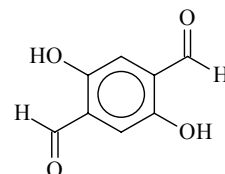


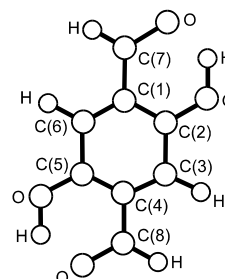
823 **C₈H₆O₄**ED, *ab initio*
calculations**2,5-Dihydroxy-1,4-benzenedicarboxaldehyde**

2,5-Dihydroxyterephthalaldehyde

C_{2h} assumed

r_g	Å ^{a)}	θ_a	deg ^{a)}
C–C (mean)	1.407(4) ^{b)}	C(6)–C(1)–C(2)	121.2(7)
C(1)–C(2)	1.422(6)	C(1)–C(2)–C(3)	119.3(3)
C(2)–C(3)	1.396(9)	C(2)–C(3)–C(4)	119.5(10)
C(3)–C(4)	1.405(5)	C(2)–C(1)–C(7)	120.5(3)
C(1)–C(7)	1.469(5)	C(1)–C(7)=O	124.6(6)
C–H (mean)	1.12(2) ^{b)}	C(1)–C(7)–H	116.0(10)
C(7)–H	1.13(2)	C(1)–C(2)–O	121.8(4)
C(7)=O	1.231(3)	C(2)–O–H	102.2(10)
C(2)–O	1.371(6)	$\tau^c)$	0 ^{d)}
O–H	0.983(9)		
O...H	1.76(1)		
O...O	2.667(8)		

There is considerable intramolecular hydrogen bonding in this molecule. The torsional motion of the formyl groups was described in terms of the potential function with coefficients assumed at the HF/6-31G* values. The nozzle was at 152 °C.

^{a)} Estimated total errors.^{b)} In the ring.^{c)} C(1)–C(2)–O–H torsional angle, $\tau = 0^\circ$ for the *syn* position.^{d)} Assumed at the value from MP2(fc)/6-31G* calculations.Borisenko, K.B., Zauer, K., Hargittai, I.: J. Phys. Chem. **100** (1996) 19303.