C1—C6		1.527 (4)	1.528 (4)	1.530 (3)
C1—C7	1.507 (11)	1.523 (4)	1.516 (4)	1.513 (3)
C2—C3	1.519 (11)	1.530 (4)	1.537 (3)	1.529 (2)
C3—C4		1.528 (4)	1.519 (3)	1.524 (3)
C4—C5		1.532 (6)	1.528 (3)	1.529 (3)
C5—C6		1.515 (4)	1.527 (4)	1.520 (3)
C3—N1—C8		109.0 (2)	111.6 (2)	110.4 (1)
C3—N1—C9		110.9 (2)	107.6 (1)	108.8 (1)
C3—N1—C10		112.7 (2)	112.6 (2)	114.2 (1)
C2—C1—C6		111.0 (2)	112.7 (2)	110.8 (1)
C2—C1—C7	111.5 (6)	110.9 (2)	109.0 (2)	112.5 (2)
C6—C1—C7		112.5 (3)	111.2 (2)	113.9 (2)
O3—C2—C1	108.7 (7)	109.3 (2)	113.7 (2)	108.9 (1)
O3—C2—C3	111.3 (7)	112.4 (2)	113.6 (2)	108.4 (1)
C1—C2—C3	107.2 (6)	111.4 (2)	108.6 (2)	109.3 (1)
N1—C3—C2	116.8 (7)	113.2 (2)	112.3 (2)	112.7 (1)
N1—C3—C4		112.7 (2)	112.1 (2)	115.2 (1)
O1—C7—O2	123.3 (8)	122.7 (3)	123.0 (3)	123.4 (2)
O1—C7—C1	111.8 (7)	111.2 (2)	111.5 (2)	112.7 (2)
O2—C7—C1	124.9 (7)	126.2 (3)	125.5 (3)	123.8 (2)
C2—C3—C4		108.4 (2)	112.3 (2)	110.1 (1)
C3—C4—C5		109.1 (3)	108.9 (2)	107.2 (2)
C4—C5—C6		111.6 (3)	110.7 (2)	113.4 (2)
C1—C6—C5		111.8 (2)	110.9 (2)	111.9 (2)
C6—C1—C2—C3		55.0 (3)	−53.6 (2)	56.6 (2)
C7—C1—C2—O3	73.4	53.9 (3)	−50.2 (2)	169.6 (2)
C7—C1—C2—C3	−166.2	−70.9 (3)	−177.6 (2)	−72.1 (2)
C2—C1—C6—C5		−51.4 (3)	54.5 (3)	−51.3 (2)
C2—C1—C7—O2	22.7	50.7 (4)	116.9 (2)	−1.83 (3)
O3—C2—C3—N1	−66.4	51.0 (3)	56.8 (2)	−74.9 (2)
C1—C2—C3—N1	174.8	174.1 (2)	−175.6 (1)	166.4 (1)
C1—C2—C3—C4		−60.1 (3)	57.0 (2)	−63.4 (2)
C2—C3—C4—C5		61.4 (3)	−60.2 (2)	62.2 (2)
C3—C4—C5—C6		−59.5 (3)	58.9 (2)	−57.0 (2)
C4—C5—C6—C1		54.4 (4)	−56.5 (2)	52.7 (2)
Cl···HO1	1.83	2.31 (4)	2.24 (4)	2.30 (3)
Cl···O1	3.00	2.988 (3)	2.973 (2)	3.025 (2)
Cl···HO3	2.23	2.31 (3)	2.40 (3)	5.96 (3)[b]
Cl···O3	3.06	3.168 (2)	3.130 (3)	5.246 (2)[b]
HO1···Cl···HO3	84	95 (1)	100 (1)	
O1···HO1···Cl	169	141 (4)	161 (3)	167 (3)
O3···HO3···Cl	138	168 (3)	153 (3)	

(*a*) Data from Tomita, Urabe, Kim & Fujiwara (1974). (*b*) Distances are much too long for hydrogen bonding.

The space groups for structures (2) ($P2_1/n$) and (4) ($P2_12_12_1$) were uniquely defined by their systematic absences. The space group for structure (3) (Cc) was not uniquely defined by the systematic absences but was proven to be correct by the successful structure refinement. The structure solutions and refinements were carried out using *MolEN* (Fair, 1990). Both linear decay corrections and empirical absorption corrections were applied to the data. The chloride ions were located in the Patterson maps and the remainder of the atoms were located by difference Fourier syntheses. All non-H atoms were refined anisotropically. The H atoms were also refined with fixed isotropic thermal parameters. Data were weighted using a non-Poisson scheme with an experimental uncertainty factor of 0.03 for all three structures. A secondary-extinction correction was applied and the extinction coefficient was refined. In the last stage of the refinements, no parameter varied by more than 0.02 of its standard deviation. The final difference Fourier maps had no interpretable peaks. For the noncentrosymmetric space groups of (3) and (4), both enantiomers were refined, and R, wR and S are reported for both refinements. Data and figures are for the enantiomers with the lower values. Corrections for anomalous dispersion were taken from Cromer (1974) and applied to the chloride ions.

ORTEP (Johnson, 1976) plots of (2), (3) and (4) are given in Figs. 1(*a*), 1(*b*) and 1(*c*), respectively. Unit-cell diagrams for (2), (3) and (4) are given in Figs. 2(*a*), 2(*b*) and 2(*c*). Note that, while (1) contains the (2*R*) configuration [numbered as in (2)–(4)], the configurations illustrated in Figs. 1(*a*–*c*) for (2)–(4) are (1*S*,2*S*,3*S*), (1*R*,2*S*,3*S*), and (1*S*,2*R*,3*S*), respectively.

Data collection and cell refinement: *CAD*-4 *Software* (Enraf–Nonius, 1989). Program used to solve structure: *MolEN* (Fair, 1990). Program used to refine structure: *MolEN*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *MolEN*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BK1049). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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4,4′-Azoxydianisole at 203 K

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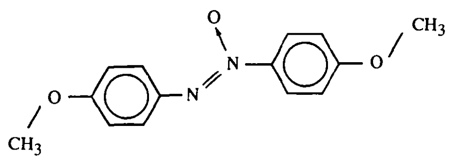
Abstract

The crystal structure determination of the title compound, $C_{14}H_{14}N_2O_3$, reinvestigated using low-

temperature X-ray diffraction data, confirms the earlier report. However, the almost planar molecule is observed in a disordered state. Two partial molecules exist in unequal proportions (75:25). They are related to one another through a pseudo-twofold axis of rotation contained in the molecular plane and normal to the molecular axis. The dihedral angle between the two aromatic systems is 22.1 (9)°.

Comment

In our study of liquid-crystal molecules and their relations to liquid-crystal polymers, we were interested in the nature of the mesomorphic transformation to the nematic phase upon heating of 4,4′-azoxydianisole (1). This molecule has been studied extensively. A paper by Krigbaum, Chatani & Barber (1970) established the crystal structure of its stable modification using diffractometer intensities measured at room temperature. The final value of R reached 0.091 when H atoms were included. Two peaks having a residual electron density of 0.7 e Å^{-3} were found in the plane of the azoxy group, in a direction perpendicular to the N=N bond. The authors suggested the possibility of a slight disorder similar to that observed in *p*-azotoluene (Brown, 1966). Carlisle & Smith (1971), using visually estimated intensities, also solved the structure which was refined to R = 0.186 without H atoms. A third determination (Bednowitz, 1970) yielded an R factor of 0.081 when H atoms were included. We were puzzled by the mediocre quality of the results and decided to reinvestigate the crystal structure of this material.



(1)

Fig. 1 shows an *ORTEP* (Johnson, 1965) drawing of the molecular structure with atomic labels, while the final atomic coordinates and the equivalent temperature factors, along with their standard deviations, are listed in Table 1. They are related through a pseudo-twofold axis of rotation, which is in the molecular plane and also passes through the azoxy O atom. The relative disposition of the two disordered molecules is shown in Fig. 2.

In the major molecule, the C—C bond distances in the two aromatic rings have an average of 1.389 Å. The N=N bond length, 1.281 (4) Å, is short enough to indicate its double-bond character; the N—O bond length is found to be 1.288 (3) Å. The two aromatic rings are planar within experimental errors. Plane I contains C(3)→C(8) (χ^2 = 1.61), and atoms O(2) and N(9) are within 6σ from this plane. The azoxy group, plane II, containing O(11), N(9), N(10) and C(6), is also planar (χ^2 = 0.04); when C(12) is included in the calculation for plane II, χ^2 is 245. This value reveals that C(12) is significantly out of plane II. Plane III is made up of C(12)→C(17) (χ^2 = 14.9). However, the overall molecule is not planar since the dihedral angles between the various groups are: I/II = 3.3 (6), I/III = 22.1 (9) and II/III = 18.8 (8)°. One can also describe the molecular conformation by the values taken by the two torsion angles N(9)—N(10)—C(12)—C(17) and N(10)—N(9)—C(6)—C(5), which have values of 18.2 (5) and 4.0 (5)°, respectively. The above shows that the molecule consists of two planar fragments twisted by *ca* 20° with respect to one another. The molecular packing of 4,4′-azoxydianisole is shown in Fig. 3.

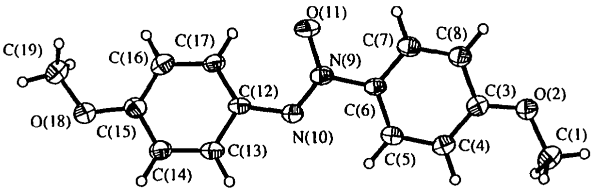


Fig. 1. *ORTEP* (Johnson, 1965) view of the molecule and atomic numbering. The displacement ellipsoids are plotted at the 40% probability level.

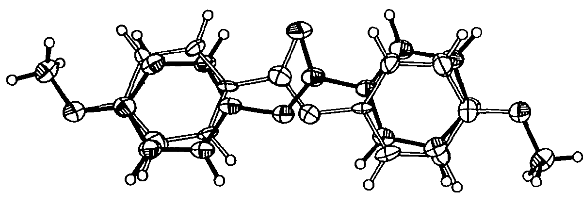


Fig. 2. Superposition of the two (major 75%, minor 25%) molecules.

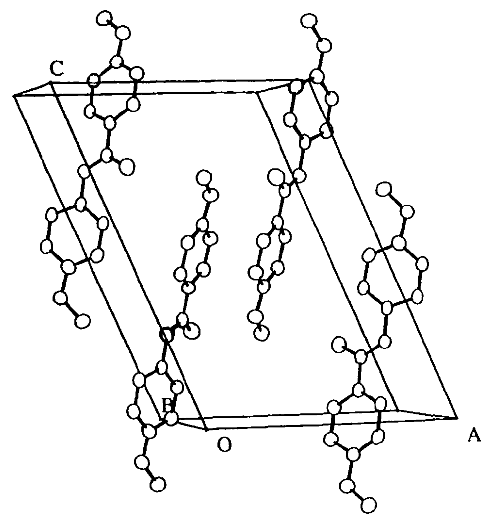


Fig. 3. Content of a unit cell.

Experimental

Single crystals of 4,4′-azoxydianisole (Aldrich) were obtained as thin platelets by slow evaporation (2 months) of a tetrahydrofuran solution at room temperature.

Crystal data

$C_{14}H_{14}N_2O_3$	Cu $K\alpha$ radiation
$M_r = 258.28$	$\lambda = 1.5418$ Å
Monoclinic	Cell parameters from 25 reflections
$P2_1/c$	$\theta = 20–24°$
$a = 10.9822$ (22) Å	$\mu = 0.71$ mm^{-1}
$b = 8.0799$ (16) Å	$T = 203$ K
$c = 15.449$ (3) Å	Platelet
$\beta = 113.28$ (12)°	0.47 × 0.46 × 0.11 mm
$V = 1259.3$ (4) Å^3	Yellow
$Z = 4$	
$D_x = 1.362$ Mg m^{-3}	
$D_m = 1.291$ Mg m^{-3}	
D_m measured by flotation in an aqueous $ZnCl_2$ solution	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.030$
$\omega/2\theta$ scans	$\theta_{max} = 70.0°$
Absorption correction: none	$h = -13 \rightarrow 13$
9667 measured reflections	$k = -9 \rightarrow 9$
2384 independent reflections	$l = -18 \rightarrow 18$
1941 observed reflections [$I \geq 2.0\sigma(I)$]	3 standard reflections frequency: 30 min intensity decay: ≤1.2%

Refinement

Refinement on F	$\Delta\rho_{max} = 0.17$ e Å^{-3}
$R = 0.052$	$\Delta\rho_{min} = -0.22$ e Å^{-3}
$wR = 0.059$	Extinction correction: none
$S = 2.68$	Atomic scattering factors from Cromer & Mann (1968) for C, N, O and Stewart, Davidson & Simpson (1965) for H atoms
1941 reflections	
301 parameters	
$w = 1/[\sigma^2(F) + 0.0001F^2]$	
$(\Delta/\sigma)_{max} = 0.06$	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{eq} = (1/3)\Sigma_i\Sigma_j B_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
C(1)	0.4867 (3)	−0.0489 (3)	0.7657 (2)	5.6 (1)
O(2)	0.4639 (2)	0.0860 (2)	0.8165 (1)	5.2 (1)
C(3)	0.5457 (4)	0.1102 (5)	0.9063 (3)	4.3 (1)
C(4)	0.6556 (4)	0.0157 (5)	0.9586 (3)	4.9 (1)
C(5)	0.7323 (3)	0.0579 (4)	1.0519 (2)	4.2 (1)
C(6)	0.6988 (3)	0.1944 (4)	1.0923 (2)	3.7 (1)
C(7)	0.5893 (3)	0.2872 (4)	1.0403 (2)	4.7 (1)
C(8)	0.5133 (3)	0.2456 (4)	0.9478 (2)	4.8 (1)
N(9)	0.7756 (3)	0.2377 (3)	1.1895 (2)	4.1 (1)
N(10)	0.8791 (3)	0.1501 (3)	1.2332 (2)	4.2 (1)
O(11)	0.7371 (2)	0.3595 (2)	1.2261 (1)	6.0 (1)
C(12)	0.9550 (3)	0.1779 (4)	1.3312 (2)	3.7 (1)
C(13)	1.0777 (3)	0.0958 (4)	1.3643 (2)	4.5 (1)
C(14)	1.1575 (3)	0.0988 (4)	1.4591 (2)	4.7 (1)
C(15)	1.1182 (4)	0.1774 (5)	1.5229 (3)	4.6 (1)
C(16)	0.9962 (4)	0.2584 (4)	1.4893 (3)	5.0 (1)
C(17)	0.9156 (3)	0.2594 (4)	1.3942 (2)	4.3 (1)
O(18)	1.2049 (1)	0.1671 (2)	1.6149 (1)	5.2 (1)
C(19)	1.1697 (2)	0.2396 (3)	1.6861 (2)	5.6 (1)
C(3′)	0.5570 (6)	0.1101 (8)	0.9080 (5)	4.0 (2)
C(4′)	0.6583 (7)	−0.0053 (8)	0.9480 (5)	4.0 (2)
C(5′)	0.7461 (7)	0.0111 (8)	1.0419 (5)	4.6 (2)
C(6′)	0.7327 (7)	0.1430 (8)	1.0958 (5)	2.8 (2)
C(7′)	0.6314 (7)	0.2584 (8)	1.0557 (5)	4.4 (2)
C(8′)	0.5435 (7)	0.2420 (8)	0.9619 (5)	5.3 (2)
N(9′)	0.8302 (8)	0.1384 (9)	1.1887 (6)	4.4 (2)
N(10′)	0.8293 (8)	0.2438 (9)	1.2496 (6)	4.4 (2)
C(12′)	0.9263 (6)	0.2223 (7)	1.3427 (4)	2.8 (2)
C(13′)	1.0399 (6)	0.1278 (7)	1.3601 (4)	3.4 (2)
C(14′)	1.1334 (6)	0.1086 (7)	1.4521 (4)	5.4 (2)
C(15′)	1.1134 (6)	0.1839 (7)	1.5267 (4)	3.2 (2)
C(16′)	0.9999 (6)	0.2785 (7)	1.5092 (4)	3.6 (2)
C(17′)	0.9063 (6)	0.2976 (7)	1.4172 (4)	3.8 (2)

Table 2. *Geometric parameters* (Å, °)

C(1)—O(2)	1.423 (4)	N(9)—O(11)	1.288 (3)
O(2)—C(3)	1.337 (3)	N(10)—C(12)	1.428 (4)
C(3)—C(4)	1.384 (6)	C(12)—C(13)	1.404 (5)
C(3)—C(8)	1.385 (5)	C(12)—C(17)	1.378 (5)
C(4)—C(5)	1.394 (5)	C(13)—C(14)	1.378 (4)
C(5)—C(6)	1.387 (5)	C(14)—C(15)	1.377 (6)
C(6)—C(7)	1.375 (5)	C(15)—C(16)	1.394 (6)
C(6)—N(9)	1.445 (4)	C(15)—O(18)	1.365 (4)
C(7)—C(8)	1.382 (5)	C(16)—C(17)	1.383 (5)
N(9)—N(10)	1.281 (4)	O(18)—C(19)	1.428 (3)
O(2)—C(3′)	1.392 (7)	N(10′)—C(12′)	1.422 (9)
C(6′)—N(9′)	1.412 (9)	C(15′)—O(18)	1.342 (6)
N(9′)—N(10′)	1.272 (9)	N(10′)—O(11)	1.319 (8)
C(1)—O(2)—C(3)	119.4 (2)	C(16)—C(15)—O(18)	126.1 (4)
O(2)—C(3)—C(4)	126.8 (4)	C(15)—C(16)—C(17)	121.0 (4)
O(2)—C(3)—C(8)	113.8 (3)	C(6)—N(9)—N(10)	116.5 (3)
C(4)—C(3)—C(8)	119.3 (4)	C(6)—N(9)—O(11)	118.9 (3)
C(3)—C(4)—C(5)	119.9 (4)	C(1)—O(2)—C(3′)	116.6 (3)
C(4)—C(5)—C(6)	119.9 (3)	O(2)—C(3′)—C(4′)	119.5 (6)
C(5)—C(6)—C(7)	119.9 (3)	O(2)—C(3′)—C(8′)	120.3 (6)
C(5)—C(6)—N(9)	120.7 (3)	C(5′)—C(6′)—N(9′)	111.7 (7)
C(7)—C(6)—N(9)	119.5 (3)	C(14′)—C(15′)—O(18)	119.7 (5)
C(6)—C(7)—C(8)	120.2 (3)	C(16′)—C(15′)—O(18)	120.3 (5)
C(3)—C(8)—C(7)	120.7 (3)	C(15′)—O(18)—C(19)	114.7 (3)
N(10)—N(9)—O(11)	124.6 (3)	C(12)—C(17)—C(16)	120.0 (3)
N(9)—N(10)—C(12)	119.8 (3)	C(15)—O(18)—C(19)	119.1 (2)
N(10)—C(12)—C(13)	112.7 (3)	C(12′)—N(10′)—O(11)	123.4 (7)
N(10)—C(12)—C(17)	127.5 (3)	N(9′)—N(10′)—C(12′)	116.4 (7)
C(13)—C(12)—C(17)	119.4 (3)	N(10′)—C(12′)—C(13′)	121.1 (6)
C(12)—C(13)—C(14)	119.6 (3)	C(7′)—C(6′)—N(9′)	128.4 (7)
C(13)—C(14)—C(15)	121.4 (4)	C(6′)—N(9′)—N(10′)	120.6 (8)
C(14)—C(15)—C(16)	118.5 (4)	O(11)—N(10′)—N(9′)	120.1 (7)
C(14)—C(15)—O(18)	115.5 (3)		

The X-ray intensities were collected at low temperature, in order to improve the quality of the data. The structure was solved by direct methods and refined using *SHELX*76 (Sheldrick, 1976). At first, the two six-membered rings could be clearly recognized while the central part of the molecule seemed disordered. Following a succession of refinements and difference Fourier syntheses, two disordered molecules were recognized in a 75:25 proportion. All but the two terminal O—CH_3 atoms and the azoxy O atom could be resolved. These five atoms were thus considered to be common to both molecules, *i.e.* not disordered. Their temperature factors are only slightly larger than those of the other atoms. The structure was refined by full-matrix least squares using anisotropic temperature factors for all non-H atoms of the major (75%) molecule. For the minor (25%) component, however, the two six-membered rings were refined as rigid groups with d(C—C) = 1.395 Å and 120° angles. The H atoms were kept at their fixed positions, d(C—H) = 0.95 Å, but their isotropic temperature factors were refined.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, least-squares-planes data and torsion angles have been deposited with the IUCr (Reference: FG1010). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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3-(4-Bromophenyl)-1-(3-thienyl)-2-propen-1-one (BTC)

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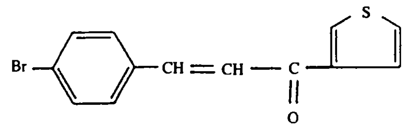
Abstract

The title chalcone derivative, $C_{13}H_9BrOS$, has a dihedral angle of 22.30° between the 4-bromobenzyl and the thienyl group planes. There is electron conjugation between the central —CH═CH—C(═O)— group and the benzyl and thienyl groups.

Comment

Chalcone derivatives are newly developed organic crystals with nonlinear optical properties (Kitaoka, Sasaki, Nakai & Goto, 1991). In an attempt to improve these properties, we have synthesized a series of substituted thiophene chalcone derivatives. Structural studies reveal that one of the products is the title compound, 3-(4-bromophenyl)-1-(3-thienyl)-2-propen-1-one, BTC.



BTC

In general, bond lengths in conjugated systems are intermediate between double- and single-bond lengths. For the title compound, BTC, the C(4)—C(7), C(9)—C(10), C(8)—C(9), C(7)—C(8) and O(1)—C(9) bond lengths are 1.47 (1), 1.49 (1), 1.483 (9), 1.29 (1) and 1.218 (7) Å, respectively. These bonds are similar to equivalent bonds found in 3-(4-chlorophenyl)-1-(3-thienyl)-2-propen-1-one (CTC) (He, Shi & Su, 1994). The C—Br distance is 1.893 (6) Å, longer than the C—Cl distance of 1.736 (4) Å in CTC. The dihedral angle between the planes of the 4-bromobenzyl group and the thienyl group is 22.30° (the equivalent dihedral angle in CTC is 21.93°). Both BTC and CTC crystallize in the same monoclinic system with space group $P2_1$. BTC exhibits nonlinear optical properties; this has been confirmed by a second harmonic generation efficiency measurement on a powder sample using the method of Kurtz & Perry (1968).

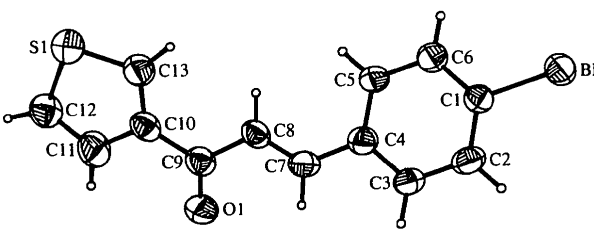


Fig. 1. The molecular structure of the title compound with the atomic numbering. The displacement ellipsoids are drawn at the 50% probability level.

Experimental

The title compound was prepared at room temperature by the condensation of 3-acetylthiophene and 4-bromobenzaldehyde in an alcoholic solution using sodium hydroxide as catalyst. A crystal was grown from alcoholic solution.

Crystal data

$C_{13}H_9BrOS$	Mo $K\alpha$ radiation
$M_r = 293.18$	$\lambda = 0.71069$ Å
Monoclinic	Cell parameters from 25 reflections
$P2_1$	$\theta = 14.8$–$16.8°$
$a = 5.978\,(2)$ Å	$\mu = 3.57$ mm^{-1}
$b = 4.945\,(2)$ Å	$T = 296$ K
$c = 20.168\,(4)$ Å	Plate
$\beta = 95.80\,(3)°$	