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The crystal structure of 4-[(2-methoxy-4-nitro-phenylazo)-phenyl]-dimethyl-amine

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Abstract

A monoazo dye, 4-[(2-methoxy-4-nitro-phenylazo)-phenyl]-dimethyl-amine ($C_{15}H_{16}N_4O_3$) was synthesized and characterized by X-ray diffraction, IR, ^{1}H NMR, and elemental analysis. The title molecule crystallizes in the triclinic system, space group *P*-1 (#2), $a = 7.301(4)$, $b = 13.854(7)$, $c = 14.575(7)$ Å, $\alpha = 90.842(9)°$, $\beta = 90.334(9)°$, $\gamma = 91.935(8)°$, $V = 1473.2(13)$ Å^3, $Z = 4$. There are two independent molecules in the asymmetric unit. They have *trans*-geometry about the azo linkage and the torsion angles of central −C−N═N−C− are 175.74° and −175.83°, respectively. The two molecules are interacted through C−H···O and C−H···N hydrogen bond. These pairs of molecules are arranged anti-parallel through π···π interaction ($1 - x$, $1 - y$, $1 - z$), and interacted through C−H···O hydrogen bond and C−H···π interaction forming 'double chains' along [010]. The 'double chains' are interacted through C−H···O, C−H···N hydrogen bonds and C−H···π interaction forming double layers along [110], which are in turn interacted by C−H···O, C−H···N hydrogen bonds and C−H···π interaction along [101] forming crystals.

Keywords: Azobenzene; π···π Interaction; Hydrogen bond

1. Introduction

Aromatic azo compounds represent the dominant class of synthetic colorants [1]; they are used extensively for dyeing fabrics and as colorants in printing. There is also interest in their biochemical applications, because of their ability to bind to proteins [2,3]. Azo dyes incorporating 'push−pull' donor−acceptor aryl rings are of much commercial importance for the dyeing of textiles [4] and some exhibit second- or third-order non-linear optical properties [5]. There is extensive literature on azo dyes, but many of these studies have provided qualitative comparisons between dyes rather than considering their detailed structure.

A good knowledge of the structure of dyes is the key to understand its properties and reactivity. But there are relatively few examples of crystallographic structures in the literatures [6−12]. The relationship between molecular structure, solid-state packing arrangements and dye/pigment performance characteristics has over recent years become an area of increasing investigation [13].

In this work, single crystal X-ray diffraction study and crystal packing analysis of the title compound have been employed to determine both the structure and the important intermolecular interactions in the solid-state of donor−acceptor azobenzene.

2. Experiment

2.1. Synthesis

A solution was formed by dissolving 1.68 g 2-methoxy-4-nitroaniline into 3 ml water in a three-necked flask, which was equipped with an efficient stirrer, a dropping funnel, and a thermometer. The stirrer was started and 3 ml of

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Table 1
Crystal data and structure refinement

Compound	$C_{15}H_{16}N_4O_3$
Color/shape	Red/polyhedron
Formula wt.	300.32
Temp. (K)	193.1 ± 1
Wavelength (Å)	0.7107
Crystal system	Triclinic
Space group	*P*-1
a (Å)	7.301(4)
b (Å)	13.854(7)
c (Å)	14.575(7)
α (°)	90.842(9)
β (°)	90.334(9)
γ (°)	91.935(8)
Cell *V* (Å^3)	1473.2(13)
Formula units/unit cell	4
D_{calc} (g/cm^3)	1.35
F_{000}	632.00
Crystal dimensions (mm)	$0.61 \times 0.30 \times 0.29$
2θ range for data collection (°)	7.2–55.0
Reflections collected	11,769
Absorption correction type	Multi-scan
Independent reflections	6648
Max. and min. transmission	1.0000–0.7481
Data/parameters	4211/429
Goodness-of-fit on F^2	1.06
R indices (all data)	0.051
$wR2[I > 3\sigma(I)]$	0.145
Largest peak and hole in final diff. map (eÅ^{-3})	0.25 and −0.25

concentrated hydrochloric acid was added, heating to 90 °C. The mixture was cooled to 0 °C and the temperature of the mixture was maintained at −5 °C to +5 °C by means of an ice-salt bath. To the stirred mixture, a solution of 0.7 g of sodium nitrite in 2 ml of water was added slowly, drop-wise. After completion of addition, the stirring was continued for 15 min. The solution of the diazonium salt was filtrated to a mixture of 1.21 g *N*,*N*-dimethylaniline and 3 ml concentrated hydrochloric acid, the above diazonium salt was added slowly. The stirring was continued 1 h. Then, the mixture was heated below 40 °C, and made neutral by the addition of hydrated sodium acetate. The solution was filtrated to title compound, washed with a lot of water and a little of ethyl alcohol, and the product was recrystallized six times from acetone. The red crystal was grown from acetone by slow evaporation at ambient temperature for a week. Melting point (uncorrected), 176–177 °C. Elemental analysis (Perkin Elmer 240C elemental analyzer) – Calcd: $C_{15}H_{16}N_4O_3$ (%), C, 60.00; H, 5.33; N, 18.67. Found: C, 59.75; H, 5.35; N, 18.59.

2.2. X-ray crystallography

A red polyhedron crystal with dimensions $0.61 \times 0.30 \times 0.29$ mm was selected for X-ray diffraction. Data were collected at -80 ± 1 °C with a Rigaku Mercury CCD area detector with graphite monochromated Mo-Kα radiation ($\lambda = 0.71070$ Å). A total of 6648 unique ($R_{\text{int}} = 0.027$) reflections was collected in the range of $7.2° < 2\theta < 55°$ with ω scans mode and used in the refinement. The structure was solved by direct methods [14] and expanded using Fourier techniques [15]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically using the riding model. All calculations were performed using the Crystal Structure Analysis Package [16,17], SHELTX-86 and SHELTX-93 programs [18,19]. The details of the X-ray analysis are listed in Table 1. The molecular structure and crystal packing are shown in Figs. 1 and 3.

3. Results and discussion

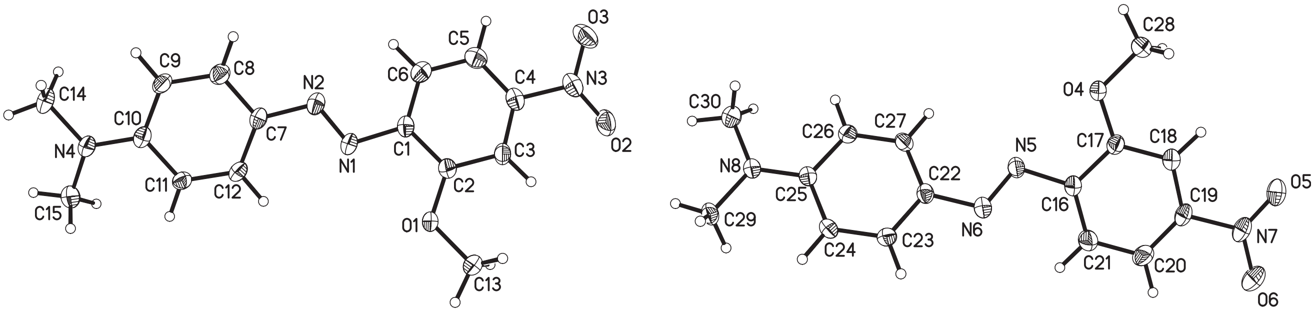
3.1. IR and NMR spectra

IR (FT-IR spectrometer with KBr pellets, cm^{-1}): 3104 (w), 2909 (s), 1602 (s), 1516 (s), 1421 (m), 1371 (s), 1339 (s, –N═N–), 1305(m), 1240 (m), 1139 (s), 1088 (s), 1018 (s), 828 (m).

^{1}H NMR data (Bruker AV-400 NMR spectrometer, DMSO-d_6 as solvent, ^{1}H (399.97 MHz), ambient temperature, ppm): 3.146 (s, 6H, $-N(CH_3)_2$), 4.100 (s, 3H, $-OCH_3$), 6.845–6.864 (d, H5, H6), 7.700–7.721 (d, H4, H7), 7.891–7.917 (d, H1, H2), 7.935–7.955 (d, H3) [20].

3.2. Molecular structure

The asymmetric unit is shown in Fig. 2. There are two molecules in the asymmetric unit, i.e. molecule A and molecule B (Fig. 1). Since the two molecules in the asymmetric unit are not related by crystallographic symmetry, and are



Molecule A Molecule B

Fig. 1. Molecular structure of the title compound.

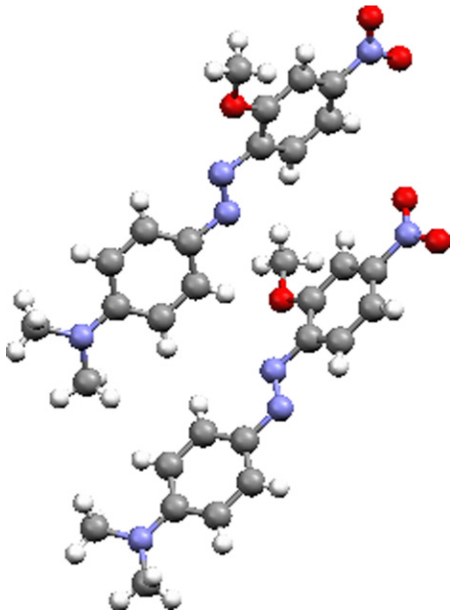


Fig. 2. Asymmetric unit viewed from axis *a*.

consequently refined separately, differences in bond distances and angles might be expected. In Table 2, the important molecular features for the two molecules in the asymmetric unit are compared with the range of reported values for donor−acceptor azobenzenes in the literatures [21,22]. The dihedral angles are listed in Table 3.

In general there is good agreement between the molecular features of the new structure and previously reported data on donor−acceptor azobenzenes. The bond lengths and bond angles all show excellent agreement with the known data, but the torsion angles are out of the reported range. The bigger values of the torsion angles are indications of the nonplanarity of the

Table 2
The important structural features in molecule A and molecule B of the asymmetric unit

Structural feature	Molecule A	Molecule B	Range reported [21,22]
Bond lengths (Å)			
N=N	1.264	1.266	1.254−1.294
C−NO_2	1.465	1.472	1.446−1.472
C−NMe_2	1.373	1.375	1.353−1.415
Bond angles (°)			
N2−N1−C1	112.6		111.0−114.5
N6−N5−C16		112.0	
N1−N2−C7	114.8		113.0−118.9
N5−N6−C22		115.4	
Torsion angles (°)			
N1−N2−C7−C12	−1.5		−1.5 to 6.0
N5−N6−C22−C27		4.9	
N2−N1−C1−C6	−18.9		−4.2 to 5.6
N6−N5−C16−C21		24.6	
C14−N4−C10−C9	0.1		8.5−12.8
C29−N8−C25−C24		−2.4	
C15−N4−C10−C11	−11.2		4.8−9.3
C30−N8−C25−C26		−1.2	

Table 3
Dihedral angles in molecule A and molecule B of the asymmetric unit

Molecule A		Molecule B	
Plane	Dihedral angles (°)	Plane	Dihedral angles (°)
1−2	21.54	6−7	29.65
1−3	18.30	6−8	23.33
2−3	5.04	7−8	6.52
1−4	8.78	6−9	6.64
2−5	7.80	7−10	4.14

Plane 1: C1−C6; Plane 2: C7−C12; Plane 3: C7−N2−N1−C1; Plane 4: NO_2 in molecule A; Plane 5: NMe_2 in molecule A; Plane 6: C16−C21; Plane 7: C22−C27; Plane 8: C22−N6−N5−C16; Plane 9: NO_2 in molecule B; Plane 10: NMe_2 in molecule B.

Table 4
Atomic coordinates and B_{iso}/B_{eq}

Atom	*x*/*a*	*y*/*b*	*z*/*c*	B_{eq} (Å^2)
O1	0.6540(3)	0.31797(13)	0.38784(11)	3.84(4)
O2	0.4116(3)	0.57467(13)	0.18652(11)	3.83(4)
O3	0.2109(3)	0.64488(13)	0.27030(12)	3.99(5)
O4	−0.1596(2)	0.21002(12)	0.00005(11)	3.30(4)
O5	0.0720(3)	0.4960(1)	−0.17653(12)	4.47(5)
O6	0.2932(3)	0.55834(13)	−0.09488(12)	3.69(4)
N1	0.4244(3)	0.30316(13)	0.52950(11)	2.31(4)
N2	0.3443(3)	0.31879(13)	0.60468(12)	2.41(4)
N3	0.3213(3)	0.5816(1)	0.25721(13)	2.86(4)
N4	0.3384(3)	0.0283(1)	0.86762(12)	2.62(4)
N5	0.0806(3)	0.18748(13)	0.13651(11)	2.22(4)
N6	0.1585(3)	0.20078(13)	0.21374(12)	2.27(4)
N7	0.1718(3)	0.4964(1)	−0.10912(13)	2.69(4)
N8	0.1689(3)	−0.10269(13)	0.46200(11)	2.17(4)
C1	0.3975(3)	0.3774(2)	0.4646(1)	2.19(4)
C2	0.5162(3)	0.3811(2)	0.3885(2)	2.44(5)
C3	0.4887(3)	0.4479(2)	0.3202(1)	2.48(5)
C4	0.3473(3)	0.5108(2)	0.3295(1)	2.43(5)
C5	0.2312(3)	0.5100(2)	0.4031(2)	3.09(5)
C6	0.2573(3)	0.4422(2)	0.4706(2)	2.95(5)
C7	0.3559(3)	0.2440(2)	0.66909(13)	2.12(4)
C8	0.2683(3)	0.2595(2)	0.7527(1)	2.57(5)
C9	0.2655(3)	0.1894(2)	0.8193(1)	2.44(5)
C10	0.3468(3)	0.1002(2)	0.80381(13)	2.09(4)
C11	0.4383(3)	0.0865(2)	0.71971(13)	2.22(4)
C12	0.4429(3)	0.1572(2)	0.6542(1)	2.19(4)
C13	0.7784(5)	0.3225(3)	0.3124(2)	6.15(9)
C14	0.2436(4)	0.0424(2)	0.9540(2)	3.29(6)
C15	0.3932(4)	−0.0685(2)	0.8440(2)	3.39(6)
C16	0.1039(3)	0.2692(2)	0.07908(13)	2.08(4)
C17	−0.0211(3)	0.2783(2)	0.0059(1)	2.16(4)
C18	0.0007(3)	0.3535(2)	−0.0551(1)	2.27(4)
C19	0.1473(3)	0.4181(2)	−0.0426(1)	2.29(4)
C20	0.2718(4)	0.4120(2)	0.0281(2)	2.98(5)
C21	0.2491(3)	0.3362(2)	0.0885(2)	2.84(5)
C22	0.1525(3)	0.1209(2)	0.27215(13)	1.96(4)
C23	0.2271(3)	0.1371(2)	0.3597(1)	2.19(4)
C24	0.2295(3)	0.0643(2)	0.4237(1)	2.12(4)
C25	0.1606(3)	−0.0296(2)	0.40129(13)	1.83(4)
C26	0.0849(3)	−0.0451(2)	0.3118(1)	2.19(4)
C27	0.0809(3)	0.0280(2)	0.2493(1)	2.20(4)
C28	−0.2919(4)	0.2197(2)	−0.0720(2)	5.14(8)
C29	0.2560(3)	−0.0883(2)	0.5518(1)	2.57(5)
C30	0.0987(4)	−0.1998(2)	0.4404(2)	3.11(5)
H1	0.5660(3)	0.4503(2)	0.2680(1)	2.95(9)

(*continued on next page*)

Table 4 (*continued*)

Atom	*x*/*a*	*y*/*b*	*z*/*c*	B_{eq} (Å^2)
H2	0.1356(3)	0.5547(2)	0.4078(2)	3.73(10)
H3	0.1776(3)	0.4401(2)	0.5219(2)	3.54(9)
H4	0.2100(3)	0.3187(2)	0.7639(1)	3.08(9)
H5	0.2079(3)	0.2017(2)	0.8764(1)	2.93(9)
H6	0.4975(3)	0.0276(2)	0.70816(13)	2.68(9)
H7	0.5061(3)	0.1467(2)	0.5983(1)	2.64(9)
H8	0.8677(5)	0.2748(3)	0.3192(2)	7.5(1)
H9	0.7128(5)	0.3110(3)	0.2565(2)	7.5(2)
H10	0.8373(5)	0.3846(3)	0.3113(2)	7.5(1)
H11	0.2994(4)	0.0956(2)	0.9867(2)	3.95(10)
H12	0.1187(4)	0.0550(2)	0.9421(2)	3.99(10)
H13	0.2510(4)	−0.0142(2)	0.9897(2)	3.96(10)
H14	0.3782(4)	−0.1088(2)	0.8958(2)	4.13(10)
H15	0.3192(4)	−0.0935(2)	0.7948(2)	4.11(10)
H16	0.5181(4)	−0.0666(2)	0.8260(2)	4.12(10)
H17	−0.0834(3)	0.3606(2)	−0.1043(1)	2.73(9)
H18	0.3702(4)	0.4582(2)	0.0353(2)	3.56(9)
H19	0.3344(3)	0.3299(2)	0.1374(2)	3.38(9)
H20	0.2770(3)	0.1994(2)	0.3757(1)	2.63(9)
H21	0.2781(3)	0.0776(2)	0.4833(1)	2.56(9)
H22	0.0361(3)	−0.1073(2)	0.2950(1)	2.63(9)
H23	0.0293(3)	0.0158(2)	0.1902(1)	2.62(9)
H24	−0.3502(4)	0.2797(2)	−0.0650(2)	6.11(12)
H25	−0.2322(4)	0.2177(2)	−0.1297(2)	6.11(12)
H26	−0.3811(4)	0.1683(2)	−0.0692(2)	6.13(12)
H27	0.2489(3)	−0.1470(2)	0.5847(1)	3.16(9)
H28	0.3809(3)	−0.0688(2)	0.5441(1)	3.14(9)
H29	0.1948(3)	−0.0397(2)	0.5852(1)	3.14(9)
H30	−0.0288(4)	−0.1982(2)	0.4273(2)	3.79(10)
H31	0.1609(4)	−0.2244(2)	0.3884(2)	3.76(10)
H32	0.1180(4)	−0.2403(2)	0.4913(2)	3.77(10)

$B_{eq} = 8/3\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$.

Table 5
Selected bond lengths and bond angles (Å, °)

Molecule A		Molecule B	
Atoms	Distances	Atoms	Distances
O1−C2	1.355(3)	O4−C17	1.362(3)
O2−N3	1.231(3)	O5−N7	1.220(3)
N1−N2	1.264(3)	N5−N6	1.266(2)
N1−C1	1.425(3)	N5−C16	1.424(3)
N2−C7	1.413(3)	N6−C22	1.406(3)
N4−C10	1.373(3)	N8−C25	1.357(3)
N3−C4	1.465(3)	N7−C19	1.472(3)
	Angles		Angles
C2−O1−C13	117.2(2)	C17−O4−C28	117.2(2)
N2−N1−C1	112.6(2)	N6−N5−C16	112.0(2)
N1−N2−C7	114.8(2)	N5−N6−C22	115.4(2)
N1−C1−C2	117.2(2)	N5−C16−C17	117.6(2)
N3−C4−C5	119.0(2)	N7−C19−C20	118.8(2)
C10−N4−C14	120.6(2)	C25−N8−C25	121.3(2)
C13−O1−C2−C1	−178.4(3)	C28−O4−C17−C16	177.9(2)
O3−N3−C4−C5	8.5(3)	O6−N7−C19−C20	−6.2(3)
N2−N1−C1−C6	−18.9(3)	N6−N5−C16−C21	24.6(3)
C1−N1−N2−C7	175.8(2)	C16−N5−N6−C22	−175.8(2)
N1−N2−C7−C8	−179.9(2)	N5−N6−C22−C23	−175.8(2)
C14−N4−C10−C11	−179.8(2)	C29−N8−C25−C26	176.4(2)

Table 6
Hydrogen bond geometries (Å, °)

D	H	A	H···A	D···A	∠D-H···A	Sym. Cod.
C20	H18	O2	2.722	3.334	122.9	*x*, *y*, *z*
C23	H20	N1	2.832	3.614	140.1	*x*, *y*, *z*
C13	H10	O5	2.659	3.380	133.2	1 − *x*, 1 − *y*, −*z*
C20	H18	O6	2.620	3.327	131.5	1 − *x*, 1 − *y*, −*z*
C3	H1	O6	2.733	3.659	165.1	1 − *x*, 1 − *y*, −*z*
C13	H9	O6	2.993	3.639	126.4	1 − *x*, 1 − *y*, −*z*
C29	H32	O1	2.532	3.398	151.6	1 − *x*, −*y*, 1 − *z*
C30	H32	O1	2.678	3.532	149.9	1 − *x*, −*y*, 1 − *z*
C12	H7	N8	2.623	3.411	140.6	1 − *x*, −*y*, 1 − *z*
C28	H24	O2	2.750	3.458	131.8	−*x*, 1 − *y*, −*z*
C28	H25	O3	2.819	3.511	130.5	−*x*, 1 − *y*, −*z*
C18	H17	O3	2.586	3.489	158.8	−*x*, 1 − *y*, −*z*
C18	H17	O2	2.850	3.730	154.4	−*x*, 1 − *y*, −*z*
C18	H17	N3	2.954	3.893	169.9	−*x*, 1 − *y*, −*z*
C30	H30	N2	2.832	3.632	142.5	−*x*, −*y*, 1 − *z*
C15	H14	O4	2.600	3.445	148.4	−*x*, −*y*, 1 − *z*
C14	H13	O4	2.778	3.603	145.7	−*x*, −*y*, 1 − *z*
C27	H23	N4	2.853	3.553	131.5	−*x*, −*y*, 1 − *z*

whole molecule, which is different from most of 4-nitro-4′-aminoazobenzenes [21,25−30]. Both molecules have *trans*-geometry about the azo linkage and the torsion angle of central −C−N═N−C− is 175.74° and −175.83°, respectively. The dihedral angle between the two aromatic rings is 21.54° in molecule A and 29.65° in molecule B (Table 3, line 1). From Table 3, lines 1−3, the data imply that the two aromatic rings rotate oppositely along the axis of N═N. The 4-nitro group is almost coplanar with the aromatic ring as indicated by the dihedral angle of 8.78° in molecule A and 6.64° in molecule B. The 4′-dimethylamino group is also coplanar to the aromatic ring with the dihedral angle of 7.8° in molecule A and 4.14° in molecule B.

3.3. Crystal structure

The atomic fractional coordinates and equivalent isotropic thermal parameters for atoms are given in Table 4. The selected bond lengths and angles are listed in Table 5.

Crystal packing analysis was done using OPEC [23] program, which was locally modified with additional calculation routines added. Given a reference molecule (FM) and the intermolecular interactions being limited within 15 Å, approximate 60−150 surrounding molecules (SM) consist of the crystal model. The molecules, which are most strongly interacted with the FM, are listed in Tables 6 and 7.

Table 7
C−H···π [24] interaction

Interaction	H···P[a]	C···P	∠C−H···P	Sym. Cod.
C11−H6···PL7	2.834	3.628	141.7	1 − *x*, −*y*, 1 − *z*
C29−H29···PL7	2.810	3.492	129.5	−*x*, −*y*, 1 − *z*
C30−H30···PL3	2.962	3.775	144.3	−*x*, −*y*, 1 − *z*
C26−H22···PL2	2.983	3.661	129.4	−*x*, −*y*, 1 − *z*
C18−H17···PL4	2.645	3.591	174.1	−*x*, 1 − *y*, −*z*
C28−H24···PL4	3.048	3.506	111.3	−*x*, 1 − *y*, −*z*
C28−H25···PL4	3.068	3.506	109.8	−*x*, 1 − *y*, −*z*
C3−H1···PL9	2.814	3.756	171.0	1 − *x*, 1 − *y*, −*z*

[a] P is the center of corresponding plane (PL).

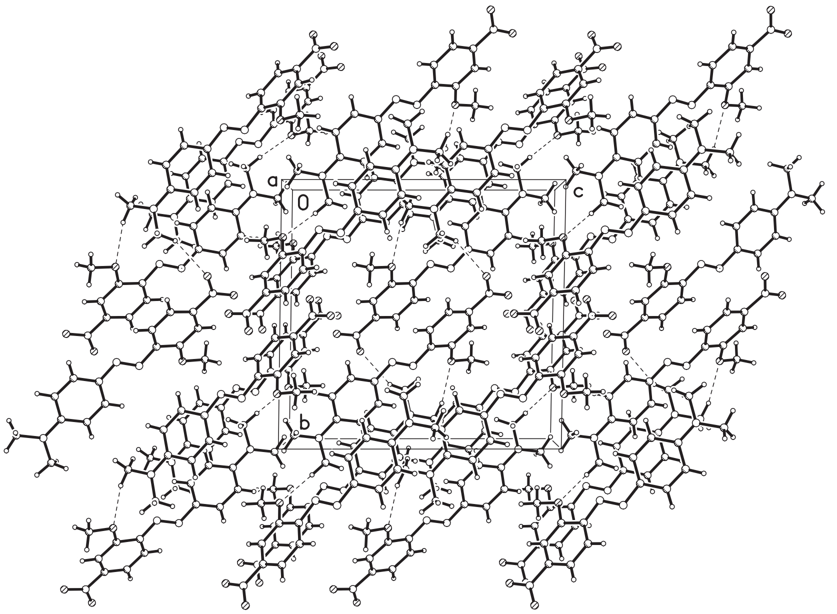


Fig. 3. Packing diagram viewed down axis *a*.

As shown from the tables, molecule A and molecule B are interacted through C−H···O and C−H···N hydrogen bonds (Table 6, lines 1, 2). These pair of molecules are arranged anti-paralleled through π···π [23] interaction (distance of plane 1-1: 3.485; distance between two centers of two planes: 3.815, $1-x$, $1-y$, $1-z$; Plane 1 is C1−C6), and interacted through C−H···O hydrogen bond (Table 6, lines 7, 8), C−H···N hydrogen bond (Table 6, line 9) and C−H···π interaction (Table 7, line 1) forming 'double chains' along [010]. The 'double chains' are interacted through C−H···O hydrogen bond (Table 6, lines 16, 17), C−H···N hydrogen bond (Table 6, lines 15, 18) and C−H···π interaction (Table 7, lines 2−4) forming 'double layers' along [110], which are in turn interacted by C−H···O hydrogen bond (Table 6, lines 10−13), C−H···N hydrogen bond (Table 6, line 14) and C−H···π interaction (Table 7, lines 5−7) along [101] forming crystals (Fig. 3).

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