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The crystal structure of (*E*)-3-chloro-2-(2-(4-methylbenzylidene)hydrazinyl)pyridine, $C_{13}H_{12}ClN_3$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.86 × 0.69 × 0.28 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.28 mm ⁻¹
Scan mode:	Ω -scans
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9647, 4032, 0.054
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2155
$N(\text{param})_{\text{refined}}$:	309
Programs:	Olex2 [1], SHELX [2, 3]

Source of material

According to our previous work [4], the 3-chloro-2-hydrazinylpyridine and 4-methylbenzaldehyde was stirred in EtOH (50 mL) at room temperature overnight. The obtained solid was, filtered and dried with 75% yield. The solid was recrystallized from ethanol to obtain colorless block crystals.

Experimental details

Coordinates of hydrogen atoms were added using the standard AFIX options of the SHELX system. Their U_{iso} values were set to 1.2 U_{eq} of the parent atoms. Using Olex2 [1], the structure was refined with the ShelXL [3].

Comment

Some pyridine derivatives possess biological activity, such as herbicidal activity [5], insecticidal activity [6], fungicidal activity [7]. While hydrazone is also a key group in some drugs or pesticides [8].

There are two crystallographically independent molecules in the asymmetric unit of the title structure (see the figure). The bond lengths and bond angles of ring systems (pyridine ring and phenyl ring) are in the normal ranges [9, 10]. The C6=N3 (C19–N6) double bond indicated the *E* configuration which is according to the normal double bond

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Abstract

$C_{13}H_{12}ClN_3$, orthorhombic, *Fdd2* (no. 43), $a = 28.7760(11)$ Å, $b = 41.7393(17)$ Å, $c = 8.5929(3)$ Å, $V = 10,320.8(7)$ Å³, $Z = 32$, $R_{\text{gt}}(F) = 0.0477$, $wR_{\text{ref}}(F^2) = 0.0976$, $T = 296$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Cl1	0.14907 (5)	0.10676 (4)	0.97745 (18)	0.0832 (6)
N1	0.25519 (17)	0.15579 (12)	1.1510 (6)	0.0668 (13)
N2	0.18239 (14)	0.14320 (11)	1.2509 (5)	0.0653 (13)
H2	0.1559	0.1338	1.2421	0.078*
N3	0.19270 (15)	0.16015 (10)	1.3844 (6)	0.0578 (12)
C1	0.20317 (17)	0.12420 (13)	0.9980 (7)	0.0590 (15)
C2	0.2350 (2)	0.12183 (14)	0.8815 (7)	0.0713 (17)
H2A	0.2279	0.1107	0.7908	0.086*
C3	0.2776 (2)	0.13613 (16)	0.9000 (8)	0.0774 (19)
H3	0.3002	0.1346	0.8231	0.093*
C4	0.2858 (2)	0.15269 (16)	1.0346 (9)	0.0770 (19)
H4	0.3146	0.1625	1.0460	0.092*
C5	0.2140 (2)	0.14132 (13)	1.1326 (7)	0.0565 (15)
C6	0.16139 (18)	0.15986 (13)	1.4911 (7)	0.0580 (15)
H6	0.1343	0.1481	1.4755	0.070*
C7	0.1674 (2)	0.17739 (13)	1.6348 (6)	0.0516 (14)
C8	0.20846 (19)	0.19301 (13)	1.6705 (6)	0.0606 (16)
H8	0.2329	0.1927	1.5997	0.073*
C9	0.2135 (2)	0.20902 (14)	1.8104 (7)	0.0688 (17)
H9	0.2414	0.2193	1.8313	0.083*
C10	0.1786 (2)	0.21023 (14)	1.9196 (7)	0.0689 (18)
C11	0.1843 (2)	0.22825 (17)	2.0705 (7)	0.102 (3)
H11A	0.1744	0.2500	2.0567	0.154*
H11B	0.2164	0.2279	2.1013	0.154*
H11C	0.1657	0.2183	2.1498	0.154*
C12	0.1377 (2)	0.19496 (16)	1.8823 (8)	0.0790 (18)
H12	0.1132	0.1956	1.9529	0.095*
C13	0.1319 (2)	0.17874 (14)	1.7433 (7)	0.0708 (16)
H13	0.1038	0.1686	1.7224	0.085*
Cl2	0.05160 (6)	0.02663 (4)	1.1392 (2)	0.1052 (7)
N4	0.11658 (18)	0.08678 (12)	1.4173 (7)	0.0792 (15)
N5	0.06095 (15)	0.09503 (12)	1.2282 (5)	0.0636 (13)
H5	0.0409	0.0878	1.1630	0.076*
N6	0.06571 (16)	0.12764 (12)	1.2492 (5)	0.0578 (12)
C14	0.0864 (2)	0.04140 (16)	1.2876 (7)	0.0622 (16)
C15	0.1106 (2)	0.02108 (16)	1.3774 (10)	0.089 (2)
H15	0.1084	−0.0010	1.3634	0.107*
C16	0.1392 (3)	0.0341 (2)	1.4923 (10)	0.110 (2)
H16	0.1567	0.0210	1.5575	0.132*
C17	0.1407 (2)	0.0665 (2)	1.5059 (9)	0.093 (2)
H17	0.1599	0.0751	1.5822	0.112*
C18	0.0882 (2)	0.07418 (15)	1.3112 (7)	0.0573 (15)
C19	0.0356 (2)	0.14463 (15)	1.1803 (7)	0.0636 (17)
H19	0.0120	0.1343	1.1257	0.076*
C20	0.0362 (2)	0.17938 (15)	1.1827 (7)	0.0627 (16)
C21	0.0651 (2)	0.19768 (19)	1.2714 (9)	0.088 (2)
H21	0.0856	0.1876	1.3395	0.105*
C22	0.0649 (3)	0.2307 (2)	1.2628 (11)	0.105 (3)
H22	0.0852	0.2425	1.3242	0.127*
C23	0.0345 (4)	0.24642 (19)	1.1632 (11)	0.107 (3)
C24	0.0060 (3)	0.2281 (2)	1.0782 (10)	0.134 (3)
H24	−0.0151	0.2379	1.0111	0.161*
C25	0.0070 (2)	0.1959 (2)	1.0874 (9)	0.108 (3)
H25	−0.0134	0.1842	1.0251	0.129*
C26	0.0362 (4)	0.28315 (18)	1.1560 (12)	0.181 (4)

Table 2: (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
H26A	0.0330	0.2900	1.0499	0.272*
H26B	0.0654	0.2905	1.1967	0.272*
H26C	0.0113	0.2919	1.2168	0.272*

length [11], and the *E* configuration is the same as in some reported structures [12–14]. The torsion angles of C7–C6–N3–N2 and C6–N3–N2–C5 are −178.3(4)° and −178.1(4)° (2. molecule: C18–N5–N6–C19–172.6(5)° and N5–N6–C19–C20–177.0(5)°).

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