Eric C. Hosten and Richard Betz*

The crystal structure of *N*-(4-(cyclohexylimino)pent-2-en-2-yl)cyclohexanamine, $C_{17}H_{30}N_2$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.47 × 0.33 × 0.26 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.06 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	28.3°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	15310, 1137, 0.017
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1039
$N(\text{param})_{\text{refined}}$:	54
Programs:	Bruker [1, 2], SHELX [3], WinGX/ORTEP [4], Mercury [5], PLATON [6]

Source of material

The compound was obtained upon condensation of cyclohexylamine with acetylacetonate under azeotropic distillation conditions. Crystals suitable for the diffraction study were taken directly from the solidified product obtained upon distillation of the crude product.

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.99 Å for methylene groups and 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 $1.5U_{\text{eq}}(C)$.

The nitrogen-bound H atom was placed in calculated positions (N–H 0.86 Å) and was included in the refinement in the riding model approximation, with $U(H)$ set to $1.5U_{\text{eq}}(N)$.

Due to the absence of a strong anomalous scatterer, the Flack parameter is meaningless. Thus, the item was removed from the CIF.

Comment

Imines are easily obtained upon condensation reaction of primary amines with carbonyles (aldehydes and

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Abstract

$C_{17}H_{30}N_2$, tetragonal, $P\bar{4}2_1m$ (no. 113), $a = 8.6755(3)$ Å, $c = 11.1611(4)$ Å, $V = 840.03(7)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0488$, $wR_{\text{ref}}(F^2) = 0.1417$, $T = 200$ 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.

*Corresponding author: Dr. 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>

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}
N1	0.39158 (18)	0.89158 (18)	0.36448 (19)	0.0420 (6)
H1 ^a	0.451763	0.951763	0.324968	0.063*
C1	0.39792 (19)	0.89792 (19)	0.4820 (2)	0.0355 (5)
C2	0.500000	1.000000	0.5396 (3)	0.0371 (7)
H2	0.500000	1.000000	0.622890	0.045*
C3	0.2970 (3)	0.7970 (3)	0.5587 (3)	0.0655 (10)
H3A ^a	0.192131	0.831667	0.553316	0.098*
H3B ^a	0.330805	0.802556	0.640481	0.098*
H3C ^a	0.303637	0.692350	0.531190	0.098*
C11	0.2909 (2)	0.7909 (2)	0.2961 (2)	0.0416 (6)
H11	0.228668	0.728667	0.351165	0.050*
C12	0.3870 (3)	0.6856 (3)	0.2174 (2)	0.0640 (7)
H12A	0.451076	0.620586	0.267528	0.077*
H12B	0.454316	0.747489	0.167399	0.077*
C13	0.2859 (4)	0.5841 (3)	0.1377 (2)	0.0705 (8)
H13A	0.351072	0.522472	0.085862	0.085*
H13B	0.226526	0.514397	0.187580	0.085*
C14	0.1781 (3)	0.6781 (3)	0.0625 (3)	0.0556 (7)
H14A	0.237044	0.737043	0.004572	0.067*
H14B	0.109783	0.609783	0.018698	0.067*

^aOccupancy: 0.5.

ketones alike). They have found application as ligands in transition metal chemistry, and their role as potential chelating agents has been confirmed on grounds of diffraction studies based on single crystals [7–11]. In continuation of our interest in the structural aspects of diverse imine compounds [12–18] the title compound was synthesized and investigated by means of a diffraction study based on single crystals.

The structure solutions shows the presence of the two-fold condensation product of cyclohexylamine and acetylacetonate. The asymmetric unit contains a quarter of a molecule. The compound is present as its enamine tautomer with the hydrogen atom on the nitrogen atom distributed evenly over both positions. C–N bond lengths of 1.314(3) and 1.452(3) Å are in good agreement with pertaining values reported for other imines derived from primary amines as found in the Cambridge Structural Database [19]. A conformational analysis according to Cremer & Pople [20] shows the cyclohexyl moiety to adopt a ¹C₄ conformation on carbon atoms C11 and C14 (¹¹C₁₄) [21].

In the crystal, only an intramolecular hydrogen bond of the N–H⋯N type is observed. In terms of graph-set analysis [22, 23], the descriptor for this interaction is S(6) at the unitary level. The absence of further intermolecular interactions is consistent with the low melting point of the title compound.

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