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The crystal structure of (E)–N-(4-chlorobenzylidene)(4-chlorophenyl)methanamine, $C_{14}H_{11}Cl_2N$

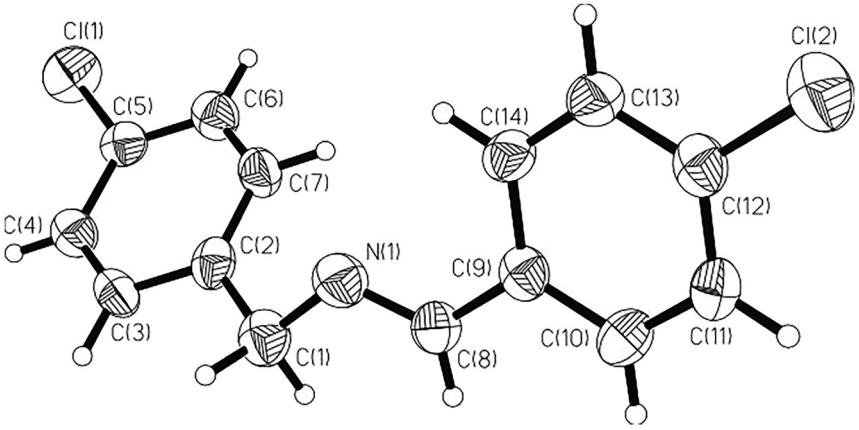

Figure 1: Molecular structure of the title compound demonstrating the atomic numbering scheme. Displacement ellipsoids are drawn at the 30 % probability level.

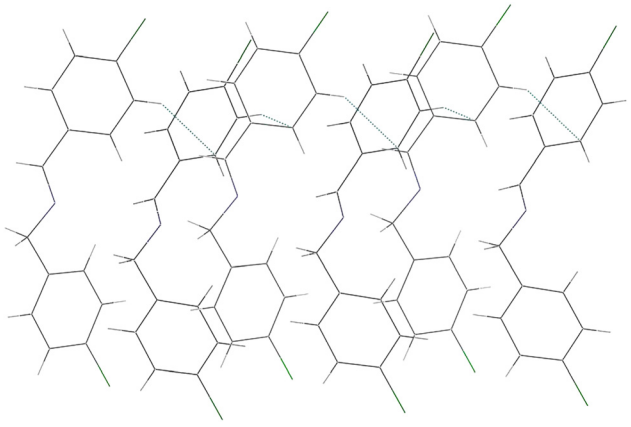

Figure 2: 1D chain structure of the title compound stretching in the b-axis.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.15 × 0.12 × 0.07 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.49 mm^{-1}
Diffractometer, scan mode:	Bruker Apex2, φ and ω scans
θ_{max}, completeness:	25.0°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2201, 2201, 0.0844
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1009
$N(param)_{refined}$:	155
Programs:	Bruker,[1] SHELX[2,3]

Abstract

$C_{14}H_{11}Cl_2N$, orthorhombic, *Pbca*, a = 14.5131(13) Å, b = 5.9090(5) Å, c = 29.470(3) Å, V = 2527.3(4) $Å^3$, Z = 8, R_{gt} (F) = 0.0825, wR_{ref} (F^2) = 0.1401, T = 298 K.

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Table 1 contains the crystallographic data.

1 Source of materials

In a representative experiment (E)–N-(4-chlorobenzylidene)(4-chlorophenyl)methanamine (26.4 mg, 0.10 mmol) was dissolved in 5 mL of 95 % ethanol understirring, then the solution was filtered into a test tube and left standing at room temperature. After ca. 12 days light yellow block crystals were collected.

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2 Experimental details

Coordinates of hydrogen atoms were refined without any constraints or restraints. The C–bound H atoms were geometrically placed (C–H = 0.95–0.97 Å) and refined as riding with U_{iso}(H) = 1.2–1.5 U_{eq}(C).[1–3]

3 Comment

Schiff bases had been synthesized for the first time by the chemist Hugo Schiff in 1864. The synthesis was conducted by an active carbonyl group and a primary amine to make the imine compounds through the condensation reaction. Schiff bases have also garnered significant attention in various research fields due to their unique structures and properties. According to the literature, researchers have continuously developed a large number of new molecules or materials with specific structures, functions, and sizes by changing Schiff base substituents, electron donor atoms, their positions and so forth.[4–6] Among these, (E)–N-(4-chlorobenzylidene)(4-chlorophenyl)methanamine, as a derivative incorporating both 4-chlorophenyl groups, represents an interesting target for investigation.

In conclusion, we have successfully designed and developed a new flexible Schiff base compound. The crystals were grown via slow evaporating its ethanol solution at room temperature and the data of the title compound were collected and analyzed by using an X-ray diffractometer. Figure 1 shows the molecular structure of the (E)–N-(4-chlorobenzylidene)(4-chlorophenyl)methanamine together with the atomic labelling scheme. The title compound crystallizes in the orthorhombic space group *Pbca*, and the asymmetric unit contains a single molecule in a general position. The (E)–N-(4-chlorobenzylidene)(4-chlorophenyl) methanamine adopted the E conformation about the C=N bond. The C=N bond was 1.264(6) Å, the C–N bond equalled 1.412(7) Å, being in alignment with the merits found in the reported Schiff base.[7] The angles C(8)–N(1)–C(1) and N(1)–C(8)–C(9) were 119.4(6)/121.5(6)°. The former was wider than the reported, yet the later was narrower than the literature merit of the similar compound of 3-benzyliminomethylphenol.[8] The planes C2–C7/C9–C14 were both planar with the rms deviations of 0.0043/0.0069 Å, both inclined at 51.7° with each other. Although there existed both Cl atoms in the title compound, the Cl-derived contacts were absent. The supramolecular aggregation is not complex; there are no classical hydrogen bonds of any kind, but a single CH-pi interaction from the aryl CH of the aldehyde and the aryl core of the amine with C–Cg = 3.616 Å links the molecules into an infinite chain (Figure 2) along the b-axis. The whole structure consisted of four such independent chains.

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