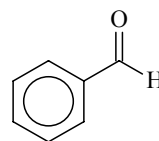
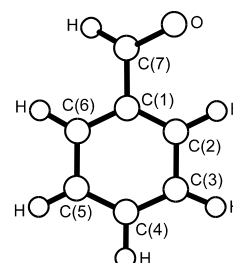


**786**      **C<sub>7</sub>H<sub>6</sub>O****Benzaldehyde**essentially C<sub>s</sub>ED, *ab initio*  
calculations

$r_g$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C–C (mean) <sup>b)</sup>	1.397(3)	C(2)–C(1)–C(6)	119.9(10)
C(1)–C(2) <sup>c)</sup>	1.400(7)	C(1)–C(2)–C(3)	120.2(14)
C–H (ring) <sup>b)</sup>	1.095(5)	C(2)–C(3)–C(4)	119.5(9)
C(1)–C(7)	1.479(4)	C(3)–C(4)–C(5)	120.7(7)
C(7)=O	1.212(3)	C(2)–C(1)–C(7)	120.9(6)
C(7)–H <sup>c)</sup>	1.12(3)	C(6)–C(1)–C(7)	119.2(6)
		C(1)–C(7)=O	123.6(4)
		C(1)–C(7)–H	115.1(16)
		O=C–H	121.2(15)
		$\tau^d)$	7(10)

Local C<sub>2v</sub> symmetry was assumed for the benzene ring. The barrier height to torsion of the formyl group around the C(1)–C(7) bond was estimated to be at least 20 kJ mol<sup>–1</sup> using a dynamic model with two-fold potential function within the Monte Carlo optimization scheme. All C–H bonds in the ring were assumed to be equal and directed along the bisectors of the respective C–C–C angles. The nozzle was at 62...66 °C.

<sup>a)</sup> Estimated total errors.<sup>b)</sup> In the benzene ring.<sup>c)</sup> Differences among the C–C bond lengths in the ring, 0.006 Å maximum, and that between C(7)–H and C–H (ring) were assumed at the values from MP2(fc)/6-31G\* calculations.<sup>d)</sup> Torsional angle around C(1)–C(7) bond, C(2)–C(1)–C(7)=O;  $\tau = 0^\circ$  for the *syn* position.Borisenko, K.B., Bock, C.W., Hargittai, I.: J. Phys. Chem. **100** (1996) 7426.