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Crystal structure of 2-(dimethylamino)ethyl 4-aminobenzoate, $C_{11}H_{16}N_2O_2$

Table 1: Data collection and handling

Crystal:	Clear light colourless
Size:	0.41 × 0.23 × 0.22 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.083 cm ⁻¹
Diffractometer, scan mode:	Xcalibur, Eos, Gemini, ω scans
2 θ max, completeness:	58.868°, 99.43%
$N(hkl)$ measured, $N(hkl)$ unique, R_{int} :	10746, 2806, 0.037
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1790
$N(param)$ refined:	140
Programs:	SHELX [1], Bruker programs [2], DIAMOND [3]

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Abstract

$C_{11}H_{16}N_2O_2$, orthorhombic, $P2_12_12_1$ (no. 19), $a = 6.1516(10)$ Å, $b = 13.711(2)$ Å, $c = 13.7392(18)$ Å, $V = 1158.8(3)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0657$, $wR_{ref}(F^2) = 0.1940$, $T = 293(2)$ K.

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The 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 materials

Following a literature procedure [4], 0.68 g 4-aminobenzoic acid, 0.71 g 2-chloro- N,N' -dimethylethylamine hydrochloride and 1.72 g anhydrous $NaHCO_3$ were added to 8 mL acetone. The mixture was stirred, cooled by an ice water bath for 5 h. After the reaction was complete, the mixture was filtered and the solvent was removed under reduced pressure. A pale yellow oil was afforded which was dissolved in 5 mL CH_2Cl_2 and washed with 2 × 5 mL saturated Na_2CO_3 and 5 mL water. The organic layer was dried by Na_2SO_4 , concentrated under

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
O1	0.5578(6)	0.5126(2)	0.6247(2)	0.0731(9)
O2	0.2857(6)	0.4716(2)	0.7217(2)	0.0739(9)
N2	0.8420(6)	0.4255(2)	0.4792(2)	0.0645(10)
N1	0.0721(7)	0.9158(3)	0.6275(3)	0.0781(12)
H1A	0.10628	0.93667	0.57015	0.094*
H1B	−0.06738	0.91827	0.63404	0.094*
C1	0.1433(7)	0.8218(3)	0.6367(3)	0.0547(10)
C2	0.0306(7)	0.7539(3)	0.6911(3)	0.0608(10)
H2	−0.09907	0.77164	0.72111	0.073*
C5	0.4165(7)	0.7005(3)	0.6054(3)	0.0581(10)
H5	0.54762	0.68293	0.57661	0.07*
C4	0.3021(7)	0.6323(3)	0.6597(2)	0.0506(9)
C7	0.3756(7)	0.5316(3)	0.6733(3)	0.0561(10)
C6	0.3389(8)	0.7933(3)	0.5935(3)	0.0636(11)
H6	0.41714	0.83782	0.55637	0.076*
C3	0.1070(7)	0.6613(3)	0.7014(3)	0.0605(11)
H3	0.02657	0.61648	0.73725	0.073*
C8	0.6362(10)	0.4137(4)	0.6317(4)	0.0963(19)
H8A	0.65576	0.39645	0.69959	0.116*
H8B	0.52991	0.36957	0.60382	0.116*
C10	0.7624(12)	0.3494(4)	0.4173(6)	0.118(2)
H10A	0.82205	0.28804	0.4378	0.176*
H10B	0.80504	0.36224	0.35132	0.176*
H10C	0.60665	0.34686	0.42128	0.176*
C9	0.8361(11)	0.4037(4)	0.5818(4)	0.103(2)
H9A	0.88523	0.33704	0.59023	0.123*
H9B	0.9415	0.44547	0.61383	0.123*
C11	1.0719(10)	0.4448(5)	0.4572(5)	0.112(2)
H11A	1.15467	0.38609	0.46606	0.168*
H11B	1.1259	0.49445	0.50011	0.168*
H11C	1.08539	0.46639	0.39099	0.168*

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reduced pressure to give a colorless oil. The residual product was recrystallized by EtOAc and the target product was obtained with a yield of 70%, m.p.: 121–122 °C. ¹H NMR (300 MHz, CDCl₃): δ 7.87 (d, *J* = 8.7 Hz, 1H), 6.64 (d, *J* = 8.7 Hz, 1H), 4.39 (t, *J* = 5.9 Hz, 1H), 4.10 (s, 1H) 2.71 (t, *J* = 5.9 Hz, 1H), 2.35 (s, 3H).

Experimental details

The structure was solved by direct methods and refined by full-matrix least-squares on *F*² using the ShelXL. All hydrogen atoms were placed in idealized positions and refined as riding on their parent atoms.

Comment

2-(Dimethylamino)ethyl 4-aminobenzoate compound has received particular attention owing to their widely application in small molecule inhibitor of the PHLPP, pharmaceutical intermediates, and local anesthesia. For example, the amino group of 2-(dimethylamino)ethyl 4-aminobenzoate compound can be used to synthesize acridine-triazenes compounds. These compounds have highly promising features for the utilization of DNA-binding of combilexins [4–6]. This paper reports the crystal structure of 2-(dimethylamino)ethyl 4-aminobenzoate which is only built up by the C₁₁H₁₆N₂O₂ molecules, in which all bond lengths are in normal ranges and are similar to parameters derived for the structures of related *p*-amin-benzoates [7, 8].

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