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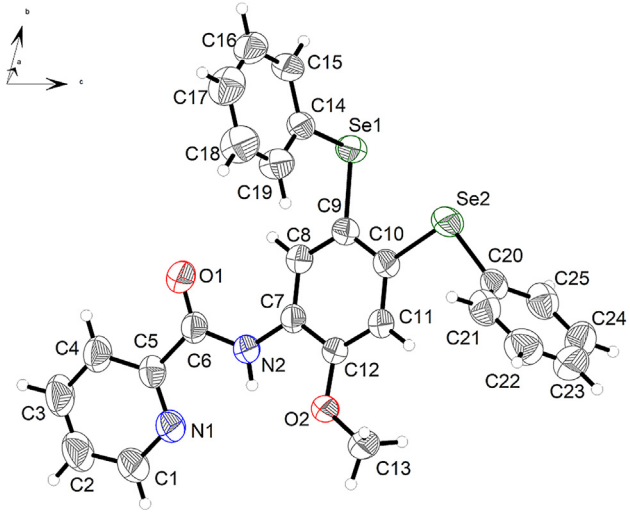
The crystal structure of *N*-(2-methoxy-4,5-bis [phenylselanyl]phenyl)picolinamide, $C_{25}H_{20}N_2O_2Se_2$



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Abstract

$C_{25}H_{20}N_2O_2Se_2$, triclinic, $P\bar{1}$ (no. 2), a = 9.6050(2) Å, b = 9.7531(2) Å, c = 13.2788(2) Å, α = 75.130(1)°, β = 81.824(1)°, γ = 72.329(2)°, V = 1142.75(4) Å^3, Z = 2, $R_{gt}(F)$ = 0.0393, $wR_{ref}(F^2)$ = 0.1092, T = 294 K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless plate
Size:	0.30 × 0.20 × 0.10 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	4.24 mm^{-1}
Diffractometer, scan mode:	XtaLAB AFC12 (RINC), ω
θ_{max}, completeness:	74.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12,742, 4516, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 4268
$N(param)_{refined}$:	281
Programs:	CrysAlis^{PRO} [1], Olex2 [2], SHELX [3, 4]

Source of material

All reagents and solvents were purchased form commercial sources and used as received. A solution of *N*-(2-methoxyphenyl)picolinamide (0.0456 g; 0.2 mmol) in acetonitrile (1 mL) was added to a mixture of diphenyl diselenide (0.1250 g; 0.4 mmol), potassium persulfate (0.0180 g; 0.4 mmol) and selectfluor *(1-(Chloromethyl)-4-fluoro-1,4-diazabicyclo[2.2.2]octane-1,4-diium ditetrafluoroborate;* 0.0350 g; 0.1 mmol) with constant stirring. The mixture was heated to 373.15 K for 24 h. The acetonitrile was evaporated under vacuum to leave a clear colourless solid. The crude product was purified by column chromatography to give the title compound (0.0656 g; 61% yield) as clear colourless crystals.

Experimental details

The carbon-bound hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

In recent years, many groups have studied the pharmacological activities and functions of diaryl selenides.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Se1	0.36316 (3)	0.81345 (3)	0.39410 (2)	0.05391 (12)
Se2	0.17160 (4)	0.68928 (3)	0.60438 (3)	0.06672 (13)
O1	0.4925 (3)	0.4638 (2)	0.15025 (16)	0.0724 (6)
O2	0.3276 (2)	0.18640 (19)	0.47048 (14)	0.0557 (5)
N1	0.5696 (3)	0.0757 (3)	0.19757 (19)	0.0573 (6)
N2	0.4670 (3)	0.2936 (2)	0.29923 (16)	0.0489 (5)
H2N	0.4832	0.2002	0.3246	0.059*
C1	0.6210 (4)	−0.0346 (4)	0.1482 (3)	0.0696 (8)
H1	0.6264	−0.1303	0.1862	0.083*
C2	0.6666 (4)	−0.0138 (4)	0.0437 (3)	0.0809 (10)
H2	0.7035	−0.0939	0.0125	0.097*
C3	0.6566 (4)	0.1266 (4)	−0.0132 (3)	0.0792 (10)
H3	0.6855	0.1436	−0.0841	0.095*
C4	0.6029 (4)	0.2432 (4)	0.0358 (2)	0.0649 (8)
H4	0.5950	0.3399	−0.0011	0.078*
C5	0.5613 (3)	0.2117 (3)	0.1412 (2)	0.0500 (6)
C6	0.5040 (3)	0.3361 (3)	0.19668 (19)	0.0502 (6)
C7	0.4047 (3)	0.3860 (3)	0.36927 (18)	0.0440 (5)
C8	0.4132 (3)	0.5296 (3)	0.35226 (19)	0.0466 (5)
H8	0.4651	0.5682	0.2927	0.056*
C9	0.3454 (3)	0.6165 (3)	0.42301 (19)	0.0464 (5)
C10	0.2681 (3)	0.5596 (3)	0.51282 (19)	0.0470 (5)
C11	0.2620 (3)	0.4140 (3)	0.53178 (19)	0.0481 (5)
H11	0.2127	0.3746	0.5925	0.058*
C12	0.3288 (3)	0.3283 (3)	0.46073 (18)	0.0447 (5)
C13	0.2467 (5)	0.1209 (4)	0.5584 (2)	0.0740 (10)
H13a	0.2521	0.0227	0.5540	0.111*
H13b	0.1462	0.1792	0.5589	0.111*
H13c	0.2873	0.1169	0.6215	0.111*
C14	0.2068 (3)	0.9151 (3)	0.30326 (19)	0.0470 (5)
C15	0.1971 (3)	1.0610 (3)	0.2539 (2)	0.0574 (7)
H15	0.2634	1.1062	0.2662	0.069*
C16	0.0879 (4)	1.1390 (3)	0.1861 (3)	0.0677 (8)
H16	0.0810	1.2371	0.1531	0.081*
C17	−0.0097 (4)	1.0731 (4)	0.1671 (3)	0.0757 (9)
H17	−0.0830	1.1261	0.1218	0.091*
C18	0.0014 (4)	0.9269 (4)	0.2160 (3)	0.0768 (9)
H18	−0.0641	0.8813	0.2029	0.092*
C19	0.1087 (3)	0.8486 (3)	0.2838 (2)	0.0606 (7)
H19	0.1151	0.7507	0.3167	0.073*
C20	0.1005 (3)	0.5560 (3)	0.7181 (2)	0.0520 (6)
C21	−0.0362 (4)	0.5370 (4)	0.7191 (3)	0.0672 (8)
H21	−0.0895	0.5779	0.6601	0.081*
C22	−0.0940 (4)	0.4567 (5)	0.8082 (3)	0.0805 (10)
H22	−0.1866	0.4447	0.8088	0.097*
C23	−0.0169 (5)	0.3957 (4)	0.8942 (3)	0.0843 (11)
H23	−0.0566	0.3423	0.9537	0.101*
C24	0.1197 (5)	0.4128 (4)	0.8933 (3)	0.0801 (10)
H24	0.1728	0.3702	0.9524	0.096*
C25	0.1790 (3)	0.4925 (4)	0.8059 (3)	0.0640 (7)
H25	0.2718	0.5036	0.8059	0.077*

Various diaryl selenides have shown good antiproliferation, antimicrobial, antiinflammatory, antihypertensive, and antiviral activities, and even had been used as scaffolds in organic synthesis and catalysis [4, 5]. Thus, it is necessary to investigate further examples of diaryl selenides.

The title compound contains one *N*-(2-methoxy-4,5-bis [phenylselanyl]phenyl) picolinamide molecule. There is a *N*-(2-methoxyphenyl) picolinamide ring and two selenophenyl groups in the structure. The nitrogen atom in *N*-(2-methoxyphenyl) picolinamide ring and the selenium atom in two selenobenzenes were coplanar, and the dihedral angles of the central aryl ring plane and the two planes defined by the selenophenyl groups were 84.49(6)° and 83.76(9)°, respectively. The Se-C distances are 1.916(3) Å and 1.922(2) Å, respectively.

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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