

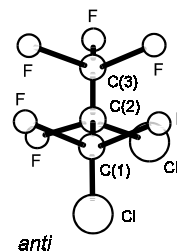
999  $\text{C}_3\text{Cl}_2\text{F}_6$   
ED, *ab initio*  
calculations (HF/6-31G\*)

1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane

$\text{C}_1$  (*gauche+*)  
 $\text{C}_1$  (near *anti*)  
 $\text{F}_2\text{ClC}-\text{CFCl}-\text{CF}_3$

$r_g$	$\text{\AA}^a$		$\theta_\alpha$	$\text{deg}^a$	
	<i>anti</i>	<i>gauche+</i>		<i>anti</i>	<i>gauche+</i>
C–F	1.335(3)	1.335(3)	C(1)–C(2)–F	107.5(6)	107.7(6)
C(1)–C(2)	1.556(15)	1.558(15)	C(2)–C(1)–F	109.2(6)	108.8(6)
C(2)–C(3)	1.555(15)	1.552(15)	C(2)–C(3)–F	110.4(6)	110.5(6)
C(1)–Cl	1.746(28)	1.751(28)	C–C–C	111.9(37)	114.6(37)
C(2)–Cl	1.762(27)	1.762(27)	C(1)–C(2)–Cl	112.1(6)	109.8(6)
			C(2)–C(1)–Cl	113.6(6)	114.9(6)
			Cl–C–F	111.1(22)	111.1(22)
			$\phi_1^b$	–4.8(33)	98.0(81)
			$\phi_2^c$	–0.9 <sup>d</sup>	0.9 <sup>d</sup>

The compound existed as a mixture of a more stable *anti* form (with the C(1)–Cl bond *anti* to the C(2)–C(3) bond) and a less stable *gauche+* form ( $\Delta E = 0.5(4)$  kcal/mol). The mole fraction of the *anti* conformer was found to be 0.67(13). Local  $\text{C}_{3v}$  symmetry was assumed for the  $\text{CF}_3$  group. The differences between corresponding parameters ( $r_\alpha$ ,  $\theta_\alpha$ ) and conformational variations within these parameters were fixed at the *ab initio* values. The nozzle temperature was 23 °C.

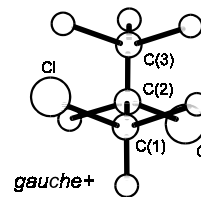


<sup>a</sup>) Twice the estimated standard errors including a systematic error.

<sup>b</sup>) Dihedral angle Cl–C(1)–C(2)–C(3), positive values for clockwise rotation from the exact *anti* position looking from C(1) to C(2).

<sup>c</sup>) Dihedral angle F–C(3)–C(2)–C(1), positive values for clockwise rotation from the exact *anti* position looking from C(2) to C(3).

<sup>d</sup>) Fixed at the *ab initio* value.



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