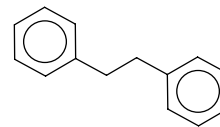


923 **C₁₄H₁₄**ED, *ab initio*
calculations**1,1'-(1,2-Ethanediy1)bisbenzene**

1,2-Diphenylethane

C₂ (*ap*)**C₂ (*sc*)**

r_g	Å ^{a)}	θ_α	deg ^{a)}
C–H ^{b)}	1.085(7)	C(2)–C(1)–C(ring)	114.7(18)
C–C (ring) ^{b)}	1.401(2)	$\varphi^c)$	67(6)
C(1')–C(2')	1.404 ^{d)}	$\tau_{ap})^e)$	165(9)
C(2')–C(3')	1.399 ^{d)}	$\tau_{sc})^f)$	61(16)
C(1)–C(ring)	1.519(9)		
C(1)–C(2)	1.549(29)		



The molecule exists predominantly as the *antiperiplanar* (*ap*) conformer (85(25)%). The presence of *synclinal* (*sc*) conformer (15(25)%) could not be excluded. The two conformers were assumed to have identical structural parameters except for τ . The nozzle was at 373 K.

^{a)} Twice the estimated standard errors.

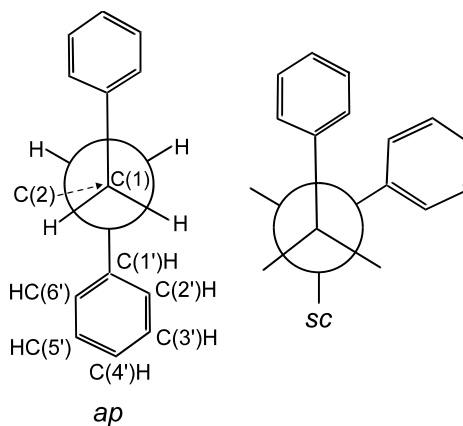
^{b)} Average value. Differences
[C(2')–H] – [C(3')–H] = 0.0011 Å
and [C(3')–H] – [C(4')–H] = 0.0003 Å
were assumed according to HF/6-31G*
calculations.

^{c)} C(1)–C(2)–C(1')–C(2') torsional angle.

^{d)} Difference between the C(1')–C(2') and
C(2')–C(3') bond lengths was assumed
at the value from HF/6-31G* calculations.
The C(2')–C(3') and C(3')–C(4') bond
lengths were assumed to be equal.

^{e)} C(ring)–C(2)–C(1)–C(ring) torsional angle
for the *ap* conformer.

^{f)} C(ring)–C(2)–C(1)–C(ring) torsional angle
for the *sc* conformer.



Shen, Q.: J. Mol. Struct. **471** (1998) 57.