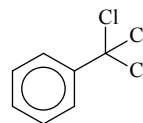


777  
ED $\text{C}_7\text{H}_5\text{Cl}_3$ **(Trichloromethyl)benzene** $\text{C}_s$  $\alpha, \alpha, \alpha$ -Trichlorotoluene

Benzylidene trichloride



$r_g$	$\text{\AA}^a$	$\theta^b$	$\text{deg}^a$
C–C (ring)	1.399(1)	C(2)–C(1)–C(6)	119.4(7)
C–H	1.096(6)	C(1)–C(2)–C(3)	119.9(7)
C(1)–C(7)	1.531(5)	C(2)–C(3)–H	119.7 <sup>c)</sup>
C–Cl	1.784(2)	C(1)–C(2)–H	120.1 <sup>c)</sup>
		tilt(CCl <sub>3</sub> ) <sup>d)</sup>	4.6(14)

Local  $\text{C}_{2v}$  symmetry for the phenyl ring and local  $\text{C}_{3v}$  symmetry for the  $\text{CCl}_3$  group were assumed. The rotational barrier height of the  $\text{CCl}_3$  group,  $V_6$ , was determined to be  $1.3(6) \text{ kJ mol}^{-1}$ , and the potential minimum of the barrier was found at the position where the C(7)–Cl(1) bond lies on the phenyl plane.

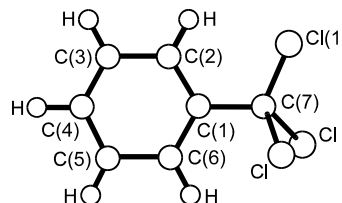
The sample was vaporized at 323 K.

<sup>a)</sup> 2.6 times the estimated standard errors including a systematic error.

<sup>b)</sup> Unidentified, possibly  $\theta_\alpha$ .

<sup>c)</sup> Assumed at the values from semiempirical PM3 molecular orbital calculations.

<sup>d)</sup> Tilt angle of the  $\text{CCl}_3$  group between the  $\text{C}_3$  axis and the C(1)–C(7) bond direction. The angle is positive when the C(7)–Cl(1) bond tilts away from C(2)–H.



Matsuyoshi, T., Iijima, K.: J. Mol. Struct. **378** (1996) 199.