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3-(4-Chlorophenyl)-6-(4-methoxybenzyl)-1,2,4,5-tetrazine

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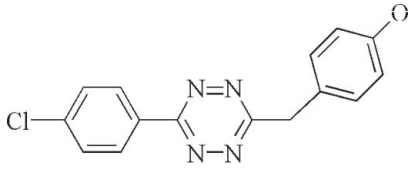
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.076; wR factor = 0.286; data-to-parameter ratio = 13.7.

The title compound, $C_{16}H_{13}ClN_4O$, crystallizes with two unique molecules in the asymmetric unit; these differ in the orientation of the methoxy group. In both molecules, the chlorophenyl ring is almost coplanar with the central tetrazine ring, but the methoxyphenyl ring is twisted. The crystal packing is governed by C—H···Cl and C—H···π interactions.

Related literature

For related literature, see: Hu *et al.* (2004); Hu *et al.* (2005); Sauer (1996).



Experimental

Crystal data

$C_{16}H_{13}ClN_4O$
M_r = 312.75
Triclinic, $P\overline{1}$
a = 9.471 (3) Å
b = 10.170 (3) Å
c = 16.911 (7) Å
α = 101.429 (6)°
β = 97.597 (6)°
γ = 107.012 (4)°
V = 1495.0 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.937, T_{max} = 0.952
8415 measured reflections
5475 independent reflections
2567 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.286
S = 0.95
5475 reflections
399 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···Cl2	0.93	2.82	3.555 (6)	137
C20—H20A···$Cg1^{i}$	0.96	2.64	3.482 (8)	147

Symmetry code: (i) $-x, -y+1, -z+1$. $Cg1$ is the centroid of the C34-C39 ring.

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2355).

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supplementary materials

Acta Cryst. (2007). E**63**, o2397 [**doi:10.1107/S1600536807017175**]

3-(4-Chlorophenyl)-6-(4-methoxybenzyl)-1,2,4,5-tetrazine

F. Xu and W.-X. Hu

Comment

1,2,4,5-Tetrazine derivatives have high potential for biological activity, possessing a wide spectrum of antiviral and antitumor properties. They have been widely used in pesticides and herbicides (Sauer, 1996). In continuation of our work on the structure-activity relationship of 1,2,4,5-tetrazine derivatives (Hu *et al.*, 2004, 2005), we present here the structure of the title compound, (I).

Compound (I) crystallizes with two unique molecules in the asymmetric unit that differ in the orientation of the methoxy group (Fig. 1). In both molecules the chlorophenyl ring is almost coplanar with the central tetrazine ring, but the methoxyphenyl ring is twisted. The C7—C12 and C14—C19 benzene rings form dihedral angles of 2.32 (3) and 76.74 (2)°, respectively, with the N1/N2/N4/N5/C3/C6 plane. The C27—C32 and C34—C39 benzene rings for dihedral angles of 2.37 (3) and 80.47 (2)°, respectively, with the N21/N22/N24/N25/C23/C26 plane.

A C—H···Cl hydrogen bonding is observed between the two independent molecules. In the crystal structure, pair of C—H···π interactions involving the C34—C39 ring (centroid Cg1) link the molecules into a dimer (Table 1).

Experimental

With sulfur (1.0 g) as catalyst, 85% hydrazine hydrate (10 ml, 170 mmol) was added dropwise to an anhydrous ethanol solution (15 ml) of *p*-methoxybenzyl cyanide (50 mmol) and *p*-chlorobenzonitrile (50 mmol) at 295 K. After refluxing for 3 h, the mixture was cooled to room temperature and the resulting solid product was filtered off. The solid product was then dissolved in diethyl ether (15 ml), and oxided by sodium nitrate (14 mmol) and acetic acid (14 mmol) over a period of 2 h to afford the product which were purified by preparative thin-layer chromatography over silica gel PF254 (2 mm) (cyclohexane-dichloromethane, 1:1) to give red single crystals of (I). The solid product was dissolved in tetrahydrofuran-anhydrous ethanol (4:1 v/v) and the solution evaporated gradually at room temperature to afford single crystals of (I) (m.p. 426-428 K).

Refinement

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles were refined to fit the electron density [U_{iso}(H) = 1.5U_{eq}(C)]. Other H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C). Owing to the large number of weak high-angle reflections, the ratio of observed to unique reflections is low (47%). The slightly large U_{eq} values and some longer C—-C distances may be as a result of the poor data set.

Figures

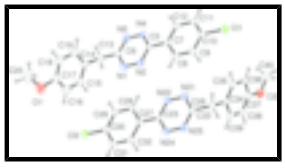


Fig. 1. The asymmetric unit of (I), with the atomic numbering. Displacement ellipsoids are drawn at the 30% probability level.

3-(4-Chlorophenyl)-6-(4-methoxybenzyl)-1,2,4,5-tetrazine

Crystal data

$C_{16}H_{13}ClN_4O$	$Z = 4$
$M_r = 312.75$	$F_{000} = 648$
Triclinic, $P\bar{1}$	$D_x = 1.390$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.471$ (3) Å	Cell parameters from 1325 reflections
$b = 10.170$ (3) Å	$\theta = 2.2$–25.1°
$c = 16.911$ (7) Å	$\mu = 0.26$ mm^{-1}
$\alpha = 101.429$ (6)°	$T = 293$ (2) K
$\beta = 97.597$ (6)°	Prism, red
$\gamma = 107.012$ (4)°	0.25 × 0.20 × 0.15 mm
$V = 1495.0$ (9) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	5475 independent reflections
Radiation source: fine-focus sealed tube	2567 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 293(2)$ K	$\theta_{max} = 25.5^\circ$
φ and ω scans	$\theta_{min} = 1.3^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.937$, $T_{max} = 0.952$	$k = -12 \rightarrow 11$
8415 measured reflections	$l = -16 \rightarrow 20$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.1771P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.076$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.286$	$\Delta\rho_{max} = 0.63$ e Å^{-3}
$S = 0.95$	$\Delta\rho_{min} = -0.31$ e Å^{-3}
5475 reflections	Extinction correction: none

399 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

Special details

Experimental. IR:(KBr cm^{-1}): 3089, 2930, 1388, 715. Analysis calculated for $C_{16}H_{13}Cl_1N_4O_1$ (312.75): C 61.44,H 4.19,*N* 17.91%; found: C 61.14, H 4.13,*N* 17.55.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.47728 (14)	1.08559 (13)	0.78131 (7)	0.1003 (5)
O1	−0.0674 (5)	0.1630 (5)	0.0080 (3)	0.1402 (15)
N1	0.4097 (4)	0.4999 (4)	0.3715 (2)	0.0863 (11)
N2	0.4047 (4)	0.5804 (4)	0.4406 (2)	0.0790 (10)
C3	0.5042 (4)	0.7185 (4)	0.4728 (2)	0.0597 (9)
N4	0.6093 (4)	0.7780 (4)	0.4411 (2)	0.0781 (10)
N5	0.6143 (4)	0.6963 (4)	0.3725 (2)	0.0833 (10)
C6	0.5145 (4)	0.5607 (5)	0.3392 (3)	0.0754 (11)
C7	0.4969 (4)	0.8087 (4)	0.5488 (2)	0.0604 (9)
C8	0.3928 (4)	0.7512 (4)	0.5873 (2)	0.0689 (11)
H8	0.3274	0.6585	0.5670	0.083*
C9	0.3869 (4)	0.8352 (4)	0.6580 (3)	0.0754 (11)
H9	0.3140	0.7980	0.6867	0.091*
C10	0.4855 (4)	0.9785 (4)	0.6922 (2)	0.0692 (10)
C11	0.5891 (4)	1.0384 (4)	0.6552 (3)	0.0733 (11)
H11	0.6546	1.1310	0.6760	0.088*
C12	0.5928 (4)	0.9531 (4)	0.5836 (3)	0.0709 (11)
H12	0.6638	0.9916	0.5542	0.085*
C13	0.5203 (5)	0.4704 (6)	0.2623 (3)	0.0964 (15)
H13A	0.5548	0.3948	0.2753	0.116*
H13B	0.5960	0.5263	0.2379	0.116*
C14	0.3661 (5)	0.3984 (5)	0.1933 (3)	0.0733 (11)
C15	0.2766 (5)	0.2587 (5)	0.1800 (3)	0.0869 (13)
H15	0.3107	0.2069	0.2131	0.104*
C16	0.1376 (6)	0.1833 (6)	0.1216 (3)	0.1084 (17)

H16	0.0870	0.0887	0.1189	0.130*
C17	0.0815 (6)	0.2496 (6)	0.0713 (3)	0.0905 (14)
C18	0.1558 (6)	0.3874 (6)	0.0769 (3)	0.0924 (15)
H18	0.1167	0.4350	0.0427	0.111*
C19	0.3072 (7)	0.4672 (6)	0.1404 (4)	0.1093 (18)
H19	0.3586	0.5616	0.1430	0.131*
C20	−0.1294 (8)	0.2308 (8)	−0.0434 (4)	0.143 (3)
H20A	−0.2000	0.2673	−0.0184	0.214*
H20B	−0.1805	0.1644	−0.0953	0.214*
H20C	−0.0508	0.3076	−0.0521	0.214*
Cl2	0.02128 (15)	−0.08105 (12)	0.23099 (7)	0.0954 (5)
O2	0.5539 (4)	0.7113 (4)	1.0099 (2)	0.1058 (11)
N21	0.0947 (4)	0.5168 (4)	0.6356 (2)	0.0788 (10)
N22	0.0969 (4)	0.4333 (3)	0.5668 (2)	0.0726 (9)
C23	−0.0032 (4)	0.2965 (4)	0.5359 (2)	0.0581 (9)
N24	−0.1086 (4)	0.2389 (4)	0.5692 (2)	0.0751 (10)
N25	−0.1113 (4)	0.3232 (4)	0.6379 (2)	0.0789 (10)
C26	−0.0098 (4)	0.4583 (5)	0.6694 (2)	0.0655 (10)
C27	0.0023 (4)	0.2033 (4)	0.4610 (2)	0.0561 (9)
C28	0.1065 (4)	0.2588 (4)	0.4221 (2)	0.0617 (10)
H28	0.1722	0.3516	0.4415	0.074*
C29	0.1117 (4)	0.1718 (4)	0.3517 (2)	0.0683 (10)
H29	0.1846	0.2072	0.3226	0.082*
C30	0.0125 (4)	0.0287 (4)	0.3190 (2)	0.0647 (10)
C31	−0.0902 (4)	−0.0287 (4)	0.3568 (2)	0.0699 (10)
H31	−0.1548	−0.1219	0.3371	0.084*
C32	−0.0957 (4)	0.0578 (4)	0.4268 (2)	0.0677 (10)
H32	−0.1685	0.0211	0.4558	0.081*
C33	−0.0099 (4)	0.5533 (5)	0.7470 (3)	0.0795 (12)
H33A	−0.0948	0.5064	0.7692	0.095*
H33B	−0.0254	0.6381	0.7351	0.095*
C34	0.1426 (4)	0.6006 (4)	0.8172 (2)	0.0635 (10)
C35	0.2527 (5)	0.7364 (4)	0.8449 (3)	0.0747 (12)
H35	0.2357	0.8071	0.8213	0.090*
C36	0.3924 (5)	0.7774 (4)	0.9077 (3)	0.0740 (11)
H36	0.4598	0.8696	0.9217	0.089*
C37	0.4201 (5)	0.6799 (5)	0.9440 (3)	0.0774 (12)
C38	0.3144 (6)	0.5426 (5)	0.9179 (3)	0.0918 (14)
H38	0.3327	0.4727	0.9418	0.110*
C39	0.1764 (5)	0.5032 (5)	0.8549 (3)	0.0837 (12)
H39	0.1108	0.4102	0.8404	0.100*
C40	0.6673 (6)	0.8493 (6)	1.0380 (3)	0.1141 (18)
H40A	0.6217	0.9186	1.0582	0.171*
H40B	0.7131	0.8732	0.9931	0.171*
H40C	0.7429	0.8482	1.0815	0.171*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1142 (10)	0.0969 (9)	0.0768 (8)	0.0206 (8)	0.0258 (7)	0.0097 (6)
O1	0.157 (4)	0.141 (4)	0.111 (3)	0.046 (3)	0.035 (3)	0.004 (3)
N1	0.080 (2)	0.081 (2)	0.088 (3)	0.0081 (19)	0.038 (2)	0.013 (2)
N2	0.076 (2)	0.072 (2)	0.081 (2)	0.0028 (18)	0.0387 (18)	0.0193 (18)
C3	0.047 (2)	0.063 (2)	0.069 (2)	0.0066 (18)	0.0169 (17)	0.0313 (19)
N4	0.075 (2)	0.078 (2)	0.081 (2)	0.0075 (18)	0.0341 (18)	0.034 (2)
N5	0.075 (2)	0.097 (3)	0.080 (2)	0.014 (2)	0.0372 (19)	0.033 (2)
C6	0.055 (2)	0.086 (3)	0.085 (3)	0.011 (2)	0.028 (2)	0.030 (2)
C7	0.051 (2)	0.060 (2)	0.071 (2)	0.0093 (18)	0.0165 (18)	0.030 (2)
C8	0.064 (2)	0.067 (2)	0.069 (3)	0.0021 (19)	0.0187 (19)	0.028 (2)
C9	0.070 (3)	0.078 (3)	0.072 (3)	0.006 (2)	0.027 (2)	0.025 (2)
C10	0.066 (2)	0.071 (3)	0.071 (3)	0.018 (2)	0.015 (2)	0.024 (2)
C11	0.068 (3)	0.059 (2)	0.083 (3)	0.007 (2)	0.014 (2)	0.017 (2)
C12	0.065 (2)	0.065 (3)	0.083 (3)	0.009 (2)	0.025 (2)	0.032 (2)
C13	0.075 (3)	0.120 (4)	0.091 (3)	0.027 (3)	0.039 (2)	0.012 (3)
C14	0.079 (3)	0.078 (3)	0.078 (3)	0.030 (2)	0.048 (2)	0.028 (2)
C15	0.102 (4)	0.087 (3)	0.077 (3)	0.029 (3)	0.045 (3)	0.017 (2)
C16	0.134 (5)	0.097 (4)	0.099 (4)	0.034 (4)	0.049 (4)	0.025 (3)
C17	0.110 (4)	0.091 (4)	0.080 (3)	0.042 (3)	0.047 (3)	0.013 (3)
C18	0.125 (4)	0.110 (4)	0.085 (3)	0.072 (4)	0.053 (3)	0.048 (3)
C19	0.139 (5)	0.102 (4)	0.124 (4)	0.055 (4)	0.084 (4)	0.049 (4)
C20	0.191 (7)	0.200 (7)	0.088 (4)	0.125 (6)	0.036 (4)	0.053 (4)
Cl2	0.1259 (10)	0.0808 (8)	0.0714 (8)	0.0269 (7)	0.0256 (7)	0.0077 (6)
O2	0.121 (3)	0.120 (3)	0.088 (2)	0.055 (2)	0.016 (2)	0.029 (2)
N21	0.082 (2)	0.073 (2)	0.076 (2)	0.0093 (18)	0.0368 (18)	0.0158 (18)
N22	0.078 (2)	0.063 (2)	0.065 (2)	0.0000 (17)	0.0345 (16)	0.0142 (16)
C23	0.052 (2)	0.063 (2)	0.061 (2)	0.0102 (18)	0.0145 (17)	0.0321 (19)
N24	0.075 (2)	0.072 (2)	0.077 (2)	0.0077 (18)	0.0347 (18)	0.0277 (19)
N25	0.074 (2)	0.093 (3)	0.072 (2)	0.016 (2)	0.0353 (18)	0.029 (2)
C26	0.056 (2)	0.079 (3)	0.067 (2)	0.019 (2)	0.0234 (19)	0.027 (2)
C27	0.055 (2)	0.057 (2)	0.057 (2)	0.0101 (17)	0.0182 (17)	0.0246 (17)
C28	0.062 (2)	0.059 (2)	0.061 (2)	0.0044 (18)	0.0206 (18)	0.0239 (18)
C29	0.080 (3)	0.067 (3)	0.061 (2)	0.017 (2)	0.0271 (19)	0.0226 (19)
C30	0.075 (3)	0.060 (2)	0.058 (2)	0.016 (2)	0.0141 (19)	0.0212 (19)
C31	0.075 (3)	0.053 (2)	0.071 (3)	0.004 (2)	0.014 (2)	0.017 (2)
C32	0.062 (2)	0.060 (2)	0.075 (3)	0.0027 (19)	0.0199 (19)	0.027 (2)
C33	0.074 (3)	0.106 (3)	0.070 (3)	0.037 (2)	0.033 (2)	0.025 (2)
C34	0.079 (3)	0.067 (2)	0.061 (2)	0.034 (2)	0.0362 (19)	0.0231 (19)
C35	0.095 (3)	0.071 (3)	0.077 (3)	0.038 (3)	0.039 (2)	0.031 (2)
C36	0.084 (3)	0.060 (2)	0.077 (3)	0.019 (2)	0.031 (2)	0.012 (2)
C37	0.093 (3)	0.091 (3)	0.063 (3)	0.045 (3)	0.029 (2)	0.022 (2)
C38	0.120 (4)	0.096 (4)	0.084 (3)	0.052 (3)	0.034 (3)	0.041 (3)
C39	0.098 (3)	0.075 (3)	0.082 (3)	0.024 (2)	0.037 (3)	0.024 (2)
C40	0.100 (4)	0.136 (5)	0.097 (4)	0.046 (4)	0.012 (3)	−0.001 (3)

Geometric parameters (Å, °)

Cl1—C10	1.701 (4)	Cl2—C30	1.703 (4)
O1—C20	1.384 (6)	O2—C40	1.438 (6)
O1—C17	1.552 (6)	O2—C37	1.482 (5)
N1—C6	1.259 (5)	N21—C26	1.266 (5)
N1—N2	1.303 (5)	N21—N22	1.303 (4)
N2—C3	1.394 (5)	N22—C23	1.385 (5)
C3—N4	1.250 (4)	C23—N24	1.263 (4)
C3—C7	1.446 (5)	C23—C27	1.441 (5)
N4—N5	1.302 (5)	N24—N25	1.308 (5)
N5—C6	1.379 (5)	N25—C26	1.377 (5)
C6—C13	1.454 (6)	C26—C33	1.467 (5)
C7—C8	1.312 (5)	C27—C28	1.311 (5)
C7—C12	1.437 (5)	C27—C32	1.449 (5)
C8—C9	1.343 (5)	C28—C29	1.351 (5)
C8—H8	0.93	C28—H28	0.93
C9—C10	1.434 (6)	C29—C30	1.431 (5)
C9—H9	0.93	C29—H29	0.93
C10—C11	1.299 (5)	C30—C31	1.294 (5)
C11—C12	1.354 (5)	C31—C32	1.345 (5)
C11—H11	0.93	C31—H31	0.93
C12—H12	0.93	C32—H32	0.93
C13—C14	1.617 (6)	C33—C34	1.625 (5)
C13—H13A	0.97	C33—H33A	0.97
C13—H13B	0.97	C33—H33B	0.97
C14—C15	1.380 (6)	C34—C39	1.370 (6)
C14—C19	1.394 (6)	C34—C35	1.409 (5)
C15—C16	1.435 (6)	C35—C36	1.478 (6)
C15—H15	0.93	C35—H35	0.93
C16—C17	1.334 (7)	C36—C37	1.334 (6)
C16—H16	0.93	C36—H36	0.93
C17—C18	1.349 (7)	C37—C38	1.403 (6)
C18—C19	1.560 (7)	C38—C39	1.469 (6)
C18—H18	0.93	C38—H38	0.93
C19—H19	0.93	C39—H39	0.93
C20—H20A	0.96	C40—H40A	0.96
C20—H20B	0.96	C40—H40B	0.96
C20—H20C	0.96	C40—H40C	0.96
C20—O1—C17	118.8 (5)	C40—O2—C37	122.4 (4)
C6—N1—N2	112.2 (4)	C26—N21—N22	112.0 (3)
N1—N2—C3	122.7 (3)	N21—N22—C23	123.3 (3)
N4—C3—N2	125.0 (4)	N24—C23—N22	124.6 (4)
N4—C3—C7	112.4 (4)	N24—C23—C27	112.3 (3)
N2—C3—C7	122.6 (3)	N22—C23—C27	123.1 (3)
C3—N4—N5	111.9 (4)	C23—N24—N25	112.0 (3)
N4—N5—C6	123.6 (3)	N24—N25—C26	123.3 (3)
N1—C6—N5	124.6 (4)	N21—C26—N25	124.8 (4)

N1—C6—C13	112.1 (4)	N21—C26—C33	111.3 (4)
N5—C6—C13	123.3 (4)	N25—C26—C33	124.0 (3)
C8—C7—C12	119.0 (4)	C28—C27—C23	115.1 (3)
C8—C7—C3	115.8 (4)	C28—C27—C32	119.1 (4)
C12—C7—C3	125.2 (3)	C23—C27—C32	125.8 (3)
C7—C8—C9	115.6 (4)	C27—C28—C29	115.3 (4)
C7—C8—H8	122.2	C27—C28—H28	122.4
C9—C8—H8	122.2	C29—C28—H28	122.4
C8—C9—C10	124.4 (4)	C28—C29—C30	124.4 (3)
C8—C9—H9	117.8	C28—C29—H29	117.8
C10—C9—H9	117.8	C30—C29—H29	117.8
C11—C10—C9	121.4 (4)	C31—C30—C29	121.4 (4)
C11—C10—Cl1	114.1 (3)	C31—C30—Cl2	114.4 (3)
C9—C10—Cl1	124.5 (3)	C29—C30—Cl2	124.1 (3)
C10—C11—C12	113.6 (4)	C30—C31—C32	114.3 (4)
C10—C11—H11	123.2	C30—C31—H31	122.8
C12—C11—H11	123.2	C32—C31—H31	122.8
C11—C12—C7	126.0 (4)	C31—C32—C27	125.5 (3)
C11—C12—H12	117.0	C31—C32—H32	117.3
C7—C12—H12	117.0	C27—C32—H32	117.3
C6—C13—C14	117.5 (3)	C26—C33—C34	115.0 (3)
C6—C13—H13A	107.9	C26—C33—H33A	108.5
C14—C13—H13A	107.9	C34—C33—H33A	108.5
C6—C13—H13B	107.9	C26—C33—H33B	108.5
C14—C13—H13B	107.9	C34—C33—H33B	108.5
H13A—C13—H13B	107.2	H33A—C33—H33B	107.5
C15—C14—C19	111.8 (5)	C39—C34—C35	113.0 (4)
C15—C14—C13	123.0 (4)	C39—C34—C33	120.1 (4)
C19—C14—C13	125.2 (5)	C35—C34—C33	126.9 (4)
C14—C15—C16	128.3 (5)	C34—C35—C36	126.3 (4)
C14—C15—H15	115.8	C34—C35—H35	116.9
C16—C15—H15	115.8	C36—C35—H35	116.9
C17—C16—C15	119.7 (5)	C37—C36—C35	118.9 (4)
C17—C16—H16	120.2	C37—C36—H36	120.6
C15—C16—H16	120.2	C35—C36—H36	120.6
C16—C17—C18	119.2 (5)	C36—C37—C38	116.9 (4)
C16—C17—O1	117.9 (5)	C36—C37—O2	123.2 (4)
C18—C17—O1	122.9 (5)	C38—C37—O2	119.9 (4)
C17—C18—C19	120.3 (5)	C37—C38—C39	123.6 (4)
C17—C18—H18	119.9	C37—C38—H38	118.2
C19—C18—H18	119.9	C39—C38—H38	118.2
C14—C19—C18	120.7 (5)	C34—C39—C38	121.3 (4)
C14—C19—H19	119.7	C34—C39—H39	119.4
C18—C19—H19	119.7	C38—C39—H39	119.4
O1—C20—H20A	109.5	O2—C40—H40A	109.5
O1—C20—H20B	109.5	O2—C40—H40B	109.5
H20A—C20—H20B	109.5	H40A—C40—H40B	109.5
O1—C20—H20C	109.5	O2—C40—H40C	109.5
H20A—C20—H20C	109.5	H40A—C40—H40C	109.5

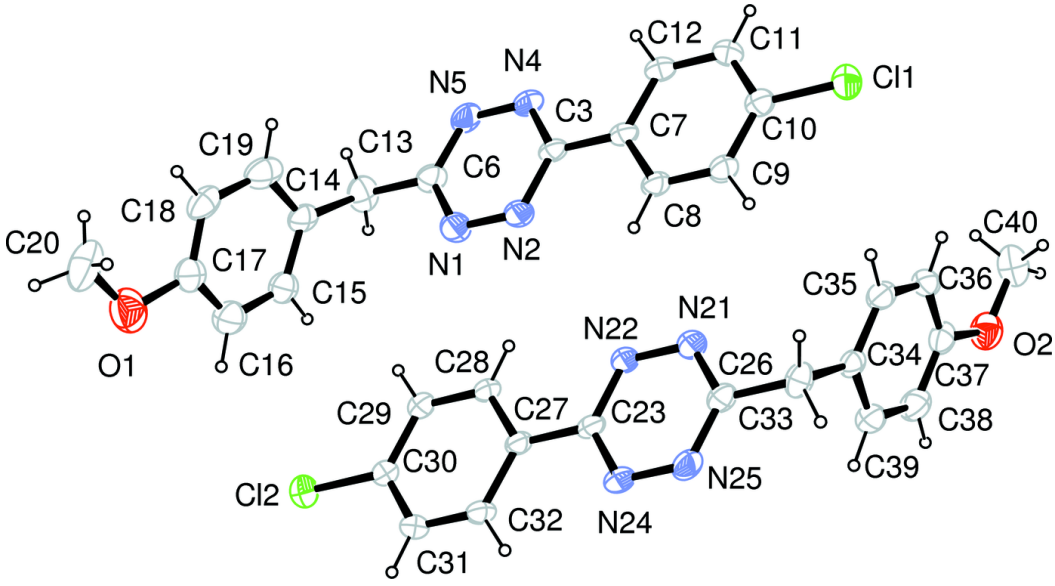
H20B—C20—H20C	109.5	H40B—C40—H40C	109.5
C6—N1—N2—C3	0.9 (6)	C26—N21—N22—C23	−0.6 (6)
N1—N2—C3—N4	−2.0 (6)	N21—N22—C23—N24	1.7 (6)
N1—N2—C3—C7	178.9 (4)	N21—N22—C23—C27	−178.3 (3)
N2—C3—N4—N5	1.2 (6)	N22—C23—N24—N25	−1.1 (6)
C7—C3—N4—N5	−179.6 (3)	C27—C23—N24—N25	178.9 (3)
C3—N4—N5—C6	0.3 (6)	C23—N24—N25—C26	−0.3 (6)
N2—N1—C6—N5	0.6 (6)	N22—N21—C26—N25	−0.8 (6)
N2—N1—C6—C13	179.7 (4)	N22—N21—C26—C33	179.6 (3)
N4—N5—C6—N1	−1.3 (7)	N24—N25—C26—N21	1.3 (6)
N4—N5—C6—C13	179.7 (4)	N24—N25—C26—C33	−179.1 (4)
N4—C3—C7—C8	−177.4 (3)	N24—C23—C27—C28	177.8 (3)
N2—C3—C7—C8	1.7 (6)	N22—C23—C27—C28	−2.2 (5)
N4—C3—C7—C12	3.0 (5)	N24—C23—C27—C32	−2.2 (5)
N2—C3—C7—C12	−177.8 (3)	N22—C23—C27—C32	177.8 (3)
C12—C7—C8—C9	−0.6 (6)	C23—C27—C28—C29	−179.9 (3)
C3—C7—C8—C9	179.8 (3)	C32—C27—C28—C29	0.1 (5)
C7—C8—C9—C10	−0.4 (6)	C27—C28—C29—C30	0.4 (6)
C8—C9—C10—C11	0.7 (7)	C28—C29—C30—C31	−1.1 (6)
C8—C9—C10—Cl1	179.5 (3)	C28—C29—C30—Cl2	−179.2 (3)
C9—C10—C11—C12	0.1 (6)	C29—C30—C31—C32	1.0 (6)
Cl1—C10—C11—C12	−178.8 (3)	Cl2—C30—C31—C32	179.3 (3)
C10—C11—C12—C7	−1.2 (6)	C30—C31—C32—C27	−0.5 (6)
C8—C7—C12—C11	1.6 (6)	C28—C27—C32—C31	−0.1 (6)
C3—C7—C12—C11	−178.9 (4)	C23—C27—C32—C31	179.9 (4)
N1—C6—C13—C14	52.1 (6)	N21—C26—C33—C34	−61.4 (5)
N5—C6—C13—C14	−128.8 (4)	N25—C26—C33—C34	118.9 (4)
C6—C13—C14—C15	−101.2 (5)	C26—C33—C34—C39	−69.2 (5)
C6—C13—C14—C19	78.9 (6)	C26—C33—C34—C35	109.4 (4)
C19—C14—C15—C16	−0.7 (6)	C39—C34—C35—C36	−0.1 (5)
C13—C14—C15—C16	179.4 (4)	C33—C34—C35—C36	−178.8 (3)
C14—C15—C16—C17	0.6 (7)	C34—C35—C36—C37	−1.0 (6)
C15—C16—C17—C18	−0.8 (7)	C35—C36—C37—C38	1.5 (6)
C15—C16—C17—O1	178.9 (4)	C35—C36—C37—O2	−177.7 (3)
C20—O1—C17—C16	178.4 (5)	C40—O2—C37—C36	−2.1 (6)
C20—O1—C17—C18	−1.9 (7)	C40—O2—C37—C38	178.8 (4)
C16—C17—C18—C19	1.1 (7)	C36—C37—C38—C39	−1.1 (6)
O1—C17—C18—C19	−178.5 (4)	O2—C37—C38—C39	178.0 (4)
C15—C14—C19—C18	0.9 (6)	C35—C34—C39—C38	0.5 (5)
C13—C14—C19—C18	−179.2 (3)	C33—C34—C39—C38	179.3 (3)
C17—C18—C19—C14	−1.3 (6)	C37—C38—C39—C34	0.1 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···Cl2	0.93	2.82	3.555 (6)	137
C20—H20A···Cg1^{i}	0.96	2.64	3.482 (8)	147

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1.

Fig. 1


C12
C11
Cl1
N4
N5
C3
C7
C10
C19
C13
C6
C9
C14
C18
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C20
C17
N1
N2
C40
C35
C36
C15
N22
N21
O2
O1
C16
C28
C26
C34
C37
C29
C27
C23
C33
C38
C30
N25
C39
Cl2
C32
N24
C31