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Crystal packing of *N, N'*-bis(4-chlorophenyl)thiourea *N, N*-dimethylformamide

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November 19, 2024.

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Introduction and background study

- Crystal packing is the arrangement of atoms, ions, and molecules in a crystalline solid. It gives the physical properties of crystalline materials.
- Suitable techniques to give detailed picture of the crystal packing are the X-ray diffraction (X-ray crystallography) and the neutron diffraction.
- The aim of this study is to examine the **crystal packing of *N, N'*-bis(4-chlorophenyl)thiourea *N, N*- dimethylformamide** with X-ray crystallography. Lattice theory is used as the theoretical framework to support the study.

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Problem statement and significance of the study

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- According to the International Union of Crystallography (IUCr), crystal packing is a subtle subject.
- The significance of this study is the application in the pharmaceuticals and materials science.

Crystal packing and lattice types

- In crystal packing where lattice theory is applicable, lattice types as essential aspect of lattice theory, are made of different crystal systems, such as cubic, hexagonal, monoclinic, orthorhombic, tetragonal, and triclinic.

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Lattice theory

- Lattice theory is the theoretical framework in line with crystal packing, which refers to the three-dimensional arrangement of atoms, ions, or molecules in a crystalline solid.
- In this framework, a lattice is a three-dimensional geometric arrangement of points, where each point represents the position of an identical component in the crystal.
- Essential aspects of lattice theory in crystal packing are ***lattice types***, unit cell, packing efficiences, Bravais Lattices, and the coordinaion number.

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Methodology

- X-ray crystallography was the methodology used to determine the crystal structure, for it to further explain the atoms in crystal lattice of ***N, N'*-bis(4-chlorophenyl)thiourea *N, N*- dimethylformamide.**
- The explanation was supported by the lattice theory.

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Synthensis of *N, N'*-bis(4-chlorophenyl)thiourea *N, N*-dimethylformamide

- *N, N'*-bis(4-chlorophenyl)thiourea is an organic compound formed from the reaction of chloroaniline, carbon(IV) sulphide, and ammonia solution in methanol at a temperature of less than 4°C.

$$2C_6H_4ClNH_{2(aq)} + CS_{2(l)} + 2NH_{3(l)} \longrightarrow C_{13}H_{10}C_{l2}N_2S_{(s)} + 3H_{2(g)}\uparrow + H_2S_{(g)}\uparrow + N_{2(g)}\uparrow$$

- *N, N*- dimethylformamide (DMF) is a polar (hydrophilic) aprotic solvent used to grow the crystals of *N, N'*-bis(4-chlorophenyl)thiourea.

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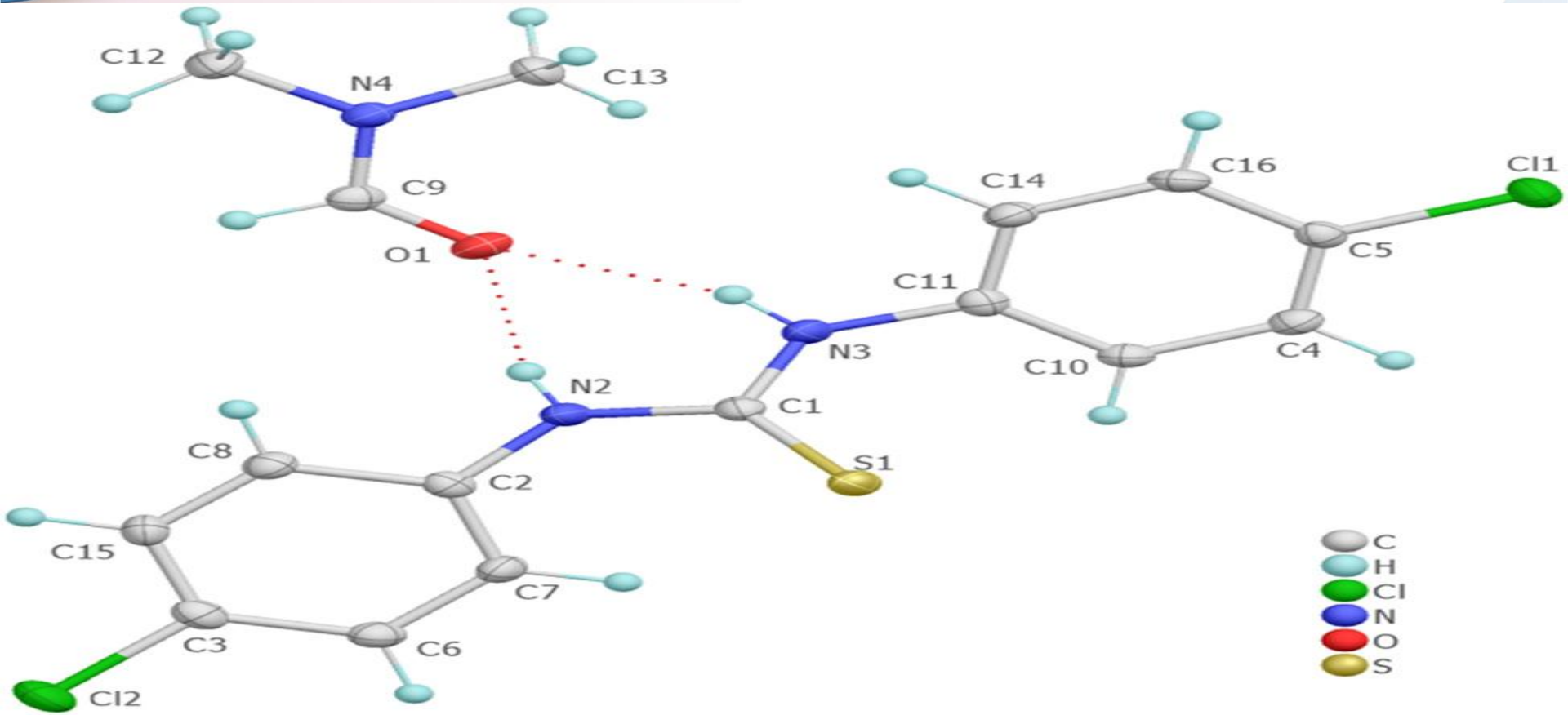
Crystal structure of $C_{16}H_{17}Cl_2N_3OS$



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Result a: Crystal packing of a

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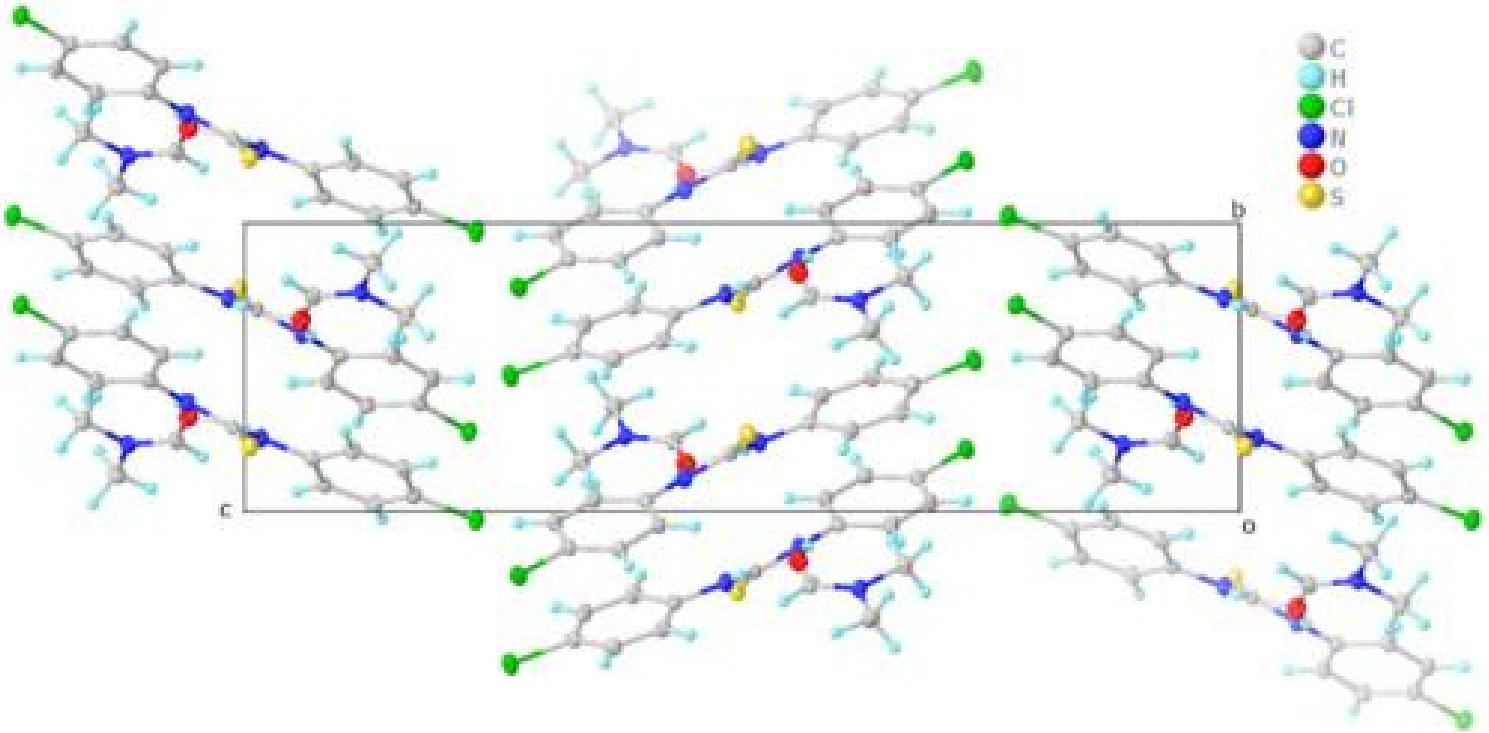

(a)

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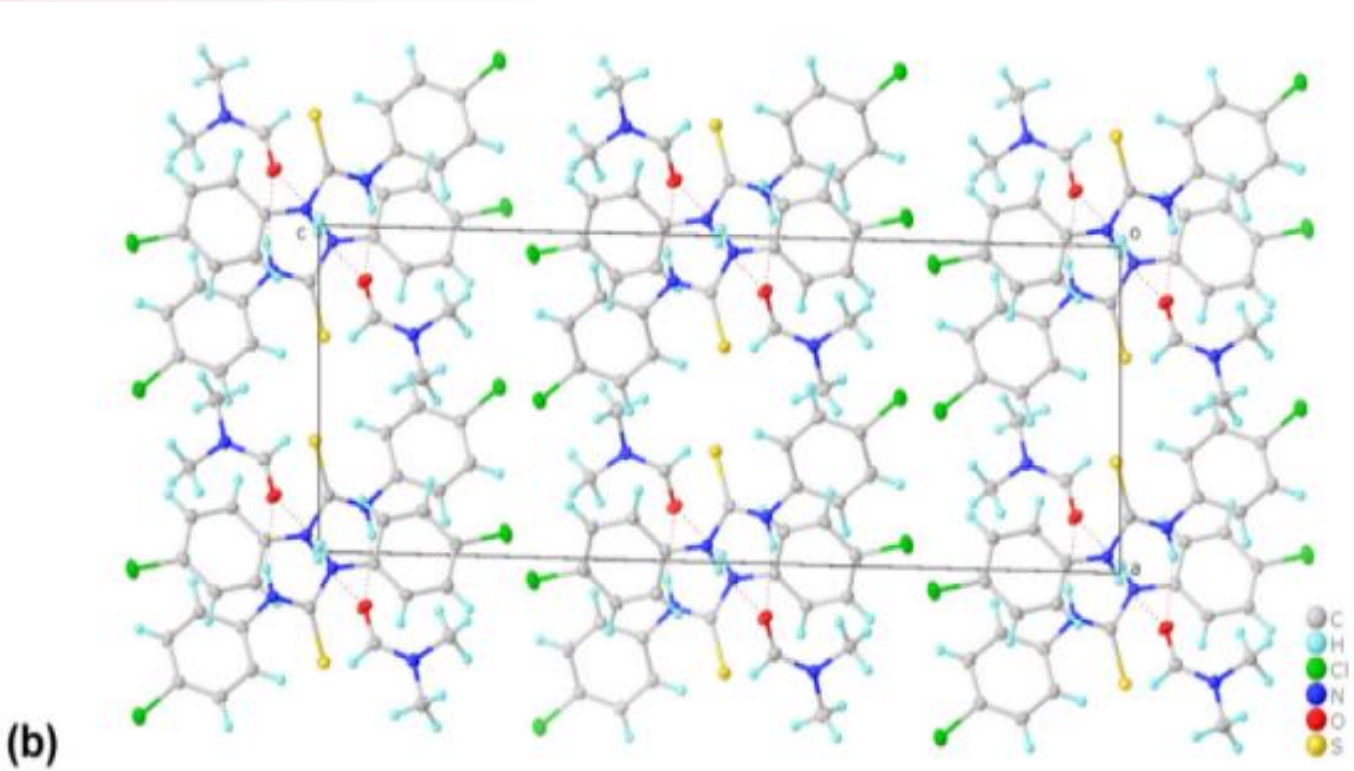
Result b: Crystal packing of b



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Result c: Crystal packing of c

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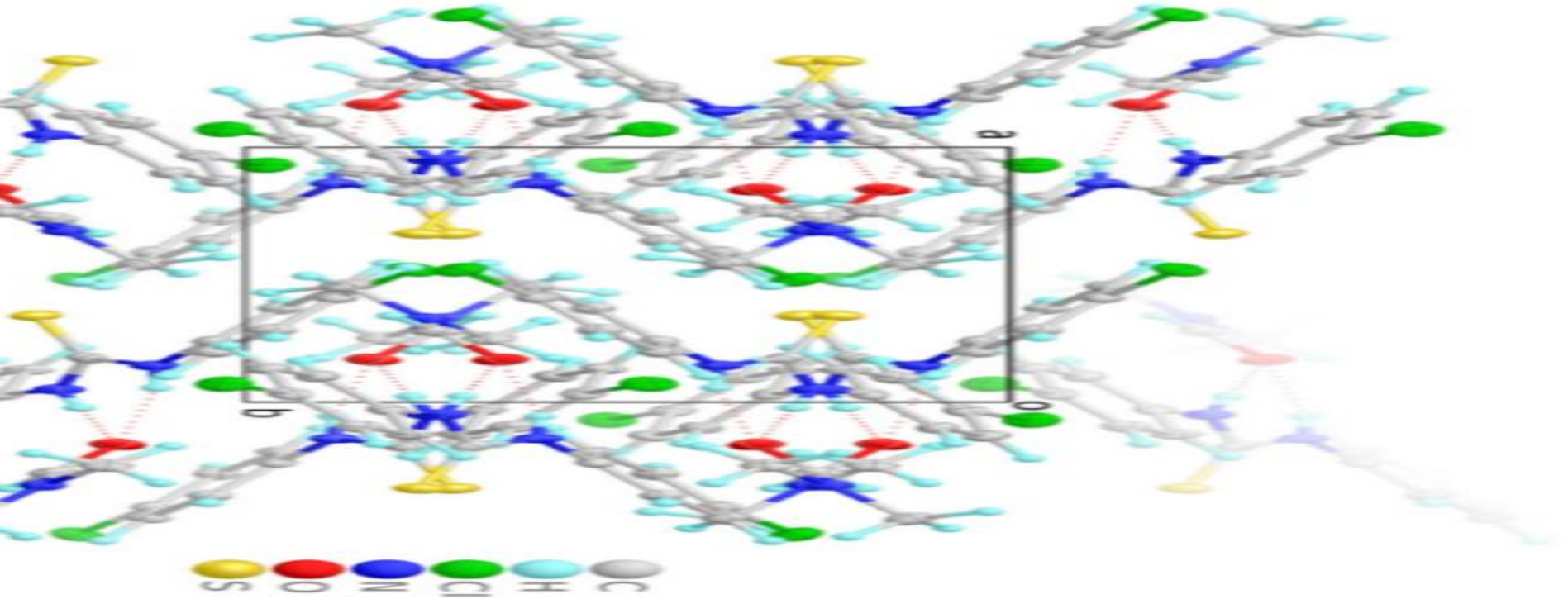

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checkCIF/PLATON (basic structural check)

Datablock

Cell a=9.2360 (4) b=7.2232 (2) c=25.55 (11)

alpha=90° beta=91.376° (3) gamma=90°

Temperature: 120K

	Calculated	Reported
Volume	1684.40(12)	1684.40(12)
Space group	P 21/c	P 1 21/c 1
Sum formula	$C_{16}H_{17}C_{l2}N_3OS$	$C_{16}H_{17}C_{l2}N_3OS$
Mr	370.29	370.30

axial lengths and angles

System	Axial lengths and angles
Cubic	a=b=c, α = β = γ = 90°
Tetragonal	a = b ≠ c, α = β = γ= 90°
Orthorhombic	a ≠ b ≠ c, α = β = γ= 90°
Rhombohedral	a = b = c, α = β = γ ≠ 90°
Hexagonal	a = b ≠ c, α = β = 90°, γ = 120°
Monoclinic	a ≠ b ≠ c, α = γ = 90°, β ≠ 90°
Triclinic	a ≠ b ≠ c, α ≠ β ≠ γ

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Conclusion and future study

- **Conclusion**

The aim of the study was achieved. Here, the lattice parameters (a, , and c wih angles) of ***N, N'*-bis(4-chlorophenyl)thiourea *N, N*-dimethylformamide** from the checkCIF dashblock gave results that validates and confirms the crystal packing of ***N, N'*-bis(4-chlorophenyl)thiourea *N, N*- dimethylformamide** as **monoclinic**.

- **Future study**

This study will involve determining the packing efficiency of ***N, N'*-bis(4-chlorophenyl)thiourea *N, N*- dimethylformamide** and comparing it with known packing types.

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Acknowledgement

- Authors sincerely appreciate the Committee and Organizers of the **African Light Source AfLS-2024** (**7th**) for allowing us as authors to participate in the AfLS-2024 conference.
- Audience for the attention.