

structure (solids and liquids)

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The Structure of Carbon Suboxide, C_3O_2 , in the Solid State. —

The title compound is prepared by heating a solid mixture of $CH_2(COOH)_2$ and P_2O_5 in vacuum to 160 °C. C_3O_2 is characterized by IR and Raman spectroscopy and by single crystal XRD (orthorhombic, space group Pnma, $Z = 8$). The crystal contains two linear, crystallographically different $O=C=C=O$ molecules in the asymmetric unit. Some systematic deviations from linearity are found by inspection of the vibrational amplitudes. Results of ab initio calculations are given. — (ELLERN, ARKADY; DREWS, THOMAS; SEPPELT, KONRAD; Z. Anorg. Allg. Chem. 627 (2001) 1, 73-76; Inst. Chem., FU Berlin, D-14195 Berlin, Germany; EN)