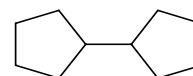


**890**      **C<sub>10</sub>H<sub>18</sub>**  
ED, MM3 and *ab initio*  
calculations

**1,1'-Bicyclopentyl**  
1,1'-Bicyclopentane

**C<sub>2h</sub> (ee-*anti*)**

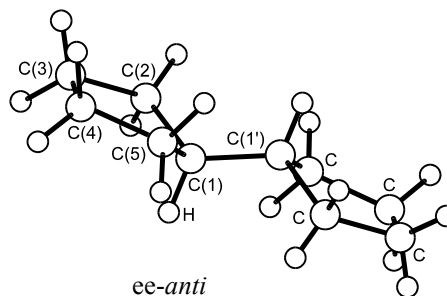


$r^a$	Å <sup>b</sup>	$\theta^a$	deg <sup>b</sup>
C–C (mean)	1.541(4)	C(2)–C(1)–C(5)	103.7(3)
C(1)–C(1')	1.545(10)	C(1)–C(2)–C(3)	107.9(5)
C–H (mean)	1.121(12)	C(2)–C(1)–C(1')	113.3(3)
		C–C–H (mean)	112.7(10)
		H–C–H (mean)	106.3(8)

The molecule exists as a mixture of equatorial-equatorial-*anti* (ee-*anti*), equatorial-axial-*anti* (ea-*anti*) and equatorial-equatorial-*gauche* (ee-*gauche*) conformers. The amount of the major conformer (ee-*anti*) was estimated to be 50(30)% by ED and 90.3% from HF/6-31G\* calculations. The ea-*anti* and ee-*gauche* conformers were estimated to be in nearly equal amounts. Only the torsional angle about the C(1)–C(1') bond was varied from one conformer to another, while all other geometric parameters were assumed to be equal in the ED analysis. The measurements were made at room temperature.

<sup>a</sup>) Unidentified, possibly  $r_a$  and  $\theta_a$ .

<sup>b</sup>) Uncertainties were unidentified, possibly estimated total errors.



Shishkov, I.F., Mastryukov, V.S., Chen, K., Allinger, N.L., Gundersen, S., Samdal, S., Volden, H.V.: J. Mol. Struct. **376** (1996) 133.