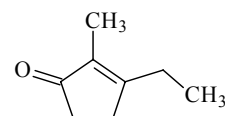


850 **C₈H₁₂O**ED, *ab initio*
calculations**3-Ethyl-2-methyl-2-cyclopenten-1-one****C₁** assumed (*gauche*)

r_a	Å ^a)	θ_a	deg ^a)
C(2)=C(3)	1.371(2)	C(5)–C(1)–C(2)	108.3(2)
C=O	1.240(2)	C(1)–C(2)=C(3)	109.0(4)
C(1)–C(2)	1.475(6)	C(2)=C(3)–C(4)	112.0(3)
C(3)–C(4)	1.530(3)	C(3)–C(4)–C(5)	104.8(3)
C(4)–C(5)	1.527(3)	C(4)–C(5)–C(1)	105.9(3)
C(1)–C(5)	1.533(3)	C(2)–C(1)=O	124.2(5)
C(2)–C(8)	1.491(2)	C(3)=C(2)–C(8)	129.8(6)
C(3)–C(6)	1.496(2)	C(2)=C(3)–C(6)	126.2(5)
C(6)–C(7)	1.559(9)	C(3)–C(6)–C(7)	111.6(6)
C(sp ³)–H	1.113(2)	τ^b	102.5 ^c)



Five-membered ring was found to be planar. A *skew (gauche)* orientation was assumed for the ethyl group relative to the ring. Differences between the C–C bond lengths and the valence and dihedral angles involving H atoms were constrained to the values from MP2/6-31G* calculations.

The temperature of the measurements was 26 °C.

^a) Estimated standard errors.

^b) C(2)=C(3)–C(6)–C(7) torsional angle
from the *syn* position.

^c) Assumed.

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Rogers, D.W.: J. Chem. Soc., Perkin Trans. 2 (1997) 1925.

