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4-(4-Chlorophenyl)-1,2,3-selenadiazole

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Keywords: crystal structure; phenyl-selenadiaxole; π–π stacking interactions.

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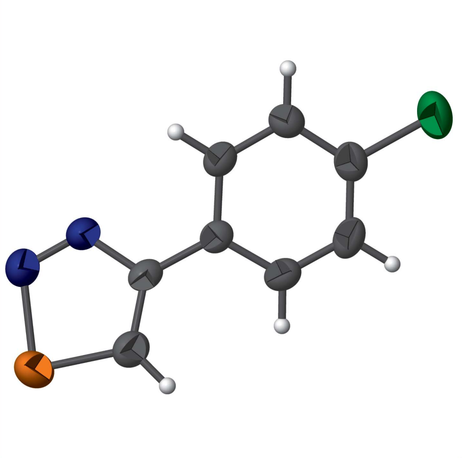
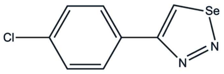
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_8H_5ClN_2Se$, the dihedral angle between the planes of the selenadiazole and chlorophenyl rings is 16.6 (2)°. In the crystal, the packing of the molecules is consolidated by weak C—H⋯N hydrogen bonds, which generate [001] chains, and π–π stacking interactions are observed between the phenyl and selenadiazole rings, with a centroid–centroid distance of 3.884 (2) Å. There is also a short Se⋯Cl contact of 3.468 (1) Å

3D view



Chemical scheme



Structure description

Selenium-containing compounds, such as 1,2,3-selenadiazoles, are of increasing interest owing to their chemical properties and biological applications, such as anti-bacterial, anti-microbial, anticancer and insecticidal activities (El-Kashef *et al.*, 1986; Khanna, 2005). Selenadiazoles are the important class of organoselenium compounds utilized in the synthesis of semiconductor nanoparticles (Padmavathi *et al.*, 2002). As part of our studies in this area, the structure of title compound has been determined.

The *ORTEP* plot of the molecule is shown in Fig. 1. The selenadiazole ring makes a dihedral angle of 16.6 (2)° with the chlorophenyl ring.

In the crystal, the packing of the molecules is consolidated by weak C—H⋯N hydrogen bonds (see Table 1), which generate [001] chains. There is also a short Se12⋯Cl1 contact of 3.468 (1) Å. The crystal structure is further augmented by π–π interactions between adjacent selenium and phenyl rings as shown in Fig. 2, with a centroid–centroid distance of 3.884 (2) Å.

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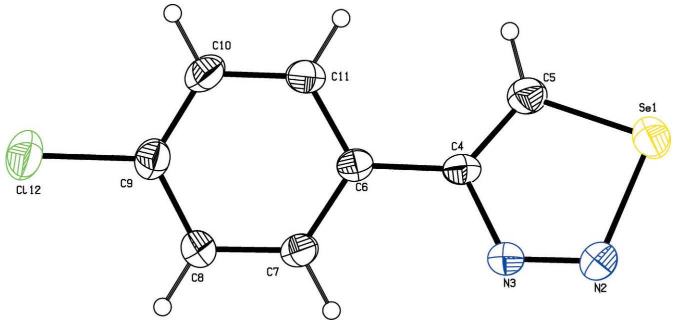

Figure 1
The molecular structure of the title compound, showing the atomic numbering scheme and displacement ellipsoids drawn at the 30% probability level.

Synthesis and crystallization

The title compound was synthesized according to the procedure of Baliah & Rangarajan, (1954)and colourless block-shaped crystals were recrystallized from a petroleum ether–ethyl acetate solvent mixture.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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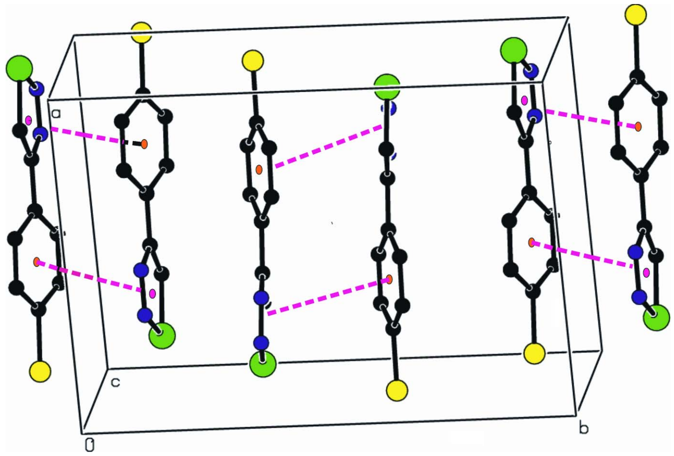

Figure 2
The π–π interactions between adjacent selenium and phenyl rings for the asymmetric molecule and its partner.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$\cdots$N2^{i}	0.93	2.62	3.528 (5)	164

Symmetry code: (i) $x, y, z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_5ClN_2Se$
M_r	243.55
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	10.3353 (9), 14.0058 (12), 5.9540 (4)
β (°)	97.320 (3)
V (Å^3)	854.84 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.64
Crystal size (mm)	0.15 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.543, 0.654
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11618, 1787, 1282
R_{int}	0.042
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.630
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.079, 1.07
No. of reflections	1787
No. of parameters	109
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.39

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/1 (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009).

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full crystallographic data

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Crystal data

$C_8H_5ClN_2Se$
$M_r = 243.55$
Monoclinic, $P2_1/c$
$a = 10.3353$ (9) Å
$b = 14.0058$ (12) Å
$c = 5.9540$ (4) Å
$\beta = 97.320$ (3)°
$V = 854.84$ (12) Å^3
$Z = 4$
$F(000) = 472$
$D_x = 1.892$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1286 reflections
$\theta = 2.0$–26.6°
$\mu = 4.64$ mm^{-1}
$T = 296$ K
Block, colorless
0.15 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{\min} = 0.543$, $T_{\max} = 0.654$
11618 measured reflections
1787 independent reflections
1282 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.042$
$\theta_{\max} = 26.6°$, $\theta_{\min} = 2.0°$
$h = -13 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -6 \rightarrow 7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.079$
$S = 1.07$
1787 reflections
109 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0166P)^2 + 1.3536P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ 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. H atoms were positioned geometrically (N—H=0.88–0.90 Å and C—H=0.93–0.98 Å) and allowed to ride on their parent atoms,with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

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

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
C4	0.4016 (4)	0.3768 (2)	0.3085 (5)	0.0370 (8)
C5	0.2945 (4)	0.3664 (3)	0.4154 (6)	0.0497 (9)
H5	0.297028	0.360609	0.571528	0.060*
C6	0.5378 (3)	0.3794 (2)	0.4058 (5)	0.0357 (8)
C7	0.6334 (4)	0.4123 (3)	0.2806 (6)	0.0447 (9)
H7	0.608413	0.435267	0.134966	0.054*
C8	0.7636 (4)	0.4121 (3)	0.3649 (6)	0.0492 (10)
H8	0.826132	0.434318	0.278261	0.059*
C9	0.7990 (4)	0.3782 (3)	0.5809 (6)	0.0475 (10)
C10	0.7070 (4)	0.3464 (3)	0.7105 (6)	0.0514 (10)
H10	0.732189	0.324180	0.856660	0.062*
C11	0.5777 (4)	0.3478 (3)	0.6230 (6)	0.0471 (10)
H11	0.515632	0.326863	0.712024	0.057*
N2	0.2534 (3)	0.3807 (3)	−0.0063 (5)	0.0589 (9)
N3	0.3723 (3)	0.3846 (2)	0.0764 (5)	0.0507 (8)
Se1	0.14713 (4)	0.36506 (3)	0.22008 (7)	0.05959 (17)
Cl12	0.96352 (11)	0.37587 (10)	0.6907 (2)	0.0761 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C4	0.048 (2)	0.033 (2)	0.0305 (17)	−0.0043 (16)	0.0080 (15)	−0.0008 (15)
C5	0.053 (2)	0.057 (2)	0.039 (2)	−0.006 (2)	0.0058 (18)	−0.0015 (19)
C6	0.043 (2)	0.0322 (19)	0.0322 (18)	−0.0001 (15)	0.0058 (15)	−0.0028 (14)
C7	0.048 (2)	0.051 (2)	0.035 (2)	−0.0035 (19)	0.0031 (17)	0.0054 (17)
C8	0.040 (2)	0.060 (3)	0.048 (2)	−0.0045 (19)	0.0066 (18)	0.0065 (19)
C9	0.043 (2)	0.052 (3)	0.046 (2)	0.0072 (19)	0.0002 (18)	−0.0043 (18)
C10	0.058 (3)	0.057 (3)	0.038 (2)	0.010 (2)	−0.0018 (19)	0.0077 (18)
C11	0.049 (2)	0.054 (3)	0.040 (2)	0.0010 (18)	0.0113 (18)	0.0072 (17)
N2	0.050 (2)	0.083 (3)	0.0423 (19)	−0.0076 (18)	−0.0005 (16)	0.0051 (17)
N3	0.044 (2)	0.072 (2)	0.0366 (17)	−0.0066 (17)	0.0060 (14)	0.0065 (15)
Se1	0.0458 (3)	0.0782 (3)	0.0553 (3)	−0.0081 (2)	0.00855 (19)	−0.0042 (2)
Cl12	0.0480 (7)	0.1104 (10)	0.0663 (7)	0.0161 (6)	−0.0065 (5)	0.0029 (7)

Geometric parameters (Å, º)

C4—C5	1.353 (5)	C8—C9	1.376 (5)
C4—N3	1.381 (4)	C8—H8	0.9300
C4—C6	1.454 (5)	C9—C10	1.372 (5)
C5—Se1	1.795 (4)	C9—Cl12	1.742 (4)
C5—H5	0.9300	C10—C11	1.371 (5)
C6—C11	1.380 (5)	C10—H10	0.9300
C6—C7	1.390 (5)	C11—H11	0.9300
C7—C8	1.376 (5)	N2—N3	1.265 (4)
C7—H7	0.9300	N2—Se1	1.857 (3)

C5—C4—N3	113.1 (3)	C9—C8—H8	120.9
C5—C4—C6	128.6 (3)	C10—C9—C8	121.1 (4)
N3—C4—C6	118.3 (3)	C10—C9—Cl12	119.7 (3)
C4—C5—Se1	111.9 (3)	C8—C9—Cl12	119.2 (3)
C4—C5—H5	124.0	C11—C10—C9	119.6 (4)
Se1—C5—H5	124.0	C11—C10—H10	120.2
C11—C6—C7	117.5 (3)	C9—C10—H10	120.2
C11—C6—C4	121.6 (3)	C10—C11—C6	121.4 (4)
C7—C6—C4	120.9 (3)	C10—C11—H11	119.3
C8—C7—C6	122.2 (3)	C6—C11—H11	119.3
C8—C7—H7	118.9	N3—N2—Se1	111.0 (2)
C6—C7—H7	118.9	N2—N3—C4	117.6 (3)
C7—C8—C9	118.2 (3)	C5—Se1—N2	86.42 (16)
C7—C8—H8	120.9		

N3—C4—C5—Se1	0.5 (4)	C8—C9—C10—C11	0.5 (6)
C6—C4—C5—Se1	−178.7 (3)	Cl12—C9—C10—C11	−179.6 (3)
C5—C4—C6—C11	16.3 (6)	C9—C10—C11—C6	0.7 (6)
N3—C4—C6—C11	−162.8 (3)	C7—C6—C11—C10	−1.6 (5)
C5—C4—C6—C7	−165.0 (4)	C4—C6—C11—C10	177.1 (3)
N3—C4—C6—C7	15.9 (5)	Se1—N2—N3—C4	0.1 (4)
C11—C6—C7—C8	1.4 (5)	C5—C4—N3—N2	−0.4 (5)
C4—C6—C7—C8	−177.4 (3)	C6—C4—N3—N2	178.9 (3)
C6—C7—C8—C9	−0.2 (6)	C4—C5—Se1—N2	−0.3 (3)
C7—C8—C9—C10	−0.8 (6)	N3—N2—Se1—C5	0.1 (3)
C7—C8—C9—Cl12	179.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···N2$^{\mathrm{i}}$	0.93	2.62	3.528 (5)	164

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