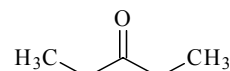


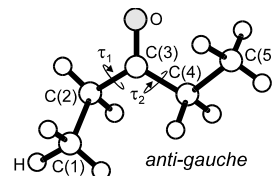
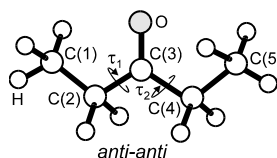
663 **C₅H₁₀O**
ED, *ab initio* calculations,
vibrational spectroscopy

3-Pentanone
Diethyl ketone

C_{2v} (*anti-anti*)
C₁ (*anti-gauche*)



r_g	$\text{\AA}^a)$	
	<i>anti-anti</i>	<i>anti-gauche</i>
C(1)–C(2)	1.524(1) ^{b)}	1.534(1)
C(2)–C(3)	1.519(1) ^{b)}	1.519(1)
C(3)–C(4)	1.519(1)	1.520(1)
C(4)–C(5)	1.524(1)	1.525(1)
C=O	1.217(2)	1.218(2)
C–H ^{c)}	1.103(3)	1.103(3)



θ_a	$\text{deg}^a)$	
	<i>anti-anti</i>	<i>anti-gauche</i>
C(1)–C(2)–C(3)	114.2(6)	114.2(6)
C(2)–C(3)–C(4)	116.0(6)	117.4(6)
C(3)–C(4)–C(5)	114.2(6)	113.9(6)
C(3)–C–H ^{c)}	108.2(7)	108.2(7)
C(2,4)–C–H ^{c)}	111.4(7)	111.6(7)
$\tau_1^d)$	180 ^{e)}	61(7)
$\tau_2^f)$	180 ^{e)}	151(14)

The molecule was found to exist as a mixture of two conformers, *anti-anti* (50(10)%) and *anti-gauche*, the former being more stable. The free energy difference ΔG° at room temperature, estimated to be 0.8(2) kcal mol^{−1}, was consistent with that estimated from vibrational spectroscopy. The structural differences between these conformers were taken from RHF/6-31G* calculations except for the dihedral angles. The measurements were made at *ca.* 27 °C.

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

^{b)} Difference between the C(2)–C(3) and C(1)–C(2) bond lengths was assumed at the RHF/6-31G* value.

^{c)} Average values.

^{d)} C(4)–C(3)–C(2)–C(1) torsional angle, $\tau_1 = 0^\circ$ for the *syn* position.

^{e)} Assumed.

^{f)} C(2)–C(3)–C(4)–C(5) torsional angle, $\tau_2 = 0^\circ$ for the *syn* position.

Kuze, N., Kojima, E., Fujiwara, H., Takeuchi, H., Egawa, T., Konaka, S.: J. Mol. Struct. **375** (1996) 231.