Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Phenyl-1,3-selenazole-4-carboxylic acid

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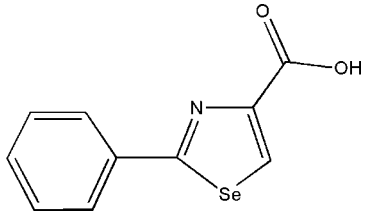
Received 23 February 2011; accepted 25 February 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.024; wR factor = 0.063; data-to-parameter ratio = 13.4.

In the title compound, $C_{10}H_7NO_2Se$, the two rings are twisted, making a dihedral angle of 12.42 (9)°. In the crystal, pairs of molecules are disposed about an inversion center, generating O—H···O hydrogen-bonded dimers.

Related literature

For the synthesis, see: Zhao *et al.* (2010). For related structures, see: Srivastava & Robins (1983); Boritzki *et al.* (1985); Shen *et al.* (2011).



Experimental

Crystal data

$C_{10}H_7NO_2Se$
M_r = 252.13
Monoclinic, $P2_1/c$
a = 8.0817 (3) Å
b = 11.5661 (4) Å
c = 11.6295 (4) Å
β = 117.168 (2)°
V = 967.12 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.85 mm^{-1}
T = 296 K
0.23 × 0.22 × 0.19 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.437, T_{max} = 0.479
7502 measured reflections
1705 independent reflections
1487 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.063
S = 1.05
1705 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H7···O2^{i}	0.82	1.81	2.623 (2)	171

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

This project was supprted by the Natural Science of Fundation of Zhejiang (Y4080256) and the Zhejiang Students' Science and Technology Innovation Plan (Young Talent Plan) Aid.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5124).

References

Boritzki, T. J., Berry, D. A., Besserer, J. A., Cook, P. D., Fry, D. W., Leopold, W. R. & Jackson, R. C. (1985). *Biochem. Pharmacol.* **34**, 1109–1114.
Bruker (2006). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shen, J.-B., Lv, X., Chen, J.-F., Zhou, Y.-F. & Zhao, G.-L. (2011). *Acta Cryst.* E**67**, m186–m187.
Srivastava, P. C. & Robins, R. K. (1983). *J. Med. Chem.* **26**, 445–448.
Zhao, G.-L., Shi, X., Zhang, J. P., Liu, J.-F., Xian, H.-D. & Shao, L. X. (2010). *Chem. Sci. China*, **40** 1525–1535.

supporting information

Acta Cryst. (2011). E**67**, o803 [doi:10.1107/S1600536811007185]

2-Phenyl-1,3-selenazole-4-carboxylic acid

Jin-Bei Shen, Xin Lv, Ji-Fei Chen, Yu-Feng Zhou and Guo-Liang Zhao

S1. Comment

It has well been confirmed that the derivatives of selenazole are important in multiple fields such as chemistry and biochemistry owing to their biological activities (Srivastava *et al.*, 1983;Boritzki *et al.*,1985). Interested in this field, we have been engaged in a major effort directed toward the development of syntheses of new selenazole carboxylic acid and their transition metal complexes. In a few of articles we have reported our partial research results (Zhao *et al.*, 2010;Shen *et al.*, 2011). Herein,we crystallize the organic ligand 2-phenyl-4-selenazole carboxylic acid.

The structure of the title, ($C_{10}H_7NO_2Se$),suitable for X-ray, was obtained by chance. The structure of the complex is shown in Fig.1, which reveals that all atoms in each molecule are nearly coplanar in the centrosymmetric unit. The molecule is essentially planar with the dihedral angle between two neighboring rings are 12.415 (89)°. In the molecule of 2-phenyl-4-selenazole carboxylic acid,the Se—C bond length range from 1.832 (2) Å-1.891 (2)Å and the angle C—Se—C is 84.78 (10)°.

The molecules arranged in the crystal at regular intervals with O—H···O hydrogen bonds. The end to end hydrogen-bonding interactions lead to the formation a one-dimensional structure framework along the *b* axis, Fig 2. Between adjacent triple-helix chains there exist weak $\pi\cdots\pi$ interactions.

S2. Experimental

Reagents and solvents used were of commercially available quality and without purified before using. $K_2Cr_2O_7$ (0.588 g, 2 mmol) was added to a mixed solution of acetic acid (50 ml) with 2-phenyl-4-selenazole carbinol (0.248 g, 1 mmol) under stirred conditions at room temperature. Few minutes later lots of red deposit appeared. After the deposit was filtered out, a light red solution was kept for evaporating. Some red single crystals were obtained about 19 days later.

S3. Refinement

The structure was solved by direct methods and successive Fourier difference synthesis. The H atoms bonded to C atoms were positioned geometrically and refined using a riding model [aromatic C—H = 0.93 Å (U_{iso}(H) = 1.2U_{eq}(C))]. The H atoms bonded to O atoms were located in difference Fourier maps and refined with O—H distance restraints of 0.85 (2) and U_{iso}(H) = 1.5U_{eq}(O).

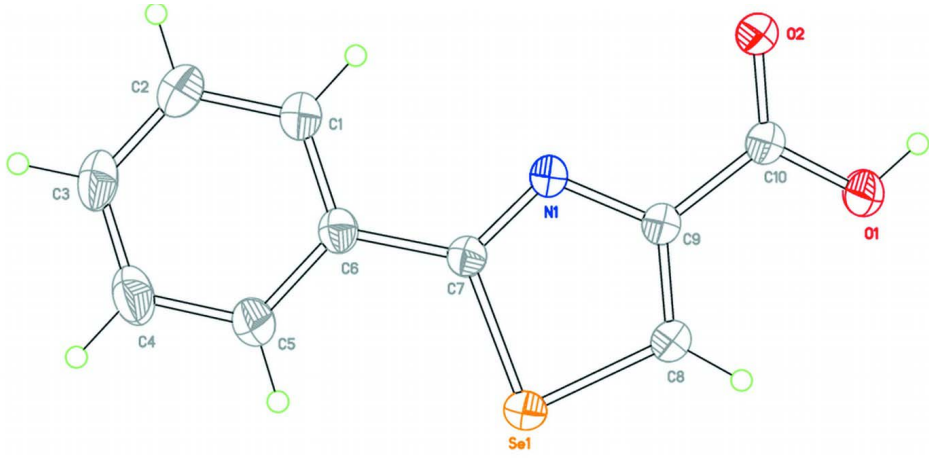


Figure 1

The molecular structure of the title complex, showing the atom- labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

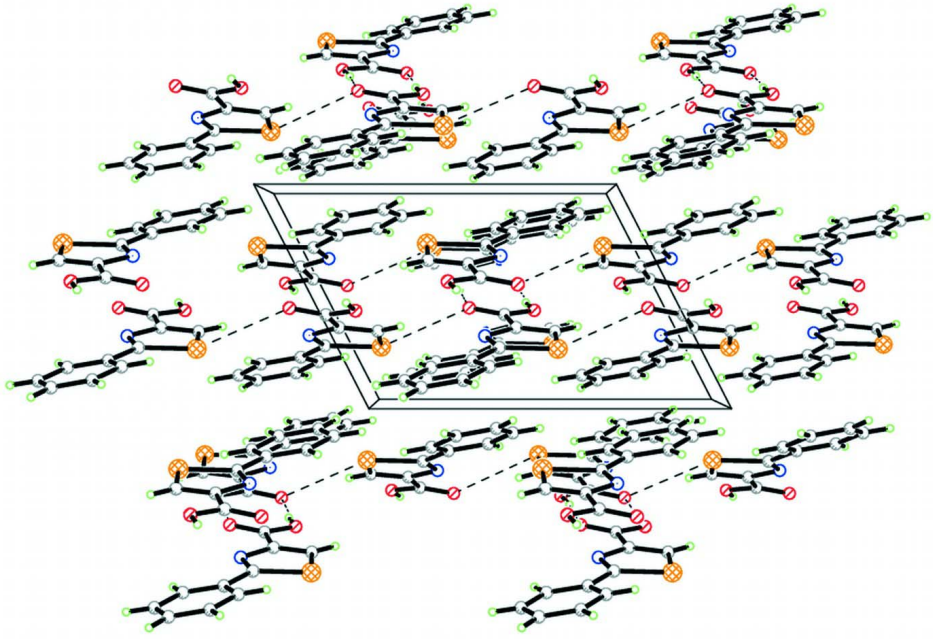


Figure 2

The stacking plot of the title compound, showing H-bond interactions (dashed lines) and $\pi\cdots\pi$ stacking interactions.

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Crystal data

$C_{10}H_7NO_2Se$
$M_r = 252.13$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.0817\ (3)$ Å
$b = 11.5661\ (4)$ Å
$c = 11.6295\ (4)$ Å
$\beta = 117.168\ (2)°$
$V = 967.12\ (6)$ Å^3
$Z = 4$
$F(000) = 496$
$D_x = 1.732$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4000 reflections

θ = 2.6–25.0°
μ = 3.85 mm^{-1}
T = 296 K

Block, red
0.23 × 0.22 × 0.19 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: none pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.437, T_{max} = 0.479

7502 measured reflections
1705 independent reflections
1487 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.0°, θ_{min} = 2.6°
h = −9→9
k = −13→13
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.063
S = 1.05
1705 reflections
127 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 0.3951P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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}
Se1	0.26583 (4)	−0.04306 (2)	0.60598 (2)	0.04992 (12)
O1	0.4357 (3)	−0.41679 (16)	0.5986 (2)	0.0685 (6)
H7	0.4714	−0.4799	0.5865	0.103*
O2	0.4478 (3)	−0.37486 (15)	0.41673 (18)	0.0661 (6)
N1	0.3215 (3)	−0.15135 (15)	0.42195 (18)	0.0382 (4)
C1	0.1846 (4)	0.0295 (2)	0.2299 (3)	0.0543 (7)
H1	0.2010	−0.0436	0.2033	0.065*
C2	0.1285 (4)	0.1208 (2)	0.1426 (3)	0.0655 (8)
H2	0.1085	0.1088	0.0581	0.079*
C3	0.1028 (4)	0.2287 (2)	0.1809 (3)	0.0595 (7)
H3	0.0630	0.2894	0.1220	0.071*
C4	0.1357 (4)	0.2467 (2)	0.3054 (3)	0.0635 (8)
H4	0.1201	0.3201	0.3315	0.076*

C5	0.1921 (4)	0.1566 (2)	0.3930 (3)	0.0538 (6)
H5	0.2141	0.1696	0.4778	0.065*
C6	0.2159 (3)	0.04648 (18)	0.3548 (2)	0.0388 (5)
C7	0.2713 (3)	−0.05191 (17)	0.4454 (2)	0.0364 (5)
C8	0.3408 (3)	−0.1944 (2)	0.6245 (2)	0.0438 (5)
H8	0.3632	−0.2404	0.6957	0.053*
C9	0.3587 (3)	−0.22941 (18)	0.5206 (2)	0.0386 (5)
C10	0.4173 (4)	−0.3472 (2)	0.5075 (2)	0.0455 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0692 (2)	0.04354 (17)	0.04006 (17)	0.01159 (11)	0.02764 (14)	0.00007 (10)
O1	0.1212 (18)	0.0434 (9)	0.0619 (13)	0.0252 (11)	0.0600 (13)	0.0203 (9)
O2	0.1187 (17)	0.0448 (10)	0.0514 (12)	0.0251 (10)	0.0533 (12)	0.0128 (8)
N1	0.0453 (11)	0.0337 (10)	0.0362 (10)	0.0043 (8)	0.0191 (8)	0.0046 (8)
C1	0.0716 (18)	0.0431 (14)	0.0488 (16)	0.0075 (12)	0.0281 (14)	0.0073 (11)
C2	0.084 (2)	0.0629 (18)	0.0483 (17)	0.0095 (15)	0.0292 (15)	0.0149 (14)
C3	0.0576 (16)	0.0517 (15)	0.068 (2)	0.0135 (12)	0.0281 (14)	0.0258 (14)
C4	0.0721 (19)	0.0394 (14)	0.084 (2)	0.0153 (13)	0.0404 (17)	0.0128 (13)
C5	0.0674 (17)	0.0421 (14)	0.0571 (17)	0.0113 (12)	0.0331 (14)	0.0054 (11)
C6	0.0363 (12)	0.0367 (12)	0.0440 (13)	0.0025 (9)	0.0187 (10)	0.0044 (9)
C7	0.0371 (11)	0.0357 (11)	0.0354 (12)	0.0012 (9)	0.0157 (9)	0.0013 (9)
C8	0.0543 (14)	0.0412 (12)	0.0357 (13)	0.0048 (11)	0.0204 (11)	0.0041 (10)
C9	0.0438 (13)	0.0357 (11)	0.0360 (12)	0.0027 (9)	0.0179 (10)	0.0031 (9)
C10	0.0620 (15)	0.0376 (12)	0.0404 (13)	0.0061 (11)	0.0264 (12)	0.0063 (10)

Geometric parameters (Å, º)

Se1—C8	1.832 (2)	C2—H2	0.9300
Se1—C7	1.891 (2)	C3—C4	1.363 (4)
O1—C10	1.284 (3)	C3—H3	0.9300
O1—H7	0.8201	C4—C5	1.382 (4)
O2—C10	1.230 (3)	C4—H4	0.9300
N1—C7	1.289 (3)	C5—C6	1.391 (3)
N1—C9	1.381 (3)	C5—H5	0.9300
C1—C6	1.370 (4)	C6—C7	1.474 (3)
C1—C2	1.390 (4)	C8—C9	1.344 (3)
C1—H1	0.9300	C8—H8	0.9300
C2—C3	1.372 (4)	C9—C10	1.473 (3)
C8—Se1—C7	84.79 (10)	C6—C5—H5	119.9
C10—O1—H7	109.5	C1—C6—C5	119.0 (2)
C7—N1—C9	112.19 (19)	C1—C6—C7	119.7 (2)
C6—C1—C2	120.4 (2)	C5—C6—C7	121.3 (2)
C6—C1—H1	119.8	N1—C7—C6	124.0 (2)
C2—C1—H1	119.8	N1—C7—Se1	114.10 (16)
C3—C2—C1	120.1 (3)	C6—C7—Se1	121.82 (15)

C3—C2—H2	120.0	C9—C8—Se1	110.35 (17)
C1—C2—H2	120.0	C9—C8—H8	124.8
C4—C3—C2	119.9 (2)	Se1—C8—H8	124.8
C4—C3—H3	120.0	C8—C9—N1	118.6 (2)
C2—C3—H3	120.0	C8—C9—C10	123.0 (2)
C3—C4—C5	120.5 (3)	N1—C9—C10	118.48 (19)
C3—C4—H4	119.8	O2—C10—O1	123.5 (2)
C5—C4—H4	119.8	O2—C10—C9	121.9 (2)
C4—C5—C6	120.1 (3)	O1—C10—C9	114.6 (2)
C4—C5—H5	119.9		

C6—C1—C2—C3	−0.5 (5)	C5—C6—C7—Se1	12.7 (3)
C1—C2—C3—C4	1.3 (5)	C8—Se1—C7—N1	−0.22 (18)
C2—C3—C4—C5	−1.0 (4)	C8—Se1—C7—C6	177.7 (2)
C3—C4—C5—C6	0.1 (4)	C7—Se1—C8—C9	−0.05 (18)
C2—C1—C6—C5	−0.5 (4)	Se1—C8—C9—N1	0.3 (3)
C2—C1—C6—C7	178.7 (3)	Se1—C8—C9—C10	179.96 (19)
C4—C5—C6—C1	0.7 (4)	C7—N1—C9—C8	−0.5 (3)
C4—C5—C6—C7	−178.4 (2)	C7—N1—C9—C10	179.8 (2)
C9—N1—C7—C6	−177.5 (2)	C8—C9—C10—O2	−173.9 (3)
C9—N1—C7—Se1	0.4 (2)	N1—C9—C10—O2	5.8 (4)
C1—C6—C7—N1	11.4 (3)	C8—C9—C10—O1	5.3 (4)
C5—C6—C7—N1	−169.5 (2)	N1—C9—C10—O1	−175.1 (2)
C1—C6—C7—Se1	−166.39 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H7···O2^{i}	0.82	1.81	2.623 (2)	171

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