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The crystal structure of 2-aminoisophthalic acid, $C_8H_7NO_4$

Table 1: Data collection and handling.

Crystal:	Needle, colorless
Size:	$0.3 \times 0.25 \times 0.1$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.13 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω -scans
θ_{max} , completeness:	25.2° , >98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5580, 675, 0.075
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 487
$N(\text{param})_{\text{refined}}$:	66
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3, 4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	1.000000	0.7890(2)	0.750000	0.0217(8)
H1	0.880(6)	0.822(2)	0.703(3)	0.036(8)*
O1	0.5330(4)	0.77617(12)	0.59221(16)	0.0241(6)
O2	0.3897(4)	0.63144(12)	0.53111(17)	0.0269(6)
H2	0.258772	0.662500	0.493303	0.040*
C1	0.5631(5)	0.68953(19)	0.5970(2)	0.0202(7)
C2	0.7898(5)	0.64106(17)	0.6751(2)	0.0182(7)
C3	0.7968(5)	0.54292(19)	0.6763(2)	0.0228(7)
H3	0.658099	0.509021	0.624983	0.027*
C4	1.000000	0.4931(3)	0.750000	0.0256(9)
H4	1.000004	0.426024	0.749999	0.031*
C5	1.000000	0.6937(3)	0.750000	0.0194(9)

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Abstract

$C_8H_7NO_4$, monoclinic, $C2/c$ (no. 15), $a = 4.9752(11)$ Å, $b = 14.167(3)$ Å, $c = 10.999(2)$ Å, $\beta = 99.066(5)^\circ$, $V = 765.6(3)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0571$, $wR_{\text{ref}}(F^2) = 0.1630$, $T = 150(2)$ K.

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The title molecular structure is shown in the figure (only the asymmetric unit is labelled). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

All of the starting materials are commercially available and used as received. The title compound, 2-aminoisophthalic acid (1.81 g, 1 mmol), was added to a THF solution (20 mL) at room temperature. After stirring for 10 min, the solution

was filtered and let evaporate. Several days later, a large number of colorless crystals were harvested, yield 83.5% (based on 2-aminoisophthalic acid).

Experimental details

The structure was solved by direct methods with the SHELXS program. All H-atoms from C, N and O atoms were positioned with idealized geometry and refined ($U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, $1.2U_{\text{eq}}(\text{N})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$, respectively), for all H atoms) using a riding model with C–H = 0.950 Å, N–H = 0.863 Å and O–H = 0.840 Å, respectively).

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Comment

To the best of our knowledge, there is no report on the crystal structure of 2-aminoisophthalic acid except a cocrystal structure with norfloxacin [5]. Some examples of mono- or di-substituted for amino group of 2-aminoisophthalic acid or its carboxylate esters have been reported [6–10]. Thus, we herein report the crystal structure of 2-aminoisophthalic acid.

As shown in the figure, 2-aminoisophthalic acid with the molecule formula of C₈H₇NO₄, crystallises in the monoclinic space group, *C2/c* with the molecule located on a twofold axis. Consequently the atoms H4, C4, C1 and N1 are located on this axis (see the figure) and non-hydrogen atoms are nearly co-planar. There are two kinds of hydrogen bonds: each molecule forms two intramolecular N—H···O hydrogen bonds. Intermolecular O—H···O link adjacent molecules to a one-dimensional supramolecular structure in a head-to-tail mode. All bond lengths and angles of the title compound are comparable to its analogue structures [5–10].

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