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N-(5-Chloro-3-methyl-1-phenylpyrazol-4-ylcarbonyl)-*N*′-(4-methylphenyl)thiourea

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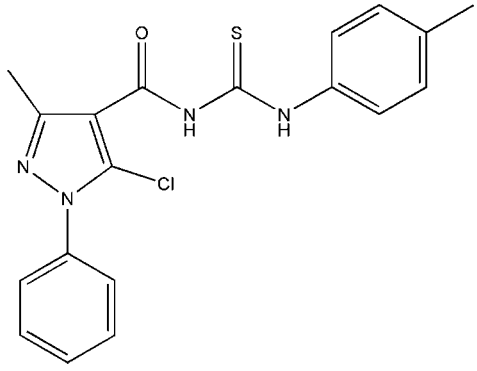
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.102; data-to-parameter ratio = 13.4.

The crystal structure of the title compound, $C_{19}H_{17}ClN_4OS$, has been determined in order to elucidate the molecular conformation. The pyrazole ring makes dihedral angles of 74.3 (3)° and 2.9 (3)° with the phenyl and tolyl rings, respectively; these two six-membered rings are twisted by 71.6 (3)° with respect to each other. The crystal packing of the title compound is stabilized by intramolcular N—H···O and intermolcular N—H···S hydrogen bonds.

Related literature

For related literature, see: Saeed & Flörke (2007); Wang *et al.* (2007).



Experimental

Crystal data

$C_{19}H_{17}ClN_4OS$
M_r = 384.88
Monoclinic, $C2/c$
a = 14.935 (6) Å
b = 16.321 (6) Å
c = 15.469 (6) Å
β = 98.786 (6)°
V = 3727 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.924, T_{max} = 0.968
7376 measured reflections
3275 independent reflections
2512 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 1.03
3275 reflections
244 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···S1^{i}	0.83 (2)	2.70 (2)	3.484 (2)	158 (2)
N4—H4A···O1	0.83 (3)	1.96 (3)	2.662 (3)	141 (2)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2200).

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supplementary materials

Acta Cryst. (2007). E**63**, o4287 [**doi:10.1107/S1600536807043541**]

N-(5-Chloro-3-methyl-1-phenylpyrazol-4-ylcarbonyl)-*N*'-(4-methylphenyl)thiourea

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Comment

In this paper, the synthesis and crystal structure of the title compound is reported. The molecular structure and the atom-numbering scheme are shown in Fig.1. The pyrazole ring makes dihedral angles of 74.3 (3)° and 2.9 (3)° with the C1—C6 ring and the C13—C18 rings, respectively; these two six-membered rings are twisted by 71.6 (3)° with respect to each other. However in the similar structure, 1-(3-methoxyphenyl)-3-(4-methylbenzoyl)thiourea (Saeed *et al.*, 2007), the dihedral angle between the two phenyl ring planes is 48.3 (1)°. All bond lengths and angles are in the normal ranges (Saeed *et al.*, 2007; Wang *et al.*, 2007). The crystal packing of the title compound is stabilized by intramolcular N—H···O and intermolecular N—H···S hydrogen bonds.

Experimental

Powdered ammonium thiocyanate (15 mmol), 5-chloro-3-methyl-1-phenylpyrazole-4-carbonyl chloride (10 mmol), PEG-400 (0.15 mmol) and acetone (25 ml) were placed in a dried round-bottomed flask containing a magnetic stirrer bar. The mixture was stirred at room temperature for 1 h, then 4-methylaniline (9.5 mmol) was added, and the mixture was stirred for 10 h. The mixture was poured into water (20 ml). The resulting solid was filtered, dried and recrystallized from DMF-EtOH to give *N*-(4-methylphenyl)-*N*'-(5-chloro-3-methyl-1-phenylpyrazol-4-yl- carbonyl)thiourea. Single crystals of the title compound were obtained by slow evaporation of a solution in DMF-EtOH (1:1, *v*/*v*).

Refinement

H atoms bonded to N atoms were located in a difference map and refined with distance restraints of N—H = 0.83 (3) Å, and with U_{iso}(H) = 1.2U_{eq}(N). Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.96 Å; U_{iso}(H) = xU_{eq}(carrier atom) where x = 1.5 for methyl groups and 1.2 for Csp^2.

Figures

Fig. 1. The molecular structure of the title compound, with the atom numbering scheme and showing displacement ellipsoids at the 50% probability level. Hydrogen atoms have been omitted.

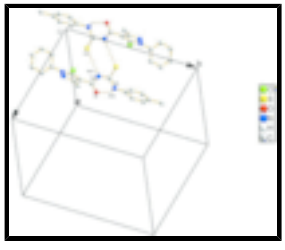

Fig. 2. The intermolecular and intramolecular hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been onitted. [Symmetry code A: −x + 1/2, −y + 1/2, −z]

N-(4-Methylphenyl)-*N*'-(5-chloro-3-methyl-1- phenylpyrazol-4-ylcarbonyl)thiourea

Crystal data

$C_{19}H_{17}ClN_4OS$	$D_x = 1.372$ Mg m^{-3}
$M_r = 384.88$	Melting point: 437 K
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 14.935 (6) Å	Cell parameters from 3035 reflections
b = 16.321 (6) Å	θ = 2.2–25.9º
c = 15.469 (6) Å	μ = 0.33 mm^{-1}
β = 98.786 (6)º	*T* = 294 (2) K
V = 3727 (2) Å^3	Prism, colourless
Z = 8	0.24 × 0.22 × 0.10 mm
F_{000} = 1600	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	3275 independent reflections
Radiation source: fine-focus sealed tube	2512 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
T = 294(2) K	$\theta_{max} = 25.0$º
phi and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −17→13
$T_{min} = 0.924$, $T_{max} = 0.968$	*k* = −19→16
7376 measured reflections	*l* = −18→18

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 3.1362P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.102$	$(\Delta/\sigma)_{max} = 0.002$
S = 1.03	$\Delta\rho_{max} = 0.26$ e Å^{-3}
3275 reflections	$\Delta\rho_{min} = -0.29$ e Å^{-3}
244 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0135 (6)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.26808 (4)	0.10959 (3)	0.18875 (4)	0.0489 (2)
S1	0.25725 (4)	0.37690 (4)	0.04136 (5)	0.0548 (2)
O1	0.52013 (11)	0.25072 (9)	0.15254 (13)	0.0601 (5)
N1	0.38841 (11)	0.00224 (10)	0.15040 (11)	0.0368 (4)
N2	0.47254 (11)	−0.00682 (11)	0.12675 (12)	0.0416 (5)
N3	0.36918 (12)	0.25941 (11)	0.10169 (13)	0.0435 (5)
H3A	0.3265 (16)	0.2329 (15)	0.0743 (16)	0.052*
N4	0.42555 (14)	0.38937 (11)	0.12986 (14)	0.0505 (5)
H4A	0.4725 (18)	0.3629 (16)	0.1476 (17)	0.061*
C1	0.33371 (14)	−0.06761 (12)	0.16252 (14)	0.0362 (5)
C2	0.26236 (16)	−0.08688 (15)	0.09905 (17)	0.0514 (6)
H2	0.2502	−0.0555	0.0484	0.062*
C3	0.20897 (16)	−0.15344 (15)	0.11148 (19)	0.0590 (7)
H3	0.1600	−0.1668	0.0692	0.071*
C4	0.22750 (16)	−0.19991 (14)	0.18540 (18)	0.0530 (6)
H4	0.1914	−0.2449	0.1932	0.064*
C5	0.29946 (17)	−0.18026 (14)	0.24817 (17)	0.0529 (6)
H5	0.3119	−0.2120	0.2985	0.064*
C6	0.35346 (15)	−0.11362 (13)	0.23706 (15)	0.0435 (5)
H6	0.4024	−0.1002	0.2794	0.052*
C7	0.59176 (15)	0.08158 (16)	0.08879 (18)	0.0533 (6)
H7A	0.6216	0.0298	0.0861	0.080*
H7B	0.6283	0.1167	0.1297	0.080*
H7C	0.5831	0.1066	0.0320	0.080*
C8	0.50222 (13)	0.06866 (13)	0.11763 (14)	0.0375 (5)
C9	0.43742 (13)	0.12760 (12)	0.13398 (14)	0.0355 (5)
C10	0.36644 (13)	0.08160 (12)	0.15463 (13)	0.0345 (5)
C11	0.44734 (14)	0.21691 (13)	0.13126 (14)	0.0397 (5)
C12	0.35583 (15)	0.34383 (13)	0.09374 (15)	0.0418 (5)
C13	0.43399 (15)	0.47650 (13)	0.12661 (15)	0.0456 (6)
C14	0.51457 (17)	0.50783 (15)	0.1089 (2)	0.0638 (8)
H14	0.5615	0.4727	0.1007	0.077*
C15	0.52592 (18)	0.59178 (16)	0.1034 (2)	0.0632 (7)

H15	0.5807	0.6123	0.0911	0.076*
C16	0.45840 (17)	0.64529 (14)	0.11565 (16)	0.0499 (6)
C17	0.37896 (19)	0.61242 (15)	0.13533 (19)	0.0615 (7)
H17	0.3325	0.6476	0.1450	0.074*
C18	0.36606 (18)	0.52902 (15)	0.14119 (18)	0.0586 (7)
H18	0.3118	0.5086	0.1549	0.070*
C19	0.4709 (2)	0.73671 (15)	0.1069 (2)	0.0743 (9)
H19A	0.4915	0.7598	0.1635	0.111*
H19B	0.4141	0.7613	0.0827	0.111*
H19C	0.5148	0.7471	0.0690	0.111*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0403 (3)	0.0417 (3)	0.0680 (4)	0.0026 (2)	0.0185 (3)	−0.0021 (3)
S1	0.0537 (4)	0.0364 (3)	0.0676 (4)	0.0055 (3)	−0.0116 (3)	0.0025 (3)
O1	0.0356 (9)	0.0367 (9)	0.1031 (15)	−0.0072 (7)	−0.0047 (9)	0.0049 (9)
N1	0.0299 (9)	0.0296 (9)	0.0509 (11)	0.0002 (7)	0.0065 (8)	0.0045 (8)
N2	0.0306 (9)	0.0356 (10)	0.0586 (12)	0.0026 (8)	0.0071 (8)	0.0041 (8)
N3	0.0365 (10)	0.0298 (10)	0.0601 (13)	−0.0037 (8)	−0.0063 (9)	0.0035 (9)
N4	0.0461 (12)	0.0318 (11)	0.0691 (14)	−0.0025 (9)	−0.0054 (10)	0.0013 (9)
C1	0.0337 (11)	0.0270 (10)	0.0480 (13)	−0.0008 (8)	0.0068 (9)	0.0008 (9)
C2	0.0478 (14)	0.0456 (14)	0.0570 (15)	−0.0052 (11)	−0.0043 (12)	0.0107 (11)
C3	0.0436 (14)	0.0480 (15)	0.0786 (19)	−0.0120 (11)	−0.0125 (13)	0.0035 (13)
C4	0.0434 (13)	0.0352 (13)	0.0799 (18)	−0.0081 (10)	0.0080 (12)	0.0083 (12)
C5	0.0569 (15)	0.0416 (13)	0.0593 (16)	−0.0058 (11)	0.0057 (12)	0.0148 (11)
C6	0.0431 (12)	0.0369 (12)	0.0482 (14)	−0.0051 (10)	0.0002 (10)	0.0032 (10)
C7	0.0370 (12)	0.0513 (14)	0.0735 (18)	−0.0021 (11)	0.0142 (12)	0.0003 (13)
C8	0.0295 (10)	0.0364 (12)	0.0453 (13)	−0.0008 (9)	0.0017 (9)	0.0040 (9)
C9	0.0304 (11)	0.0323 (11)	0.0420 (12)	−0.0029 (9)	−0.0005 (9)	0.0043 (9)
C10	0.0302 (10)	0.0314 (11)	0.0411 (12)	0.0019 (9)	0.0032 (9)	0.0010 (9)
C11	0.0347 (12)	0.0348 (12)	0.0485 (13)	−0.0027 (9)	0.0030 (10)	0.0029 (10)
C12	0.0478 (13)	0.0313 (11)	0.0455 (13)	−0.0015 (10)	0.0041 (10)	0.0029 (10)
C13	0.0492 (14)	0.0312 (12)	0.0535 (14)	−0.0044 (10)	−0.0018 (11)	−0.0024 (10)
C14	0.0417 (14)	0.0396 (14)	0.107 (2)	0.0002 (11)	0.0025 (14)	−0.0073 (14)
C15	0.0478 (15)	0.0444 (15)	0.097 (2)	−0.0118 (12)	0.0092 (14)	−0.0041 (14)
C16	0.0573 (15)	0.0365 (13)	0.0533 (15)	−0.0059 (11)	0.0002 (12)	−0.0042 (11)
C17	0.0652 (17)	0.0389 (14)	0.085 (2)	0.0006 (12)	0.0254 (15)	−0.0131 (13)
C18	0.0616 (16)	0.0401 (14)	0.0791 (19)	−0.0066 (12)	0.0266 (14)	−0.0096 (13)
C19	0.087 (2)	0.0382 (15)	0.097 (2)	−0.0115 (14)	0.0136 (18)	−0.0058 (14)

Geometric parameters (Å, °)

Cl1—C10	1.698 (2)	C6—H6	0.9300
S1—C12	1.659 (2)	C7—C8	1.488 (3)
O1—C11	1.219 (2)	C7—H7A	0.9600
N1—C10	1.340 (3)	C7—H7B	0.9600
N1—N2	1.369 (2)	C7—H7C	0.9600
N1—C1	1.431 (3)	C8—C9	1.415 (3)

N2—C8	1.324 (3)	C9—C10	1.376 (3)
N3—C11	1.375 (3)	C9—C11	1.466 (3)
N3—C12	1.395 (3)	C13—C18	1.373 (3)
N3—H3A	0.83 (2)	C13—C14	1.373 (3)
N4—C12	1.331 (3)	C14—C15	1.385 (4)
N4—C13	1.429 (3)	C14—H14	0.9300
N4—H4A	0.83 (3)	C15—C16	1.369 (4)
C1—C6	1.370 (3)	C15—H15	0.9300
C1—C2	1.371 (3)	C16—C17	1.378 (4)
C2—C3	1.378 (3)	C16—C19	1.512 (3)
C2—H2	0.9300	C17—C18	1.380 (3)
C3—C4	1.365 (4)	C17—H17	0.9300
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.372 (3)	C19—H19A	0.9600
C4—H4	0.9300	C19—H19B	0.9600
C5—C6	1.380 (3)	C19—H19C	0.9600
C5—H5	0.9300		
C10—N1—N2	111.03 (16)	C10—C9—C8	104.05 (18)
C10—N1—C1	127.92 (17)	C10—C9—C11	129.34 (19)
N2—N1—C1	120.95 (16)	C8—C9—C11	126.59 (19)
C8—N2—N1	105.29 (16)	N1—C10—C9	108.24 (18)
C11—N3—C12	129.08 (19)	N1—C10—Cl1	120.34 (15)
C11—N3—H3A	116.9 (17)	C9—C10—Cl1	131.25 (16)
C12—N3—H3A	112.4 (17)	O1—C11—N3	122.6 (2)
C12—N4—C13	127.5 (2)	O1—C11—C9	122.16 (19)
C12—N4—H4A	114.4 (19)	N3—C11—C9	115.26 (18)
C13—N4—H4A	116.9 (19)	N4—C12—N3	114.99 (19)
C6—C1—C2	121.4 (2)	N4—C12—S1	127.06 (17)
C6—C1—N1	119.54 (19)	N3—C12—S1	117.95 (16)
C2—C1—N1	119.06 (19)	C18—C13—C14	119.5 (2)
C1—C2—C3	118.9 (2)	C18—C13—N4	123.0 (2)
C1—C2—H2	120.5	C14—C13—N4	117.5 (2)
C3—C2—H2	120.5	C13—C14—C15	120.0 (2)
C4—C3—C2	120.5 (2)	C13—C14—H14	120.0
C4—C3—H3	119.8	C15—C14—H14	120.0
C2—C3—H3	119.8	C16—C15—C14	121.5 (2)
C3—C4—C5	120.0 (2)	C16—C15—H15	119.2
C3—C4—H4	120.0	C14—C15—H15	119.2
C5—C4—H4	120.0	C15—C16—C17	117.4 (2)
C4—C5—C6	120.4 (2)	C15—C16—C19	120.9 (2)
C4—C5—H5	119.8	C17—C16—C19	121.7 (2)
C6—C5—H5	119.8	C16—C17—C18	122.2 (2)
C1—C6—C5	118.8 (2)	C16—C17—H17	118.9
C1—C6—H6	120.6	C18—C17—H17	118.9
C5—C6—H6	120.6	C13—C18—C17	119.4 (2)
C8—C7—H7A	109.5	C13—C18—H18	120.3
C8—C7—H7B	109.5	C17—C18—H18	120.3
H7A—C7—H7B	109.5	C16—C19—H19A	109.5
C8—C7—H7C	109.5	C16—C19—H19B	109.5

H7A—C7—H7C	109.5	H19A—C19—H19B	109.5
H7B—C7—H7C	109.5	C16—C19—H19C	109.5
N2—C8—C9	111.37 (18)	H19A—C19—H19C	109.5
N2—C8—C7	119.65 (19)	H19B—C19—H19C	109.5
C9—C8—C7	128.9 (2)		
C10—N1—N2—C8	0.8 (2)	C11—C9—C10—N1	−178.5 (2)
C1—N1—N2—C8	177.37 (18)	C8—C9—C10—Cl1	175.06 (17)
C10—N1—C1—C6	−107.7 (3)	C11—C9—C10—Cl1	−3.3 (4)
N2—N1—C1—C6	76.3 (3)	C12—N3—C11—O1	−3.0 (4)
C10—N1—C1—C2	72.2 (3)	C12—N3—C11—C9	178.1 (2)
N2—N1—C1—C2	−103.8 (2)	C10—C9—C11—O1	144.7 (2)
C6—C1—C2—C3	0.8 (4)	C8—C9—C11—O1	−33.4 (4)
N1—C1—C2—C3	−179.0 (2)	C10—C9—C11—N3	−36.4 (3)
C1—C2—C3—C4	−0.7 (4)	C8—C9—C11—N3	145.5 (2)
C2—C3—C4—C5	0.3 (4)	C13—N4—C12—N3	175.1 (2)
C3—C4—C5—C6	0.0 (4)	C13—N4—C12—S1	−4.7 (4)
C2—C1—C6—C5	−0.5 (4)	C11—N3—C12—N4	−9.3 (4)
N1—C1—C6—C5	179.3 (2)	C11—N3—C12—S1	170.60 (19)
C4—C5—C6—C1	0.1 (4)	C12—N4—C13—C18	45.8 (4)
N1—N2—C8—C9	−0.8 (2)	C12—N4—C13—C14	−134.9 (3)
N1—N2—C8—C7	−177.85 (19)	C18—C13—C14—C15	−1.9 (4)
N2—C8—C9—C10	0.6 (2)	N4—C13—C14—C15	178.8 (2)
C7—C8—C9—C10	177.3 (2)	C13—C14—C15—C16	0.3 (4)
N2—C8—C9—C11	179.1 (2)	C14—C15—C16—C17	1.2 (4)
C7—C8—C9—C11	−4.3 (4)	C14—C15—C16—C19	−178.3 (3)
N2—N1—C10—C9	−0.4 (2)	C15—C16—C17—C18	−1.2 (4)
C1—N1—C10—C9	−176.71 (19)	C19—C16—C17—C18	178.3 (3)
N2—N1—C10—Cl1	−176.19 (14)	C14—C13—C18—C17	1.9 (4)
C1—N1—C10—Cl1	7.5 (3)	N4—C13—C18—C17	−178.9 (2)
C8—C9—C10—N1	−0.1 (2)	C16—C17—C18—C13	−0.3 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···S1^{i}	0.83 (2)	2.70 (2)	3.484 (2)	158 (2)
N4—H4A···O1	0.83 (3)	1.96 (3)	2.662 (3)	141 (2)

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

Fig. 1

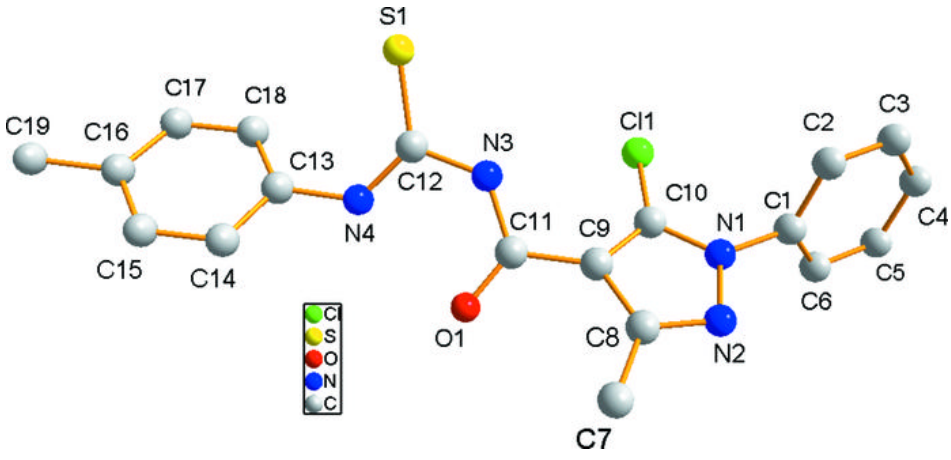
S1
C17
C18
C19
C16
C13
C12
N3
Cl1
C2
C3
C10
C1
C4
N4
C11
C9
N1
C15
C14
C5
C6
O1
C8
N2
C7
Cl
S
O
N
C

Fig. 2