

1660  
ED

**C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>**

**2,3-Butanedione**

Biacetyl

Dimethylglyoxal

**C<sub>2h</sub> (s-*trans*)**

H<sub>3</sub>C–C(O)–C(O)–CH<sub>3</sub>

$r_{\alpha}$	Å <sup>a)</sup>	$\theta_{\alpha}$	deg <sup>a)</sup>
C=O	1.210(2)	C–C=O	119.5(6)
C–C (average)	1.520(2)	C–C–C	116.6(2)
$\Delta(\text{C–C})$ <sup>b)</sup>	–0.015(21)	C–C–H	109.6(12)
C–H	1.057(4)	$\tau$ <sup>c)</sup>	180.0 <sup>d)</sup>
		$\delta$ <sup>e)</sup>	24.1(34)

There is no evidence for the presence of any but the *trans* conformer.  
The nozzle temperatures were 228 and 525 °C. The parameters are given for 228 °C.

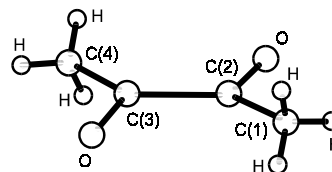
<sup>a)</sup> Twice the estimated standard errors.

<sup>b)</sup>  $\Delta(\text{C–C}) = [\text{C}(3)\text{–C}(4)] - [\text{C}(2)\text{–C}(3)]$ .

<sup>c)</sup> Dihedral angle C–C–C–H.

<sup>d)</sup> Assumed.

<sup>e)</sup> Root-mean-square amplitude of the torsional vibration.



Danielson, D.D., Hedberg, K.: J. Am. Chem. Soc. **101** (1979) 3730.

See also: Hagen, K., Hedberg, K.: J. Am. Chem. Soc. **95** (1973) 8266.