Supplementary Material

Acylation of \textit{trans}-2-substituted cyclohexanols: the impact of substituent variation on the pyridine-induced reversal of diastereoselectivity

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$^1$H NMR of **Compound 7** [(±)-*trans*-2-(2,6-dimethylphenyloxy)cyclohexanol]
$^1$H NMR of Compound 8 [(±)-trans-2-(cyclohexyloxy)cyclohexanol]
$^1$H NMR of **Compound 9** [(±)-trans-2-(t-butoxy)cyclohexanol]
$^1$H NMR of **Compound 10** [(±)-*trans*-2-(pyridine-2-ylthio)cyclohexanol]
$^{1}$H NMR of **Compound 11** [$(\pm)-\text{trans-2-}(p$-tolylsulfonyl)cy clohexanol]
\[ ^1H \text{NMR of Compound 12 [}(\pm)-\text{trans-2-(benzyl)cyclohexanol}] \]
$^1$H NMR of **Compound 16a+b** [(±)-(trans-2-(p-tolylsulfanyl)cyclohexyl) 2-chloropropanoate]
$^1$H NMR of Compound 17a+b[(±)-(trans-2-(p-tolyloxy)cyclohexyl) 2-chloropropanoate]
$^1$H NMR of **Compound 18a+b** [(±)-(trans-2-(phenyloxy)cyclohexyl 2-chloropropanoate)]
$^1$H NMR of Compound 19a+b [(±)-trans-2-(napthalen-2-yloxy)cyclohexyl) 2-chloropropanoate]
$^1$H NMR of **Compound 20a+b** [(±)-(*trans*-2-(3,4,5-trimethoxyphenyloxy)cyclohexanol]
$^1$H NMR of **Compound 21a+b** [(±)-(trans-2-(p-tert-butyl-phenyloxy)cyclohexyl 2-chloropropanoate]
$^1$H NMR of **Compound 22a+b** [(±)-(trans-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloropropanoate)]
$^1$H NMR of **Compound 23a+b** [(±)-\textit{trans}-2-(cyclohexyloxy)cyclohexyl 2-chloropropanoate]
$^1$H NMR of **Compound 24a+b** [(±)-(trans-2-(tert-butoxy)cyclohexyl 2-chloropropanoate)]
$^1$H NMR of Compound 25a+b [(±)-trans-2-(pyridin-2-ylthio)cyclohexyl 2-chloropropanoate]
$^1$H NMR of **Compound 26a+b** [(±)-\(trans\)-2-(\(p\)-tolylsulfonyl)cyclohexyl 2-chloropropanoate]
$^1$H NMR of Compound 27a+b [(±)-(trans-2-benzylcyclohexyl) 2-chloropropanoate]
$^1$H NMR of **Compound 28a+b** [(±)-(trans-2-methylcyclohexyl) 2-chloropropanoate]
$^1$H NMR of **Compound 29a+b** [(±)-(trans-2-(p-tolylsulfanyl)cyclohexyl 2-chloro-2-phenylethanoate)]
$^1$H NMR of **Compound 30a+b** [(±)-(trans-2-(p-tolyloxy)cyclohexyl 2-chloro-2-phenylethanoate)]
$^1$H NMR of Compound 31a+b [(±)-(trans-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloro-2-phenylethanoate]
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$^1$H NMR of **Compound 34a+b** [($\pm$)-trans-2-(methyl)cyclohexyl 2-chloro-2-phenylethanoate]
$^{13}$C NMR of Compound 1 [(±)-trans-2-(p-tolylsulfanyl)cyclohexanol]
$^{13}$C NMR of **Compound 2** [(±)-trans-2-(p-tolyloxy)cyclohexanol]
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$^{13}$C NMR of Compound 4 [(±)-trans-2-(napthalen-2-yloxy)cyclohexanol]
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$^{13}$C NMR of **Compound 7** [(±)-trans-2-(2,6-dimethylphenyloxy)cyclohexanol]
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\[13\text{C NMR of Compound 9 [(±)-\textit{trans}-2-(t-butoxy)cyclohexanol]}\]
$^{13}$C NMR of **Compound 10** [(±)-trans-2-(pyridine-2-yithio)cyclohexanol]
$^{13}\text{C}$ NMR of Compound 11 [(±)-trans-2-(p-tolylsulfonyl)cyclohexanol]
$^{13}$C NMR of **Compound 12** [($\pm$)-*trans*-2-(benzyl)cyclohexanol]
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$^{13}$C NMR of Compound 17a+b [(±)-trans-2-(p-tolyloxy)cyclohexyl) 2-chloropropanoate]
$^{13}$C NMR of **Compound 18a+b** [(±)-(trans-2-(phenyloxy)cyclohexyl 2-chloropropanoate)]

$^{13}$C NMR of **Compound 19a+b** [(±)-(trans-2-(napthalen-2-ylxy)cyclohexyl) 2-chloropropanoate]
13C NMR of Compound 20a+b [(±)-trans-2-(3,4,5-trimethoxyphenyloxy)cyclohexanol]
\(^{13}\)C NMR of **Compound 21a+b**\([(\pm)-(trans-2-(p-tert-butyl-phenyloxy)cyclohexyl 2-chloropropanoate)]\)
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$^{13}$C NMR of Compound 25a+b [(±)-trans-2-(pyridin-2-ylthio)cyclohexyl 2-chloropropanoate]
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$^{13}$C NMR of **Compound 29a+b** [(±)-(*trans*-2-(*p*-tolylsulfanyl)cyclohexyl 2-chloro-2-phenylethanoate)]

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$^{13}$C NMR of **Compound 30a+b** [(±)-trans-2-(p-tolyloxy)cyclohexyl 2-chloro-2-phenylethanoate]
$^{13}$C NMR of **Compound 31a+b** [(±)-trans-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloro-2-phenylethanoate]
$^{13}$C NMR of **Compound 32a+b** [(±)-*trans*-2-(cyclohexyloxy)cyclohexyl 2-chloro-2-phenylethanoate]
$^{13}$C NMR of **Compound 33a+b** [(±)-(*trans*-2-(*p*-tolylsulfonyl)cyclohexyl 2-chloro-2-phenylethanoate)]
$^{13}$C NMR of **Compound 34a+b [(±)-trans-2-(methyl)cyclohexyl 2-chloro-2-phenylethanoate]**

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HRMS of Compound 1 [(±)-trans-2-(p-tolylsulfanyl)cyclohexanol]
HRMS of Compound 2 [(±)-trans-2-(p-tolyloxy)cyclohexanol]
HRMS of **Compound 3** [(±)-*trans*-2-(phenyloxy)cyclohexanol]
HRMS of **Compound 4** [(±)-*trans*-2-(napthalen-2-yloxy)cyclohexanol]
HRMS of Compound 5 [(±)-trans-2-(3,4,5-trimethylphenyloxy)cyclohexanol]
HRMS of **Compound 6** [(±)-*trans*-2-(*tert*-butoxy)phenyloxy)cyclohexanol]
The graph shows the relative intensity (y-axis) plotted against mass-to-charge ratio (m/z) on the x-axis. Key m/z values are labeled:

- 203.1440
- 221.1513
- 238.1846
- 441.2979
HRMS of **Compound 7** [(±)-*trans*-2-(2,6-dimethylphenyloxy)cyclohexanol]
HRMS of Compound 8 [(±)-trans-2-(cyclohexyloxy)cyclohexanol]
HRMS of **Compound 9** [(±)-*trans*-2-(*t*-butoxy)cyclohexanol]
HRMS of **Compound 10** [(±)-*trans*-2-(pyridine-2-ylthio)cyclohexanol]
The mass spectrum shows a peak at m/z 255.079 with relative intensity.
HRMS of **Compound 11** [(±)-trans-2-(p-tolylsulfonyl)cyclohexanol]
The diagram shows a mass spectroscopy graph with the y-axis labeled 'Rel. Intensity' and the x-axis labeled 'm/z'. Key peaks are labeled at their respective m/z values: 173.1319, 191.1432, 208.1712, and 381.2769.
HRMS of Compound 12 [(+)-trans-2-(benzyl)cyclohexanol]
HRMS of Compound 16a+b [(±)-(trans-2-(p-tolylsulfanyl)cyclohexyl) 2-chloropropanoate]
HRMS of Compound 17a+b [(±)-(trans-2-(p-tolyloxy)cyclohexyl) 2-chloropropanoate]
HRMS NMR of **Compound 18a+b** [(±)-(trans-2-(phenyloxy)cyclohexyl 2-chloropropanoate)]
HRMS of **Compound 19a+b** [(±)-(trans-2-(napthalen-2-yloxy)cyclohexyl) 2-chloropropanoate]
HRMS of Compound 20a+b [(±)-(trans-2-(3,4,5-trimethoxyphenyloxy)cyclohexanol]
HRMS of **Compound 21a+b** [(±)-**(trans-2-(p-tert-butyl-phenyloxy)cyclohexyl 2-chloropropanoate)**]
HRMS of Compound 22a+b [(±)-(trans-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloropropanoate]
HRMS of **Compound 23a+b** [(±)-(trans-2-(cyclohexyloxy)cyclohexyl 2-chloropropanoate]
207.0774
263.1426
HRMS of **Compound 24a+b** [(±)-(trans-2-(tert-butoxy)cyclohexyl 2-chloropropanoate)
HRMS of Compound 25a+b [(±)-trans-2-(pyridin-2-ylthio)cyclohexyl 2-chloropropanoate]
HRMS of **Compound 26a+b** [(±)-(trans-2-(p-tolylsulfonyl)cyclohexyl 2-chloropropanoate)]
HRMS of Compound 27a+b [(±)-trans-2-benzylcyclohexyl) 2-chloropropanoate]
HRMS of **Compound 28a+b** [(±)-(trans-2-methylcyclohexyl) 2-chloropropanoate]
HRMS of Compound 29a+b [(±)-(trans-2-(p-tolylsulfanyl)cyclohexyl 2-chloro-2-phenylethanoate]
HRMS of **Compound 30a+b** [(±)-(trans-2-(p-tolyloxy)cyclohexyl 2-chloro-2-phenylethanoate)]
HRMS of **Compound 31a+b** [(±)-**(trans-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloro-2-phenylethanoate)**]
HRMS of **Compound 32a+b** [(±)-*trans*-2-(cyclohexyloxy)cyclohexyl 2-chloro-2-phenylethanoate]
HRMS of Compound 33a+b [(±)-(trans-2-(p-tolylsulfonyl)cyclohexyl 2-chloro-2-phenylethanoate]
HRMS of **Compound 34a+b** [(±)-*trans*-2-(methyl)cyclohexyl 2-chloro-2-phenylethanoate]
Summary of Molecular Modeling results – computed energies:

Absolute energies of transition states:

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Relative energies (lowest respective diastereomeric transition state in bold) of transition states:

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Nomenclature examples:

2-Methyl \((R,R,S,R)\)

\((1S,2R)-1,2\)-dichloro-1-\(((1R,2R)-2\text{-methylcyclohexyl})\)propan-1-olate

2-Methyl \((R,R,R)-(a,a)\)
LUMO representation and Cartesian coordinates of pyridinium transition state structures (catalyzed reaction):

2-Methyl \((R,R,R,R)\)-(a,a)

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2-Methyl (R,R,R,R)-(e,e)
2-Methyl (R,R,R,S)-(a,a)

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H(39) -3.5297  -5.883  -6.491  
H(40) -1.2373  -1.685  -4.3653  
H(41) -2.5107 -5.3396  -5.1195  

H(37) -3.6628 -1.2239 -4.0683  
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H(39) -3.5297 -5.883 -6.491  
H(40) -1.2373 -1.685 -4.3653  
H(41) -2.5107 -5.3396 -5.1195  

2-Methyl (R,R,S,S)-(e,e)

C(1)  -9.1639  -4.4263  -8.8309  
C(2)  -8.3604  -4.8671  -9.8833  
C(3)  -7.0825  -4.3233 -10.0257  
C(4)  -6.6516  -3.3553 -10.1172  
N(5)  -7.4139  -2.8860  -8.0616  
C(6)  -8.6706  -3.4558  -7.9551  
C(7)  -8.8905  -1.820  -7.0941  
O(8)  -7.8541  -1.4974  -6.121  
O(9)  -5.6775  -2.2147 -10.5873  
C(10) -6.6135  -0.5163  -7.8517  
C(11) -5.7127  -3.4235  -5.7746  
C(12) -6.1427  0.629  -6.9516  
Cl(13) -8.0429  -0.0055  -8.7944  
H(14) -10.1755 -4.8403  -8.6932  
H(15) -8.7267 -5.6311 -10.5873  
H(16) -6.4237  -4.6547  -10.8443  
H(17) -5.6406  -2.9359  -9.2375  
H(18) -9.3203  -3.1243  -7.1306  
H(19) -5.8233  -0.691  -8.6142  
C(20) -6.1739  -3.1955  -4.329  
H(21) -6.3927  -4.148  -6.2764  
C(22) -4.2982  -4.0333  -5.7703  
H(23) -5.9183  1.5462  -7.5434  
H(24) -6.9068  0.902  -6.1892  
H(25) -5.2077  0.3621  -6.4091  
Lp(26) -5.319  -2.3261  -6.9559  
Lp(27) -5.5846  -1.8017  -6.0644  
C(28) -4.2804  -5.3465  -4.9654  
H(29) -3.6039  -3.31  -5.2728  
C(30) -3.7605  -4.2929 -10.1891  
C(31) -6.156  -4.4978  -3.5161  
H(32) -7.2101  -2.7898  -4.2918  
H(33) -5.5122  -2.4419  -3.8398  
H(34) -3.2492  -5.7731  -4.9482
|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

2-OTol \((R,R,R)\)-(a,a)

\[
\begin{align*}
H(35) &\quad -4.9376 & -6.0972 & -5.4648 \\
C(36) &\quad -4.7584 & -5.1268 & -3.5248 \\
H(37) &\quad -6.4734 & -4.2967 & -2.4647 \\
H(38) &\quad -2.7544 & -4.7699 & -7.1563 \\
H(39) &\quad -6.8919 & -5.2163 & -3.9497 \\
H(40) &\quad -4.7736 & -6.0977 & -2.974 \\
H(41) &\quad -3.6446 & -3.3498 & -7.7688 \\
\end{align*}
\]

\[
\begin{align*}
H(35) &\quad -4.9376 & -6.0972 & -5.4648 \\
C(36) &\quad -4.7584 & -5.1268 & -3.5248 \\
H(37) &\quad -6.4734 & -4.2967 & -2.4647 \\
H(38) &\quad -2.7544 & -4.7699 & -7.1563 \\
H(39) &\quad -6.8919 & -5.2163 & -3.9497 \\
H(40) &\quad -4.7736 & -6.0977 & -2.974 \\
H(41) &\quad -3.6446 & -3.3498 & -7.7688 \\
\end{align*}
\]

2-OTol \((R,R,R)\)-(a,a)

\[
\begin{align*}
C(1) &\quad -10.4885 & 2.1198 & -5.8188 \\
C(2) &\quad -11.4643 & 1.3239 & -6.4198 \\
C(3) &\quad -11.0592 & 0.2369 & -7.1958 \\
C(4) &\quad -9.6956 & -0.0191 & -7.3484 \\
N(5) &\quad -8.693 & 0.7448 & -6.775 \\
C(6) &\quad -9.1398 & 1.8109 & -6.0151 \\
C(7) &\quad -7.2087 & 0.4333 & -6.9907 \\
O(8) &\quad -6.3861 & 1.3167 & -6.2649 \\
O(9) &\quad -6.8123 & 0.4574 & -8.3449 \\
C(10) &\quad -6.8773 & -0.9643 & -6.4526 \\
C(11) &\quad -7.3281 & 1.4939 & -9.1395 \\
C(12) &\quad -5.4036 & -1.3504 & -6.6046 \\
C(13) &\quad -7.3844 & -1.1293 & -4.7473 \\
H(14) &\quad -10.7795 & 2.9866 & -5.2046 \\
H(15) &\quad -12.5336 & 1.5526 & -6.288 \\
H(16) &\quad -11.8075 & -0.4053 & -7.6874 \\
H(17) &\quad -9.3865 & -0.8675 & -7.9793 \\
H(18) &\quad -8.388 & 2.4606 & -5.5414 \\
H(19) &\quad -7.4775 & -1.7246 & -6.9984 \\
C(20) &\quad -6.982 & 1.164 & -10.5987 \\
H(21) &\quad -8.4385 & 1.4694 & -9.0628 \\
C(22) &\quad -6.7907 & 2.8773 & -8.7577 \\
H(23) &\quad -5.2136 & -2.3849 & -6.2361 \\
H(24) &\quad -4.7317 & -0.6653 & -6.0402 \\
H(25) &\quad -5.0848 & -1.3292 & -7.6715 \\
C(26) &\quad -5.2923 & 3.0015 & -9.0484 \\
H(27) &\quad -6.9465 & 3.0827 & -7.6741 \\
O(28) &\quad -7.4705 & 3.8861 & -9.457 \\
C(29) &\quad -5.4747 & 1.2682 & -10.8691 \\
H(30) &\quad -7.3385 & 0.1365 & -10.8509 \\
H(31) &\quad -7.5217 & 1.8583 & -11.2852 \\
H(32) &\quad -4.9426 & 4.0341 & -8.8084 \\
\end{align*}
\]
2-OTol (R,R,R)-(e,e)

C(1)  -10.2922  -3.4244  -7.6843
C(2)  -10.0539  -4.2178  -8.8071
C(3)  -8.7509   -4.3078  -9.2979
C(4)  -7.7290   -3.6031  -8.6572
N(5)  -7.9168   -2.7965  -7.5469
C(6)  -9.2255   -2.7428  -7.0938
C(7)  -6.7884   -2.0166  -6.8565
O(8)  -7.1376   -1.9087  -5.4910
O(9)  -6.7183   -0.6744  -7.2926
C(10) -5.4072   -2.6795  -6.8489
C(11) -6.4711   -0.4649  -8.6617
C(12) -4.3713   -1.9558  -5.9815
C(13) -5.5242   -4.3816  -6.3104
H(14) -11.3115  -3.3272  -7.2779
H(15) -10.8785  -4.7578  -9.2985
H(16) -8.5333   -4.9235  -10.1853
H(17) -6.7137   -3.6837  -9.0732
H(18) -9.4424   -2.1007  -6.2256
H(19) -4.9963   -2.7418  -7.8781
C(20) -5.2991   -0.5162  -8.7905
H(21) -6.1822   -1.4147  -9.1701
C(22) -7.7220   -0.1054  -9.3417
H(23) -3.3678   -2.4339  -6.0625
H(24) -4.6516   -1.9546  -4.9042
H(25) -4.2411   -0.8941  -6.2847
C(26) -7.4395   -0.5063  -10.7939
H(27) -8.0689   0.9957   -8.7658
O(28) -8.7119   -0.8779  -9.3059
C(29) -5.0143   0.8829  -10.2522
H(30) -5.5228   1.4447  -8.2132
2-OTol \((R,R,S)-(a,a)\)

\[
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C(1) & -10.6181 & 2.01 \\
C(2) & -11.5424 & 1.577 \\
C(3) & -11.0706 & 0.0683 \\
C(4) & -9.6931 & -0.1341 \\
N(5) & 8.421 & 0.6861 \\
C(6) & -9.253 & 1.7538 \\
C(7) & -7.2391 & 0.436 \\
O(8) & 6.826 & 1.3711 \\
O(9) & 6.8315 & 0.4378 \\
C(10) & -6.8794 & -0.9344 \\
C(11) & 7.3469 & 1.4622 \\
C(12) & 7.3468 & 1.1047 \\
C(13) & 5.1205 & 1.25 \\
H(14) & 10.962 & 2.8805 \\
H(15) & 12.6237 & 1.3445 \\
H(16) & 11.7772 & 0.617 \\
H(17) & 9.3299 & -0.9846 \\
H(18) & 8.5423 & 2.4484 \\
H(19) & 7.3391 & -1.7404 \\
C(20) & 7.0719 & 1.076 \\
H(21) & 8.4535 & 1.4771 \\
C(22) & -6.7522 & 2.8386 \\
H(23) & 7.0331 & 2.1154 \\
H(24) & 8.4512 & -0.9993 \\
H(25) & 6.8823 & -0.3512 \\
C(26) & -5.2652 & 2.9079 \\
H(27) & 6.8515 & 3.0792 \\
O(28) & -7.4365 & 3.8472
\end{array}
\]
C(29) -5.5753 1.1248 -10.9492
H(30) -7.4701 0.0531 -10.8178
H(31) -7.6183 1.7655 -11.2997
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H(37) -5.0273 0.3624 -10.3466
H(38) -3.9119 2.5369 -10.8692
C(39) -9.8271 3.6872 -9.8586
H(40) -5.4837 3.2671 -11.3347
C(41) -11.1345 3.9172 -9.4281

2-OTol (R,R,R,S)-(e,e)

C(1) -10.1128 -3.5835 -8.0496
C(2) -9.6656 -4.4425 -9.0541
C(3) -8.2985 -4.4971 -9.3284
C(4) -7.4218 -3.6933 -8.5957
N(5) -7.8175 -2.8238 -7.593
C(6) -9.183 -2.8054 -7.3561
C(7) -6.8509 -1.9238 -6.8102
O(8) -7.4006 -1.7595 -5.5186
O(9) -6.8209 -0.6166 -7.3502
C(10) -5.4519 -2.5041 -6.5661
C(11) -6.3166 -0.4795 -8.6557
C(12) -5.4884 -3.8867 -5.9047
Cl(13) -4.4456 -1.4228 -5.5539
H(14) -11.1876 -3.5085 -7.8193
H(15) -10.3788 -5.0569 -9.6261
H(16) -7.9178 -5.1583 -10.1232
H(17) -6.3516 -3.7398 -8.8467
H(18) -9.5613 -2.1107 -6.5896
H(19) -4.8806 -2.5988 -7.5121
C(20) -5.2511 0.6235 -8.6423
H(21) -5.8419 -1.4207 -9.0063
C(22) -7.4372 -0.1041 -9.6299
H(23) -4.4631 -4.3061 -5.7812
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H(25) -5.9613 -3.855 -4.8972
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2-OTol \((R,R,S,R)-(a,a)\)

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2-OTol (R,R,S,S)-(a,a)

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©ARKAT-USA, Inc.
2-STol \((R,R,S,S)-(a,a)\)

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USA, Inc.
LUMO representation and Cartesian coordinates of chloride transition state structures (uncatalyzed reaction):

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\end{align*}
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\text{S(12)} & : 2.2944, -0.4702, 1.6925 \\
\text{C(13)} & : 1.7794, 2.9407, -0.2172 \\
\text{C(14)} & : 2.6909, 1.8032, -0.6936 \\
\text{C(15)} & : 1.0469, -1.3063, 2.722 \\
\text{C(16)} & : 0.6378, -0.7319, 3.9268 \\
\text{C(17)} & : -0.3277, -1.3703, 4.7081 \\
\text{C(18)} & : -0.8876, -2.5885, 4.3058 \\
\text{C(19)} & : -0.4562, -3.1588, 3.1026 \\
\text{C(20)} & : 0.5091, -2.5294, 2.3151 \\
\text{C(21)} & : -1.9488, -3.2729, 5.1301 \\
\text{H(22)} & : -4.04, 0.6073, 0.0182 \\
\text{H(23)} & : -0.1698, 1.0399, 1.9501 \\
\text{H(24)} & : -4.364, 2.9046, -0.9012 \\
\text{H(25)} & : -3.2961, 1.9812, -1.9914 \\
\text{H(26)} & : -2.5933, 3.206, -0.8846 \\
\text{H(27)} & : 0.4071, 3.3885, 1.4141 \\
\text{H(28)} & : 1.834, 2.4316, 1.8937 \\
\text{H(29)} & : 0.4759, -0.7692, 0.1425 \\
\text{H(30)} & : 2.5654, -0.325, -1.1822 \\
\text{H(31)} & : 1.1637, 0.6505, -1.6903
\end{align*}
\]
2-STol \((R,R,S,S)-(e,e)\)

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