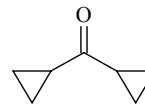


807 **C₇H₁₀O**
ED, *ab initio*
calculations

Dicyclopropyl ketone
Dicyclopropylmethanone

C_{2v} assumed (*syn-syn*)
C_s assumed (*syn-anti*)

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)=O	1.221(1)	O=C(1)–C(1')	121.59(13)
C(1)–C(1')	1.502(3)	C(1)–C(1')...D	121.33(22)
C(1')–C(2')	1.519(1)	H–C(ring)–H	111.4(13)
C(2')–C(3')	1.488 ^{b)}	C(1)–C(1')–H	115.8(28)
C(ring)–H	1.087(2)	τ^c	0.0



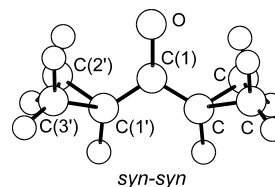
A mixture of *syn-syn* and *syn-anti* conformers was predicted by MP2/6-31G* calculations, and their populations were estimated by ED analysis to be 93(3) and 7%, respectively. The *syn-anti* conformer was described by the same parameters as those for the *syn-syn* conformer, except for two different C(1)–C(1')...D angles, where D is a dummy atom on the bisector of the C(2')–C(1')–C(3') angle, with the difference of 5° estimated by *ab initio* calculations and the torsional angle τ .

The nozzle temperature was 360 K.

^{a)} Estimated standard errors.

^{b)} Difference between the C(1')–C(2') and C(2')–C(3') bonds was assumed at the value from MP2/6-31G* calculations.

^{c)} Torsional angle C(2)=C(1)–C(1')...D, $\tau = 0^\circ$ for the *syn* position.



Traetteberg, M., Bakken, P., Quesada, J.V., Mastryukov, V.S., Boggs, J.E.: J. Mol. Struct. **485-486** (1999) 73.