Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-1-(2,4-Dichlorophenyl)-3-(1,3-diphenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one

Hoong-Kun Fun,[a]*‡ Ching Kheng Quah,[a]§ Shridhar Malladi,[b] Arun M. Isloor[b] and Kammasandra N. Shivananda[c]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Medicinal Chemistry Division, Department of Chemistry, National Institute of Technology-Karnataka, Surathkal, Mangalore 575 025, India, and [c]Schulich Faculty of Chemistry, Technion Israel Institute of Technology, Haifa 32000, Israel
Correspondence e-mail: hkfun@usm.my

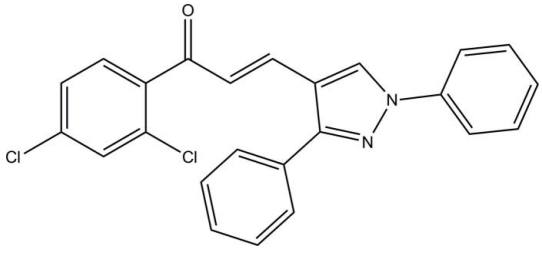
Received 19 October 2011; accepted 25 October 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.134; data-to-parameter ratio = 23.1.

In the title molecule, $C_{24}H_{16}Cl_2N_2O$, the dihedral angles between the pyrazole ring and its N- and C-bonded phenyl rings are 7.06 (10) and 53.15 (10)°, respectively. The dihedral angle between the two pendant rings is 52.32 (10)°. The molecule exists in a *trans* conformation with respect to the acyclic C=C bond. In the crystal, inversion dimers occur in which each molecule is linked to the other by two C—H···O hydrogen bonds to the same acceptor O atom. There are also short Cl···Cl contacts [3.3492 (9) Å] and C—H···π interactions.

Related literature

For general background to and the biological activity of pyrazoles, see: Patel *et al.* (2004); Isloor *et al.* (2009); Vijesh *et al.* (2010); Sharma *et al.* (2010); Rostom *et al.* (2003); Ghorab *et al.* (2010); Amnekar & Bhusari (2010). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For standard bond-length data, see: Allen *et al.* (1987).



‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5525-2009.

Experimental

Crystal data

$C_{24}H_{16}Cl_2N_2O$
M_r = 419.29
Triclinic, $P\overline{1}$
a = 9.6185 (8) Å
b = 10.6596 (9) Å
c = 11.8537 (10) Å
α = 67.377 (2)°
β = 75.777 (1)°
γ = 69.934 (2)°
V = 1044.64 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 296 K
0.31 × 0.21 × 0.08 mm

Data collection

Bruker SMART APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.904, T_{max} = 0.973
22059 measured reflections
6053 independent reflections
3980 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.134
S = 1.04
6053 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C19–C24 and C13–C18 benzene rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11*A*···O1^{i}	0.93	2.30	3.230 (2)	174
C20—H20*A*···O1^{i}	0.93	2.59	3.509 (3)	168
C2—H2*A*···*Cg*1^{ii}	0.93	2.75	3.585 (2)	149
C23—H23*A*···*Cg*2^{iii}	0.93	2.90	3.655 (2)	140

Symmetry codes: (i) $-x, -y+1, -z+2$; (ii) $-x+1, -y+1, -z+2$; (iii) $-x+1, -y+2, -z+2$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and CKQ thank Universiti Sains Malaysia for the Research University Grant (No. 1001/PFIZIK/811160). AMI is thankful to the Department of Atomic Energy, Board for Research in Nuclear Sciences, Government of India, for the Young scientist award.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6456).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Amnekar, N. D. & Bhusari, K. P. (2010). *Eur. J. Med. Chem.* **45**, 149–159.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ghorab, M. M., Ragab, F. A., Alqasoumi, S. I., Alafeefy, A. M. & Aboulmagd, S. A. (2010). *Eur. J. Med. Chem.* **45**, 171–178.

Isloor, A. M., Kalluraya, B. & Shetty, P. (2009). *Eur. J. Med. Chem.* **44**, 3784–3787.
Patel, M. V., Bell, R., Majest, S., Henry, R. & Kolasa, T. (2004). *J. Org. Chem.* **69**, 7058–7065.
Rostom, S. A. F., Shalaby, M. A. & El-Demellawy, M. A. (2003). *Eur. J. Med. Chem.* **38**, 959–974.
Sharma, P. K., Kumar, S., Kumar, P., Kaushik, P., Kaushik, D., Dhingra, Y. & Aneja, K. R. (2010). *Eur. J. Med. Chem.* **45**, 2650–2655.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Vijesh, A. M., Isloor, A. M., Prabhu, V., Ahmad, S. & Malladi, S. (2010). *Eur. J. Med. Chem.* **45**, 5460–5464.

supplementary materials

Acta Cryst. (2011). E**67**, o3102-o3103 [**doi:10.1107/S1600536811044382**]

(*E*)-1-(2,4-Dichlorophenyl)-3-(1,3-diphenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one

H.-K. Fun, C. K. Quah, S. Malladi, A. M. Isloor and K. N. Shivananda

Comment

Pyrazoles are novel class of heterocyclic compounds possessing wide variety of application in the agrochemical and pharmaceutical industries (Patel *et al.*, 2004). Derivatives of pyrazoles are found to show good antibacterial (Isloor *et al.*, 2009; Vijesh *et al.*, 2010), anti-inflammatory (Sharma *et al.*, 2010), analgesic (Rostom *et al.*, 2003), anticancer, radioprotective (Ghorab *et al.*, 2010) and anti-convulsant activity (Amnekar & Bhusari, 2010). Prompted by the diverse activities of pyrazole derivatives, we have synthesized the title compound to study its crystal structure.

In the title molecule (Fig. 1), the phenyl (C1-C6) ring and the two benzene (C13-C18 and C19-C24) rings form dihedral angles of 64.29 (9), 53.15 (10) and 7.06 (10)°, respectively, with the pyrazole ring (N1/N2/C10-C12). The phenyl ring also forms dihedral angles of 65.06 (10) and 67.80 (10)° with the two benzene rings (C13-C18 and C19-C24), respectively. The benzene rings form a dihedral angle of 52.32 (10)°. The title molecule exists in *trans* conformation with respect to the acyclic C8═C9 bond [bond length = 1.330 (2) Å]. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. There is a short Cl2···Cl2 contact (symmetry code : -x, 1-y, 1-z) with distance = 3.3492 (9) Å which is shorter than the sum of van der Waals radii of the Cl atoms.

In the crystal (Fig. 2), molecules are linked into inversion dimers by intermolecular bifurcated C11–H11A···O1 and C20–H20A···O1 acceptor bonds (Table 1), generating six-membered $R^1_2(6)$ ring motifs (Bernstein *et al.*, 1995). The crystal structure is further consolidated by C2–H2A···Cg1 and C23–H23A···Cg2 (Table 1) interactions, where Cg1 and Cg2 are the centroids of C19-C24 and C13-C18 benzene rings, respectively.

Experimental

To a cold, stirred mixture of methanol (20 ml) and sodium hydroxide (12.09 mmol), 2,4-dichloroacetophenone (4.03 mmol) was added. The reaction mixture was stirred for 10 min. 1,3-Diphenyl-1H-pyrazole-4-carbaldehyde (4.03 mmol) was added to this solution followed by tetrahydrofuran (30 ml). The solution was further stirred for 2 h at 273 K and then at room temperature for 5 h. It was then poured into ice cold water. The resulting solution was neutralized with Dil. HCl. The solid that separated was filtered, washed with water, dried and crystallized from ethanol to yield colourless blocks of (I). Yield: 1.28 g, 76.19 %. *M.p.*: 406-408 K.

Refinement

All H atoms were positioned geometrically and refined using a riding model with C–H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C).

Figures

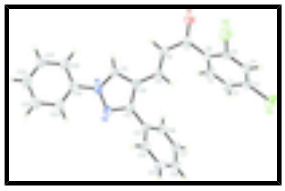


Fig. 1. The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms.

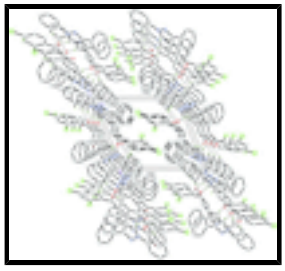


Fig. 2. The crystal structure of the title compound, viewed along the *a* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

(*E*)-1-(2,4-Dichlorophenyl)-3-(1,3-diphenyl-1*H*- pyrazol-4-yl)prop-2-en-1-one

Crystal data

$C_{24}H_{16}Cl_2N_2O$	$Z = 2$
$M_r = 419.29$	$F(000) = 432$
Triclinic, $P\overline{1}$	$D_x = 1.333$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.6185$ (8) Å	Cell parameters from 5364 reflections
$b = 10.6596$ (9) Å	$\theta = 2.4$–$28.8°$
$c = 11.8537$ (10) Å	$\mu = 0.33$ mm^{-1}
$\alpha = 67.377$ (2)°	$T = 296$ K
$\beta = 75.777$ (1)°	Block, colourless
$\gamma = 69.934$ (2)°	0.31 × 0.21 × 0.08 mm
$V = 1044.64$ (15) Å^3	

Data collection

Bruker SMART APEXII DUO CCD diffractometer	6053 independent reflections
Radiation source: fine-focus sealed tube	3980 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.027$
φ and ω scans	$\theta_{max} = 30.0°$, $\theta_{min} = 1.9°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$h = -13 \rightarrow 13$
$T_{min} = 0.904$, $T_{max} = 0.973$	$k = -14 \rightarrow 14$
22059 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods

Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.043$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.134$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 0.1623P]$ where $P = (F_o^2 + 2F_c^2)/3$
6053 reflections	$(\Delta/\sigma)_{max} = 0.001$
262 parameters	$\Delta\rho_{max} = 0.22$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

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	0.72422 (6)	0.23879 (6)	0.46250 (5)	0.08035 (18)
Cl2	0.14184 (5)	0.45480 (9)	0.57917 (6)	0.1019 (3)
O1	0.10827 (16)	0.35212 (16)	0.86276 (14)	0.0787 (4)
N1	0.22996 (13)	0.84151 (14)	1.00579 (11)	0.0461 (3)
N2	0.35901 (14)	0.86410 (14)	0.93127 (12)	0.0496 (3)
C1	0.4853 (2)	0.3081 (2)	0.76848 (16)	0.0634 (5)
H1A	0.5039	0.2962	0.8459	0.076*
C2	0.6034 (2)	0.2677 (2)	0.68476 (17)	0.0677 (5)
H2A	0.7000	0.2286	0.7056	0.081*
C3	0.57655 (18)	0.28591 (17)	0.57036 (15)	0.0537 (4)
C4	0.43478 (18)	0.34217 (18)	0.53839 (16)	0.0565 (4)
H4A	0.4175	0.3541	0.4606	0.068*
C5	0.31849 (17)	0.38071 (18)	0.62408 (16)	0.0526 (4)
C6	0.33961 (17)	0.36581 (16)	0.74104 (14)	0.0470 (3)
C7	0.21224 (19)	0.40361 (18)	0.83561 (15)	0.0536 (4)
C8	0.21287 (19)	0.50151 (19)	0.89386 (15)	0.0570 (4)
H8A	0.1421	0.5086	0.9621	0.068*
C9	0.30613 (17)	0.58143 (16)	0.85751 (13)	0.0466 (3)
H9A	0.3819	0.5680	0.7937	0.056*
C10	0.30113 (16)	0.68689 (16)	0.90744 (13)	0.0452 (3)
C11	0.19295 (17)	0.73726 (17)	0.99304 (14)	0.0481 (3)
H11A	0.1098	0.7049	1.0343	0.058*
C12	0.40123 (16)	0.77075 (16)	0.87221 (14)	0.0452 (3)

C13	0.53890 (16)	0.76264 (17)	0.78363 (14)	0.0478 (3)
C14	0.5637 (2)	0.8813 (2)	0.68817 (19)	0.0703 (5)
H14A	0.4923	0.9684	0.6784	0.084*
C15	0.6947 (3)	0.8706 (3)	0.6070 (2)	0.0862 (7)
H15A	0.7098	0.9505	0.5420	0.103*
C16	0.8019 (2)	0.7449 (3)	0.6209 (2)	0.0785 (6)
H16A	0.8902	0.7395	0.5666	0.094*
C17	0.7792 (2)	0.6270 (2)	0.71462 (19)	0.0711 (5)
H17A	0.8523	0.5410	0.7244	0.085*
C18	0.64774 (18)	0.6348 (2)	0.79530 (16)	0.0580 (4)
H18A	0.6323	0.5535	0.8580	0.070*
C19	0.15658 (16)	0.92254 (17)	1.08631 (14)	0.0488 (4)
C20	0.03696 (19)	0.8896 (2)	1.17154 (17)	0.0612 (4)
H20A	0.0011	0.8173	1.1752	0.073*
C21	−0.0289 (2)	0.9666 (3)	1.25176 (19)	0.0756 (6)
H21A	−0.1097	0.9455	1.3097	0.091*
C22	0.0236 (2)	1.0730 (3)	1.2467 (2)	0.0799 (6)
H22A	−0.0205	1.1228	1.3018	0.096*
C23	0.1411 (2)	1.1064 (2)	1.1603 (2)	0.0755 (6)
H23A	0.1757	1.1797	1.1561	0.091*
C24	0.2084 (2)	1.03114 (19)	1.07925 (17)	0.0609 (4)
H24A	0.2880	1.0538	1.0205	0.073*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0657 (3)	0.0801 (3)	0.0695 (3)	0.0003 (2)	0.0118 (2)	−0.0280 (3)
Cl2	0.0469 (3)	0.1805 (7)	0.1026 (4)	0.0004 (3)	−0.0210 (3)	−0.0934 (5)
O1	0.0746 (8)	0.1027 (10)	0.0849 (10)	−0.0569 (8)	0.0247 (7)	−0.0516 (8)
N1	0.0409 (6)	0.0555 (7)	0.0445 (7)	−0.0107 (5)	−0.0034 (5)	−0.0228 (6)
N2	0.0432 (6)	0.0584 (8)	0.0514 (7)	−0.0148 (6)	0.0002 (5)	−0.0258 (6)
C1	0.0607 (10)	0.0753 (11)	0.0465 (9)	−0.0052 (9)	−0.0152 (8)	−0.0190 (8)
C2	0.0498 (9)	0.0772 (12)	0.0580 (10)	0.0050 (8)	−0.0153 (8)	−0.0180 (9)
C3	0.0512 (8)	0.0471 (8)	0.0515 (9)	−0.0044 (7)	0.0001 (7)	−0.0165 (7)
C4	0.0537 (9)	0.0680 (10)	0.0519 (9)	−0.0095 (8)	−0.0069 (7)	−0.0306 (8)
C5	0.0435 (8)	0.0643 (10)	0.0600 (9)	−0.0117 (7)	−0.0080 (7)	−0.0330 (8)
C6	0.0491 (8)	0.0494 (8)	0.0472 (8)	−0.0172 (6)	−0.0011 (6)	−0.0210 (6)
C7	0.0549 (9)	0.0619 (9)	0.0507 (9)	−0.0251 (8)	0.0054 (7)	−0.0255 (7)
C8	0.0576 (9)	0.0704 (10)	0.0515 (9)	−0.0284 (8)	0.0132 (7)	−0.0321 (8)
C9	0.0467 (8)	0.0563 (9)	0.0390 (7)	−0.0165 (7)	0.0010 (6)	−0.0200 (6)
C10	0.0448 (7)	0.0514 (8)	0.0404 (7)	−0.0147 (6)	−0.0022 (6)	−0.0171 (6)
C11	0.0446 (7)	0.0584 (9)	0.0446 (8)	−0.0175 (7)	−0.0006 (6)	−0.0209 (7)
C12	0.0414 (7)	0.0522 (8)	0.0430 (8)	−0.0118 (6)	−0.0037 (6)	−0.0190 (6)
C13	0.0444 (8)	0.0591 (9)	0.0471 (8)	−0.0187 (7)	0.0000 (6)	−0.0250 (7)
C14	0.0740 (12)	0.0622 (11)	0.0730 (12)	−0.0283 (9)	0.0118 (10)	−0.0255 (9)
C15	0.0974 (16)	0.0867 (15)	0.0792 (14)	−0.0554 (13)	0.0292 (12)	−0.0311 (12)
C16	0.0657 (12)	0.1101 (17)	0.0835 (14)	−0.0461 (12)	0.0260 (10)	−0.0599 (14)
C17	0.0497 (9)	0.0921 (14)	0.0775 (13)	−0.0128 (9)	0.0048 (9)	−0.0482 (12)

C18	0.0497 (9)	0.0676 (10)	0.0536 (9)	−0.0132 (8)	−0.0020 (7)	−0.0223 (8)
C19	0.0430 (7)	0.0575 (9)	0.0451 (8)	−0.0012 (6)	−0.0116 (6)	−0.0238 (7)
C20	0.0487 (9)	0.0821 (12)	0.0594 (10)	−0.0145 (8)	−0.0031 (7)	−0.0360 (9)
C21	0.0540 (10)	0.1103 (17)	0.0666 (12)	−0.0113 (10)	0.0016 (9)	−0.0495 (12)
C22	0.0712 (12)	0.0989 (16)	0.0786 (14)	−0.0009 (11)	−0.0085 (11)	−0.0595 (13)
C23	0.0809 (13)	0.0743 (12)	0.0820 (14)	−0.0099 (10)	−0.0114 (11)	−0.0467 (11)
C24	0.0642 (10)	0.0610 (10)	0.0605 (10)	−0.0121 (8)	−0.0050 (8)	−0.0297 (8)

Geometric parameters (Å, °)

Cl1—C3	1.7369 (16)	C11—H11A	0.9300
Cl2—C5	1.7304 (16)	C12—C13	1.474 (2)
O1—C7	1.2196 (19)	C13—C14	1.382 (2)
N1—C11	1.346 (2)	C13—C18	1.385 (2)
N1—N2	1.3718 (17)	C14—C15	1.385 (3)
N1—C19	1.4283 (19)	C14—H14A	0.9300
N2—C12	1.3282 (19)	C15—C16	1.360 (3)
C1—C2	1.378 (3)	C15—H15A	0.9300
C1—C6	1.388 (2)	C16—C17	1.362 (3)
C1—H1A	0.9300	C16—H16A	0.9300
C2—C3	1.370 (3)	C17—C18	1.384 (2)
C2—H2A	0.9300	C17—H17A	0.9300
C3—C4	1.371 (2)	C18—H18A	0.9300
C4—C5	1.378 (2)	C19—C24	1.377 (2)
C4—H4A	0.9300	C19—C20	1.379 (2)
C5—C6	1.391 (2)	C20—C21	1.388 (3)
C6—C7	1.501 (2)	C20—H20A	0.9300
C7—C8	1.458 (2)	C21—C22	1.368 (3)
C8—C9	1.330 (2)	C21—H21A	0.9300
C8—H8A	0.9300	C22—C23	1.371 (3)
C9—C10	1.441 (2)	C22—H22A	0.9300
C9—H9A	0.9300	C23—C24	1.384 (3)
C10—C11	1.385 (2)	C23—H23A	0.9300
C10—C12	1.416 (2)	C24—H24A	0.9300
C11—N1—N2	111.74 (12)	N2—C12—C13	120.29 (14)
C11—N1—C19	128.80 (13)	C10—C12—C13	127.91 (13)
N2—N1—C19	119.42 (13)	C14—C13—C18	118.39 (15)
C12—N2—N1	104.76 (12)	C14—C13—C12	121.32 (15)
C2—C1—C6	122.13 (16)	C18—C13—C12	120.28 (15)
C2—C1—H1A	118.9	C13—C14—C15	119.99 (19)
C6—C1—H1A	118.9	C13—C14—H14A	120.0
C3—C2—C1	119.06 (16)	C15—C14—H14A	120.0
C3—C2—H2A	120.5	C16—C15—C14	121.0 (2)
C1—C2—H2A	120.5	C16—C15—H15A	119.5
C2—C3—C4	121.28 (15)	C14—C15—H15A	119.5
C2—C3—Cl1	119.79 (13)	C15—C16—C17	119.70 (18)
C4—C3—Cl1	118.92 (13)	C15—C16—H16A	120.1
C3—C4—C5	118.53 (15)	C17—C16—H16A	120.1
C3—C4—H4A	120.7	C16—C17—C18	120.23 (19)

C5—C4—H4A	120.7	C16—C17—H17A	119.9
C4—C5—C6	122.56 (14)	C18—C17—H17A	119.9
C4—C5—Cl2	117.16 (12)	C17—C18—C13	120.67 (17)
C6—C5—Cl2	120.25 (12)	C17—C18—H18A	119.7
C1—C6—C5	116.43 (14)	C13—C18—H18A	119.7
C1—C6—C7	121.05 (14)	C24—C19—C20	120.82 (15)
C5—C6—C7	122.46 (14)	C24—C19—N1	119.36 (15)
O1—C7—C8	120.46 (15)	C20—C19—N1	119.81 (15)
O1—C7—C6	119.38 (15)	C19—C20—C21	118.66 (19)
C8—C7—C6	120.16 (14)	C19—C20—H20A	120.7
C9—C8—C7	125.46 (15)	C21—C20—H20A	120.7
C9—C8—H8A	117.3	C22—C21—C20	120.8 (2)
C7—C8—H8A	117.3	C22—C21—H21A	119.6
C8—C9—C10	126.31 (14)	C20—C21—H21A	119.6
C8—C9—H9A	116.8	C21—C22—C23	120.02 (19)
C10—C9—H9A	116.8	C21—C22—H22A	120.0
C11—C10—C12	104.10 (13)	C23—C22—H22A	120.0
C11—C10—C9	128.48 (14)	C22—C23—C24	120.2 (2)
C12—C10—C9	127.26 (13)	C22—C23—H23A	119.9
N1—C11—C10	107.60 (13)	C24—C23—H23A	119.9
N1—C11—H11A	126.2	C19—C24—C23	119.49 (18)
C10—C11—H11A	126.2	C19—C24—H24A	120.3
N2—C12—C10	111.80 (13)	C23—C24—H24A	120.3
C11—N1—N2—C12	−0.17 (16)	N1—N2—C12—C13	−179.30 (13)
C19—N1—N2—C12	177.93 (12)	C11—C10—C12—N2	0.29 (17)
C6—C1—C2—C3	0.5 (3)	C9—C10—C12—N2	175.95 (14)
C1—C2—C3—C4	−0.6 (3)	C11—C10—C12—C13	179.43 (15)
C1—C2—C3—Cl1	178.80 (15)	C9—C10—C12—C13	−4.9 (3)
C2—C3—C4—C5	0.1 (3)	N2—C12—C13—C14	−52.8 (2)
Cl1—C3—C4—C5	−179.29 (13)	C10—C12—C13—C14	128.08 (19)
C3—C4—C5—C6	0.5 (3)	N2—C12—C13—C18	126.52 (17)
C3—C4—C5—Cl2	178.65 (14)	C10—C12—C13—C18	−52.6 (2)
C2—C1—C6—C5	0.1 (3)	C18—C13—C14—C15	0.1 (3)
C2—C1—C6—C7	177.56 (17)	C12—C13—C14—C15	179.44 (18)
C4—C5—C6—C1	−0.7 (3)	C13—C14—C15—C16	−1.3 (4)
Cl2—C5—C6—C1	−178.70 (14)	C14—C15—C16—C17	1.2 (4)
C4—C5—C6—C7	−178.03 (16)	C15—C16—C17—C18	0.1 (3)
Cl2—C5—C6—C7	3.9 (2)	C16—C17—C18—C13	−1.3 (3)
C1—C6—C7—O1	−123.5 (2)	C14—C13—C18—C17	1.2 (3)
C5—C6—C7—O1	53.8 (2)	C12—C13—C18—C17	−178.17 (16)
C1—C6—C7—C8	56.8 (2)	C11—N1—C19—C24	−176.03 (15)
C5—C6—C7—C8	−125.95 (18)	N2—N1—C19—C24	6.2 (2)
O1—C7—C8—C9	−168.14 (18)	C11—N1—C19—C20	5.2 (2)
C6—C7—C8—C9	11.6 (3)	N2—N1—C19—C20	−172.51 (14)
C7—C8—C9—C10	174.67 (16)	C24—C19—C20—C21	−1.1 (3)
C8—C9—C10—C11	−7.0 (3)	N1—C19—C20—C21	177.64 (16)
C8—C9—C10—C12	178.37 (17)	C19—C20—C21—C22	0.0 (3)
N2—N1—C11—C10	0.35 (17)	C20—C21—C22—C23	1.0 (3)
C19—N1—C11—C10	−177.52 (14)	C21—C22—C23—C24	−1.0 (3)

C12—C10—C11—N1	−0.37 (16)	C20—C19—C24—C23	1.2 (3)
C9—C10—C11—N1	−175.96 (14)	N1—C19—C24—C23	−177.55 (16)
N1—N2—C12—C10	−0.08 (16)	C22—C23—C24—C19	−0.1 (3)

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C19–C24 and C13–C18 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11A···O1^{i}	0.93	2.30	3.230 (2)	174
C20—H20A···O1^{i}	0.93	2.59	3.509 (3)	168
C2—H2A···Cg1^{ii}	0.93	2.75	3.585 (2)	149
C23—H23A···Cg2^{iii}	0.93	2.90	3.655 (2)	140

Symmetry codes: (i) −*x*, −*y*+1, −*z*+2; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) −*x*+1, −*y*+2, −*z*+2.

Fig. 1

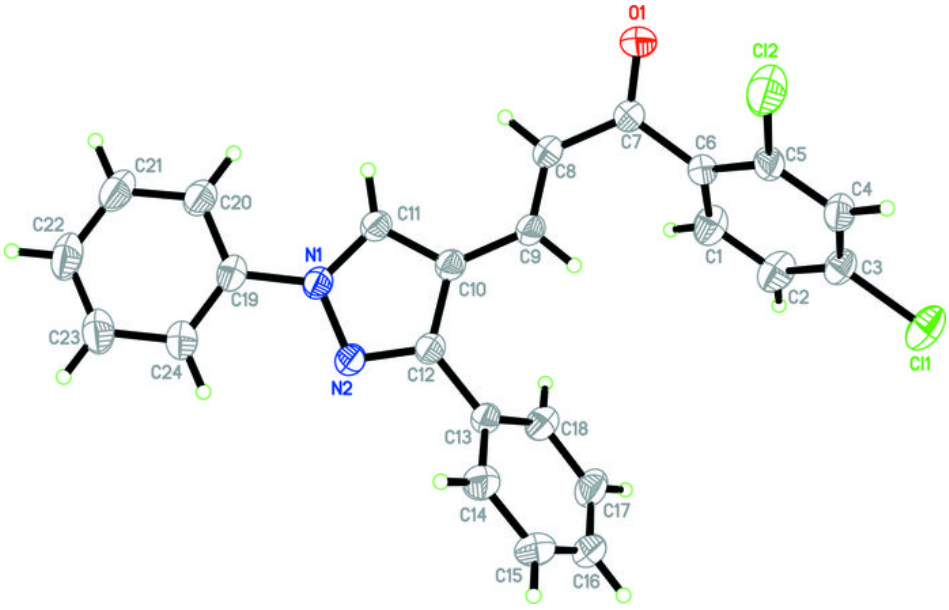

O1
Cl2
C7
C6
C5
C8
C4
C21
C20
C11
C22
N1
C9
C1
C3
C19
C10
C2
Cl1
C23
C24
N2
C12
C13
C18
C14
C17
C15
C16

Fig. 2