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4-(4-Chlorophenylsulfanyl)-1-[(*E*)-2-(4-chlorophenylsulfanyl)-1-phenylethenyl]-3-phenyl-1*H*-pyrazole

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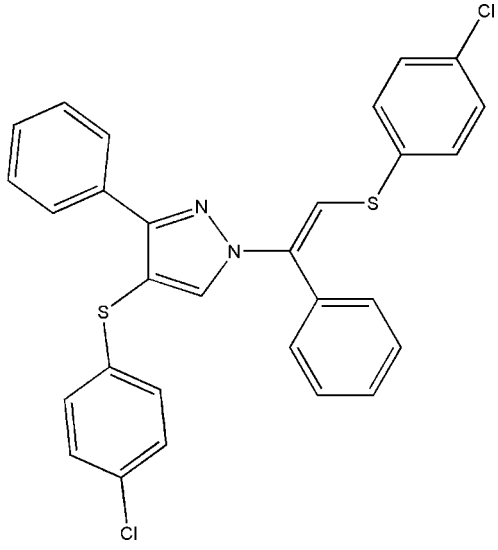
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.142; data-to-parameter ratio = 20.9.

In the title compound, $C_{29}H_{20}Cl_2N_2S_2$, the pyrazole ring adopts a planar conformation. The chlorophenyl rings are twisted from the pyrazole ring at angles of 52.74 (14) and 29.92 (13)°, respectively. The crystal structure is stabilized by C—H···N and C—H···π interactions.

Related literature

For the pharmacological and medicinal properties of the title compound, see: Baraldi *et al.* (1998); Bruno *et al.* (1990); Cottineau *et al.* (2002); Londershausen (1996); Chen & Li (1998); Mishra *et al.* (1998); Smith *et al.* (2001). For hybridization, see: Beddoes *et al.* (1986). For a related structure, see: Jin *et al.* (2004).



Experimental

Crystal data

$C_{29}H_{20}Cl_2N_2S_2$
M_r = 531.49
Monoclinic, $P2_1/c$
a = 12.3808 (4) Å
b = 21.4667 (7) Å
c = 10.4281 (4) Å
β = 108.181 (2)°
V = 2633.16 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.883, T_{max} = 0.927
31420 measured reflections
6594 independent reflections
4292 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.142
S = 1.02
6594 reflections
316 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

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

Cg is the centroid of the C26–C31 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···N1	0.93	2.44	2.772 (3)	101
C21—H21···Cg^{i}	0.93	2.96	3.808 (3)	153

Symmetry code: (i) $x, \frac{1}{2}-y, \frac{1}{2}+z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

PR thanks Dr Babu Varghese, SAIF, IIT Madras, Chennai, India, for his help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2789).

References

Baraldi, P. G., Manfredini, S., Romagnoli, R., Stevanato, L., Zaid, A. N. & Manservigi, R. (1998). *Nucleosides Nucleotides*, **17**, 2165–2171.
Beddoes, R. L., Dalton, L., Joule, T. A., Mills, O. S., Street, J. D. & Watt, C. I. F. (1986). *J. Chem. Soc. Perkin Trans. 2*, pp. 787–797.
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruno, O., Bondavalli, F., Ranise, A., Schenone, P., Losasso, C., Cilenti, L., Matera, C. & Marmo, E. (1990). *Il Farmaco*, **45**, 147–166.
Chen, H. S. & Li, Z. M. (1998). *Chem. J. Chin. Univ.* **19**, 572–576.
Cottineau, B., Toto, P., Marot, C., Pipaud, A. & Chenault, J. (2002). *Bioorg. Med. Chem.* **12**, 2105–2108.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Jin, Z.-M., Li, L., Li, M.-C., Hu, M.-L. & Shen, L. (2004). *Acta Cryst.* C**60**, o642–o643.
Londershausen, M. (1996). *Pestic. Sci.* **48**, 269–274.
Mishra, P. D., Wahidullah, S. & Kamat, S. Y. (1998). *Indian J. Chem. Sect. B*, **37**, 199.

Sheldrick, G. M. (2001). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Smith, S. R., Denhardt, G. & Terminelli, C. (2001). *Eur. J. Pharmacol.* **432**, 107–119.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2008). E**64**, o2054-o2055 [**doi:10.1107/S1600536808031231**]

4-(4-Chlorophenylsulfanyl)-1-[(*E*)-2-(4-chlorophenylsulfanyl)-1-phenylethenyl]-3-phenyl-1*H*-pyrazole

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Comment

Pyrazole derivatives possess significant antiarrhythmic and sedative (Bruno *et al.*, 1990), hypoglycemic (Cottineau *et al.*, 2002), antiviral (Baraldi *et al.*, 1998), and pesticidal (Londershausen *et al.*, 1996) properties. Some pyrazole derivatives are successfully tested for their antifungal (Chen & Li, 1998), antihistaminic (Mishra *et al.*, 1998) and anti-inflammatory (Smith *et al.*, 2001) activities.

An *ORTEP* plot of the molecule is shown in Fig. 1. The pyrazole ring adopts a planar conformation. The sum of the bond angles at N2 of the pyrazole ring (359.34°) is in accordance with sp^2 hybridization (Beddoes *et al.*, 1986). The C—N bond lengths in the pyrazole ring are 1.340 (3) and 1.325 (3) Å, which are shorter than a C—N single bond length of 1.443 Å, but longer than a double bond length of 1.269 Å (Jin *et al.*, 2004), indicating electron delocalization. The chlorophenyl rings are twisted from the pyrazole ring at angles of 52.74 (14)° and 29.92 (13), respectively. The crystal packing shows weak C—H···N (Tab. 1) and C—H···π interactions [C21-H21···cog^{i}(C26,C27,C28,C29,C30,C31); symmetry operator (i) x, 1/2-y, 1/2+z: H···cog 2.956Å, C21···cog 3.808Å, C21-H21···cog 152.9°] in addition to van der Waals forces.

Experimental

To a mixture of 2-[(4-chlorophenyl)sulfanyl]-1-phenyl-1-ethanone N-(E)-2- [(4-chlorophenyl)sulfanyl]-1-phenylethyl-idenehydrazone (0.003 mole) and 3 ml of dimethyl formamide kept in ice bath at 0° C, phosphorus oxycholride (0.024 mole) was added dropwise for 5–10 minutes. The reaction mixture was then kept in a microwave oven at 600 W for 30–60 sec. The process of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was poured into crushed ice and extracted with dichloromethane. The organic layer was dried in anhydrous sodium sulfate. The different compounds present in the mixture were separated by column chromatography using petroleum ether and ethyl acetate mixture as eluent. This isolated compound was recrystallized in dichloromethane to obtain 4-[(4-chlorophenyl)sulfanyl]-1-(*E*)-2-[(4-chlorophenyl)sulfanyl]-1-phenylethenyl-3-phenyl-1*H*-pyrazole in 86% yield.

Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) for all H atoms. The atom S1 was restrained within an effective standard deviation of 0.1 so that their U_{ij} components approximate to isotropic bahavior.

Figures

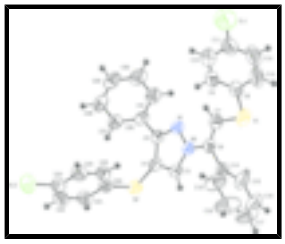


Fig. 1. Molecular structure of the title compound, showing the atomic numbering and 50% probability displacement ellipsoids.

4-(4-Chlorophenylsulfanyl)-1-[(*E*)-2-(4-chlorophenylsulfanyl)-1- phenylethenyl]-3-phenyl-1*H*-pyrazole

Crystal data

$C_{29}H_{20}Cl_2N_2S_2$	F_{000} = 1096
M_r = 531.49	D_x = 1.341 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4538 reflections
a = 12.3808 (4) Å	θ = 1.9–28.4º
b = 21.4667 (7) Å	μ = 0.43 mm^{-1}
c = 10.4281 (4) Å	T = 293 (2) K
β = 108.181 (2)º	Block, colorless
V = 2633.16 (16) Å^3	0.30 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker Kappa APEXII diffractometer	6594 independent reflections
Radiation source: fine-focus sealed tube	4292 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 293(2) K	θ_{max} = 28.4º
ω and φ scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	h = −9→16
T_{min} = 0.883, T_{max} = 0.927	k = −28→28
31420 measured reflections	l = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H-atom parameters constrained
$wR(F^2)$ = 0.142	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 1.5769P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
6594 reflections	$\Delta\rho_{max}$ = 0.58 e Å^{-3}
316 parameters	$\Delta\rho_{min}$ = −0.56 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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	−0.05360 (11)	0.97426 (6)	1.29295 (10)	0.1304 (4)
Cl2	0.49992 (8)	0.55063 (4)	0.67733 (9)	0.0936 (3)
S1	−0.22821 (6)	0.89305 (5)	0.68804 (10)	0.0988 (3)
S2	0.13985 (5)	0.72882 (3)	0.29751 (6)	0.05543 (17)
N2	−0.03047 (14)	0.82027 (8)	0.48954 (18)	0.0442 (4)
N1	0.06227 (14)	0.85803 (8)	0.52541 (18)	0.0458 (4)
C4	0.08940 (18)	0.77699 (10)	0.4007 (2)	0.0457 (5)
C5	0.13504 (17)	0.83241 (10)	0.4710 (2)	0.0432 (5)
C3	−0.01665 (18)	0.77170 (10)	0.4154 (2)	0.0474 (5)
H3	−0.0692	0.7402	0.3804	0.057*
C6	−0.12269 (18)	0.83142 (11)	0.5402 (2)	0.0487 (5)
C7	−0.1128 (2)	0.87324 (13)	0.6357 (3)	0.0660 (7)
H7	−0.0430	0.8924	0.6756	0.079*
C8	−0.1672 (2)	0.91670 (13)	0.8564 (3)	0.0708 (7)
C9	−0.0600 (2)	0.90247 (14)	0.9387 (3)	0.0749 (8)
H9	−0.0108	0.8804	0.9040	0.090*
C10	−0.0243 (3)	0.92044 (15)	1.0718 (4)	0.0844 (9)
H10	0.0490	0.9110	1.1262	0.101*
C11	−0.0963 (3)	0.95220 (14)	1.1244 (3)	0.0815 (9)
C12	−0.2020 (3)	0.96751 (19)	1.0443 (4)	0.1049 (12)
H12	−0.2504	0.9899	1.0797	0.126*
C13	−0.2377 (3)	0.95004 (19)	0.9112 (4)	0.1074 (13)
H13	−0.3104	0.9608	0.8570	0.129*
C14	−0.22593 (18)	0.79358 (11)	0.4766 (2)	0.0521 (5)
C15	−0.3037 (2)	0.81280 (15)	0.3589 (3)	0.0748 (8)
H15	−0.2918	0.8497	0.3186	0.090*

C16	−0.4000 (3)	0.7778 (2)	0.2995 (4)	0.0977 (11)
H16	−0.4524	0.7911	0.2192	0.117*
C17	−0.4182 (3)	0.7247 (2)	0.3572 (4)	0.1013 (13)
H17	−0.4834	0.7014	0.3171	0.122*
C18	−0.3416 (4)	0.7046 (2)	0.4741 (4)	0.1147 (15)
H18	−0.3544	0.6677	0.5137	0.138*
C19	−0.2445 (3)	0.73921 (16)	0.5344 (3)	0.0901 (10)
H19	−0.1919	0.7254	0.6141	0.108*
C20	0.23637 (18)	0.67789 (10)	0.4109 (2)	0.0465 (5)
C21	0.3060 (2)	0.64266 (12)	0.3584 (3)	0.0584 (6)
H21	0.2985	0.6456	0.2670	0.070*
C22	0.3863 (2)	0.60336 (12)	0.4394 (3)	0.0656 (7)
H22	0.4333	0.5801	0.4035	0.079*
C23	0.3961 (2)	0.59894 (11)	0.5732 (3)	0.0615 (6)
C24	0.3265 (2)	0.63248 (13)	0.6277 (3)	0.0653 (7)
H24	0.3333	0.6286	0.7187	0.078*
C25	0.2463 (2)	0.67213 (12)	0.5457 (2)	0.0571 (6)
H25	0.1989	0.6950	0.5817	0.069*
C26	0.24546 (18)	0.86348 (11)	0.4912 (2)	0.0471 (5)
C27	0.34364 (19)	0.83066 (12)	0.5004 (2)	0.0544 (6)
H27	0.3402	0.7878	0.4864	0.065*
C28	0.4473 (2)	0.86127 (14)	0.5304 (3)	0.0653 (7)
H28	0.5130	0.8389	0.5364	0.078*
C29	0.4531 (2)	0.92423 (15)	0.5512 (3)	0.0738 (8)
H29	0.5228	0.9445	0.5725	0.089*
C30	0.3564 (2)	0.95734 (14)	0.5405 (3)	0.0780 (8)
H30	0.3604	1.0003	0.5534	0.094*
C31	0.2524 (2)	0.92733 (12)	0.5107 (3)	0.0637 (7)
H31	0.1870	0.9502	0.5039	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1506 (10)	0.1492 (10)	0.0782 (6)	0.0227 (8)	0.0167 (6)	−0.0108 (6)
Cl2	0.0875 (6)	0.0736 (5)	0.1054 (6)	0.0208 (4)	0.0094 (5)	0.0060 (4)
S1	0.0426 (4)	0.1458 (8)	0.1049 (6)	0.0127 (4)	0.0184 (4)	−0.0526 (6)
S2	0.0496 (3)	0.0730 (4)	0.0426 (3)	0.0013 (3)	0.0128 (2)	−0.0085 (3)
N2	0.0340 (9)	0.0478 (10)	0.0491 (10)	−0.0018 (7)	0.0103 (7)	0.0014 (8)
N1	0.0401 (9)	0.0447 (9)	0.0511 (10)	−0.0051 (7)	0.0119 (8)	0.0017 (8)
C4	0.0388 (11)	0.0537 (12)	0.0425 (11)	−0.0019 (9)	0.0097 (9)	−0.0018 (9)
C5	0.0382 (11)	0.0498 (12)	0.0404 (10)	−0.0024 (9)	0.0103 (8)	0.0055 (9)
C3	0.0373 (11)	0.0513 (12)	0.0504 (12)	−0.0036 (9)	0.0089 (9)	−0.0035 (10)
C6	0.0351 (11)	0.0543 (13)	0.0546 (13)	0.0051 (9)	0.0109 (9)	0.0013 (10)
C7	0.0375 (12)	0.0774 (17)	0.0822 (18)	0.0019 (11)	0.0173 (12)	−0.0179 (15)
C8	0.0533 (15)	0.0706 (17)	0.089 (2)	0.0111 (13)	0.0222 (14)	−0.0161 (15)
C9	0.0548 (16)	0.0710 (18)	0.099 (2)	0.0148 (13)	0.0241 (15)	−0.0101 (16)
C10	0.0685 (19)	0.084 (2)	0.092 (2)	0.0161 (16)	0.0113 (16)	0.0015 (18)
C11	0.091 (2)	0.0686 (18)	0.080 (2)	0.0153 (16)	0.0203 (17)	−0.0020 (15)

C12	0.103 (3)	0.118 (3)	0.092 (2)	0.049 (2)	0.028 (2)	−0.021 (2)
C13	0.074 (2)	0.142 (3)	0.098 (3)	0.051 (2)	0.0150 (18)	−0.031 (2)
C14	0.0384 (11)	0.0631 (14)	0.0565 (13)	−0.0014 (10)	0.0175 (10)	−0.0032 (11)
C15	0.0466 (14)	0.087 (2)	0.0811 (19)	−0.0006 (13)	0.0055 (13)	0.0086 (16)
C16	0.0480 (16)	0.140 (3)	0.090 (2)	−0.0098 (19)	−0.0007 (15)	−0.009 (2)
C17	0.072 (2)	0.147 (4)	0.092 (3)	−0.055 (2)	0.0362 (19)	−0.042 (2)
C18	0.135 (4)	0.118 (3)	0.096 (3)	−0.071 (3)	0.043 (3)	−0.011 (2)
C19	0.099 (2)	0.091 (2)	0.0697 (19)	−0.0358 (19)	0.0118 (17)	0.0075 (17)
C20	0.0432 (11)	0.0498 (12)	0.0489 (12)	−0.0083 (9)	0.0177 (9)	−0.0106 (10)
C21	0.0645 (15)	0.0629 (15)	0.0545 (14)	−0.0016 (12)	0.0283 (12)	−0.0093 (12)
C22	0.0661 (16)	0.0593 (15)	0.0797 (18)	0.0048 (13)	0.0347 (14)	−0.0102 (13)
C23	0.0583 (15)	0.0484 (13)	0.0731 (17)	−0.0009 (11)	0.0136 (13)	−0.0042 (12)
C24	0.0750 (18)	0.0684 (16)	0.0510 (14)	0.0034 (14)	0.0175 (12)	−0.0034 (12)
C25	0.0569 (14)	0.0674 (15)	0.0510 (13)	0.0055 (12)	0.0227 (11)	−0.0067 (11)
C26	0.0421 (11)	0.0585 (13)	0.0391 (11)	−0.0097 (10)	0.0103 (9)	0.0051 (9)
C27	0.0453 (12)	0.0629 (14)	0.0555 (13)	−0.0062 (11)	0.0164 (10)	−0.0006 (11)
C28	0.0421 (13)	0.0853 (19)	0.0682 (16)	−0.0075 (12)	0.0167 (11)	0.0051 (14)
C29	0.0478 (15)	0.085 (2)	0.0841 (19)	−0.0233 (14)	0.0140 (13)	0.0101 (16)
C30	0.0644 (18)	0.0612 (16)	0.102 (2)	−0.0207 (14)	0.0169 (16)	0.0073 (15)
C31	0.0503 (14)	0.0570 (15)	0.0802 (18)	−0.0086 (11)	0.0150 (12)	0.0087 (13)

Geometric parameters (Å, °)

Cl1—C11	1.735 (3)	C15—H15	0.9300
Cl2—C23	1.742 (3)	C16—C17	1.340 (5)
S1—C7	1.734 (3)	C16—H16	0.9300
S1—C8	1.756 (3)	C17—C18	1.360 (6)
S2—C4	1.742 (2)	C17—H17	0.9300
S2—C20	1.772 (2)	C18—C19	1.386 (5)
N2—C3	1.340 (3)	C18—H18	0.9300
N2—N1	1.359 (2)	C19—H19	0.9300
N2—C6	1.420 (3)	C20—C25	1.378 (3)
N1—C5	1.325 (3)	C20—C21	1.382 (3)
C4—C3	1.373 (3)	C21—C22	1.375 (4)
C4—C5	1.419 (3)	C21—H21	0.9300
C5—C26	1.476 (3)	C22—C23	1.366 (4)
C3—H3	0.9300	C22—H22	0.9300
C6—C7	1.318 (3)	C23—C24	1.374 (4)
C6—C14	1.485 (3)	C24—C25	1.383 (4)
C7—H7	0.9300	C24—H24	0.9300
C8—C9	1.371 (4)	C25—H25	0.9300
C8—C13	1.383 (4)	C26—C27	1.382 (3)
C9—C10	1.374 (4)	C26—C31	1.384 (3)
C9—H9	0.9300	C27—C28	1.388 (3)
C10—C11	1.366 (4)	C27—H27	0.9300
C10—H10	0.9300	C28—C29	1.367 (4)
C11—C12	1.355 (5)	C28—H28	0.9300
C12—C13	1.371 (5)	C29—C30	1.367 (4)
C12—H12	0.9300	C29—H29	0.9300

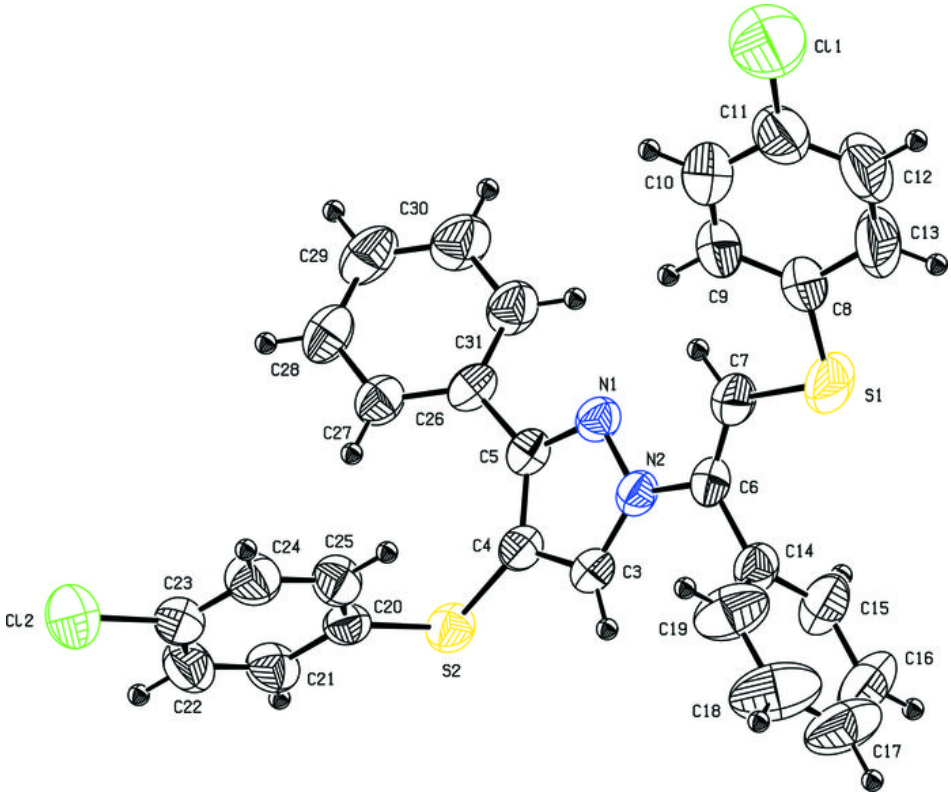
C13—H13	0.9300	C30—C31	1.386 (3)
C14—C19	1.365 (4)	C30—H30	0.9300
C14—C15	1.366 (4)	C31—H31	0.9300
C15—C16	1.382 (4)		
C7—S1—C8	104.26 (13)	C15—C16—H16	119.9
C4—S2—C20	104.53 (10)	C16—C17—C18	120.2 (3)
C3—N2—N1	111.96 (17)	C16—C17—H17	119.9
C3—N2—C6	127.43 (18)	C18—C17—H17	119.9
N1—N2—C6	120.35 (17)	C17—C18—C19	120.0 (4)
C5—N1—N2	105.27 (17)	C17—C18—H18	120.0
C3—C4—C5	104.59 (19)	C19—C18—H18	120.0
C3—C4—S2	124.02 (17)	C14—C19—C18	120.0 (3)
C5—C4—S2	130.90 (16)	C14—C19—H19	120.0
N1—C5—C4	110.79 (18)	C18—C19—H19	120.0
N1—C5—C26	118.32 (19)	C25—C20—C21	119.2 (2)
C4—C5—C26	130.9 (2)	C25—C20—S2	124.29 (17)
N2—C3—C4	107.39 (19)	C21—C20—S2	116.56 (18)
N2—C3—H3	126.3	C22—C21—C20	120.9 (2)
C4—C3—H3	126.3	C22—C21—H21	119.6
C7—C6—N2	120.0 (2)	C20—C21—H21	119.6
C7—C6—C14	125.0 (2)	C23—C22—C21	119.2 (2)
N2—C6—C14	114.93 (19)	C23—C22—H22	120.4
C6—C7—S1	120.9 (2)	C21—C22—H22	120.4
C6—C7—H7	119.5	C22—C23—C24	121.3 (2)
S1—C7—H7	119.5	C22—C23—Cl2	119.4 (2)
C9—C8—C13	117.9 (3)	C24—C23—Cl2	119.3 (2)
C9—C8—S1	126.3 (2)	C23—C24—C25	119.2 (2)
C13—C8—S1	115.7 (2)	C23—C24—H24	120.4
C8—C9—C10	120.9 (3)	C25—C24—H24	120.4
C8—C9—H9	119.6	C20—C25—C24	120.3 (2)
C10—C9—H9	119.6	C20—C25—H25	119.8
C11—C10—C9	120.1 (3)	C24—C25—H25	119.8
C11—C10—H10	120.0	C27—C26—C31	118.8 (2)
C9—C10—H10	120.0	C27—C26—C5	122.3 (2)
C12—C11—C10	119.9 (3)	C31—C26—C5	118.7 (2)
C12—C11—Cl1	119.3 (3)	C26—C27—C28	120.4 (2)
C10—C11—Cl1	120.8 (3)	C26—C27—H27	119.8
C11—C12—C13	120.1 (3)	C28—C27—H27	119.8
C11—C12—H12	119.9	C29—C28—C27	120.2 (3)
C13—C12—H12	119.9	C29—C28—H28	119.9
C12—C13—C8	121.0 (3)	C27—C28—H28	119.9
C12—C13—H13	119.5	C30—C29—C28	120.0 (2)
C8—C13—H13	119.5	C30—C29—H29	120.0
C19—C14—C15	119.1 (3)	C28—C29—H29	120.0
C19—C14—C6	120.7 (2)	C29—C30—C31	120.4 (3)
C15—C14—C6	120.2 (2)	C29—C30—H30	119.8
C14—C15—C16	120.4 (3)	C31—C30—H30	119.8
C14—C15—H15	119.8	C26—C31—C30	120.2 (3)
C16—C15—H15	119.8	C26—C31—H31	119.9

C17—C16—C15	120.2 (3)	C30—C31—H31	119.9
C17—C16—H16	119.9		
C3—N2—N1—C5	0.5 (2)	C7—C6—C14—C15	94.6 (3)
C6—N2—N1—C5	175.07 (18)	N2—C6—C14—C15	−84.7 (3)
C20—S2—C4—C3	−104.7 (2)	C19—C14—C15—C16	0.2 (5)
C20—S2—C4—C5	84.6 (2)	C6—C14—C15—C16	−179.9 (3)
N2—N1—C5—C4	−0.8 (2)	C14—C15—C16—C17	0.3 (5)
N2—N1—C5—C26	179.40 (17)	C15—C16—C17—C18	−0.5 (6)
C3—C4—C5—N1	0.8 (2)	C16—C17—C18—C19	0.1 (7)
S2—C4—C5—N1	172.85 (17)	C15—C14—C19—C18	−0.5 (5)
C3—C4—C5—C26	−179.5 (2)	C6—C14—C19—C18	179.6 (3)
S2—C4—C5—C26	−7.4 (4)	C17—C18—C19—C14	0.3 (6)
N1—N2—C3—C4	−0.1 (2)	C4—S2—C20—C25	11.8 (2)
C6—N2—C3—C4	−174.1 (2)	C4—S2—C20—C21	−167.52 (18)
C5—C4—C3—N2	−0.4 (2)	C25—C20—C21—C22	−1.6 (4)
S2—C4—C3—N2	−173.19 (16)	S2—C20—C21—C22	177.8 (2)
C3—N2—C6—C7	164.7 (2)	C20—C21—C22—C23	0.6 (4)
N1—N2—C6—C7	−8.9 (3)	C21—C22—C23—C24	0.7 (4)
C3—N2—C6—C14	−15.9 (3)	C21—C22—C23—Cl2	−178.5 (2)
N1—N2—C6—C14	170.50 (18)	C22—C23—C24—C25	−1.0 (4)
N2—C6—C7—S1	173.84 (18)	Cl2—C23—C24—C25	178.2 (2)
C14—C6—C7—S1	−5.5 (4)	C21—C20—C25—C24	1.2 (4)
C8—S1—C7—C6	152.2 (2)	S2—C20—C25—C24	−178.1 (2)
C7—S1—C8—C9	−19.9 (3)	C23—C24—C25—C20	0.0 (4)
C7—S1—C8—C13	163.8 (3)	N1—C5—C26—C27	147.7 (2)
C13—C8—C9—C10	0.5 (5)	C4—C5—C26—C27	−32.0 (3)
S1—C8—C9—C10	−175.8 (3)	N1—C5—C26—C31	−27.8 (3)
C8—C9—C10—C11	0.9 (5)	C4—C5—C26—C31	152.5 (2)
C9—C10—C11—C12	−1.8 (6)	C31—C26—C27—C28	0.8 (3)
C9—C10—C11—Cl1	179.0 (3)	C5—C26—C27—C28	−174.7 (2)
C10—C11—C12—C13	1.4 (6)	C26—C27—C28—C29	0.0 (4)
Cl1—C11—C12—C13	−179.4 (3)	C27—C28—C29—C30	−0.9 (4)
C11—C12—C13—C8	0.0 (7)	C28—C29—C30—C31	1.0 (5)
C9—C8—C13—C12	−1.0 (6)	C27—C26—C31—C30	−0.7 (4)
S1—C8—C13—C12	175.7 (4)	C5—C26—C31—C30	174.9 (2)
C7—C6—C14—C19	−85.5 (4)	C29—C30—C31—C26	−0.1 (5)
N2—C6—C14—C19	95.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···N1	0.93	2.44	2.772 (3)	101

Fig. 1


Cl1
C11
C10
C12
C13
C9
C8
C30
C29
C31
C28
C27
C26
C7
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N1
C5
N2
C6
C4
C3
C14
C24
C25
C23
C20
C15
Cl2
C19
C16
S2
C21
C18
C22
C17