Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-(2,4-Dichlorophenyl)-3-(4-nitrophenyl)-1,2,4-oxadiazole

Hoong-Kun Fun,[a]*‡ Mohd Mustaqim Rosli,[a] Sankappa Rai,[b] Arun M Isloor[c] and Prakash Shetty[d]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Syngene International Ltd, Biocon Park, Plot No. 2 & 3, Bommasandra 4th Phase, Jigani Link Rd, Bangalore 560 100, India, [c]Department of Chemistry, Organic Chemistry Division, National Institute of Technology-Karnataka, Surathkal, Mangalore 575 025, India, and [d]Department of Printing, Manipal Institute of Technology, Manipal 576 104, India
Correspondence e-mail: hkfun@usm.my

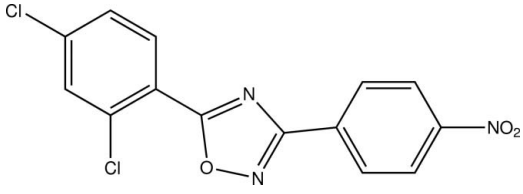
Received 20 March 2010; accepted 24 March 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.048; wR factor = 0.091; data-to-parameter ratio = 13.4.

In the title compound, $C_{14}H_7Cl_2N_3O_3$, the dichlorophenyl and nitrophenyl rings form dihedral angles of 5.4 (2) and 4.0 (2)°, respectively, with the oxadiazole ring. The nitro group is twisted out of the attached benzene ring by a dihedral angle of 10.4 (3)°. In the crystal, molecules are linked into a chain along the a axis by C—H···N hydrogen bonds.

Related literature

For the biological activity of heterocyclic compounds including oxadiazoles, see: Andersen *et al.* (1994); Showell *et al.* (1991); Watjen *et al.* (1989); Swain *et al.* (1991); Clitherow *et al.* (1996); Isloor *et al.* (2010); Chandrakantha *et al.* (2010). For related structures, see: Wang *et al.* (2006); Fun *et al.* (2010*a*,*b*).



Experimental

Crystal data

$C_{14}H_7Cl_2N_3O_3$
M_r = 336.13
Orthorhombic, $Pca2_1$
a = 13.5272 (5) Å
b = 6.5362 (2) Å
c = 15.6880 (5) Å
V = 1387.08 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 296 K
0.37 × 0.11 × 0.04 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.843, T_{max} = 0.980
9845 measured reflections
2658 independent reflections
2029 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.091
S = 1.06
2658 reflections
199 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 1243 Friedel pairs
Flack parameter: −0.01 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13A···N1^{i}	0.93	2.54	3.338 (5)	144

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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).

AMI is grateful to Professor Sandeep Sancheti, Director, National Institute of Technology-Karnataka, India, for providing research facilities and encouragement. HKF and MMR thank Universiti Sains Malaysia for the Research University Golden Goose Grant (No. 1001/PFIZIK/811012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5063).

References

Andersen, K. E., Jørgensen, A. S. & Braestrup, C. (1994). *Eur. J. Med. Chem.* **29**, 393–399.
Bruker (2005). *APEX2* , *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chandrakantha, B., Shetty, P., Nambiyar, V., Isloor, N. & Isloor, A. M. (2010). *Eur. J. Med. Chem.* **45**, 1206–1210.
Clitherow, J. W., Beswick, P., Irving, W. J., Scopes, D. I. C., Barnes, J. C., Clapham, J., Brown, J. D., Evans, D. J. & Hayes, A. G. (1996). *Bioorg. Med. Chem. Lett.* **6**, 833–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Fun, H.-K., Rosli, M. M., Rai, S., Isloor, A. M. & Shetty, P. (2010*a*). *Acta Cryst.* E**66**, o772.
Fun, H.-K., Rosli, M. M., Rai, S., Isloor, A. M. & Shetty, P. (2010*b*). *Acta Cryst.* E**66**, o851.
Isloor, A. M., Kalluraya, B. & Pai, K. S. (2010). *Eur. J. Med. Chem.* **45**, 825–830.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Showell, G. A., Gibbons, T. L., Kneen, C. O., MacLeod, A. M., Merchant, K., Saunders, J., Freedman, S. B., Patel, S. & Baker, R. (1991). *J. Med. Chem.* **34**, 1086–1094.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

‡ Thomson Reuters ResearcherID: A-3561-2009.

Swain, C. J., Baker, R., Kneen, C., Moseley, J., Saunders, J., Seward, E. M., Stevenson, G., Beer, M., Stanton, J. & Watling, K. (1991). *J. Med. Chem.* **34**, 140–151.
Wang, H.-B., Liu, Z.-Q., Wang, H.-B. & Yan, X.-C. (2006). *Acta Cryst.* E**62**, o4715–o4716.
Watjen, F., Baker, R., Engelstoff, M., Herbert, R., MacLeod, A., Knight, A., Merchant, K., Moseley, J., Saunders, J., Swain, C. J., Wong, E. & Springer, J. P. (1989). *J. Med. Chem.* **32**, 2282–2291.

supplementary materials

Acta Cryst. (2010). E**66**, o1196-o1197 [**doi:10.1107/S1600536810011153**]

5-(2,4-Dichlorophenyl)-3-(4-nitrophenyl)-1,2,4-oxadiazole

H.-K. Fun, M. M. Rosli, S. Rai, A. M. Isloor and P. Shetty

Comment

Heterocyclic compounds are becoming increasingly important in recent years due to their pharmacological activities (Isloor *et al.*, 2010). Nitrogen- and oxygen-containing five/six-membered heterocyclic compounds are of enormous significance in the field of medicinal chemistry (Chandrakantha *et al.*, 2010). Oxadiazoles play a very vital role in the preparation of various biologically active drugs with anti-inflammatory (Andersen *et al.*, 1994), anti-cancer (Showell *et al.*, 1991), anti-HIV (Watjen *et al.*, 1989), anti-diabetic and anti-microbial (Swain *et al.*, 1991) activities. The results of biological studies showed that oxadiazole derivatives also possess maximum anti-inflammatory, analgesic and minimum ulcerogenic and lipid per-oxidation (Clitherow *et al.*, 1996) properties.

Bond lengths and angles in the title molecule (Fig.1) are within the normal range and comparable to those observed in related structures (Wang *et al.*, 2006; Fun *et al.*, 2010*a*,b). The oxadiazole ring (C7/C8/N1/N2/O1) forms dihedral angles of 5.4 (2)° and 4.0 (2)°, respectively, with with the C1–C6 and C9–C14 benzene rings. The plane of the nitro group is twisted out of the C9–C14 benzene ring by a dihedral of 10.4 (3)°.

In the crystal structure (Fig. 2), the molecules are connected by intermolecular C13—H13A···N1 hydrogen bonds (Table 1) forming chains along the *a* axis.

Experimental

The title compound was prepared by heating a solution of 2,4-dichlorobenzoyl chloride (1.15 g, 0.02 mol) and N'-hydroxy-4-nitrobenzamidine (1 g, 0.02 mol) in pyridine (30 ml). The reaction mixture was heated at 114°C for 1.5 h and concentrated under vacuum. Further purification was done by column chromatography. The solid obtained was recrystallized using dichloromethane (yield: 1.0 g (55%), m.p 458-461 K).

Refinement

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

Figures

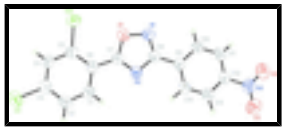


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

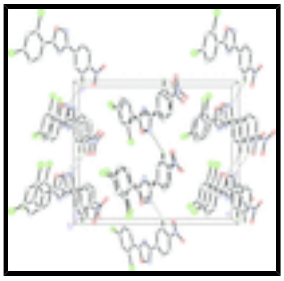


Fig. 2. The crystal packing of the title compound, showing hydrogen-bonded (dashed lines) chains along the *a* axis. H atoms not involved in the interactions have been omitted.

5-(2,4-Dichlorophenyl)-3-(4-nitrophenyl)-1,2,4-oxadiazole

Crystal data

$C_{14}H_7Cl_2N_3O_3$	$F(000) = 680$
$M_r = 336.13$	$D_x = 1.610$ Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2c -2ac	Cell parameters from 2389 reflections
$a = 13.5272$ (5) Å	$\theta = 2.6$–$30.1°$
$b = 6.5362$ (2) Å	$\mu = 0.48$ mm^{-1}
$c = 15.6880$ (5) Å	$T = 296$ K
$V = 1387.08$ (8) Å^3	Plate, colourless
$Z = 4$	0.37 × 0.11 × 0.04 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	2658 independent reflections
Radiation source: fine-focus sealed tube	2029 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.045$
φ and ω scans	$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -13\rightarrow16$
$T_{min} = 0.843$, $T_{max} = 0.980$	$k = -7\rightarrow8$
9845 measured reflections	$l = -17\rightarrow19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 0.1623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
2658 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
1 restraint	Absolute structure: Flack (1983), 1243 Friedel pairs

Primary atom site location: structure-invariant direct methods

Flack parameter: −0.01 (7)

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.37074 (7)	1.17134 (15)	0.20371 (7)	0.0672 (3)
Cl2	0.08039 (7)	0.73697 (16)	0.34239 (10)	0.0814 (4)
O1	0.15793 (17)	0.3687 (4)	0.41360 (18)	0.0643 (8)
O2	0.3673 (2)	−0.6615 (5)	0.6679 (2)	0.0975 (12)
O3	0.5067 (2)	−0.5915 (5)	0.6109 (2)	0.0959 (11)
N1	0.1636 (2)	0.1879 (5)	0.4615 (2)	0.0653 (10)
N2	0.3154 (2)	0.2966 (4)	0.4278 (2)	0.0454 (7)
N3	0.4200 (3)	−0.5541 (5)	0.6249 (2)	0.0646 (9)
C1	0.3731 (2)	0.6429 (5)	0.3289 (2)	0.0515 (10)
H1A	0.4198	0.5472	0.3463	0.062*
C2	0.4043 (3)	0.8143 (5)	0.2848 (3)	0.0562 (10)
H2A	0.4709	0.8346	0.2729	0.067*
C3	0.3342 (3)	0.9546 (5)	0.2589 (2)	0.0478 (9)
C4	0.2351 (3)	0.9269 (5)	0.2767 (2)	0.0493 (9)
H4A	0.1888	1.0233	0.2594	0.059*
C5	0.2060 (2)	0.7551 (5)	0.3204 (2)	0.0484 (9)
C6	0.2735 (2)	0.6087 (4)	0.3481 (2)	0.0417 (8)
C7	0.2522 (2)	0.4235 (5)	0.3964 (2)	0.0423 (8)
C8	0.2581 (3)	0.1536 (5)	0.4676 (2)	0.0434 (8)
C9	0.2984 (2)	−0.0278 (5)	0.5105 (2)	0.0411 (8)
C10	0.2372 (2)	−0.1701 (5)	0.5499 (2)	0.0463 (9)
H10A	0.1692	−0.1493	0.5501	0.056*
C11	0.2759 (3)	−0.3416 (5)	0.5887 (2)	0.0491 (10)
H11A	0.2350	−0.4357	0.6158	0.059*
C12	0.3767 (3)	−0.3693 (5)	0.5861 (2)	0.0457 (9)
C13	0.4388 (3)	−0.2323 (5)	0.5472 (2)	0.0547 (10)
H13A	0.5066	−0.2559	0.5458	0.066*
C14	0.3995 (2)	−0.0590 (5)	0.5103 (2)	0.0508 (9)
H14A	0.4411	0.0369	0.4851	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0778 (7)	0.0595 (6)	0.0642 (6)	−0.0179 (5)	0.0002 (6)	0.0100 (6)
Cl2	0.0403 (4)	0.0675 (6)	0.1363 (11)	−0.0026 (5)	−0.0083 (7)	0.0236 (7)
O1	0.0468 (14)	0.0596 (15)	0.086 (2)	0.0041 (12)	0.0112 (14)	0.0228 (15)
O2	0.089 (2)	0.0758 (19)	0.127 (3)	0.0000 (18)	0.006 (2)	0.045 (2)
O3	0.070 (2)	0.094 (2)	0.124 (3)	0.0193 (18)	−0.001 (2)	0.035 (2)
N1	0.0445 (17)	0.0621 (19)	0.089 (3)	0.0045 (15)	0.0144 (19)	0.0230 (19)
N2	0.0442 (16)	0.0428 (15)	0.0493 (18)	−0.0004 (14)	0.0019 (15)	−0.0026 (15)
N3	0.066 (2)	0.061 (2)	0.066 (2)	0.0007 (19)	−0.007 (2)	0.0065 (19)
C1	0.046 (2)	0.0437 (19)	0.065 (3)	0.0046 (14)	0.0124 (19)	−0.0034 (18)
C2	0.051 (2)	0.054 (2)	0.065 (3)	−0.0046 (18)	0.015 (2)	−0.009 (2)
C3	0.061 (2)	0.044 (2)	0.038 (2)	−0.0077 (17)	0.0005 (18)	−0.0042 (17)
C4	0.050 (2)	0.0450 (19)	0.053 (2)	0.0004 (16)	−0.0104 (18)	0.0052 (18)
C5	0.0418 (18)	0.0520 (19)	0.052 (2)	−0.0054 (16)	−0.0026 (17)	−0.0072 (19)
C6	0.0440 (18)	0.0357 (15)	0.046 (2)	0.0000 (13)	0.0014 (17)	−0.0082 (18)
C7	0.0402 (18)	0.0428 (17)	0.044 (2)	−0.0013 (16)	0.0029 (17)	−0.0085 (17)
C8	0.0472 (19)	0.0424 (17)	0.040 (2)	−0.0011 (17)	0.0037 (19)	−0.0072 (16)
C9	0.0462 (19)	0.0400 (17)	0.0370 (19)	0.0007 (15)	0.0012 (17)	−0.0081 (16)
C10	0.0367 (18)	0.052 (2)	0.050 (2)	0.0023 (16)	0.0099 (17)	−0.0048 (18)
C11	0.054 (2)	0.0464 (19)	0.047 (2)	−0.0071 (16)	0.0106 (19)	0.0000 (18)
C12	0.050 (2)	0.0432 (19)	0.043 (2)	−0.0008 (16)	−0.0008 (17)	0.0002 (17)
C13	0.045 (2)	0.059 (2)	0.060 (3)	−0.0018 (18)	−0.0032 (19)	0.006 (2)
C14	0.044 (2)	0.053 (2)	0.055 (2)	−0.0082 (16)	0.0048 (18)	0.0032 (19)

Geometric parameters (Å, °)

Cl1—C3	1.732 (3)	C4—C5	1.373 (5)
Cl2—C5	1.739 (3)	C4—H4A	0.93
O1—C7	1.352 (4)	C5—C6	1.392 (4)
O1—N1	1.403 (4)	C6—C7	1.458 (4)
O2—N3	1.207 (4)	C8—C9	1.468 (4)
O3—N3	1.218 (4)	C9—C14	1.384 (4)
N1—C8	1.302 (5)	C9—C10	1.390 (4)
N2—C7	1.289 (4)	C10—C11	1.378 (4)
N2—C8	1.366 (4)	C10—H10A	0.93
N3—C12	1.474 (5)	C11—C12	1.377 (5)
C1—C2	1.383 (5)	C11—H11A	0.93
C1—C6	1.398 (4)	C12—C13	1.371 (5)
C1—H1A	0.93	C13—C14	1.379 (5)
C2—C3	1.380 (5)	C13—H13A	0.93
C2—H2A	0.93	C14—H14A	0.93
C3—C4	1.381 (5)		
C7—O1—N1	106.2 (2)	N2—C7—O1	112.3 (3)
C8—N1—O1	103.8 (3)	N2—C7—C6	127.0 (3)
C7—N2—C8	103.8 (3)	O1—C7—C6	120.7 (3)

O2—N3—O3	123.6 (4)	N1—C8—N2	113.9 (3)
O2—N3—C12	118.2 (3)	N1—C8—C9	122.5 (3)
O3—N3—C12	118.2 (4)	N2—C8—C9	123.5 (3)
C2—C1—C6	122.1 (3)	C14—C9—C10	119.4 (3)
C2—C1—H1A	119.0	C14—C9—C8	119.0 (3)
C6—C1—H1A	119.0	C10—C9—C8	121.6 (3)
C3—C2—C1	118.4 (3)	C11—C10—C9	121.0 (3)
C3—C2—H2A	120.8	C11—C10—H10A	119.5
C1—C2—H2A	120.8	C9—C10—H10A	119.5
C2—C3—C4	121.3 (3)	C10—C11—C12	118.0 (3)
C2—C3—Cl1	119.6 (3)	C10—C11—H11A	121.0
C4—C3—Cl1	119.1 (3)	C12—C11—H11A	121.0
C5—C4—C3	119.1 (3)	C13—C12—C11	122.3 (3)
C5—C4—H4A	120.4	C13—C12—N3	118.4 (3)
C3—C4—H4A	120.4	C11—C12—N3	119.3 (3)
C4—C5—C6	122.0 (3)	C12—C13—C14	119.2 (3)
C4—C5—Cl2	115.8 (3)	C12—C13—H13A	120.4
C6—C5—Cl2	122.1 (3)	C14—C13—H13A	120.4
C5—C6—C1	117.0 (3)	C13—C14—C9	120.1 (3)
C5—C6—C7	127.1 (3)	C13—C14—H14A	120.0
C1—C6—C7	115.8 (3)	C9—C14—H14A	120.0
C7—O1—N1—C8	−0.2 (4)	O1—N1—C8—N2	0.1 (4)
C6—C1—C2—C3	−0.3 (5)	O1—N1—C8—C9	−177.5 (3)
C1—C2—C3—C4	0.4 (5)	C7—N2—C8—N1	0.2 (4)
C1—C2—C3—Cl1	179.9 (3)	C7—N2—C8—C9	177.7 (3)
C2—C3—C4—C5	−0.6 (5)	N1—C8—C9—C14	176.5 (4)
Cl1—C3—C4—C5	179.9 (3)	N2—C8—C9—C14	−0.8 (5)
C3—C4—C5—C6	0.7 (5)	N1—C8—C9—C10	−2.4 (5)
C3—C4—C5—Cl2	178.3 (3)	N2—C8—C9—C10	−179.7 (3)
C4—C5—C6—C1	−0.6 (5)	C14—C9—C10—C11	0.0 (5)
Cl2—C5—C6—C1	−178.0 (3)	C8—C9—C10—C11	178.9 (3)
C4—C5—C6—C7	178.5 (3)	C9—C10—C11—C12	−1.0 (5)
Cl2—C5—C6—C7	1.0 (5)	C10—C11—C12—C13	0.6 (5)
C2—C1—C6—C5	0.4 (5)	C10—C11—C12—N3	−178.3 (3)
C2—C1—C6—C7	−178.8 (3)	O2—N3—C12—C13	171.1 (4)
C8—N2—C7—O1	−0.3 (4)	O3—N3—C12—C13	−9.9 (6)
C8—N2—C7—C6	179.1 (3)	O2—N3—C12—C11	−9.9 (5)
N1—O1—C7—N2	0.4 (4)	O3—N3—C12—C11	169.0 (4)
N1—O1—C7—C6	−179.1 (3)	C11—C12—C13—C14	0.8 (6)
C5—C6—C7—N2	−174.0 (4)	N3—C12—C13—C14	179.7 (3)
C1—C6—C7—N2	5.0 (5)	C12—C13—C14—C9	−1.8 (6)
C5—C6—C7—O1	5.3 (5)	C10—C9—C14—C13	1.4 (6)
C1—C6—C7—O1	−175.6 (3)	C8—C9—C14—C13	−177.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13A···N1^{i}	0.93	2.54	3.338 (5)	144

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

Fig. 1

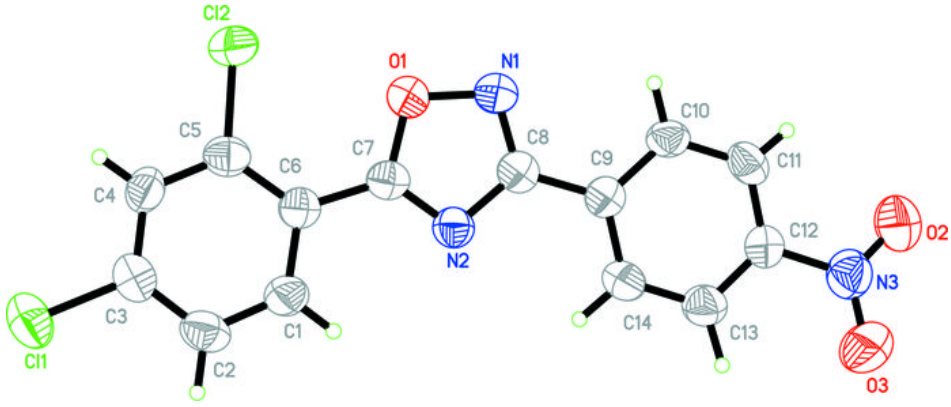

Cl2
O1
N1
C5
C7
C8
C10
C6
C9
C11
C4
N2
C12
O2
N3
C3
C1
C14
C13
Cl1
C2
O3

Fig. 2