Eric C. Hosten and Richard Betz*

The crystal structure of 2-*iso*-propylimidazole, $C_6H_{10}N_2$

Table 1: Data collection and handling.

Crystal:	Colourless platelet
Size:	0.57 × 0.36 × 0.36 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.07 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	28.4°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	11,379, 3298, 0.024
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2837
$N(\text{param})_{\text{refined}}$:	164
Programs:	Bruker [1, 2], SHELX [3], WinGX/ORTEP [4], Mercury [5], PLATON [6]

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Abstract

$C_6H_{10}N_2$, triclinic, $P\bar{1}$ (no. 2), $a = 7.4423(5)$ Å, $b = 7.9420(5)$ Å, $c = 11.6711(8)$ Å, $\alpha = 96.667(3)^\circ$, $\beta = 95.650(3)^\circ$, $\gamma = 100.999(3)^\circ$, $V = 667.42(8)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0620$, $wR_{\text{ref}}(F^2) = 0.1681$, $T = 200$ K.

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The asymmetric unit of the title 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.

***Corresponding author: Richard Betz**, Department of Chemistry, Nelson Mandela University, Summerstrand Campus (South), University Way, Summerstrand, PO Box 77000, Port Elizabeth, 6031, South Africa, E-mail: Richard.Betz@mandela.ac.za. <https://orcid.org/0000-0002-5730-2152>

Eric C. Hosten, Department of Chemistry, Nelson Mandela University, Summerstrand Campus (South), University Way, Summerstrand, PO Box 77000, Port Elizabeth, 6031, South Africa. <https://orcid.org/0000-0003-4173-2550>

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.95 Å for aromatic carbon atoms, C–H 1.00 Å for methine groups) and were included in the refinement in the riding model approximation, with $U(H)$ set to $1.2U_{\text{eq}}(C)$. 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 $U(H)$ set to $1.5U_{\text{eq}}(C)$. All nitrogen-bound H atoms were located on a difference Fourier map and refined freely.

One of the *iso*-propyl groups shows orientational 3-fold disorder that was resolved by means of a disorder model showing a distribution of 50.8% for the major component as well as 35.4 and 13.7% for the other two orientations.

Comment

Imidazole is 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

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
N11	0.39683 (17)	0.29685 (16)	0.18912 (11)	0.0355 (3)
N12	0.19887 (17)	0.05819 (16)	0.20147 (11)	0.0368 (3)
N21	0.83962 (18)	0.86244 (16)	0.21919 (11)	0.0353 (3)
N22	0.62231 (17)	0.63402 (16)	0.22126 (12)	0.0392 (3)
C11	0.30405 (18)	0.20039 (17)	0.26070 (12)	0.0308 (3)
C12	0.3488 (2)	0.2120 (2)	0.07865 (13)	0.0415 (4)
H12	0.391540	0.248536	0.009712	0.050*
C13	0.2282 (2)	0.0657 (2)	0.08739 (13)	0.0418 (4)
H13	0.171407	−0.020035	0.023909	0.050*
C14	0.3284 (2)	0.2513 (2)	0.38974 (13)	0.0408 (4)
H14	0.310794	0.373339	0.404627	0.049*
C15	0.5220 (3)	0.2491 (4)	0.44266 (17)	0.0725 (7)
H15A	0.544801	0.131423	0.428343	0.109*
H15B	0.535169	0.286600	0.526612	0.109*
H15C	0.611397	0.327979	0.407257	0.109*
C16	0.1862 (4)	0.1417 (4)	0.44722 (18)	0.0882 (9)
H16A	0.062796	0.153208	0.415765	0.132*
H16B	0.206053	0.180048	0.531203	0.132*
H16C	0.197009	0.020267	0.432223	0.132*
C21	0.8002 (2)	0.68992 (18)	0.21647 (14)	0.0361 (3)
C22	0.6794 (2)	0.92056 (19)	0.22464 (14)	0.0405 (4)
H22	0.664175	1.036926	0.226901	0.049*
C23	0.5471 (2)	0.7795 (2)	0.22616 (14)	0.0397 (4)
H23	0.420380	0.780409	0.230055	0.048*
H11	0.470 (3)	0.403 (3)	0.206 (2)	0.065 (6)*
H21	0.949 (3)	0.926 (3)	0.2195 (19)	0.063 (6)*
C24 ^a	0.9472 (3)	0.5847 (3)	0.2081 (2)	0.0670 (5)
H24 ^a	1.026224	0.634220	0.150740	0.080*
C25 ^a	1.0715 (7)	0.6162 (7)	0.3232 (5)	0.0670 (5)
H25A ^a	1.163342	0.542902	0.318938	0.101*
H25B ^a	0.996893	0.587681	0.385656	0.101*
H25C ^a	1.134262	0.738181	0.339205	0.101*
C26 ^a	0.8827 (7)	0.4014 (6)	0.1635 (6)	0.0670 (5)
H26A ^a	0.808379	0.389416	0.087763	0.101*
H26B ^a	0.807439	0.344778	0.217963	0.101*
H26C ^a	0.989009	0.346816	0.154762	0.101*
C27 ^b	0.9472 (3)	0.5847 (3)	0.2081 (2)	0.0670 (5)
H27 ^b	1.053028	0.658193	0.179014	0.080*
C28 ^b	1.0171 (11)	0.5498 (11)	0.3250 (6)	0.0670 (5)
H28A ^b	0.922419	0.466245	0.352982	0.101*
H28B ^b	1.046207	0.657932	0.379133	0.101*
H28C ^b	1.128582	0.502102	0.319805	0.101*
C29 ^b	0.8727 (10)	0.4263 (9)	0.1121 (9)	0.0670 (5)
H29A ^b	0.767657	0.350559	0.136789	0.101*
H29B ^b	0.970497	0.361667	0.099678	0.101*
H29C ^b	0.833001	0.466974	0.039515	0.101*
C30 ^c	0.9472 (3)	0.5847 (3)	0.2081 (2)	0.0670 (5)
H30 ^c	1.066124	0.668241	0.236423	0.080*
C31 ^c	0.929 (2)	0.4513 (19)	0.2963 (14)	0.0670 (5)
H31A ^c	0.815256	0.363752	0.272622	0.101*
H31B ^c	0.924769	0.511264	0.374019	0.101*
H31C ^c	1.035205	0.394973	0.297881	0.101*
C32 ^c	0.964 (2)	0.518 (2)	0.0923 (12)	0.0670 (5)
H32A ^c	0.842954	0.455436	0.053519	0.101*
H32B ^c	1.050078	0.438787	0.093398	0.101*

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H32C ^c	1.010578	0.613751	0.050186	0.101*

^aOccupancy: 0.508 (6). ^bOccupancy: 0.354 (6). ^cOccupancy: 0.137 (3).

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 for several coordination compounds featuring the title compound as a ligand is apparent in the literature such as for copper [7], nickel [8] or zinc [9].

The structure solution shows the presence of an imidazole scaffold bearing an *iso*-propyl substituent on the carbon atom between the two heteroatoms. The asymmetric unit consists of two complete molecules. C–N bond lengths of 1.3497(17) Å and 1.364(2) Å as well as 1.3413(18) Å and 1.363(2) Å for the amine-type nitrogen are in good agreement with the values reported for other imidazole derivatives whose structural parameters have been deposited with the Cambridge Structural Database [10]. Intracyclic angles cover a range of 105.35(12)–110.74(12)° and 105.37(12)–110.74(13)°, respectively, with the smallest angle invariably found on the imine-type nitrogen atom. The least-squares planes as defined by the non-hydrogen atom of the imidazole scaffold of each of the two molecules present in the asymmetric unit enclose an angle of 80.00(9)°.

In the structure, classical hydrogen bonds of the N–H...N type are observed. These are supported by the amino group of one of the two molecules present in the asymmetric unit and have the imine-type nitrogen of the other molecule as acceptor. In terms of graph-set-analysis [11, 12], the descriptor for these contacts is *DD* on the unary and *C*₂(8) on the binary level. In total, the molecules are connected to undulated chains along [1 1 0]. In addition, it is possible to discuss the presence of two C–H...π contacts that stem from the CH group in *ortho* position to the amine-type nitrogen as well as one of the hydrogen atoms of the CH₃ groups of the *iso*-propyl substituent on the same molecule present in the asymmetric unit and exclusively employ the aromatic system of the other molecule as acceptor. π Stacking is not an important stabilizing feature in the crystal structure of the title compound with the shortest distance in between two centers of gravity measured at 4.5711(10)° between the imidazole systems of the two different molecules present in the asymmetric unit.

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