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(*S*)-*N*-Nitrosoazetidine-2-carboxylic acid

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.100
Data-to-parameter ratio = 7.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure determination of the title compound, $C_4H_6N_2O_3$, reveals that the *N*-nitrosamine moiety adopts the *E* conformation. The azetidine N atom is slightly pyramidalized, as evidenced by its displacement from the plane containing the three attached atoms by 0.038 (2) Å.

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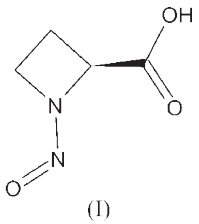
Comment

N-Nitrosamines are of widespread interest due to their strong carcinogenic and mutagenic properties (Loeppky & Outram, 1982). Since the molecular geometry of these compounds critically influences their biological activity, the stereochemistry of *N*-nitrosamines has been studied using various experimental techniques (Połoński *et al.*, 1996, and references therein). Particularly, non-planarity and, connected with it, inherent chirality of the *N*-nitrosamine chromophore strongly influence the circular dichroism spectra (Shustov *et al.*, 1992). As a correct interpretation of these spectra is assisted by a detailed knowledge of the chromophore geometry, we performed an X-ray crystallographic study of (*S*)-*N*-nitrosoazetidine-2-carboxylic acid, (I). The N atom of the *N*-nitrosamino group in (I) is included in the strained four-membered ring that may lead to its pyramidal configuration and the intrinsic chirality of the chromophore (Shustov & Rauk, 1995). Additionally, due to a restricted rotation about the partially double N—N bond, the molecules of (I) can exist as either the *E* or *Z* stereoisomer. In aqueous solution, the equilibrium between these two forms is shifted towards the *E* conformer (Gaffield *et al.*, 1981).



(I)

Nitroso groups are known to exhibit orientational disorder in the solid state (Gdaniec *et al.*, 1995; Połoński *et al.*, 1996; Olszewska *et al.*, 2001), which often leads to situations in which both stereoisomers, *Z* and *E*, occupy the same site in the crystal. However, the crystal structure of (I) reveals that the *N*-nitrosamine moiety is ordered, and adopts the *E* conformation (Fig. 1). No residual electron-density peaks were found in the nearest vicinity of this group, indicating that the crystal indeed consists solely of the *E* stereoisomer. Bond lengths and angles of the azetidine-2-carboxylic acid fragment of (I)