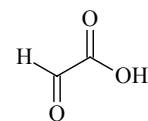


**226**      **C<sub>2</sub>H<sub>2</sub>O<sub>3</sub>**MW, *ab initio* calculations  
(CCSD(T)/cc-pVQZ *etc.*)**Glyoxylic acid**

Oxoacetic acid

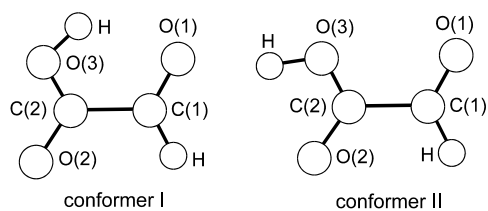
**C<sub>s</sub>** (conformer I)**C<sub>s</sub>** (conformer II)

$r_e^a)$	$\text{\AA}^b)$	$\theta_e^a)$	$\text{deg}^b)$
C–C	1.5256(50)	C–C–H	115.41(50)
C–H	1.0963(50)	C(2)–C(1)=O(1)	120.66(50)
C(1)=O(1)	1.2087(50)	C(1)–C(2)=O(2)	121.90(50)
C(2)=O(2)	1.1977(50)	C(1)–C(2)–O(3)	113.35(50)
C(2)–O(3)	1.3317(50)	O(2)=C(2)–O(3)	124.75(50)
O–H	0.9697(50)	C–C–H	106.74(50)

The energy difference between the two low-energy *anti* conformers, I and II, is 5.0(2) kJ mol<sup>−1</sup>.

<sup>a)</sup> Equilibrium structural parameters for the most stable conformer I estimated by combining the observed data with results of *ab initio* calculations.

<sup>b)</sup> Uncertainties were not estimated in the original paper.



Bakri, B., Demaison, J., Margulès, L., Møllendal, H.: J. Mol. Spectrosc. **208** (2001) 92.