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CRYSTAL STRUCTURE AND HIRSHFELD SURFACE ANALYSIS OF 4-{2,2-DICHLORO-1-[(E)-(2,4-DICHLOROPHENYL)DIAZENYL]ETHENYL}-N,N-DIMETHYLANILINE

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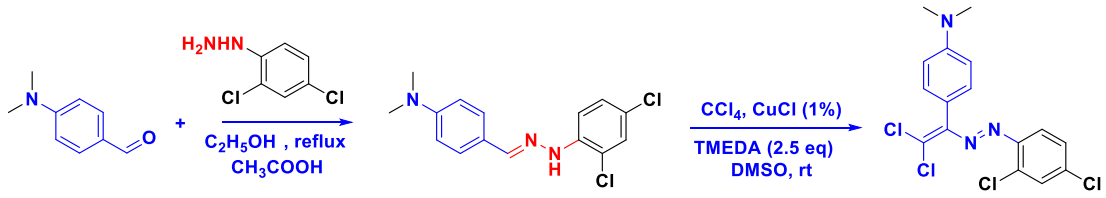
Abstract: *In the title compound, $C_{16}H_{13}Cl_4N_3$, the dihedral angle between the benzene rings of the dichlorophenyl and dimethylaniline groups is 50.85 (13)°. The central –N=N– unit shows an E configuration. In the crystal, molecules form parallel layers to the (100) plane by C—H···π and face-to-face π-π [centroid-to-centroid distances = 4.0538 (17) and 4.0537 (17) Å] interactions. These layers are connected by Van der Waals interactions to stabilize the crystal structure. Hirshfeld surface analysis indicates that the most important contributions for the crystal packing are from Cl···H/H···Cl (36.4%), H···H (23.3%) and C···H/H···C (15.2%) contacts.*
Key words: *Molecule structure, Dichlorodiazadienes, Fingerprint, Dimethylaniline group, Van der Waals interactions*

1. Introduction

Corresponding dihalodiazabutadiene derivatives were synthesized from the reaction of N-substituted hydrazones of various benzoic aldehyde derivatives with polyhalogen alkanes in the presence of CuCl catalyst [1-2]. The synthesized compounds were studied as dyes [3-4]. At the same time, due to strong reactivity, they have been applied as convenient synthons in the synthesis of many compounds [5]. Similar studies were also conducted on the basis of dimethylamino benzoic aldehyde and corresponding new diazo dyes were synthesized [6-8]. In this article, we provide information about the synthesis and structural features of a new diazo dye *"4-{2,2-dichloro-1-[(E)-(2,4-dichlorophenyl)diazenyl]ethenyl}-N,N-dimethylaniline"* (**Scheme 1**).



Scheme 1. Synthesis of 4-{2,2-dichloro-1-[(E)-(2,4-dichlorophenyl)diazenyl]ethenyl}-N,N-dimethylaniline

Investigation of intermolecular interactions of title compound was provided by Hirschfeld surface analysis [9-10], which has been widely used to study intermolecular interactions in the crystal structure in recent years [11-12].

2. Material and Methods

The syntheses of compounds were carried out at the Organic Chemistry Department of Baku State University (Baku, Azerbaijan). Every reagent utilized in this investigation came from commercial source (Aldrich, TCI-Europe, Strem, ABCR). NMR spectra were recorded on a Bruker Avance 300 (1H: 300 MHz, Karlsruhe, Germany); chemical shifts (δ) are given in *ppm* relative to TMS, coupling constants (J) in *Hz*. The solvent signals were used as references ($CDCl_3$ δH = 7.26 ppm, δC = 77.16 pp). The X-ray analyses of compound was carried out using the Bruker APEX II CCD diffractometer (T = 296 K, λ(MoKα) - radiation, graphite monochromator, φ- and ω-scan).

Dye was synthesized according to a literature protocol [1]. A 20 ml screw-neck vial was charged with dimethyl sulfoxide (DMSO; 10 ml), (E)-4-((2-(2,4-dichlorophenyl)hydrazineylidene)methyl)-N,N-dimethylaniline (308 mg, 1 mmol), tetramethylethylenediamine (TMEDA; 295 mg, 2.5 mmol), CuCl (2 mg, 0.02 mmol) and CCl4 (20 mmol, 10 equiv). After 1–3 h (until TLC analysis showed complete consumption of the corresponding Schiff base), the reaction mixture was poured into a 0.01 M solution of HCl (100 mL, pH = 2-3), and extracted with dichloromethane (3 20 ml). The combined organic phase was washed with water (3 * 50 ml), brine (30 ml), dried over anhydrous Na_2SO_4 and concentrated in vacuo in a rotary evaporator. The residue was purified by column chromatography on silica gel using appropriate mixtures of hexane and dichloromethane (v/v = 3/1–1/1). white solid (yield 75%); m.p. 405 K. Analysis calculated for $C_{16}H_{13}Cl_4N_3$ (M = 389.10). ^{1}H NMR (300 MHz, Chloroform-d) δ 7.61 – 7.46 (m, 3H), 7.28 (s, 1H), 7.21 (d, *J* = 8.5 Hz, 1H), 7.01 (d, *J* = 8.5 Hz, 1H), 6.77 (s, 1H), 3.08 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 127.0, 125.7, 125.4, 125.3, 123.4, 123.3, 123.1, 113.9, 113.9, 111.3, 111.2, 25.1. Compound was dissolved in dichloromethane and then left at room temperature for slow evaporation; red crystal of compound suitable for X-rays started to form after ca 2 d.

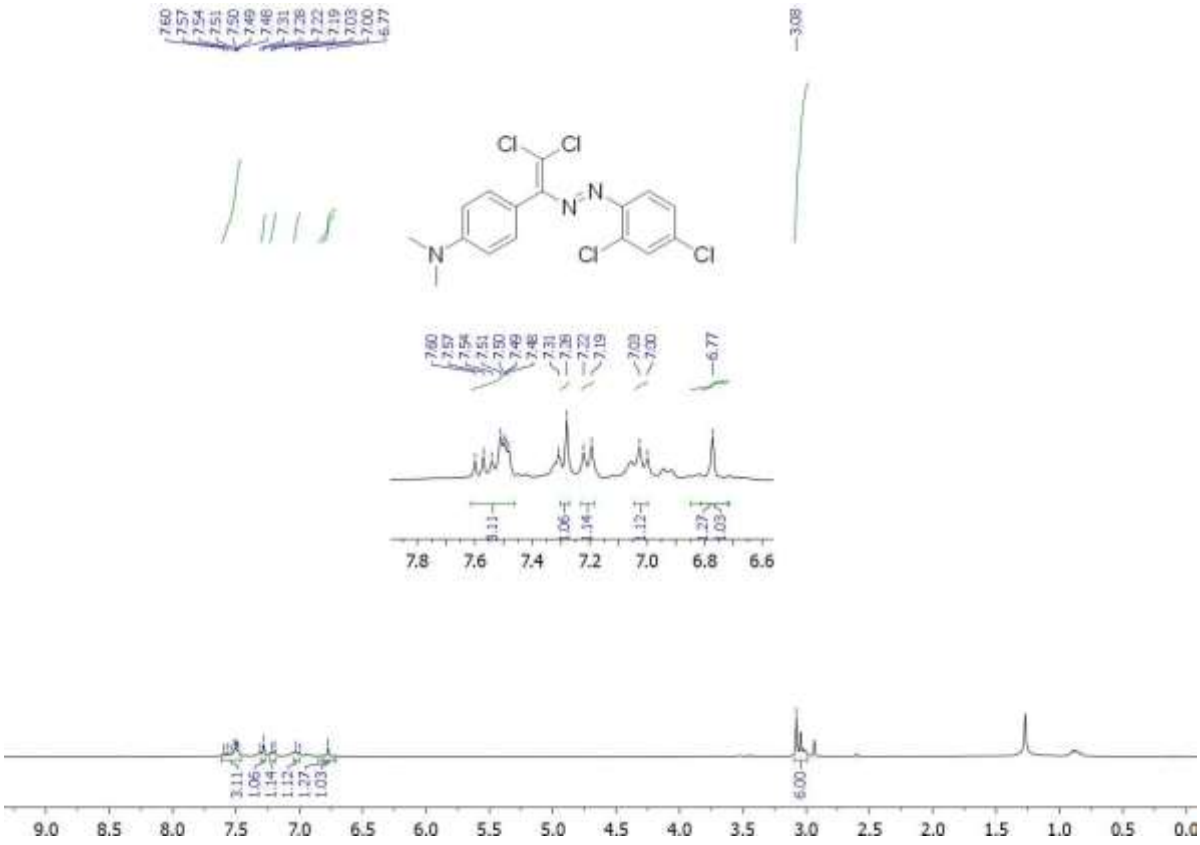


Fig. 1. ^{1}H NMR spectrum of synthesized compound in $CDCl_3$ solution**.**

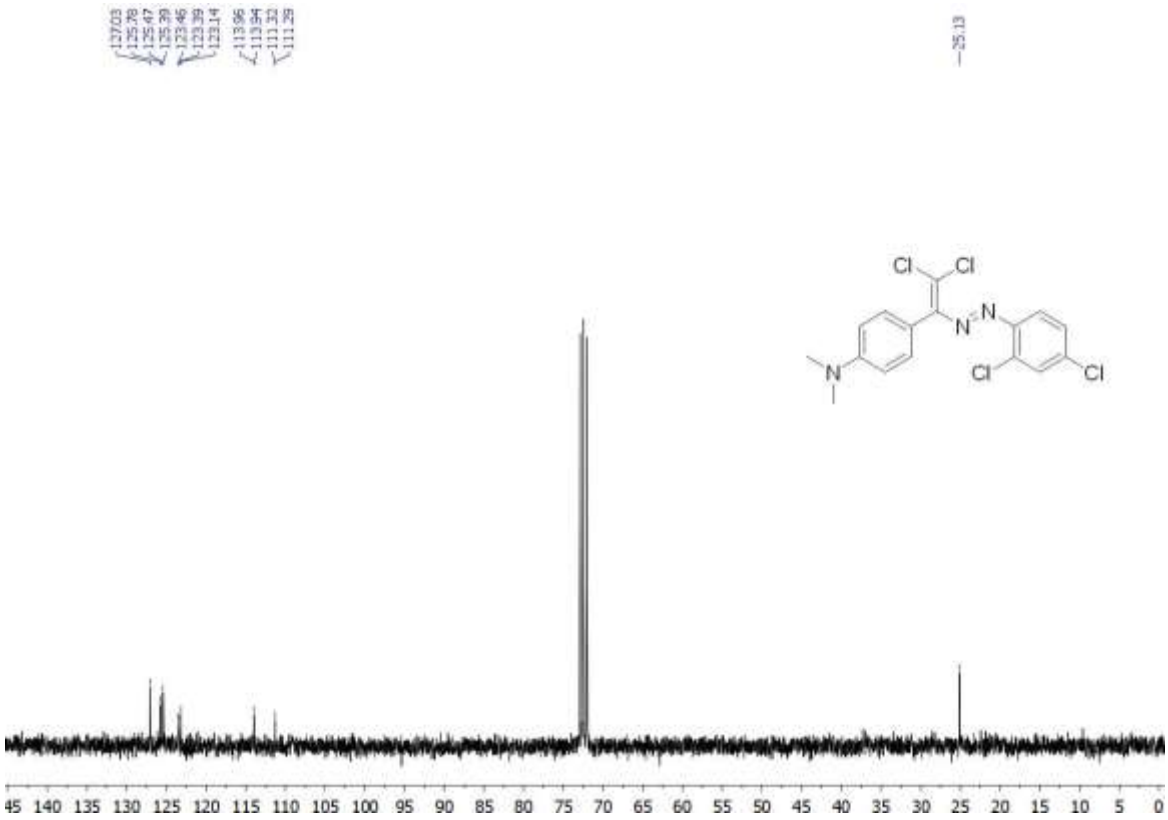


Fig. 2. ^{13}C NMR spectrum of synthesized compound in $CDCl_3$ solution.

3. Result and discussion

3.1. Stuructural commentary

In the title compound, (Fig. 3), the dihedral angle between the benzene rings (C3–C8 and C11–C16) of the dichlorophenyl and dimethylaniline groups is 50.85 (13)°. The title molecule adopts an *E* configuration with respect to the N1=N2 bond. The N1/N2/C1–C3/Cl1/Cl2 unit is approximately planar with a maximum deviation of -0.165 (2) Å, and makes dihedral angles of 57.37 (10) and 16.91 (11)°, respectively, with the C3–C8 and C11–C16 benzene rings. CCDC no:2333616.

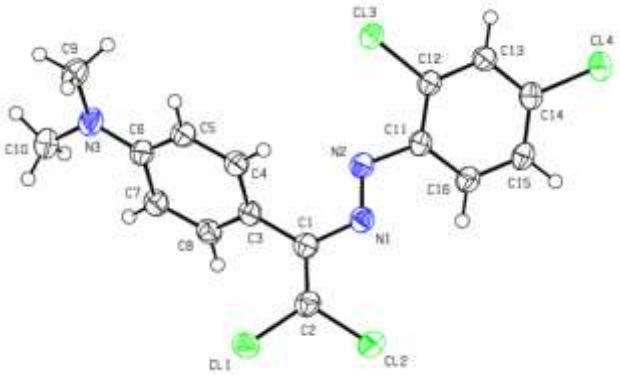


Fig. 3. The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

3.2. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules form parallel layers to the (100) plane by C—H···π (Table 1) and face-to-face π-π [Cg2···Cg2^{a} = 4.0538 (17) Å and Cg2···Cg2^{b} = 4.0537 (17) Å; symmetry codes (a) x, 3/2 - y, - 1/2 + z and (b) x, 3/2 - y, 1/2 + z; Cg2 is a centroid of the dichlorophenyl ring (C11-C16)] interactions (Figures 4, 5 and 6).

Table 1. Hydrogen-bond geometry (Å, °)
("D" and "A" are donor and acceptor, respectively.)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···Cg1^{i}	0.95	2.98	3.789 (3)	144

Symmetry code: (i) *x*, −*y*−1/2, *z*−3/2.

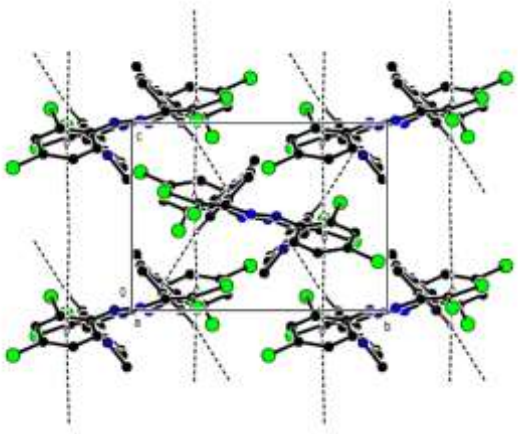


Fig. 4. The crystal packing of the title compound viewed along the *a*-axis with intermolecular C—H···π interactions and face-to-face π-π interactions shown as dashed lines.

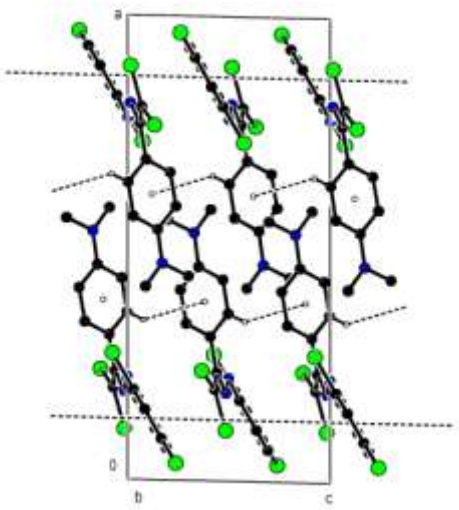


Fig. 5. The crystal packing of the title compound viewed along the *b*-axis with intermolecular C—H···π interactions and face-to-face π-π interactions shown as dashed lines.

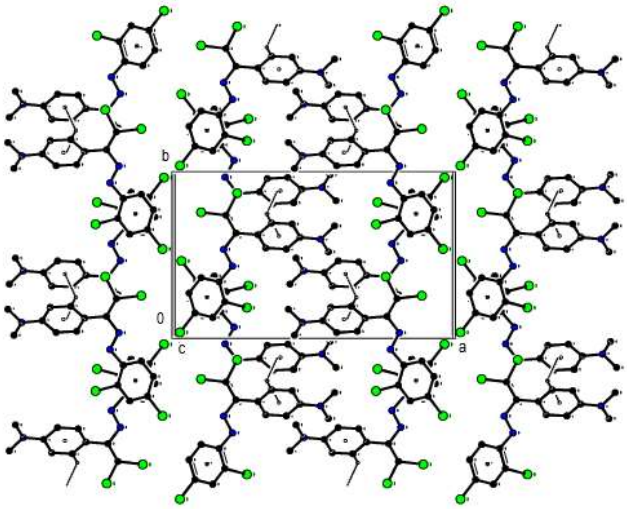


Fig. 6. The crystal packing of the title compound viewed along the *c*-axis with intermolecular C—H···π interactions and face-to-face π-π interactions shown as dashed lines.

These layers are additionally bound by the Van der Waals interactions stabilizing the crystal structure (Table 2).

Table 2. Summary of short interatomic contacts (Å) in the title compound

Cl1···H13	2.86	x,-1+y,z
C4···H8	2.90	x,1/2-y,1/2+z
H15···Cl2	3.14	2-x,1-y,1-z
H5···H10C	2.52	1-x,1/2+y,3/2-z
H10A···C5	2.90	1-x,1-y,1-z
C11···C14	3.47	x,1/2-y,-1/2+z

To visualize the intermolecular interactions in the title molecule, *CrystalExplorer17.5* [13] was used to compute Hirshfeld surfaces and their corresponding two-dimensional fingerprint plots. In the Hirshfeld surface mapped over d_{norm} (Fig. 7).

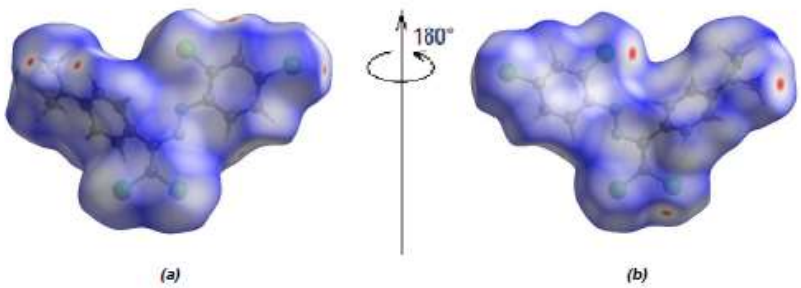


Fig. 7. (a) Front and (b) back sides of the three-dimensional Hirshfeld surface of the title compound mapped over d_{norm}, with a fixed colour scale of -0.0653 to +1.0161 a.u.

Fig. 8 depicts the two-dimensional fingerprint plots of (d_i, d_e) points from all the contacts contributing to the Hirshfeld surface analysis in normal mode for all atoms. The most important

intermolecular interactions are Cl···H/H···Cl contacts, contributing 36.4% to the overall crystal packing. Other interactions and their respective contributions are H···H (23.3%), C···H/H···C (15.2%), Cl···C/C···Cl (6.2%), Cl···Cl (5.7%), C···C (4.0%), Cl···N/N···Cl (3.9%) and N···C/C···N (2.0%), respectively

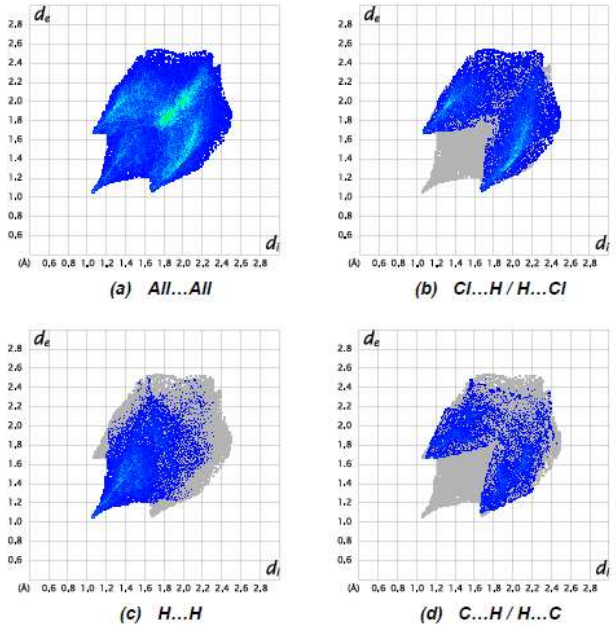


Fig. 8. The full two-dimensional fingerprint plots for the title compound, showing (a) all interactions, and delineated into (b) Cl···H/H···Cl, (c) H···H and (d) C···H/H···C interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

3.3. Database Survey

A search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; [14]) for structures having an (*E*)-1-(2,2-dichloro-1-phenylethenyl)-2-phenyldiazene unit gave 26 hits. Six compounds closely resemble the title compound, *viz.* HAFXOF, DULTAI [15]), HODQAV [15], HONBOE, HONBUK and XIZREG.

In the crystal of HAFXOF, C—H···N interactions, C—Cl···π and π-π stacking interactions [centroid-to-centroid distance = 3.7719 (14) Å] link the molecules, forming molecular layers approximately parallel to the (002) plane. Additional weak Van der Waals interactions between the layers consolidate the three-dimensional packing. In the crystal of DULTAI, the molecules are connected by a short Cl···H contact (2.96 Å) and C—Cl···π interactions, which contribute to the overall packing energy stabilization, into infinite columns along the *a*-axis direction. In HODQAV, molecules are stacked in columns along the *a* axis *via* weak C—H···Cl hydrogen bonds and face-to-face π–π stacking interactions. The crystal packing is further stabilized by short Cl···Cl contacts. In the crystals of HONBOE and HONBUK, molecules are linked through weak *X*···Cl contacts [*X* = Br for HONBOE and Cl for HONBUK] and C—H···Cl and C—Cl···π interactions into sheets parallel to the *ab* plane. In XIZREG, molecules are linked by C—H···O hydrogen bonds into chains running parallel to the *c* axis. The crystal packing is further stabilized by C—Cl···π, C—F···π and N—O···π interactions

3.4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and treated as riding atoms, C—H = 0.95 Å with U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms and C—H = 0.98 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms. Owing to poor agreement between observed and calculated intensities, twenty four outliers (1 14 0,

-1 13 2, 1 12 2, 2 12 1, 1 12 0, 1 12 3, 0 12 1, 0 13 4, 1 9 2, 0 10 0, 1 10 3, 2 10 0, -2 13 3, 0 14 2, 0 12 2, -1 12 3, -2 12 2, 2 9 0, 1 13 2, -2 13 4, 0 13 3, 0 11 3, -1 10 3, 3 9 2) were omitted during the final refinement cycle.

Table 3. Experimental details

Chemical formula	$C_{16}H_{13}Cl_4N_3$
M_r	389.09
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a; *b; c* (Å)	18.6030 (17); 11.0500 (12); 8.1050 (7)
β (°)	91.393 (8)
V (Å^3)	1665.6 (3)
Z	4
Radiation type	Synchrotron, λ = 0.79313 Å
μ (mm^{-1})	0.96
Crystal size (mm)	0.23 × 0.15 × 0.12
Diffractometer	Rayonix SX165 CCD
Absorption correction	Multi-scan *SCALA [16]*
T_{min}, T_{max}	0.789, 0.876
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12533, 3761, 3040
R_{int}	0.064
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.649
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.150, 1.03
No. of reflections	3761
No. of parameters	211
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.64, −0.57

Computer programs: Marccd [17]), iMosflm [18],, SHELXT [19] , SHELXL [20], ORTEP-3 for Windows [21], PLATON [22].

4. Conclusion

The dihedral angle between the benzene rings of the dichlorophenyl and dimethylaniline groups in the title compound, $C_{16}H_{13}Cl_4N_3$, is 50.85 (13)°. The title molecule shows an *E*

configuration with respect to the –N=N– unit between the aromatic rings. If the two groups of higher priority are on opposite sides of the double bond (*trans* to each other), the bond is assigned the configuration *E* (from *entgegen,* the German word for "opposite"). The molecules ensure the stability of the crystal structure by forming layers parallel to the (100) plane through C—H···π and face-to-face π-π stacking interactions. Thus, important information was obtained about the synthesis and structural properties of a new diazo dye, *"4-{2,2-dichloro-1-[(E)-(2,4-dichlorophenyl)diazenyl]ethenyl}-N,N-dimethylaniline"*.

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КРИСТАЛЛИЧЕСКАЯ СТРУКТУРА И АНАЛИЗ ПОВЕРХНОСТИ ПО ХИРШФЕЛЬДУ 4-{2,2-ДИХЛОР-1-[(E)-(2,4-ДИХЛОРФЕНИЛ)ДИАЗЕНИЛ]ЭТЕНИЛ}-N,N-ДИМЕТИЛАНИЛИНА

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Резюме: В исследуемом соединении $C_{16}H_{13}Cl_4N_3$ двугранный угол между бензольными кольцами дихлорфенильной и диметиланилиновой групп равен 50,85 (13)°. Центральный блок –N=N– имеет конфигурацию E. В кристалле молекулы образуют слои, параллельные плоскости (100) посредством C—H···π и встречных π-π [расстояния между центроидами = 4,0538 (17) и 4,0537 (17) Å] взаимодействий. Эти слои соединены взаимодействиями Ван-

дер-Ваальса для стабилизации кристаллической структуры. Анализ поверхности Хиршфельда показывает, что наиболее важный вклад в кристаллическую упаковку вносят Cl···H/H···Cl (36,4%), H···H (23,3%) и C···H/H··. ·C (15,2%) контакты.

Ключевые слова: Молекулярная структура, Дихлордиазадиены, Отпечаток пальца, Диметиланилиновая группа, Ван-дер-Ваальсовые взаимодействия

4-{2,2-DİXLOR-1-[(E)-(2,4-DİXLORFENİL)DİAZENİL]ETENİL}-N,N-DİMETİLANİLİN KRİSTAL QURULUŞU VƏ HİRŞFELD SƏTH ANALIZI

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Xülasə: Tədqiq edilən $C_{16}H_{13}Cl_4N_3$ birləşməsində, dixlorofenil və dimetilanilin qruplarının benzol halqaları arasındakı dihedral bucaq 50,85 (13) ° bərabərdir. Mərkəzi –N=N– fraqmenti E konfiqurasiyasına malikdir. Kristalda molekullar C—H···π və üz-üzə π-π qarşılıqlı təsirlər [mərkəzdən mərkəzə məsafələr = 4,0538 (17) və 4,0537 (17) Å] ilə (100) müstəvisinə paralel təbəqələr əmələ gətirirlər. Bu təbəqələr kristal quruluşu sabitləşdirmək üçün Van der Waals qarşılıqlı qüvvələri ilə əlaqələnir. Hirshfeld səthinin təhlili göstərir ki, kristal qablaşdırma üçün ən mühüm töhfələr Cl···H/H···Cl (36,4%), H···H (23,3%) və C···H/H·· ·C (15,2%) əlaqələr verir.

Açar sözlər: Molekul quruluşu, Dichlorodiazadienes, Barmaq izi, Dimetilanilin qrupu, Van der Waals qarşılıqlı təsirləri