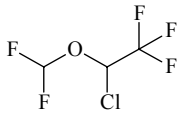
**345** **$C_3H_2ClF_5O$** **2-Chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane** **$C_1$** (*anti-anti*) **$C_1$** (*anti-gauche*$^-$)

ED, *ab initio* and DFT calculations

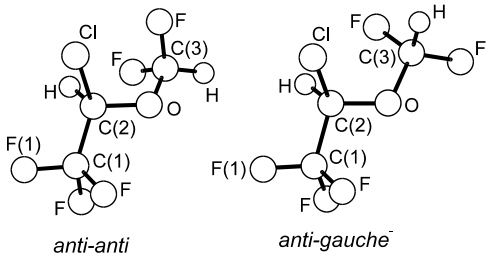


| $r_a$ | Å [a]) |
|---|---|
| O–C(2) | 1.401(15) |
| O–C(3) | 1.372 [b]) |
| C(1)–C(2) | 1.536(11) |
| C(1)–F | 1.332(3) |
| C(3)–F | 1.350 [b]) |
| C(2)–Cl | 1.773(8) |
| C–H (mean) | 1.100 [e]) |

| $\theta_a$ | deg [a]) |
|---|---|
| C(1)–C(2)–O | 108.5(19) |
| C(2)–O–C(3) | 113.4(28) |
| F–C(l)–F | 107.6(7) |
| C(1)–C(2)–Cl | 109.9(7) |
| O–C(2)–Cl | 111.4 [c]) |
| O–C(3)–F | 111.8 [d]) |
| F–C(3)–F | 106.4 [f]) |
| tilt ($CF_3$) [g]) | 1.6 [f]) |
| $\tau_1$ [h]) | –136(5) |
| $\tau_2$ [i]) | 170(9) |
| $\tau_3$ [j]) | –177.2 [e]) |

The molecule was found to exist as a mixture of *anti-anti* and *anti-gauche*$^-$ conformers in the ratio of 83(11):17. These conformers possess near *anti* configuration of the C–C–O–C skeleton and *anti* or *gauche*$^-$ configuration of C–O–C(3)–H unit. Local $C_{3v}$ symmetry was assumed for the $CF_3$ group and $C_{2v}$ for $CHF_2$. The structural parameters of the *anti-gauche*$^-$ conformer were coupled to those of the *anti-anti* conformer using the respective theoretical differences. All angles involving hydrogen atoms were assumed at the calculated values. The structural parameters are listed for the *anti-anti* conformer.

The nozzle was at room temperature.




[a]) Three times the estimated standard errors.
[b]) Differences in the O–C and C–F bond lengths were assumed at the values from MP2/6-311G(2d) calculations.
[c]) Difference between the O–C(2)–Cl and C(1)–C(2)–Cl bond angles was assumed at the value from MP2/6-311G(2d) calculations.
[d]) Difference between the O–C(3)–F and C(2)–C(1)–F (mean) bond angles was assumed.
[e]) Assumed.
[f]) Assumed at the value from MP2/6-311G(2d) calculations.
[g]) Angle between the $C_3$ axis of $CF_3$ group and C(1)–C(2) bond, away from the Cl atom.
[h]) Torsional angle C(1)–C(2)–O–C(3), $\tau_1 = 0°$ for the *syn* position.
[i]) Torsional angle C(2)–O–C(3)–H, $\tau_2 = 0°$ for the *syn* position.
[j]) Torsional angle F(1)–C(1)–C(2)–O, $\tau_3 = 0°$ for the *syn* position.

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