Crystal structure of 2,5-diiodo-4-nitro-1H-imidazole hemihydrate, C$_6$H$_4$I$_4$N$_6$O$_5$

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Abstract

C$_6$H$_4$I$_4$N$_6$O$_5$, orthorhombic, Pna2$_1$ (no. 33), $a = 16.6477(8)$ Å, $b = 8.1899(4)$ Å, $c = 12.2143(6)$ Å, $V = 1665.33(14)$ Å$^3$, $Z = 4$, $R_{	ext{gt}}(F) = 0.0406$, $wR_{	ext{gt}}(F^2) = 0.0859$, $T = 105$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared by nitrifying 2,4,5-triiodoimidazole. It was recrystallized from ether solution at room temperature to give colorless crystals.

Experimental details

All H atoms were positioned geometrically and treated as riding, with O–H bond lengths constrained to 0.85 Å and $U_{	ext{iso}}$(H) = 1.5$U_{	ext{eq}}$(O), N–H bond 0.88 Å and $U_{	ext{iso}}$(H) = 1.2$U_{	ext{eq}}$(N).

Discussion

Polynitroimidazole systems have been used as antifungal, antibacterial, antiviral, antitumor drugs [1–3]. Recently,
these so called “high energy density materials” have attracted renewed attention in conjunction with their favorable detonation performance [4, 5]. As a promising candidate, 1-methyl-2,4,5-trinitroimidazole was synthesized by the nitration of 2,4,5-triiodoimidazole and alkylation of 2,4,5-triiodoimidazole [6, 7]. 2,5-Diido-4-nitroimidzole is an intermediate, but the position of the nitro group was not known [8, 9]. So, it was recrystallized to determine the position of the nitro group. Here we report the crystal structure of the title compound (cf. the figure).

As shown in the figure, the asymmetric unit of the title compound contains two title molecules and one water molecule. The two crystallographically independent 2,5-diido-4-nitroimidzole molecules and the water molecule are connected by two hydrogen bonds. The imidazole rings are planar and the dihedral angle of the two imidazole rings is 60.3°.

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References