

1749 **C₄H₈O₂**
ED, *ab initio* calculations
(HF/4-21G)

Ethyl acetate

C_s (*trans*)
C₁ (*gauche*)
H₃C–C(O)–O–CH₂–CH₃

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(3)–H(7)	1.105(3)	O(2)–C(1)–C(3)	124.1(10)
C(1)=O(2)	1.203(2)	O(2)=C(1)–O(4)	124.0(3)
C(1)–C(3)	1.508(2)	C(3)–C(1)–O(4) ^{b)}	111.9
C(1)–O(4)	1.345(3)	C(1)–O(4)–C(5)	115.7(5)
O(4)–C(5)	1.448(3)	O(4)–C(5)–C(6)	108.2(11)
C(5)–C(6)	1.515(2) ^{g)}	C(1)–C(3)–H	107.7(13)
		H–C(5)–H ^{b)}	108.1
		O(4)–C(5)–H ^{b)}	108.3
		C(5)–C(6)–H	108.1(13)
		ϕ_1 ^{c)}	0° ^{e)}
		ϕ_2 ^{d)}	0° ^{e)}
		ϕ_3 ^{f)}	180° ^{e)}
		ϕ_4 ^{g)}	180° ^{e)}

Two stable conformers, *trans* and *gauche*, with ϕ_3 of 180° and 79°, respectively, were observed; the fraction of the *trans* conformer was estimated to be 38(7)%. With the aid of *ab initio* calculations [1], the potential function for the torsional motion of the ethyl group, $V(\phi_3) = 1/2[V_1(1 + \cos \phi_3) + V_2(1 - \cos 2\phi_3) + (h - V_1)(1 + \cos 3\phi_3)]$ was estimated to be (in units of kcal mol^{–1}) $V_1 = 3.5(4)$ and $V_2 = -2.7(3)$, where h was assumed to be 5.7.

The parameters for the *trans* conformer are listed.

The nozzle was at room temperature.

^{a)} Estimated limits of error.

^{b)} Dependent parameter.

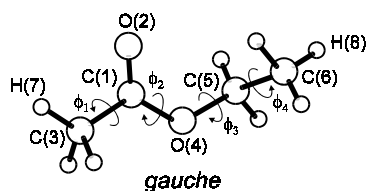
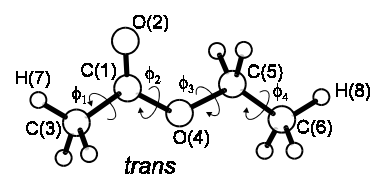
^{c)} Dihedral angle H(7)–C(3)–C(1)=O(2).

^{d)} Dihedral angle O(2)=C(1)–O(4)–C(5).

^{e)} Assumed.

^{f)} Dihedral angle C(1)–O(4)–C(5)–C(6).

^{g)} Dihedral angle O(4)–C(5)–C(6)–H(8).



Sugino, M., Takeuchi, H., Egawa, T., Konaka, S.: J. Mol. Struct. **245** (1991) 357.

[1] Manning, J., Klimkowski, V.J., Siam, K., Ewbank, J.D., Schäfer, L.: J. Mol. Struct. (Theochem) **139** (1986) 305.