ELECTRONIC SUPPLEMENTARY INFORMATION

# NMR and molecular modeling of the dimeric self-association of the enantiomers of 1,1′-bi-2-napthol and 1-phenyl-2,2,2-trifluoroethanol in the solution state and their relevance to enantiomer self-disproportionation on achiral-phase chromatography (ESDAC)

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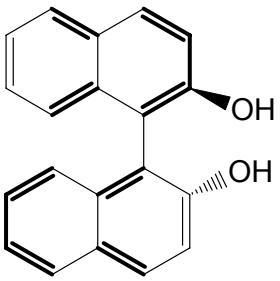
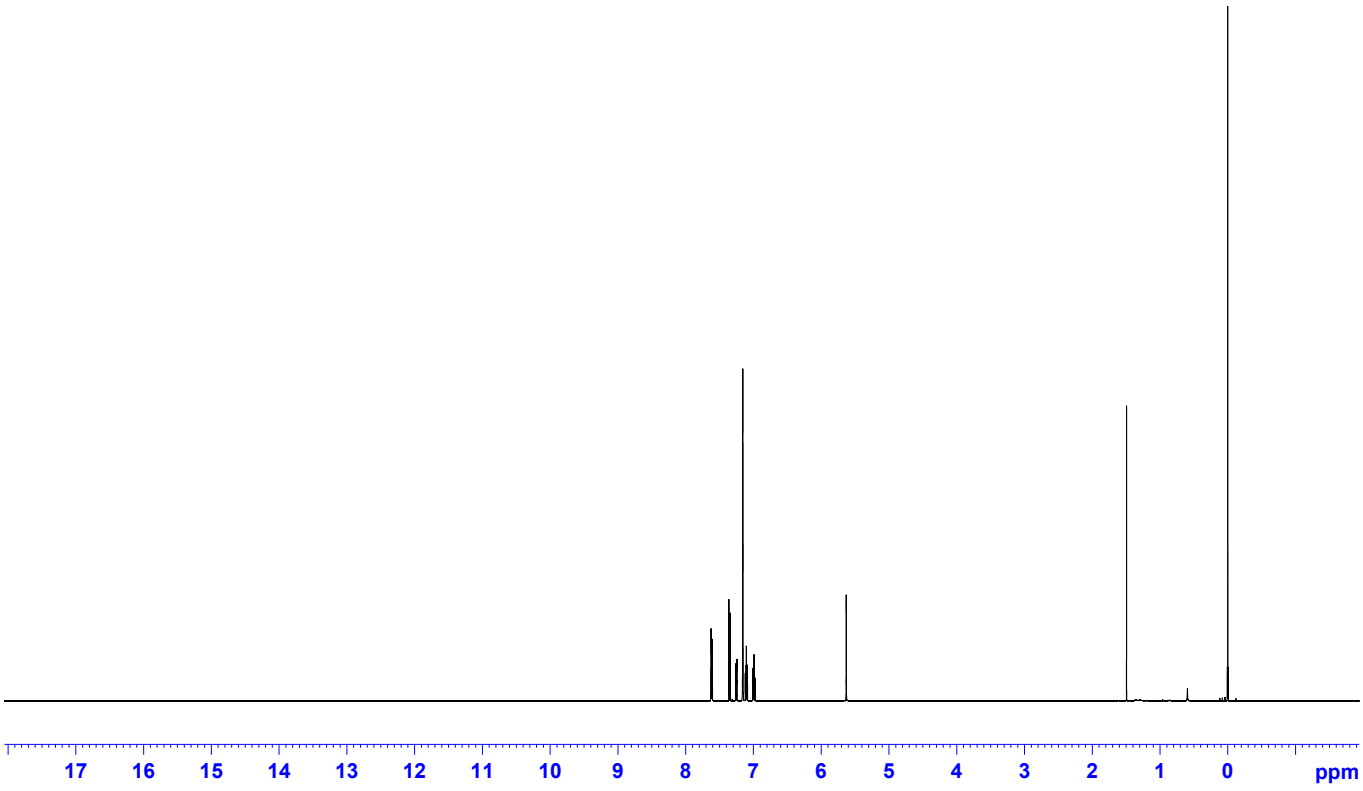
*Signal assignments of 1,1′-bi-2-napthol* (**1**)



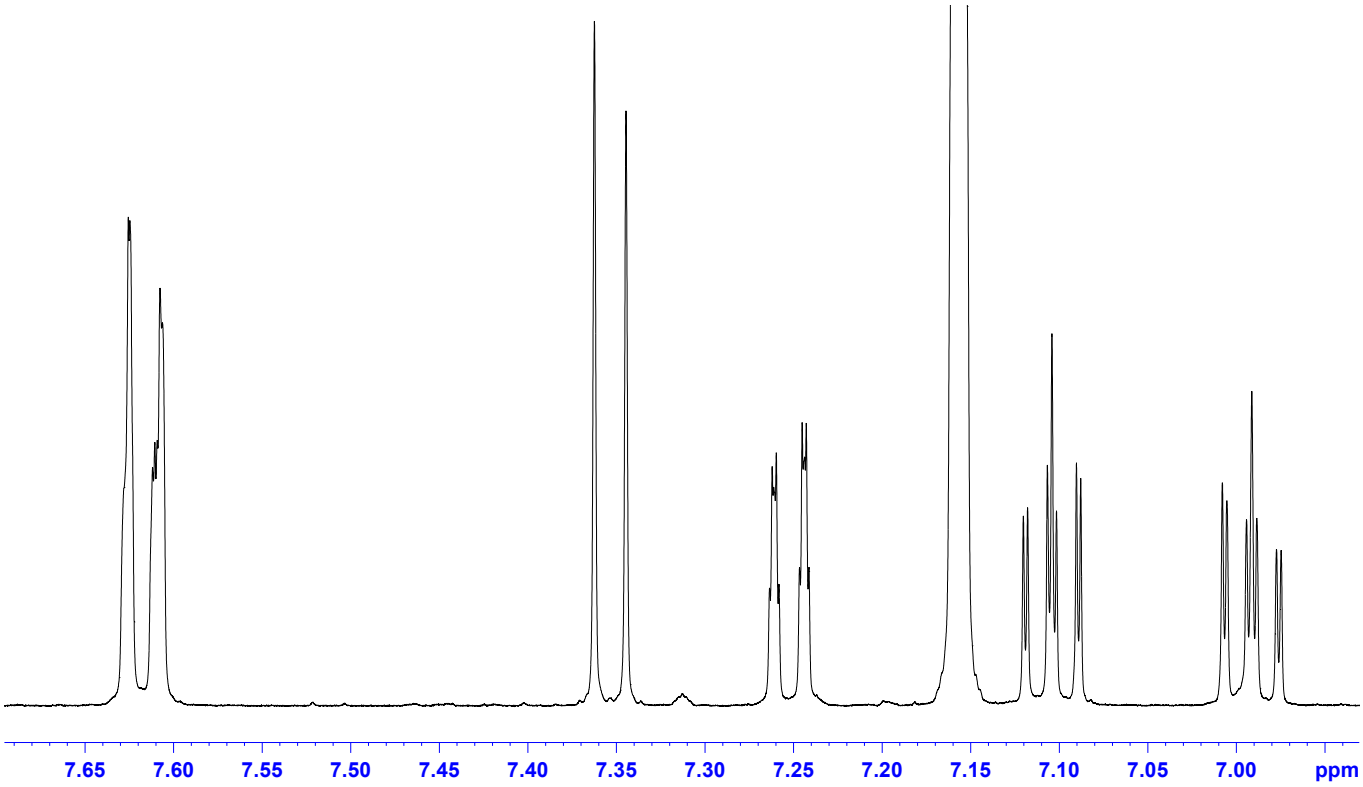

*R*-(+)-1,1'-bi-2-napthol (**1**)

$^1$H NMR (racemic sample in $C_6D_6$, $\delta$): 7.619 (dm, $J_{H6}$ = 8.21, $J_{H7}$ = –1.37, $J_{H8}$ = 0.71, $J_{H4}$ = –0.45, $J_{H3}$ = 0.28 Hz, H-5), 7.615 (dm, $J_{H3}$ = 8.92, $J_{H8}$ = 0.80, $J_{H5}$ = –0.45, $J_{H7}$ = –0.21, $J_{OH}$ = 0.15 Hz, H-4), 7.355 (d, $J_{H4}$ = 8.92, $J_{H5}$ = 0.28 Hz, H-3), 7.253 (ddt, $J_{H7}$ = 8.49, $J_{H6}$ = –1.25, $J_{H4}$ = 0.80, $J_{H5}$ = 0.71 Hz, H-8), 7.104 (ddd, $J_{H5}$ = 8.21, $J_{H7}$ = 6.83, $J_{H8}$ = –1.25 Hz, H-6), 6.992 (ddd, $J_{H8}$ = 8.49, $J_{H6}$ = 6.83, $J_{H5}$ = –1.37 Hz, H-7), 5.635 (s, $J_{H4}$ = 0.15 Hz, HO).

50% R in C6D6 at 25 deg., proton

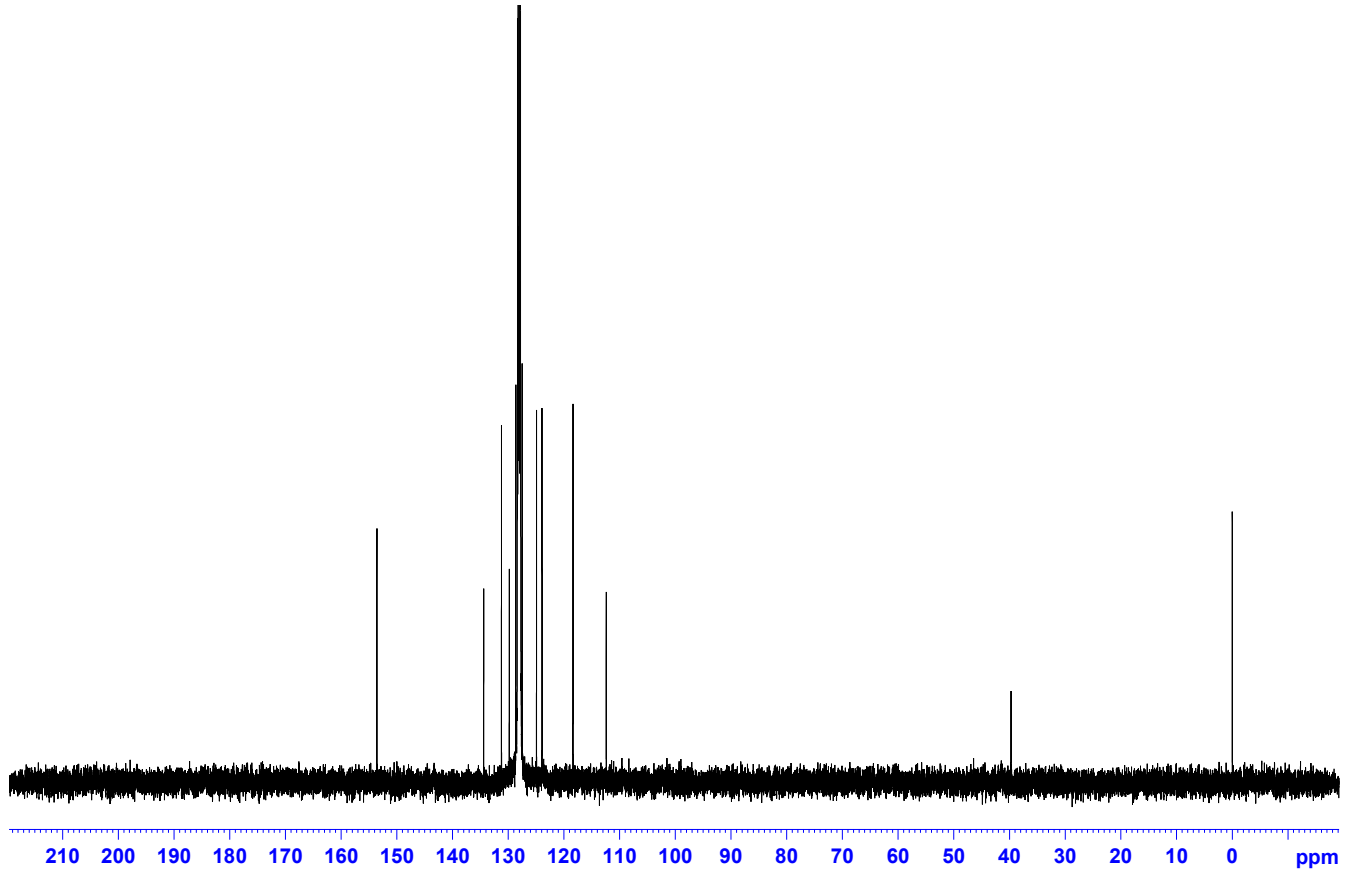


50% R in C6D6 at 25 deg., proton

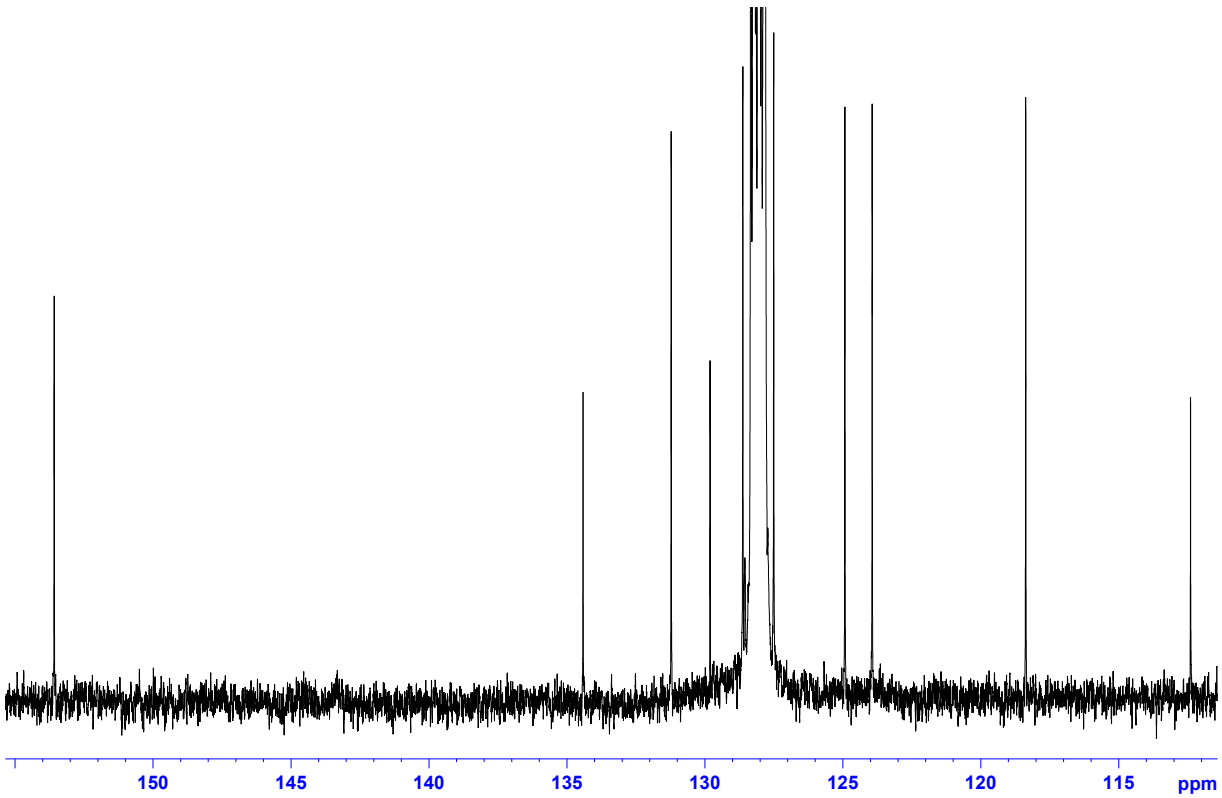



$^{13}$C NMR (racemic sample in $C_6D_6$, $\delta$): 153.58 (C-2), 134.41 (C-8a), 131.22 (C-4), 129.81 (C-4a), 128.62 (C-5), 127.50 (C-7), 124.92 (C-8), 123.93 (C-6), 118.37 (C-3), 112.40 (C-1).

50% R in C6D6 at 25 deg., carbon

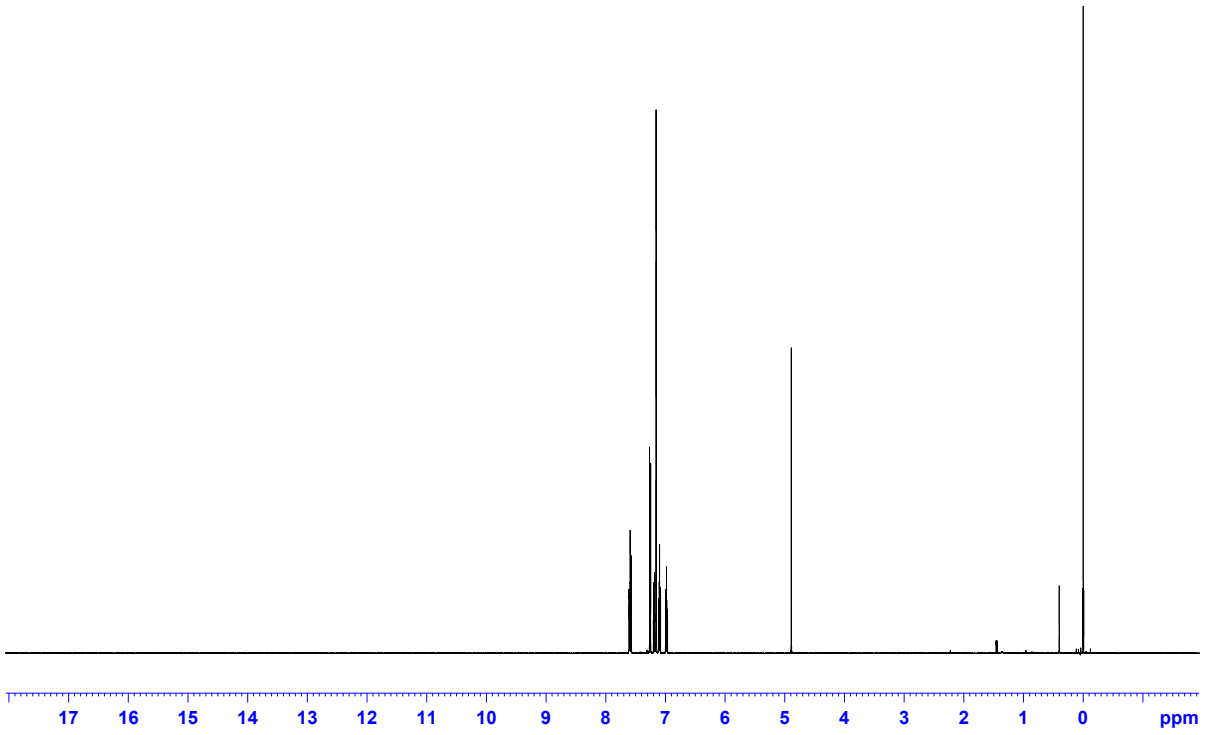


50% R in C6D6 at 25 deg., carbon

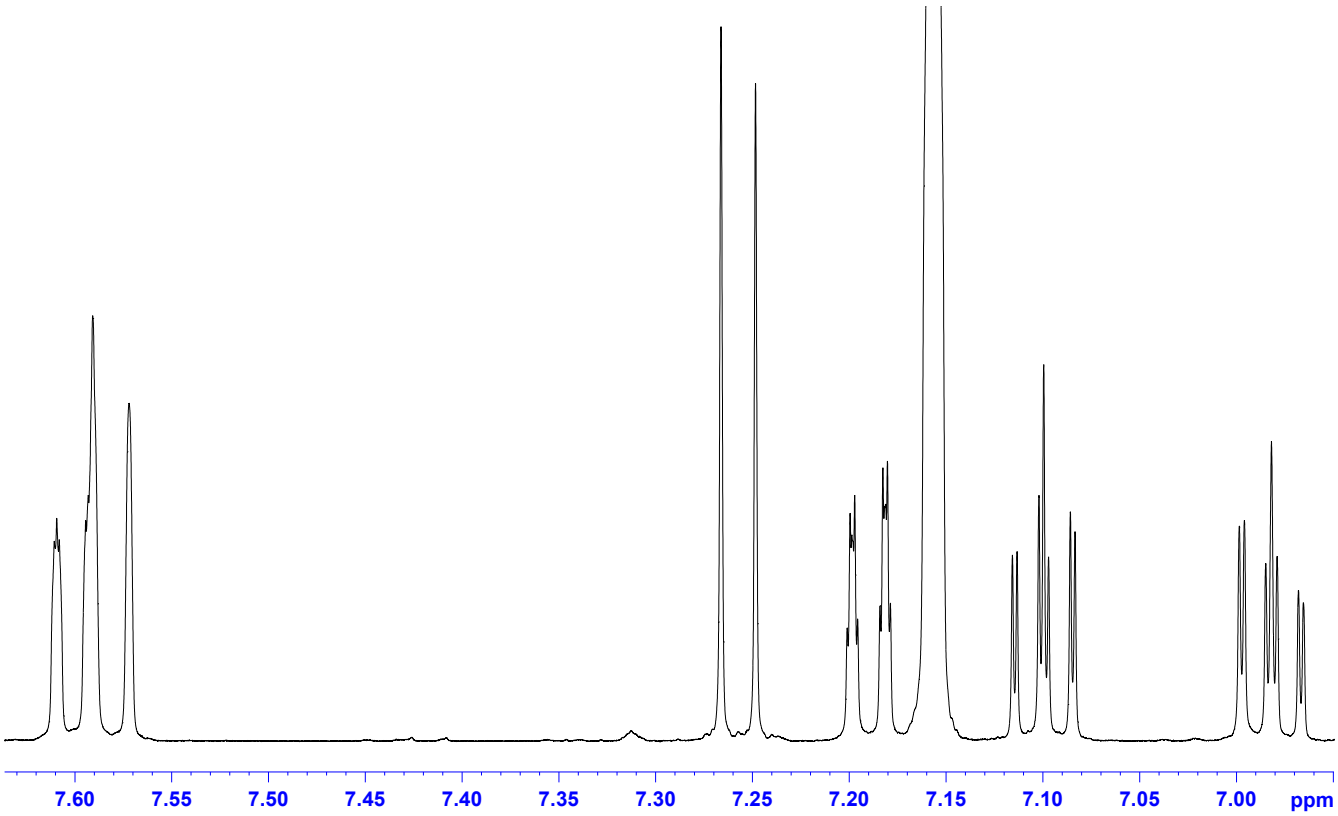



$^1$H NMR (100% *R* sample in $C_6D_6$, $\delta$): 7.601 (dm, $J_{H6}$ = 8.19, $J_{H7}$ = –1.37, $J_{H8}$ = 0.71, $J_{H4}$ = –0.42, $J_{H3}$ = 0.24 Hz, H-5), 7.581 (dm, $J_{H3}$ = 8.93, $J_{H8}$ = 0.80, $J_{H5}$ = –0.42, $J_{OH}$ = 0.41, $J_{H7}$ = –0.24 Hz, H-4), 7.258 (d, $J_{H4}$ = 8.93, $J_{H5}$ = 0.24 Hz, H-3), 7.190 (ddt, $J_{H7}$ = 8.48, $J_{H6}$ = –1.25, $J_{H4}$ = 0.80, $J_{H5}$ = 0.71 Hz, H-8), 7.099 (ddd, $J_{H5}$ = 8.19, $J_{H7}$ = 6.85, $J_{H8}$ = –1.25 Hz, H-6), 6.983 (ddd, $J_{H8}$ = 8.48, $J_{H6}$ = 6.85, $J_{H5}$ = –1.37 Hz, H-7), 4.891 (d, $J_{H4}$ = 0.41 Hz, HO).

100% R in C6D6 at 25 deg., proton

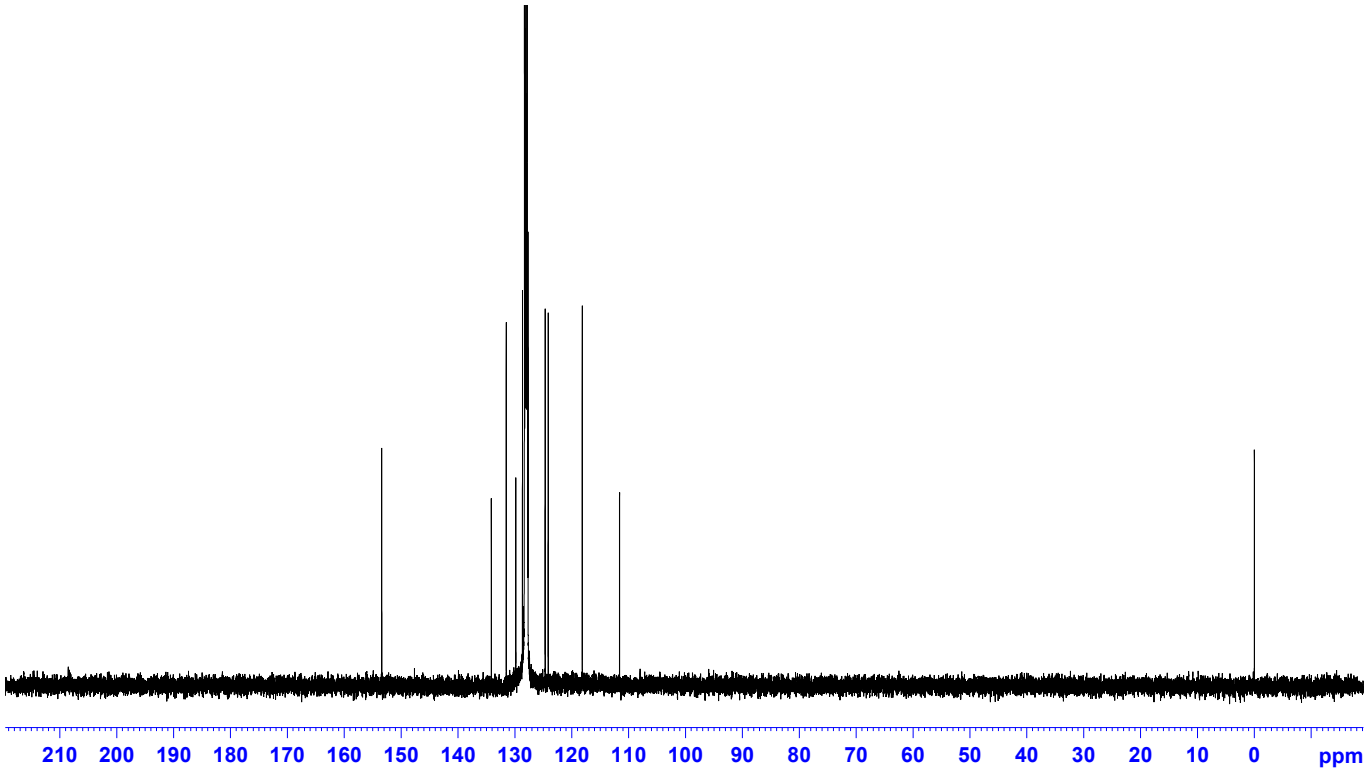


100% R in C6D6 at 25 deg., proton

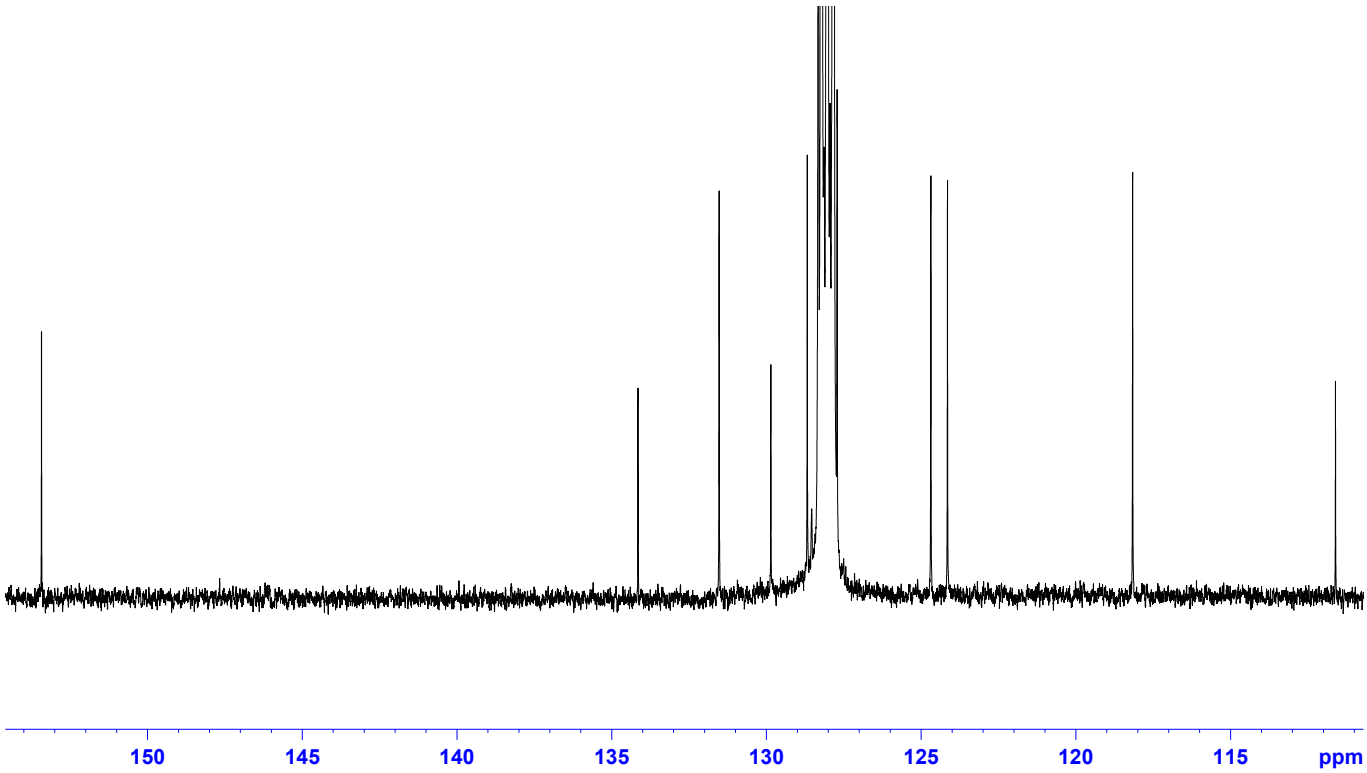



$^{13}$C NMR (100% *R* sample in $C_6D_6$, $\delta$): 153.43 (C-2), 134.15 (C-8a), 131.53 (C-4), 129.86 (C-4a), 128.68 (C-5), 127.72 (C-7), 124.69 (C-8), 124.15 (C-6), 118.17 (C-3), 111.61 (C-1).

100% R in C6D6 at 25 deg., carbon



100% R in C6D6 at 25 deg., carbon



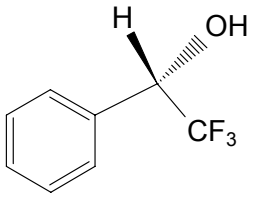

$^{1}$H NMR (racemic sample in $CDCl_3$, $\delta$): 7.973 (dm, $J_{H3}$ = 8.93, $J_{H8}$ = 0.78, $J_{OH}$ = 0.46, $J_{H5}$ = –0.41, $J_{H7}$ = –0.28 Hz, H-4), 7.890 (dm, $J_{H6}$ = 8.24, $J_{H7}$ = –1.48, $J_{H8}$ = 0.71, $J_{H4}$ = –0.41, $J_{H3}$ = 0.27 Hz, H-5), 7.381 (d, $J_{H4}$ = 8.93, $J_{H5}$ = 0.27 Hz, H-3), 7.370 (ddd, $J_{H5}$ = 8.24, $J_{H7}$ = 6.84, $J_{H8}$ = –1.40 Hz, H-6), 7.305 (ddd, $J_{H8}$ = 8.54, $J_{H6}$ = 6.84, $J_{H5}$ = –1.48 Hz, H-7), 7.150 (ddt, $J_{H7}$ = 8.54, $J_{H6}$ = –1.40, $J_{H4}$ = 0.78, $J_{H5}$ = 0.71 Hz, H-8), 5.053 (d, $J_{H4}$ = 0.46 Hz, HO).

$^{13}$C NMR (racemic sample in $CDCl_3$, $\delta$): 152.75 (C-2), 133.40 (C-8a), 131.44 (C-4), 129.46 (C-4a), 128.42 (C-5), 127.50 (C-7), 124.21 (C-8), 124.05 (C-6), 117.76 (C-3), 110.80 (C-1).

$^{1}$H NMR (100% *R* sample in $CDCl_3$, $\delta$): 7.973 (dm, $J_{H3}$ = 8.96, $J_{H8}$ = 0.77, $J_{OH}$ = 0.46, $J_{H5}$ = –0.39, $J_{H7}$ = –0.25 Hz, H-4), 7.892 (dm, $J_{H6}$ = 8.22, $J_{H7}$ = –1.49, $J_{H8}$ = 0.72, $J_{H4}$ = –0.39, $J_{H3}$ = 0.23 Hz, H-5), 7.379 (d, $J_{H4}$ = 8.96, $J_{H5}$ = 0.23 Hz, H-3), 7.372 (ddd, $J_{H5}$ = 8.22, $J_{H7}$ = 6.85, $J_{H8}$ = –1.41 Hz, H-6), 7.306 (ddd, $J_{H8}$ = 8.54, $J_{H6}$ = 6.85, $J_{H5}$ = –1.49 Hz, H-7), 7.151 (ddt, $J_{H7}$ = 8.54, $J_{H6}$ = –1.41, $J_{H4}$ = 0.77, $J_{H5}$ = 0.72 Hz, H-8), 5.052 (d, $J_{H4}$ = 0.46 Hz, HO).

$^{13}$C NMR (100% *R* sample in $CDCl_3$, $\delta$): 152.75 (C-2), 133.40 (C-8a), 131.44 (C-4), 129.46 (C-4a), 128.42 (C-5), 127.50 (C-7), 124.21 (C-8), 124.05 (C-6), 117.76 (C-3), 110.80 (C-1).

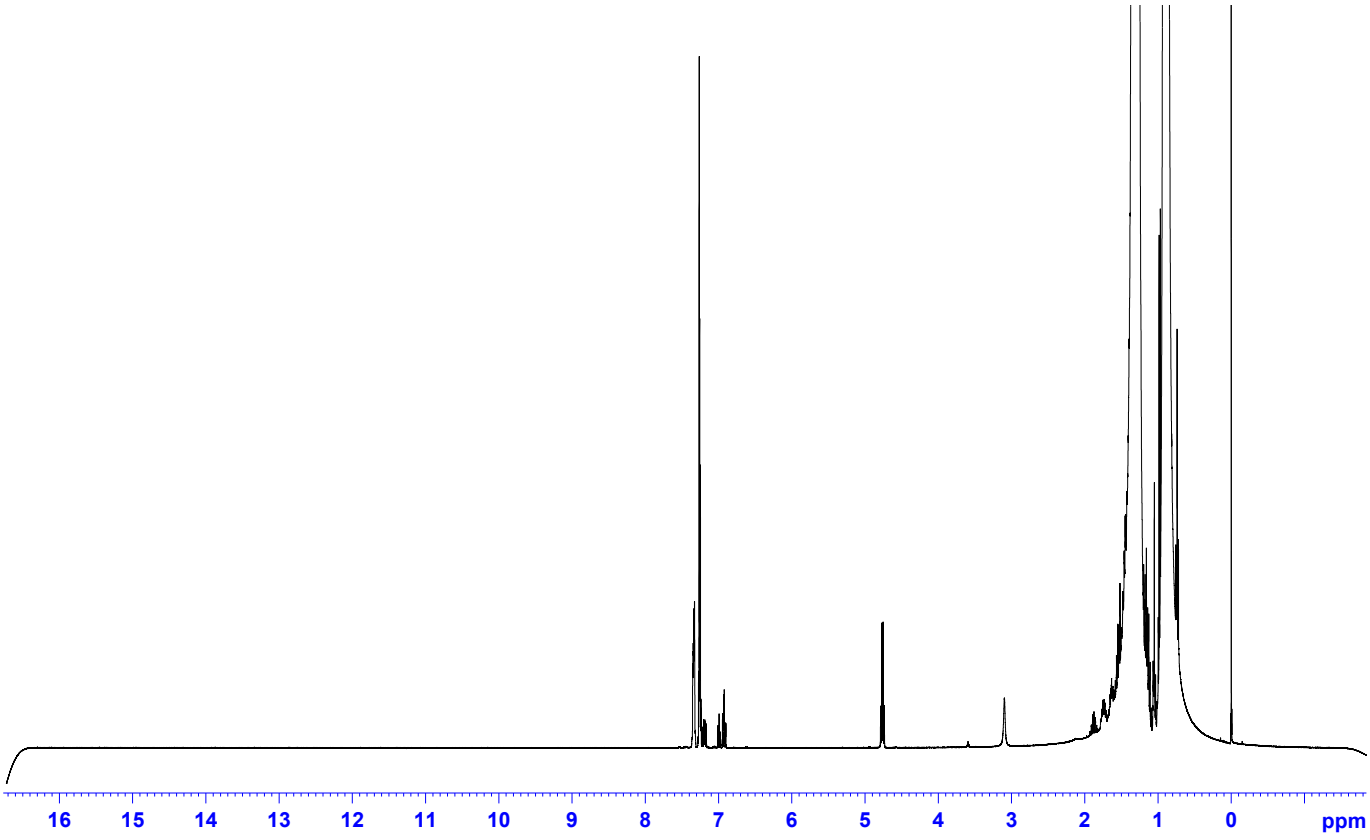
*Signal assignments of 1-phenyl-2,2,2-trifluoroethanol* (**2**)



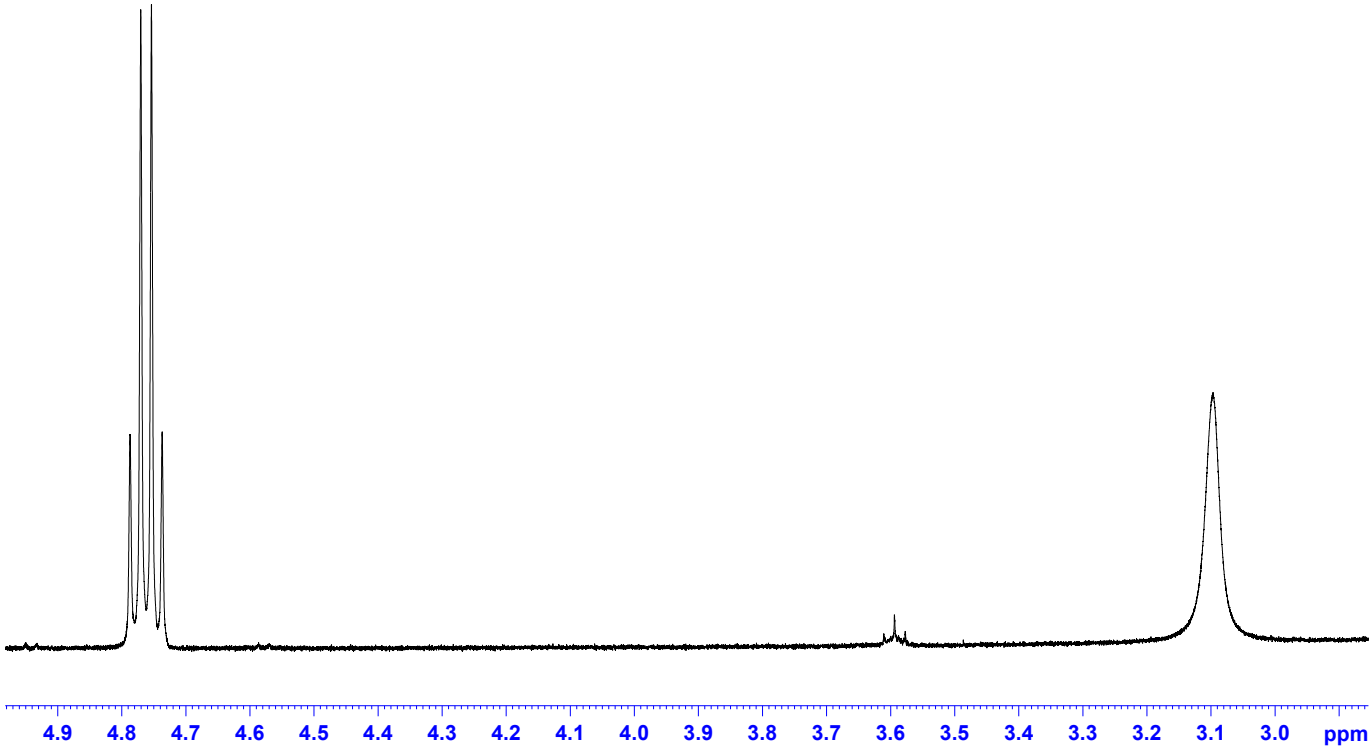

*S*-(+)-1-phenyl-
2,2,2-trifluoroethanol (**2**)

$^1$H NMR (racemic sample in *n*-hexane, $\delta$): 7.340 (m, 2 × H-*o*), 7.258 (om, 2 × H-*m*), 7.258 (om, H-*p*), 4.762 (qt, $J_F$ = 6.67 Hz, H-1), HO not observed.

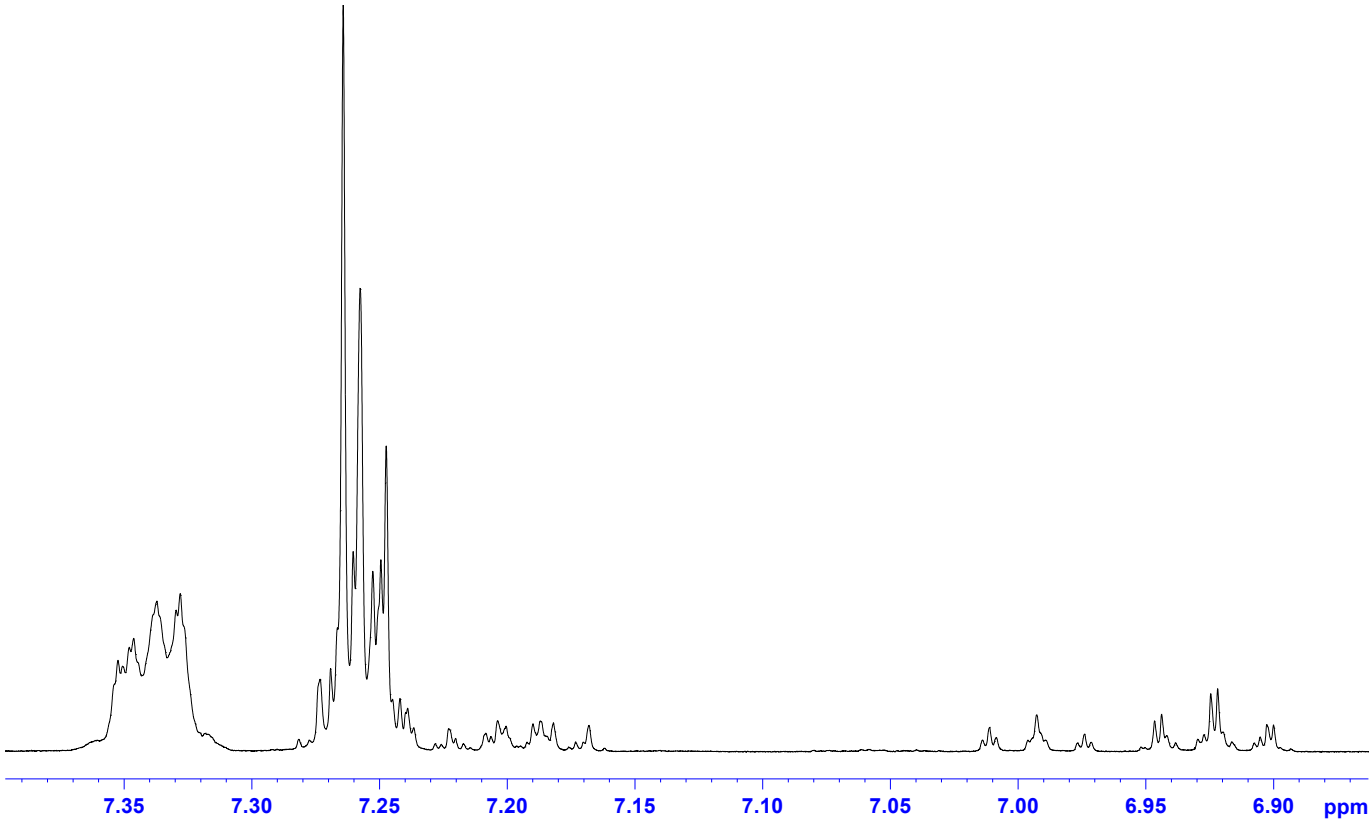
50% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., proton



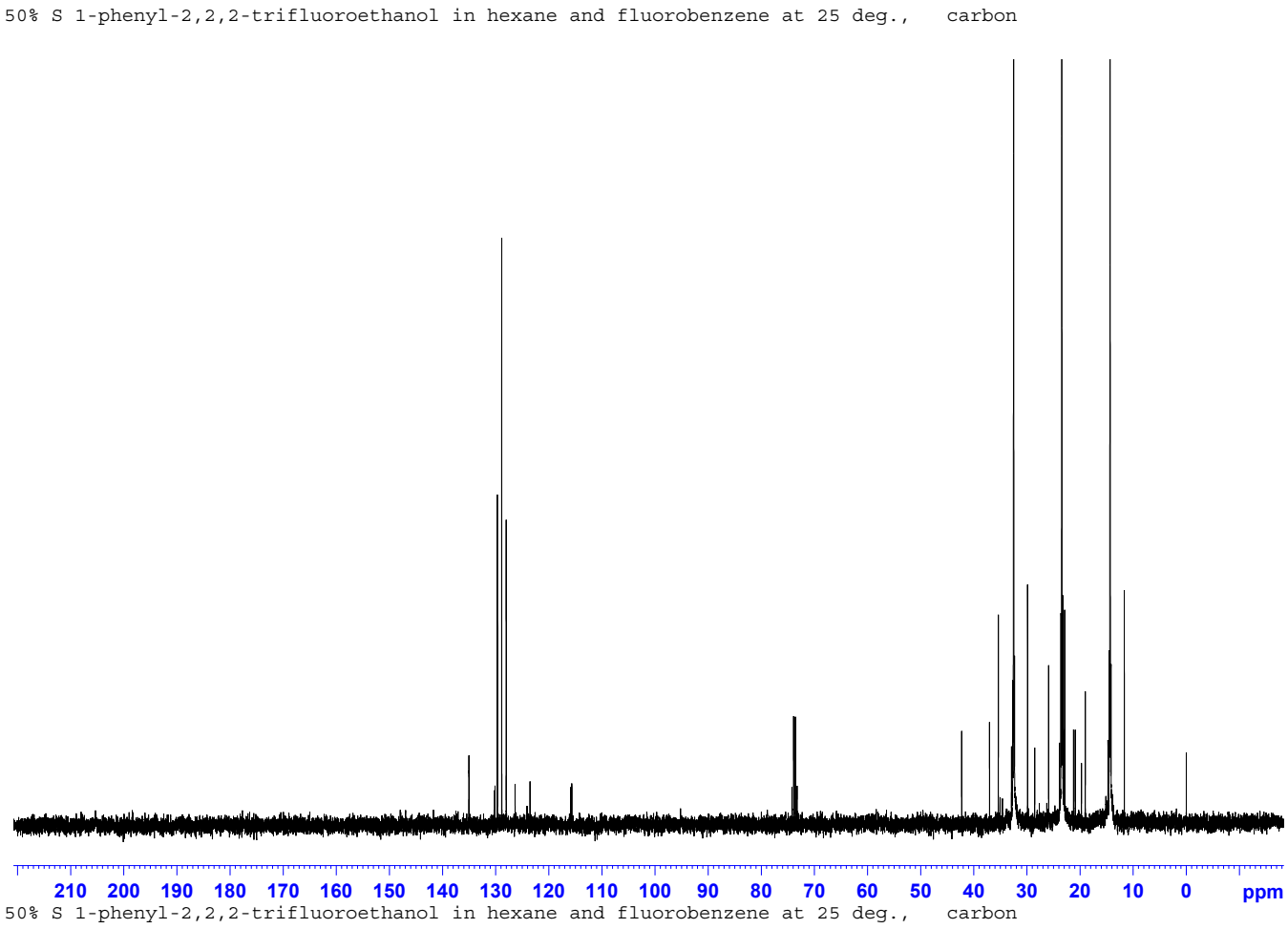
50% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., proton



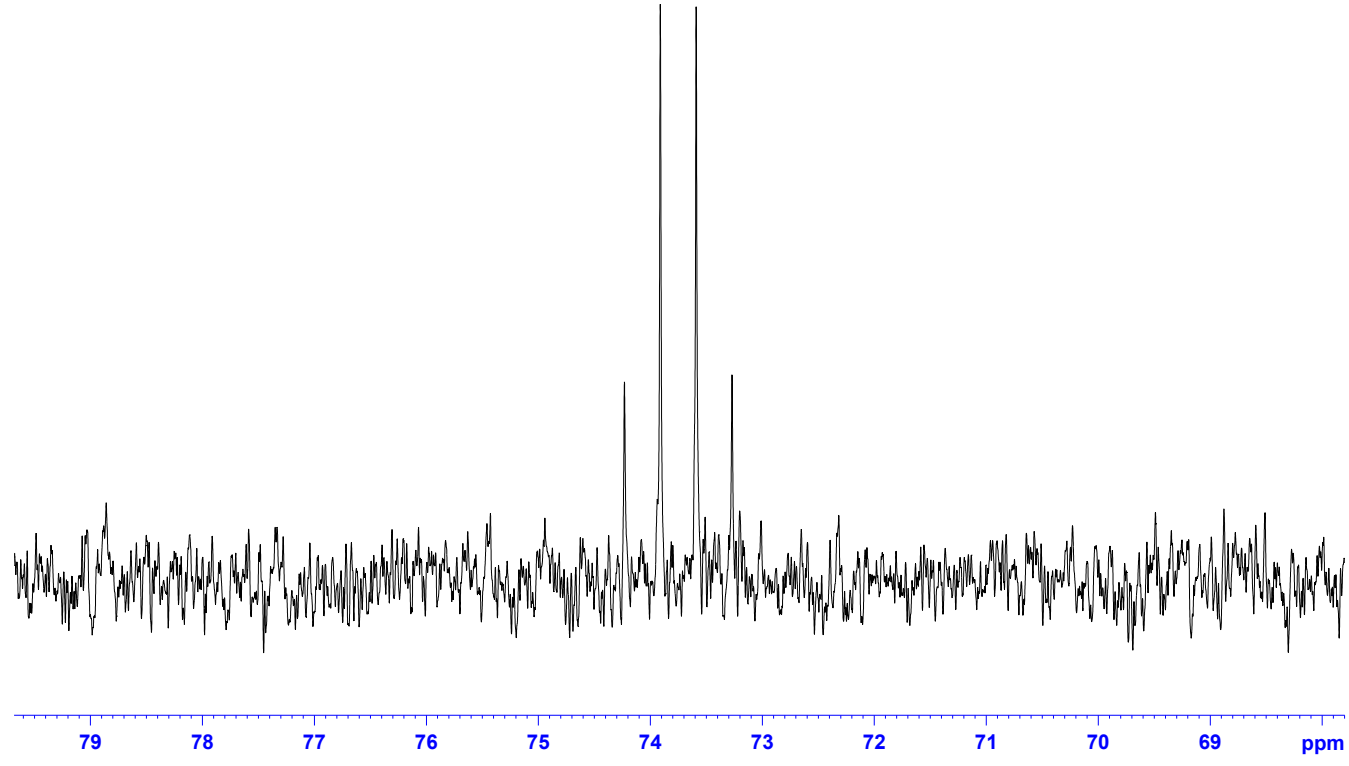

50% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., proton



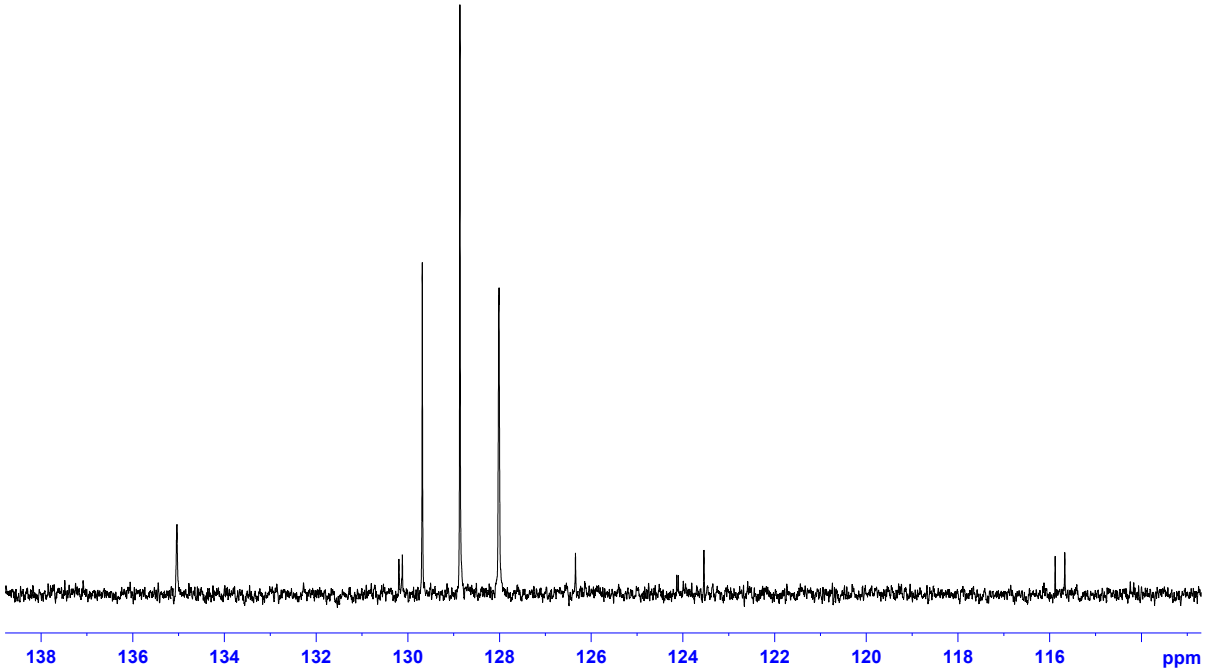
$^{13}$C NMR (racemic sample in *n*-hexane, $\delta$): 135.04 (C-*i*, $J_F$ = 1.17 Hz), 129.68 (C-*p*), 128.86 (C-*m*), 128.01 (C-*o*, $J_F$ = 1.05 Hz), 124.94 (C-2, $J_F$ = 281.53 Hz), 73.75 (C-1, $J_F$ = 32.21 Hz).




50% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., carbon



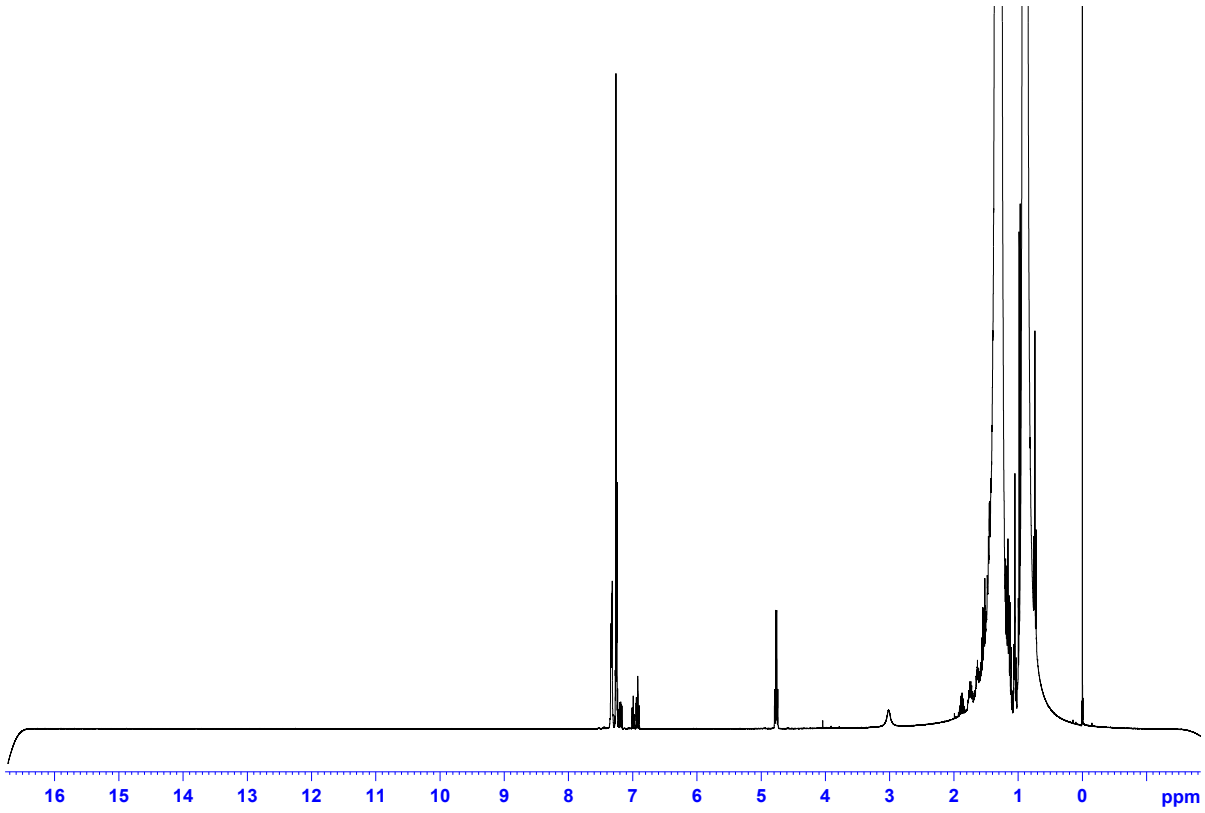
50% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., carbon



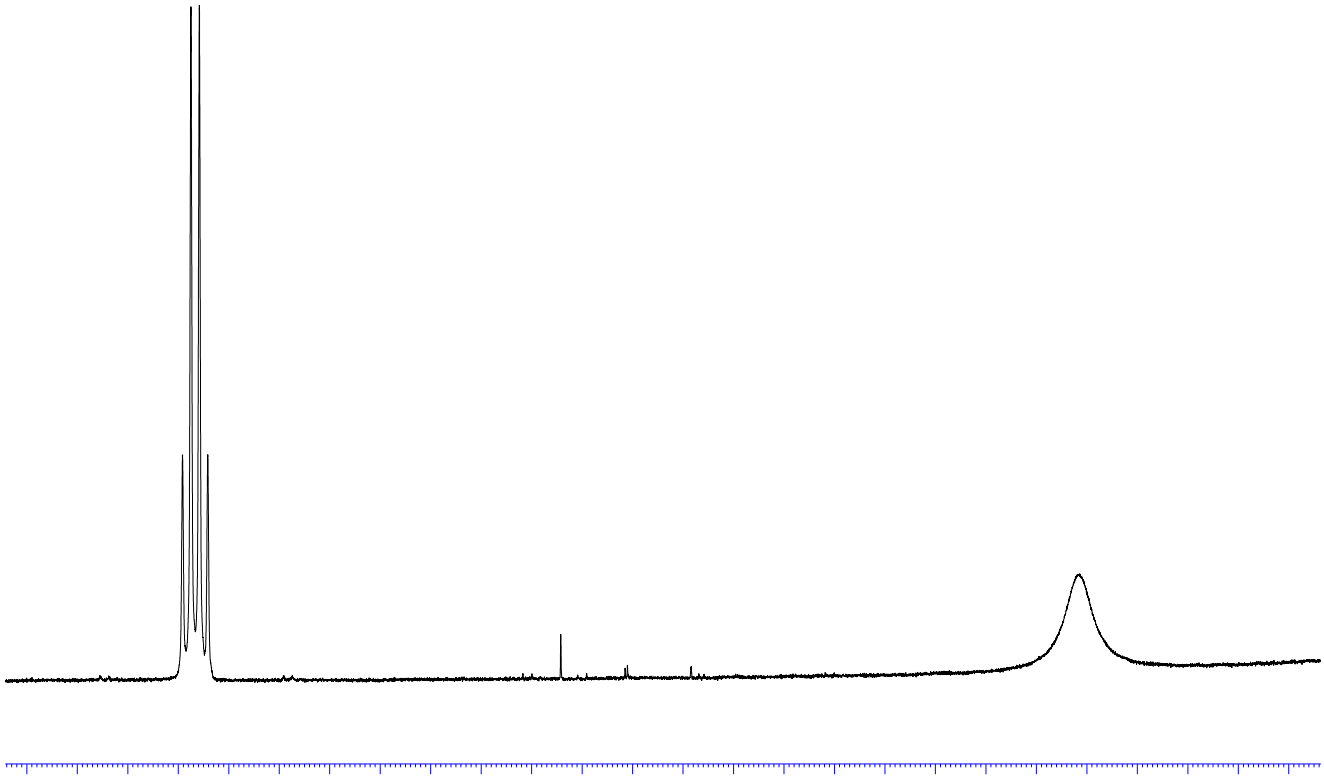

$^{19}$F NMR (racemic sample in *n*-hexane, $\delta$): –82.4176, dt, $J_{H1}$ = 6.67 Hz, $J_{Ho}$ = 1.39 Hz..

$^{1}$H NMR (100% *S* sample in *n*-hexane, $\delta$): 7.331 (m, 2 × H-*o*), 7.256 (om, 2 × H-*m*), 7.256 (om, H-*p*), 4.767 (qt, $J_F$ = 6.66 Hz, H-1), HO not observed.

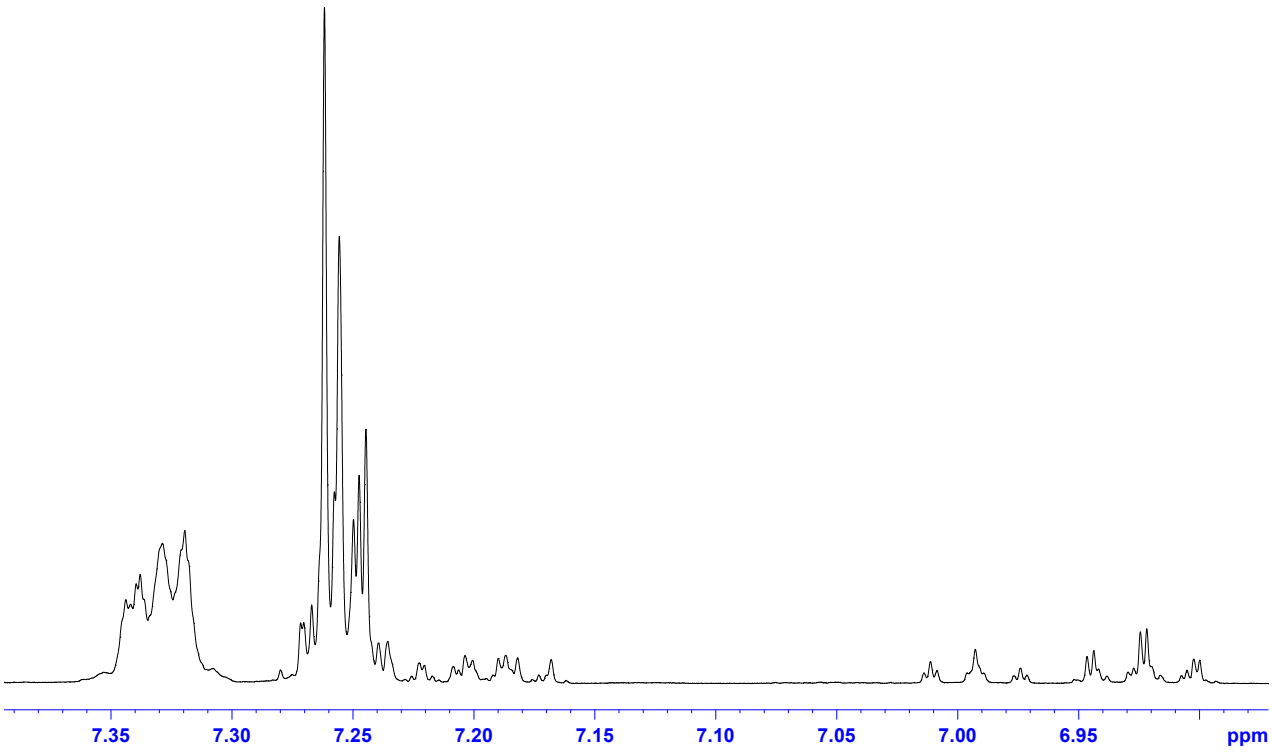
100% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., proton



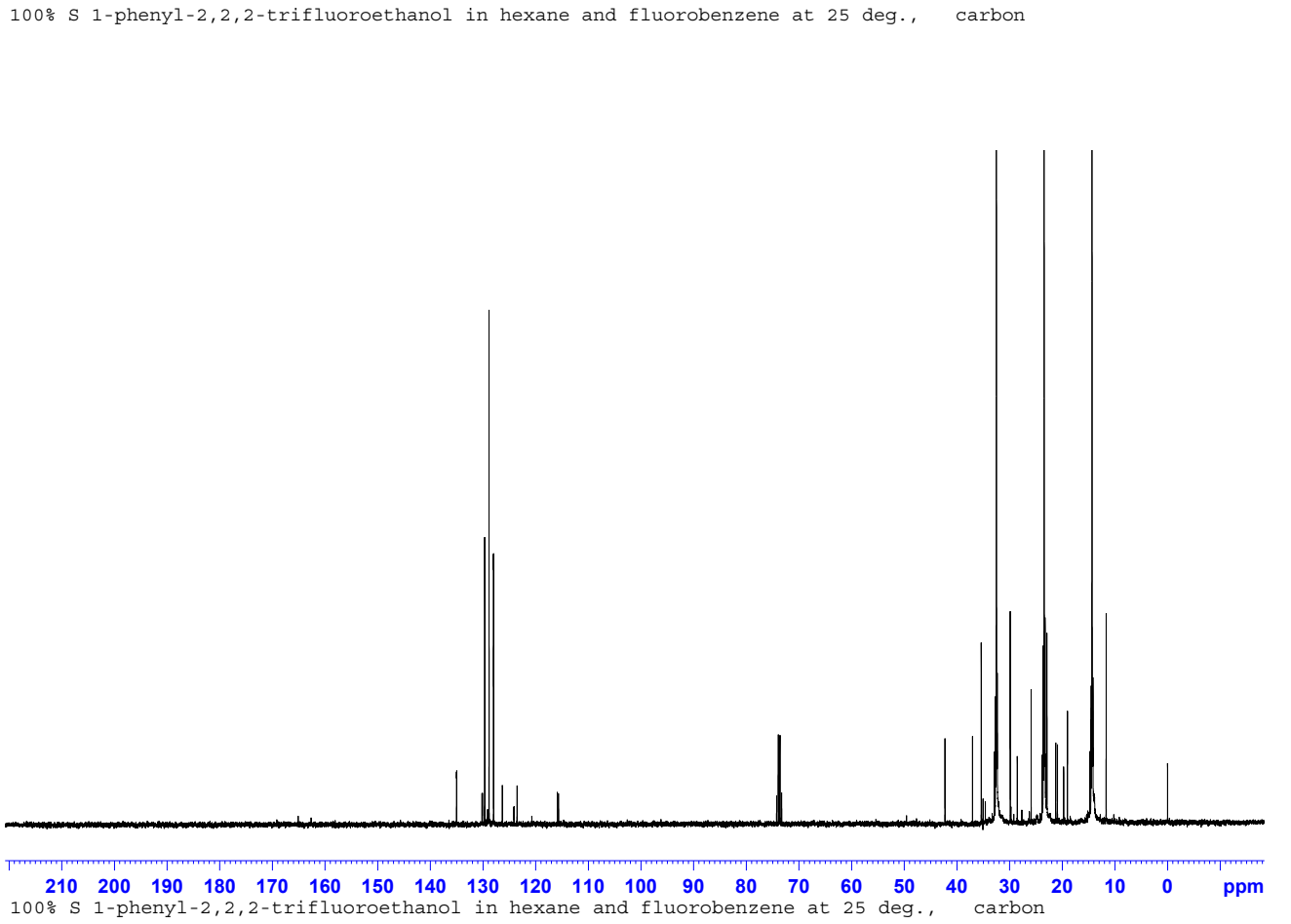
100% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., proton

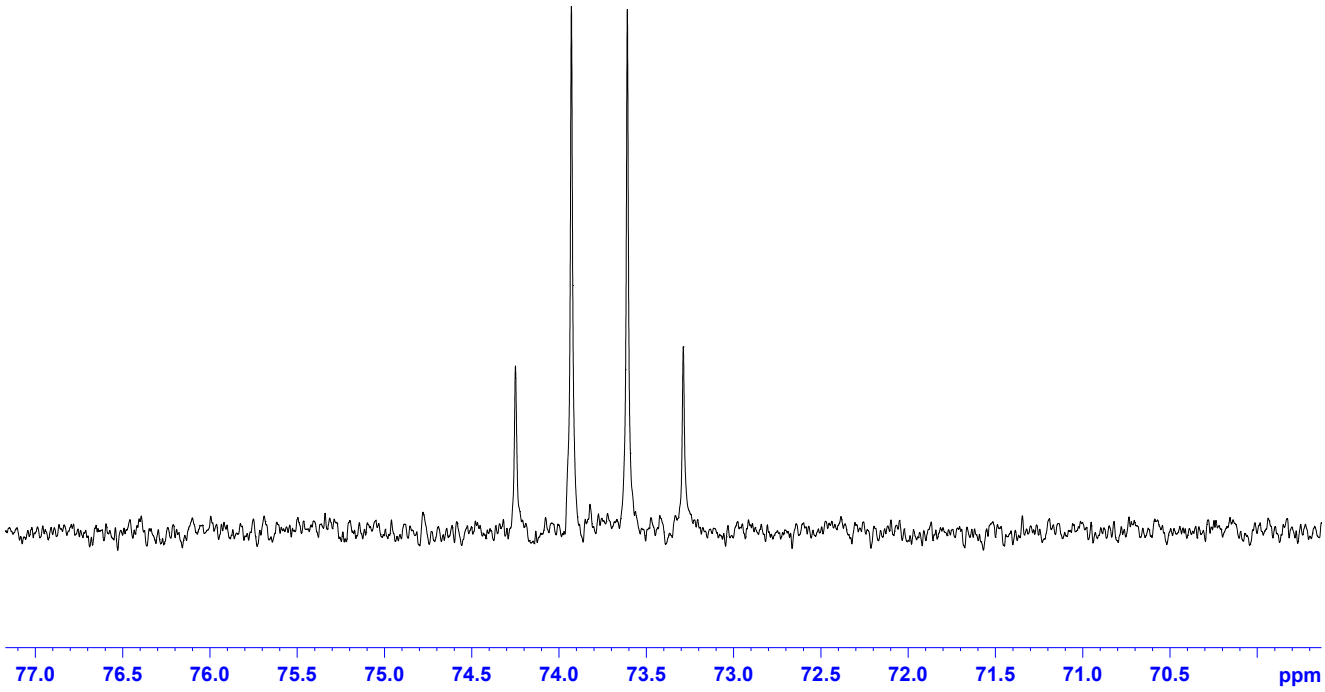



100% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., proton

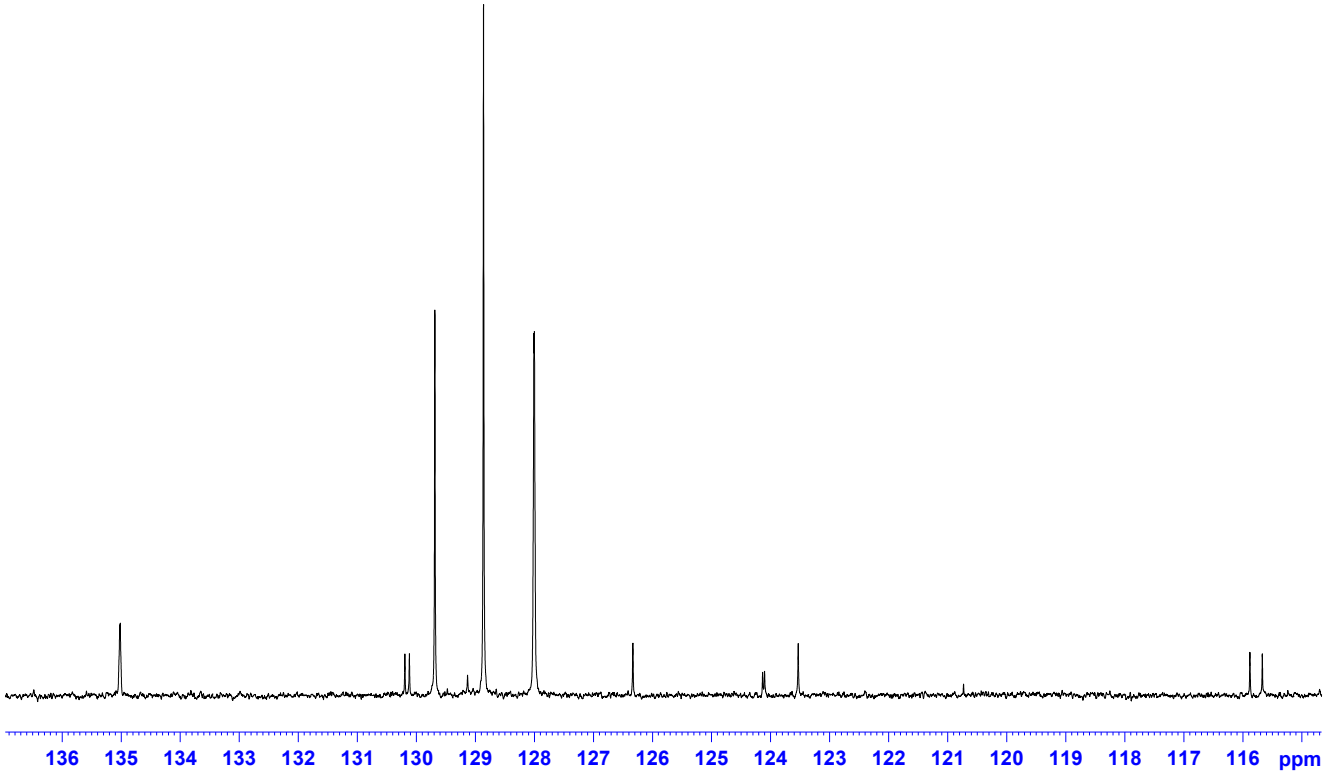


$^{13}$C NMR (100% *S* sample in *n*-hexane, $\delta$): 135.02 ($C_i$, $J_F$ = 1.17 Hz), 129.69 ($C_p$), 128.86 ($C_m$), 128.01 ($C_o$, $J_F$ = 1.05 Hz), 124.93 (C-2, $J_F$ = 281.50 Hz), 73.77 (C-1, $J_F$ = 32.22 Hz).



100% S 1-phenyl-2,2,2-trifluoroethanol in hexane and fluorobenzene at 25 deg., carbon




$^{19}$F NMR (100% *S* sample in *n*-hexane, $\delta$): –82.4265, dt, $J_{H1}$ = 6.67 Hz, $J_{Ho}$ = 1.37 Hz.

*Cartesian coordinates of the heterochiral complex of 1,1′-bi-2-napthol* (**1**$_{2het}$)

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!DATE Fri May 18 09:44:13 2007

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| C7 | -0.295841231 | -2.819074490 | 0.693603784 | XXX | ND | c | C 0.000 |
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| | | | | | | | | |
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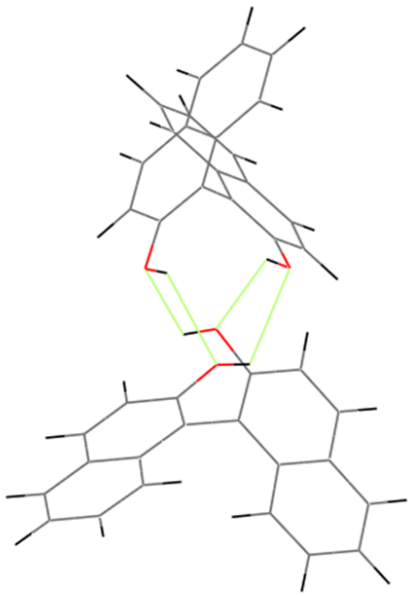
| C49 | 1.007735992 | 3.787168081 | 1.340036741 | XXX | ND | c | C | 0.000 |
| C50 | 2.324153337 | 3.807916381 | 1.908946090 | XXX | ND | c | C | 0.000 |
| C51 | 2.623474250 | 4.736607716 | 2.940034739 | XXX | ND | c | C | 0.000 |
| C52 | 1.668805394 | 5.614467522 | 3.403269334 | XXX | ND | c | C | 0.000 |
| C53 | 3.296629231 | 2.891660131 | 1.421320310 | XXX | ND | c | C | 0.000 |
| C54 | 2.989330295 | 1.989979001 | 0.437369888 | XXX | ND | c | C | 0.000 |
| C55 | 1.684386222 | 1.961457715 | -0.120760378 | XXX | ND | c | C | 0.000 |
| C56 | 0.697362320 | 2.847794057 | 0.295941541 | XXX | ND | c | C | 0.000 |
| O57 | -1.360275031 | 0.927600949 | 0.952105076 | XXX | ND | o | O | 0.000 |
| O58 | 1.479473302 | 1.011071013 | -1.078453183 | XXX | ND | o | O | 0.000 |
| H59 | -1.983667217 | 6.396790487 | -4.140091626 | XXX | ND | h | H | 0.000 |
| H60 | -3.643457956 | 4.719059070 | -3.371476073 | XXX | ND | h | H | 0.000 |
| H61 | 0.936100900 | 4.792400525 | -1.407281099 | XXX | ND | h | H | 0.000 |
| H62 | 0.309330922 | 6.418904586 | -3.148976900 | XXX | ND | h | H | 0.000 |
| H63 | -3.616995273 | 1.144842200 | -0.191683210 | XXX | ND | h | H | 0.000 |
| H64 | -4.245966384 | 2.812301803 | -1.928787502 | XXX | ND | h | H | 0.000 |
| H65 | -0.387156670 | 6.288930874 | 3.216155658 | XXX | ND | h | H | 0.000 |
| H66 | -0.958096153 | 4.701798440 | 1.420357160 | XXX | ND | h | H | 0.000 |
| H67 | 3.630795387 | 4.740414315 | 3.362792925 | XXX | ND | h | H | 0.000 |
| H68 | 1.909998636 | 6.323108299 | 4.197245116 | XXX | ND | h | H | 0.000 |
| H69 | 4.300732982 | 2.910814644 | 1.849921292 | XXX | ND | h | H | 0.000 |
| H70 | 3.725749503 | 1.279093002 | 0.061644924 | XXX | ND | h | H | 0.000 |
| H71 | -0.453180183 | 1.021760892 | 1.301877732 | XXX | ND | h | H | 0.000 |
| H72 | 0.553888166 | 1.036235067 | -1.388631050 | XXX | ND | h | H | 0.000 |

end

end



*Cartesian coordinates of the homochiral complex of 1,1′-bi-2-napthol* (**1**$_{2hom}$)

!BIOSYM archive 3

PBC=OFF

Materials Studio Generated CAR File

!DATE Fri May 18 09:44:21 2007

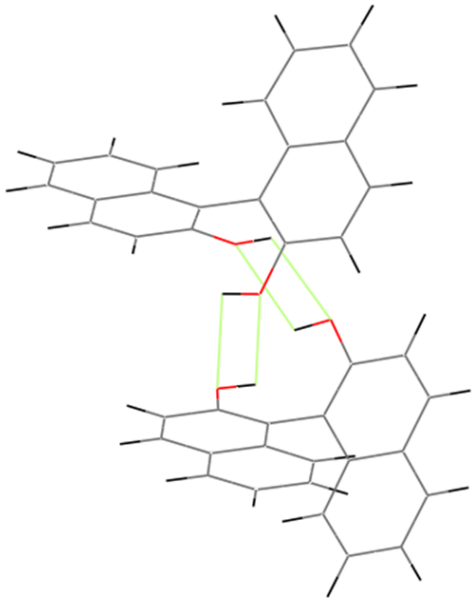
| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C1 | -5.543593526 | -2.816669274 | 2.647402339 | XXX | ND | c | C | 0.000 |
| C2 | -4.687269855 | -3.531269290 | 1.839490132 | XXX | ND | c | C | 0.000 |
| C3 | -3.787953038 | -2.870793035 | 0.961726995 | XXX | ND | c | C | 0.000 |
| C4 | -3.772341228 | -1.436951823 | 0.919190963 | XXX | ND | c | C | 0.000 |
| C5 | -4.671540112 | -0.730420809 | 1.764893625 | XXX | ND | c | C | 0.000 |
| C6 | -5.532204639 | -1.403400167 | 2.605515440 | XXX | ND | c | C | 0.000 |
| C7 | -2.863402914 | -0.762833404 | 0.033676368 | XXX | ND | c | C | 0.000 |
| C8 | -2.017624022 | -1.523127397 | -0.767415189 | XXX | ND | c | C | 0.000 |
| C9 | -2.034749315 | -2.941635603 | -0.725082589 | XXX | ND | c | C | 0.000 |
| C10 | -2.898396308 | -3.591760365 | 0.117601565 | XXX | ND | c | C | 0.000 |
| C11 | -5.396343466 | 1.518028192 | -2.679522954 | XXX | ND | c | C | 0.000 |
| C12 | -4.591980317 | 0.798671950 | -1.821847284 | XXX | ND | c | C | 0.000 |
| C13 | -3.675067900 | 1.454756807 | -0.955063641 | XXX | ND | c | C | 0.000 |
| C14 | -3.612362570 | 2.887423687 | -0.994266396 | XXX | ND | c | C | 0.000 |
| C15 | -4.455882902 | 3.596568882 | -1.889497333 | XXX | ND | c | C | 0.000 |
| C16 | -5.331071826 | 2.930023100 | -2.717992387 | XXX | ND | c | C | 0.000 |
| C17 | -2.704241960 | 3.558309743 | -0.129123822 | XXX | ND | c | C | 0.000 |
| C18 | -1.893387344 | 2.861469528 | 0.728884883 | XXX | ND | c | C | 0.000 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C19 | -1.952785058 | 1.444360157 | 0.765885637 | XXX | ND | c | C | 0.000 |
| C20 | -2.822346396 | 0.731561558 | -0.052775000 | XXX | ND | c | C | 0.000 |
| O21 | -1.130743668 | -0.968143610 | -1.639976065 | XXX | ND | o | O | 0.000 |
| O22 | -1.111848618 | 0.837757403 | 1.651637319 | XXX | ND | o | O | 0.000 |
| H23 | -6.230210853 | -3.336082786 | 3.317738779 | XXX | ND | h | H | 0.000 |
| H24 | -4.687383839 | -4.623444121 | 1.861757753 | XXX | ND | h | H | 0.000 |
| H25 | -4.672182459 | 0.359296999 | 1.739325857 | XXX | ND | h | H | 0.000 |
| H26 | -6.212952433 | -0.838942205 | 3.245331291 | XXX | ND | h | H | 0.000 |
| H27 | -1.348797159 | -3.484767055 | -1.375523085 | XXX | ND | h | H | 0.000 |
| H28 | -2.911521808 | -4.683403098 | 0.148825362 | XXX | ND | h | H | 0.000 |
| H29 | -6.091747382 | 0.991730754 | -3.335868258 | XXX | ND | h | H | 0.000 |
| H30 | -4.651201091 | -0.289462496 | -1.798857028 | XXX | ND | h | H | 0.000 |
| H31 | -4.397286327 | 4.687289858 | -1.908873411 | XXX | ND | h | H | 0.000 |
| H32 | -5.973785603 | 3.486293535 | -3.402170916 | XXX | ND | h | H | 0.000 |
| H33 | -2.659681143 | 4.649194589 | -0.156432583 | XXX | ND | h | H | 0.000 |
| H34 | -1.193341834 | 3.366183509 | 1.394881544 | XXX | ND | h | H | 0.000 |
| H35 | -1.181329118 | 0.005436681 | -1.590399158 | XXX | ND | h | H | 0.000 |
| H36 | -1.229923044 | -0.129890180 | 1.603706812 | XXX | ND | h | H | 0.000 |
| C37 | 5.334084446 | 2.927325062 | 2.717842174 | XXX | ND | c | C | 0.000 |
| C38 | 4.459526803 | 3.594624298 | 1.889265824 | XXX | ND | c | C | 0.000 |
| C39 | 3.615107987 | 2.886175321 | 0.994326951 | XXX | ND | c | C | 0.000 |
| C40 | 3.676019526 | 1.453416324 | 0.955676288 | XXX | ND | c | C | 0.000 |
| C41 | 4.592194680 | 0.796541089 | 1.822660070 | XXX | ND | c | C | 0.000 |
| C42 | 5.397635068 | 1.515226668 | 2.679885240 | XXX | ND | c | C | 0.000 |
| C43 | 2.822686493 | 0.730835272 | 0.053476854 | XXX | ND | c | C | 0.000 |
| C44 | 1.954122108 | 1.444417311 | -0.765542438 | XXX | ND | c | C | 0.000 |
| C45 | 1.895834702 | 2.861564674 | -0.728469477 | XXX | ND | c | C | 0.000 |
| C46 | 2.707244175 | 3.557829376 | 0.129494059 | XXX | ND | c | C | 0.000 |
| C47 | 5.527606284 | -1.405009011 | -2.608969011 | XXX | ND | c | C | 0.000 |
| C48 | 4.668161741 | -0.731729235 | -1.767337487 | XXX | ND | c | C | 0.000 |
| C49 | 3.770274887 | -1.437966277 | -0.919986653 | XXX | ND | c | C | 0.000 |
| C50 | 3.785290555 | -2.871820222 | -0.962587689 | XXX | ND | c | C | 0.000 |
| C51 | 4.683332523 | -3.532598293 | -1.841434082 | XXX | ND | c | C | 0.000 |
| C52 | 5.538654021 | -2.818286305 | -2.650660395 | XXX | ND | c | C | 0.000 |
| C53 | 2.897181803 | -3.592492895 | -0.116704589 | XXX | ND | c | C | 0.000 |
| C54 | 2.035105988 | -2.942090927 | 0.727385658 | XXX | ND | c | C | 0.000 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C55 | 2.018088815 | -1.523573969 | 0.769309793 | XXX | ND | c | C | 0.000 |
| C56 | 2.862884046 | -0.763565287 | -0.033070199 | XXX | ND | c | C | 0.000 |
| O57 | 1.112847858 | 0.838624789 | -1.651540167 | XXX | ND | o | O | 0.000 |
| O58 | 1.132447240 | -0.968319614 | 1.642939594 | XXX | ND | o | O | 0.000 |
| H59 | 5.977533184 | 3.483069588 | 3.401759229 | XXX | ND | h | H | 0.000 |
| H60 | 4.402104614 | 4.685409480 | 1.908384616 | XXX | ND | h | H | 0.000 |
| H61 | 4.649955690 | -0.291690852 | 1.800168902 | XXX | ND | h | H | 0.000 |
| H62 | 6.092486244 | 0.988315480 | 3.336324356 | XXX | ND | h | H | 0.000 |
| H63 | 1.196103820 | 3.366798956 | -1.394408583 | XXX | ND | h | H | 0.000 |
| H64 | 2.663586307 | 4.648746126 | 0.156754180 | XXX | ND | h | H | 0.000 |
| H65 | 6.207649351 | -0.840777941 | -3.249731438 | XXX | ND | h | H | 0.000 |
| H66 | 4.669106940 | 0.357995715 | -1.741863721 | XXX | ND | h | H | 0.000 |
| H67 | 4.683257963 | -4.624777685 | -1.863489635 | XXX | ND | h | H | 0.000 |
| H68 | 6.224538155 | -3.337940420 | -3.321558783 | XXX | ND | h | H | 0.000 |
| H69 | 2.910123217 | -4.684142247 | -0.147719004 | XXX | ND | h | H | 0.000 |
| H70 | 1.350323298 | -3.485051857 | 1.379198958 | XXX | ND | h | H | 0.000 |
| H71 | 1.230494895 | -0.129099823 | -1.604004988 | XXX | ND | h | H | 0.000 |
| H72 | 1.182981433 | 0.005243150 | 1.592939210 | XXX | ND | h | H | 0.000 |

end

end



*Cartesian coordinates of the heterochiral complex of 1-phenyl-2,2,2-trifluoroethanol* (**2**$_{2het}$)

!BIOSYM archive 3

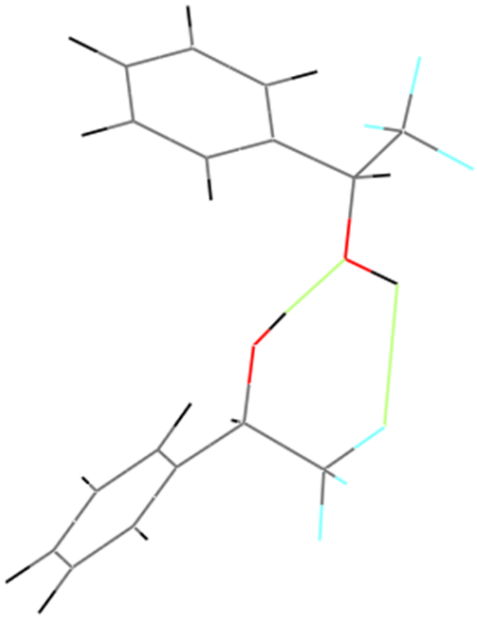
PBC=OFF

Materials Studio Generated CAR File

!DATE Fri May 18 09:55:32 2007

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C1 | 0.564267760 | 0.634676751 | 2.717460695 | XXX | ND | c | C | 0.000 |
| C2 | 1.326154948 | -0.585969528 | 3.271566438 | XXX | ND | c | C | 0.000 |
| O3 | 0.816197053 | 0.748279387 | 1.320565756 | XXX | ND | o | O | 0.000 |
| H4 | 0.981647004 | 1.497738129 | 3.246327996 | XXX | ND | h | H | 0.000 |
| F5 | 1.234189598 | -0.642223028 | 4.612752113 | XXX | ND | f | F | 0.000 |
| F6 | 2.644757460 | -0.482184139 | 2.960876885 | XXX | ND | f | F | 0.000 |
| F7 | 0.889619114 | -1.749908954 | 2.772322443 | XXX | ND | f | F | 0.000 |
| H8 | 1.757231664 | 0.913565878 | 1.174201704 | XXX | ND | h | H | 0.000 |
| C9 | 1.567465998 | 0.666948729 | -2.436232099 | XXX | ND | c | C | 0.000 |
| C10 | 0.090370762 | 0.385099744 | -2.083434686 | XXX | ND | c | C | 0.000 |
| O11 | 0.025284222 | -0.598545550 | -1.077399787 | XXX | ND | o | O | 0.000 |
| F12 | 2.194801266 | -0.383989915 | -2.979323446 | XXX | ND | f | F | 0.000 |
| F13 | 2.265394321 | 1.009113435 | -1.314218485 | XXX | ND | f | F | 0.000 |
| F14 | 1.678757876 | 1.704006129 | -3.291623107 | XXX | ND | f | F | 0.000 |
| H15 | -0.303164325 | 1.345410410 | -1.730278170 | XXX | ND | h | H | 0.000 |
| H16 | 0.298492001 | -0.206576530 | -0.230150162 | XXX | ND | h | H | 0.000 |
| C17 | -0.692498885 | -0.056739980 | -3.302458564 | XXX | ND | c | C | 0.000 |
| C18 | -0.842797098 | -1.412104122 | -3.591237022 | XXX | ND | c | C | 0.000 |
| C19 | -1.549168009 | -1.810060819 | -4.721033044 | XXX | ND | c | C | 0.000 |
| C20 | -2.107992771 | -0.860095755 | -5.571595623 | XXX | ND | c | C | 0.000 |
| C21 | -1.962350282 | 0.493759691 | -5.284226382 | XXX | ND | c | C | 0.000 |
| C22 | -1.259330158 | 0.892468293 | -4.152366966 | XXX | ND | c | C | 0.000 |
| C23 | -0.920459447 | 0.562514734 | 2.988067690 | XXX | ND | c | C | 0.000 |
| C24 | -1.432525528 | 1.180775654 | 4.129017123 | XXX | ND | c | C | 0.000 |
| C25 | -2.789742372 | 1.106105532 | 4.423493470 | XXX | ND | c | C | 0.000 |
| C26 | -3.647917723 | 0.420373906 | 3.570270272 | XXX | ND | c | C | 0.000 |
| C27 | -3.142655403 | -0.190751061 | 2.426554855 | XXX | ND | c | C | 0.000 |
| C28 | -1.784795556 | -0.126201164 | 2.135896564 | XXX | ND | c | C | 0.000 |
| H29 | -0.416403429 | -2.147438277 | -2.922674167 | XXX | ND | h | H | 0.000 |
| H30 | -1.663288264 | -2.866028628 | -4.937152715 | XXX | ND | h | H | 0.000 |
| H31 | -2.658324742 | -1.172949305 | -6.451106040 | XXX | ND | h | H | 0.000 |
| H32 | -2.400120785 | 1.239442084 | -5.936717720 | XXX | ND | h | H | 0.000 |
| H33 | -1.151277378 | 1.948483665 | -3.932085223 | XXX | ND | h | H | 0.000 |
| H34 | -0.768795792 | 1.721111808 | 4.795209300 | XXX | ND | h | H | 0.000 |

H35 -3.175133434 1.587566405 5.314186275 XXX ND h H 0.000
H36 -4.706636821 0.364351293 3.793697684 XXX ND h H 0.000
H37 -3.806889527 -0.722659392 1.757041912 XXX ND h H 0.000
H38 -1.408315365 -0.607446520 1.243530327 XXX ND h H 0.000
end
end



*Cartesian coordinates of the homochiral complex of 1-phenyl-2,2,2-trifluoroethanol* (**2**$_{2hom}$)

!BIOSYM archive 3
PBC=OFF
Materials Studio Generated CAR File
!DATE Fri May 18 09:55:26 2007

C1 1.425346135 -0.881151481 -2.295172169 XXX ND c C 0.000
C2 0.156534953 -0.121992169 -1.852784235 XXX ND c C 0.000
O3 -0.608598229 -0.937564148 -0.995898855 XXX ND o O 0.000
F4 1.161356413 -2.015207011 -2.956650074 XXX ND f F 0.000
F5 2.174429549 -1.225799109 -1.204243048 XXX ND f F 0.000
F6 2.213264461 -0.116295755 -3.074743760 XXX ND f F 0.000
H7 0.527688067 0.771935079 -1.336736259 XXX ND h H 0.000
H8 -0.148736733 -1.036976635 -0.144106596 XXX ND h H 0.000
C9 1.433540102 0.976178888 2.493614782 XXX ND c C 0.000
C10 0.857517137 -0.437983638 2.702971341 XXX ND c C 0.000
O11 0.865761975 -1.132800459 1.460170477 XXX ND o O 0.000

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| F12 | 0.694456908 | 1.726024406 | 1.659298779 | XXX | ND | f | F | 0.000 |
| F13 | 2.677611655 | 0.888261103 | 1.954761789 | XXX | ND | f | F | 0.000 |
| F14 | 1.546718244 | 1.633822699 | 3.659733110 | XXX | ND | f | F | 0.000 |
| H15 | 1.537640818 | -0.921225715 | 3.412006632 | XXX | ND | h | H | 0.000 |
| H16 | 1.774886205 | -1.224985636 | 1.144201235 | XXX | ND | h | H | 0.000 |
| C17 | -3.081763715 | -0.356624955 | 4.429402159 | XXX | ND | c | C | 0.000 |
| C18 | -1.963042237 | -0.536504930 | 5.236058516 | XXX | ND | c | C | 0.000 |
| C19 | -0.695156666 | -0.571881229 | 4.666209541 | XXX | ND | c | C | 0.000 |
| C20 | -0.534186237 | -0.418525798 | 3.289241166 | XXX | ND | c | C | 0.000 |
| C21 | -1.659149798 | -0.234985968 | 2.483487843 | XXX | ND | c | C | 0.000 |
| C22 | -2.926484983 | -0.209527658 | 3.054154728 | XXX | ND | c | C | 0.000 |
| C23 | -1.186361466 | 1.919688440 | -4.767927831 | XXX | ND | c | C | 0.000 |
| C24 | -0.440270926 | 1.533514431 | -3.659462312 | XXX | ND | c | C | 0.000 |
| C25 | -0.673846340 | 0.303778379 | -3.045361683 | XXX | ND | c | C | 0.000 |
| C26 | -1.668578983 | -0.535226989 | -3.547234688 | XXX | ND | c | C | 0.000 |
| C27 | -2.416280717 | -0.146402639 | -4.652957778 | XXX | ND | c | C | 0.000 |
| C28 | -2.175659580 | 1.079068859 | -5.267592951 | XXX | ND | c | C | 0.000 |
| H29 | -4.071322127 | -0.334900672 | 4.869859073 | XXX | ND | h | H | 0.000 |
| H30 | -2.076056803 | -0.656913939 | 6.306655642 | XXX | ND | h | H | 0.000 |
| H31 | 0.173163623 | -0.720206883 | 5.298371358 | XXX | ND | h | H | 0.000 |
| H32 | -1.555036238 | -0.120562587 | 1.412909079 | XXX | ND | h | H | 0.000 |
| H33 | -3.794284291 | -0.073602071 | 2.420394667 | XXX | ND | h | H | 0.000 |
| H34 | -0.997717232 | 2.877956368 | -5.236980694 | XXX | ND | h | H | 0.000 |
| H35 | 0.327152094 | 2.194107785 | -3.271580515 | XXX | ND | h | H | 0.000 |
| H36 | -1.859336459 | -1.481874261 | -3.059671756 | XXX | ND | h | H | 0.000 |
| H37 | -3.189071099 | -0.802530667 | -5.035638461 | XXX | ND | h | H | 0.000 |
| H38 | -2.759713395 | 1.379436131 | -6.129431638 | XXX | ND | h | H | 0.000 |

end

end