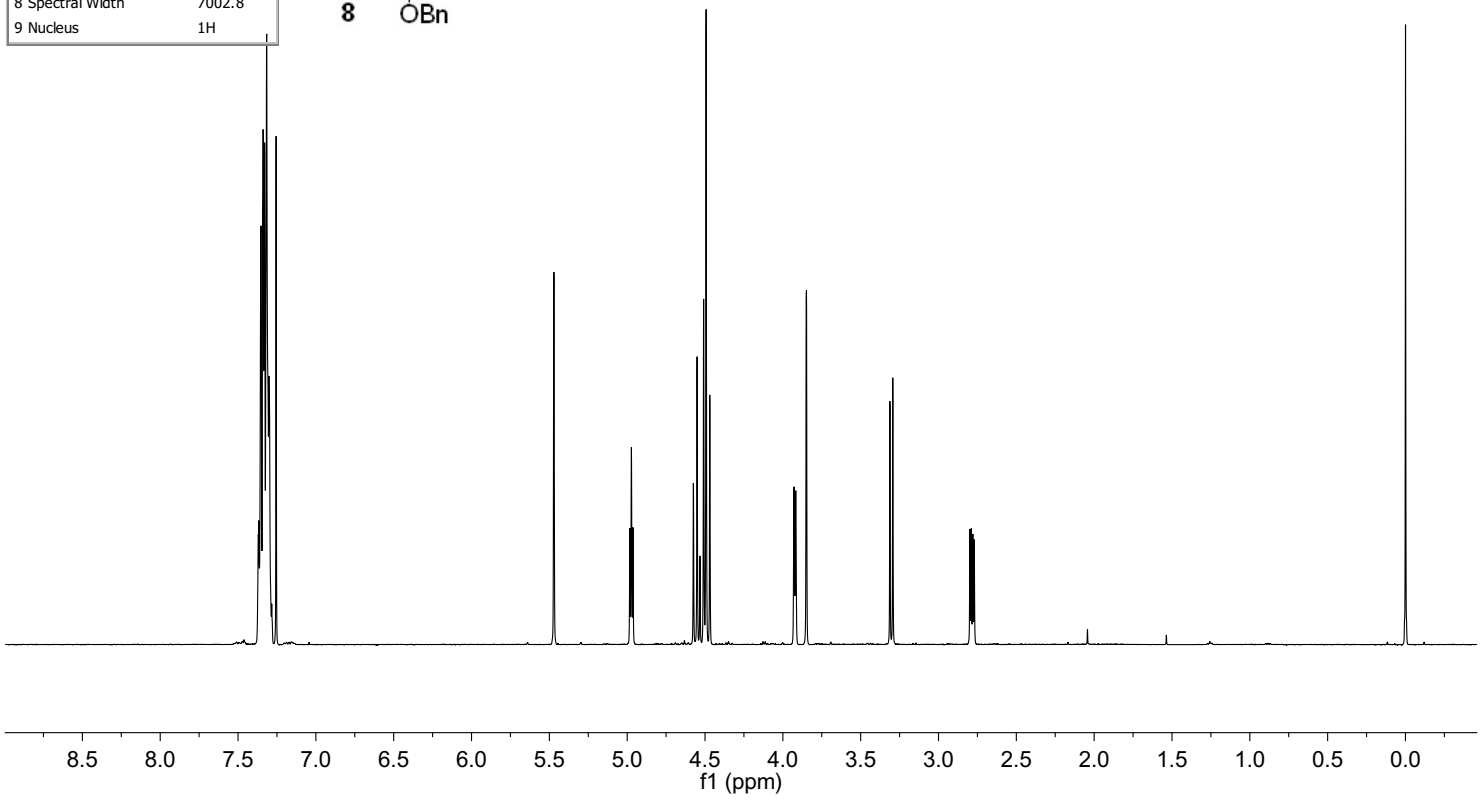



**7**

| Parameter | Value |
|---|---|
| 1 Title | Sam47698 |
| 2 Spectrometer | avance500 |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg30 |
| 6 Number of Scans | 32 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |

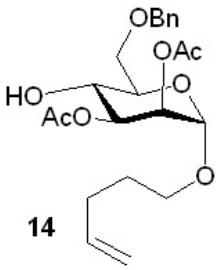



**8**

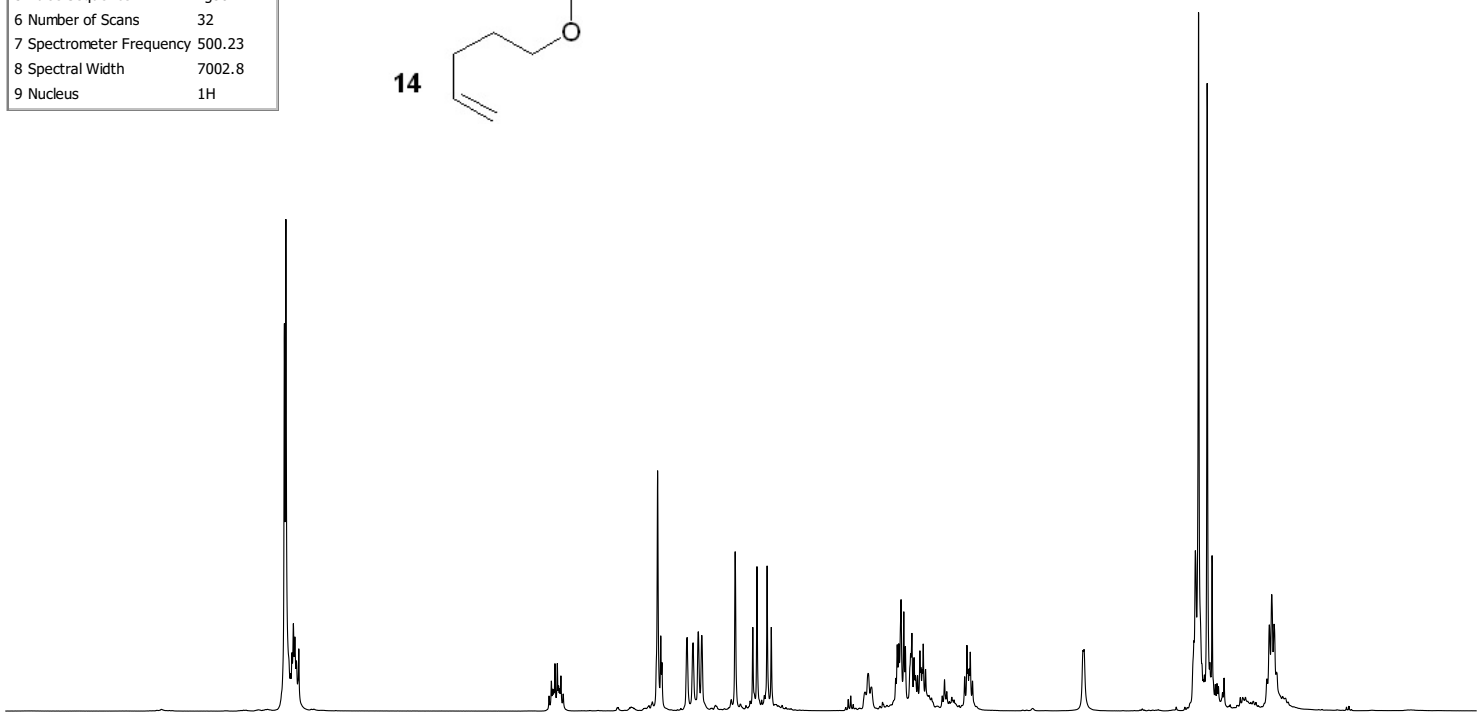




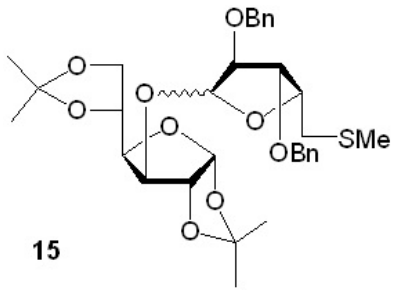

| Parameter | Value |
|---|---|
| 1 Title | Sam63512 |
| 2 Spectrometer | avance500 |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg30 |
| 6 Number of Scans | 32 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |




**14**



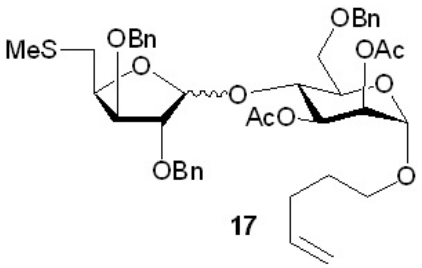
| Parameter | Value |
|---|---|
| 1 Title | Sam3863 |
| 2 Spectrometer | av500lc |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg30 |
| 6 Number of Scans | 512 |
| 7 Spectrometer Frequency | 500.57 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |




15

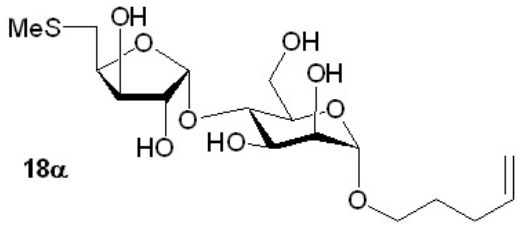



| Parameter | Value |
|---|---|
| 1 Title | Sam50300 |
| 2 Spectrometer | avance500 |
| 3 Solvent | CDCl3 |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg30 |
| 6 Number of Scans | 32 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |




17

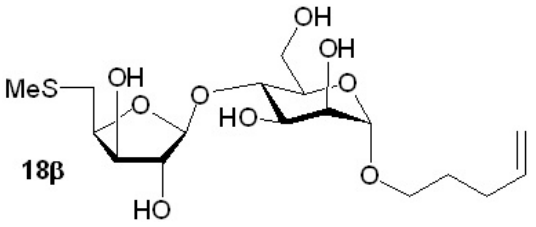
| Parameter | Value |
|---|---|
| 1 Title | Sam50456 |
| 2 Spectrometer | avance500 |
| 3 Solvent | MeOD |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg0f2pr |
| 6 Number of Scans | 64 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |




**18α**




| Parameter | Value |
|---|---|
| 1 Title | Sam50455 |
| 2 Spectrometer | avance500 |
| 3 Solvent | MeOD |
| 4 Temperature | 300.0 |
| 5 Pulse Sequence | zg0f2pr |
| 6 Number of Scans | 64 |
| 7 Spectrometer Frequency | 500.23 |
| 8 Spectral Width | 7002.8 |
| 9 Nucleus | 1H |




**18β**