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Crystal structure of 2-amino-3-[2-(1,3,3-trimethyl-1,3-dihydro-indol-2-ylidene)-ethylideneamino]-but-2-enedinitrile, $C_{17}H_{17}N_5$

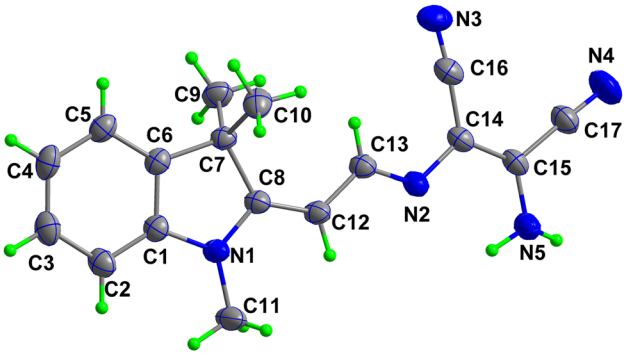

Table 1: Data collection and handling.

Crystal:	Red rod
Size:	0.25 × 0.12 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.08 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8087, 2837, 0.023
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2179
$N(param)_{refined}$:	214
Programs:	SHELX [1], Bruker [2]

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Abstract

$C_{17}H_{17}N_5$, monoclinic, $P2_1/c$ (no. 14), a = 9.4347(9) Å, b = 15.6392(15) Å, c = 11.0939(11) Å, β = 100.215(2)°, V = 1611.0(3) Å^3, Z = 4, $R_{gt}(F)$ = 0.0392, $wR_{ref}(F^2)$ = 0.1105, T = 296 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.

1 Source of material

The starting materials 1,3,3-trimethyl-2-(formylmethylene) indoline (2.01 g, 10 mmol) and diaminomaleonitrile (1.08 g, 10 mmol) in an ethanol solution (100 mL) were stirred for 5 h under refluxing. The formed red powder was filtered, and the

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
N1	0.45302 (14)	−0.05812 (7)	0.22928 (11)	0.0542 (3)
N2	0.82583 (13)	0.02201 (8)	0.55349 (10)	0.0508 (3)
N3	0.93074 (19)	−0.13704 (11)	0.76901 (16)	0.0837 (5)
N4	1.1906 (2)	0.06644 (13)	0.90620 (16)	0.1033 (6)
N5	0.99322 (17)	0.15520 (10)	0.65207 (14)	0.0648 (4)
H5A	0.915 (2)	0.1593 (12)	0.5930 (18)	0.078 (6)*
H5B	1.024 (2)	0.2030 (14)	0.6964(18)	0.091 (7)*
C1	0.35602 (16)	−0.12407 (9)	0.18802 (13)	0.0505(4)
C2	0.24188 (18)	−0.12403 (11)	0.09088 (15)	0.0617 (4)
H2	0.2211	−0.0763	0.0408	0.074*
C3	0.15956 (19)	−0.19771 (12)	0.07087 (16)	0.0681 (5)
H3	0.0817	−0.1995	0.0065	0.082*
C4	0.19108 (19)	−0.26816 (12)	0.14460 (16)	0.0670(5)
H4	0.1350	−0.3172	0.1290	0.080*
C5	0.30601(18)	−0.26709(10)	0.24244(15)	0.0582(4)
H5	0.3262	−0.3148	0.2926	0.070*
C6	0.38949 (16)	−0.19447 (9)	0.26406 (13)	0.0477 (4)
C7	0.51933 (16)	−0.17412 (9)	0.36154(13)	0.0466 (4)
C8	0.54813 (16)	−0.08085 (9)	0.33193 (12)	0.0458 (4)
C9	0.4809 (2)	−0.18485 (11)	0.48919 (14)	0.0656 (5)
H9A	0.4030	−0.1471	0.4976	0.098*
H9B	0.5633	−0.1713	0.5503	0.098*
H9C	0.4523	−0.2429	0.4997	0.098*
C10	0.64776 (18)	−0.23082 (11)	0.34572 (18)	0.0686 (5)
H10A	0.6249	−0.2896	0.3585	0.103*
H10B	0.7308	−0.2144	0.4044	0.103*
H10C	0.6678	−0.2239	0.2644	0.103*
C11	0.4462 (2)	0.02617 (11)	0.17427 (17)	0.0765 (6)
H11A	0.3665	0.0286	0.1072	0.111 (7)*

Table 2: (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
H11B	0.5341	0.0374	0.1448	0.118 (9)*
H11C	0.4334	0.0683	0.2344	0.129 (9)*
C12	0.64775 (16)	−0.02544 (9)	0.39179 (13)	0.0514 (4)
H12	0.6512	0.0282	0.3562	0.062*
C13	0.74614 (16)	−0.03963 (9)	0.50105 (13)	0.0498 (4)
H13	0.7540	−0.0939	0.5360	0.060*
C14	0.92156 (16)	0.00967 (10)	0.66198 (13)	0.0494 (4)
C15	1.00174 (16)	0.07803 (10)	0.70943 (13)	0.0521 (4)
C16	0.93162 (17)	−0.07085 (11)	0.72491(15)	0.0588 (4)
C17	1.10605 (19)	0.07038 (12)	0.81975 (16)	0.0674 (5)

mother liquid was left in air for a few days, yielding red rod crystals.

2 Experimental details

The structure was solved by Direct Methods and refined with the SHELX crystallographic software package [1]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

3 Comment

Schiff bases have been extensively studied due to their excellent coordinative abilities, biological activities, and fluorescence properties, etc. [3]. Particularly, diaminomaleonitrile-based Schiff bases have been developed as fluorescent probes for the detection of Cu^{2+} [4] or ClO^- [5]. The title compound, derived from 1,3,3-trimethyl-2-(formylmethylene)indoline and diaminomaleonitrile, could act as a fluorescence turn-on probe for detecting Cu^{2+} [6].

In the title structure, the bond length of C13–N2 is 1.2953(18) Å (see the Figure), indicating the Schiff base formation. Bond lengths and angles are all in the expected ranges [7]. In the solid state, intermolecular N–H···N hydrogen bonds link the molecules into a chain along the *b* axis, which are further connected with each other by two types of intermolecular C–H···N hydrogen bonds to form a two-dimensional wave-like supermolecular network.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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