

## Theoretically mechanistic insights on the polar hydrohalogenation of olefins

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### Supporting Information

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## 1. Details of Calculation

All of the DFT calculations were performed with the Gaussian 09 program package.<sup>1</sup> The geometry optimization of all the minima and transition states involved were performed at the M06-2X levels of theory<sup>2</sup> with the def2TZVP basis set for all atoms. The solution conditions are given by SMD model.<sup>3</sup> The vibrational frequencies were computed at the same level of theory to check whether every optimized geometrical structure is an energy minimum or a transition state and get the correction of the Gibbs free energy. IRC calculations<sup>4-5</sup> were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. The high accurate zero-point energy is given under the level DLPNO-CCSD(T)/aug-cc-pVTZ using ORCA 5 package.<sup>6-14</sup> Solvent effects were computed by the uESE software<sup>15-18</sup> at the B3LYP/def2-TZVP level using the optimized structures. CM5 charges are given by Multiwfn program.<sup>19-23</sup> The Mayer bond order, Hirshfeld atomic charges, and Electron Localization Function (ELF) analysis are all given by Multiwfn program. The general order of Gaussian and ORCA are given below:

Gaussian: opt freq scrf = (smd, solvent = aceticacid) def2tzvp int = (ultrafine, acc2e = 12) m062x.

ORCA: ! DLPNO-CCSD(T) normal PNO RIJK aug-cc-pVTZ aug-cc-pVTZ/JK aug-cc-pVTZ/C tightSCF miniprint nopop.

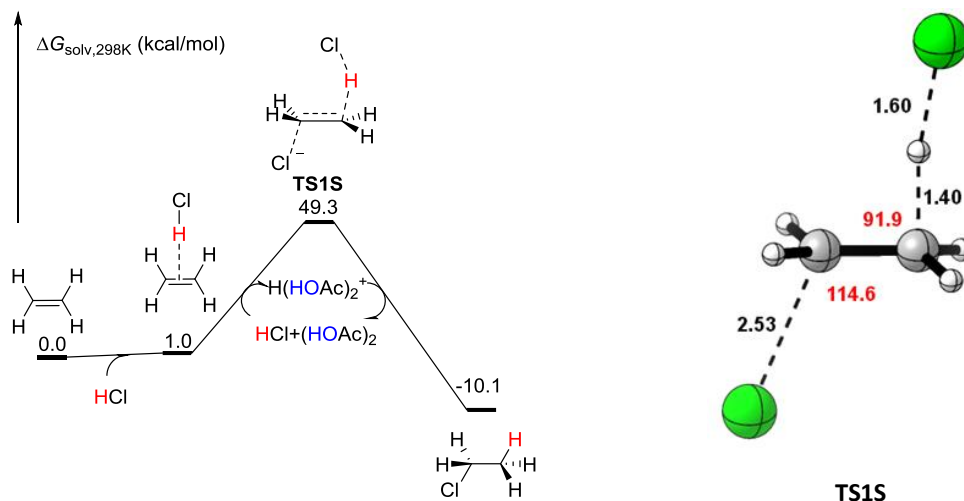
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## 2. Other Structures and Details of Cyclic Proton Transferring Mechanism

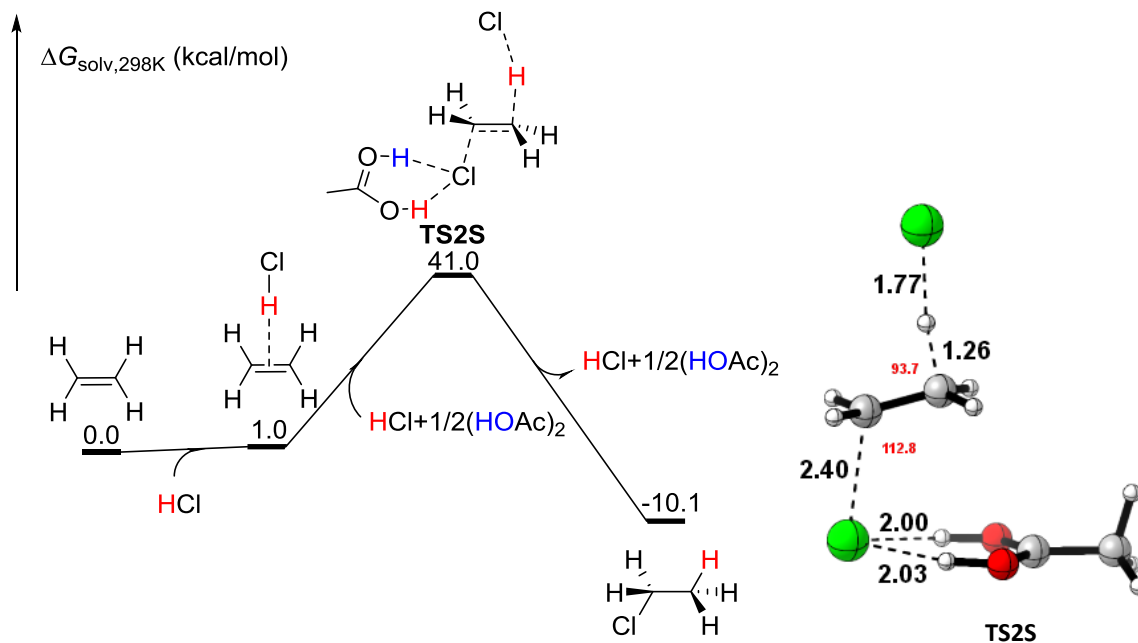
To find the most reasonable transition state structure for the *anti*-addition, we have tried many structures (more than 10), some of them were given below.

### (1) Ionic mechanism

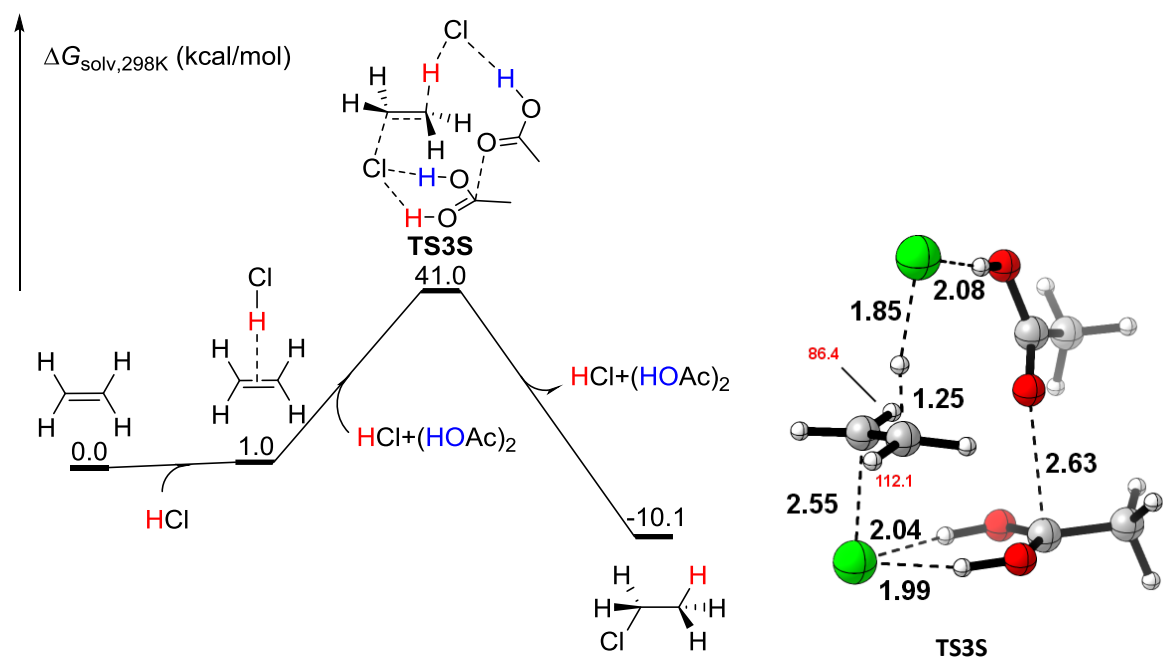


Note: The structure  $\text{H}(\text{HOAc})_2^+$  has a small imaginary vibrational mode and cannot be removed

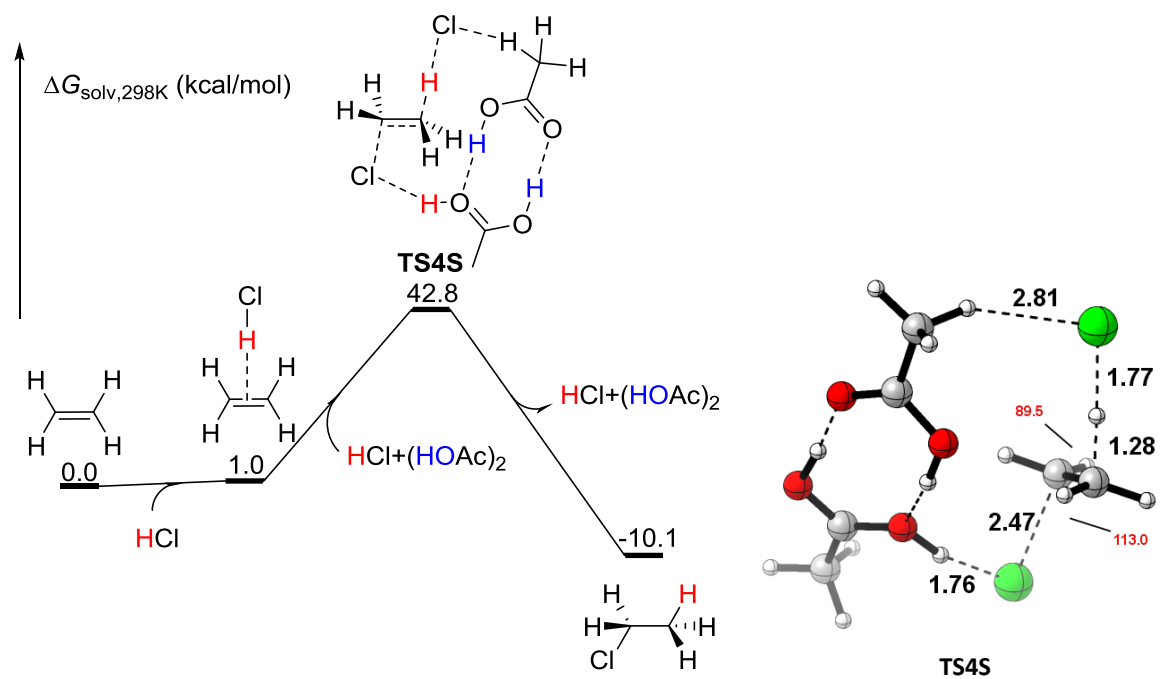
### (2) Reaction involving one molecule of acetic acid



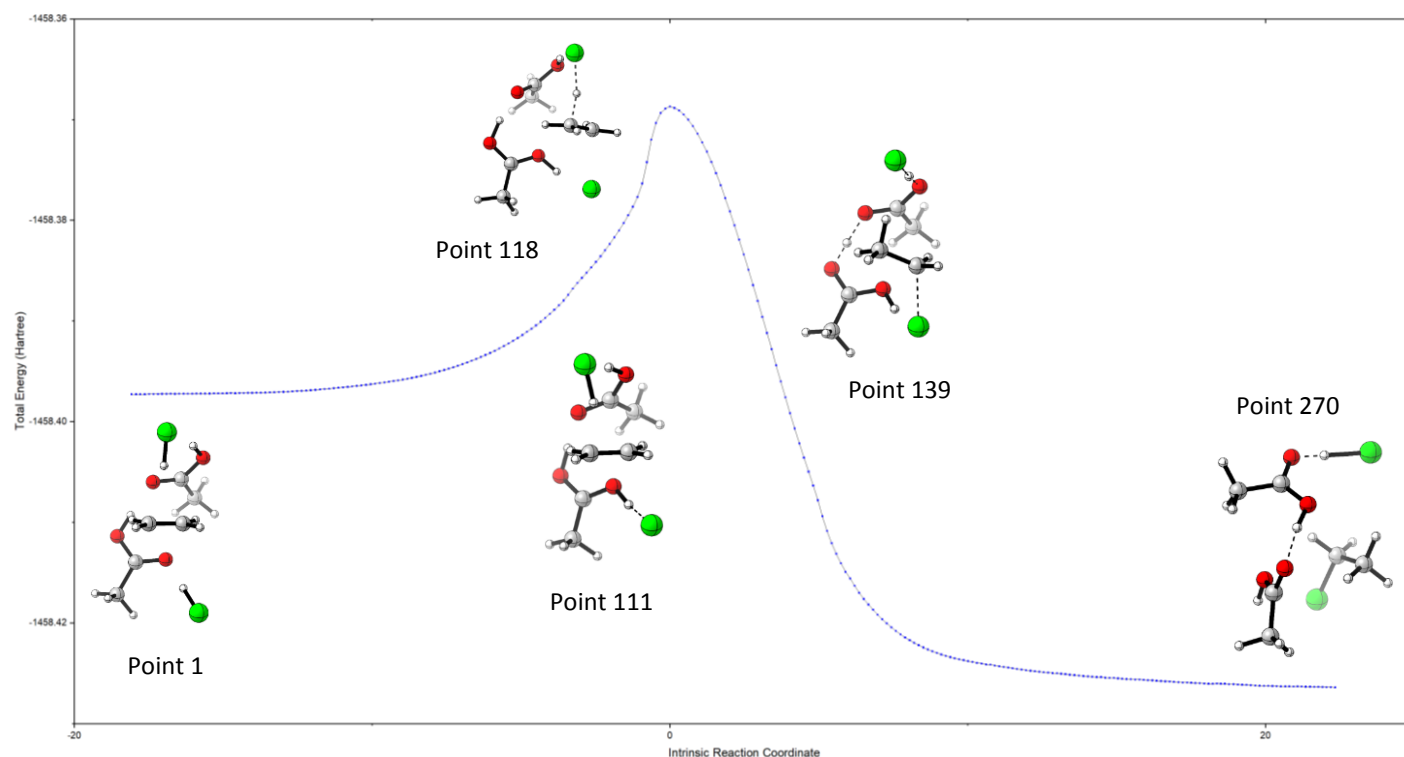
**(3) Reaction involving two molecules of acetic acid in another combination mode**



**(4) Reaction involving one acetic acid dimer.**

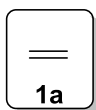


The *anti*-addition follows the Cyclic Proton Transferring Mechanism. Details of the mechanism are shown below according to the IRC path way.



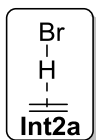
At the starting of the reaction (Point 1), HCl coordinates with ethene to form a  $\pi$ -complex. Then hydrogen chloride which gives its chloride to ethene breaks its H-Cl bond first and generates chloride (Point 111). Then the coordinated hydrogen chloride breaks its H-Cl bond to give its proton to ethene (Point 118). After addition, two protons from acetic acid transfer (Point 139) to get the product (Point 270).

### 3. Coordinates of All Stationary Points



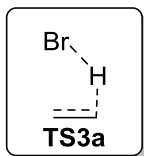
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.000000               | -0.000000 | 0.661508  |
| 2                | 1                | 0              | 0.000000                | 0.923959  | 1.228852  |
| 3                | 1                | 0              | -0.000000               | -0.923959 | 1.228852  |
| 4                | 6                | 0              | 0.000000                | -0.000000 | -0.661508 |
| 5                | 1                | 0              | -0.000000               | -0.923959 | -1.228852 |
| 6                | 1                | 0              | 0.000000                | 0.923959  | -1.228852 |



Standard orientation:

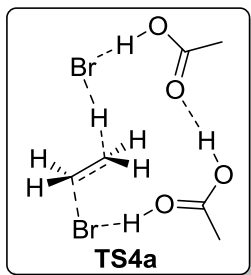
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.575590               | -0.662613 | 0.002350  |
| 2                | 1                | 0              | -2.548387               | -1.229223 | 0.926565  |
| 3                | 1                | 0              | -2.605523               | -1.229161 | -0.921741 |
| 4                | 6                | 0              | -2.575826               | 0.662747  | 0.002338  |
| 5                | 1                | 0              | -2.605942               | 1.229245  | -0.921771 |
| 6                | 1                | 0              | -2.548827               | 1.229372  | 0.926539  |
| 7                | 1                | 0              | -0.250100               | -0.004115 | -0.008384 |
| 8                | 35               | 0              | 1.184779                | 0.000088  | -0.000838 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

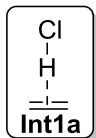
|   |    |   |           |           |           |
|---|----|---|-----------|-----------|-----------|
| 1 | 6  | 0 | 1.765372  | 0.738022  | 0.000292  |
| 2 | 6  | 0 | 2.387171  | -0.497164 | 0.000190  |
| 3 | 1  | 0 | 1.509888  | 1.237769  | 0.924946  |
| 4 | 1  | 0 | 2.746505  | -0.912367 | -0.932753 |
| 5 | 1  | 0 | 2.746217  | -0.912671 | 0.933109  |
| 6 | 1  | 0 | 1.185453  | -0.687770 | -0.000027 |
| 7 | 35 | 0 | -0.988956 | -0.040233 | -0.000111 |
| 8 | 1  | 0 | 1.510154  | 1.238042  | -0.924290 |



Standard orientation:

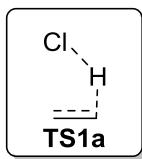
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|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.344649               | -1.284351 | -1.010867 |
| 2                | 6                | 0              | 0.048661                | -1.576643 | 0.271747  |
| 3                | 1                | 0              | -0.274199               | -0.265289 | -1.377335 |
| 4                | 1                | 0              | -1.578314               | -1.280260 | -0.604719 |
| 5                | 1                | 0              | 2.220644                | 0.212207  | 0.291744  |
| 6                | 6                | 0              | 1.892056                | 1.686530  | -0.956662 |
| 7                | 8                | 0              | 1.624458                | 1.050513  | 0.114667  |
| 8                | 8                | 0              | 1.049592                | 2.531748  | -1.374600 |
| 9                | 1                | 0              | 0.126290                | 2.445119  | -0.856720 |
| 10               | 6                | 0              | 3.136053                | 1.445799  | -1.715586 |
| 11               | 1                | 0              | 3.990190                | 1.467218  | -1.039188 |
| 12               | 1                | 0              | 3.074471                | 0.439640  | -2.140584 |
| 13               | 1                | 0              | 3.241411                | 2.178766  | -2.509258 |
| 14               | 6                | 0              | -1.238160               | 1.946916  | 0.939118  |
| 15               | 8                | 0              | -1.099993               | 2.002706  | -0.280864 |
| 16               | 8                | 0              | -2.157442               | 1.195485  | 1.485020  |
| 17               | 1                | 0              | -2.641005               | 0.650630  | 0.806114  |
| 18               | 6                | 0              | -0.405759               | 2.698682  | 1.917100  |
| 19               | 1                | 0              | 0.131635                | 1.984892  | 2.543436  |
| 20               | 1                | 0              | 0.294868                | 3.352939  | 1.406015  |
| 21               | 1                | 0              | -1.063334               | 3.279241  | 2.565044  |
| 22               | 1                | 0              | -0.334539               | -2.071097 | -1.756894 |
| 23               | 1                | 0              | 0.060837                | -2.599567 | 0.624780  |
| 24               | 1                | 0              | 0.088454                | -0.802055 | 1.028152  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 25 | 35 | 0 | -3.454939 | -1.026146 | -0.419405 |
| 26 | 35 | 0 | 2.849238  | -1.623499 | 0.556449  |



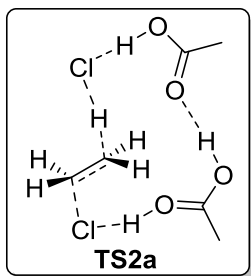
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| 1                | 6                | 0              | 1.851722                | 0.662760  | 0.002410  |
| 2                | 1                | 0              | 1.821045                | 1.229258  | 0.926531  |
| 3                | 1                | 0              | 1.885083                | 1.229197  | -0.921581 |
| 4                | 6                | 0              | 1.852645                | -0.662706 | 0.002455  |
| 5                | 1                | 0              | 1.886945                | -1.229169 | -0.921468 |
| 6                | 1                | 0              | 1.822818                | -1.229146 | 0.926636  |
| 7                | 17               | 0              | -1.718639               | -0.000322 | -0.001528 |
| 8                | 1                | 0              | -0.425237               | 0.005010  | -0.013336 |



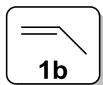
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| 1                | 6                | 0              | -1.143030               | 0.736794  | 0.000238  |
| 2                | 6                | 0              | -1.806651               | -0.475712 | 0.000148  |
| 3                | 1                | 0              | -0.870000               | 1.226765  | -0.924466 |
| 4                | 1                | 0              | -2.184024               | -0.874726 | 0.932969  |
| 5                | 1                | 0              | -2.184169               | -0.874507 | -0.932708 |
| 6                | 17               | 0              | 1.436876                | -0.091464 | -0.000185 |
| 7                | 1                | 0              | -0.620761               | -0.715674 | 0.000025  |
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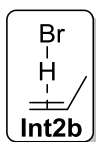
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| 1                | 6                | 0              | 0.421929                | 1.791931  | -0.933922 |
| 2                | 6                | 0              | 0.242220                | 1.983025  | 0.416250  |
| 3                | 1                | 0              | 0.186481                | 0.827093  | -1.371266 |
| 4                | 1                | 0              | 1.669325                | 1.628697  | -0.706151 |
| 5                | 1                | 0              | -1.992667               | 0.417277  | 0.600263  |
| 6                | 6                | 0              | -2.015422               | -1.083519 | -0.692506 |
| 7                | 8                | 0              | -1.516658               | -0.479986 | 0.308019  |
| 8                | 8                | 0              | -1.318495               | -1.973093 | -1.265559 |
| 9                | 1                | 0              | -0.310124               | -1.942054 | -0.929681 |
| 10               | 6                | 0              | -3.360588               | -0.758479 | -1.210519 |
| 11               | 1                | 0              | -4.057970               | -0.633150 | -0.383679 |
| 12               | 1                | 0              | -3.283731               | 0.199161  | -1.734278 |
| 13               | 1                | 0              | -3.694529               | -1.525260 | -1.902805 |
| 14               | 6                | 0              | 1.336914                | -1.639038 | 0.635483  |
| 15               | 8                | 0              | 1.013933                | -1.582023 | -0.550390 |
| 16               | 8                | 0              | 2.362783                | -0.978334 | 1.095379  |
| 17               | 1                | 0              | 2.771991                | -0.390103 | 0.396182  |
| 18               | 6                | 0              | 0.613925                | -2.440168 | 1.661101  |
| 19               | 1                | 0              | 0.200297                | -1.760916 | 2.408248  |
| 20               | 1                | 0              | -0.179790               | -3.025042 | 1.205151  |
| 21               | 1                | 0              | 1.325798                | -3.094804 | 2.164686  |
| 22               | 1                | 0              | 0.376656                | 2.650507  | -1.594179 |
| 23               | 17               | 0              | 3.402714                | 1.149536  | -0.774169 |
| 24               | 17               | 0              | -2.308761               | 2.116696  | 1.005826  |
| 25               | 1                | 0              | 0.372977                | 2.964306  | 0.854339  |
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Standard orientation:

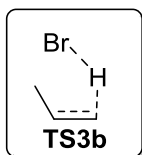
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|        |        |        |                         |  |  |

| Number | Number | Type | X         | Y         | Z         |
|--------|--------|------|-----------|-----------|-----------|
| 1      | 6      | 0    | 0.133259  | -0.455035 | 0.000001  |
| 2      | 6      | 0    | 1.273357  | 0.221101  | -0.000002 |
| 3      | 1      | 0    | 2.231119  | -0.285578 | -0.000000 |
| 4      | 1      | 0    | 1.287474  | 1.306464  | -0.000005 |
| 5      | 6      | 0    | -1.226888 | 0.163272  | 0.000001  |
| 6      | 1      | 0    | -1.169195 | 1.252273  | -0.000009 |
| 7      | 1      | 0    | -1.797039 | -0.153644 | -0.876979 |
| 8      | 1      | 0    | -1.797032 | -0.153627 | 0.876992  |
| 9      | 1      | 0    | 0.166299  | -1.541917 | 0.000005  |



Standard orientation:

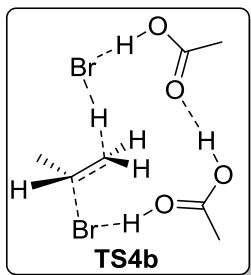
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| 1                | 6                | 0              | -2.250488               | 0.168932  | -0.428883 |
| 2                | 6                | 0              | -1.998410               | 1.290261  | 0.238238  |
| 3                | 1                | 0              | -2.016021               | 2.256320  | -0.251964 |
| 4                | 1                | 0              | -1.781163               | 1.277387  | 1.302286  |
| 5                | 1                | 0              | 0.113644                | 0.403146  | -0.111102 |
| 6                | 6                | 0              | -2.242026               | -1.198448 | 0.170119  |
| 7                | 1                | 0              | -1.984369               | -1.170136 | 1.229507  |
| 8                | 1                | 0              | -3.221098               | -1.672002 | 0.062012  |
| 9                | 1                | 0              | -1.526213               | -1.843473 | -0.346693 |
| 10               | 1                | 0              | -2.472353               | 0.228867  | -1.491495 |
| 11               | 35               | 0              | 1.480946                | -0.029845 | -0.007697 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 6                | 0              | -1.759286               | 0.078967 | 0.478504  |
| 2                | 6                | 0              | -1.729922               | 1.318336 | -0.174015 |
| 3                | 1                | 0              | -1.495791               | 0.048329 | 1.531664  |

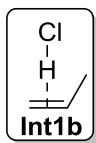
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 4  | 1  | 0 | -2.163112 | 1.368404  | -1.167843 |
| 5  | 1  | 0 | -1.786882 | 2.210207  | 0.440775  |
| 6  | 6  | 0 | -2.085719 | -1.176870 | -0.174017 |
| 7  | 1  | 0 | -2.030631 | -1.115022 | -1.258795 |
| 8  | 1  | 0 | -1.517346 | -2.012568 | 0.226053  |
| 9  | 1  | 0 | -3.142551 | -1.340596 | 0.103915  |
| 10 | 1  | 0 | -0.580925 | 1.118274  | -0.316674 |
| 11 | 35 | 0 | 1.319052  | -0.045704 | -0.009769 |



Standard orientation:

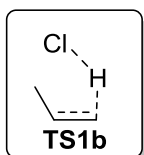
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.395942               | -1.135096 | -1.089273 |
| 2                | 6                | 0              | -0.098948               | -1.492074 | 0.212771  |
| 3                | 1                | 0              | -0.135448               | -0.141111 | -1.435689 |
| 4                | 1                | 0              | -1.593357               | -1.004290 | -0.764918 |
| 5                | 1                | 0              | 2.255331                | 0.234064  | 0.235887  |
| 6                | 6                | 0              | 1.965770                | 1.877354  | -0.815666 |
| 7                | 8                | 0              | 1.639787                | 1.091738  | 0.128664  |
| 8                | 8                | 0              | 1.136712                | 2.766246  | -1.173180 |
| 9                | 1                | 0              | 0.190948                | 2.611454  | -0.722571 |
| 10               | 6                | 0              | 3.266833                | 1.770506  | -1.507907 |
| 11               | 1                | 0              | 4.070125                | 1.729009  | -0.772567 |
| 12               | 1                | 0              | 3.275125                | 0.825932  | -2.058558 |
| 13               | 1                | 0              | 3.399254                | 2.603113  | -2.191583 |
| 14               | 6                | 0              | -1.222662               | 2.021723  | 0.994297  |
| 15               | 8                | 0              | -1.056875               | 2.124849  | -0.218878 |
| 16               | 8                | 0              | -2.164040               | 1.264748  | 1.492243  |
| 17               | 1                | 0              | -2.657229               | 0.765659  | 0.781400  |
| 18               | 6                | 0              | -0.393754               | 2.716473  | 2.017867  |
| 19               | 1                | 0              | 0.168978                | 1.966712  | 2.577222  |
| 20               | 1                | 0              | 0.287690                | 3.420795  | 1.549236  |
| 21               | 1                | 0              | -1.050796               | 3.230539  | 2.719377  |
| 22               | 1                | 0              | -0.436136               | -1.919078 | -1.839315 |
| 23               | 1                | 0              | 0.075689                | -0.697902 | 0.934218  |
| 24               | 35               | 0              | -3.556824               | -0.752221 | -0.539633 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 25 | 35 | 0 | 2.987336  | -1.522985 | 0.341010  |
| 26 | 6  | 0 | -0.312970 | -2.839309 | 0.750685  |
| 27 | 1  | 0 | -0.262251 | -3.609079 | -0.016167 |
| 28 | 1  | 0 | 0.375940  | -3.047716 | 1.567022  |
| 29 | 1  | 0 | -1.326409 | -2.834007 | 1.181384  |



Standard orientation:

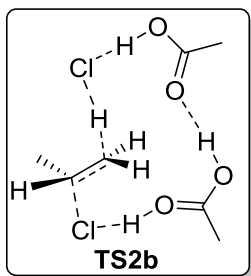
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.559549               | 0.185338  | -0.421006 |
| 2                | 6                | 0              | -1.257166               | 1.296382  | 0.242328  |
| 3                | 1                | 0              | -1.270234               | 2.265485  | -0.241917 |
| 4                | 1                | 0              | -1.001050               | 1.272181  | 1.297476  |
| 5                | 17               | 0              | 2.016956                | -0.075705 | -0.017711 |
| 6                | 1                | 0              | 0.808748                | 0.364113  | -0.169254 |
| 7                | 6                | 0              | -1.565097               | -1.185813 | 0.170324  |
| 8                | 1                | 0              | -1.260221               | -1.171492 | 1.217294  |
| 9                | 1                | 0              | -2.562446               | -1.627762 | 0.103405  |
| 10               | 1                | 0              | -0.893083               | -1.848370 | -0.381528 |
| 11               | 1                | 0              | -1.819097               | 0.257388  | -1.474274 |



Standard orientation:

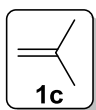
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.120318               | 0.087179  | 0.477342  |
| 2                | 6                | 0              | -1.086513               | 1.326659  | -0.170786 |
| 3                | 1                | 0              | -0.831745               | 0.049748  | 1.523381  |
| 4                | 1                | 0              | -1.534596               | 1.389679  | -1.156850 |
| 5                | 1                | 0              | -1.101783               | 2.218359  | 0.446191  |
| 6                | 6                | 0              | -1.478573               | -1.162838 | -0.170867 |
| 7                | 1                | 0              | -1.461471               | -1.094651 | -1.256428 |
| 8                | 1                | 0              | -0.898326               | -2.002304 | 0.204020  |
| 9                | 1                | 0              | -2.523659               | -1.325189 | 0.146686  |

|    |    |   |          |           |           |
|----|----|---|----------|-----------|-----------|
| 10 | 17 | 0 | 1.788972 | -0.107253 | -0.023117 |
| 11 | 1  | 0 | 0.051472 | 1.081667  | -0.328138 |



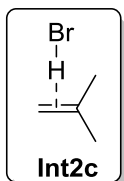
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.561677                | 1.457774  | -1.160812 |
| 2                | 6                | 0              | 0.497619                | 1.807338  | 0.182020  |
| 3                | 1                | 0              | 0.073064                | 0.543302  | -1.480078 |
| 4                | 1                | 0              | 1.715992                | 1.099336  | -1.008695 |
| 5                | 1                | 0              | -2.037629               | 0.509134  | 0.473635  |
| 6                | 6                | 0              | -2.203759               | -1.167487 | -0.593410 |
| 7                | 8                | 0              | -1.622487               | -0.468510 | 0.289770  |
| 8                | 8                | 0              | -1.600653               | -2.182988 | -1.058460 |
| 9                | 1                | 0              | -0.586223               | -2.198342 | -0.751479 |
| 10               | 6                | 0              | -3.545619               | -0.819948 | -1.108269 |
| 11               | 1                | 0              | -4.202803               | -0.557426 | -0.280454 |
| 12               | 1                | 0              | -3.434891               | 0.065913  | -1.740230 |
| 13               | 1                | 0              | -3.950145               | -1.639482 | -1.694228 |
| 14               | 6                | 0              | 1.125208                | -1.885380 | 0.747323  |
| 15               | 8                | 0              | 0.783781                | -1.938582 | -0.433752 |
| 16               | 8                | 0              | 2.225017                | -1.291222 | 1.115587  |
| 17               | 1                | 0              | 2.689806                | -0.837844 | 0.345115  |
| 18               | 6                | 0              | 0.340470                | -2.472628 | 1.869467  |
| 19               | 1                | 0              | 0.024682                | -1.668382 | 2.535903  |
| 20               | 1                | 0              | -0.526000               | -3.010739 | 1.494737  |
| 21               | 1                | 0              | 0.985356                | -3.142338 | 2.439182  |
| 22               | 1                | 0              | 0.616776                | 2.260304  | -1.889835 |
| 23               | 1                | 0              | 0.309732                | 1.018598  | 0.905273  |
| 24               | 6                | 0              | 0.974449                | 3.086860  | 0.709362  |
| 25               | 1                | 0              | 0.934891                | 3.885729  | -0.027430 |
| 26               | 1                | 0              | 0.444382                | 3.354488  | 1.621522  |
| 27               | 1                | 0              | 2.024449                | 2.916203  | 0.993405  |
| 28               | 17               | 0              | 3.508807                | 0.415319  | -0.966076 |
| 29               | 17               | 0              | -2.324511               | 2.197198  | 0.665159  |



Standard orientation:

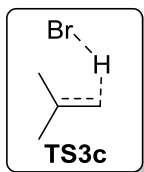
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.000000               | 0.124939  | -0.000061 |
| 2                | 6                | 0              | -0.000003               | 1.453982  | 0.000003  |
| 3                | 1                | 0              | -0.925540               | 2.018874  | 0.000152  |
| 4                | 1                | 0              | 0.925533                | 2.018878  | -0.000084 |
| 5                | 6                | 0              | -1.267723               | -0.676659 | 0.000001  |
| 6                | 1                | 0              | -2.151217               | -0.038736 | 0.000360  |
| 7                | 1                | 0              | -1.309592               | -1.328237 | -0.877380 |
| 8                | 1                | 0              | -1.309238               | -1.328735 | 0.877032  |
| 9                | 6                | 0              | 1.267726                | -0.676655 | -0.000005 |
| 10               | 1                | 0              | 2.151217                | -0.038730 | -0.001606 |
| 11               | 1                | 0              | 1.310131                | -1.327165 | 0.878152  |
| 12               | 1                | 0              | 1.308710                | -1.329797 | -0.876257 |



Standard orientation:

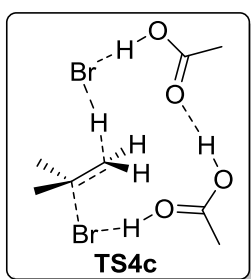
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.902606                | 0.002121  | 0.177252  |
| 2                | 6                | 0              | 1.563216                | -0.139873 | 1.458746  |
| 3                | 1                | 0              | 1.491887                | -1.119583 | 1.918307  |
| 4                | 1                | 0              | 1.367295                | 0.720652  | 2.089251  |
| 5                | 6                | 0              | 2.176679                | -1.173205 | -0.710011 |
| 6                | 1                | 0              | 2.072071                | -2.118138 | -0.177861 |
| 7                | 1                | 0              | 1.493132                | -1.174096 | -1.564277 |
| 8                | 1                | 0              | 3.188629                | -1.111483 | -1.119570 |
| 9                | 1                | 0              | -0.397031               | -0.091048 | 0.449785  |
| 10               | 6                | 0              | 1.996830                | 1.345985  | -0.477413 |
| 11               | 1                | 0              | 1.776106                | 2.154866  | 0.218355  |
| 12               | 1                | 0              | 2.998057                | 1.500010  | -0.888731 |
| 13               | 1                | 0              | 1.300242                | 1.408290  | -1.318936 |

14                      35                      0                      -1.746468                      -0.010847                      -0.065650



Standard orientation:

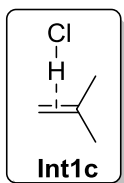
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.704781               | 0.000100  | 0.086894  |
| 2                | 6                | 0              | -1.396291               | -0.001350 | 1.467788  |
| 3                | 1                | 0              | -1.591411               | 0.920577  | 2.007823  |
| 4                | 1                | 0              | -1.591844               | -0.924176 | 2.006118  |
| 5                | 6                | 0              | -1.846416               | 1.266892  | -0.633684 |
| 6                | 1                | 0              | -1.386641               | 2.095069  | -0.098890 |
| 7                | 1                | 0              | -1.490768               | 1.199765  | -1.659268 |
| 8                | 1                | 0              | -2.931653               | 1.452919  | -0.667451 |
| 9                | 1                | 0              | -0.259305               | -0.001265 | 1.225580  |
| 10               | 35               | 0              | 1.595376                | -0.000099 | -0.059709 |
| 11               | 6                | 0              | -1.847866               | -1.265201 | -0.636097 |
| 12               | 1                | 0              | -1.386558               | -2.094261 | -0.103927 |
| 13               | 1                | 0              | -2.933096               | -1.451688 | -0.667164 |
| 14               | 1                | 0              | -1.494753               | -1.196119 | -1.662412 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.543096               | -1.134312 | -1.042096 |
| 2                | 6                | 0              | -0.343793               | -1.849365 | 0.107678  |
| 3                | 1                | 0              | -0.391223               | -0.060987 | -1.046095 |
| 4                | 1                | 0              | -1.858877               | -1.116257 | -0.735644 |
| 5                | 1                | 0              | 2.271459                | 0.188761  | 0.111752  |

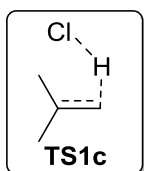
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 6  | 6  | 0 | 2.044004  | 1.931209  | -0.822331 |
| 7  | 8  | 0 | 1.620392  | 1.037391  | -0.033355 |
| 8  | 8  | 0 | 1.246494  | 2.855166  | -1.180342 |
| 9  | 1  | 0 | 0.276015  | 2.682993  | -0.830100 |
| 10 | 6  | 0 | 3.427749  | 1.934713  | -1.344279 |
| 11 | 1  | 0 | 4.126710  | 1.917804  | -0.507288 |
| 12 | 1  | 0 | 3.581753  | 1.016342  | -1.914781 |
| 13 | 1  | 0 | 3.592401  | 2.805512  | -1.970696 |
| 14 | 6  | 0 | -1.318523 | 2.290853  | 0.809367  |
| 15 | 8  | 0 | -1.050494 | 2.238106  | -0.386264 |
| 16 | 8  | 0 | -2.343729 | 1.646980  | 1.310543  |
| 17 | 1  | 0 | -2.783902 | 1.078128  | 0.629831  |
| 18 | 6  | 0 | -0.515691 | 3.039114  | 1.815227  |
| 19 | 1  | 0 | 0.084496  | 2.314534  | 2.371614  |
| 20 | 1  | 0 | 0.139615  | 3.754267  | 1.325411  |
| 21 | 1  | 0 | -1.175381 | 3.538435  | 2.522784  |
| 22 | 6  | 0 | -0.326555 | -3.330497 | 0.101146  |
| 23 | 1  | 0 | -0.586549 | -3.744642 | -0.870676 |
| 24 | 1  | 0 | 0.691089  | -3.642283 | 0.360528  |
| 25 | 1  | 0 | -0.989071 | -3.727652 | 0.873775  |
| 26 | 1  | 0 | -0.522521 | -1.644915 | -1.998320 |
| 27 | 6  | 0 | -0.316147 | -1.185427 | 1.432725  |
| 28 | 1  | 0 | -0.065525 | -0.129591 | 1.367893  |
| 29 | 1  | 0 | -1.316972 | -1.287329 | 1.873148  |
| 30 | 1  | 0 | 0.382062  | -1.693166 | 2.098650  |
| 31 | 35 | 0 | 3.221149  | -1.413216 | 0.311557  |
| 32 | 35 | 0 | -3.617852 | -0.719607 | -0.531301 |



Standard orientation:

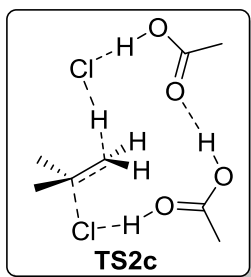
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.213926                | 0.000038  | 0.186207  |
| 2                | 6                | 0              | 0.842648                | -0.001796 | 1.466657  |
| 3                | 1                | 0              | 0.696274                | -0.928828 | 2.010183  |
| 4                | 1                | 0              | 0.694458                | 0.923704  | 2.012309  |
| 5                | 6                | 0              | 1.420376                | -1.266928 | -0.586437 |
| 6                | 1                | 0              | 1.231651                | -2.150585 | 0.022243  |
| 7                | 1                | 0              | 0.759864                | -1.293387 | -1.458080 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 8  | 1  | 0 | 2.443873  | -1.316139 | -0.968086 |
| 9  | 17 | 0 | -2.267319 | -0.000336 | -0.147208 |
| 10 | 1  | 0 | -1.077517 | -0.000513 | 0.379600  |
| 11 | 6  | 0 | 1.417950  | 1.269159  | -0.583537 |
| 12 | 1  | 0 | 1.226297  | 2.151044  | 0.026804  |
| 13 | 1  | 0 | 2.441754  | 1.321807  | -0.963906 |
| 14 | 1  | 0 | 0.758377  | 1.295779  | -1.455880 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.142734               | 0.006587  | 0.108500  |
| 2                | 6                | 0              | -0.745770               | -0.098283 | 1.470690  |
| 3                | 1                | 0              | -0.942212               | 0.769383  | 2.092819  |
| 4                | 1                | 0              | -0.929362               | -1.062289 | 1.937709  |
| 5                | 6                | 0              | -1.236391               | 1.311020  | -0.534099 |
| 6                | 1                | 0              | -1.511995               | 2.111537  | 0.147716  |
| 7                | 1                | 0              | -0.189737               | 1.480678  | -0.850465 |
| 8                | 1                | 0              | -1.844605               | 1.292388  | -1.436555 |
| 9                | 17               | 0              | 2.106081                | -0.010505 | -0.141715 |
| 10               | 1                | 0              | 0.370828                | -0.084743 | 1.207352  |
| 11               | 6                | 0              | -1.300922               | -1.195571 | -0.705975 |
| 12               | 1                | 0              | -0.819568               | -2.066443 | -0.267417 |
| 13               | 1                | 0              | -2.388329               | -1.375955 | -0.719159 |
| 14               | 1                | 0              | -0.993504               | -1.028490 | -1.737552 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

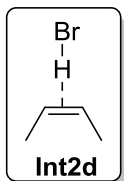
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 1  | 6  | 0 | 0.794760  | 1.247444  | -1.121082 |
| 2  | 6  | 0 | 0.899801  | 1.996456  | 0.036679  |
| 3  | 1  | 0 | 0.324311  | 0.271456  | -1.070651 |
| 4  | 1  | 0 | 1.998985  | 0.893596  | -0.998289 |
| 5  | 1  | 0 | -2.077939 | 0.654545  | 0.350646  |
| 6  | 6  | 0 | -2.380699 | -1.089260 | -0.628669 |
| 7  | 8  | 0 | -1.688930 | -0.370790 | 0.141675  |
| 8  | 8  | 0 | -1.876706 | -2.165965 | -1.091331 |
| 9  | 1  | 0 | -0.866211 | -2.252460 | -0.840699 |
| 10 | 6  | 0 | -3.757639 | -0.720876 | -1.028600 |
| 11 | 1  | 0 | -4.335985 | -0.461026 | -0.142483 |
| 12 | 1  | 0 | -3.697577 | 0.171011  | -1.657051 |
| 13 | 1  | 0 | -4.223069 | -1.533037 | -1.578175 |
| 14 | 6  | 0 | 0.918020  | -2.186927 | 0.640907  |
| 15 | 8  | 0 | 0.569401  | -2.156898 | -0.536008 |
| 16 | 8  | 0 | 2.098706  | -1.773399 | 1.019481  |
| 17 | 1  | 0 | 2.603227  | -1.344938 | 0.272266  |
| 18 | 6  | 0 | 0.049758  | -2.656727 | 1.756801  |
| 19 | 1  | 0 | -0.267503 | -1.781720 | 2.329195  |
| 20 | 1  | 0 | -0.822431 | -3.177971 | 1.371556  |
| 21 | 1  | 0 | 0.622141  | -3.302004 | 2.421892  |
| 22 | 6  | 0 | 1.229756  | 3.433783  | -0.010396 |
| 23 | 1  | 0 | 1.519922  | 3.764038  | -1.005113 |
| 24 | 1  | 0 | 0.315630  | 3.963796  | 0.285666  |
| 25 | 1  | 0 | 1.994770  | 3.684930  | 0.726405  |
| 26 | 1  | 0 | 0.755854  | 1.767687  | -2.071995 |
| 27 | 6  | 0 | 0.861796  | 1.355082  | 1.366782  |
| 28 | 1  | 0 | 0.313617  | 0.416668  | 1.368343  |
| 29 | 1  | 0 | 1.906406  | 1.155464  | 1.644580  |
| 30 | 1  | 0 | 0.456861  | 2.038703  | 2.112593  |
| 31 | 17 | 0 | 3.579382  | 0.021421  | -0.936079 |
| 32 | 17 | 0 | -2.463741 | 2.245275  | 0.591152  |



Standard orientation:

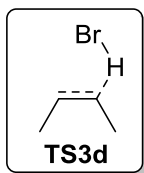
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.665079               | 0.663359  | 0.000545  |
| 2                | 6                | 0              | 0.665075                | 0.663357  | -0.000546 |
| 3                | 1                | 0              | 1.164098                | 1.628976  | -0.002178 |
| 4                | 6                | 0              | -1.577369               | -0.522513 | -0.000364 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 5  | 1 | 0 | -1.043234 | -1.470357 | -0.031697 |
| 6  | 1 | 0 | -2.210738 | -0.518876 | 0.890854  |
| 7  | 1 | 0 | -2.250152 | -0.484825 | -0.861119 |
| 8  | 6 | 0 | 1.577371  | -0.522512 | 0.000364  |
| 9  | 1 | 0 | 2.250151  | -0.484817 | 0.861121  |
| 10 | 1 | 0 | 1.043245  | -1.470361 | 0.031694  |
| 11 | 1 | 0 | 2.210741  | -0.518864 | -0.890853 |
| 12 | 1 | 0 | -1.164098 | 1.628979  | 0.002183  |



Standard orientation:

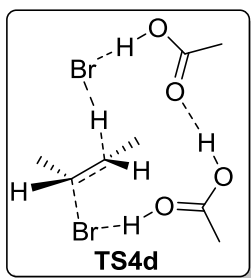
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.877052               | -0.662951 | 0.651132  |
| 2                | 6                | 0              | -1.867580               | 0.671505  | 0.651096  |
| 3                | 1                | 0              | -1.913114               | 1.169095  | 1.616236  |
| 4                | 6                | 0              | -1.832149               | -1.574123 | -0.533618 |
| 5                | 1                | 0              | -1.752546               | -1.042261 | -1.479919 |
| 6                | 1                | 0              | -0.986648               | -2.263112 | -0.454936 |
| 7                | 1                | 0              | -2.733502               | -2.191813 | -0.565663 |
| 8                | 6                | 0              | -1.806071               | 1.581975  | -0.533731 |
| 9                | 1                | 0              | -0.983265               | 2.293526  | -0.424868 |
| 10               | 1                | 0              | -1.674520               | 1.051356  | -1.475029 |
| 11               | 1                | 0              | -2.722379               | 2.174516  | -0.601618 |
| 12               | 1                | 0              | -1.927077               | -1.159884 | 1.616405  |
| 13               | 1                | 0              | 0.284937                | -0.000632 | 0.382080  |
| 14               | 35               | 0              | 1.677292                | -0.003692 | -0.000627 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |          |
|------------------|------------------|----------------|-------------------------|----------|----------|
|                  |                  |                | X                       | Y        | Z        |
| 1                | 6                | 0              | 1.239494                | 0.698359 | 0.697863 |

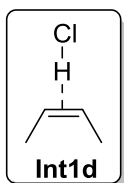
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 2  | 6  | 0 | 1.696626  | -0.626976 | 0.626480  |
| 3  | 1  | 0 | 0.753142  | 1.004596  | 1.618397  |
| 4  | 1  | 0 | 1.827594  | -1.109154 | 1.592713  |
| 5  | 6  | 0 | 1.357883  | 1.686626  | -0.364190 |
| 6  | 1  | 0 | 1.462936  | 1.245095  | -1.352193 |
| 7  | 1  | 0 | 0.562966  | 2.425301  | -0.331810 |
| 8  | 1  | 0 | 2.310057  | 2.196317  | -0.130197 |
| 9  | 1  | 0 | 0.558237  | -0.818839 | 0.398384  |
| 10 | 35 | 0 | -1.625174 | -0.143508 | -0.059261 |
| 11 | 6  | 0 | 2.553169  | -1.119309 | -0.513874 |
| 12 | 1  | 0 | 2.656391  | -2.200973 | -0.454946 |
| 13 | 1  | 0 | 2.117458  | -0.874850 | -1.482349 |
| 14 | 1  | 0 | 3.549271  | -0.676924 | -0.461529 |



Standard orientation:

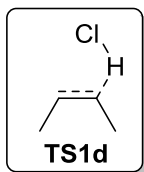
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.366580                | -1.137660 | 0.869206  |
| 2                | 6                | 0              | 0.071504                | -1.388376 | -0.466488 |
| 3                | 1                | 0              | 0.067721                | -0.160367 | 1.238982  |
| 4                | 1                | 0              | 1.505767                | -0.900538 | 0.477687  |
| 5                | 1                | 0              | -2.265708               | 0.344079  | -0.309638 |
| 6                | 6                | 0              | -2.042583               | 1.892399  | 0.885836  |
| 7                | 8                | 0              | -1.677181               | 1.193175  | -0.115088 |
| 8                | 8                | 0              | -1.233297               | 2.745493  | 1.348630  |
| 9                | 1                | 0              | -0.255284               | 2.637604  | 0.914355  |
| 10               | 6                | 0              | -3.368796               | 1.717799  | 1.514441  |
| 11               | 1                | 0              | -4.142142               | 1.715306  | 0.746581  |
| 12               | 1                | 0              | -3.382093               | 0.738738  | 2.001057  |
| 13               | 1                | 0              | -3.542340               | 2.499239  | 2.247611  |
| 14               | 6                | 0              | 1.134417                | 2.291703  | -0.817130 |
| 15               | 8                | 0              | 0.977414                | 2.239907  | 0.403055  |
| 16               | 8                | 0              | 2.087358                | 1.629877  | -1.410339 |
| 17               | 1                | 0              | 2.599431                | 1.045307  | -0.776246 |
| 18               | 6                | 0              | 0.279488                | 3.094742  | -1.733964 |
| 19               | 1                | 0              | -0.179996               | 2.428171  | -2.465005 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 20 | 1  | 0 | -0.484969 | 3.631117  | -1.177556 |
| 21 | 1  | 0 | 0.914362  | 3.796556  | -2.276486 |
| 22 | 1  | 0 | -0.076721 | -0.525586 | -1.109284 |
| 23 | 35 | 0 | 3.539431  | -0.605587 | 0.290104  |
| 24 | 35 | 0 | -2.904671 | -1.461436 | -0.576903 |
| 25 | 6  | 0 | 0.280372  | -2.689945 | -1.118971 |
| 26 | 1  | 0 | -0.085371 | -3.516395 | -0.512279 |
| 27 | 1  | 0 | -0.163315 | -2.714239 | -2.110103 |
| 28 | 1  | 0 | 1.369544  | -2.809744 | -1.228829 |
| 29 | 6  | 0 | 0.474910  | -2.242894 | 1.886642  |
| 30 | 1  | 0 | 1.070646  | -3.076401 | 1.515644  |
| 31 | 1  | 0 | 0.945964  | -1.869121 | 2.794406  |
| 32 | 1  | 0 | -0.521806 | -2.612144 | 2.139563  |



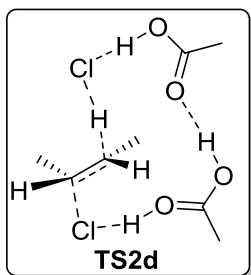
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.276319               | -0.658206 | 0.626847  |
| 2                | 6                | 0              | -1.259410               | 0.675832  | 0.626331  |
| 3                | 1                | 0              | -1.411448               | 1.175658  | 1.579259  |
| 4                | 6                | 0              | -1.106060               | -1.571930 | -0.545162 |
| 5                | 1                | 0              | -0.898005               | -1.042975 | -1.473551 |
| 6                | 1                | 0              | -0.292618               | -2.279489 | -0.363710 |
| 7                | 1                | 0              | -2.010762               | -2.168356 | -0.689927 |
| 8                | 6                | 0              | -1.063145               | 1.584084  | -0.546129 |
| 9                | 1                | 0              | -0.258784               | 2.296553  | -0.345712 |
| 10               | 1                | 0              | -0.824609               | 1.051318  | -1.465025 |
| 11               | 1                | 0              | -1.966635               | 2.174683  | -0.720283 |
| 12               | 1                | 0              | -1.438893               | -1.153449 | 1.580442  |
| 13               | 17               | 0              | 2.141543                | -0.013131 | 0.026400  |
| 14               | 1                | 0              | 0.925134                | -0.009390 | 0.478379  |



Standard orientation:

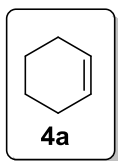
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.520110                | 0.671761  | 0.697235  |
| 2                | 6                | 0              | 1.105949                | -0.601285 | 0.617336  |
| 3                | 1                | 0              | -0.020496               | 0.909650  | 1.607679  |
| 4                | 1                | 0              | 1.254830                | -1.086495 | 1.579341  |
| 5                | 6                | 0              | 0.575142                | 1.689755  | -0.341470 |
| 6                | 1                | 0              | 0.747624                | 1.282558  | -1.334913 |
| 7                | 1                | 0              | -0.284452               | 2.352630  | -0.316978 |
| 8                | 1                | 0              | 1.469854                | 2.278313  | -0.069669 |
| 9                | 1                | 0              | 0.000960                | -0.893697 | 0.351818  |
| 10               | 6                | 0              | 2.041419                | -0.983374 | -0.502911 |
| 11               | 1                | 0              | 2.253371                | -2.049694 | -0.456477 |
| 12               | 1                | 0              | 1.609420                | -0.768318 | -1.479683 |
| 13               | 1                | 0              | 2.984912                | -0.442463 | -0.414354 |
| 14               | 17               | 0              | -2.086573               | -0.367272 | -0.134583 |



Standard orientation:

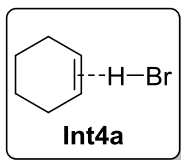
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.809556                | 1.347309  | -0.790409 |
| 2                | 6                | 0              | 0.707810                | 1.498666  | 0.593322  |
| 3                | 1                | 0              | 0.164105                | 0.582069  | -1.216324 |
| 4                | 1                | 0              | 1.811487                | 0.708798  | -0.589452 |
| 5                | 1                | 0              | -1.987263               | 0.631712  | 0.560738  |
| 6                | 6                | 0              | -2.434801               | -0.875317 | -0.662598 |
| 7                | 8                | 0              | -1.740881               | -0.367526 | 0.271849  |
| 8                | 8                | 0              | -2.001800               | -1.917380 | -1.238345 |
| 9                | 1                | 0              | -0.991170               | -2.124874 | -0.950101 |
| 10               | 6                | 0              | -3.713467               | -0.273635 | -1.098088 |
| 11               | 1                | 0              | -4.320544               | -0.031098 | -0.226662 |
| 12               | 1                | 0              | -3.480378               | 0.662298  | -1.613344 |
| 13               | 1                | 0              | -4.236583               | -0.944342 | -1.772642 |
| 14               | 6                | 0              | 0.647452                | -2.291905 | 0.590468  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 15 | 8  | 0 | 0.367756  | -2.141186 | -0.600563 |
| 16 | 8  | 0 | 1.814486  | -1.968663 | 1.064799  |
| 17 | 1  | 0 | 2.404514  | -1.518062 | 0.376848  |
| 18 | 6  | 0 | -0.295587 | -2.849816 | 1.599988  |
| 19 | 1  | 0 | -0.413103 | -2.132875 | 2.413114  |
| 20 | 1  | 0 | -1.258645 | -3.072142 | 1.148589  |
| 21 | 1  | 0 | 0.141965  | -3.757958 | 2.017439  |
| 22 | 1  | 0 | 0.355690  | 0.639724  | 1.156617  |
| 23 | 6  | 0 | 1.332078  | 2.591026  | 1.349040  |
| 24 | 1  | 0 | 1.205939  | 3.554431  | 0.858446  |
| 25 | 1  | 0 | 0.971416  | 2.622816  | 2.373322  |
| 26 | 1  | 0 | 2.409388  | 2.366186  | 1.376310  |
| 27 | 6  | 0 | 1.170520  | 2.506030  | -1.684935 |
| 28 | 1  | 0 | 2.042999  | 3.042859  | -1.312952 |
| 29 | 1  | 0 | 1.398041  | 2.145923  | -2.686948 |
| 30 | 1  | 0 | 0.333080  | 3.204490  | -1.749731 |
| 31 | 17 | 0 | 3.517628  | -0.291996 | -0.684749 |
| 32 | 17 | 0 | -1.953440 | 2.331051  | 0.947931  |



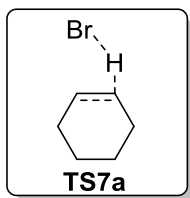
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.489363                | 0.041742  | -0.111318 |
| 2                | 6                | 0              | 0.688491                | -1.181577 | 0.327022  |
| 3                | 6                | 0              | -0.689600               | -1.180987 | -0.327047 |
| 4                | 6                | 0              | -1.489308               | 0.043005  | 0.111355  |
| 5                | 6                | 0              | -0.661462               | 1.296872  | 0.060300  |
| 6                | 6                | 0              | 0.662664                | 1.296345  | -0.060334 |
| 7                | 1                | 0              | 2.374003                | 0.164859  | 0.519070  |
| 8                | 1                | 0              | 1.233382                | -2.095499 | 0.083401  |
| 9                | 1                | 0              | -0.566540               | -1.159570 | -1.414809 |
| 10               | 1                | 0              | -2.373896               | 0.167010  | -0.518916 |
| 11               | 1                | 0              | -1.190371               | 2.243473  | 0.119716  |
| 12               | 1                | 0              | 1.192297                | 2.242533  | -0.119732 |
| 13               | 1                | 0              | -1.866787               | -0.099488 | 1.130723  |
| 14               | 1                | 0              | -1.235248               | -2.094466 | -0.083476 |
| 15               | 1                | 0              | 0.565466                | -1.160105 | 1.414779  |
| 16               | 1                | 0              | 1.866806                | -0.101149 | -1.130628 |



Standard orientation:

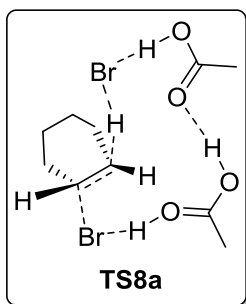
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.520751               | 1.443913  | 0.520322  |
| 2                | 6                | 0              | -1.754475               | 0.980230  | -0.915874 |
| 3                | 6                | 0              | -2.544787               | -0.324114 | -0.941209 |
| 4                | 6                | 0              | -1.765845               | -1.434469 | -0.241771 |
| 5                | 6                | 0              | -1.199722               | -0.972752 | 1.070968  |
| 6                | 6                | 0              | -1.111433               | 0.311603  | 1.419153  |
| 7                | 1                | 0              | -0.753927               | 2.223474  | 0.551214  |
| 8                | 1                | 0              | -2.271281               | 1.758430  | -1.479838 |
| 9                | 1                | 0              | -3.498425               | -0.174842 | -0.424865 |
| 10               | 1                | 0              | -2.403666               | -2.305108 | -0.070376 |
| 11               | 1                | 0              | -0.859134               | -1.735672 | 1.764952  |
| 12               | 1                | 0              | -0.722513               | 0.570519  | 2.399806  |
| 13               | 1                | 0              | -0.949170               | -1.786400 | -0.884467 |
| 14               | 1                | 0              | -2.776004               | -0.615866 | -1.966950 |
| 15               | 1                | 0              | -0.789107               | 0.819917  | -1.407453 |
| 16               | 1                | 0              | -2.429599               | 1.904817  | 0.923519  |
| 17               | 35               | 0              | 2.170536                | -0.014787 | -0.152194 |
| 18               | 1                | 0              | 0.866134                | -0.168180 | 0.451718  |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |          |
|------------------|------------------|----------------|-------------------------|----------|----------|
|                  |                  |                | X                       | Y        | Z        |
| 1                | 6                | 0              | 0.610518                | 0.101414 | 1.241071 |
| 2                | 6                | 0              | 1.039482                | 1.280223 | 0.594511 |
| 3                | 1                | 0              | 0.958362                | 2.186456 | 1.190378 |

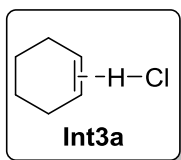
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 4  | 1  | 0 | -0.006221 | 1.213949  | 0.101808  |
| 5  | 35 | 0 | -2.080504 | 0.011845  | -0.201651 |
| 6  | 1  | 0 | -0.048791 | 0.191370  | 2.097355  |
| 7  | 6  | 0 | 1.010812  | -1.232373 | 0.810177  |
| 8  | 1  | 0 | 1.721629  | -1.507399 | 1.615508  |
| 9  | 1  | 0 | 0.178069  | -1.927383 | 0.904566  |
| 10 | 6  | 0 | 2.125901  | 1.228087  | -0.474655 |
| 11 | 1  | 0 | 1.694868  | 1.531176  | -1.430528 |
| 12 | 1  | 0 | 2.883630  | 1.970692  | -0.225286 |
| 13 | 6  | 0 | 1.707155  | -1.256484 | -0.541203 |
| 14 | 1  | 0 | 2.155487  | -2.236848 | -0.698535 |
| 15 | 1  | 0 | 0.954963  | -1.108093 | -1.321334 |
| 16 | 6  | 0 | 2.760755  | -0.155625 | -0.604363 |
| 17 | 1  | 0 | 3.320223  | -0.213364 | -1.537892 |
| 18 | 1  | 0 | 3.477687  | -0.306572 | 0.208506  |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.414289                | -0.872446 | 0.769221  |
| 2                | 6                | 0              | 0.128918                | -1.006457 | -0.583889 |
| 3                | 1                | 0              | 0.019328                | 0.010702  | 1.264953  |
| 4                | 1                | 0              | 1.523208                | -0.481236 | 0.410827  |
| 5                | 1                | 0              | -2.374814               | 0.384657  | -0.244549 |
| 6                | 6                | 0              | -2.301774               | 1.969800  | 0.927773  |
| 7                | 8                | 0              | -1.869906               | 1.289192  | -0.058188 |
| 8                | 8                | 0              | -1.583712               | 2.914244  | 1.363768  |
| 9                | 1                | 0              | -0.606212               | 2.896573  | 0.921636  |
| 10               | 6                | 0              | -3.598627               | 1.670525  | 1.570739  |
| 11               | 1                | 0              | -4.367786               | 1.545634  | 0.809379  |
| 12               | 1                | 0              | -3.496330               | 0.718438  | 2.098958  |
| 13               | 1                | 0              | -3.860435               | 2.455807  | 2.272926  |
| 14               | 6                | 0              | 0.826463                | 2.696211  | -0.812941 |
| 15               | 8                | 0              | 0.663177                | 2.622475  | 0.404852  |

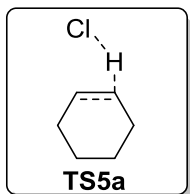
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 16 | 8  | 0 | 1.858544  | 2.154425  | -1.396451 |
| 17 | 1  | 0 | 2.424246  | 1.629660  | -0.756545 |
| 18 | 6  | 0 | -0.111561 | 3.387386  | -1.739390 |
| 19 | 1  | 0 | -0.509945 | 2.658353  | -2.446681 |
| 20 | 1  | 0 | -0.920917 | 3.859218  | -1.188783 |
| 21 | 1  | 0 | 0.443168  | 4.133518  | -2.309441 |
| 22 | 1  | 0 | -0.145400 | -0.117633 | -1.144978 |
| 23 | 35 | 0 | 3.512327  | 0.075368  | 0.318544  |
| 24 | 35 | 0 | -2.846571 | -1.466350 | -0.538820 |
| 25 | 6  | 0 | 0.485434  | -2.216833 | -1.346648 |
| 26 | 1  | 0 | -0.168937 | -2.299736 | -2.214301 |
| 27 | 1  | 0 | 1.490001  | -1.999665 | -1.748874 |
| 28 | 6  | 0 | 0.649651  | -2.103626 | 1.617657  |
| 29 | 1  | 0 | 1.283797  | -1.837497 | 2.464421  |
| 30 | 1  | 0 | -0.318423 | -2.416018 | 2.021223  |
| 31 | 6  | 0 | 0.511050  | -3.477108 | -0.489410 |
| 32 | 1  | 0 | -0.519858 | -3.763358 | -0.264403 |
| 33 | 1  | 0 | 0.962037  | -4.291605 | -1.056743 |
| 34 | 6  | 0 | 1.276666  | -3.235017 | 0.807883  |
| 35 | 1  | 0 | 2.313294  | -2.973579 | 0.574248  |
| 36 | 1  | 0 | 1.300648  | -4.145140 | 1.408558  |



Standard orientation:

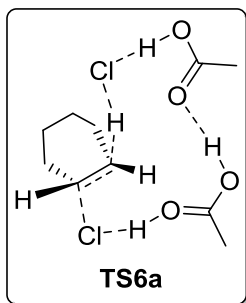
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.857129               | 1.452152  | 0.503044  |
| 2                | 6                | 0              | -1.179475               | 0.959697  | -0.906142 |
| 3                | 6                | 0              | -1.953046               | -0.353953 | -0.855555 |
| 4                | 6                | 0              | -1.114509               | -1.442514 | -0.191466 |
| 5                | 6                | 0              | -0.466119               | -0.950052 | 1.071474  |
| 6                | 6                | 0              | -0.371551               | 0.341131  | 1.390929  |
| 7                | 1                | 0              | -0.101264               | 2.242027  | 0.468905  |
| 8                | 1                | 0              | -1.742309               | 1.721465  | -1.448092 |
| 9                | 1                | 0              | -2.871578               | -0.206247 | -0.278609 |
| 10               | 1                | 0              | -1.728481               | -2.316803 | 0.038473  |
| 11               | 1                | 0              | -0.068808               | -1.696192 | 1.753474  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 12 | 1  | 0 | 0.080610  | 0.622333  | 2.337712  |
| 13 | 1  | 0 | -0.338690 | -1.796232 | -0.881745 |
| 14 | 1  | 0 | -2.249229 | -0.666959 | -1.858096 |
| 15 | 1  | 0 | -0.246438 | 0.801122  | -1.457042 |
| 16 | 1  | 0 | -1.743794 | 1.907504  | 0.958645  |
| 17 | 17 | 0 | 2.654680  | -0.029127 | -0.352756 |
| 18 | 1  | 0 | 1.531406  | -0.155634 | 0.289524  |



Standard orientation:

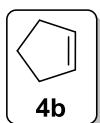
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.120290               | 0.105591  | 1.136777  |
| 2                | 6                | 0              | 0.372384                | 1.281604  | 0.532806  |
| 3                | 1                | 0              | 0.228590                | 2.190442  | 1.112333  |
| 4                | 1                | 0              | -0.615950               | 1.207838  | -0.062208 |
| 5                | 1                | 0              | -0.859314               | 0.197898  | 1.924724  |
| 6                | 6                | 0              | 0.313553                | -1.230336 | 0.746752  |
| 7                | 1                | 0              | 0.920497                | -1.521727 | 1.626916  |
| 8                | 1                | 0              | -0.534948               | -1.913197 | 0.739993  |
| 9                | 6                | 0              | 1.566407                | 1.224854  | -0.414698 |
| 10               | 1                | 0              | 1.238928                | 1.512933  | -1.415006 |
| 11               | 1                | 0              | 2.289793                | 1.974294  | -0.093755 |
| 12               | 6                | 0              | 1.160583                | -1.257429 | -0.515568 |
| 13               | 1                | 0              | 1.622379                | -2.238678 | -0.619548 |
| 14               | 1                | 0              | 0.507065                | -1.107867 | -1.379695 |
| 15               | 6                | 0              | 2.215100                | -0.157169 | -0.457235 |
| 16               | 1                | 0              | 2.885087                | -0.219538 | -1.314607 |
| 17               | 1                | 0              | 2.825627                | -0.301133 | 0.439763  |
| 18               | 17               | 0              | -2.562010               | 0.024473  | -0.419524 |



Standard orientation:

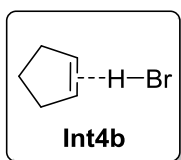
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.146528               | -0.195460 | -0.752774 |
| 2                | 6                | 0              | -1.148415               | -0.348232 | 0.635821  |
| 3                | 1                | 0              | -0.169061               | -0.171630 | -1.229063 |
| 4                | 1                | 0              | -1.352065               | 0.973351  | -0.565180 |
| 5                | 1                | 0              | 1.257761                | -1.806907 | 0.554903  |
| 6                | 6                | 0              | 2.649905                | -1.124886 | -0.695294 |
| 7                | 8                | 0              | 1.831857                | -0.955071 | 0.260937  |
| 8                | 8                | 0              | 3.121016                | -0.102692 | -1.276332 |
| 9                | 1                | 0              | 2.607252                | 0.785550  | -0.970156 |
| 10               | 6                | 0              | 3.047286                | -2.474495 | -1.150546 |
| 11               | 1                | 0              | 3.303768                | -3.090853 | -0.289565 |
| 12               | 1                | 0              | 2.180067                | -2.928065 | -1.638337 |
| 13               | 1                | 0              | 3.872771                | -2.409612 | -1.852544 |
| 14               | 6                | 0              | 1.670148                | 2.126155  | 0.586144  |
| 15               | 8                | 0              | 1.716190                | 1.804938  | -0.602785 |
| 16               | 8                | 0              | 0.656222                | 2.774430  | 1.079542  |
| 17               | 1                | 0              | -0.085189               | 2.907274  | 0.402553  |
| 18               | 6                | 0              | 2.744892                | 1.815353  | 1.569830  |
| 19               | 1                | 0              | 2.324554                | 1.216387  | 2.378690  |
| 20               | 1                | 0              | 3.563833                | 1.284353  | 1.092097  |
| 21               | 1                | 0              | 3.103563                | 2.750761  | 2.001379  |
| 22               | 1                | 0              | -0.263930               | -0.046463 | 1.188657  |
| 23               | 6                | 0              | -2.383854               | -0.581516 | 1.400055  |
| 24               | 1                | 0              | -2.136174               | -1.078336 | 2.338195  |
| 25               | 1                | 0              | -2.714428               | 0.433263  | 1.681375  |
| 26               | 6                | 0              | -2.303875               | -0.740522 | -1.564958 |
| 27               | 1                | 0              | -2.379262               | -0.179147 | -2.497070 |
| 28               | 1                | 0              | -2.071270               | -1.776768 | -1.827978 |
| 29               | 6                | 0              | -3.463339               | -1.298604 | 0.597770  |
| 30               | 1                | 0              | -3.184468               | -2.351356 | 0.501354  |
| 31               | 1                | 0              | -4.405315               | -1.259102 | 1.145017  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 32 | 6  | 0 | -3.614650 | -0.675540 | -0.786386 |
| 33 | 1  | 0 | -3.918678 | 0.370689  | -0.682444 |
| 34 | 1  | 0 | -4.399710 | -1.185042 | -1.346427 |
| 35 | 17 | 0 | -1.736008 | 2.936014  | -0.665384 |
| 36 | 17 | 0 | -0.031386 | -2.913938 | 0.952776  |



Standard orientation:

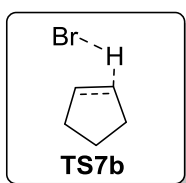
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.295432               | -1.189857 | 0.000000  |
| 2                | 6                | 0              | 0.075902                | -0.331612 | -1.224733 |
| 3                | 6                | 0              | 0.075902                | 1.067706  | -0.663923 |
| 4                | 6                | 0              | 0.075902                | 1.067706  | 0.663923  |
| 5                | 6                | 0              | 0.075902                | -0.331612 | 1.224733  |
| 6                | 1                | 0              | 0.191432                | -2.164206 | 0.000000  |
| 7                | 1                | 0              | -0.622154               | -0.458598 | -2.054050 |
| 8                | 1                | 0              | 1.070954                | -0.580268 | -1.609791 |
| 9                | 1                | 0              | 0.117821                | 1.953518  | -1.286190 |
| 10               | 1                | 0              | 0.117821                | 1.953518  | 1.286190  |
| 11               | 1                | 0              | -0.622154               | -0.458598 | 2.054050  |
| 12               | 1                | 0              | 1.070954                | -0.580268 | 1.609791  |
| 13               | 1                | 0              | -1.373743               | -1.359084 | 0.000000  |



Standard orientation:

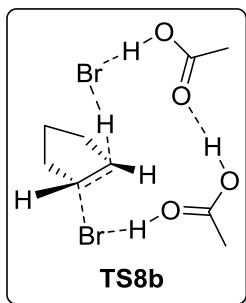
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.871699               | 0.126583  | -1.180505 |
| 2                | 6                | 0              | -1.895281               | 1.260703  | -0.134797 |
| 3                | 6                | 0              | -1.522426               | 0.556776  | 1.143653  |
| 4                | 6                | 0              | -1.562836               | -0.767651 | 1.013566  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 5  | 6  | 0 | -1.970109 | -1.185754 | -0.375058 |
| 6  | 1  | 0 | -0.921562 | 0.150118  | -1.716489 |
| 7  | 1  | 0 | -2.889646 | 1.707423  | -0.034462 |
| 8  | 1  | 0 | -1.210571 | 2.074645  | -0.382169 |
| 9  | 1  | 0 | -1.294780 | 1.083009  | 2.063197  |
| 10 | 1  | 0 | -1.373219 | -1.474849 | 1.812347  |
| 11 | 1  | 0 | -2.990496 | -1.581813 | -0.357850 |
| 12 | 1  | 0 | -1.334088 | -1.975591 | -0.780031 |
| 13 | 1  | 0 | -2.663644 | 0.223426  | -1.921250 |
| 14 | 1  | 0 | 0.576465  | -0.079743 | 0.479283  |
| 15 | 35 | 0 | 1.915304  | -0.002016 | -0.056107 |



Standard orientation:

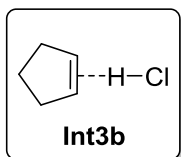
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.935647               | 0.748224  | -0.844473 |
| 2                | 6                | 0              | -1.490157               | 1.183261  | 0.558767  |
| 3                | 6                | 0              | -1.003597               | -0.044286 | 1.186907  |
| 4                | 6                | 0              | -1.359884               | -1.176725 | 0.439800  |
| 5                | 6                | 0              | -2.297970               | -0.735221 | -0.676544 |
| 6                | 1                | 0              | -1.084712               | 0.847702  | -1.519790 |
| 7                | 1                | 0              | -2.369272               | 1.424025  | 1.186646  |
| 8                | 1                | 0              | -0.802975               | 2.022981  | 0.625773  |
| 9                | 1                | 0              | -0.431042               | -0.071683 | 2.105734  |
| 10               | 1                | 0              | -1.386348               | -2.159355 | 0.898202  |
| 11               | 1                | 0              | -3.330545               | -0.859770 | -0.343226 |
| 12               | 1                | 0              | -2.161418               | -1.312788 | -1.587926 |
| 13               | 1                | 0              | -2.757296               | 1.349883  | -1.224707 |
| 14               | 1                | 0              | -0.255052               | -1.043884 | 0.046981  |
| 15               | 35               | 0              | 1.802920                | -0.001389 | -0.119269 |



Standard orientation:

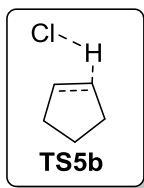
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.353598               | -1.038308 | -0.753783 |
| 2                | 6                | 0              | -0.070521               | -1.211955 | 0.604809  |
| 3                | 1                | 0              | 0.089340                | -0.218304 | -1.308774 |
| 4                | 1                | 0              | -1.451940               | -0.655789 | -0.469580 |
| 5                | 1                | 0              | 2.351937                | 0.362375  | 0.201173  |
| 6                | 6                | 0              | 2.156839                | 1.974656  | -0.918494 |
| 7                | 8                | 0              | 1.786416                | 1.227445  | 0.047666  |
| 8                | 8                | 0              | 1.372964                | 2.886442  | -1.299605 |
| 9                | 1                | 0              | 0.398298                | 2.787380  | -0.834349 |
| 10               | 6                | 0              | 3.459451                | 1.781415  | -1.589889 |
| 11               | 1                | 0              | 4.248594                | 1.699416  | -0.842650 |
| 12               | 1                | 0              | 3.418177                | 0.834444  | -2.135087 |
| 13               | 1                | 0              | 3.652454                | 2.597273  | -2.279351 |
| 14               | 6                | 0              | -0.938676               | 2.373106  | 0.912428  |
| 15               | 8                | 0              | -0.816618               | 2.417807  | -0.313124 |
| 16               | 8                | 0              | -1.915403               | 1.721984  | 1.474254  |
| 17               | 1                | 0              | -2.489069               | 1.234705  | 0.802674  |
| 18               | 6                | 0              | -0.015397               | 3.046291  | 1.867856  |
| 19               | 1                | 0              | 0.385003                | 2.307984  | 2.563218  |
| 20               | 1                | 0              | 0.791050                | 3.546990  | 1.338778  |
| 21               | 1                | 0              | -0.590020               | 3.770685  | 2.447345  |
| 22               | 1                | 0              | 0.215891                | -0.409681 | 1.274409  |
| 23               | 6                | 0              | -0.468413               | -2.554227 | 1.070750  |
| 24               | 1                | 0              | 0.449228                | -3.051529 | 1.403052  |
| 25               | 1                | 0              | -1.117791               | -2.489977 | 1.947427  |
| 26               | 6                | 0              | -0.572902               | -2.417088 | -1.361894 |
| 27               | 1                | 0              | -1.274181               | -2.394033 | -2.194003 |
| 28               | 1                | 0              | 0.385907                | -2.797979 | -1.721035 |
| 29               | 6                | 0              | -1.094799               | -3.227856 | -0.165445 |
| 30               | 1                | 0              | -0.842778               | -4.283794 | -0.228318 |
| 31               | 1                | 0              | -2.179704               | -3.134841 | -0.112078 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 32 | 35 | 0 | -3.553948 | -0.173280 | -0.399716 |
| 33 | 35 | 0 | 2.911914  | -1.486461 | 0.481876  |



Standard orientation:

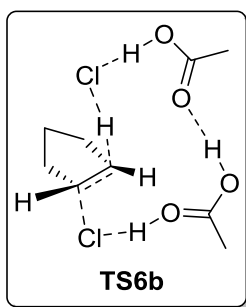
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.274682                | 0.000025  | -1.165490 |
| 2                | 6                | 0              | 1.289094                | -1.229194 | -0.233223 |
| 3                | 6                | 0              | 0.825607                | -0.665670 | 1.084797  |
| 4                | 6                | 0              | 0.825596                | 0.665628  | 1.084822  |
| 5                | 6                | 0              | 1.289072                | 1.229210  | -0.233178 |
| 6                | 1                | 0              | 0.351560                | 0.000027  | -1.747319 |
| 7                | 1                | 0              | 2.294000                | -1.649024 | -0.122149 |
| 8                | 1                | 0              | 0.649492                | -2.037144 | -0.593960 |
| 9                | 1                | 0              | 0.571023                | -1.285836 | 1.936162  |
| 10               | 1                | 0              | 0.571001                | 1.285758  | 1.936210  |
| 11               | 1                | 0              | 2.293970                | 1.649055  | -0.122089 |
| 12               | 1                | 0              | 0.649454                | 2.037160  | -0.593885 |
| 13               | 1                | 0              | 2.103295                | 0.000045  | -1.871930 |
| 14               | 17               | 0              | -2.426996               | -0.000004 | -0.144247 |
| 15               | 1                | 0              | -1.249175               | 0.000028  | 0.404791  |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.393116               | 0.756777  | -0.791321 |
| 2                | 6                | 0              | -0.819723               | 1.178733  | 0.569153  |
| 3                | 6                | 0              | -0.284746               | -0.057177 | 1.141122  |
| 4                | 6                | 0              | -0.712681               | -1.180092 | 0.419809  |
| 5                | 6                | 0              | -1.745784               | -0.726301 | -0.602986 |

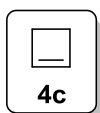
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 6  | 1  | 0 | -0.608383 | 0.858012  | -1.542354 |
| 7  | 1  | 0 | -1.635927 | 1.421126  | 1.275263  |
| 8  | 1  | 0 | -0.123074 | 2.013278  | 0.579115  |
| 9  | 1  | 0 | 0.368155  | -0.096146 | 2.003924  |
| 10 | 1  | 0 | -0.694065 | -2.168969 | 0.864351  |
| 11 | 1  | 0 | -2.743970 | -0.849352 | -0.177184 |
| 12 | 1  | 0 | -1.696285 | -1.296698 | -1.527464 |
| 13 | 1  | 0 | -2.242984 | 1.364797  | -1.090714 |
| 14 | 17 | 0 | 2.279913  | -0.002781 | -0.278851 |
| 15 | 1  | 0 | 0.354310  | -1.030400 | -0.059130 |



Standard orientation:

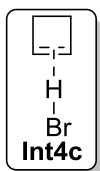
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.052976                | 0.829691  | -0.737571 |
| 2                | 6                | 0              | 1.007770                | 1.002712  | 0.659650  |
| 3                | 1                | 0              | 0.156996                | 0.532598  | -1.274022 |
| 4                | 1                | 0              | 1.678731                | -0.152267 | -0.624484 |
| 5                | 1                | 0              | -1.803698               | 1.233038  | 0.509657  |
| 6                | 6                | 0              | -2.757426               | -0.031610 | -0.685609 |
| 7                | 8                | 0              | -1.936241               | 0.211678  | 0.254520  |
| 8                | 8                | 0              | -2.738263               | -1.178065 | -1.220151 |
| 9                | 1                | 0              | -1.875905               | -1.738817 | -0.904722 |
| 10               | 6                | 0              | -3.708262               | 0.992089  | -1.169149 |
| 11               | 1                | 0              | -4.198741               | 1.467960  | -0.320710 |
| 12               | 1                | 0              | -3.129972               | 1.758881  | -1.692401 |
| 13               | 1                | 0              | -4.430049               | 0.548219  | -1.847644 |
| 14               | 6                | 0              | -0.386745               | -2.397671 | 0.654227  |
| 15               | 8                | 0              | -0.623858               | -2.233264 | -0.545519 |
| 16               | 8                | 0              | 0.827334                | -2.480832 | 1.106419  |
| 17               | 1                | 0              | 1.532777                | -2.345361 | 0.381013  |
| 18               | 6                | 0              | -1.445814               | -2.528679 | 1.694793  |
| 19               | 1                | 0              | -1.260815               | -1.813207 | 2.495871  |
| 20               | 1                | 0              | -2.431298               | -2.373389 | 1.264906  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 21 | 1  | 0 | -1.380282 | -3.531031 | 2.121907  |
| 22 | 1  | 0 | 0.344282  | 0.458104  | 1.319937  |
| 23 | 6  | 0 | 2.147936  | 1.799872  | 1.138061  |
| 24 | 1  | 0 | 1.712729  | 2.721431  | 1.544241  |
| 25 | 1  | 0 | 2.658200  | 1.309779  | 1.969984  |
| 26 | 6  | 0 | 2.022037  | 1.871689  | -1.287592 |
| 27 | 1  | 0 | 2.513008  | 1.536516  | -2.198956 |
| 28 | 1  | 0 | 1.472409  | 2.790837  | -1.502381 |
| 29 | 6  | 0 | 2.998938  | 2.059945  | -0.118100 |
| 30 | 1  | 0 | 3.462012  | 3.043597  | -0.103587 |
| 31 | 1  | 0 | 3.786923  | 1.308320  | -0.177798 |
| 32 | 17 | 0 | 2.968702  | -1.813248 | -0.776542 |
| 33 | 17 | 0 | -1.123263 | 2.819156  | 0.857999  |



Standard orientation:

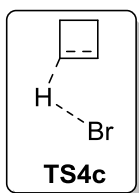
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.696640               | 0.779697  | 0.000001  |
| 2                | 6                | 0              | 0.809548                | 0.666030  | -0.000002 |
| 3                | 6                | 0              | 0.809541                | -0.666038 | -0.000001 |
| 4                | 6                | 0              | -0.696648               | -0.779691 | -0.000001 |
| 5                | 1                | 0              | -1.136174               | 1.236528  | 0.888208  |
| 6                | 1                | 0              | -1.136187               | 1.236528  | -0.888201 |
| 7                | 1                | 0              | 1.594977                | 1.412257  | 0.000000  |
| 8                | 1                | 0              | 1.594963                | -1.412272 | 0.000001  |
| 9                | 1                | 0              | -1.136184               | -1.236517 | 0.888208  |
| 10               | 1                | 0              | -1.136201               | -1.236517 | -0.888201 |



Standard orientation:

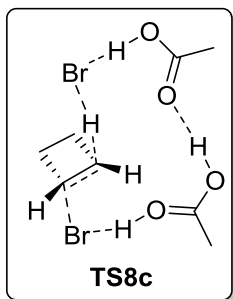
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 1  | 6  | 0 | 2.051321  | -0.673336 | -0.781380 |
| 2  | 6  | 0 | 1.868308  | 0.821732  | -0.665844 |
| 3  | 6  | 0 | 1.867584  | 0.818111  | 0.670347  |
| 4  | 6  | 0 | 2.050946  | -0.677455 | 0.778047  |
| 5  | 1  | 0 | 1.225648  | -1.218165 | -1.243703 |
| 6  | 1  | 0 | 2.987460  | -0.995153 | -1.239184 |
| 7  | 1  | 0 | 1.782515  | 1.605558  | -1.409121 |
| 8  | 1  | 0 | 1.780808  | 1.597869  | 1.417780  |
| 9  | 1  | 0 | 1.225711  | -1.225392 | 1.237509  |
| 10 | 1  | 0 | 2.987249  | -1.001055 | 1.234286  |
| 11 | 35 | 0 | -1.676680 | -0.028301 | -0.000065 |
| 12 | 1  | 0 | -0.334544 | 0.492576  | -0.002310 |



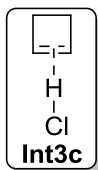
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.832213                | 1.049000  | 0.021966  |
| 2                | 6                | 0              | 1.256573                | 0.093966  | 0.990389  |
| 3                | 6                | 0              | 1.631263                | -1.038773 | 0.241184  |
| 4                | 6                | 0              | 2.343465                | -0.165784 | -0.800557 |
| 5                | 1                | 0              | 1.138269                | 1.752118  | -0.433639 |
| 6                | 1                | 0              | 2.633098                | 1.607217  | 0.522089  |
| 7                | 1                | 0              | 0.743427                | 0.220571  | 1.935023  |
| 8                | 1                | 0              | 1.814104                | -2.049808 | 0.587972  |
| 9                | 1                | 0              | 1.963446                | -0.246734 | -1.815830 |
| 10               | 1                | 0              | 3.425472                | -0.267926 | -0.794216 |
| 11               | 1                | 0              | 0.498214                | -0.981161 | -0.075282 |
| 12               | 35               | 0              | -1.559917               | 0.009579  | -0.075543 |



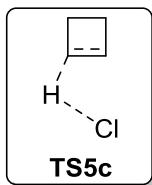
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.377365               | -1.089596 | -0.807931 |
| 2                | 6                | 0              | -0.069186               | -1.253515 | 0.539430  |
| 3                | 1                | 0              | -0.093103               | -0.294055 | -1.488840 |
| 4                | 1                | 0              | -1.553684               | -0.822204 | -0.499760 |
| 5                | 1                | 0              | 2.256247                | 0.309796  | 0.220969  |
| 6                | 6                | 0              | 2.002682                | 1.889958  | -0.934576 |
| 7                | 8                | 0              | 1.658252                | 1.157071  | 0.047283  |
| 8                | 8                | 0              | 1.188356                | 2.768809  | -1.339311 |
| 9                | 1                | 0              | 0.230860                | 2.651760  | -0.875956 |
| 10               | 6                | 0              | 3.307487                | 1.726718  | -1.609546 |
| 11               | 1                | 0              | 4.101028                | 1.652325  | -0.866709 |
| 12               | 1                | 0              | 3.280450                | 0.784363  | -2.163650 |
| 13               | 1                | 0              | 3.482201                | 2.550546  | -2.294567 |
| 14               | 6                | 0              | -1.113904               | 2.218565  | 0.891876  |
| 15               | 8                | 0              | -0.996055               | 2.239837  | -0.332040 |
| 16               | 8                | 0              | -2.068843               | 1.541714  | 1.470790  |
| 17               | 1                | 0              | -2.607269               | 1.019679  | 0.811751  |
| 18               | 6                | 0              | -0.216669               | 2.942409  | 1.833909  |
| 19               | 1                | 0              | 0.199532                | 2.234236  | 2.550928  |
| 20               | 1                | 0              | 0.579146                | 3.449994  | 1.295172  |
| 21               | 1                | 0              | -0.814175               | 3.666624  | 2.390167  |
| 22               | 1                | 0              | 0.161918                | -0.555604 | 1.335055  |
| 23               | 6                | 0              | -0.422795               | -2.698884 | 0.541630  |
| 24               | 1                | 0              | 0.306774                | -3.361007 | 1.003089  |
| 25               | 1                | 0              | -1.404189               | -2.863468 | 0.998055  |
| 26               | 6                | 0              | -0.463185               | -2.606314 | -1.008720 |
| 27               | 1                | 0              | -1.350078               | -2.988199 | -1.508916 |
| 28               | 1                | 0              | 0.442327                | -3.008154 | -1.459708 |
| 29               | 35               | 0              | -3.524746               | -0.600800 | -0.386601 |
| 30               | 35               | 0              | 2.914630                | -1.480975 | 0.532393  |



Standard orientation:

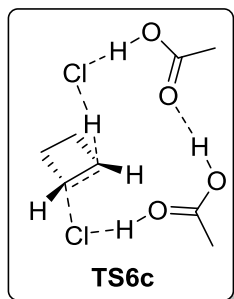
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.380721                | -0.668003 | -0.779921 |
| 2                | 6                | 0              | 1.168072                | 0.823666  | -0.667784 |
| 3                | 6                | 0              | 1.167960                | 0.823335  | 0.668213  |
| 4                | 6                | 0              | 1.380570                | -0.668393 | 0.779642  |
| 5                | 1                | 0              | 0.566117                | -1.230162 | -1.240719 |
| 6                | 1                | 0              | 2.323398                | -0.971794 | -1.236692 |
| 7                | 1                | 0              | 1.067117                | 1.603833  | -1.412979 |
| 8                | 1                | 0              | 1.066874                | 1.603134  | 1.413776  |
| 9                | 1                | 0              | 0.565883                | -1.230786 | 1.240007  |
| 10               | 1                | 0              | 2.323166                | -0.972413 | 1.236429  |
| 11               | 1                | 0              | -1.022228               | 0.464703  | -0.000030 |
| 12               | 17               | 0              | -2.204368               | -0.066479 | -0.000041 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.194992                | 1.048692  | 0.034883  |
| 2                | 6                | 0              | 0.575391                | 0.091969  | 0.972998  |
| 3                | 6                | 0              | 0.989699                | -1.039550 | 0.242721  |
| 4                | 6                | 0              | 1.740097                | -0.163668 | -0.769511 |
| 5                | 1                | 0              | 0.530517                | 1.764168  | -0.444057 |
| 6                | 1                | 0              | 1.977874                | 1.593627  | 0.577163  |
| 7                | 1                | 0              | 0.019026                | 0.216078  | 1.893252  |
| 8                | 1                | 0              | 1.164428                | -2.048258 | 0.599824  |
| 9                | 1                | 0              | 1.395843                | -0.243567 | -1.797404 |
| 10               | 1                | 0              | 2.821327                | -0.263481 | -0.724726 |
| 11               | 17               | 0              | -2.046129               | 0.020198  | -0.169103 |

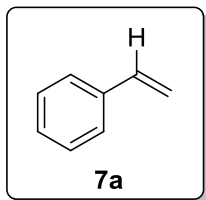
12                      1                      0                      -0.125895                      -0.986588                      -0.115843



Standard orientation:

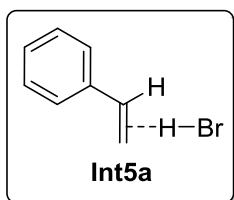
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.684245                | 1.266728  | -0.770464 |
| 2                | 6                | 0              | 0.586761                | 1.421565  | 0.616435  |
| 3                | 1                | 0              | 0.105216                | 0.620514  | -1.422140 |
| 4                | 1                | 0              | 1.750238                | 0.697331  | -0.640634 |
| 5                | 1                | 0              | -2.007032               | 0.535041  | 0.576106  |
| 6                | 6                | 0              | -2.341771               | -0.941664 | -0.706337 |
| 7                | 8                | 0              | -1.716992               | -0.447496 | 0.281987  |
| 8                | 8                | 0              | -1.850622               | -1.956795 | -1.285229 |
| 9                | 1                | 0              | -0.853541               | -2.140363 | -0.956309 |
| 10               | 6                | 0              | -3.603471               | -0.354171 | -1.205775 |
| 11               | 1                | 0              | -4.246546               | -0.086880 | -0.368763 |
| 12               | 1                | 0              | -3.346618               | 0.565721  | -1.739438 |
| 13               | 1                | 0              | -4.096701               | -1.042256 | -1.885628 |
| 14               | 6                | 0              | 0.776381                | -2.201544 | 0.627606  |
| 15               | 8                | 0              | 0.508536                | -2.100084 | -0.569814 |
| 16               | 8                | 0              | 1.916413                | -1.794384 | 1.109319  |
| 17               | 1                | 0              | 2.484122                | -1.342331 | 0.411127  |
| 18               | 6                | 0              | -0.144164               | -2.792241 | 1.638678  |
| 19               | 1                | 0              | -0.315869               | -2.068674 | 2.436036  |
| 20               | 1                | 0              | -1.085487               | -3.081621 | 1.179689  |
| 21               | 1                | 0              | 0.341400                | -3.664093 | 2.080056  |
| 22               | 1                | 0              | 0.305109                | 0.747595  | 1.415793  |
| 23               | 6                | 0              | 1.271050                | 2.741271  | 0.610879  |
| 24               | 1                | 0              | 0.773468                | 3.523950  | 1.180281  |
| 25               | 1                | 0              | 2.306125                | 2.649773  | 0.953429  |
| 26               | 6                | 0              | 1.108171                | 2.732521  | -0.933953 |
| 27               | 1                | 0              | 1.997518                | 2.922760  | -1.529753 |
| 28               | 1                | 0              | 0.283688                | 3.365100  | -1.256849 |
| 29               | 17               | 0              | 3.495017                | -0.064112 | -0.742995 |

30                      17                      0                      -2.040721                      2.237860                      0.979141



Standard orientation:

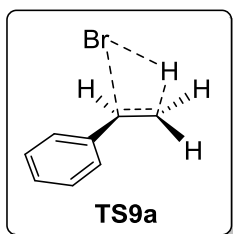
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.344949                | 1.325438  | -0.000022 |
| 2                | 6                | 0              | -0.017964               | 1.082245  | -0.000082 |
| 3                | 6                | 0              | -0.509103               | -0.226689 | -0.000060 |
| 4                | 6                | 0              | 0.407993                | -1.278452 | -0.000001 |
| 5                | 6                | 0              | 1.775097                | -1.036264 | 0.000060  |
| 6                | 6                | 0              | 2.248728                | 0.267451  | 0.000052  |
| 7                | 1                | 0              | 1.707541                | 2.346002  | -0.000044 |
| 8                | 1                | 0              | -0.705512               | 1.918651  | -0.000165 |
| 9                | 1                | 0              | 0.041156                | -2.298632 | 0.000001  |
| 10               | 1                | 0              | 2.469688                | -1.867181 | 0.000107  |
| 11               | 1                | 0              | 3.313975                | 0.461582  | 0.000094  |
| 12               | 6                | 0              | -1.948734               | -0.536998 | -0.000101 |
| 13               | 6                | 0              | -2.947190               | 0.340213  | 0.000134  |
| 14               | 1                | 0              | -2.187369               | -1.597001 | -0.000338 |
| 15               | 1                | 0              | -3.976088               | 0.003151  | 0.000075  |
| 16               | 1                | 0              | -2.786054               | 1.411769  | 0.000393  |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.181431                | -1.042867 | 1.188541  |
| 2                | 6                | 0              | 1.287671                | 0.009590  | 1.085185  |
| 3                | 6                | 0              | 1.266471                | 0.813990  | -0.058021 |

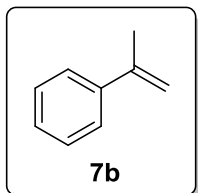
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 4  | 6  | 0 | 2.154136  | 0.523304  | -1.094606 |
| 5  | 6  | 0 | 3.050421  | -0.531133 | -0.991759 |
| 6  | 6  | 0 | 3.067574  | -1.316528 | 0.151575  |
| 7  | 1  | 0 | 2.185406  | -1.657516 | 2.080085  |
| 8  | 1  | 0 | 0.599747  | 0.201371  | 1.899598  |
| 9  | 1  | 0 | 2.139459  | 1.134756  | -1.989720 |
| 10 | 1  | 0 | 3.732820  | -0.740025 | -1.806148 |
| 11 | 1  | 0 | 3.763750  | -2.141543 | 0.235580  |
| 12 | 6  | 0 | 0.338034  | 1.943990  | -0.218476 |
| 13 | 6  | 0 | -0.489358 | 2.432091  | 0.704710  |
| 14 | 1  | 0 | 0.346831  | 2.406263  | -1.201750 |
| 15 | 1  | 0 | -1.138337 | 3.267742  | 0.474170  |
| 16 | 1  | 0 | -0.539629 | 2.041241  | 1.714946  |
| 17 | 35 | 0 | -2.474459 | -0.629311 | -0.170386 |
| 18 | 1  | 0 | -1.622263 | 0.518982  | -0.046152 |



Standard orientation:

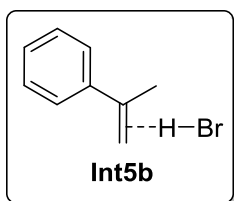
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.755472               | -0.070412 | -1.338900 |
| 2                | 6                | 0              | -1.687562               | 0.707066  | -0.956873 |
| 3                | 6                | 0              | -1.202998               | 0.626643  | 0.367178  |
| 4                | 6                | 0              | -1.823180               | -0.246110 | 1.286884  |
| 5                | 6                | 0              | -2.896422               | -1.016050 | 0.896643  |
| 6                | 6                | 0              | -3.356497               | -0.926919 | -0.414223 |
| 7                | 1                | 0              | -3.130183               | -0.022665 | -2.352329 |
| 8                | 1                | 0              | -1.216912               | 1.370152  | -1.670146 |
| 9                | 1                | 0              | -1.435942               | -0.302375 | 2.297041  |
| 10               | 1                | 0              | -3.373180               | -1.688665 | 1.596514  |
| 11               | 1                | 0              | -4.197293               | -1.535233 | -0.724787 |
| 12               | 6                | 0              | -0.096378               | 1.369630  | 0.811685  |
| 13               | 6                | 0              | 0.747208                | 2.224680  | 0.040183  |
| 14               | 1                | 0              | 0.195724                | 1.206874  | 1.846204  |
| 15               | 1                | 0              | 1.231141                | 2.999010  | 0.632067  |
| 16               | 1                | 0              | 1.568280                | 1.460960  | -0.181146 |
| 17               | 35               | 0              | 2.526679                | -0.630833 | -0.134084 |

18                      1                      0                      0.352422                      2.579942                      -0.905931



Standard orientation:

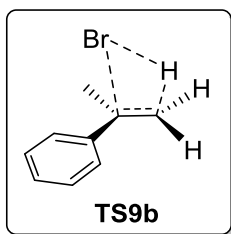
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.955960                | 1.139310  | 0.197460  |
| 2                | 6                | 0              | 0.571976                | 1.203430  | 0.202315  |
| 3                | 6                | 0              | -0.203098               | 0.058439  | -0.006292 |
| 4                | 6                | 0              | 0.458443                | -1.157727 | -0.189545 |
| 5                | 6                | 0              | 1.845586                | -1.222769 | -0.197164 |
| 6                | 6                | 0              | 2.600759                | -0.074776 | -0.007866 |
| 7                | 1                | 0              | 2.534700                | 2.039264  | 0.365783  |
| 8                | 1                | 0              | 0.084985                | 2.151511  | 0.393266  |
| 9                | 1                | 0              | -0.111041               | -2.066094 | -0.339111 |
| 10               | 1                | 0              | 2.336207                | -2.176261 | -0.349712 |
| 11               | 1                | 0              | 3.682434                | -0.125133 | -0.009173 |
| 12               | 6                | 0              | -1.687664               | 0.125355  | -0.023071 |
| 13               | 6                | 0              | -2.333041               | 1.237596  | -0.371927 |
| 14               | 1                | 0              | -3.415963               | 1.274832  | -0.367983 |
| 15               | 1                | 0              | -1.813723               | 2.133051  | -0.690245 |
| 16               | 6                | 0              | -2.440932               | -1.122545 | 0.344479  |
| 17               | 1                | 0              | -2.322140               | -1.894363 | -0.420001 |
| 18               | 1                | 0              | -2.078069               | -1.541872 | 1.285474  |
| 19               | 1                | 0              | -3.505321               | -0.912812 | 0.441367  |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

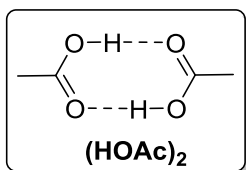
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 1  | 6  | 0 | 2.440932  | -1.650686 | 0.645120  |
| 2  | 6  | 0 | 1.401504  | -0.765450 | 0.882476  |
| 3  | 6  | 0 | 1.351659  | 0.472376  | 0.234708  |
| 4  | 6  | 0 | 2.362539  | 0.782309  | -0.677227 |
| 5  | 6  | 0 | 3.407302  | -0.101303 | -0.910155 |
| 6  | 6  | 0 | 3.452293  | -1.319986 | -0.248529 |
| 7  | 1  | 0 | 2.456840  | -2.607050 | 1.152876  |
| 8  | 1  | 0 | 0.608986  | -1.049944 | 1.563979  |
| 9  | 1  | 0 | 2.344487  | 1.727387  | -1.204526 |
| 10 | 1  | 0 | 4.186705  | 0.164305  | -1.613523 |
| 11 | 1  | 0 | 4.263502  | -2.012558 | -0.434707 |
| 12 | 6  | 0 | 0.248958  | 1.432913  | 0.494299  |
| 13 | 6  | 0 | -0.399640 | 1.456809  | 1.662304  |
| 14 | 1  | 0 | -1.211805 | 2.154989  | 1.830232  |
| 15 | 1  | 0 | -0.124573 | 0.814338  | 2.489906  |
| 16 | 35 | 0 | -2.716249 | -0.666839 | -0.293617 |
| 17 | 1  | 0 | -1.708906 | 0.130063  | 0.359065  |
| 18 | 6  | 0 | -0.119360 | 2.381032  | -0.611251 |
| 19 | 1  | 0 | 0.667853  | 3.122190  | -0.768530 |
| 20 | 1  | 0 | -0.254214 | 1.851088  | -1.557032 |
| 21 | 1  | 0 | -1.037277 | 2.916492  | -0.371635 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.366980                | -1.545364 | 0.768809  |
| 2                | 6                | 0              | 1.335476                | -0.658601 | 0.995200  |
| 3                | 6                | 0              | 1.227913                | 0.512965  | 0.220862  |
| 4                | 6                | 0              | 2.189919                | 0.768775  | -0.774652 |
| 5                | 6                | 0              | 3.240021                | -0.104085 | -0.967473 |
| 6                | 6                | 0              | 3.322801                | -1.263764 | -0.202906 |
| 7                | 1                | 0              | 2.431396                | -2.458800 | 1.344625  |
| 8                | 1                | 0              | 0.584033                | -0.892414 | 1.736595  |
| 9                | 1                | 0              | 2.127218                | 1.668952  | -1.371062 |
| 10               | 1                | 0              | 3.989604                | 0.106945  | -1.718188 |
| 11               | 1                | 0              | 4.137327                | -1.957863 | -0.369560 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 12 | 6  | 0 | 0.147349  | 1.425351  | 0.433510  |
| 13 | 6  | 0 | -0.688716 | 1.355962  | 1.604130  |
| 14 | 1  | 0 | -1.215769 | 2.287469  | 1.801853  |
| 15 | 1  | 0 | -1.475673 | 0.631100  | 1.216592  |
| 16 | 35 | 0 | -2.486197 | -0.744292 | -0.334856 |
| 17 | 1  | 0 | -0.233118 | 0.930022  | 2.491542  |
| 18 | 6  | 0 | -0.212187 | 2.435623  | -0.577136 |
| 19 | 1  | 0 | 0.310296  | 3.364046  | -0.305240 |
| 20 | 1  | 0 | 0.063531  | 2.160844  | -1.590623 |
| 21 | 1  | 0 | -1.279292 | 2.648756  | -0.518638 |



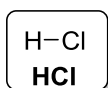
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.917794                | -0.056265 | -0.000088 |
| 2                | 8                | 0              | 1.241207                | -1.074974 | -0.000136 |
| 3                | 8                | 0              | 1.390940                | 1.146845  | -0.000028 |
| 4                | 1                | 0              | 0.388598                | 1.099751  | -0.000069 |
| 5                | 6                | 0              | 3.409176                | -0.064126 | 0.000105  |
| 6                | 1                | 0              | 3.768718                | 0.470660  | -0.879812 |
| 7                | 1                | 0              | 3.768407                | 0.469672  | 0.880760  |
| 8                | 1                | 0              | 3.779170                | -1.084719 | -0.000376 |
| 9                | 6                | 0              | -1.917793               | 0.056265  | 0.000023  |
| 10               | 8                | 0              | -1.241244               | 1.074999  | -0.000014 |
| 11               | 8                | 0              | -1.390898               | -1.146827 | 0.000081  |
| 12               | 1                | 0              | -0.388541               | -1.099756 | -0.000029 |
| 13               | 6                | 0              | -3.409186               | 0.064090  | 0.000024  |
| 14               | 1                | 0              | -3.768499               | -0.469636 | -0.880640 |
| 15               | 1                | 0              | -3.768620               | -0.470785 | 0.879930  |
| 16               | 1                | 0              | -3.779219               | 1.084670  | 0.000631  |



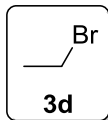
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 1                | 0              | 0.000000                | 0.000000 | -1.384183 |
| 2                | 35               | 0              | 0.000000                | 0.000000 | 0.039548  |



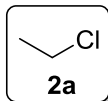
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 17               | 0              | 0.000000                | 0.000000 | 0.071342  |
| 2                | 1                | 0              | 0.000000                | 0.000000 | -1.212808 |



Standard orientation:

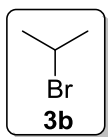
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.022360                | 0.684919  | 0.000008  |
| 2                | 6                | 0              | 2.067910                | -0.400409 | 0.000030  |
| 3                | 1                | 0              | 1.984416                | -1.030282 | -0.885416 |
| 4                | 1                | 0              | 3.056723                | 0.064775  | -0.000655 |
| 5                | 1                | 0              | 1.985223                | -1.029661 | 0.885931  |
| 6                | 1                | 0              | 1.072127                | 1.310509  | -0.886773 |
| 7                | 35               | 0              | -0.791774               | -0.066659 | -0.000001 |
| 8                | 1                | 0              | 1.071978                | 1.310653  | 0.886722  |



Standard orientation:

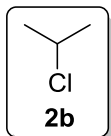
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

|   |    |   |           |           |           |
|---|----|---|-----------|-----------|-----------|
| 1 | 6  | 0 | 0.483794  | 0.656709  | -0.000025 |
| 2 | 6  | 0 | 1.599098  | -0.357580 | -0.000045 |
| 3 | 1  | 0 | 1.552674  | -0.990259 | 0.886419  |
| 4 | 1  | 0 | 1.552441  | -0.991072 | -0.885839 |
| 5 | 1  | 0 | 2.556559  | 0.167669  | -0.000302 |
| 6 | 17 | 0 | -1.127237 | -0.150288 | 0.000004  |
| 7 | 1  | 0 | 0.502119  | 1.286786  | 0.886127  |
| 8 | 1  | 0 | 0.501896  | 1.287002  | -0.886044 |



Standard orientation:

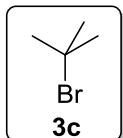
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.917156               | -0.427685 | 0.000000  |
| 2                | 6                | 0              | -0.917156               | -1.257662 | 1.262547  |
| 3                | 1                | 0              | -0.912976               | -0.634407 | 2.155898  |
| 4                | 1                | 0              | -1.820197               | -1.873872 | 1.276936  |
| 5                | 1                | 0              | -0.050654               | -1.920109 | 1.292284  |
| 6                | 6                | 0              | -0.917156               | -1.257662 | -1.262547 |
| 7                | 1                | 0              | -0.912976               | -0.634407 | -2.155898 |
| 8                | 1                | 0              | -0.050654               | -1.920109 | -1.292284 |
| 9                | 1                | 0              | -1.820197               | -1.873872 | -1.276936 |
| 10               | 1                | 0              | -1.743721               | 0.278997  | 0.000000  |
| 11               | 35               | 0              | 0.680577                | 0.749595  | -0.000000 |



Standard orientation:

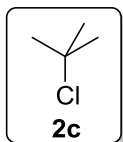
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |          |
|------------------|------------------|----------------|-------------------------|-----------|----------|
|                  |                  |                | X                       | Y         | Z        |
| 1                | 6                | 0              | -0.574098               | -0.062909 | 0.000000 |
| 2                | 6                | 0              | -0.574098               | -0.894767 | 1.261939 |
| 3                | 1                | 0              | -0.562694               | -0.267232 | 2.152515 |
| 4                | 1                | 0              | -1.476917               | -1.509474 | 1.283465 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 5  | 1  | 0 | 0.293793  | -1.556058 | 1.285991  |
| 6  | 6  | 0 | -0.574098 | -0.894767 | -1.261939 |
| 7  | 1  | 0 | -0.562694 | -0.267232 | -2.152515 |
| 8  | 1  | 0 | 0.293793  | -1.556058 | -1.285991 |
| 9  | 1  | 0 | -1.476917 | -1.509474 | -1.283465 |
| 10 | 17 | 0 | 0.896152  | 1.008538  | -0.000000 |
| 11 | 1  | 0 | -1.409182 | 0.635034  | 0.000000  |



Standard orientation:

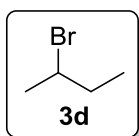
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |           |           |
|---------------|---------------|-------------|-------------------------|-----------|-----------|
|               |               |             | X                       | Y         | Z         |
| 1             | 6             | 0           | -0.000000               | 0.000000  | -0.839640 |
| 2             | 6             | 0           | 0.000000                | 1.448829  | -1.284738 |
| 3             | 1             | 0           | -0.886605               | 1.974179  | -0.929744 |
| 4             | 1             | 0           | 0.886605                | 1.974179  | -0.929744 |
| 5             | 6             | 0           | -1.254723               | -0.724415 | -1.284738 |
| 6             | 1             | 0           | -2.152992               | -0.219267 | -0.929744 |
| 7             | 1             | 0           | -1.277791               | -0.737733 | -2.378284 |
| 8             | 1             | 0           | -1.266387               | -1.754912 | -0.929744 |
| 9             | 6             | 0           | 1.254723                | -0.724415 | -1.284738 |
| 10            | 1             | 0           | 2.152992                | -0.219267 | -0.929744 |
| 11            | 1             | 0           | 1.266387                | -1.754912 | -0.929744 |
| 12            | 1             | 0           | 1.277791                | -0.737733 | -2.378284 |
| 13            | 1             | 0           | 0.000000                | 1.475466  | -2.378284 |
| 14            | 35            | 0           | -0.000000               | 0.000000  | 1.167898  |



Standard orientation:

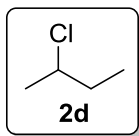
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |           |           |
|---------------|---------------|-------------|-------------------------|-----------|-----------|
|               |               |             | X                       | Y         | Z         |
| 1             | 6             | 0           | -0.360121               | 0.000036  | -0.000053 |
| 2             | 6             | 0           | -0.807717               | -0.144872 | 1.441921  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 3  | 1  | 0 | -0.447223 | -1.079616 | 1.872221  |
| 4  | 1  | 0 | -0.446937 | 0.685220  | 2.049902  |
| 5  | 6  | 0 | -0.808221 | -1.176502 | -0.846195 |
| 6  | 1  | 0 | -0.447284 | -2.118088 | -0.431485 |
| 7  | 1  | 0 | -1.900648 | -1.203193 | -0.864580 |
| 8  | 1  | 0 | -0.448232 | -1.082120 | -1.871049 |
| 9  | 6  | 0 | -0.808299 | 1.321319  | -0.595369 |
| 10 | 1  | 0 | -0.447060 | 2.161513  | -0.001735 |
| 11 | 1  | 0 | -0.448573 | 1.432554  | -1.618612 |
| 12 | 1  | 0 | -1.900734 | 1.351276  | -0.607780 |
| 13 | 1  | 0 | -1.900105 | -0.148088 | 1.474526  |
| 14 | 17 | 0 | 1.476056  | 0.000039  | -0.000190 |



Standard orientation:

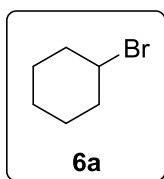
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.467370                | 0.626849  | 0.570050  |
| 2                | 6                | 0              | 0.816189                | 1.758304  | -0.370220 |
| 3                | 1                | 0              | 0.041821                | 2.524421  | -0.369231 |
| 4                | 1                | 0              | 1.753349                | 2.214898  | -0.038622 |
| 5                | 1                | 0              | 0.949576                | 1.404740  | -1.392339 |
| 6                | 6                | 0              | 1.555184                | -0.421818 | 0.731208  |
| 7                | 1                | 0              | 1.197230                | -1.204541 | 1.402122  |
| 8                | 1                | 0              | 2.381168                | 0.079784  | 1.247505  |
| 9                | 1                | 0              | 0.186558                | 1.014253  | 1.546394  |
| 10               | 35               | 0              | -1.215126               | -0.229505 | -0.054497 |
| 11               | 6                | 0              | 2.064640                | -1.032459 | -0.565113 |
| 12               | 1                | 0              | 2.798487                | -1.810381 | -0.351228 |
| 13               | 1                | 0              | 1.251975                | -1.487596 | -1.134084 |
| 14               | 1                | 0              | 2.548956                | -0.288161 | -1.198668 |



Standard orientation:

| Center | Atomic | Atomic | Coordinates (Angstroms) |  |  |
|--------|--------|--------|-------------------------|--|--|
|--------|--------|--------|-------------------------|--|--|

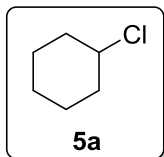
| Number | Number | Type | X         | Y         | Z         |
|--------|--------|------|-----------|-----------|-----------|
| 1      | 6      | 0    | 0.182604  | 0.472156  | 0.552680  |
| 2      | 6      | 0    | -1.141522 | -0.252831 | 0.735862  |
| 3      | 1      | 0    | -0.971909 | -1.135658 | 1.355130  |
| 4      | 1      | 0    | -1.782709 | 0.419346  | 1.315062  |
| 5      | 6      | 0    | 0.111088  | 1.698085  | -0.330400 |
| 6      | 1      | 0    | 1.066334  | 2.221915  | -0.346716 |
| 7      | 1      | 0    | -0.155107 | 1.434389  | -1.353935 |
| 8      | 1      | 0    | -0.649686 | 2.377783  | 0.061915  |
| 9      | 17     | 0    | 1.420258  | -0.673171 | -0.136660 |
| 10     | 1      | 0    | 0.588687  | 0.732436  | 1.528097  |
| 11     | 6      | 0    | -1.843854 | -0.643854 | -0.555541 |
| 12     | 1      | 0    | -1.200411 | -1.261069 | -1.185155 |
| 13     | 1      | 0    | -2.744187 | -1.218593 | -0.335084 |
| 14     | 1      | 0    | -2.145288 | 0.232022  | -1.131710 |



Standard orientation:

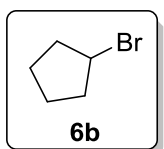
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.640427               | 1.260199  | -0.141703 |
| 2                | 6                | 0              | -2.133590               | 1.256570  | 0.195707  |
| 3                | 6                | 0              | -2.817532               | 0.000000  | -0.334360 |
| 4                | 6                | 0              | -2.133590               | -1.256568 | 0.195708  |
| 5                | 6                | 0              | -0.640428               | -1.260201 | -0.141706 |
| 6                | 6                | 0              | 0.008745                | -0.000002 | 0.398900  |
| 7                | 1                | 0              | -3.873835               | -0.000001 | -0.057612 |
| 8                | 1                | 0              | -2.258132               | 1.306140  | 1.282556  |
| 9                | 1                | 0              | -2.599186               | 2.152960  | -0.218635 |
| 10               | 1                | 0              | -0.509294               | 1.289838  | -1.227609 |
| 11               | 1                | 0              | -0.154121               | 2.143973  | 0.273325  |
| 12               | 1                | 0              | -2.258128               | -1.306133 | 1.282558  |
| 13               | 1                | 0              | -2.599191               | -2.152959 | -0.218626 |
| 14               | 1                | 0              | -0.154125               | -2.143977 | 0.273323  |
| 15               | 1                | 0              | -0.509295               | -1.289840 | -1.227611 |
| 16               | 1                | 0              | -0.007821               | -0.000003 | 1.488652  |
| 17               | 1                | 0              | -2.773347               | 0.000001  | -1.428762 |

18                      35                      0                      1.938211                      0.000000                      -0.035909



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.055685                | -1.259335 | -0.155751 |
| 2                | 6                | 0              | 1.542679                | -1.257024 | 0.202499  |
| 3                | 6                | 0              | 2.234561                | -0.000001 | -0.316899 |
| 4                | 6                | 0              | 1.542679                | 1.257022  | 0.202496  |
| 5                | 6                | 0              | 0.055685                | 1.259338  | -0.155751 |
| 6                | 6                | 0              | -0.605152               | 0.000001  | 0.374036  |
| 7                | 1                | 0              | 3.286487                | 0.000001  | -0.023930 |
| 8                | 1                | 0              | 1.651910                | -1.306724 | 1.291061  |
| 9                | 1                | 0              | 2.015301                | -2.152830 | -0.204834 |
| 10               | 1                | 0              | -0.062751               | -1.286487 | -1.243412 |
| 11               | 1                | 0              | -0.440218               | -2.141121 | 0.252912  |
| 12               | 1                | 0              | 1.651909                | 1.306723  | 1.291059  |
| 13               | 1                | 0              | 2.015305                | 2.152828  | -0.204833 |
| 14               | 1                | 0              | -0.440211               | 2.141124  | 0.252921  |
| 15               | 1                | 0              | -0.062757               | 1.286496  | -1.243411 |
| 16               | 1                | 0              | -0.596150               | 0.000002  | 1.464634  |
| 17               | 1                | 0              | 2.207116                | -0.000004 | -1.411855 |
| 18               | 17               | 0              | -2.363692               | -0.000001 | -0.066123 |

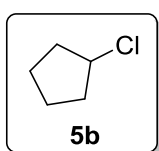


Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.822304               | 0.774803  | -0.687628 |
| 2                | 6                | 0              | -1.099492               | 1.192066  | 0.603368  |
| 3                | 6                | 0              | -0.227570               | 0.000058  | 0.956437  |
| 4                | 6                | 0              | -1.099478               | -1.192000 | 0.603508  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 5  | 6  | 0 | -1.822171 | -0.774926 | -0.687602 |
| 6  | 1  | 0 | -1.286806 | 1.153417  | -1.557983 |
| 7  | 1  | 0 | -1.818669 | 1.305028  | 1.420460  |
| 8  | 1  | 0 | -0.546191 | 2.125347  | 0.516637  |
| 9  | 1  | 0 | 0.155359  | 0.000120  | 1.971795  |
| 10 | 1  | 0 | -1.818723 | -1.304803 | 1.420564  |
| 11 | 1  | 0 | -2.829764 | -1.186996 | -0.724765 |
| 12 | 1  | 0 | -1.286438 | -1.153467 | -1.557844 |
| 13 | 1  | 0 | -2.829981 | 1.186683  | -0.724622 |
| 14 | 1  | 0 | -0.546191 | -2.125308 | 0.516974  |
| 15 | 35 | 0 | 1.406671  | -0.000001 | -0.171706 |

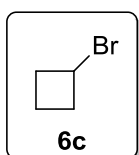
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Standard orientation:

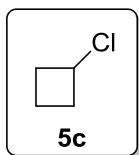
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.412374               | 0.774883  | -0.588764 |
| 2                | 6                | 0              | -0.531210               | 1.191867  | 0.600444  |
| 3                | 6                | 0              | 0.381667                | 0.000039  | 0.833512  |
| 4                | 6                | 0              | -0.531190               | -1.191821 | 0.600540  |
| 5                | 6                | 0              | -1.412277               | -0.774968 | -0.588760 |
| 6                | 1                | 0              | -0.992397               | 1.153506  | -1.520439 |
| 7                | 1                | 0              | -1.137856               | 1.308049  | 1.502821  |
| 8                | 1                | 0              | 0.012565                | 2.121626  | 0.441176  |
| 9                | 1                | 0              | 0.886033                | 0.000083  | 1.795342  |
| 10               | 1                | 0              | -1.137888               | -1.307889 | 1.502898  |
| 11               | 1                | 0              | -2.416514               | -1.187085 | -0.498206 |
| 12               | 1                | 0              | -0.992125               | -1.153536 | -1.520378 |
| 13               | 1                | 0              | -2.416655               | 1.186864  | -0.498081 |
| 14               | 17               | 0              | 1.718503                | -0.000001 | -0.399317 |
| 15               | 1                | 0              | 0.012592                | -2.121601 | 0.441411  |

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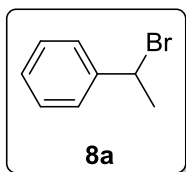
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.434367               | 1.077799  | -0.094092 |
| 2                | 6                | 0              | -0.518286               | 0.000000  | 0.481294  |
| 3                | 6                | 0              | -1.434368               | -1.077799 | -0.094091 |
| 4                | 6                | 0              | -2.544295               | 0.000000  | -0.087080 |
| 5                | 1                | 0              | -1.570777               | 1.985974  | 0.489225  |
| 6                | 1                | 0              | -1.149138               | 1.329456  | -1.115201 |
| 7                | 1                | 0              | -0.513607               | 0.000000  | 1.567774  |
| 8                | 1                | 0              | -1.570778               | -1.985974 | 0.489225  |
| 9                | 1                | 0              | -1.149140               | -1.329456 | -1.115202 |
| 10               | 1                | 0              | -3.097129               | 0.000000  | 0.851244  |
| 11               | 1                | 0              | -3.241214               | 0.000000  | -0.922273 |
| 12               | 35               | 0              | 1.367991                | -0.000000 | -0.042314 |



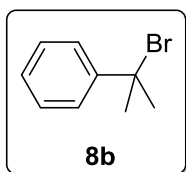
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.867836                | -1.076526 | -0.096028 |
| 2                | 6                | 0              | -0.065533               | 0.000000  | 0.455767  |
| 3                | 6                | 0              | 0.867837                | 1.076526  | -0.096028 |
| 4                | 6                | 0              | 1.977702                | -0.000001 | -0.064201 |
| 5                | 1                | 0              | 0.991442                | -1.985728 | 0.488551  |
| 6                | 1                | 0              | 0.601119                | -1.325465 | -1.123120 |
| 7                | 1                | 0              | -0.093860               | 0.000001  | 1.542524  |
| 8                | 1                | 0              | 0.991446                | 1.985726  | 0.488553  |
| 9                | 1                | 0              | 0.601122                | 1.325468  | -1.123120 |
| 10               | 1                | 0              | 2.508846                | 0.000000  | 0.886702  |
| 11               | 1                | 0              | 2.694755                | -0.000002 | -0.881878 |
| 12               | 17               | 0              | -1.775407               | 0.000000  | -0.086781 |



Standard orientation:

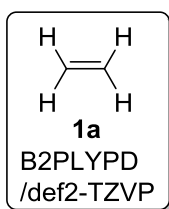
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.481583               | -0.047939 | -1.326486 |
| 2                | 6                | 0              | -1.170852               | 0.311675  | -1.058761 |
| 3                | 6                | 0              | -0.693076               | 0.314039  | 0.251121  |
| 4                | 6                | 0              | -1.549463               | -0.054080 | 1.283338  |
| 5                | 6                | 0              | -2.865612               | -0.411840 | 1.016564  |
| 6                | 6                | 0              | -3.334355               | -0.408768 | -0.288420 |
| 7                | 1                | 0              | -2.840952               | -0.048815 | -2.348027 |
| 8                | 1                | 0              | -0.510966               | 0.578804  | -1.875872 |
| 9                | 1                | 0              | -1.184478               | -0.058240 | 2.304109  |
| 10               | 1                | 0              | -3.522058               | -0.693220 | 1.830527  |
| 11               | 1                | 0              | -4.358909               | -0.688248 | -0.499785 |
| 12               | 6                | 0              | 0.710553                | 0.738438  | 0.568867  |
| 13               | 6                | 0              | 1.104688                | 2.085383  | 0.001628  |
| 14               | 1                | 0              | 2.120043                | 2.348603  | 0.295432  |
| 15               | 1                | 0              | 1.042969                | 2.097760  | -1.086376 |
| 16               | 1                | 0              | 0.420454                | 2.842057  | 0.393464  |
| 17               | 1                | 0              | 0.866315                | 0.715192  | 1.644078  |
| 18               | 35               | 0              | 1.989879                | -0.635867 | -0.095562 |



Standard orientation:

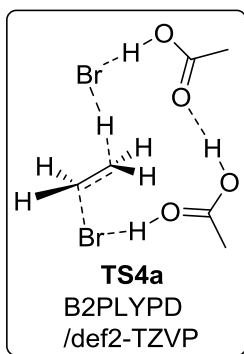
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.554584                | -1.306066 | 0.495850  |
| 2                | 6                | 0              | 1.234585                | -0.929723 | 0.670216  |
| 3                | 6                | 0              | 0.755849                | 0.276685  | 0.152993  |
| 4                | 6                | 0              | 1.640048                | 1.093273  | -0.545271 |
| 5                | 6                | 0              | 2.968473                | 0.716718  | -0.720040 |
| 6                | 6                | 0              | 3.431048                | -0.480589 | -0.201195 |
| 7                | 1                | 0              | 2.901823                | -2.248255 | 0.901429  |
| 8                | 1                | 0              | 0.560391                | -1.592910 | 1.198638  |
| 9                | 1                | 0              | 1.309181                | 2.035204  | -0.960511 |
| 10               | 1                | 0              | 3.638810                | 1.368399  | -1.266676 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 11 | 1  | 0 | 4.464113  | -0.774174 | -0.339071 |
| 12 | 6  | 0 | -0.682357 | 0.689317  | 0.398765  |
| 13 | 6  | 0 | -1.022122 | 0.680168  | 1.881237  |
| 14 | 1  | 0 | -2.067760 | 0.945467  | 2.037035  |
| 15 | 1  | 0 | -0.834472 | -0.287932 | 2.341944  |
| 16 | 1  | 0 | -0.395344 | 1.424435  | 2.380349  |
| 17 | 35 | 0 | -1.854825 | -0.699191 | -0.475395 |
| 18 | 6  | 0 | -1.071254 | 2.016197  | -0.224660 |
| 19 | 1  | 0 | -0.482926 | 2.815093  | 0.234305  |
| 20 | 1  | 0 | -0.903762 | 2.030545  | -1.300739 |
| 21 | 1  | 0 | -2.124297 | 2.219922  | -0.035228 |



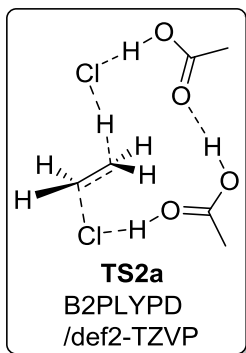
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |          |
|------------------|------------------|----------------|-------------------------|-----------|----------|
|                  |                  |                | X                       | Y         | Z        |
| 1                | 6                | 0              | 0.000000                | 0.664292  | 0.000000 |
| 2                | 1                | 0              | 0.923685                | 1.231158  | 0.000000 |
| 3                | 1                | 0              | -0.923679               | 1.231164  | 0.000000 |
| 4                | 6                | 0              | -0.000000               | -0.664292 | 0.000000 |
| 5                | 1                | 0              | -0.923685               | -1.231158 | 0.000000 |
| 6                | 1                | 0              | 0.923679                | -1.231164 | 0.000000 |



Standard orientation:

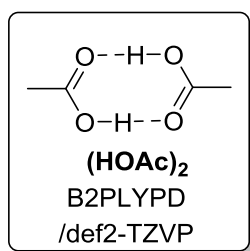
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.500828               | -1.395957 | -0.871573 |
| 2                | 6                | 0              | -0.030256               | -1.748615 | 0.370296  |
| 3                | 1                | 0              | -0.387268               | -0.371024 | -1.207850 |
| 4                | 1                | 0              | -1.773383               | -1.328915 | -0.500833 |
| 5                | 1                | 0              | 2.181268                | 0.021914  | 0.164759  |
| 6                | 6                | 0              | 2.053812                | 1.729776  | -0.830014 |
| 7                | 8                | 0              | 1.595138                | 0.884299  | 0.004060  |
| 8                | 8                | 0              | 1.287613                | 2.673634  | -1.217720 |
| 9                | 1                | 0              | 0.318900                | 2.544954  | -0.860920 |
| 10               | 6                | 0              | 3.430497                | 1.653007  | -1.361919 |
| 11               | 1                | 0              | 4.137135                | 1.639521  | -0.530860 |
| 12               | 1                | 0              | 3.540309                | 0.710463  | -1.902660 |
| 13               | 1                | 0              | 3.630209                | 2.490282  | -2.023618 |
| 14               | 6                | 0              | -1.211211               | 2.058516  | 0.832885  |
| 15               | 8                | 0              | -1.036060               | 2.106570  | -0.385525 |
| 16               | 8                | 0              | -2.162217               | 1.325858  | 1.374254  |
| 17               | 1                | 0              | -2.642655               | 0.780553  | 0.694463  |
| 18               | 6                | 0              | -0.370073               | 2.779451  | 1.830431  |
| 19               | 1                | 0              | 0.282759                | 2.052137  | 2.317918  |
| 20               | 1                | 0              | 0.233282                | 3.539373  | 1.341042  |
| 21               | 1                | 0              | -1.001615               | 3.227707  | 2.596570  |
| 22               | 1                | 0              | -0.530894               | -2.153598 | -1.647971 |
| 23               | 1                | 0              | -0.009395               | -2.785034 | 0.678029  |
| 24               | 1                | 0              | 0.078256                | -1.010050 | 1.152299  |
| 25               | 35               | 0              | -3.557431               | -0.958796 | -0.409487 |
| 26               | 35               | 0              | 2.821307                | -1.776583 | 0.458299  |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

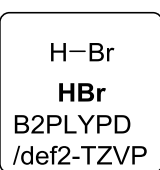
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 1  | 6  | 0 | 0.617436  | 1.762004  | -0.874642 |
| 2  | 6  | 0 | 0.367159  | 2.065854  | 0.445544  |
| 3  | 1  | 0 | 0.353929  | 0.776611  | -1.243251 |
| 4  | 1  | 0 | 1.880788  | 1.560863  | -0.672856 |
| 5  | 1  | 0 | -1.940984 | 0.578583  | 0.498099  |
| 6  | 6  | 0 | -2.102914 | -1.026255 | -0.668553 |
| 7  | 8  | 0 | -1.502374 | -0.353147 | 0.225016  |
| 8  | 8  | 0 | -1.488847 | -2.011029 | -1.205815 |
| 9  | 1  | 0 | -0.490756 | -2.031628 | -0.920549 |
| 10 | 6  | 0 | -3.473516 | -0.704659 | -1.118223 |
| 11 | 1  | 0 | -4.107217 | -0.505269 | -0.255033 |
| 12 | 1  | 0 | -3.422654 | 0.211508  | -1.712646 |
| 13 | 1  | 0 | -3.874779 | -1.511032 | -1.724969 |
| 14 | 6  | 0 | 1.236495  | -1.714876 | 0.639518  |
| 15 | 8  | 0 | 0.945217  | -1.746763 | -0.557847 |
| 16 | 8  | 0 | 2.258720  | -1.024098 | 1.093680  |
| 17 | 1  | 0 | 2.703757  | -0.493696 | 0.372139  |
| 18 | 6  | 0 | 0.482021  | -2.436142 | 1.704445  |
| 19 | 1  | 0 | 0.096144  | -1.714192 | 2.425334  |
| 20 | 1  | 0 | -0.334895 | -3.008556 | 1.273534  |
| 21 | 1  | 0 | 1.165205  | -3.101248 | 2.234887  |
| 22 | 1  | 0 | 0.597511  | 2.566799  | -1.602171 |
| 23 | 17 | 0 | 3.522640  | 1.011215  | -0.780830 |
| 24 | 17 | 0 | -2.223302 | 2.265995  | 0.905442  |
| 25 | 1  | 0 | 0.493024  | 3.077137  | 0.807295  |
| 26 | 1  | 0 | 0.330378  | 1.286276  | 1.192960  |



Standard orientation:

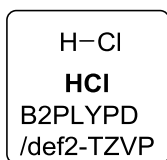
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.926514                | -0.062615 | -0.000025 |
| 2                | 8                | 0              | 1.262875                | -1.097018 | -0.000224 |
| 3                | 8                | 0              | 1.383418                | 1.141358  | -0.000604 |
| 4                | 1                | 0              | 0.380693                | 1.082469  | -0.000680 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 5  | 6 | 0 | 3.419391  | -0.045119 | 0.000639  |
| 6  | 1 | 0 | 3.774022  | 0.493992  | -0.879149 |
| 7  | 1 | 0 | 3.773111  | 0.492804  | 0.881528  |
| 8  | 1 | 0 | 3.806590  | -1.059993 | 0.000194  |
| 9  | 6 | 0 | -1.926519 | 0.062619  | -0.000011 |
| 10 | 8 | 0 | -1.262868 | 1.097010  | -0.000008 |
| 11 | 8 | 0 | -1.383418 | -1.141360 | -0.000410 |
| 12 | 1 | 0 | -0.380694 | -1.082457 | -0.000561 |
| 13 | 6 | 0 | -3.419393 | 0.045125  | 0.000547  |
| 14 | 1 | 0 | -3.773778 | -0.492014 | -0.880561 |
| 15 | 1 | 0 | -3.773358 | -0.494769 | 0.880116  |
| 16 | 1 | 0 | -3.806592 | 1.059998  | 0.002182  |



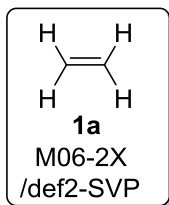
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 1                | 0              | 0.000000                | 0.000000 | -1.381724 |
| 2                | 35               | 0              | 0.000000                | 0.000000 | 0.039478  |



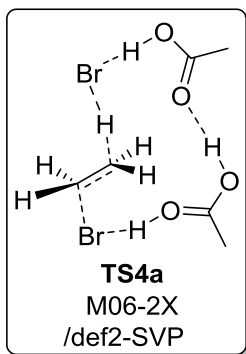
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 17               | 0              | 0.000000                | 0.000000 | 0.071342  |
| 2                | 1                | 0              | 0.000000                | 0.000000 | -1.212808 |



Standard orientation:

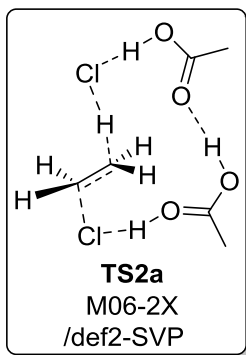
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.664818               | 0.000000  | 0.000003  |
| 2                | 6                | 0              | 0.664818                | -0.000000 | -0.000004 |
| 3                | 1                | 0              | -1.237734               | -0.931570 | -0.000009 |
| 4                | 1                | 0              | -1.237732               | 0.931571  | 0.000025  |
| 5                | 1                | 0              | 1.237734                | 0.931570  | 0.000012  |
| 6                | 1                | 0              | 1.237732                | -0.931571 | -0.000022 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.337611               | -1.280012 | -1.043493 |
| 2                | 6                | 0              | 0.079360                | -1.655012 | 0.213872  |
| 3                | 1                | 0              | -0.317582               | -0.225056 | -1.334380 |
| 4                | 1                | 0              | -1.595217               | -1.319801 | -0.617726 |
| 5                | 1                | 0              | 2.162021                | 0.189465  | 0.382860  |
| 6                | 6                | 0              | 1.875832                | 1.677758  | -0.865676 |
| 7                | 8                | 0              | 1.549003                | 1.020049  | 0.177142  |
| 8                | 8                | 0              | 1.033845                | 2.475242  | -1.363650 |
| 9                | 1                | 0              | 0.053323                | 2.342790  | -0.923851 |
| 10               | 6                | 0              | 3.212867                | 1.527722  | -1.485313 |
| 11               | 1                | 0              | 3.970834                | 1.875410  | -0.767867 |
| 12               | 1                | 0              | 3.398717                | 0.458248  | -1.665396 |

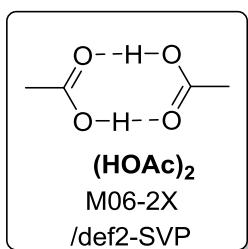
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 13 | 1  | 0 | 3.267889  | 2.103895  | -2.413290 |
| 14 | 6  | 0 | -1.290583 | 1.968014  | 0.825156  |
| 15 | 8  | 0 | -1.128543 | 1.892507  | -0.395009 |
| 16 | 8  | 0 | -2.190170 | 1.253189  | 1.433204  |
| 17 | 1  | 0 | -2.654715 | 0.624848  | 0.803848  |
| 18 | 6  | 0 | -0.496519 | 2.862705  | 1.715925  |
| 19 | 1  | 0 | -0.030300 | 2.260870  | 2.507797  |
| 20 | 1  | 0 | 0.263382  | 3.404269  | 1.141616  |
| 21 | 1  | 0 | -1.183750 | 3.572523  | 2.198032  |
| 22 | 1  | 0 | -0.321752 | -2.016859 | -1.851239 |
| 23 | 1  | 0 | 0.127924  | -2.709937 | 0.490192  |
| 24 | 1  | 0 | 0.088887  | -0.936506 | 1.036977  |
| 25 | 35 | 0 | -3.407972 | -1.058147 | -0.362033 |
| 26 | 35 | 0 | 2.847891  | -1.609256 | 0.534493  |



Standard orientation:

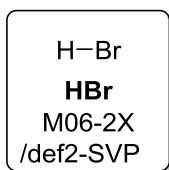
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.337833               | -1.727120 | -0.959630 |
| 2                | 6                | 0              | -0.135301               | -1.964638 | 0.384820  |
| 3                | 1                | 0              | -0.202587               | -0.718017 | -1.361274 |
| 4                | 1                | 0              | -1.629573               | -1.650450 | -0.725313 |
| 5                | 1                | 0              | 1.950254                | -0.295640 | 0.731159  |
| 6                | 6                | 0              | 1.929976                | 1.057571  | -0.704464 |
| 7                | 8                | 0              | 1.467905                | 0.593310  | 0.384866  |
| 8                | 8                | 0              | 1.216681                | 1.858986  | -1.375769 |
| 9                | 1                | 0              | 0.203634                | 1.855726  | -1.021073 |
| 10               | 6                | 0              | 3.282408                | 0.690471  | -1.185900 |
| 11               | 1                | 0              | 4.020881                | 1.199994  | -0.548156 |
| 12               | 1                | 0              | 3.421177                | -0.391570 | -1.051090 |
| 13               | 1                | 0              | 3.414359                | 0.992723  | -2.228772 |
| 14               | 6                | 0              | -1.375475               | 1.597247  | 0.597727  |
| 15               | 8                | 0              | -1.070548               | 1.493568  | -0.593001 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 16 | 8  | 0 | -2.341003 | 0.899856  | 1.114179  |
| 17 | 1  | 0 | -2.736925 | 0.251232  | 0.445787  |
| 18 | 6  | 0 | -0.683197 | 2.506407  | 1.557914  |
| 19 | 1  | 0 | -0.225039 | 1.900372  | 2.351896  |
| 20 | 1  | 0 | 0.079168  | 3.104841  | 1.048390  |
| 21 | 1  | 0 | -1.430827 | 3.159941  | 2.028292  |
| 22 | 1  | 0 | -0.231049 | -2.555244 | -1.665349 |
| 23 | 17 | 0 | -3.304148 | -1.237758 | -0.707538 |
| 24 | 17 | 0 | 2.335949  | -1.964859 | 1.043946  |
| 25 | 1  | 0 | -0.207004 | -2.979769 | 0.779475  |
| 26 | 1  | 0 | -0.234828 | -1.155043 | 1.112090  |



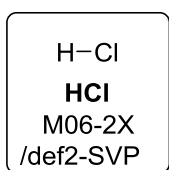
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.889059                | 0.048309  | -0.000192 |
| 2                | 8                | 0              | 1.209692                | 1.068519  | -0.000048 |
| 3                | 8                | 0              | 1.372465                | -1.151952 | -0.000457 |
| 4                | 1                | 0              | 0.360428                | -1.109864 | -0.000843 |
| 5                | 6                | 0              | 3.383862                | 0.073246  | 0.000544  |
| 6                | 1                | 0              | 3.750689                | -0.463031 | 0.886881  |
| 7                | 1                | 0              | 3.751422                | -0.462007 | -0.886107 |
| 8                | 1                | 0              | 3.744272                | 1.106363  | 0.001277  |
| 9                | 6                | 0              | -1.889063               | -0.048304 | -0.000172 |
| 10               | 8                | 0              | -1.209663               | -1.068493 | -0.000288 |
| 11               | 8                | 0              | -1.372488               | 1.151967  | -0.000226 |
| 12               | 1                | 0              | -0.360455               | 1.109906  | -0.000511 |
| 13               | 6                | 0              | -3.383862               | -0.073285 | 0.000637  |
| 14               | 1                | 0              | -3.750595               | 0.462168  | 0.887516  |
| 15               | 1                | 0              | -3.751545               | 0.462768  | -0.885474 |
| 16               | 1                | 0              | -3.744237               | -1.106415 | 0.000512  |



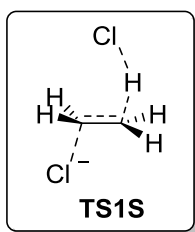
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 1                | 0              | 0.000000                | 0.000000 | -1.382953 |
| 2                | 35               | 0              | 0.000000                | 0.000000 | 0.039513  |



Standard orientation:

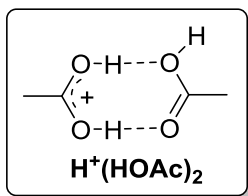
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 17               | 0              | 0.000000                | 0.000000 | 0.071701  |
| 2                | 1                | 0              | 0.000000                | 0.000000 | -1.218914 |



Standard orientation:

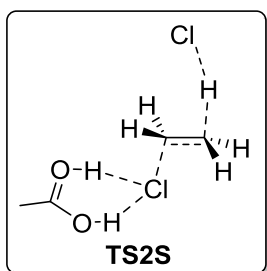
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.215478                | 0.898985  | 0.000142  |
| 2                | 6                | 0              | -0.446236               | -0.298864 | 0.000800  |
| 3                | 1                | 0              | 0.286459                | 1.466268  | -0.921567 |
| 4                | 1                | 0              | 1.466407                | 0.259577  | 0.000170  |
| 5                | 1                | 0              | 0.286452                | 1.467291  | 0.921218  |
| 6                | 1                | 0              | -0.562167               | -0.856881 | 0.919074  |
| 7                | 17               | 0              | -2.969326               | -0.109184 | -0.000261 |

|   |    |   |           |           |           |
|---|----|---|-----------|-----------|-----------|
| 8 | 17 | 0 | 2.996934  | -0.189580 | -0.000194 |
| 9 | 1  | 0 | -0.561936 | -0.857996 | -0.916817 |



Standard orientation:

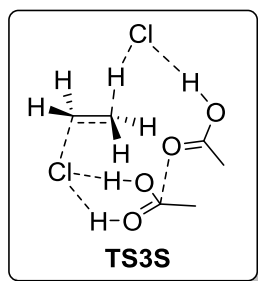
| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.934935                | -0.092688 | -0.000075 |
| 2                | 8                | 0              | 1.336174                | 1.094476  | -0.000424 |
| 3                | 8                | 0              | 1.224308                | -1.082029 | -0.000067 |
| 4                | 1                | 0              | -0.196449               | -1.000712 | -0.000159 |
| 5                | 6                | 0              | 3.418053                | -0.135372 | 0.000320  |
| 6                | 1                | 0              | 3.753807                | -1.167122 | 0.000356  |
| 7                | 1                | 0              | 3.791997                | 0.385096  | -0.883187 |
| 8                | 1                | 0              | 3.791468                | 0.384967  | 0.884132  |
| 9                | 6                | 0              | -1.949420               | -0.021518 | 0.000041  |
| 10               | 8                | 0              | -1.256379               | -1.069552 | -0.000185 |
| 11               | 8                | 0              | -1.452113               | 1.163413  | 0.000253  |
| 12               | 1                | 0              | -0.468070               | 1.205924  | 0.000128  |
| 13               | 6                | 0              | -3.421435               | -0.112744 | 0.000080  |
| 14               | 1                | 0              | -3.798257               | 0.410698  | 0.880397  |
| 15               | 1                | 0              | -3.798320               | 0.410974  | -0.880046 |
| 16               | 1                | 0              | -3.738727               | -1.149706 | -0.000075 |
| 17               | 1                | 0              | 1.953836                | 1.843338  | -0.000364 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

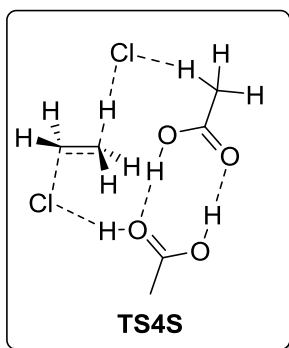
|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 1  | 6  | 0 | 1.120946  | -0.187944 | 0.001799  |
| 2  | 6  | 0 | 1.162540  | 1.203596  | 0.000667  |
| 3  | 1  | 0 | 0.839226  | -0.689812 | 0.922802  |
| 4  | 1  | 0 | 2.377794  | -0.307581 | 0.000798  |
| 5  | 1  | 0 | 0.838221  | -0.691037 | -0.918246 |
| 6  | 1  | 0 | 1.392677  | 1.728201  | -0.917666 |
| 7  | 1  | 0 | -1.695445 | 0.598495  | -0.994186 |
| 8  | 6  | 0 | -2.208943 | -0.940856 | 0.000326  |
| 9  | 8  | 0 | -2.022480 | -0.348430 | -1.111372 |
| 10 | 8  | 0 | -2.018895 | -0.368110 | 1.123348  |
| 11 | 1  | 0 | -1.693631 | 0.577233  | 1.023630  |
| 12 | 6  | 0 | -2.625721 | -2.349927 | -0.010372 |
| 13 | 1  | 0 | -3.191494 | -2.566336 | -0.912572 |
| 14 | 1  | 0 | -1.708677 | -2.948182 | -0.018971 |
| 15 | 1  | 0 | -3.185389 | -2.582555 | 0.891558  |
| 16 | 17 | 0 | -1.020074 | 2.197262  | -0.001249 |
| 17 | 17 | 0 | 4.094908  | -0.754026 | -0.001438 |
| 18 | 1  | 0 | 1.392600  | 1.729672  | 0.918211  |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.888527               | -1.987555 | 0.871045  |
| 2                | 6                | 0              | -0.589756               | -1.926943 | -0.475611 |
| 3                | 1                | 0              | -1.024437               | -2.959684 | 1.330465  |
| 4                | 1                | 0              | -2.028697               | -1.578897 | 0.555856  |
| 5                | 1                | 0              | -0.574983               | -1.173450 | 1.515537  |
| 6                | 1                | 0              | -0.442068               | -0.967692 | -0.954027 |
| 7                | 1                | 0              | 2.294729                | -0.325491 | -1.021935 |
| 8                | 6                | 0              | 2.231103                | 0.656927  | 0.601314  |
| 9                | 8                | 0              | 2.393355                | 0.608651  | -0.663806 |
| 10               | 8                | 0              | 2.022517                | -0.386855 | 1.300560  |
| 11               | 1                | 0              | 1.984359                | -1.222464 | 0.735294  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 12 | 6  | 0 | 2.383672  | 1.946762  | 1.290405  |
| 13 | 1  | 0 | 3.414591  | 1.992289  | 1.654605  |
| 14 | 1  | 0 | 2.211015  | 2.766822  | 0.600161  |
| 15 | 1  | 0 | 1.710546  | 1.987128  | 2.143028  |
| 16 | 17 | 0 | 1.893591  | -2.320360 | -0.925793 |
| 17 | 17 | 0 | -3.666670 | -0.725430 | 0.431776  |
| 18 | 6  | 0 | -0.270684 | 3.003599  | -1.070744 |
| 19 | 1  | 0 | -0.822985 | 3.326777  | -1.949424 |
| 20 | 1  | 0 | -0.249508 | 3.823440  | -0.349164 |
| 21 | 1  | 0 | 0.753529  | 2.746204  | -1.333563 |
| 22 | 6  | 0 | -0.932671 | 1.832852  | -0.415950 |
| 23 | 8  | 0 | -0.358183 | 1.065086  | 0.332993  |
| 24 | 8  | 0 | -2.213191 | 1.718089  | -0.714182 |
| 25 | 1  | 0 | -2.628867 | 0.938031  | -0.255262 |
| 26 | 1  | 0 | -0.809681 | -2.768204 | -1.120567 |



Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.252225               | 2.258434  | 0.745293  |
| 2                | 6                | 0              | -0.416002               | 2.153628  | -0.350413 |
| 3                | 1                | 0              | -1.216322               | 1.491049  | 1.511339  |
| 4                | 1                | 0              | -2.219184               | 1.811978  | 0.036466  |
| 5                | 1                | 0              | 1.913048                | 0.801728  | 0.355924  |
| 6                | 6                | 0              | 2.516342                | -1.013827 | -0.192219 |
| 7                | 8                | 0              | 1.660229                | -0.229115 | 0.337662  |
| 8                | 8                | 0              | 2.180113                | -2.209267 | -0.412164 |
| 9                | 1                | 0              | 1.151387                | -2.399361 | -0.238161 |
| 10               | 6                | 0              | 3.866421                | -0.546558 | -0.564934 |
| 11               | 1                | 0              | 3.759140                | 0.111188  | -1.432066 |
| 12               | 1                | 0              | 4.293146                | 0.039493  | 0.248304  |
| 13               | 1                | 0              | 4.498034                | -1.391702 | -0.820163 |
| 14               | 1                | 0              | -1.546054               | 3.248192  | 1.075509  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 15 | 1  | 0 | -0.372734 | 2.957251  | -1.074189 |
| 16 | 1  | 0 | -0.119771 | 1.176591  | -0.710817 |
| 17 | 6  | 0 | -1.157613 | -2.113627 | 0.349191  |
| 18 | 8  | 0 | -0.241640 | -2.721341 | -0.196726 |
| 19 | 8  | 0 | -0.957226 | -1.035462 | 1.074319  |
| 20 | 1  | 0 | -0.011539 | -0.790933 | 1.072420  |
| 21 | 6  | 0 | -2.580384 | -2.516941 | 0.246610  |
| 22 | 1  | 0 | -2.986942 | -2.650711 | 1.249766  |
| 23 | 1  | 0 | -3.132302 | -1.698213 | -0.223068 |
| 24 | 1  | 0 | -2.670112 | -3.430667 | -0.332144 |
| 25 | 17 | 0 | -3.625544 | 1.029720  | -0.707017 |
| 26 | 17 | 0 | 1.959025  | 2.556100  | 0.204369  |

---

#### 4. Source Data of Figure 7.

Table S1. Source data of ethene.

| Ethene    |                |                 |             |
|-----------|----------------|-----------------|-------------|
| IRC point | C-H bond order | C-Br bond order | Charge on C |
| 1         | 0.92836862     | 0.93466567      | -0.00366766 |
| 2         | 0.92714938     | 0.93172073      | -0.00245013 |
| 3         | 0.92617046     | 0.93148322      | -0.00247128 |
| 4         | 0.92413847     | 0.92811435      | -0.00118905 |
| 5         | 0.92302199     | 0.9267072       | -0.00051744 |
| 6         | 0.92108909     | 0.92357318      | 0.00078907  |
| 7         | 0.9191297      | 0.92093583      | 0.00198496  |
| 8         | 0.91735864     | 0.91760732      | 0.00366679  |
| 9         | 0.91486846     | 0.91365871      | 0.00553981  |
| 10        | 0.91295328     | 0.90958744      | 0.00774383  |
| 11        | 0.91010536     | 0.90480344      | 0.01010891  |
| 12        | 0.90821198     | 0.90014138      | 0.01263936  |
| 13        | 0.90469489     | 0.89482604      | 0.01519868  |
| 14        | 0.90218874     | 0.88930127      | 0.01807842  |
| 15        | 0.89856309     | 0.88304988      | 0.02114188  |
| 16        | 0.89563369     | 0.87658727      | 0.02445035  |
| 17        | 0.89170393     | 0.8696556       | 0.02779805  |
| 18        | 0.88878195     | 0.86266843      | 0.03137824  |
| 19        | 0.8841007      | 0.85541198      | 0.03457532  |
| 20        | 0.88177032     | 0.84823574      | 0.03811572  |
| 21        | 0.87523803     | 0.84057532      | 0.04071139  |
| 22        | 0.87265291     | 0.83188369      | 0.04464496  |
| 23        | 0.86621603     | 0.82330299      | 0.04765693  |
| 24        | 0.86137164     | 0.8126851       | 0.05162599  |
| 25        | 0.85684483     | 0.80365476      | 0.05520326  |
| 26        | 0.84951917     | 0.79130644      | 0.05879356  |
| 27        | 0.84642609     | 0.78225319      | 0.06256616  |
| 28        | 0.83672353     | 0.76792131      | 0.06566113  |
| 29        | 0.83367366     | 0.75812258      | 0.06939843  |
| 30        | 0.82324383     | 0.74263786      | 0.07221631  |
| 31        | 0.81827737     | 0.73066084      | 0.07569193  |
| 32        | 0.80798154     | 0.71442366      | 0.07840097  |
| 33        | 0.80087985     | 0.70000327      | 0.08153678  |
| 34        | 0.79030526     | 0.68256068      | 0.08409048  |
| 35        | 0.78150564     | 0.66589213      | 0.0868758   |
| 36        | 0.77001774     | 0.64675123      | 0.08912968  |
| 37        | 0.7596855      | 0.62795641      | 0.091504    |
| 38        | 0.74664067     | 0.60668759      | 0.09327235  |

|    |            |            |             |
|----|------------|------------|-------------|
| 39 | 0.73512408 | 0.58604177 | 0.09523969  |
| 40 | 0.7199152  | 0.56226723 | 0.09634331  |
| 41 | 0.70878273 | 0.54098161 | 0.0982145   |
| 42 | 0.68853443 | 0.51293303 | 0.09787445  |
| 43 | 0.68283595 | 0.49518774 | 0.10067471  |
| 44 | 0.65004262 | 0.45852118 | 0.09665358  |
| 45 | 0.64489123 | 0.44130609 | 0.09909601  |
| 46 | 0.61695964 | 0.40744865 | 0.09595399  |
| 47 | 0.5994258  | 0.38111802 | 0.09511056  |
| 48 | 0.57509366 | 0.35058083 | 0.09212659  |
| 49 | 0.55206377 | 0.32200904 | 0.0889274   |
| 50 | 0.52353573 | 0.29145757 | 0.08352148  |
| 51 | 0.48475266 | 0.25632738 | 0.07426428  |
| 52 | 0.44672006 | 0.22383819 | 0.06448048  |
| 53 | 0.40077026 | 0.1904286  | 0.05123388  |
| 54 | 0.34266882 | 0.15595796 | 0.03315788  |
| 55 | 0.2837591  | 0.1245628  | 0.01406188  |
| 56 | 0.22972172 | 0.09781043 | -0.00398702 |
| 57 | 0.18574576 | 0.07632149 | -0.01884351 |
| 58 | 0.17014228 | 0.06535205 | -0.02381414 |
| 59 | 0.16241943 | 0.05877205 | -0.02546474 |
| 60 | 0.15398046 | 0.05268091 | -0.02764828 |
| 61 | 0.14873325 | 0.04808206 | -0.02866982 |

**Table S2. Source data of propene.**

| propene   |                |                 |             |
|-----------|----------------|-----------------|-------------|
| IRC point | C-H bond order | C-Br bond order | Charge on C |
| 1         | 0.93525493     | 0.93870549      | 0.02523639  |
| 2         | 0.93481026     | 0.93698121      | 0.02607684  |
| 3         | 0.93497146     | 0.93853029      | 0.02557863  |
| 4         | 0.93478283     | 0.93764907      | 0.02588212  |
| 5         | 0.9346884      | 0.93781623      | 0.02604474  |
| 6         | 0.93479931     | 0.9379908       | 0.02591258  |
| 7         | 0.93455361     | 0.93729019      | 0.02620298  |
| 8         | 0.93482831     | 0.93821468      | 0.02612933  |
| 9         | 0.9341831      | 0.9362209       | 0.02655499  |
| 10        | 0.9348964      | 0.938804        | 0.02619171  |
| 11        | 0.93455971     | 0.93718173      | 0.02640682  |
| 12        | 0.934577       | 0.93798694      | 0.02664279  |
| 13        | 0.93488497     | 0.938728        | 0.02615045  |
| 14        | 0.93443445     | 0.93749676      | 0.02697872  |
| 15        | 0.93500049     | 0.94002176      | 0.02607428  |

|    |            |            |            |
|----|------------|------------|------------|
| 16 | 0.93446799 | 0.9381931  | 0.0269513  |
| 17 | 0.93471706 | 0.93997384 | 0.0266246  |
| 18 | 0.93466069 | 0.93995143 | 0.02667141 |
| 19 | 0.9343607  | 0.93926439 | 0.02728598 |
| 20 | 0.93459886 | 0.9407919  | 0.02670844 |
| 21 | 0.93427198 | 0.93887328 | 0.02762155 |
| 22 | 0.93438727 | 0.94047872 | 0.02698986 |
| 23 | 0.93432117 | 0.93912361 | 0.02754447 |
| 24 | 0.93425924 | 0.9394255  | 0.0273985  |
| 25 | 0.93438273 | 0.9392075  | 0.0275106  |
| 26 | 0.93417439 | 0.93825363 | 0.02775597 |
| 27 | 0.93433944 | 0.93932762 | 0.0276357  |
| 28 | 0.93394766 | 0.93750134 | 0.02799751 |
| 29 | 0.93422683 | 0.93830516 | 0.02822579 |
| 30 | 0.93363642 | 0.93855661 | 0.02796792 |
| 31 | 0.93365021 | 0.93660043 | 0.02884528 |
| 32 | 0.93314912 | 0.9378387  | 0.02834307 |
| 33 | 0.93288175 | 0.93562285 | 0.02923271 |
| 34 | 0.93208478 | 0.93494997 | 0.0292799  |
| 35 | 0.93194581 | 0.93365015 | 0.02984107 |
| 36 | 0.93051006 | 0.9307816  | 0.0306767  |
| 37 | 0.93070126 | 0.92968996 | 0.03114066 |
| 38 | 0.92848608 | 0.9254655  | 0.03257967 |
| 39 | 0.92864448 | 0.92350468 | 0.03317383 |
| 40 | 0.92644742 | 0.91875783 | 0.03504745 |
| 41 | 0.92582464 | 0.91499816 | 0.03618762 |
| 42 | 0.92404402 | 0.90977775 | 0.03838892 |
| 43 | 0.92271582 | 0.90439686 | 0.04026985 |
| 44 | 0.92107031 | 0.89840107 | 0.04275985 |
| 45 | 0.91939412 | 0.89184295 | 0.04527681 |
| 46 | 0.91760452 | 0.88518307 | 0.04794784 |
| 47 | 0.91576271 | 0.87776202 | 0.05094585 |
| 48 | 0.91370111 | 0.87055045 | 0.05370378 |
| 49 | 0.91169432 | 0.86241483 | 0.05705409 |
| 50 | 0.90942384 | 0.85437577 | 0.06011845 |
| 51 | 0.90719835 | 0.84560976 | 0.06363244 |
| 52 | 0.90475201 | 0.83680874 | 0.06699016 |
| 53 | 0.90231703 | 0.82741239 | 0.07060452 |
| 54 | 0.89969404 | 0.81795518 | 0.07412682 |
| 55 | 0.89709613 | 0.80790712 | 0.07781184 |
| 56 | 0.89429561 | 0.79782499 | 0.08142596 |
| 57 | 0.89160902 | 0.78712729 | 0.08515562 |
| 58 | 0.88854494 | 0.7764285  | 0.0888055  |
| 59 | 0.88599613 | 0.76542679 | 0.09244224 |

|     |            |            |            |
|-----|------------|------------|------------|
| 60  | 0.88206715 | 0.75388416 | 0.09602226 |
| 61  | 0.87995412 | 0.74376649 | 0.09923429 |
| 62  | 0.87587371 | 0.73061966 | 0.10286721 |
| 63  | 0.87277281 | 0.71904648 | 0.10634069 |
| 64  | 0.86984989 | 0.70601429 | 0.10991737 |
| 65  | 0.86576885 | 0.69263636 | 0.11347384 |
| 66  | 0.86479631 | 0.68205729 | 0.11679222 |
| 67  | 0.85889666 | 0.66618046 | 0.11989676 |
| 68  | 0.85743557 | 0.65809713 | 0.12265052 |
| 69  | 0.85234642 | 0.64217743 | 0.12554234 |
| 70  | 0.84685484 | 0.62904886 | 0.12818635 |
| 71  | 0.84372154 | 0.61363466 | 0.13166934 |
| 72  | 0.83624366 | 0.59696221 | 0.13431959 |
| 73  | 0.83434675 | 0.58213479 | 0.13810627 |
| 74  | 0.82619087 | 0.56435763 | 0.14053516 |
| 75  | 0.82356843 | 0.54889305 | 0.14421259 |
| 76  | 0.81621738 | 0.5309866  | 0.14681069 |
| 77  | 0.81224201 | 0.51476745 | 0.15014009 |
| 78  | 0.80544624 | 0.49692884 | 0.15284119 |
| 79  | 0.80048623 | 0.48056022 | 0.15580737 |
| 80  | 0.79356822 | 0.46282686 | 0.15832361 |
| 81  | 0.78784085 | 0.44692625 | 0.16088234 |
| 82  | 0.78018463 | 0.42941087 | 0.16282837 |
| 83  | 0.77356678 | 0.41450373 | 0.16492389 |
| 84  | 0.76469542 | 0.39740064 | 0.16584511 |
| 85  | 0.75640627 | 0.38284224 | 0.16742603 |
| 86  | 0.747206   | 0.36698226 | 0.16764876 |
| 87  | 0.73668228 | 0.35158516 | 0.16834997 |
| 88  | 0.72823702 | 0.33752091 | 0.1684089  |
| 89  | 0.71557316 | 0.32154402 | 0.16812005 |
| 90  | 0.70963347 | 0.3099572  | 0.16840585 |
| 91  | 0.68621728 | 0.29114201 | 0.16437906 |
| 92  | 0.69473266 | 0.29009011 | 0.16778821 |
| 93  | 0.66122741 | 0.2676599  | 0.16067266 |
| 94  | 0.65548782 | 0.258538   | 0.16065257 |
| 95  | 0.6360061  | 0.24258471 | 0.15684048 |
| 96  | 0.62209436 | 0.22983703 | 0.15434714 |
| 97  | 0.60479216 | 0.21603288 | 0.15065103 |
| 98  | 0.58822779 | 0.20323528 | 0.14694789 |
| 99  | 0.56974468 | 0.19026347 | 0.14237338 |
| 100 | 0.55158923 | 0.17856358 | 0.13779107 |
| 101 | 0.53110679 | 0.16580435 | 0.13232125 |
| 102 | 0.51082954 | 0.1537531  | 0.12662463 |
| 103 | 0.49315481 | 0.14402832 | 0.12143983 |

|     |            |            |            |
|-----|------------|------------|------------|
| 104 | 0.46775331 | 0.13188291 | 0.11367898 |
| 105 | 0.43673457 | 0.11875869 | 0.1039599  |
| 106 | 0.39970845 | 0.10477238 | 0.09220115 |
| 107 | 0.35116477 | 0.08905393 | 0.0766838  |
| 108 | 0.29159823 | 0.0721862  | 0.05767403 |
| 109 | 0.23247856 | 0.05664787 | 0.03865771 |
| 110 | 0.18203926 | 0.0439872  | 0.02226548 |
| 111 | 0.16401964 | 0.03910477 | 0.01635307 |

**Table S3. Source data of isobutene.**

| isobutene |                |                 |             |
|-----------|----------------|-----------------|-------------|
| IRC point | C-H bond order | C-Br bond order | Charge on C |
| 1         | 0.16522502     | 0.01828208      | 0.05234647  |
| 2         | 0.17448964     | 0.0198416       | 0.05462775  |
| 3         | 0.17486739     | 0.02028444      | 0.05477326  |
| 4         | 0.18720221     | 0.02218935      | 0.05777467  |
| 5         | 0.19326232     | 0.02311385      | 0.05931889  |
| 6         | 0.21773493     | 0.02570654      | 0.06604615  |
| 7         | 0.2531913      | 0.02934164      | 0.07594678  |
| 8         | 0.294474       | 0.0335998       | 0.08738194  |
| 9         | 0.33759403     | 0.03805749      | 0.09931308  |
| 10        | 0.37850605     | 0.04244247      | 0.1107511   |
| 11        | 0.46141027     | 0.05144018      | 0.134082    |
| 12        | 0.47977575     | 0.05342031      | 0.139443    |
| 13        | 0.48437915     | 0.05424931      | 0.14106473  |
| 14        | 0.51361494     | 0.05784659      | 0.14940773  |
| 15        | 0.51031376     | 0.0579057       | 0.14878291  |
| 16        | 0.53245389     | 0.0609818       | 0.15510978  |
| 17        | 0.53946748     | 0.06237681      | 0.15726654  |
| 18        | 0.55438854     | 0.06474971      | 0.16154267  |
| 19        | 0.56105869     | 0.06613303      | 0.16355158  |
| 20        | 0.57607198     | 0.06858586      | 0.16778973  |
| 21        | 0.57794727     | 0.06942812      | 0.1684116   |
| 22        | 0.59617405     | 0.07238407      | 0.17340134  |
| 23        | 0.59497738     | 0.07287024      | 0.1731641   |
| 24        | 0.61072192     | 0.07565143      | 0.17737829  |
| 25        | 0.61371101     | 0.07675998      | 0.178295    |
| 26        | 0.62542103     | 0.07914891      | 0.18132136  |
| 27        | 0.63095717     | 0.08061754      | 0.18292546  |
| 28        | 0.64115077     | 0.08283954      | 0.18546067  |
| 29        | 0.64770267     | 0.08448962      | 0.18737168  |
| 30        | 0.6561636      | 0.08649115      | 0.18931936  |

|    |            |            |            |
|----|------------|------------|------------|
| 31 | 0.66403334 | 0.08844347 | 0.19159718 |
| 32 | 0.67017436 | 0.09010975 | 0.19288135 |
| 33 | 0.68008517 | 0.09248769 | 0.19560706 |
| 34 | 0.68427411 | 0.09376582 | 0.19642203 |
| 35 | 0.6967423  | 0.09653418 | 0.19961992 |
| 36 | 0.69833753 | 0.09735118 | 0.1999324  |
| 37 | 0.71385919 | 0.10042643 | 0.20363266 |
| 38 | 0.71163053 | 0.10076946 | 0.20309711 |
| 39 | 0.72680375 | 0.10367482 | 0.2067497  |
| 40 | 0.72720745 | 0.10463597 | 0.20677634 |
| 41 | 0.735018   | 0.10675204 | 0.20874449 |
| 42 | 0.73977615 | 0.10848394 | 0.20962308 |
| 43 | 0.74461675 | 0.11012331 | 0.21102407 |
| 44 | 0.7508875  | 0.1120675  | 0.21210008 |
| 45 | 0.75422698 | 0.11346306 | 0.21321963 |
| 46 | 0.7603909  | 0.11544751 | 0.21434106 |
| 47 | 0.76299454 | 0.11678851 | 0.21507602 |
| 48 | 0.7684565  | 0.11880332 | 0.21622782 |
| 49 | 0.77075106 | 0.12005722 | 0.21670273 |
| 50 | 0.77561295 | 0.12201332 | 0.21765374 |
| 51 | 0.77789931 | 0.12327001 | 0.21827541 |
| 52 | 0.78120164 | 0.12490499 | 0.21873996 |
| 53 | 0.78318205 | 0.12654322 | 0.21928898 |
| 54 | 0.78556322 | 0.12811503 | 0.21969277 |
| 55 | 0.78758231 | 0.129992   | 0.22001352 |
| 56 | 0.79019505 | 0.13148276 | 0.22067474 |
| 57 | 0.79168309 | 0.13313797 | 0.22060007 |
| 58 | 0.7964341  | 0.13511861 | 0.22182638 |
| 59 | 0.79513712 | 0.13560772 | 0.22134055 |
| 60 | 0.8020962  | 0.13861126 | 0.22250308 |
| 61 | 0.79972174 | 0.13846553 | 0.22237554 |
| 62 | 0.80364664 | 0.14113535 | 0.22257261 |
| 63 | 0.8045776  | 0.14216296 | 0.22313546 |
| 64 | 0.80518292 | 0.14358441 | 0.22286425 |
| 65 | 0.8078441  | 0.1454568  | 0.22345456 |
| 66 | 0.80797761 | 0.14683887 | 0.22345333 |
| 67 | 0.81024762 | 0.14850203 | 0.22367285 |
| 68 | 0.81076115 | 0.15017588 | 0.22388205 |
| 69 | 0.81189253 | 0.15175672 | 0.22384507 |
| 70 | 0.81275339 | 0.15375256 | 0.22407195 |
| 71 | 0.81362979 | 0.15557972 | 0.22408334 |
| 72 | 0.81446846 | 0.15748493 | 0.22425452 |
| 73 | 0.81534671 | 0.15935873 | 0.22431344 |
| 74 | 0.81587878 | 0.16124728 | 0.22435781 |

|     |            |            |            |
|-----|------------|------------|------------|
| 75  | 0.81654653 | 0.16326182 | 0.22437809 |
| 76  | 0.81702585 | 0.16531291 | 0.22440958 |
| 77  | 0.8174982  | 0.16722999 | 0.22436676 |
| 78  | 0.81803805 | 0.1690904  | 0.22441793 |
| 79  | 0.81813323 | 0.17079043 | 0.22428983 |
| 80  | 0.8186397  | 0.17246193 | 0.22433611 |
| 81  | 0.81863391 | 0.17418682 | 0.22418594 |
| 82  | 0.81908176 | 0.17576137 | 0.22419555 |
| 83  | 0.81898343 | 0.17748291 | 0.22395256 |
| 84  | 0.81967457 | 0.17903456 | 0.22397304 |
| 85  | 0.819276   | 0.18051666 | 0.22360583 |
| 86  | 0.82053846 | 0.18233666 | 0.2237546  |
| 87  | 0.820088   | 0.18371753 | 0.22337348 |
| 88  | 0.82143515 | 0.18596455 | 0.22358941 |
| 89  | 0.82146861 | 0.18776825 | 0.22323525 |
| 90  | 0.8226219  | 0.19016422 | 0.22343747 |
| 91  | 0.8231695  | 0.19219428 | 0.22295145 |
| 92  | 0.82403732 | 0.19403256 | 0.22327511 |
| 93  | 0.82483573 | 0.19613529 | 0.22263501 |
| 94  | 0.82563368 | 0.19781453 | 0.22298532 |
| 95  | 0.82652554 | 0.20025423 | 0.22243498 |
| 96  | 0.82745476 | 0.2022579  | 0.22253436 |
| 97  | 0.82824368 | 0.20464449 | 0.22221402 |
| 98  | 0.82938253 | 0.20690936 | 0.22192989 |
| 99  | 0.83015254 | 0.2086274  | 0.22190382 |
| 100 | 0.83116789 | 0.21152813 | 0.22151126 |
| 101 | 0.8325124  | 0.21338459 | 0.22126065 |
| 102 | 0.83291986 | 0.21633007 | 0.22130305 |
| 103 | 0.8342629  | 0.21717254 | 0.22076716 |
| 104 | 0.83515418 | 0.2199736  | 0.22078562 |
| 105 | 0.83591859 | 0.22328691 | 0.22041643 |
| 106 | 0.83753775 | 0.2270118  | 0.22018198 |
| 107 | 0.83750467 | 0.23058014 | 0.21973892 |
| 108 | 0.83980796 | 0.23447529 | 0.2195664  |
| 109 | 0.83888887 | 0.23762346 | 0.21907307 |
| 110 | 0.84179356 | 0.24189913 | 0.21900903 |
| 111 | 0.84064314 | 0.24509473 | 0.21845692 |
| 112 | 0.84329182 | 0.24985342 | 0.21839958 |
| 113 | 0.84265601 | 0.2537162  | 0.21779597 |
| 114 | 0.8446204  | 0.25873842 | 0.2177051  |
| 115 | 0.84440865 | 0.26285184 | 0.21697772 |
| 116 | 0.84581745 | 0.26727059 | 0.2170645  |
| 117 | 0.84586735 | 0.27052932 | 0.21621692 |
| 118 | 0.84698377 | 0.27471728 | 0.21631253 |

|     |            |            |            |
|-----|------------|------------|------------|
| 119 | 0.8473028  | 0.27848375 | 0.21574264 |
| 120 | 0.84839004 | 0.28376487 | 0.21530416 |
| 121 | 0.84907283 | 0.28896834 | 0.21491831 |
| 122 | 0.8498154  | 0.29395686 | 0.21412719 |
| 123 | 0.8506758  | 0.29983161 | 0.21376342 |
| 124 | 0.85130571 | 0.30587576 | 0.21291102 |
| 125 | 0.85220857 | 0.31216147 | 0.21228227 |
| 126 | 0.85299109 | 0.31936794 | 0.21132569 |
| 127 | 0.85377665 | 0.32532766 | 0.21068361 |
| 128 | 0.85488644 | 0.33313617 | 0.20972985 |
| 129 | 0.85571384 | 0.33939948 | 0.20889028 |
| 130 | 0.85707122 | 0.34737045 | 0.208179   |
| 131 | 0.8582752  | 0.35319981 | 0.20748797 |
| 132 | 0.85976702 | 0.36056502 | 0.20697962 |
| 133 | 0.86101167 | 0.36498229 | 0.20673027 |
| 134 | 0.86200206 | 0.37110967 | 0.20604225 |
| 135 | 0.86261828 | 0.37555542 | 0.20535204 |
| 136 | 0.8634902  | 0.38226634 | 0.20442704 |
| 137 | 0.86377014 | 0.38667046 | 0.20348098 |
| 138 | 0.8646857  | 0.3935413  | 0.20229056 |
| 139 | 0.86562469 | 0.40134108 | 0.20083489 |
| 140 | 0.86660394 | 0.40912631 | 0.19935337 |
| 141 | 0.86771958 | 0.41763388 | 0.19769671 |
| 142 | 0.86881791 | 0.42610207 | 0.1960428  |
| 143 | 0.87002299 | 0.43508237 | 0.19425673 |
| 144 | 0.87117827 | 0.44401361 | 0.19247786 |
| 145 | 0.87243291 | 0.45334863 | 0.19058429 |
| 146 | 0.87361947 | 0.46260114 | 0.18870451 |
| 147 | 0.87491171 | 0.47222278 | 0.18671888 |
| 148 | 0.87611458 | 0.48171017 | 0.18475967 |
| 149 | 0.87743691 | 0.49158809 | 0.18269943 |
| 150 | 0.87864385 | 0.50123809 | 0.18068408 |
| 151 | 0.87998951 | 0.51134593 | 0.17856628 |
| 152 | 0.88119173 | 0.52106375 | 0.17651487 |
| 153 | 0.88255154 | 0.53135108 | 0.17436081 |
| 154 | 0.88374844 | 0.54102647 | 0.17229003 |
| 155 | 0.8851066  | 0.55141946 | 0.17011848 |
| 156 | 0.88630932 | 0.56097116 | 0.1680314  |
| 157 | 0.88764393 | 0.5713585  | 0.16585977 |
| 158 | 0.88887424 | 0.58077736 | 0.1637512  |
| 159 | 0.89016956 | 0.59102863 | 0.16158735 |
| 160 | 0.89144132 | 0.60035799 | 0.15944887 |
| 161 | 0.89269887 | 0.61037758 | 0.15728746 |
| 162 | 0.89400834 | 0.61963076 | 0.15511645 |

|     |            |            |            |
|-----|------------|------------|------------|
| 163 | 0.89523909 | 0.62936104 | 0.15295048 |
| 164 | 0.89657424 | 0.63849756 | 0.15075163 |
| 165 | 0.89778807 | 0.64789261 | 0.14857829 |
| 166 | 0.89913227 | 0.65685106 | 0.14636149 |
| 167 | 0.9003356  | 0.6658768  | 0.14418055 |
| 168 | 0.9016729  | 0.67461756 | 0.14195341 |
| 169 | 0.90287429 | 0.68327619 | 0.13975926 |
| 170 | 0.90419264 | 0.69179623 | 0.1375239  |
| 171 | 0.90540133 | 0.7001212  | 0.13530623 |
| 172 | 0.90669078 | 0.70842746 | 0.1330601  |
| 173 | 0.90791243 | 0.71645386 | 0.13080764 |
| 174 | 0.90916478 | 0.72453771 | 0.12854983 |
| 175 | 0.91039893 | 0.73227392 | 0.12626188 |
| 176 | 0.91160492 | 0.74009081 | 0.12400342 |
| 177 | 0.91284441 | 0.74753435 | 0.12169098 |
| 178 | 0.91399643 | 0.75504195 | 0.11944734 |
| 179 | 0.91523027 | 0.76221714 | 0.11712444 |
| 180 | 0.91633006 | 0.76940744 | 0.11490329 |
| 181 | 0.91754739 | 0.7763681  | 0.11257856 |
| 182 | 0.91860334 | 0.78325602 | 0.11037552 |
| 183 | 0.91979316 | 0.79004841 | 0.10805295 |
| 184 | 0.92081409 | 0.79663512 | 0.10586396 |
| 185 | 0.92196007 | 0.80325956 | 0.10355838 |
| 186 | 0.92294856 | 0.8095146  | 0.10139394 |
| 187 | 0.92403059 | 0.81593247 | 0.09913578 |
| 188 | 0.92498887 | 0.82183904 | 0.0970166  |
| 189 | 0.92599252 | 0.82802221 | 0.09483775 |
| 190 | 0.92692402 | 0.83361716 | 0.09277748 |
| 191 | 0.92784648 | 0.83955556 | 0.09069535 |
| 192 | 0.92875675 | 0.84489918 | 0.08870022 |
| 193 | 0.92960226 | 0.85056921 | 0.08672051 |
| 194 | 0.93049306 | 0.85568155 | 0.08480285 |
| 195 | 0.93126207 | 0.86101503 | 0.08293902 |
| 196 | 0.93213522 | 0.86584076 | 0.08113349 |
| 197 | 0.93280977 | 0.87071288 | 0.07942434 |
| 198 | 0.93367857 | 0.87515029 | 0.07779564 |
| 199 | 0.9342034  | 0.87941177 | 0.07629478 |
| 200 | 0.93511672 | 0.88338377 | 0.07492882 |
| 201 | 0.93537684 | 0.88685467 | 0.07367817 |
| 202 | 0.93642884 | 0.89030283 | 0.07267541 |
| 203 | 0.93632468 | 0.89281241 | 0.07168427 |
| 204 | 0.93742246 | 0.89560699 | 0.07105042 |
| 205 | 0.9371903  | 0.89732015 | 0.07035117 |
| 206 | 0.93795306 | 0.89931253 | 0.06989396 |

|     |            |            |            |
|-----|------------|------------|------------|
| 207 | 0.93787516 | 0.90033123 | 0.06956851 |
| 208 | 0.93830325 | 0.90181514 | 0.06907083 |
| 209 | 0.93833743 | 0.90196529 | 0.06909071 |
| 210 | 0.93860974 | 0.90336268 | 0.06849485 |

## 5. Computed Energies and Charges

**Table S4.** Electronic energies ( $E_{gas}$  in Hartree), thermal corrections to Gibbs free energy ( $\Delta G_{correction}$  in Hartree), Gibbs free energies in gas phase ( $G_{gas}$  in Hartree,  $G_{gas} = E_{gas} + \Delta G_{correction}$ ), solvation free energies ( $G_{uESE}$  in kcal/mol), Gibbs free energies about molecule converts from the gas-phase standard state to the solution-phase standard state of 1M  $RT\ln(RT/p)$  in kcal/mol (for (HOAc)<sub>2</sub> is 8.75 mol/L because acetic acid is the solvent), free energies in solution ( $\Delta G_{solv}$  in Hartree,  $\Delta G_{solv} = G_{gas} + G_{uESE} + RT\ln(RT/p)$ ). Relative energies ( $\Delta G$ ) at 298 K are reported in kcal/mol.

| Structure                 | $E_{gas}$    | $\Delta G_{correction}$ | $G_{gas}$    | $RT\ln(RT/p)$ | $G_{uESE}$ | $\Delta G_{solv}$ | $\Delta G$  |
|---------------------------|--------------|-------------------------|--------------|---------------|------------|-------------------|-------------|
| <b>HCl</b>                | -460.3431378 | -0.011204               | -460.3543418 | 1.89          | -1.613     | -460.3539004      | <b>0.0</b>  |
| <b>HBr</b>                | -2573.316191 | -0.01317                | -2573.329361 | 1.89          | -1.735     | -2573.329114      | <b>0.0</b>  |
| <b>(HOAc)<sub>2</sub></b> | -457.5633139 | 0.087906                | -457.4754079 | 4.06          | -6.67      | -457.4795672      | <b>0.0</b>  |
| <b>1a</b>                 | -78.44284252 | 0.029848                | -78.41299452 | 1.89          | -0.508     | -78.41079216      | <b>0.0</b>  |
| <b>Int1a</b>              | -538.7911349 | 0.029231                | -538.7619039 | 1.89          | -2.659     | -538.7631294      | <b>1.0</b>  |
| <b>TS1a</b>               | -538.714237  | 0.032842                | -538.681395  | 1.89          | -12.47     | -538.6982553      | <b>41.7</b> |
| <b>TS2a</b>               | -1456.653563 | 0.14882                 | -1456.504743 | 1.89          | -20.045    | -1456.533675      | <b>40.5</b> |
| <b>Int2a</b>              | -2651.764216 | 0.028237                | -2651.735979 | 1.89          | -2.667     | -2651.737217      | <b>1.7</b>  |
| <b>TS3a</b>               | -2651.692592 | 0.031559                | -2651.661033 | 1.89          | -11.277    | -2651.675992      | <b>40.1</b> |
| <b>TS4a</b>               | -5682.611172 | 0.14569                 | -5682.465482 | 1.89          | -19.577    | -5682.493668      | <b>34.5</b> |
| <b>1b</b>                 | -117.6889851 | 0.055019                | -117.6339661 | 1.89          | -1.263     | -117.6329669      | <b>0.0</b>  |
| <b>Int1b</b>              | -578.0386552 | 0.056605                | -577.9820502 | 1.89          | -3.036     | -577.9838765      | <b>1.9</b>  |
| <b>TS1b</b>               | -577.9681266 | 0.058633                | -577.9094936 | 1.89          | -16.066    | -577.9320845      | <b>34.4</b> |
| <b>TS2b</b>               | -1495.907738 | 0.174591                | -1495.733147 | 1.89          | -21.706    | -1495.764726      | <b>34.9</b> |
| <b>Int2b</b>              | -2691.012172 | 0.054958                | -2690.957214 | 1.89          | -3.232     | -2690.959353      | <b>1.7</b>  |
| <b>TS3b</b>               | -2690.947545 | 0.057168                | -2690.890377 | 1.89          | -14.266    | -2690.9101        | <b>32.6</b> |
| <b>TS4b</b>               | -5721.866063 | 0.172795                | -5721.693268 | 1.89          | -20.921    | -5721.723595      | <b>29.6</b> |
| <b>1c</b>                 | -156.936319  | 0.079894                | -156.856425  | 1.89          | -2.029     | -156.8566465      | <b>0.0</b>  |
| <b>Int1c</b>              | -617.2873811 | 0.081589                | -617.2057921 | 1.89          | -3.861     | -617.2089331      | <b>1.0</b>  |
| <b>TS1c</b>               | -617.2247077 | 0.084973                | -617.1397347 | 1.89          | -19.757    | -617.1682075      | <b>26.6</b> |
| <b>TS2c</b>               | -1535.168227 | 0.197967                | -1534.97026  | 1.89          | -21.688    | -1535.00181       | <b>26.5</b> |
| <b>Int2c</b>              | -2730.261043 | 0.081577                | -2730.179466 | 1.89          | -4.032     | -2730.182879      | <b>1.8</b>  |
| <b>TS3c</b>               | -2730.205825 | 0.08313                 | -2730.122695 | 1.89          | -17.229    | -2730.14714       | <b>24.2</b> |
| <b>TS4c</b>               | -5761.128171 | 0.195334                | -5760.932837 | 1.89          | -21.381    | -5760.963898      | <b>19.2</b> |
| <b>1d</b>                 | -156.9327607 | 0.080519                | -156.8522417 | 1.89          | -2.272     | -156.8528504      | <b>0.0</b>  |
| <b>Int1d</b>              | -617.28377   | 0.083909                | -617.199861  | 1.89          | -3.867     | -617.2030116      | <b>2.3</b>  |
| <b>TS1d</b>               | -617.2118217 | 0.085097                | -617.1267247 | 1.89          | -17.287    | -617.1512614      | <b>34.8</b> |
| <b>TS2d</b>               | -1535.153242 | 0.201851                | -1534.951391 | 1.89          | -23.116    | -1534.985216      | <b>34.5</b> |
| <b>Int2d</b>              | -2730.257788 | 0.081756                | -2730.176032 | 1.89          | -4.146     | -2730.179627      | <b>1.5</b>  |
| <b>TS3d</b>               | -2730.192017 | 0.082956                | -2730.109061 | 1.89          | -15.565    | -2730.130853      | <b>32.1</b> |
| <b>TS4d</b>               | -5761.11338  | 0.199645                | -5760.913735 | 1.89          | -22.297    | -5760.946256      | <b>27.9</b> |

|              |              |          |              |      |         |              |              |
|--------------|--------------|----------|--------------|------|---------|--------------|--------------|
| <b>4a</b>    | -234.2074064 | 0.118496 | -234.0889104 | 1.89 | -4.077  | -234.0923956 | <b>0.0</b>   |
| <b>Int3a</b> | -694.5549373 | 0.121689 | -694.4332483 | 1.89 | -5.658  | -694.4392529 | <b>4.4</b>   |
| <b>TS5a</b>  | -694.4984566 | 0.122529 | -694.3759276 | 1.89 | -18.616 | -694.4025822 | <b>27.4</b>  |
| <b>TS6a</b>  | -1612.442733 | 0.239648 | -1612.203085 | 1.89 | -24.649 | -1612.239353 | <b>25.4</b>  |
| <b>Int4a</b> | -2807.545026 | 0.119299 | -2807.425727 | 1.89 | -5.919  | -2807.432148 | <b>-6.7</b>  |
| <b>TS7a</b>  | -2807.479214 | 0.120804 | -2807.35841  | 1.89 | -16.897 | -2807.382325 | <b>31.3</b>  |
| <b>TS8a</b>  | -5838.403551 | 0.23793  | -5838.165621 | 1.89 | -23.782 | -5838.200509 | <b>25.3</b>  |
| <b>4b</b>    | -194.969167  | 0.090139 | -194.879028  | 1.89 | -3.04   | -194.8808607 | <b>0.0</b>   |
| <b>Int3b</b> | -655.3204024 | 0.093134 | -655.2272684 | 1.89 | -4.742  | -655.2318133 | <b>1.8</b>   |
| <b>TS5b</b>  | -655.249717  | 0.094366 | -655.155351  | 1.89 | -17.501 | -655.1802287 | <b>34.2</b>  |
| <b>TS6b</b>  | -1573.187667 | 0.210614 | -1572.977053 | 1.89 | -24.853 | -1573.013647 | <b>34.3</b>  |
| <b>Int4b</b> | -2768.294271 | 0.091569 | -2768.202702 | 1.89 | -4.916  | -2768.207524 | <b>1.5</b>   |
| <b>TS7b</b>  | -2768.232226 | 0.092925 | -2768.139301 | 1.89 | -15.875 | -2768.161587 | <b>30.4</b>  |
| <b>TS8b</b>  | -5799.147658 | 0.209343 | -5798.938315 | 1.89 | -23.556 | -5798.972842 | <b>28.7</b>  |
| <b>4c</b>    | -155.685393  | 0.061113 | -155.624263  | 1.89 | -1.997  | -155.6244335 | <b>0.0</b>   |
| <b>Int3c</b> | -616.0358487 | 0.063808 | -615.9720407 | 1.89 | -3.702  | -615.9749283 | <b>2.1</b>   |
| <b>TS5c</b>  | -615.9634503 | 0.064988 | -615.8984623 | 1.89 | -15.124 | -615.919552  | <b>36.9</b>  |
| <b>TS6c</b>  | -1533.90452  | 0.182387 | -1533.722133 | 1.89 | -22.021 | -1533.754214 | <b>36.1</b>  |
| <b>Int4c</b> | -2729.009635 | 0.061153 | -2728.948482 | 1.89 | -3.892  | -2728.951672 | <b>1.2</b>   |
| <b>TS7c</b>  | -2728.943237 | 0.063617 | -2728.87962  | 1.89 | -13.497 | -2728.898116 | <b>34.8</b>  |
| <b>TS8c</b>  | -5759.863491 | 0.179039 | -5759.684452 | 1.89 | -20.509 | -5759.714123 | <b>30.2</b>  |
| <b>7a</b>    | -309.0739836 | 0.103571 | -308.9704126 | 1.89 | -5.686  | -308.9764619 | <b>0.0</b>   |
| <b>Int5a</b> | -2882.397831 | 0.104666 | -2882.293165 | 1.89 | -7.695  | -2882.302416 | <b>2.0</b>   |
| <b>TS9a</b>  | -2882.336969 | 0.107452 | -2882.229517 | 1.89 | -19.349 | -2882.25734  | <b>30.3</b>  |
| <b>7b</b>    | -348.3199844 | 0.130129 | -348.1898554 | 1.89 | -6.474  | -348.1971605 | <b>0.0</b>   |
| <b>Int5b</b> | -2921.644995 | 0.131487 | -2921.513508 | 1.89 | -8.498  | -2921.524039 | <b>1.4</b>   |
| <b>TS9b</b>  | -2921.593374 | 0.133175 | -2921.460199 | 1.89 | -20.755 | -2921.490262 | <b>22.6</b>  |
| <b>2a</b>    | -538.820519  | 0.040774 | -538.779745  | 1.89 | -2.496  | -538.7807108 | <b>-10.1</b> |
| <b>3a</b>    | -2651.797894 | 0.039089 | -2651.758805 | 1.89 | -2.68   | -2651.760064 | <b>-12.6</b> |
| <b>2b</b>    | -578.0674203 | 0.067132 | -578.0002883 | 1.89 | -3.103  | -578.0022213 | <b>-9.6</b>  |
| <b>3b</b>    | -2691.044983 | 0.06544  | -2690.979543 | 1.89 | -3.319  | -2690.981821 | <b>-12.4</b> |
| <b>2c</b>    | -617.3147524 | 0.093532 | -617.2212204 | 1.89 | -3.856  | -617.2243534 | <b>-8.7</b>  |
| <b>3c</b>    | -2730.292914 | 0.092994 | -2730.19992  | 1.89 | -4.037  | -2730.203342 | <b>-11.0</b> |
| <b>2d</b>    | -617.3092022 | 0.093886 | -617.2153162 | 1.89 | -3.93   | -617.2185671 | <b>-7.4</b>  |
| <b>3d</b>    | -2730.28734  | 0.092197 | -2730.195143 | 1.89 | -4.168  | -2730.198773 | <b>-10.5</b> |
| <b>5a</b>    | -694.596807  | 0.131219 | -694.465588  | 1.89 | -5.483  | -694.4713138 | <b>-15.7</b> |
| <b>6a</b>    | -2807.575423 | 0.129544 | -2807.445879 | 1.89 | -5.795  | -2807.452102 | <b>-19.2</b> |
| <b>5b</b>    | -655.3434493 | 0.102245 | -655.2412043 | 1.89 | -4.877  | -655.2459644 | <b>-7.0</b>  |
| <b>6b</b>    | -2768.32181  | 0.100618 | -2768.221192 | 1.89 | -5.149  | -2768.226386 | <b>-10.3</b> |
| <b>5c</b>    | -616.0689093 | 0.073969 | -615.9949403 | 1.89 | -3.843  | -615.9980526 | <b>-12.4</b> |
| <b>6c</b>    | -2729.046446 | 0.07229  | -2728.974156 | 1.89 | -4.114  | -2728.977701 | <b>-15.2</b> |
| <b>8a</b>    | -2882.42643  | 0.112768 | -2882.313662 | 1.89 | -7.714  | -2882.322943 | <b>-10.9</b> |
| <b>8b</b>    | -2921.672257 | 0.140763 | -2921.531494 | 1.89 | -8.711  | -2921.542364 | <b>-10.1</b> |