

Structure Data of Free Polyatomic Molecules

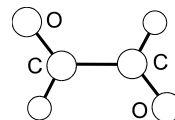
225 **C₂H₂O₂**
 IR, *ab initio* calculations
 (CCSD(T)/cc-pVTZ)

Glyoxal
 Ethanedial

C_{2h} (*anti*)



r_e	\AA^a	θ_e	deg^a
C–C	1.51453(38)	C–C–H	115.251(24)
C–H	1.10071(26)	O=C–H	123.472(19)
C=O	1.20450(27)		



^a) Estimated standard errors.

Wugt Larsen, R., Pawlowski, F., Hegelund, F., Jørgensen, P., Gauss, J., Nelander, B.: Phys. Chem. Chem. Phys. **5** (2003) 5031.

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