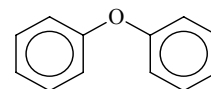


906 **C₁₂H₁₀O**ED,
DFT calculations**1,1'-Oxybisbenzene**

Diphenyl ether

C₁

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)–C(2)	1.396(3)	C–O–C	123.2(13)
C(2)–C(3)	1.395 ^{b)}	C(2)–C(1)–O	120.5 ^{c)}
C(3)–C(4)	1.402 ^{b)}	C(6)–C(1)–O	118.9 ^{c)}
C(4)–C(5)	1.404 ^{b)}	C(1)–C(2)–C(3)	119.5 ^{d)}
C(5)–C(6)	1.397 ^{b)}	C(2)–C(3)–C(4)	120.5 ^{d)}
C(6)–C(1)	1.395 ^{b)}	C(3)–C(4)–C(5)	119.5 ^{d)}
C–C (mean)	1.396(3)	τ_1 ^{e)}	64.0(73)
C–O	1.382(14)	τ_2 ^{f)}	32.0 ^{c)}
C–H	1.104(16)		

The experimental data from [1] were reanalyzed. The corresponding parameters of two rings were assumed to be equal.

The nozzle temperature was 90...100 °C.

^{a)} Three times the estimated standard errors.

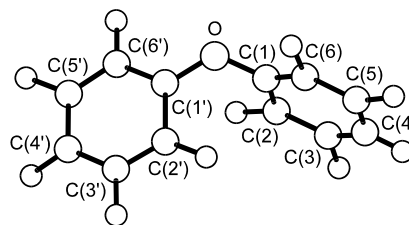
^{b)} Differences between the C–C bond lengths were probably assumed at the values from B3LYP/6-31G(d) calculations.

^{c)} Uncertainties were not given in the original paper.

^{d)} Assumed at the value from B3LYP/6-31G(d) calculations.

^{e)} Torsional angle C(2)–C(1)–O–C(1'), $\tau_1 = 0^\circ$ from the *syn* position.

^{f)} Torsional angle C(2')–C(1')–O–C(1), $\tau_2 = 0^\circ$ from the *syn* position.



Naumov, V.A., Ziatdinova, R.N., Naumov, A.V., Hagen, K.: Zh. Obshch. Khim. **70** No.2 (2000) 294; Russ. J. Gen. Chem. (Engl. Transl.) **70** (2000) 273.

[1] Naumov, V.A., Ziatdinova, R.N.: Zh. Strukt. Khim. **25** No.1 (1984) 88; J. Struct. Chem. (Engl. Transl.) **25** (1984) 77.

Replaces [II/25D \(3, 2803\)](#)