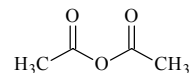


543 **C₄H₆O₃**ED, *ab initio* and
DFT calculations**Acetic anhydride****C₁ (*sp-ac*)**
C₂ assumed (*sp-sp*)

r_g	\AA^a		θ_α	deg^a	
	<i>sp-ac</i>	<i>sp-sp</i>		<i>sp-ac</i>	<i>sp-sp</i>
O(1)–C(1)	1.406(6)	1.370(15)	C(1)–O(1)–C(1')	121.0(15)	116.5(20)
O(1)–C(1')	1.370(13)	1.370(15)	O(1)–C(1)=O(2)	124.2(18)	124.8(20)
C(1)=O(2)	1.182(3)	1.182(3)	O(1)–C(1)–C(2)	111.1(22)	114.6(23)
C(1')=O(2')	1.194(3) ^b	1.182(3) ^b	O(1)–C(1')=O(2')	117.1(10)	124.8(20)
C–C ^c	1.489(2)	1.489(2)	O(1)–C(1')–C(2')	110.9(17)	114.6(23)
C–H ^c	1.099(4)	1.099(4)	τ_1^d	–27.4(53)	30.9(67)
			τ_2^e	122.0(39)	30.9(67)

Molecular structure from [1] was reinvestigated. It was found that the molecule exists as a mixture of *sp-ac* (63(15)%) and *sp-sp* (37(15)%) conformers at the nozzle temperature of 70 °C. Local C_{3v} symmetry was assumed for the CH₃ group and C_s for C–C(O)–O. The large-amplitude motions around the O–C bonds were described by the method of pseudoconformers.

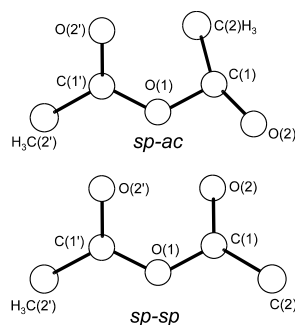
^a) Estimated standard errors.

^b) Difference between the C(1')=O(2') bond lengths of *sp-ac* and *sp-sp* conformers was assumed at the value from MP2/6-31G** calculations.

^c) Average value.

^d) Torsional angle O(2')=C(1')–O(1)–C(1),
 $\tau_1 = 0^\circ$ for the *syn* position.

^e) Torsional angle O(2)=C(1)–O(1)–C(1'),
 $\tau_2 = 0^\circ$ for the *syn* position.



Wu, G., Van Alsenoy, C., Geise, H.J., Sluyts, E., Van der Veken, B.J., Shishkov, I.F.,
Khristenko, L.V.: J. Phys. Chem. A **104** (2000) 1576.

[1] Vledder, H.J., Mijlhoff, F.C., Leyte, J.C., Romers, C.: J. Mol. Struct. **7** (1971) 421.

Replaces [II/25C \(3, 1669\)](#)