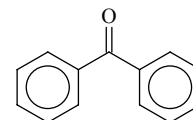
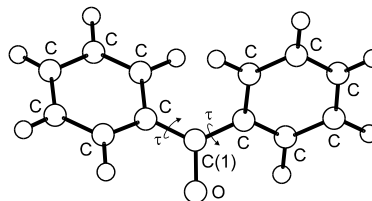


917
MW $C_{13}H_{10}O$ **Benzophenone**
Diphenylmethanone C_2

r_0	$\text{\AA}^a)$	θ_0	$\text{deg}^a)$
C(1)–C	1.4757(100)	C–C(1)–C	122.44(100)



The molecule exhibits C_2 symmetry, with two phenyl groups tilted by 31.74° . The lowest torsional frequency is estimated to be 17 cm^{-1} . The phenyl group bond lengths were obtained by scaling those based on STO/3-21G calculations with known empirical corrections, and the torsional angle τ , the C–C(1)–C angle, and the C–C(1) bond length were refined to reproduce the observed rotational constants.



^{a)} Uncertainties were not estimated in the original paper.

Maris, A., Melandri, S., Caminati, W., Favero, P.G.: Chem. Phys. Lett. **256** (1996) 509.