Crystal structure of *P,P*-dicyclohexyl-*N*-cyclohexyl-selenophosphinyl-thioformamide, $C_{19}H_{34}NPSSe$

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Source of material: Prepared using the literature method (ref. 1); mp 403 K–404 K.

Significant deviations from planarity are found in the central chromophore with the Se(2), P(1), C(1), S(1) and N(1) atoms lying $-0.009(1)$ Å, $0.051(2)$ Å, $0.106(8)$ Å, $-0.044(2)$ Å and $0.224(7)$ Å, respectively out of their least-squares plane; the conformation about the C(1)–N(1) bond is *Z*. With the exception of the relatively long N(1)–C(31) Å distance of $1.51(1)$ Å, the derived interatomic parameters are in essential agreement with the literature values for related systems (see refs. 1 and 2).

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

Crystal:	yellow plate, size 0.08 x 0.48 x 0.53 mm
Wavelength:	Mo $K\alpha$ radiation (0.7107 Å)
μ :	19.99 cm ⁻¹
Diffractometer:	AFC6R
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	1957
Criterion for F_o :	$F_o > 6 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	208
Program:	teXsan

$C_{19}H_{34}NPSSe$, monoclinic, $P12_1/c1$ (No. 14), $a = 12.591(4)$ Å, $b = 12.868(4)$ Å, $c = 12.888(3)$ Å, $\beta = 98.79(2)^\circ$, $V = 2063.6$ Å³, $Z = 4$, $R(F) = 0.059$, $R_w(F) = 0.054$.

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	0.7221	0.2529	0.4411	0.0603
H(11)	4e	0.7110	-0.0864	0.3620	0.0490
H(21)	4e	0.9553	0.0280	0.3623	0.0424
H(31)	4e	0.5241	0.2799	0.3070	0.0490
H(12a)	4e	0.8767	-0.1372	0.4405	0.0743
H(12b)	4e	0.8541	-0.0946	0.5503	0.0743
H(13a)	4e	0.7539	-0.2678	0.4440	0.0980
H(13b)	4e	0.8340	-0.2712	0.5514	0.0908
H(14a)	4e	0.6577	-0.2904	0.5751	0.1052
H(14b)	4e	0.7130	-0.1926	0.6356	0.1052
H(15a)	4e	0.5692	-0.1872	0.4483	0.0942
H(15b)	4e	0.5469	-0.1451	0.5583	0.0942
H(16a)	4e	0.6684	-0.0140	0.5548	0.0644
H(16b)	4e	0.5878	-0.0106	0.4477	0.0424
H(22a)	4e	0.8525	-0.0896	0.2574	0.0635
H(22b)	4e	0.8033	0.0014	0.1823	0.0635
H(23a)	4e	1.0203	-0.0598	0.2143	0.0733
H(23b)	4e	0.9388	-0.0761	0.1092	0.0733
H(24a)	4e	1.0523	0.0622	0.0967	0.0847
H(24b)	4e	0.9303	0.0971	0.0804	0.0847
H(25a)	4e	1.0787	0.1266	0.2636	0.0695
H(25b)	4e	1.0270	0.2157	0.1873	0.0695
H(26a)	4e	0.8626	0.1881	0.2351	0.0589
H(26b)	4e	0.9463	0.2029	0.3391	0.0662
H(32a)	4e	0.5067	0.4250	0.4020	0.0664
H(32b)	4e	0.5571	0.3392	0.4830	0.0664
H(33a)	4e	0.6402	0.5037	0.5104	0.1019
H(33b)	4e	0.7214	0.4123	0.4975	0.1019
H(34a)	4e	0.6464	0.5599	0.3437	0.1085
H(34b)	4e	0.7662	0.5497	0.4019	0.1085
H(35a)	4e	0.7475	0.4807	0.2362	0.0776
H(35b)	4e	0.7843	0.3954	0.3228	0.0776
H(36a)	4e	0.6547	0.3268	0.2002	0.0846
H(36b)	4e	0.5762	0.4199	0.2152	0.0855

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

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Se(2)	4e	0.85872(8)	0.14752(8)	0.54611(7)	0.0545(6)	0.0511(6)	0.0483(5)	0.0032(6)	0.0043(4)	-0.0094(6)
S(1)	4e	0.6095(2)	0.0930(2)	0.2345(2)	0.038(2)	0.055(2)	0.052(1)	-0.001(1)	-0.006(1)	-0.021(1)
P(1)	4e	0.7924(2)	0.0692(2)	0.4068(2)	0.041(2)	0.037(1)	0.052(1)	0.003(1)	0.016(1)	0.002(1)
N(1)	4e	0.6736(6)	0.2361(5)	0.3795(5)	0.051(5)	0.033(5)	0.067(5)	0.013(4)	0.009(4)	-0.004(4)
C(1)	4e	0.6821(7)	0.1450(7)	0.3357(6)	0.050(6)	0.043(6)	0.056(6)	0.009(6)	0.026(5)	0.008(5)
C(11)	4e	0.7372(7)	-0.0559(6)	0.4299(6)	0.035(6)	0.033(5)	0.058(6)	0.000(5)	0.015(5)	-0.001(4)
C(12)	4e	0.8221(7)	-0.1270(7)	0.4850(7)	0.054(7)	0.044(7)	0.091(7)	0.001(5)	0.019(6)	0.010(6)
C(13)	4e	0.7776(9)	-0.2315(7)	0.5094(9)	0.060(8)	0.035(6)	0.15(1)	0.004(6)	0.009(7)	0.028(7)
C(14)	4e	0.687(1)	-0.2218(9)	0.5669(9)	0.068(9)	0.074(8)	0.13(1)	-0.012(7)	0.025(8)	0.047(8)
C(15)	4e	0.6012(8)	-0.1544(9)	0.5133(9)	0.057(8)	0.060(7)	0.128(9)	-0.005(7)	0.036(7)	0.021(7)
C(16)	4e	0.6450(7)	-0.0499(7)	0.4891(7)	0.046(7)	0.049(6)	0.073(7)	0.015(5)	0.027(6)	0.012(5)
C(21)	4e	0.8914(6)	0.0548(6)	0.3190(6)	0.025(5)	0.041(5)	0.043(5)	0.008(4)	0.015(4)	-0.001(4)
C(22)	4e	0.8665(7)	-0.0220(7)	0.2292(7)	0.051(7)	0.051(6)	0.058(6)	-0.003(5)	0.018(5)	-0.006(5)
C(23)	4e	0.9591(8)	-0.0306(8)	0.1689(7)	0.061(8)	0.074(8)	0.054(6)	0.000(6)	0.026(5)	-0.018(6)
C(24)	4e	0.9894(8)	0.0709(9)	0.1308(7)	0.057(8)	0.11(1)	0.053(6)	0.000(7)	0.023(5)	-0.002(7)
C(25)	4e	1.0145(7)	0.1485(8)	0.2174(7)	0.045(6)	0.068(7)	0.066(6)	-0.002(6)	0.022(5)	0.011(6)
C(26)	4e	0.9240(7)	0.1578(7)	0.2795(6)	0.058(7)	0.040(6)	0.055(5)	-0.001(5)	0.025(5)	0.004(5)
C(31)	4e	0.5900(8)	0.3152(7)	0.3362(7)	0.053(7)	0.051(7)	0.063(6)	-0.009(6)	0.008(5)	0.003(5)
C(32)	4e	0.5699(7)	0.3829(7)	0.4249(8)	0.039(7)	0.042(7)	0.092(8)	0.013(5)	0.032(6)	-0.008(5)
C(33)	4e	0.663(1)	0.4537(9)	0.4617(8)	0.11(1)	0.082(9)	0.062(7)	0.008(8)	0.015(7)	-0.023(7)
C(34)	4e	0.702(1)	0.5116(8)	0.374(1)	0.09(1)	0.059(8)	0.12(1)	-0.019(7)	0.030(8)	-0.022(8)
C(35)	4e	0.7258(8)	0.4405(8)	0.2930(8)	0.065(8)	0.053(7)	0.080(8)	-0.020(6)	0.028(6)	-0.001(6)
C(36)	4e	0.6328(9)	0.3755(8)	0.2503(7)	0.081(9)	0.076(8)	0.059(6)	0.010(7)	0.016(6)	0.008(6)

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