The Crystal Structure of Dimethyl (2Z, 6Z)-2,7-bis-(benzyloxycarbonyl-amino)octa-2,6-diendioate: A Useful Precursor for Optically Pure 2,7-Diaminosuberic Acid

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Needle shaped single crystals of the dimethyl ester of (2Z, 6Z)-2,7-bis-(benzyloxycarbonyl-amino)-octa-2,6-diendioic acid (**1**), $C_{26}H_{28}N_2O_8$ were obtained by very slow cooling from methanol/ethylacetate solution 20:1. **1** crystallizes in the anorthic space group P$\bar{1}$ (No.2) with a = 4.813(5), b = 12.277(6), c = 12.340(7) Å, α =117.15(3)°, β = 97.52(4)°, γ = 92.02(4)°, Z =1. The crystal structure was determined from diffractometer data (MoKα-radiation). It was solved by direct methods and refined to a conventional R of 0.054 for 1452 Fo's and 178 refined parameters. The molecule is characterized by the presence of an inversion center. In the crystal structure the molecules are stacked along the crystallographic a-axis. In this direction - which coincides with the needle axis of the crystals - each molecule is connected with its neighbors through almost linear N-H···O-hydrogen bonds.

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