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The crystal structure of 1,2-dimethylimidazole, $C_5H_8N_2$

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Abstract

$C_5H_8N_2$, monoclinic, $P2_1/n$ (no. 14), $a = 8.2492(6)$ Å, $b = 7.2496(5)$ Å, $c = 9.2882(7)$ Å, $\beta = 99.214(2)^\circ$, $V = 548.30(7)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0477$, $wR_{ref}(F^2) = 0.1400$, $T = 200$ K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The compound was obtained commercially (Aldrich). Crystals suitable for the diffraction study were taken directly from the provided product.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.58 \times 0.57 \times 0.53$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.07 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	28.3° , 99%
$N(hkl)_{\text{measured}}$,	4863, 1348, 0.014
$N(hkl)_{\text{unique}}$, R_{int} :	
Criterion for I_{obs} ,	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1256
$N(hkl)_{\text{gt}}$:	
$N(\text{param})_{\text{refined}}$:	66
Programs:	Bruker [1, 2], SHELX [3], WinGX/ORTEP [4], Mercury [5], PLATON [6]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.38435 (12)	0.09522 (14)	0.63048 (10)	0.0311 (3)
N2	0.59954 (13)	0.19446 (15)	0.78426 (11)	0.0369 (3)
C1	0.50008 (13)	0.05372 (16)	0.74707 (12)	0.0306 (3)
C2	0.54442 (17)	0.33158 (18)	0.68596 (14)	0.0391 (3)
H2	0.592303	0.450670	0.685048	0.047*
C3	0.41255 (16)	0.27345 (18)	0.59070 (13)	0.0364 (3)
H3	0.352165	0.341689	0.512672	0.044*
C4	0.25650 (16)	−0.0255 (2)	0.55711 (15)	0.0440 (4)
H4A	0.306764	−0.126763	0.509961	0.066*
H4B	0.183489	0.044761	0.483286	0.066*
H4C	0.193048	−0.076021	0.628621	0.066*
C5	0.51149 (18)	−0.1298 (2)	0.81983 (17)	0.0460 (4)
H5A	0.554805	−0.220360	0.757511	0.069*
H5B	0.402101	−0.168322	0.836368	0.069*
H5C	0.585072	−0.121420	0.913535	0.069*

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.95 Å for aromatic carbon atoms) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$.

The H atoms of the methyl groups were allowed to rotate with a fixed angle around the C–C bond to best fit the experimental electron density (HFIX 137 in the SHELX program suite [3]), with $U(\text{H})$ set to $1.5U_{\text{eq}}(\text{C})$.

Comment

Imidazole is a versatile aromatic heterocycle that has found ample use as ligand in coordination compounds or basic agent in synthesis reactions where acid products shall be scavenged. Being an aromatic compound, imidazole can be functionalized over a broad range – including substitution on the acidic nitrogen atom – which allows for tweaking the steric pretense as well as the basicity in comparison to the pristine mother compound. At the onset of a study about coordination compounds of various imidazoles, the structure of the title compound was determined to allow for comparisons of metrical parameters in relation to coordination numbers and oxidation states of various central atoms. Structural information featuring the title compound is only apparent for a mixed hydrochloride salt [7].

According to the structure solution, the crystal contains an imidazole derivative featuring a methyl each substituent at the 1 and 2 positions of the heterocycle. Intracyclic C–N bond lengths for the methylated pnitrogen atom are found at 1.3577(14) and 1.3739(17) Å while the pertaining exocyclic bond length measures 1.4536(15) Å. Both value ranges are in good agreement with other imidazole derivatives as well as tertiary amines whose metrical parameters have been deposited with the Cambridge Structural Database [8]. Intracyclic angles cover a range of 105.02(11)–111.45(11)° with the smallest angle on the imine-type nitrogen and the largest angle on the carbon atom in between the two heteroatoms.

In the crystal there are C–H $\cdots\pi$ interactions supported by one of the hydrogen atoms of the nitrogen-bonded methyl group. In total, these contacts connect the

molecules to centrosymmetric dimers. π -Stacking is not a prominent stabilizing feature as the shortest distance between two centers of gravity was measured at 4.4695(8) Å.

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