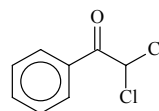


822 C₈H₆Cl₂OED, *ab initio*
calculations**2,2-Dichloro-1-phenylethanone**

2,2-Dichloroacetophenone

Dichloromethyl phenyl ketone

C_s (conformer I)**C₁** (conformer II)

r_a	\AA^a		θ_a	deg^a	
	both conformers			both conformers	
C(1)–C(2,6)	1.409(2)		C–C–H (ring)	120.0 ^b	
C(2)–C(3) =	1.399(2)			conformer I	conformer II
C(5)–C(6)			C(2)–C(1)–C(1')	116.8(7)	117.1 ^c
C(3,5)–C(4)	1.402(2)		O=C(1')–C(1)	120.1(7)	120.1 ^d
C–H (ring)	1.099(6)		C(1)–C(1')–C(2')	120.7(5)	115.8 ^c
C(2')–H	1.087 ^b		C–C–Cl(1)	112.2(2)	111.8 ^c
	conformer I	conformer II	C–C–Cl(2)	112.2(2)	108.5 ^c
C=O	1.206(3)	1.200 ^c	H–C(2')–Cl	107.1(5)	107.1 ^c
C(1)–C(1')	1.494(6)	1.500 ^c	H–C(2')–C(1')	106.2 ^c	111.5 ^c
C(1')–C(2')	1.548(5)	1.549 ^c	Cl–C–Cl ^f	111.6(3)	110.7
C–Cl(1)	1.778(3)	1.763 ^c	C(2')–C(1')=O ^f	119.2(9)	124.1
C–Cl(2)	1.778(3)	1.784 ^c	C(2)–C(1)–C(6)	119.1 ^c	119.2 ^c
			C(1)–C(2)–C(3)	120.5 ^c	120.4 ^c
			C(5)–C(6)–C(1)	120.2 ^c	120.3 ^c
			C(2)–C(3)–C(4)	119.8 ^c	119.9 ^c
			C(4)–C(5)–C(6)	120.1 ^c	120.0 ^c
			C(3)–C(4)–C(5)	120.1 ^c	120.1 ^c
			τ^g	0 ^c	130.2(40)

The molecule exists as a mixture of two conformers with C_s and C₁ symmetry in the ratio of 65(6):35. The energy difference was estimated to be 6.3 kJ mol^{−1}. The fragment C(O)C–phenyl was assumed to be planar.

The nozzle temperature was 170 ... 175 °C.

^a) Twice the estimated standard errors.

^b) Assumed.

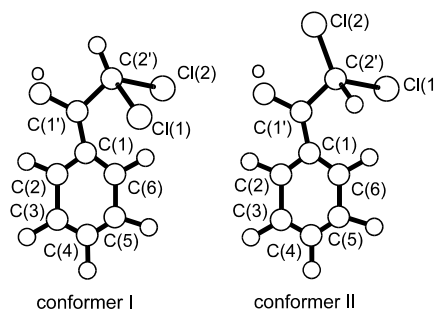
^c) Differences between parameters of the conformers were assumed at the values from HF/6-31G* calculations.

^d) Assumed to be equal for both conformers.

^e) Assumed at the value from HF/6-31G* calculations.

^f) Dependent parameter.

^g) Torsional angle H–C(2')–C(1')=O; 0° for the *syn* position.



Naumov, V.A., Hagen, K.: Zh. Obshch. Khim. **68** (1998) 1847; Russ. J. Gen. Chem. (Engl. Transl.) **68** (1998) 1768.

See also: Naumov, V.A., Hagen, K.: Zh. Org. Khim. **35** No.3 (1999) 356; Russ. J. Org. Chem. (Engl. Transl.) **35** (1999) 331.