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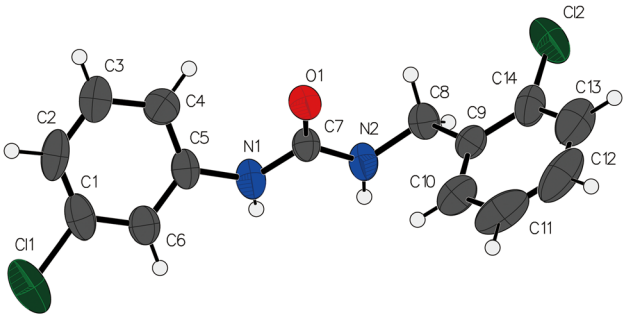
The crystal structure of 1-(2-chlorobenzyl)-3-(3-chlorophenyl)urea, $C_{14}H_{12}Cl_2N_2O$



https://doi.org/10.1515/ncrs-2024-0037
Received January 23, 2024; accepted February 22, 2024;
published online March 12, 2024

Abstract

$C_{14}H_{12}Cl_2N_2O$, orthorhombic, $P2_12_12_1$ (no. 19), a = 8.5344(8) Å, b = 12.0204(16) Å, c = 13.4504(13) Å, V = 1379.8(3) Å^3, Z = 4, $R_{gt}(F)$ = 0.0896, $wR_{ref}(F^2)$ = 0.2327, T = 293 K.

CCDC no.: 2334472

The crystal 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.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.32 × 0.28 × 0.23 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.46 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
θ_{max}, completeness:	59,1°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4412, 2897, 0.025
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1867
$N(param)_{refined}$:	160
Programs:	Bruker programs [1], SHELX [2, 3], OLEX2 [4]

1 Source of materials

3-Chlorophenyl isocyanate (0.15 g, 1 mmol) and 2-chlorobenzylamine (0.14 g, 1 mmol) were mixed in a 25 mL glass bottle. Subsequently, 15 mL of dichloromethane was added, and the resulting solution was stirred at room temperature for 10 min. Stirring was continued for an additional 5 h to ensure complete reaction at 50 °C. The solvent was then evaporated using a rotary evaporator to obtain the crude product. The crude product was dissolved in a minimal amount of hot ethanol under controlled heating and gradually cooled to room temperature. During the cooling process, the formation of a single crystal of the desired compound was observed.

2 Experimental details

The crystal structure was determined using SHELXT [2] and refined using SHELXL [3] with anisotropic refinement for non-hydrogen atoms and isotropic refinement for hydrogen atoms. The resulting crystal structure was visualized using the OLEX2 software package [4].

3 Comment

Urea and its derivatives play a crucial role in drug development and medicinal chemistry, owing to their capacity to form multiple stable hydrogen bonds with proteins and receptor targets [5]. This urea functionality acts as a core feature that facilitates effective interactions with biomolecules, enabling the design and synthesis of novel drug candidates. Despite the multitude of reported crystal structures of similar urea derivatives [6–8], the development of innovative structures continues to play a pivotal role in drug discovery. This article presents a novel structure of a urea derivative, aiming to contribute to the advancement of pharmaceutical research.

The crystal structure of the titled compound shows that the Cl atom and C atom in the chlorobenzene group are almost coplanar. The two benzene rings exhibit significant

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.5601 (4)	0.1198 (3)	0.06867 (17)	0.1034 (11)
Cl2	0.5454 (4)	0.3444 (2)	0.90046 (16)	0.0951 (10)
O1	0.6653 (4)	0.1909 (4)	0.5500 (3)	0.0427 (12)
N1	0.4689 (6)	0.1929 (5)	0.4347 (4)	0.0491 (15)
H1	0.377822	0.219441	0.420862	0.059*
N2	0.4406 (6)	0.2844 (5)	0.5819 (4)	0.0458 (15)
H2	0.358413	0.314890	0.556823	0.055*
C1	0.5867 (9)	0.0860 (8)	0.1919 (6)	0.059 (2)
C2	0.6776 (10)	−0.0048 (8)	0.2149 (7)	0.065 (2)
H2A	0.724007	−0.046979	0.164969	0.078*
C3	0.6985 (9)	−0.0320 (8)	0.3135 (7)	0.062 (2)
H3	0.758671	−0.093626	0.330606	0.074*
C4	0.6286 (8)	0.0333 (6)	0.3887 (6)	0.0522 (19)
H4	0.641768	0.014547	0.455218	0.063*
C5	0.5414 (7)	0.1245 (6)	0.3629 (5)	0.0414 (16)
C6	0.5191 (8)	0.1516 (6)	0.2631 (5)	0.0484 (18)
H6	0.459370	0.213181	0.245255	0.058*
C7	0.5325 (7)	0.2200 (5)	0.5241 (5)	0.0384 (15)
C8	0.4786 (7)	0.3030 (6)	0.6863 (5)	0.0434 (16)
H8A	0.533783	0.238157	0.711024	0.052*
H8B	0.381360	0.309073	0.723252	0.052*
C9	0.5760 (5)	0.4040 (3)	0.7076 (3)	0.0416 (16)
C10	0.6318 (6)	0.4733 (4)	0.6329 (3)	0.058 (2)
H10	0.607474	0.458546	0.566837	0.069*
C11	0.7240 (6)	0.5647 (4)	0.6570 (5)	0.083 (3)
H11	0.761392	0.611153	0.607000	0.099*
C12	0.7604 (5)	0.5868 (4)	0.7558 (6)	0.090 (4)
H12	0.822119	0.647999	0.771870	0.108*
C13	0.7046 (6)	0.5175 (5)	0.8305 (4)	0.080 (3)
H13	0.728931	0.532239	0.896578	0.096*
C14	0.6124 (6)	0.4260 (4)	0.8064 (3)	0.056 (2)

twists relative to the urea group, with dihedral angles of 83.6° and 38.5°, respectively. The dihedral angle between the two benzene rings is 69.6°. All bond lengths, bond angles, and dihedral angles in the molecule fall within reasonable ranges and are similar to those reported in the literature for crystal structures of similar compounds [9–13].

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This work was financially supported by the projects of key research and development project of Shaanxi Provincial Science and Technology Department (2022SF-448), Scientific research plan project of Shaanxi Provincial Department of Education (22JK0276), the Xianyang Key Laboratory of Molecular Imaging and Drug Synthesis (2021QXNL–PT-0008), the 2023 key research and development project of the Xianyang Science and Technology Bureau (L2023–ZDYF–SF-030), the key research and development project of Shaanxi Provincial Science and Technology Department (2023-YBSF-036) and the youth innovation team of Shaanxi University 2023 – "Key technology development and application innovation team of the industrialization of traditional Chinese medicine with northwest characteristics".

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

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