Research Square

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Synthesis, crystal structure and Hirshfeld surface analysis of Schiff base Bis ((1-chlorophenyl) methylene) carbonohydrazide

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Research Article

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Abstract

A organic Schiff base, bis((1-chlorophenyl)methylene)carbohydrazide, was synthesized by condensation of carbohydrazide with 2-chlorobenzaldehyde. After slow evaporation for one week, colorless crystals suitable for X-ray diffraction analysis were obtained. producing crystals suitable for X-ray diffraction analysis. The compound crystallizes in the monoclinic system with space group $P2_1/c$ and has a non-planar conformation due to ortho-chlorinated aromatic rings, which induce significant torsion angles. Hirshfeld surface and contact enrichment analysis reveal that O...H-N hydrogen bonds are the most abundant and dominant intermolecular interactions, while hydrophobic and hydrophilic contacts are clearly separated in the crystal stacking. The crystal structure is stabilized by a combination of strong hydrogen bonds (particularly O...H-N), van der Waals forces, and specific halogen interactions (Cl...π, C–H...Cl). These structural characteristics suggest that the synthesized Schiff base could serve as an effective chelating agent, with its stability and interaction profile showing promise for applications in coordination chemistry and materials science. Electrostatic complementarity shows that the Cl1B…H4A interaction (Cl1B…H4A distance = 2.828 Å) also appears as two inverted images in Fig. 5c. The angle C1B–Cl1B…H4A = 164.4° is close to 180°, but is not optimal, as the electropositive region of the sigma hole of the chlorine atom faces the hydrogen atom, which is also electropositive.

1. Introduction

A Schiff base is defined as the product resulting from the condensation of a primary amine with a ketone or aldehyde, featuring a C = N double bond with the nitrogen atom linked to an aryl or alkyl group. It is named after its inventor Hugo Schiff (1834–1915), who was the first chemist to synthesize this type of compound in 1864 [1]. The great interest in these compounds is due to their ease of synthesis, high stability and coordination properties. For example, Schiff bases containing the aryl group as a substituent are considered to be the most stable, due to their greater electron delocalization on the surface of the molecule [2]. Schiff bases derived from the condensation of aliphatic aldehydes are relatively less stable and easily polymerized [3].

Schiff bases have played a vital role in various fields of chemistry, namely the pharmaceutical industry due to their antibacterial, antifungal, anti-inflammatory properties [4] as well as in corrosion control [5]. They may also have wide application in the field of water treatment due to their high capacity for transition metal complexation particularly in the recovery of heavy metals from industrial noxious effluents [6]. These compounds can be classified as monodentate, bidentate and polydentate depending on the number of coordination sites available; they are often polydentate, capable of accommodating one or more metal cations [7]. Their ability to stabilize metal ions in different oxidation states has enhanced their use in metal complexes [8]. However, despite their potential, only a small number of these technologies are applied industrially. To increase their use in industry, it is necessary to develop low-cost, environmentally friendly and efficient processes. Salen-type metal complexes, used in catalytic cycles, must be stable to the reaction medium, but demetallization can occur as a result of competition with reactants and products, or a change in the metal oxidation state. Furthermore, ligand degradation,

exacerbated by the use of strong acids or oxidizing/reducing agents, can result in demetallization by protonation of oxygen atoms, leading to the formation of a metal-free ligand susceptible to hydrolysis [8–9–10].

In this article, we explore a known [11] type of Schiff base and evaluate its properties in a specific context, including its effectiveness as a chelating agent. To this end, we investigate the electrostatic complementarity between molecules, analyze intermolecular interactions using the Hirshfeld surface method, and examine contact enrichment.

2. Materials and Methods

2.1. Crystallization

In a 250 ml flask, carbonohydrazide (0.60 g; 6.66 mmol) was added and 10 ml of ethanol was added. After dissolution, 1-chlorobenzaldehyde (1.5 ml; 13.32 mmol), previously dissolved in 10 ml of ethanol, was also added. The mixture obtained was heated under reflux for 24 hours according to the reaction scheme below. A whitish precipitate was obtained, collected by filtration, washed with 2 x 10 ml of ethanol, and dried in air. The reaction yield was 94.43%. The precipitate was dissolved in a solution of nickel chloride with ethanol. After slow evaporation for one week, colorless crystals, analyzable by X-ray diffraction, were obtained.

Scheme. *Synthesis of the Bis((1-chlorophenyl) methylene) carbonohydrazide ligand Schiff base*

2.2. Crystal data collection

A single crystal was carefully selected under a polarizing microscope to perform its structural analysis. X-ray diffraction data were collected on a Super Nova, Bruker SMART X2S benchtop diffractometer [12] at 298 K, using graphite-monochromated (MoKα λ = 0.71073 Å) radiation. The structure was solved using a direct method with the SHELXT program [13] and initially refined by successive differential Fourier syntheses and a full-matrix least-squares procedure using the SHELXL program [14]. Crystal data and experimental parameters used for the intensity data collection are summarized in Table 1.

Table 1
Crystal data and structure parameters of the title compound.

Chemical formula	**$C_{15}H_{13}Cl_2N_4O$**
MW ($g.mol^{-1}$)	335.19
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, *b*, *c* (Å)	10.8475 (11), 15.7797 (12), 9.0947 (6)
β (°)	91.014 (7)
V ($Å^3$) ; Z	1556.5 (2); 4
μ (mm^{-1})	0.42
Data collection	
Radiation type	Mo Ka
Wavelength *λ* (Å)	0,71073
Diffractometer	Bruker SMART X2S benchtop
Absorption correction	Multi-scan (SADABS; Bruker, 2016)
T_{min}, T_{max}	0.568, 1.000
# measured, independent, observed with [$I > 2\sigma(I)$] reflections	13397, 3496, 2244
R_{int} (%)	4.6
$sin\theta_{max}/\lambda$ ($Å^{-1}$)	0.649
Refinement	
$wR^2[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, gof	0.048, 0.120, 1.04
No. of reflections	3496
No. of parameters	211
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$(\Delta/\sigma)_{max}$	0.147
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.17, − 0.27

2.3. Structure Refinement

The structure was solved by direct methods with XT and refined by full-matrix least-squares methods against F^2 using SHELXL 2018/3 [13–14]. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined with isotropic displacement parameters. Some of their coordinates were refined freely and some on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms

3. Results and discussion

X-ray diffraction analysis of the crystal structure shows that the compound in question crystallizes in the monoclinic space group $P2_1/c$ with Z = 4 (Table 1). The interatomic distances and selected angles are listed in Tables S1 and S2, respectively. Table 2 lists the hydrogen bonds identified in the crystal structure, and Table S3 gives the atomic coordinates and equivalent isotropic displacement parameters.

Table 2. List of intermolecular hydrogen bonds (distance in Å, angles in °)

D H	A	dAD	dAH	DHA	Sym.
C7A–H7A ...	N1B	3.432(2)	2.755	130.42	i
N2A–H2A ...	N1B	3.472(2)	2.758	143.74	i
N2A–H2A ...	O2	2.932(2)	2.192	146.72	i
N2B–H2B ...	O2	2.871(2)	2.135	157.73	i
C5A–H5A ...	Cl1B	3.556(2)	2.945	124.61	ii
C4A–H4A ...	Cl1B	3.500(2)	2.833	129.60	ii
C2A–H2A ...	O2	3.294(2)	2.753	118.04	iii

Symmetry operators applying on the acceptor atom: (i) X ; -Y + 3/2 ; Z-½ ; (ii) X ; -Y + 3/2 ; Z+½ ; (iii) -X + 1 ; -Y + 1 ; -Z + 1

Hydroxyl groups form more polar hydrogen bonds than chlorophenyls, influencing the compactness of the crystal lattice [15]. The presence of chlorophenyls leads to C–Cl···π interactions and N-H···O hydrogen bonds, forming R_2^2 (8) dimers (Fig. 2). This suggests that the compound could adopt similar models, with stacking stabilized by weak interactions [16]. Cl groups promote van der Waals interactions and halogen contacts (Cl···π) [16–17]. OH groups allow directional hydrogen bonds, while Cl induces crystalline organization via more diffuse interactions (e.g., aromatic stacking) [15].

The estimated length of the azomethine bond (C = N) (~ 1.27 Å) corresponds to typical values for Schiff bases, confirming the nature of the bond and the electronic conjugation in the molecule [15–16] (Fig. 1). Compounds containing halogen or hydroxide substituents form 1D or 2D networks via recurring synthons (e.g., O–H···N, N–H···O, C–Cl···π) [15–16–18]. In our case, the compound has a 1D network structure (Fig. 2). The Cl substituents replace strong hydrogen bonds with weaker interactions, such as Cl···π or C–H···Cl, thereby modifying the interaction network and crystal stacking. These weak interactions stabilize the structure, but with less directionality than conventional hydrogen bonds [15–16].

3.1. Structure description

The crystal structure presented and described here corresponds to that already published by Li et al (2009) [11].

The compound $C_{15}H_{11}C_{l2}N_4O$ crystallizes in the monoclinic system, with space group $P2_1/c$. This compound is characterized by the presence of chlorinated aromatic rings in the ortho position (1-chloro), which significantly influence the molecular conformation and crystal lattice. Phenyl rings substituted with a chlorine atom often adopt dihedral angles that are not coplanar with the rest of the molecule, resulting in dihedral angles typically between 60 ° and 80 °. This torsion limits the overall flatness, giving the structure a non-planar three-dimensional (3D) conformation, stabilized by interactions such as hydrogen bonds (N-H...O) or Van der Waals interactions (Fig. 2). These hydrogen interactions stabilize the three-dimensional structure and influence the formation of dimers or networks in columns parallel to a crystallographic axis $\overrightarrow{b}$.

In addition, van der Waals contacts between alkyls or hydrophobic aromatic groups play a key role in crystal compaction, particularly through dispersive contacts between hydrogen atoms of parallel chains, as observed in saturated fatty acids or chlorophenyl derivatives.

Typical crystallographic parameters include C–C and C–N bond distances in the range of 1.3 to 1.5 Å, bond angles between 100 ° and 130 °, and intermolecular hydrogen bond distances in the range of 2.5 to 3.0 Å.

Figure 2. Crystallographic autostereogram [20] showing the projection of a two-dimensional layer of the crystal structure along the **a** axis of the Bis((1-chlorophenyl) methylene) carbonohydrazide molecule.

3.2. Hirshfeld surface analysis.

The Hirshfeld representation of the Schiff base ligand of the asymmetric unit highlights intermolecular interactions in the crystal structure (Fig. 3).

The 2D fingerprint plots of the Hirshfeld surface allows to highlight the atoms participating in contacts (Fig. 4). The graph shown in Fig. 4c represents the H...O/O…H contacts. It is characterized by two

symmetrical spikes at short distance d_i+d_e ~1.9 Å. These spikes are characteristic of the strong O-H…O hydrogen bond present in the structure, but there are also c-H…O contacts at longer distance. The graph in Fig. 4f representing H…H contacts is characterized by an end pointing towards the origin along the diagonal corresponding to $d_i = d_i$ ~ 1.2 Å. These are c-H...H-c contacts representing 12.6% of intermolecular contacts (Table 3). The 2D fingerprint decomposition also shows other contacts: Cl…H (17.4%) which is the first major contact and C…H-c which is in second position at 15.6%. The preferred and disadvantaged contacts from the point of view of chemical elements can be highlighted in a crystal structure by means of contacts enrichment ratios [23] which are shown in Table 3. The O…H-c electrostatic interactions is the most strongly enriched contacts (E > 10) and constitute the strongest electrostatic interactions stabilizing the crystal packing.

Table 3

Statistical analysis of intermolecular contacts on the Hirshfeld surface around compound. The second/third row shows the inner/external chemical content on the Hirshfeld surface. The next 6 + 6 rows show the % *C*xy of the contact types on the surface followed by the contacts enrichments *E*xy. The major *C*xy contacts and the significantly enriched contacts (E_{XY}>1) are in bold characters. In the last 3 rows, the contact statistics are regrouped in hydrophobic (Hphob, C, H-c and Cl) and in hydrophilic (Hphil, O, N, H) atoms. H-c and H-n hydrogen atoms bound to carbon and nitrogen have been distinguished.

atom	**C**	**H-c**	**Cl**	**N**	**O**	**H-n**
surf_int%	30.8	33.8	18.1	7.4	4.2	5.7
surf_ext%	29.7	34.8	19.2	6.4	4.6	5.4
C	**14.9**					
H-c	**15.6**	**12.6**				% *C*xy
Cl	7.6	**17.4**	5.0		actual	contacts
N	4.7	6.3	1.3	0		
O	1.3	2.2	0.2	0	0	
H-n	1.6	2.0	0.8	1.5	5.2	0
C	**1.63**					
H-c	0.75	1.07				*E*xy
Cl	0.67	**1.36**	**1.44**			enrichment
N	1.13	**1.32**	0.52	0		
O	0.48	0.73	0.10	0	0	
H-n	0.47	0.53	0.40	**1.93**	**10.6**	0
surface		82.7		17.3	Hphob	
% contact	Hphob	73.0	Hphil	7	x	20.3
enrichment		1.05		**5.94**	Hphil	0.73

The Hirshfeld surface [24] was calculated using MoProViewer [21] for the contacts enrichments and with CrystalExplorer17 [25] for the fingerprint plots. This surface enables intermolecular interactions to be analyzed and visualized. The E_{XY} contact enrichment ratio between chemical species X and Y is obtained by comparing actual C_{XY} contacts with those calculated as if all contact types had the same probability of forming [21]. Equiprobable proportions R_{XY} are derived from probability products based on chemical proportions on the Hirshfeld surface. An E_{XY} enrichment ratio greater than unity for a particular contact between chemical species X and Y indicates that these contacts are over-represented. The chemical

nature of the contacts and their enrichment in the molecule are shown in Table 3. The less polar, carbon-bonded H-c hydrogen atoms are distinguished from the more electropositive, nitrogen-bonded H-n atoms.

Electrostatically highly attractive O...H-n hydrogen bonds are extremely over-represented (*E* = 10.6, Table 3). Representing 5.2% of the interaction surface, they are recognized as the most favored contacts. These are the bifurcated interactions between the C = O acceptor and the two n-H hydrogen bond donors. The other potentially strong n-H...N hydrogen bond is only enriched at *E* = 1.93. One of the 2 H-n atoms makes a bifurcated H-bond with O = C and N1B. Cl...H-c bond contacts account for 17.4% of the interaction surface and can be defined as slightly favored contacts, with an enrichment ratio of *E* = 1.36.

Occupying 14.39% of the contact surface, non-polar C...C contacts are significantly over-represented (E_{CC} = 1.63) due to the occurrence of aromatic stacking of C_6ClH_4 rings. Aromatic cycles substituted with electronegative atoms such as halogens have a high likelihood to be in stacking interaction, as they have the possibility to be in electrostatic complementarity [26]. Hc...Hc contacts account for 12.6% of the surface and can be considered as weakly favored contacts (*E* = 1.07), due in part to aromatic stacking. Some near-zero enrichment ratios concern the O...Cl, H-n...Cl and N...Cl contacts, which are at *E* = 0.10, 0.40 and 0.52 respectively. These contacts are underrepresented because the favored contact for weakly negatively charged organic chlorine is the H-c atom [26].

Hydrophobic (Hphob) and hydrophilic (Hphil) atoms were grouped together to analyze interactions between the two subgroups. The contact surface of the C, H-c and Cl atoms was considered hydrophobic, the other atoms being hydrophilic. Hydrophobic and hydrophilic interactions make up 82.7% and 17.3% of the Hirshfeld surface, respectively. The crystal structure shows an enrichment of hydrophilic contacts (*E* = 5.94) and hydrophobic contacts (*E* = 1.05) in accordance with the presence of hydrophobic and hydrophilic layers in the crystal packing. Conversely, Hphob x Hphil cross-contacts are strongly under-represented (*E* = 0.73), indicating a significant separation of hydrophilic and hydrophobic contacts, which are made by the central part and by the ends of the molecule, respectively.

In summary, molecules in the crystal are mainly held together by strong interactions of the O...H-n and, to a lesser extent, H-N...N hydrogen bond type. Secondly, more moderately enriched interactions also play an important role, such as hydrophobic contacts H-C...H-c, C...C and Cl...H-c. The enrichment values found agree with trends observed in studies of interactions in several families of oxygenated and nitrogenous hydrocarbon molecules [27 – 23].

3.3. Electrostatic complementarity

(a) **(b)** **(b)**

The electrostatic potential generated by a molecule inside the Hirshfeld surface V_{int} can be displayed on the Hirshfeld surface to highlight the electrostatic nature of interactions in the crystal packing [25–26].

The electrostatic complementarity can be illustrated qualitatively by coloring the Hirshfeld surface according to V_{int} and V_{ext}, where the latter property is computed from a cluster of surrounding molecules (Fig. 5a,b). The two surfaces show qualitatively the electrostatic complementarity with electropositive regions facing generally electronegative ones and vice versa. A large electronegative potential is generated in the vicinity of the oxygen and the two non-protonated nitrogen atoms. The region around the H-N groups and to a lesser extend around the C-H group show electropositive potential;

The electrostatic energy density scatterplots (E_{int},E_{ext}), where the E value is obtained by the product between V and ρ, the total electron density have been described by Jelsch *et al*. (2023). The interactions which are attractive from an electrostatic point of view are located in the (E^+, E^-) and (E^-, E^+) quadrants. These plots allow to highlight by spikes the strong intermolecular interactions which are characterized by high values of the electron density on the Hirshfeld surface (Fig. 5c). The spikes correspond to the 3 strong hydrogen bonds and have been highlighted in color and appear twice as reciprocal contacts in the crystal packing. The two N-H…O hydrogen bonds correspond to points with stronger electrostatic energy points than the N-H…H hydrogen bond.

Moreover the Cl1B…H4A interaction (CL1B…H4A distance = 2.828) Å appears also as two reciprocal spikes in Fig. 5c. The C1B-Cl1B…H4A = 164.4 ° angle is not far from 180° and is not optimal as it results in the electropositive sigma-hole region of the chlorine atom facing the electropositive hydrogen atom. The CL1B…H4A interaction appears in the (+,+) quadrant and is not attractive from an electrostatic perspective.

The correlation coefficient between the inner and outer E values reaches − 0.57, suggesting however a global good electrostatic complementarity at the Hirshfeld surface.

Conclusion

The study presents the successful synthesis and crystallographic characterization of the bis((1-chlorophenyl)methylene) carbonohydrazide Schiff base, highlighting its unique structural attributes influenced by ortho-chlorinated aromatic rings. Detailed analysis of intermolecular interactions via Hirshfeld surfaces demonstrates that strong hydrogen bonds and aromatic stacking are key factors in stabilizing the crystal lattice, with a notable enrichment of hydrophilic contacts. Electrostatic analysis on the Hirshfeld surface highlights the role of two bifurcated O…H-N and one N…H-N strong hydrogen bonds. The clear separation between hydrophobic and hydrophilic regions within the crystal further highlights the compound's potential for selective molecular recognition and complexation. These results not only advance the understanding of structure-property relationships in Schiff bases but also open prospects for their targeted use in metal coordination and the design of functional materials.

Declarations

Compliance with Ethical Standards

Conflicts of interest/Competing interests None.

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Scheme

Scheme is available in the Supplementary Files section.

Figures

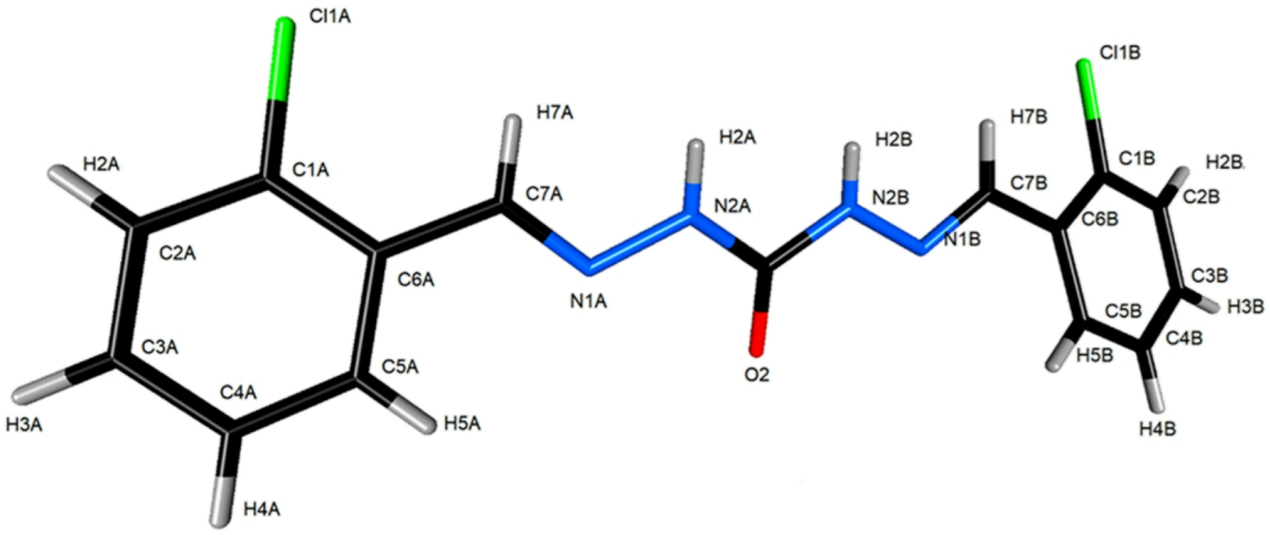


Figure 1

Structural view of the molecule bis((1-chlorophenyl) methylene) carbonohydrazide,

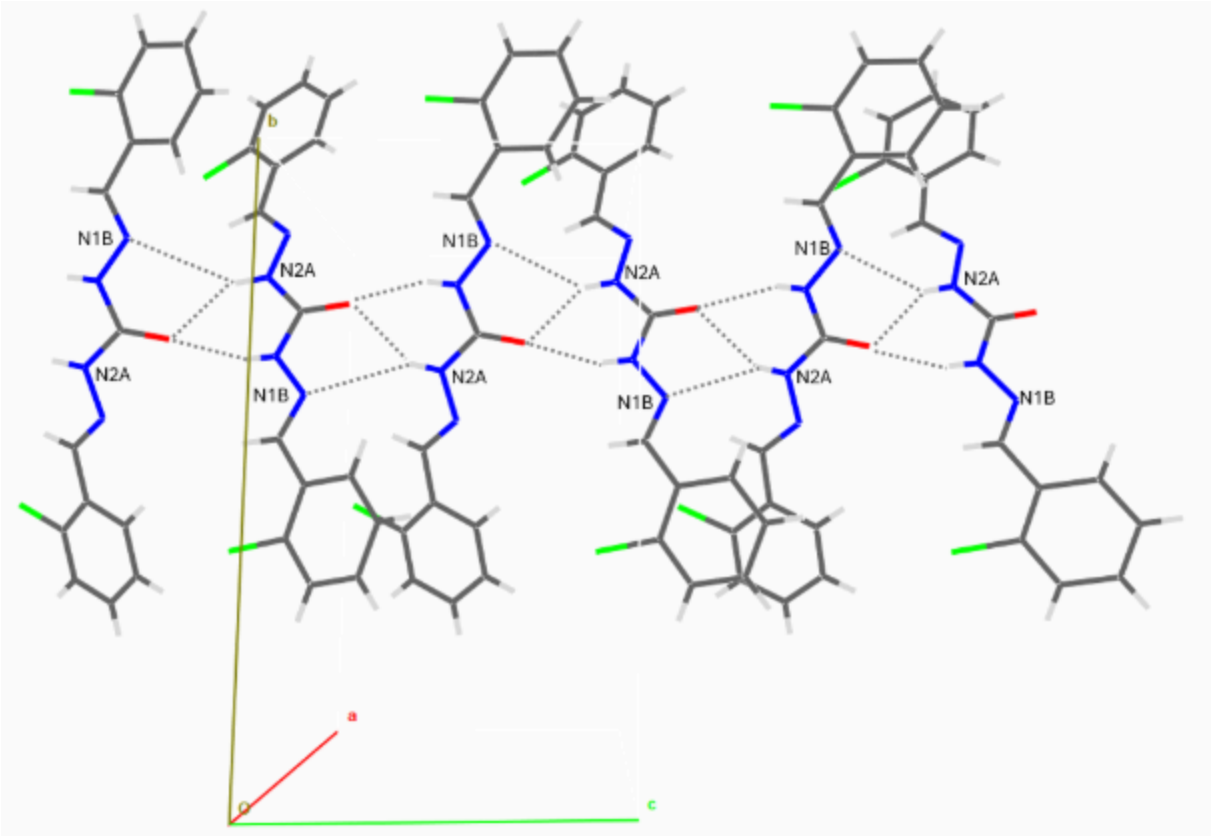


Figure 2

Crystallographic autostereogram [20] showing the projection of a two-dimensional layer of the crystal structure along the **a** axis of the Bis((1-chlorophenyl) methylene) carbonohydrazide molecule.

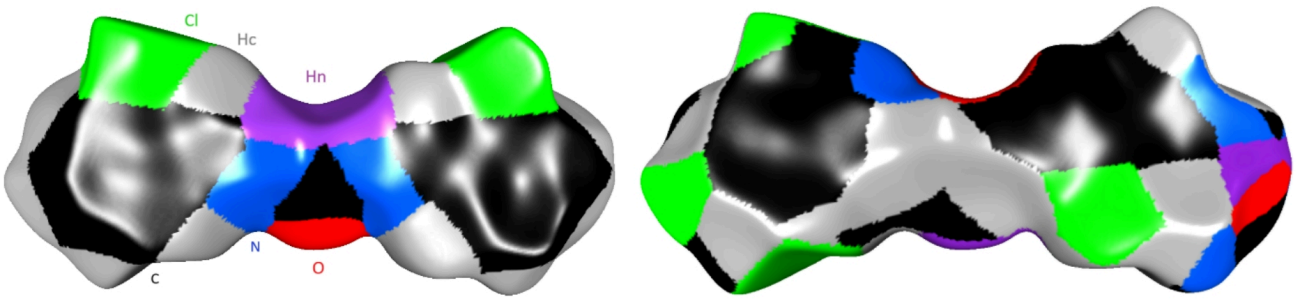


Figure 3

Hirshfeld Surface around the Schiff base ligand, of the asymmetric unit. Left/Right: the surface is colored according to the internal /external chemical type: hydrogen H-C: grey, hydrogen H-N: purple, carbon: black, oxygen: red, chlorine: green, nitrogen blue. The view was made with MoProViewer [21].

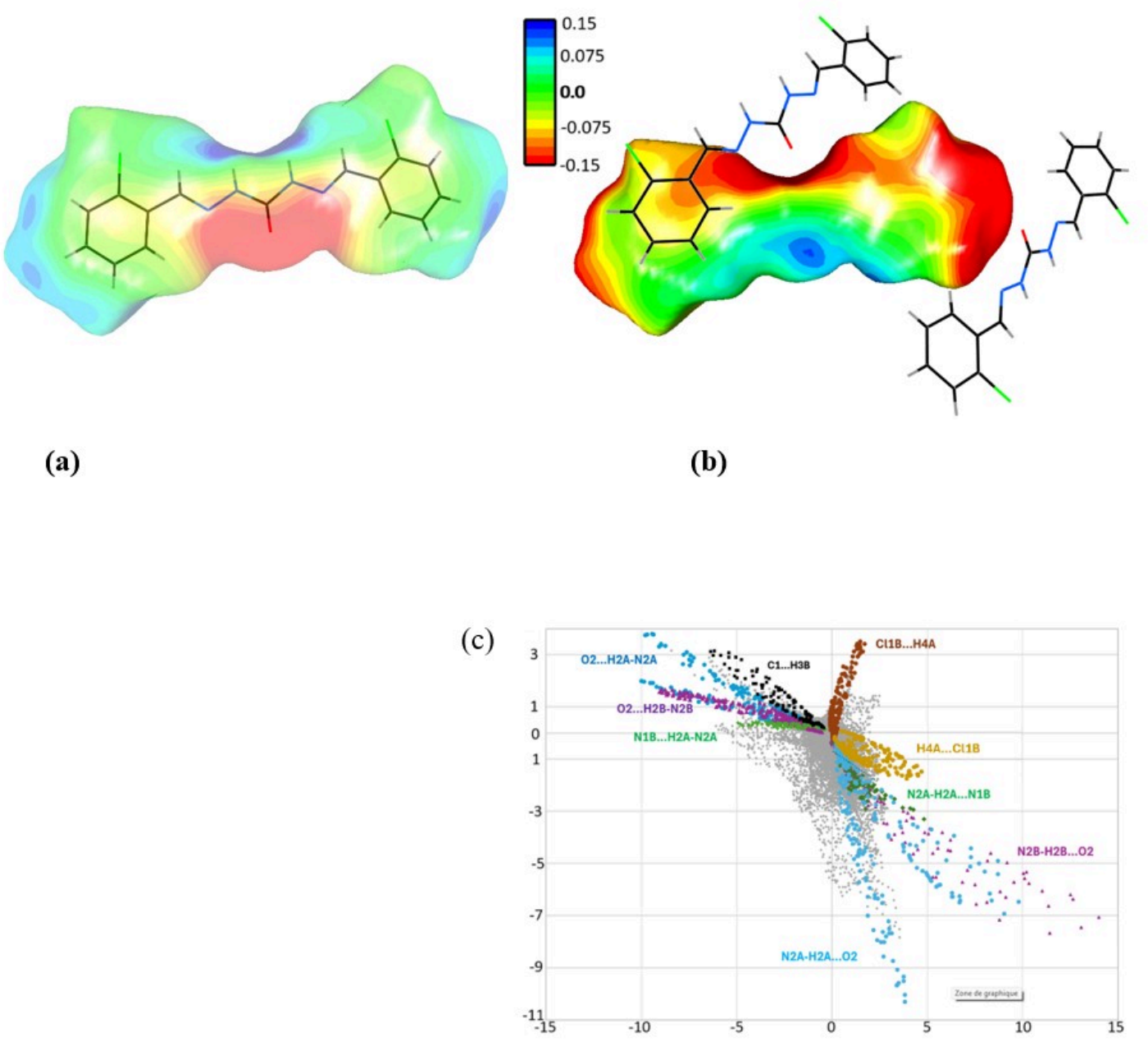


Figure 4

(a) View of the Hirshfeld surface colored according the total electrostatic potential $V(\mathbf{r})$ value (unit is in e/Å). (a) $V_{int}(\mathbf{r})$ generated by the inner molecule, (b) $V_{ext}(\mathbf{r})$ generated by the cluster of molecules forming contacts with the inner molecule. (c) Scatterplot of electrostatic energy density ($E_{int}(\mathbf{r})$,$E_{ext}(\mathbf{r})$). $E = r*V$, where $r(\mathbf{r})$ is the total electron density and its unit is in $e^2/Å^4$.

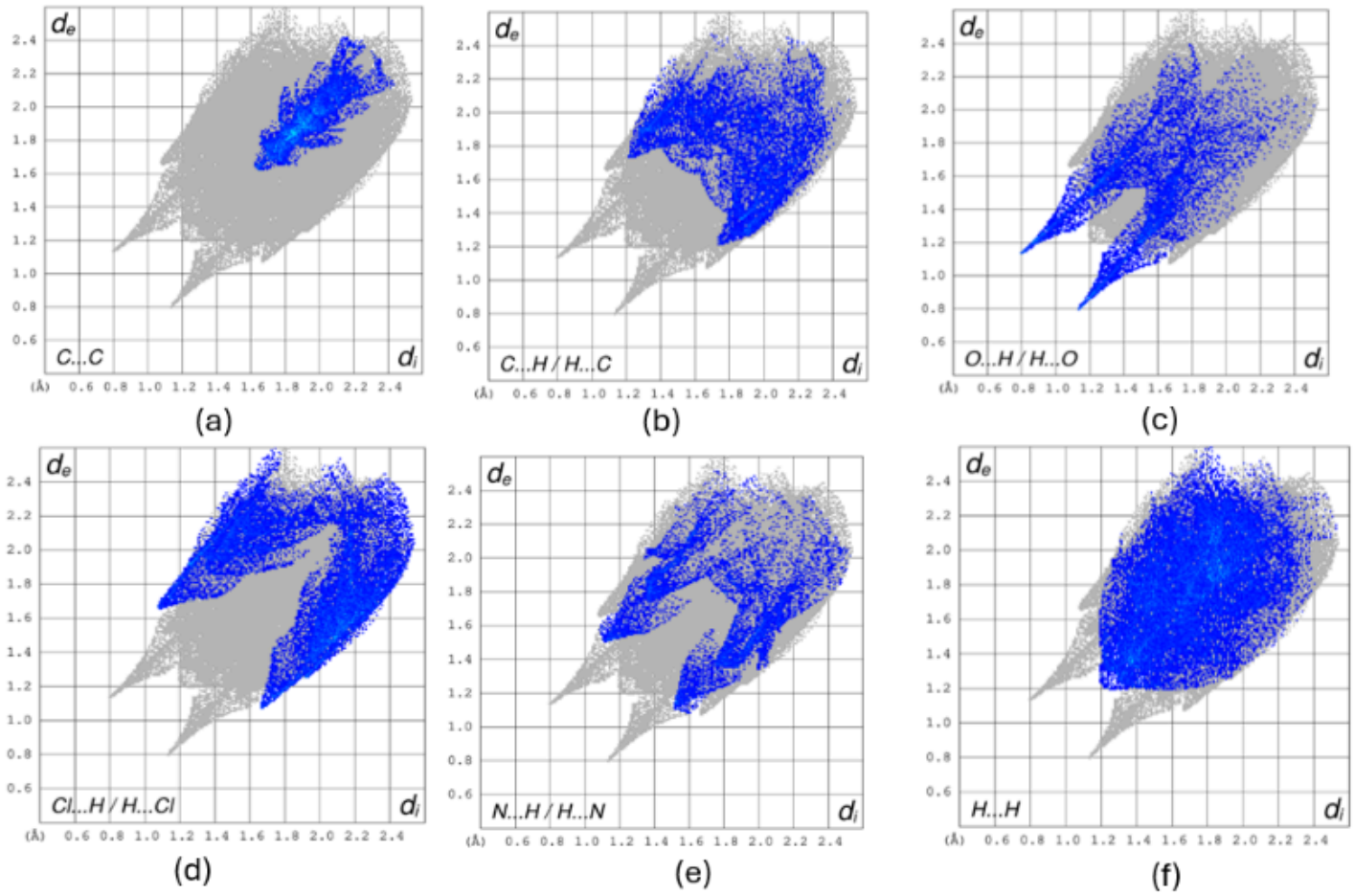


Figure 5

Fingerprint plots in (d_i,d_e) of the main contacts on the Hirshfeld surface. The graphs were obtained with CrystalExplorer17 program [22].

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- floatimage1.jpeg