Crystal structure of *P,P*-diphenyl-*N*-ethyl-selenophosphinythioformamide, $C_{15}H_{16}NPSSe$

R. Kramolowsky, J. Sawluk

Universität Hamburg, Institut für Anorganische und Angewandte Chemie, D-20146 Hamburg, Germany

G. Siasios and E. R. T. Tiekink

The University of Adelaide, Department of Chemistry, South Australia 5005, Australia

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Source of material: Prepared using the literature method (see ref. 1); mp 371 K.

The conformation about the C(1)–N(1) bond is *Z* and the central chromophore is planar as seen in the values of the Se(2)/P(1)/C(1)/S(1) and Se(2)/P(1)/C(1)/N(1) torsion angles of 178.8(6)° and –0.3(4)°, respectively. The derived interatomic parameters are equal within experimental error to those of a methyl analogue (see ref. 2), indicating that the substitution of a methyl group for an ethyl has little effect on the electronic structures of the compounds.

$C_{15}H_{16}NPSSe$, monoclinic, $P12_1/c1$ (No. 14), $a = 11.944(3)$ Å, $b = 8.999(7)$ Å, $c = 14.882(3)$ Å, $\beta = 100.71(2)^\circ$, $V = 1571.7$ Å³, $Z = 4$, $R(F) = 0.036$, $R_w(F) = 0.034$.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow block, size 0.19 x 0.23 x 0.24 mm
Wavelength:	Mo $K\alpha$ radiation (0.7107 Å)
μ :	26.10 cm ⁻¹
Diffractometer:	AFC6R
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	1761
Criterion for F_o :	$F_o > 6 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	236
Program:	teXsan

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4e	0.556(3)	0.399(4)	0.635(3)	0.04(1)
H(12)	4e	0.808(3)	0.261(4)	0.394(2)	0.03(1)
H(13)	4e	0.883(4)	0.406(6)	0.299(3)	0.08(1)
H(14)	4e	0.873(4)	0.663(5)	0.299(3)	0.07(1)
H(15)	4e	0.778(4)	0.767(5)	0.407(3)	0.07(1)
H(16)	4e	0.709(3)	0.608(4)	0.504(3)	0.04(1)
H(22)	4e	0.930(4)	0.244(5)	0.573(3)	0.05(1)
H(23)	4e	1.049(4)	0.044(5)	0.614(3)	0.07(1)
H(24)	4e	0.972(4)	–0.179(6)	0.639(3)	0.09(1)
H(25)	4e	0.767(3)	–0.208(5)	0.616(3)	0.05(1)
H(26)	4e	0.651(3)	0.004(4)	0.562(3)	0.06(1)
H(31a)	4e	0.635(5)	0.461(6)	0.799(4)	0.10(1)
H(31b)	4e	0.614(6)	0.612(8)	0.742(5)	0.162(8)
H(32a)	4e	0.469(4)	0.582(6)	0.816(4)	0.11(1)
H(32b)	4e	0.441(5)	0.579(7)	0.711(4)	0.12(1)
H(32c)	4e	0.477(8)	0.43(1)	0.786(6)	0.229(7)

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Se(2)	4e	0.52365(4)	0.24677(6)	0.48055(3)	0.0362(2)	0.0694(4)	0.0668(3)	–0.0088(3)	–0.0009(2)	–0.0074(3)
S(1)	4e	0.8292(1)	0.4600(2)	0.69682(9)	0.0520(8)	0.087(1)	0.0619(8)	–0.0098(7)	–0.0024(6)	–0.0211(8)
P(1)	4e	0.69252(9)	0.3011(1)	0.53392(8)	0.0331(6)	0.0424(7)	0.0421(7)	–0.0025(5)	0.0052(5)	–0.0035(5)
N(1)	4e	0.6091(4)	0.4327(5)	0.6665(3)	0.047(3)	0.080(3)	0.052(3)	0.001(2)	0.008(2)	–0.017(3)
C(1)	4e	0.7051(4)	0.4083(5)	0.6418(3)	0.043(3)	0.044(3)	0.042(3)	0.002(2)	0.006(2)	0.000(2)
C(11)	4e	0.7563(3)	0.4165(5)	0.4602(3)	0.036(2)	0.044(3)	0.039(3)	–0.004(2)	0.005(2)	–0.003(2)
C(12)	4e	0.8086(4)	0.3560(7)	0.3938(4)	0.061(3)	0.050(4)	0.056(3)	0.006(3)	0.017(3)	0.011(3)
C(13)	4e	0.8500(5)	0.4461(8)	0.3346(4)	0.076(4)	0.085(5)	0.051(4)	0.009(4)	0.025(3)	0.005(4)

Table 3. (Continued)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(14)	4e	0.8413(5)	0.5953(8)	0.3401(4)	0.084(4)	0.082(5)	0.057(4)	−0.027(4)	0.021(3)	0.010(4)
C(15)	4e	0.7888(5)	0.6571(7)	0.4038(4)	0.106(5)	0.054(4)	0.068(4)	−0.018(4)	0.021(4)	0.003(3)
C(16)	4e	0.7461(5)	0.5668(6)	0.4631(4)	0.075(4)	0.055(4)	0.053(3)	−0.008(3)	0.024(3)	−0.006(3)
C(21)	4e	0.7826(3)	0.1440(5)	0.5639(3)	0.039(3)	0.048(3)	0.041(3)	0.003(2)	0.009(2)	−0.003(2)
C(22)	4e	0.8998(4)	0.1550(6)	0.5778(3)	0.049(3)	0.060(4)	0.045(3)	0.003(3)	0.010(2)	0.003(3)
C(23)	4e	0.9657(5)	0.0333(7)	0.6036(3)	0.057(4)	0.081(5)	0.055(3)	0.027(3)	0.009(3)	0.011(3)
C(24)	4e	0.9168(6)	−0.0984(7)	0.6162(3)	0.095(5)	0.065(4)	0.048(3)	0.039(4)	0.009(3)	0.002(3)
C(25)	4e	0.8018(6)	−0.1118(6)	0.6018(4)	0.095(5)	0.036(3)	0.067(4)	0.003(3)	0.009(3)	−0.004(3)
C(26)	4e	0.7342(5)	0.0093(6)	0.5753(3)	0.059(3)	0.049(3)	0.057(3)	0.001(3)	0.009(3)	−0.006(3)
C(31)	4e	0.5966(6)	0.5125(8)	0.7489(4)	0.079(4)	0.121(6)	0.058(4)	0.016(4)	0.015(3)	−0.031(4)
C(32)	4e	0.4770(6)	0.5243(9)	0.7584(5)	0.095(5)	0.145(7)	0.061(5)	0.042(5)	0.026(4)	−0.008(5)

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