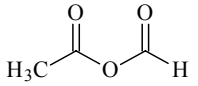
375 **$C_3H_4O_3$** **Acetic formic anhydride** **C_s** (*sp-ap*)

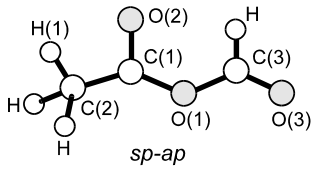
ED, IR, *ab initio* calculations



r_g	Å [a])
C(1)=O(2)	1.195(8)
C(3)=O(3)	1.187(8)
C(1)–O(1)	1.380(8)
C(3)–O(1)	1.380(8)
C(1)–C(2)	1.500(8)
C(3)–H	1.082(15)
C(2)–H [b])	1.069(15)

θ_α^0	deg [a])
C(1)–O(1)–C(3)	119.8(5)
O(2)=C(1)–O(1)	122.4(5)
O(2)=C(1)–C(2)	127.4(5)
O(1)–C(1)–C(2)	110.2(5)
O(3)=C(3)–O(1)	121.7(5)
O(3)=C(3)–H	120.4(10)
O(1)–C(3)–H	117.9(10)
C(1)–C(2)–H [b])	109.1(10)
O(2)=C(1)–O(1)–C(3)	0.0(5)
O(3)=C(3)–O(1)–C(1)	180.0(5)
H(1)–C(2)–C(1)–O(1)	180.0(10)

The molecule exists as a *sp-ap* conformer (planar skeleton). Best results were obtained using geometrical constraints derived from HF/4-21G calculations.
The measurements were made at 300 K.



sp-ap

[a]) Estimated total errors.
[b]) Mean value.

Wu, G., Shlykov, S., Van Alsenoy, C., Geise, H.J., Sluyts, E., Van der Veken, B.J.:
J. Phys. Chem. **100** (1996) 11620.

Replaces II/25C (**3**, 1169)