

Supplementary material for:

Amine substitution into sulfuric acid - ammonia clusters

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Cartesian coordinates for the most stable structure of each cluster, optimized at the B3LYP/CBSB7 level.

$[\text{H}_2\text{SO}_4 \cdot \text{NH}_4]^+$

| | | | |
|---|-----------|-----------|-----------|
| H | 3.753482 | -0.087396 | 0.945444 |
| S | -0.681440 | -0.025187 | 0.123569 |
| O | -1.375673 | -0.943847 | -0.969993 |
| O | -1.461063 | -0.014165 | 1.314451 |
| O | -0.675779 | 1.391217 | -0.590636 |
| O | 0.711939 | -0.393562 | 0.136213 |
| H | -2.160364 | -1.372627 | -0.589747 |
| H | -1.542683 | 1.823734 | -0.510432 |
| N | 3.366374 | -0.032204 | 0.000108 |
| H | 2.315005 | -0.097422 | 0.043749 |
| H | 3.731086 | -0.807956 | -0.558330 |
| H | 3.646501 | 0.852946 | -0.428815 |

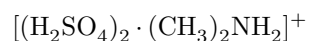
$[\text{H}_2\text{SO}_4 \cdot (\text{CH}_3)_2\text{NH}_2]^+$

| | | | |
|---|-----------|-----------|-----------|
| H | -2.696159 | 0.014717 | -1.437322 |
| S | 1.347121 | 0.028635 | 0.003181 |
| O | 2.472549 | -0.041593 | -1.109667 |
| O | 1.108724 | 1.408694 | 0.254558 |
| O | 2.016112 | -0.678890 | 1.257546 |
| O | 0.264400 | -0.855871 | -0.363164 |
| H | 2.594261 | -0.952942 | -1.425941 |
| H | 2.649337 | -0.078067 | 1.686884 |
| N | -2.426603 | -0.043369 | -0.453004 |
| H | -1.438121 | -0.364919 | -0.442704 |
| C | -3.281284 | -1.068493 | 0.232870 |
| H | -4.320280 | -0.745248 | 0.201826 |
| H | -2.946601 | -1.159330 | 1.264408 |
| H | -3.165476 | -2.021614 | -0.280124 |
| C | -2.491092 | 1.328013 | 0.156054 |
| H | -3.512181 | 1.699058 | 0.089244 |
| H | -1.807985 | 1.982947 | -0.381402 |
| H | -2.184546 | 1.254976 | 1.197548 |

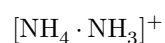
$[(\text{H}_2\text{SO}_4)_2 \cdot \text{NH}_4]^+$

| | | | |
|---|----------|-----------|-----------|
| S | 1.919215 | -0.272124 | -0.052576 |
| O | 1.856012 | 1.147228 | 0.168730 |
| O | 1.623659 | -1.055378 | 1.278711 |
| O | 1.135895 | -0.833155 | -1.128114 |
| H | 0.832504 | 2.602849 | 0.024990 |
| H | 0.646815 | -1.102509 | 1.410423 |

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|---|-----------|-----------|-----------|
| S | -1.919373 | -0.271765 | 0.052571 |
| O | -1.624186 | -1.055423 | -1.278544 |
| O | -1.136794 | -0.833287 | 1.128411 |
| O | -3.439069 | -0.598578 | 0.231815 |
| O | -1.855041 | 1.147509 | -0.168914 |
| H | -0.647381 | -1.103170 | -1.410331 |
| H | -3.577255 | -1.524024 | 0.497527 |
| N | 0.001063 | 3.224780 | -0.000005 |
| H | -0.830356 | 2.602884 | -0.025335 |
| O | 3.438604 | -0.600142 | -0.232088 |
| H | 3.576053 | -1.525769 | -0.497565 |
| H | -0.021527 | 3.813895 | 0.834099 |
| H | 0.023609 | 3.814404 | -0.833750 |



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|---|-----------|-----------|-----------|
| S | -1.978644 | -0.668544 | 0.056018 |
| O | -1.817112 | 0.744372 | -0.140500 |
| O | -1.725237 | -1.453297 | -1.284482 |
| O | -1.247180 | -1.303404 | 1.128834 |
| H | 0.971555 | 2.075355 | -0.033211 |
| H | -0.752033 | -1.568636 | -1.405444 |
| S | 1.856489 | -0.945064 | -0.058156 |
| O | 1.481932 | -1.681552 | 1.281136 |
| O | 1.033131 | -1.454203 | -1.131326 |
| O | 3.341080 | -1.419381 | -0.223964 |
| O | 1.922213 | 0.475301 | 0.140593 |
| H | 0.500990 | -1.657041 | 1.394959 |
| H | 3.388136 | -2.358928 | -0.470121 |
| N | 0.210604 | 2.770173 | -0.005952 |
| H | -0.645901 | 2.196986 | 0.000976 |
| C | 0.240670 | 3.602878 | -1.249279 |
| H | 1.179741 | 4.152417 | -1.284312 |
| H | -0.598528 | 4.295968 | -1.230555 |
| H | 0.159965 | 2.944631 | -2.112457 |
| C | 0.302779 | 3.551010 | 1.267804 |
| H | 1.236858 | 4.109983 | 1.272650 |
| H | 0.281370 | 2.855836 | 2.105105 |
| H | -0.543070 | 4.233769 | 1.326281 |
| O | -3.519463 | -0.902380 | 0.220601 |
| H | -3.714446 | -1.820807 | 0.473717 |

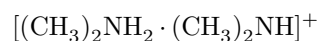


| | | | |
|---|-----------|-----------|-----------|
| N | 1.345451 | -0.000039 | -0.000025 |
| H | 1.733292 | 0.887206 | 0.319069 |
| H | 1.733813 | -0.719610 | 0.608825 |
| H | 1.734374 | -0.167164 | -0.927515 |
| N | -1.335672 | -0.000009 | -0.000012 |
| H | -1.695304 | 0.862191 | -0.413384 |
| H | -0.184341 | -0.000001 | -0.000189 |
| H | -1.695034 | -0.073121 | 0.953416 |
| H | -1.695250 | -0.789161 | -0.539964 |

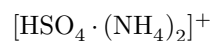


| | | | |
|---|-----------|----------|-----------|
| H | 0.626694 | 0.000070 | -1.416776 |
| H | -2.718852 | 0.865278 | -0.244890 |
| N | 0.496381 | 0.000194 | -0.403398 |
| H | -0.569503 | 0.001730 | -0.234288 |
| C | 1.087005 | 1.254364 | 0.160956 |

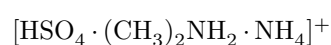
| | | | |
|---|-----------|-----------|-----------|
| H | 2.158746 | 1.272420 | -0.031351 |
| H | 0.904429 | 1.271857 | 1.234240 |
| H | 0.610302 | 2.113260 | -0.309059 |
| C | 1.082558 | -1.256184 | 0.160699 |
| H | 2.153854 | -1.279094 | -0.033511 |
| H | 0.601103 | -2.113282 | -0.307757 |
| H | 0.901947 | -1.272109 | 1.234339 |
| N | -2.271376 | 0.001515 | 0.057159 |
| H | -2.749068 | -0.749907 | -0.437570 |
| H | -2.512063 | -0.111269 | 1.040363 |



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|---|-----------|-----------|-----------|
| N | 1.330701 | -0.295503 | -0.326201 |
| H | 1.489898 | -0.970859 | -1.071637 |
| C | 2.119495 | 0.917041 | -0.644586 |
| C | 1.761214 | -0.921993 | 0.945208 |
| H | 1.935855 | 1.679506 | 0.115221 |
| H | 3.194515 | 0.712717 | -0.669548 |
| H | 1.817390 | 1.310308 | -1.616857 |
| H | 1.562667 | -0.237703 | 1.772520 |
| H | 2.830603 | -1.156145 | 0.945683 |
| H | 1.202916 | -1.844893 | 1.110872 |
| N | -1.347901 | 0.281036 | -0.341527 |
| H | -1.495782 | 0.917217 | -1.126530 |
| H | -0.258006 | 0.045606 | -0.330816 |
| C | -2.121187 | -0.973348 | -0.589085 |
| C | -1.726998 | 0.983060 | 0.922170 |
| H | -2.785640 | 1.239942 | 0.900627 |
| H | -1.129947 | 1.888687 | 1.019270 |
| H | -1.528778 | 0.320046 | 1.763000 |
| H | -3.186170 | -0.749494 | -0.640226 |
| H | -1.791788 | -1.415072 | -1.528659 |
| H | -1.932478 | -1.667152 | 0.228939 |

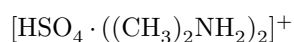


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|---|-----------|-----------|-----------|
| S | 0.001296 | -0.460925 | -0.105845 |
| O | 0.000304 | -1.455865 | 1.166249 |
| O | 0.003023 | 0.865666 | 0.536280 |
| O | -1.229063 | -0.729758 | -0.856184 |
| O | 1.229183 | -0.733662 | -0.857889 |
| H | 0.001320 | -2.373630 | 0.851157 |
| N | -2.800901 | 1.193797 | 0.042578 |
| H | -3.534741 | 0.922798 | 0.697384 |
| H | -1.993453 | 1.587236 | 0.546855 |
| H | -2.382307 | 0.340514 | -0.443148 |
| H | -3.166985 | 1.864937 | -0.632579 |
| N | 2.796522 | 1.196962 | 0.042791 |
| H | 1.979291 | 1.577990 | 0.542253 |
| H | 2.391515 | 0.341127 | -0.446697 |
| H | 3.158352 | 1.874072 | -0.628670 |
| H | 3.529346 | 0.933403 | 0.701736 |



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|---|-----------|-----------|-----------|
| H | -1.565967 | 0.836299 | -0.589150 |
| S | 0.849785 | -0.500248 | 0.264168 |
| O | -0.221611 | -0.871030 | 1.181274 |
| O | 0.504409 | 0.632255 | -0.618169 |
| O | 0.999287 | -1.713589 | -0.802161 |

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|---|-----------|-----------|-----------|
| O | 2.164370 | -0.337386 | 0.897942 |
| H | -1.764697 | -0.206156 | 0.602436 |
| H | 1.243456 | -2.520633 | -0.322610 |
| N | -2.320649 | 0.366467 | -0.068957 |
| C | -3.075692 | -0.536918 | -0.988238 |
| H | -3.587243 | 0.061258 | -1.740748 |
| H | -3.800662 | -1.104816 | -0.407461 |
| H | -2.368759 | -1.214044 | -1.464544 |
| C | -3.157504 | 1.363088 | 0.661073 |
| H | -3.661504 | 2.007295 | -0.057876 |
| H | -2.511552 | 1.955183 | 1.307077 |
| H | -3.893107 | 0.832434 | 1.263399 |
| N | 3.136662 | 1.658909 | -0.515946 |
| H | 2.208532 | 1.726301 | -0.962168 |
| H | 2.995093 | 0.850662 | 0.168149 |
| H | 3.854104 | 1.439357 | -1.206569 |
| H | 3.371202 | 2.524165 | -0.030395 |

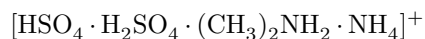


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|---|-----------|-----------|-----------|
| S | 0.093795 | -0.181845 | -0.001433 |
| O | -0.902850 | 0.888078 | -0.001331 |
| O | 0.900018 | -0.275985 | -1.217770 |
| O | 0.900099 | -0.275581 | 1.215024 |
| N | 3.354843 | 0.174368 | -0.000146 |
| H | 2.706317 | 0.020580 | -0.795594 |
| H | 2.702441 | 0.021126 | 0.792521 |
| C | 4.436799 | -0.851108 | 0.002902 |
| C | 3.832061 | 1.588251 | 0.000420 |
| H | 5.051483 | -0.725747 | -0.887220 |
| H | 5.046889 | -0.725049 | 0.896074 |
| H | 3.981451 | -1.839871 | 0.002139 |
| H | 4.433823 | 1.762142 | -0.890327 |
| H | 4.429601 | 1.762755 | 0.893879 |
| H | 2.965886 | 2.247498 | -0.001843 |
| N | -3.428898 | 0.008308 | 0.000773 |
| H | -3.186754 | -0.985657 | -0.000102 |
| H | -2.481561 | 0.474110 | 0.000026 |
| C | -4.154696 | 0.351238 | 1.259267 |
| C | -4.157473 | 0.352876 | -1.255660 |
| H | -5.106142 | -0.181326 | -1.286089 |
| H | -3.538394 | 0.070449 | -2.105390 |
| H | -4.334172 | 1.427019 | -1.272071 |
| H | -5.103271 | -0.183048 | 1.291096 |
| H | -3.533719 | 0.067723 | 2.107248 |
| H | -4.331393 | 1.425351 | 1.277454 |
| O | -0.904835 | -1.504943 | -0.001159 |
| H | -0.364410 | -2.307345 | -0.002957 |

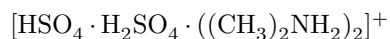


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|---|-----------|-----------|-----------|
| S | -1.087114 | -1.366873 | 1.417527 |
| O | -0.452215 | -0.647491 | 2.492698 |
| O | -2.294341 | -0.808535 | 0.851623 |
| N | 2.067075 | 0.561518 | 2.591676 |
| H | 2.888414 | -0.042648 | 2.628209 |
| H | 1.204382 | 0.002325 | 2.732892 |
| N | -2.785095 | 1.601023 | -0.624856 |
| H | -3.553172 | 2.157369 | -0.249914 |
| H | -2.678147 | 0.724172 | -0.083544 |
| S | 0.645168 | 1.673045 | -0.817728 |

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|---|-----------|-----------|-----------|
| O | 1.274362 | 2.067323 | -2.233335 |
| O | 1.761481 | 1.557866 | 0.122133 |
| O | -0.026480 | 0.399229 | -1.126985 |
| O | -0.325928 | 2.708787 | -0.448116 |
| H | 1.783133 | 2.888611 | -2.146825 |
| O | -1.369808 | -2.804352 | 1.994285 |
| H | -1.879425 | -3.340217 | 1.364116 |
| H | 2.140201 | 1.277778 | 3.314350 |
| H | 1.989130 | 1.009950 | 1.636851 |
| H | -2.975468 | 1.367414 | -1.599724 |
| H | -1.869115 | 2.134234 | -0.570474 |
| O | -0.063760 | -1.696779 | 0.292983 |
| H | 0.027819 | -0.895344 | -0.341672 |



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|---|-----------|-----------|-----------|
| S | -2.192333 | -0.298221 | -1.001468 |
| O | -2.077121 | 1.107596 | -0.694105 |
| O | -1.624879 | -0.772566 | -2.239852 |
| N | 0.415947 | -2.672622 | -2.362314 |
| H | 1.037977 | -2.216773 | -1.638182 |
| H | 0.894853 | -2.711879 | -3.262048 |
| C | 0.127933 | 3.270055 | 1.390712 |
| H | 0.092351 | 2.368089 | 1.998022 |
| H | -0.763519 | 3.874297 | 1.552285 |
| H | 1.019356 | 3.847307 | 1.630708 |
| N | 0.190823 | 2.859309 | -0.044963 |
| C | 0.255655 | 3.992712 | -1.013497 |
| H | -0.625894 | 2.269076 | -0.259258 |
| H | 1.017088 | 2.235509 | -0.173664 |
| H | 0.300297 | 3.589179 | -2.023621 |
| H | -0.632140 | 4.613099 | -0.900849 |
| H | 1.149307 | 4.580818 | -0.811011 |
| S | 1.779064 | -0.246604 | 0.345777 |
| O | 2.691949 | -0.511886 | 1.635002 |
| O | 1.891273 | -1.436440 | -0.501506 |
| O | 2.243413 | 0.981979 | -0.293250 |
| O | 0.444663 | -0.074357 | 0.955781 |
| H | 3.615321 | -0.620236 | 1.358923 |
| O | -3.710017 | -0.724940 | -1.062170 |
| H | -4.200039 | -0.372766 | -0.301146 |
| H | 0.170554 | -3.617739 | -2.067113 |
| H | -0.440902 | -2.089428 | -2.440213 |
| O | -1.687363 | -1.160126 | 0.190994 |
| H | -0.804091 | -0.773947 | 0.565673 |

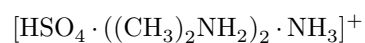


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|---|-----------|-----------|-----------|
| S | -1.007059 | 0.824322 | 0.753006 |
| C | 0.660146 | -3.780141 | 0.782921 |
| H | 1.430736 | -4.534111 | 0.935757 |
| H | -0.325544 | -4.216964 | 0.936288 |
| H | 0.740562 | -3.361775 | -0.218104 |
| O | -1.062223 | -0.520828 | 1.277928 |
| O | -0.420115 | 1.857887 | 1.564547 |
| N | 0.865589 | -2.672715 | 1.764387 |
| C | 0.793650 | -3.087790 | 3.195498 |
| H | 1.788507 | -2.225663 | 1.570304 |
| H | 0.169045 | -1.934794 | 1.584960 |
| H | -0.187793 | -3.514180 | 3.397524 |
| H | 0.953600 | -2.212532 | 3.822816 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.568555 | -3.827605 | 3.389844 |
| C | 1.541275 | 3.983694 | -0.724589 |
| H | 0.942383 | 3.327416 | -1.353383 |
| H | 2.471261 | 4.237150 | -1.230695 |
| H | 0.982963 | 4.889118 | -0.491273 |
| N | 1.860278 | 3.260621 | 0.542482 |
| C | 2.670462 | 4.044651 | 1.520461 |
| H | 2.363749 | 2.378194 | 0.311313 |
| H | 0.982656 | 2.947364 | 0.985437 |
| H | 2.849664 | 3.427154 | 2.398811 |
| H | 3.619536 | 4.312221 | 1.058941 |
| H | 2.124783 | 4.944181 | 1.801550 |
| S | 2.872474 | -0.531327 | -0.142019 |
| O | 3.774703 | -1.086866 | -1.347730 |
| O | 1.508453 | -0.825803 | -0.637419 |
| O | 3.151946 | 0.896849 | -0.014032 |
| O | 3.191694 | -1.314088 | 1.049900 |
| H | 4.710175 | -1.020174 | -1.101416 |
| O | -0.366762 | 0.819546 | -0.666224 |
| H | 0.427657 | 0.146086 | -0.713242 |
| O | -2.466241 | 1.341085 | 0.429544 |
| H | -2.971188 | 0.666549 | -0.052755 |

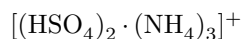


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|---|-----------|-----------|-----------|
| S | 0.676339 | 0.093594 | -0.166614 |
| O | 1.859729 | 0.709071 | -0.804307 |
| O | -0.152613 | -0.671162 | -1.103668 |
| O | -0.118274 | 1.111659 | 0.579037 |
| O | 1.187528 | -0.883712 | 0.946546 |
| N | 2.707572 | -2.753750 | -0.074670 |
| H | 2.207352 | -3.279392 | -0.787266 |
| H | 3.520433 | -2.339804 | -0.524358 |
| H | 1.793729 | -1.635067 | 0.534430 |
| H | 3.046336 | -3.419561 | 0.615003 |
| N | -2.565438 | -0.126259 | 0.009951 |
| C | -3.657325 | 0.505819 | -0.780836 |
| C | -3.012695 | -1.133056 | 1.014510 |
| H | -4.336900 | 1.027741 | -0.108267 |
| H | -3.215778 | 1.208845 | -1.485183 |
| H | -4.197764 | -0.267511 | -1.324827 |
| H | -1.847697 | -0.551332 | -0.619609 |
| H | -1.978425 | 0.589908 | 0.472750 |
| H | -3.682471 | -0.657189 | 1.729565 |
| H | -3.531148 | -1.942000 | 0.501876 |
| H | -2.133821 | -1.519830 | 1.527636 |
| N | 1.857504 | 3.023075 | 0.388790 |
| H | 2.551541 | 3.188776 | 1.115758 |
| H | 2.103566 | 2.164380 | -0.210867 |
| H | 0.957392 | 2.709894 | 0.796486 |
| H | 1.733914 | 3.859761 | -0.178706 |

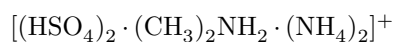


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|---|-----------|-----------|-----------|
| S | -0.014894 | 0.247385 | 0.259257 |
| O | 0.920264 | -0.152715 | 1.323717 |
| O | -0.461326 | -0.903220 | -0.548473 |
| O | -1.132226 | 1.078540 | 0.730699 |
| N | -3.129585 | -0.650220 | -0.064243 |
| H | -2.240062 | -1.039698 | -0.447749 |
| H | -2.754078 | 0.213708 | 0.371302 |

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|---|-----------|-----------|-----------|
| C | -4.078250 | -0.320800 | -1.163049 |
| C | -3.672609 | -1.555098 | 0.987519 |
| H | -4.382312 | -1.240004 | -1.661883 |
| H | -4.951887 | 0.180644 | -0.748560 |
| H | -3.575291 | 0.334188 | -1.872449 |
| H | -3.955357 | -2.503493 | 0.532863 |
| H | -4.543145 | -1.090559 | 1.448720 |
| H | -2.899452 | -1.718294 | 1.736242 |
| N | 3.065065 | -0.749295 | -0.175423 |
| H | 2.822788 | 0.007287 | -0.824079 |
| H | 2.338632 | -0.617922 | 0.582846 |
| C | 4.441439 | -0.558203 | 0.360867 |
| C | 2.822954 | -2.063325 | -0.844868 |
| H | 3.492826 | -2.165375 | -1.697755 |
| H | 1.782228 | -2.090169 | -1.163831 |
| H | 3.011315 | -2.858622 | -0.125339 |
| H | 5.163888 | -0.624165 | -0.451806 |
| H | 4.501156 | 0.419689 | 0.835927 |
| H | 4.641758 | -1.334791 | 1.097325 |
| O | 0.846415 | 1.141263 | -0.750827 |
| H | 0.693123 | 2.156963 | -0.556329 |
| N | 0.345335 | 3.650285 | -0.194950 |
| H | 0.022479 | 4.211766 | -0.978084 |
| H | 1.070457 | 4.179443 | 0.281302 |
| H | -0.432699 | 3.539467 | 0.451804 |

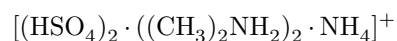


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| S | 2.202481 | -0.026478 | 0.001099 |
| O | 1.560829 | 0.440145 | -1.233462 |
| N | -0.013134 | -2.328094 | -1.377575 |
| H | 0.904099 | -2.147965 | -0.902575 |
| H | -0.739716 | -2.280953 | -0.640379 |
| O | 2.034699 | -1.467053 | 0.217829 |
| O | 1.834018 | 0.773252 | 1.180012 |
| N | -0.077755 | 2.569861 | -1.101384 |
| H | 0.356263 | 3.438630 | -0.793310 |
| H | 0.647667 | 1.805408 | -1.195630 |
| N | -0.191669 | -0.112973 | 2.761997 |
| H | 0.054540 | -0.646247 | 3.594228 |
| H | 0.669375 | 0.209545 | 2.245139 |
| S | -2.139270 | -0.006976 | -0.069571 |
| O | -3.718970 | -0.245559 | 0.092732 |
| O | -1.816381 | 0.032394 | -1.488872 |
| O | -1.586608 | -1.189162 | 0.628982 |
| O | -1.806084 | 1.245070 | 0.634254 |
| H | -4.203153 | 0.423009 | -0.415389 |
| O | 3.755372 | 0.250685 | -0.287010 |
| H | 4.288014 | -0.083816 | 0.450703 |
| H | -0.781065 | 2.232903 | -0.404596 |
| H | -0.539605 | 2.709449 | -1.999252 |
| H | -0.212639 | -1.546341 | -2.009216 |
| H | -0.023868 | -3.216116 | -1.875699 |
| H | -0.755940 | -0.683655 | 2.091961 |
| H | -0.752446 | 0.701664 | 3.012582 |



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|---|-----------|-----------|-----------|
| S | -2.160272 | -0.391844 | -0.102858 |
| O | -1.784207 | 0.560939 | -1.150430 |
| N | -0.158679 | -1.903686 | 2.364280 |

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|---|-----------|-----------|-----------|
| H | -0.629043 | -2.807663 | 2.370248 |
| H | -0.830469 | -1.162769 | 2.030855 |
| O | -1.720674 | 0.007437 | 1.238621 |
| O | -1.776304 | -1.775141 | -0.438496 |
| N | 0.159169 | -1.904695 | -2.363804 |
| H | 0.830787 | -1.163447 | -2.030808 |
| H | -0.176630 | -1.684606 | -3.300048 |
| C | -0.783984 | 3.258352 | 0.981869 |
| H | -1.334671 | 2.569814 | 1.619301 |
| H | -1.477802 | 3.900898 | 0.441577 |
| H | -0.100653 | 3.864884 | 1.574549 |
| N | -0.000232 | 2.454301 | -0.000209 |
| C | 0.783756 | 3.258036 | -0.982365 |
| H | -0.649705 | 1.821631 | -0.505820 |
| H | 0.649121 | 1.821517 | 0.505434 |
| H | 1.334197 | 2.569273 | -1.619770 |
| H | 0.100606 | 3.864761 | -1.575052 |
| H | 1.477813 | 3.900367 | -0.442126 |
| S | 2.160246 | -0.391627 | 0.102861 |
| O | 3.760963 | -0.363174 | -0.038560 |
| O | 1.720706 | 0.007257 | -1.238748 |
| O | 1.783800 | 0.561304 | 1.150149 |
| O | 1.776599 | -1.774945 | 0.438807 |
| H | 4.165963 | -0.563245 | 0.818759 |
| O | -3.760989 | -0.363744 | 0.038769 |
| H | -4.166026 | -0.563613 | -0.818580 |
| H | 0.629662 | -2.808611 | -2.368926 |
| H | -0.644342 | -1.920345 | -1.683486 |
| H | 0.177309 | -1.682792 | 3.300266 |
| H | 0.644696 | -1.919737 | 1.683787 |

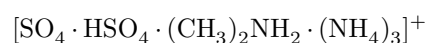


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|---|-----------|-----------|-----------|
| S | 2.038046 | -0.737343 | 0.384577 |
| O | 1.912289 | -0.289919 | -1.009346 |
| N | 0.899027 | 2.334445 | -1.086096 |
| H | 0.147501 | 2.221792 | -0.373494 |
| H | 1.327981 | 1.389470 | -1.154996 |
| C | 1.919256 | 3.297299 | -0.583985 |
| C | 0.274158 | 2.702726 | -2.388137 |
| H | -0.191540 | 3.683079 | -2.295217 |
| H | -0.483858 | 1.957783 | -2.623355 |
| H | 1.039740 | 2.727397 | -3.162719 |
| H | 1.447291 | 4.264224 | -0.414307 |
| H | 2.323653 | 2.905078 | 0.347164 |
| H | 2.713465 | 3.397739 | -1.322915 |
| O | 1.071417 | -1.762881 | 0.777817 |
| O | 2.074740 | 0.394268 | 1.328035 |
| N | 0.007399 | -0.012400 | 3.111373 |
| H | 0.213575 | -0.834134 | 3.677632 |
| H | 0.830994 | 0.197577 | 2.493178 |
| C | -1.931776 | -3.293493 | -0.591499 |
| H | -2.341522 | -2.899201 | 0.336485 |
| H | -1.465647 | -4.262615 | -0.417909 |
| H | -2.720676 | -3.390840 | -1.336664 |
| N | -0.903398 | -2.334885 | -1.086272 |
| C | -0.272024 | -2.705236 | -2.384952 |
| H | -0.154698 | -2.225795 | -0.370423 |
| H | -1.327847 | -1.387971 | -1.156457 |
| H | 0.489217 | -1.962071 | -2.615793 |
| H | 0.190610 | -3.686714 | -2.288126 |

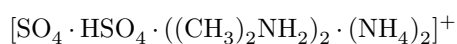
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|---|-----------|-----------|-----------|
| H | -1.033294 | -2.728764 | -3.163918 |
| S | -2.037033 | 0.740094 | 0.390104 |
| O | -3.440515 | 1.518236 | 0.519542 |
| O | -2.068281 | -0.391524 | 1.333648 |
| O | -1.069253 | 1.765743 | 0.779133 |
| O | -1.917738 | 0.292499 | -1.004602 |
| H | -4.160300 | 0.934933 | 0.236285 |
| O | 3.441262 | -1.516650 | 0.509678 |
| H | 4.163098 | -0.925662 | 0.248621 |
| H | -0.823175 | -0.200245 | 2.494942 |
| H | -0.191039 | 0.784835 | 3.714236 |



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|---|-----------|-----------|-----------|
| S | 1.884192 | -0.076190 | -1.260217 |
| O | 0.951264 | -1.204906 | -1.232511 |
| C | 1.042951 | 3.292035 | 0.938365 |
| H | 1.802628 | 4.005117 | 0.620381 |
| H | 0.433800 | 3.723448 | 1.731465 |
| H | 1.519539 | 2.376014 | 1.279270 |
| N | 1.521374 | -1.389638 | 2.123490 |
| H | 1.998933 | -0.861259 | 1.361622 |
| H | 0.581763 | -0.940556 | 2.185830 |
| C | 2.241720 | -1.188110 | 3.410381 |
| C | 1.373519 | -2.814923 | 1.714848 |
| H | 2.359753 | -3.273897 | 1.655605 |
| H | 0.898954 | -2.835042 | 0.736946 |
| H | 0.761697 | -3.337330 | 2.449023 |
| H | 3.254439 | -1.579415 | 3.322844 |
| H | 2.275151 | -0.122545 | 3.630836 |
| H | 1.709881 | -1.708627 | 4.205766 |
| O | 2.456970 | 0.217815 | 0.063064 |
| O | 1.375776 | 1.124501 | -1.930099 |
| N | 0.171397 | 2.954684 | -0.222056 |
| C | -0.471985 | 4.127970 | -0.874171 |
| H | 0.721272 | 2.408753 | -0.918350 |
| H | -0.569185 | 2.282482 | 0.077953 |
| H | -1.104045 | 4.639576 | -0.149497 |
| H | -1.079966 | 3.777218 | -1.706259 |
| H | 0.298040 | 4.805860 | -1.240080 |
| C | -1.796846 | -2.907914 | -2.471055 |
| H | -1.248354 | -3.583397 | -1.817122 |
| H | -1.365662 | -2.937018 | -3.470797 |
| H | -2.845416 | -3.200224 | -2.509169 |
| N | -1.689306 | -1.524892 | -1.930431 |
| C | -2.392506 | -0.488984 | -2.737891 |
| H | -0.681841 | -1.280328 | -1.831735 |
| H | -2.037808 | -1.495436 | -0.949050 |
| H | -2.302412 | 0.460041 | -2.214893 |
| H | -1.934298 | -0.430175 | -3.724327 |
| H | -3.443249 | -0.761168 | -2.830956 |
| S | -1.882255 | 0.065593 | 1.271585 |
| O | -3.204123 | 0.595095 | 2.031956 |
| O | -1.744914 | 1.038112 | 0.182005 |
| O | -2.167756 | -1.293028 | 0.799337 |
| O | -0.788564 | 0.116101 | 2.249718 |
| H | -3.411555 | -0.010532 | 2.758960 |
| O | 3.079510 | -0.646624 | -2.182800 |
| H | 3.706275 | 0.069947 | -2.361405 |

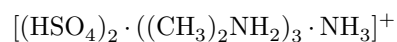


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| S | -3.281223 | -0.320687 | 0.183762 |
| O | -2.332063 | -1.205606 | 0.876371 |
| N | -0.969669 | -1.952505 | -1.657763 |
| H | -1.925385 | -1.533318 | -1.716970 |
| H | -0.282643 | -1.131894 | -1.580752 |
| O | -3.259482 | -0.503946 | -1.272693 |
| O | -3.168822 | 1.087562 | 0.577910 |
| N | -0.346111 | -0.170785 | 2.431664 |
| H | -0.298775 | -0.363601 | 3.428827 |
| H | -1.219646 | -0.554837 | 1.998978 |
| N | -1.401935 | 2.519646 | -0.989723 |
| H | -1.547611 | 3.507256 | -1.185200 |
| H | -2.225078 | 2.093676 | -0.509775 |
| S | 1.323016 | 0.610440 | -0.307496 |
| O | 2.625382 | 1.144828 | -0.764394 |
| O | 1.554849 | -0.619576 | 0.542010 |
| O | 0.458073 | 0.255969 | -1.478114 |
| O | 0.587608 | 1.625732 | 0.522630 |
| H | 3.831168 | 0.261623 | -0.267908 |
| O | -4.699474 | -0.853777 | 0.723790 |
| H | -5.407962 | -0.321930 | 0.331087 |
| H | -0.296269 | 0.834244 | 2.228592 |
| H | 0.469308 | -0.555226 | 1.889385 |
| H | -0.943924 | -2.491881 | -0.793048 |
| H | -0.764712 | -2.544835 | -2.458945 |
| H | -1.208612 | 2.003178 | -1.849077 |
| H | -0.559254 | 2.344001 | -0.359555 |
| C | 5.208936 | 0.021092 | 1.312982 |
| H | 5.694301 | -0.793476 | 1.850347 |
| H | 4.558380 | 0.577981 | 1.985119 |
| H | 5.962018 | 0.690887 | 0.900242 |
| N | 4.386099 | -0.524096 | 0.201033 |
| C | 5.143555 | -1.301840 | -0.814601 |
| H | 3.601196 | -1.075150 | 0.573429 |
| H | 5.623756 | -2.159851 | -0.344495 |
| H | 4.450711 | -1.636872 | -1.584699 |
| H | 5.898135 | -0.656836 | -1.262701 |



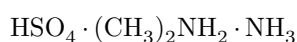
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| S | 2.941102 | -0.985477 | -0.075658 |
| O | 2.674781 | -0.413553 | -1.377805 |
| N | 1.668978 | 2.311321 | -0.115186 |
| H | 0.849911 | 1.769307 | -0.501629 |
| H | 2.232634 | 1.601710 | 0.380975 |
| C | 1.154566 | 3.319442 | 0.852995 |
| C | 2.471288 | 2.876829 | -1.235432 |
| H | 1.842258 | 3.549368 | -1.817350 |
| H | 2.817304 | 2.050784 | -1.852731 |
| H | 3.322468 | 3.423785 | -0.830676 |
| H | 0.540931 | 4.041959 | 0.316427 |
| H | 0.541304 | 2.801340 | 1.587817 |
| H | 1.991674 | 3.826766 | 1.331743 |
| O | 2.059778 | -2.146994 | 0.239358 |
| O | 2.948206 | -0.028722 | 1.043546 |
| N | 0.717363 | -1.217503 | 2.504952 |
| H | 1.147820 | -1.778216 | 1.741409 |
| H | 1.478034 | -0.688403 | 2.930284 |
| C | -5.392434 | -0.533404 | 1.121480 |
| H | -4.729297 | -0.472215 | 1.982784 |

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|---|-----------|-----------|-----------|
| H | -5.928935 | -1.482073 | 1.129327 |
| H | -6.102914 | 0.291700 | 1.151548 |
| N | -4.575008 | -0.424112 | -0.114613 |
| C | -5.346252 | -0.468522 | -1.383789 |
| H | -3.823095 | -1.131208 | -0.120762 |
| H | -3.961778 | 0.449020 | -0.079522 |
| H | -4.651264 | -0.365563 | -2.215443 |
| H | -5.883019 | -1.414101 | -1.459531 |
| H | -6.054554 | 0.358832 | -1.398788 |
| S | -1.421755 | 0.458007 | 0.060134 |
| O | -1.825641 | -0.992329 | -0.154890 |
| O | -0.418841 | 0.813871 | -0.985699 |
| O | -0.792127 | 0.593818 | 1.413556 |
| O | -2.625841 | 1.315279 | -0.024820 |
| H | -0.745413 | -1.672317 | -1.210310 |
| O | 4.435828 | -1.570078 | -0.211986 |
| H | 4.740491 | -1.882320 | 0.652446 |
| H | 0.021572 | -0.511407 | 2.053454 |
| H | 0.261371 | -1.808274 | 3.195940 |
| N | 0.123065 | -1.885301 | -1.783638 |
| H | 0.853811 | -2.261899 | -1.151112 |
| H | 0.469870 | -0.975127 | -2.103279 |
| H | -0.053688 | -2.509159 | -2.566878 |

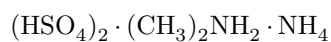


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|---|-----------|-----------|-----------|
| S | 2.463601 | 0.551691 | 0.072081 |
| O | 1.797311 | 1.565144 | 0.906744 |
| N | 0.406481 | -1.014343 | 2.622773 |
| H | -0.419055 | -0.555474 | 2.178328 |
| H | 1.129623 | -1.033980 | 1.876834 |
| C | 0.034308 | -2.406923 | 2.997680 |
| C | 0.907603 | -0.175494 | 3.746538 |
| H | 0.121917 | -0.064866 | 4.493057 |
| H | 1.192736 | 0.794894 | 3.344449 |
| H | 1.776985 | -0.657109 | 4.192515 |
| H | -0.745904 | -2.375425 | 3.757232 |
| H | -0.337157 | -2.905395 | 2.105121 |
| H | 0.911442 | -2.921699 | 3.388275 |
| O | 2.121978 | 0.704447 | -1.351160 |
| O | 2.311702 | -0.814598 | 0.567143 |
| N | -5.403178 | 0.285013 | -0.101371 |
| H | -5.487906 | 0.905698 | -0.901744 |
| H | -4.032308 | -0.577997 | -0.113818 |
| C | 1.860121 | -2.797983 | -2.150356 |
| H | 2.374465 | -2.752001 | -1.192541 |
| H | 2.577312 | -2.683514 | -2.962392 |
| H | 1.331196 | -3.744730 | -2.253364 |
| N | 0.877420 | -1.679993 | -2.199392 |
| C | 0.110217 | -1.572957 | -3.470485 |
| H | 1.374709 | -0.788457 | -2.008955 |
| H | 0.198793 | -1.771518 | -1.407577 |
| H | -0.609173 | -0.763122 | -3.363558 |
| H | 0.796071 | -1.373635 | -4.293107 |
| H | -0.417462 | -2.509520 | -3.646800 |
| S | -1.836835 | -0.595546 | -0.052396 |
| O | -1.685913 | 0.325801 | -1.201767 |
| O | -1.722245 | 0.137304 | 1.228179 |
| O | -0.904606 | -1.733308 | -0.114577 |
| O | -3.252779 | -1.253108 | -0.132262 |
| H | -0.901269 | 1.786704 | -0.774096 |

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| O | 4.052568 | 0.795737 | 0.212794 |
| H | 4.266823 | 1.687534 | -0.097802 |
| H | -5.513885 | 0.848077 | 0.737545 |
| H | -6.191045 | -0.357295 | -0.136343 |
| C | 0.099662 | 3.430147 | -1.589893 |
| H | -0.736032 | 3.718556 | -2.226666 |
| H | 0.798562 | 2.803275 | -2.139979 |
| H | 0.610104 | 4.320995 | -1.225061 |
| N | -0.409506 | 2.646599 | -0.431404 |
| C | -1.328172 | 3.391239 | 0.471823 |
| H | 0.403071 | 2.292611 | 0.115598 |
| H | -2.172420 | 3.765134 | -0.107046 |
| H | -1.679319 | 2.699620 | 1.235180 |
| H | -0.794228 | 4.225873 | 0.924914 |

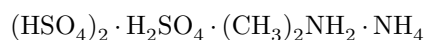


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|---|-----------|-----------|-----------|
| S | -0.393481 | 0.937791 | -0.599382 |
| O | 0.189991 | 2.445577 | -0.826649 |
| O | 0.412330 | 0.049813 | -1.440112 |
| O | -1.802773 | 0.985110 | -1.070902 |
| O | -0.266432 | 0.733697 | 0.831748 |
| H | 0.356098 | 2.537423 | -1.774347 |
| N | -0.412938 | -2.281757 | 0.587009 |
| H | -0.511106 | -2.939693 | 1.354183 |
| H | 0.475698 | -2.469979 | 0.130554 |
| H | -1.639070 | -1.997395 | -0.657913 |
| H | -0.318692 | -1.339838 | 0.979225 |
| C | -1.764631 | -2.005235 | -2.745859 |
| H | -1.737901 | -3.092145 | -2.837583 |
| H | -0.763690 | -1.585125 | -2.829197 |
| H | -2.405460 | -1.586437 | -3.522446 |
| N | -2.293604 | -1.625516 | -1.412719 |
| C | -3.681635 | -2.059463 | -1.142577 |
| H | -2.212385 | -0.569286 | -1.313807 |
| H | -3.746921 | -3.147613 | -1.186597 |
| H | -3.969762 | -1.715544 | -0.149679 |
| H | -4.353647 | -1.623610 | -1.882335 |

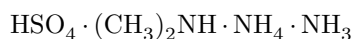


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|---|-----------|-----------|-----------|
| S | -0.780281 | -1.116603 | 1.731516 |
| O | -0.765034 | -2.317697 | 2.513413 |
| O | -0.109279 | 0.058822 | 2.372890 |
| O | -2.087176 | -0.684720 | 1.194262 |
| N | -2.016535 | 1.952218 | 1.287707 |
| H | -2.883206 | 2.450479 | 1.103275 |
| H | -1.738293 | 2.061410 | 2.261577 |
| S | 0.831410 | 1.910037 | -0.936330 |
| O | 2.211997 | 1.593268 | -0.546938 |
| O | 0.023095 | 0.721999 | -1.223080 |
| O | 0.172877 | 2.872387 | -0.050644 |
| O | 0.145438 | -1.450740 | 0.440424 |
| H | 0.031802 | -0.734165 | -0.229521 |
| H | 1.495398 | 0.115095 | 2.106522 |
| H | -2.126232 | 0.895007 | 1.138471 |
| H | -1.234844 | 2.320126 | 0.688507 |
| N | 2.510750 | 0.227140 | 1.823107 |

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|---|----------|-----------|-----------|
| C | 3.154821 | -1.111062 | 1.769812 |
| C | 3.164157 | 1.200833 | 2.731392 |
| H | 2.466272 | 0.647832 | 0.868793 |
| H | 3.148952 | -1.551202 | 2.766792 |
| H | 2.573668 | -1.736238 | 1.095133 |
| H | 4.179525 | -1.008160 | 1.412242 |
| H | 3.125618 | 0.825381 | 3.753773 |
| H | 4.200419 | 1.348091 | 2.427243 |
| H | 2.628883 | 2.146643 | 2.663412 |
| O | 0.935602 | 2.734731 | -2.330030 |
| H | 1.272841 | 2.126633 | -3.002879 |

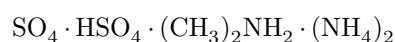


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|---|-----------|-----------|-----------|
| N | -3.615647 | -5.002409 | 0.865570 |
| H | -2.902888 | -4.379682 | 0.430576 |
| H | -3.249000 | -5.633996 | 1.593619 |
| H | -4.085121 | -5.544224 | 0.143476 |
| S | -3.028006 | -1.749177 | -0.319097 |
| O | -2.216745 | -2.966975 | -0.365579 |
| O | -2.903107 | -1.013537 | 0.950897 |
| O | -4.424492 | -1.934572 | -0.720083 |
| H | -2.925970 | -1.969471 | 2.371063 |
| S | -4.550160 | -2.705524 | 3.579042 |
| O | -3.032070 | -2.642900 | 3.095366 |
| O | -4.502912 | -3.366027 | 4.868395 |
| O | -5.075151 | -1.341707 | 3.576284 |
| O | -5.262015 | -3.538533 | 2.545680 |
| H | -4.304965 | -4.395047 | 1.361144 |
| O | -2.447471 | -0.769978 | -1.470533 |
| H | -1.491305 | -0.691487 | -1.340253 |
| S | -4.838488 | -6.720508 | 4.014828 |
| O | -4.723972 | -5.988976 | 5.403313 |
| O | -6.063070 | -5.992730 | 3.304813 |
| O | -5.230471 | -8.063316 | 4.260025 |
| O | -3.643412 | -6.437891 | 3.239777 |
| H | -4.539561 | -5.020679 | 5.269839 |
| H | -5.829644 | -5.049918 | 3.086578 |
| H | -5.659109 | -0.867205 | 2.053295 |
| H | -5.479749 | -1.146968 | 0.416996 |
| N | -6.054076 | -0.624795 | 1.114969 |
| C | -5.873164 | 0.831263 | 0.876462 |
| C | -7.458766 | -1.106523 | 1.060699 |
| H | -8.051012 | -0.572601 | 1.803193 |
| H | -7.865031 | -0.935264 | 0.064202 |
| H | -7.458465 | -2.170363 | 1.290891 |
| H | -6.241942 | 1.084002 | -0.117212 |
| H | -6.420377 | 1.391590 | 1.633884 |
| H | -4.809260 | 1.050659 | 0.944587 |

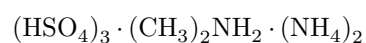


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|---|-----------|-----------|-----------|
| S | 1.399007 | -0.603519 | 0.000230 |
| O | 2.919816 | -1.118453 | -0.307625 |
| O | 1.446132 | -0.019418 | 1.357584 |
| O | 0.546924 | -1.787967 | -0.075493 |
| O | 1.171209 | 0.392412 | -1.041714 |
| H | 3.059697 | -1.910726 | 0.228453 |
| N | -0.827542 | 1.485888 | 1.401661 |
| H | -1.250846 | 1.842315 | 2.253349 |
| H | 0.050520 | 0.945202 | 1.603978 |

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|---|-----------|-----------|-----------|
| H | -1.477204 | 0.798220 | 0.895351 |
| H | -0.539257 | 2.268731 | 0.750598 |
| N | 0.363330 | 3.188636 | -0.507559 |
| H | -0.119422 | 3.601444 | -1.299908 |
| H | 1.062123 | 3.858899 | -0.200704 |
| H | 0.858374 | 2.356900 | -0.845811 |
| C | -3.413435 | -1.132926 | 0.515487 |
| H | -4.226311 | -0.400208 | 0.520596 |
| H | -3.238711 | -1.457165 | 1.543975 |
| H | -3.748751 | -2.002943 | -0.067192 |
| N | -2.195736 | -0.523980 | -0.025578 |
| C | -2.320505 | -0.150788 | -1.441345 |
| H | -1.417645 | -1.184285 | 0.048012 |
| H | -3.032068 | 0.674282 | -1.549156 |
| H | -1.343226 | 0.166773 | -1.806812 |
| H | -2.670761 | -0.985260 | -2.064939 |

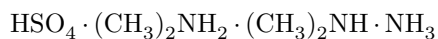


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|---|-----------|-----------|-----------|
| S | -2.241362 | -0.408613 | -0.019719 |
| O | -3.636553 | -0.701872 | -0.164317 |
| N | 0.198638 | -1.000940 | 2.706801 |
| H | -0.727801 | -0.689693 | 2.328783 |
| H | 0.417067 | -1.920963 | 2.318788 |
| O | -1.818982 | 0.130992 | 1.294228 |
| O | -1.673199 | 0.453737 | -1.109761 |
| N | -0.004957 | -1.069431 | -2.684995 |
| H | 0.093910 | -0.997603 | -3.693331 |
| H | -0.816884 | -0.519823 | -2.331091 |
| S | 2.092393 | -0.636998 | 0.038320 |
| O | 3.451548 | -1.089791 | 0.193438 |
| O | 1.723481 | 0.407150 | 1.107835 |
| O | 1.088573 | -1.759219 | 0.179812 |
| O | 1.835279 | 0.034733 | -1.294253 |
| O | -1.480841 | -1.819500 | -0.180967 |
| H | -0.487330 | -1.717340 | -0.025682 |
| H | -0.545287 | 1.671148 | -0.512471 |
| H | 0.918676 | -0.347705 | 2.240627 |
| H | 0.228244 | -0.999413 | 3.721756 |
| H | -0.140960 | -2.039935 | -2.408810 |
| H | 0.871704 | -0.657273 | -2.139359 |
| N | 0.152416 | 2.281706 | -0.033175 |
| C | -0.555123 | 3.101456 | 0.982235 |
| C | 0.929923 | 3.065160 | -1.026208 |
| H | 0.805208 | 1.593454 | 0.442742 |
| H | -1.209166 | 3.815093 | 0.480261 |
| H | -1.152453 | 2.431475 | 1.596931 |
| H | 0.176890 | 3.636195 | 1.587955 |
| H | 0.252667 | 3.678967 | -1.621151 |
| H | 1.638141 | 3.704028 | -0.498270 |
| H | 1.474956 | 2.360279 | -1.649991 |



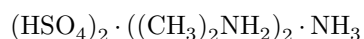
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|---|-----------|-----------|-----------|
| S | -3.681499 | 0.049504 | 0.245008 |
| O | -3.568652 | 1.414648 | -0.271151 |
| O | -5.286923 | -0.165568 | 0.294265 |
| O | -3.159046 | -0.967952 | -0.675862 |
| H | -5.453166 | -1.067977 | 0.601488 |
| S | 1.942930 | 2.106100 | 0.061404 |
| O | 2.310772 | 1.109370 | 1.094906 |

| | | | |
|---|-----------|-----------|-----------|
| O | 2.821942 | 3.228905 | -0.072583 |
| O | 2.052911 | 1.309771 | -1.351088 |
| S | 0.233272 | -1.801708 | -0.524788 |
| O | 0.070279 | -0.475851 | -1.183909 |
| O | 0.309721 | -1.653466 | 0.938980 |
| O | 1.360348 | -2.556880 | -1.060859 |
| O | -1.059597 | -2.630208 | -0.884052 |
| H | -1.864947 | -2.060173 | -0.745666 |
| O | -3.197647 | -0.106104 | 1.619164 |
| N | -0.578161 | 0.669668 | 2.097838 |
| N | -1.354315 | 1.801362 | -1.766258 |
| H | -2.286569 | 1.751345 | -1.281573 |
| H | -1.418631 | 2.281525 | -2.659664 |
| H | -0.660398 | 2.259636 | -1.135508 |
| H | -1.024157 | 0.829333 | -1.882231 |
| H | 1.375844 | 0.585141 | -1.343932 |
| H | -1.611145 | 0.557146 | 2.035281 |
| H | -0.233967 | 1.442926 | 1.490166 |
| H | -0.159860 | -0.217065 | 1.732189 |
| H | -0.282370 | 0.830483 | 3.056718 |
| O | 0.492691 | 2.440652 | 0.199844 |
| N | 3.447003 | -1.240697 | 0.306190 |
| H | 2.974576 | -0.348315 | 0.604313 |
| H | 2.769069 | -1.747290 | -0.301716 |
| C | 4.663656 | -0.883684 | -0.470329 |
| C | 3.688718 | -2.075399 | 1.512529 |
| H | 5.137838 | -1.791066 | -0.843506 |
| H | 4.361950 | -0.244413 | -1.298218 |
| H | 5.351208 | -0.338700 | 0.175564 |
| H | 4.185653 | -2.999879 | 1.219384 |
| H | 4.311615 | -1.520586 | 2.213508 |
| H | 2.721884 | -2.300769 | 1.958591 |

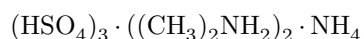


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|---|-----------|-----------|-----------|
| S | 0.220973 | -0.418896 | -0.492254 |
| O | 1.463090 | -0.451889 | -1.480291 |
| O | -0.730132 | -1.399465 | -1.005181 |
| O | -0.333788 | 0.968472 | -0.565734 |
| O | 0.727658 | -0.713124 | 0.857816 |
| H | 2.267464 | -0.023566 | -1.023222 |
| N | -2.054604 | -1.562399 | 1.767169 |
| H | -2.347721 | -1.841234 | 2.698330 |
| H | -2.099337 | -2.380418 | 1.164871 |
| H | -2.704225 | -0.217136 | 0.784576 |
| H | -1.058922 | -1.321009 | 1.795296 |
| C | -3.577703 | 0.062163 | -1.096214 |
| H | -4.560885 | -0.314604 | -0.808408 |
| H | -2.965868 | -0.731746 | -1.520964 |
| H | -3.691052 | 0.866518 | -1.824001 |
| N | -2.864095 | 0.577198 | 0.097385 |
| C | -3.520234 | 1.714135 | 0.775087 |
| H | -1.866406 | 0.842246 | -0.196729 |
| H | -4.510037 | 1.420320 | 1.128617 |
| H | -2.906498 | 2.020176 | 1.621965 |
| H | -3.615640 | 2.550026 | 0.081241 |
| N | 3.584697 | 0.566905 | -0.183632 |
| C | 4.098826 | -0.569637 | 0.593209 |
| C | 3.142716 | 1.684862 | 0.661844 |
| H | 4.300807 | 0.890964 | -0.826680 |
| H | 3.275877 | -0.985321 | 1.176398 |

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|---|----------|-----------|-----------|
| H | 4.456942 | -1.342222 | -0.090117 |
| H | 4.917003 | -0.286278 | 1.271164 |
| H | 2.309621 | 1.341546 | 1.276281 |
| H | 3.942106 | 2.063095 | 1.315619 |
| H | 2.782964 | 2.497964 | 0.028953 |



| | | | |
|---|-----------|-----------|-----------|
| S | -2.241362 | -0.408613 | -0.019719 |
| O | -3.636553 | -0.701872 | -0.164317 |
| N | 0.198638 | -1.000940 | 2.706801 |
| H | -0.727801 | -0.689693 | 2.328783 |
| H | 0.417067 | -1.920963 | 2.318788 |
| O | -1.818982 | 0.130992 | 1.294228 |
| O | -1.673199 | 0.453737 | -1.109761 |
| N | -0.004957 | -1.069431 | -2.684995 |
| H | 0.093910 | -0.997603 | -3.693331 |
| H | -0.816884 | -0.519823 | -2.331091 |
| S | 2.092393 | -0.636998 | 0.038320 |
| O | 3.451548 | -1.089791 | 0.193438 |
| O | 1.723481 | 0.407150 | 1.107835 |
| O | 1.088573 | -1.759219 | 0.179812 |
| O | 1.835279 | 0.034733 | -1.294253 |
| O | -1.480841 | -1.819500 | -0.180967 |
| H | -0.487330 | -1.717340 | -0.025682 |
| H | -0.545287 | 1.671148 | -0.512471 |
| H | 0.918676 | -0.347705 | 2.240627 |
| H | 0.228244 | -0.999413 | 3.721756 |
| H | -0.140960 | -2.039935 | -2.408810 |
| H | 0.871704 | -0.657273 | -2.139359 |
| N | 0.152416 | 2.281706 | -0.033175 |
| C | -0.555123 | 3.101456 | 0.982235 |
| C | 0.929923 | 3.065160 | -1.026208 |
| H | 0.805208 | 1.593454 | 0.442742 |
| H | -1.209166 | 3.815093 | 0.480261 |
| H | -1.152453 | 2.431475 | 1.596931 |
| H | 0.176890 | 3.636195 | 1.587955 |
| H | 0.252667 | 3.678967 | -1.621151 |
| H | 1.638141 | 3.704028 | -0.498270 |
| H | 1.474956 | 2.360279 | -1.649991 |



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|---|-----------|-----------|-----------|
| S | -3.681499 | 0.049504 | 0.245008 |
| O | -3.568652 | 1.414648 | -0.271151 |
| O | -5.286923 | -0.165568 | 0.294265 |
| O | -3.159046 | -0.967952 | -0.675862 |
| H | -5.453166 | -1.067977 | 0.601488 |
| S | 1.942930 | 2.106100 | 0.061404 |
| O | 2.310772 | 1.109370 | 1.094906 |
| O | 2.821942 | 3.228905 | -0.072583 |
| O | 2.052911 | 1.309771 | -1.351088 |
| S | 0.233272 | -1.801708 | -0.524788 |
| O | 0.070279 | -0.475851 | -1.183909 |
| O | 0.309721 | -1.653466 | 0.938980 |
| O | 1.360348 | -2.556880 | -1.060859 |
| O | -1.059597 | -2.630208 | -0.884052 |
| H | -1.864947 | -2.060173 | -0.745666 |
| O | -3.197647 | -0.106104 | 1.619164 |
| N | -0.578161 | 0.669668 | 2.097838 |
| N | -1.354315 | 1.801362 | -1.766258 |

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|---|-----------|-----------|-----------|
| H | -2.286569 | 1.751345 | -1.281573 |
| H | -1.418631 | 2.281525 | -2.659664 |
| H | -0.660398 | 2.259636 | -1.135508 |
| H | -1.024157 | 0.829333 | -1.882231 |
| H | 1.375844 | 0.585141 | -1.343932 |
| H | -1.611145 | 0.557146 | 2.035281 |
| H | -0.233967 | 1.442926 | 1.490166 |
| H | -0.159860 | -0.217065 | 1.732189 |
| H | -0.282370 | 0.830483 | 3.056718 |
| O | 0.492691 | 2.440652 | 0.199844 |
| N | 3.447003 | -1.240697 | 0.306190 |
| H | 2.974576 | -0.348315 | 0.604313 |
| H | 2.769069 | -1.747290 | -0.301716 |
| C | 4.663656 | -0.883684 | -0.470329 |
| C | 3.688718 | -2.075399 | 1.512529 |
| H | 5.137838 | -1.791066 | -0.843506 |
| H | 4.361950 | -0.244413 | -1.298218 |
| H | 5.351208 | -0.338700 | 0.175564 |
| H | 4.185653 | -2.999879 | 1.219384 |
| H | 4.311615 | -1.520586 | 2.213508 |
| H | 2.721884 | -2.300769 | 1.958591 |