parameters are presented in Table 1* and bond lengths and angles in Table 2. A view of the molecule is shown in Fig. 1.

Related literature. In the molecules of the α-pyridonate-bridged cis-diammineplatinum isomers (Hollis & Lippard, 1983a), the Pt—Pt distance is 2·8981 (5) Å for the head-to-tail dimer, 2·8767 (7) and 3·1294 (4) Å for the head-to-head tetramer; the dihedral angle between the coordination plane is 28·8° for the head-to-tail dimer, 30·0° for the head-to-head tetramer.

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* Lists of structure factors, anisotropic thermal parameters, and complete lists of bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51650 (25 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

In the head-to-head isomer of bis(μ-2-pyridonate-N,O)-bis|(ethylenediamine)platinum(II)| (Hollis & Lippard, 1983b), the Pt—Pt distance is 2·9915 (4) and 3·2355 (5) Å and the dihedral angle between the coordination planes is 39·6°.

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Structure of Bis(N,N-diisobutyldiselenocarbamato)palladium(II), Pd[Se₂CN(ᶦBu)₂]₂

BY JU-CHUN WANG AND JOHN P. FACKLER JR*

Department of Chemistry and Laboratory for Molecular Structure and Bonding, Texas A&M University, College Station, TX 77843, USA

Abstract. |Pd(C₉H₁₈NSe₂)₂|, $M_r = 702·7$, monoclinic, $P2_1/c$, $a = 6·684$ (1), $b = 12·393$ (3), $c = 15·648$ (3) Å, $\beta = 99·12$ (1)°, $V = 1279·8$ (4) Å³, $Z = 2$, $D_x = 1·83$ g cm⁻³, $\lambda(Mo\ K\alpha) = 0·71073$ Å, $\mu = 63·5$ cm⁻¹, $F(000) = 680$, $T = 295$ K. Final $R = 0·0325$ for 1274 unique observed reflections. The Pd atom occupies a center of symmetry in the molecule. The N—C bond distance |1·310 (8) Å| shows significant double-bond character.

Experimental. Crystals of bis(N,N-diisobutyldiselenocarbamato)palladium(II) were prepared according to Pan & Fackler (1978). An orange-red irregularly shaped crystal of dimensions 0·3 × 0·3 × 0·5 mm was mounted on a glass fiber. Cell constants were derived from least-squares refinement of 25 reflections having $10 < 2\theta < 26°$. Intensity data were collected using ω-scan technique with $0 < 2\theta < 45°$ ($h = 0$ to 14, $k = 0$ to 14, $l = -17$ to 17) on a Nicolet R3m/E diffractometer using graphite-monochromated Mo Kα radiation. Three standard reflections (032, 1̄22, 12̄3), measured every 197 reflections, showed small (<4%) random variations. Data were corrected for Lorentz

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* To whom correspondence should be addressed.

and polarization effects, and for absorption effects using the empirical method: $T_{min} = 0·472$, $T_{max} = 0·571$. 1963 data were collected and averaged to 1274 unique observed reflections |$F_o^2 > 3\sigma(F_o^2)$; $R_{int}(F_o) = 0·039$|. Scattering factors, including terms for anomalous dispersion, were taken from International Tables for X-ray Crystallography (1974). All computations were carried out using the SHELXTL crystallographic package (Sheldrick, 1986).

Pd was assigned to the special position $(0,\frac{1}{2},0)$; all other non-H atoms were located by Fourier synthesis. Some (ten out of 18) of the H atoms were revealed by difference Fourier maps. These H atoms were not included in the least-squares refinements but they were included in the final structure-factor calculations. Non-H atoms were refined anisotropically. A partial correction for secondary extinction was applied by multiplying F_c by |1 + 0·002xF_c^2(sin 2θ)|⁻¹/⁴; refinement gave $x = 0·00095$. $\sum w(|F_o| - |F_c|)^2$ was minimized, where $w = |\sigma^2(F_o) + 0·00046F_o^2|^{-1}$; the final R value was 0·033, $wR = 0·043$ and $S = 1·396$ for 116 variables. The largest shift/e.s.d. in the final least-squares cycle was 0·005; the maximum and minimum residual electron densities in the difference Fourier map were less than 0·5 e Å⁻³. The molecule and the atomic

labeling scheme are shown in Fig. 1. Fig. 2 shows a stereoscopic view of the unit cell. Final positional and equivalent isotropic thermal parameters are given in Table 1;* some selected bond distances and angles are listed in Table 2.

Related literature. The crystal structure of the Pt analog has been reported (Pan, Fackler & Chen, 1981). The structure of the corresponding thiocarbamate Pd^{II} complex (Riekkola, Pakkanen & Niinisto, 1983) and those of a few other alkylselenocarbamate transition-metal complexes (Bonamico & Dessy, 1971; Noordik & Smits, 1974) have also been reported.

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* Lists of structure factors, anisotropic thermal parameters and hydrogen parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51609 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
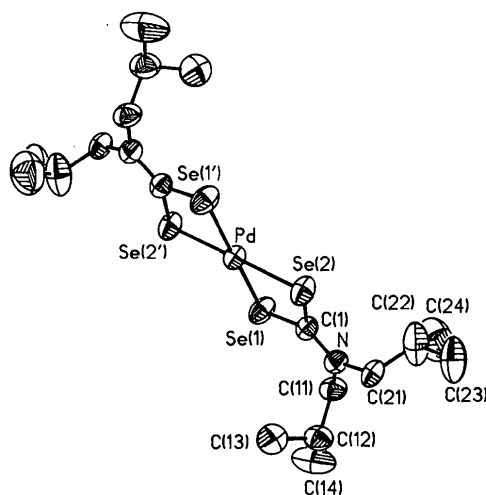

Fig. 1. A perspective view of the Pd[Se$_2$CN(^{i}Bu)$_2$]$_2$ structure. Thermal ellipsoids have been drawn at the 50% probability level.
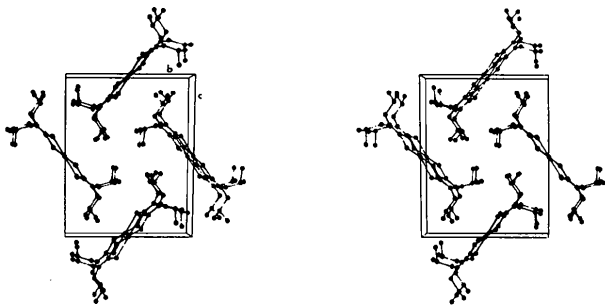

Fig. 2. A stereoview packing diagram viewed down the *a* axis.

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($\text{Å}^2 \times 10^3$) *for* Pd[Se$_2$CN(^{i}Bu)$_2$]$_2$

E.s.d.'s in the least-significant digits are given in parentheses.

	x	y	z	U_{eq}
Pd	0	5000	0	47 (1)*
Se(1)	2803 (1)	4109 (1)	−539 (1)	62 (1)*
Se(2)	−1733 (1)	4039 (1)	−1256 (1)	57 (1)*
N	1151 (8)	2735 (4)	−1936 (3)	49 (2)*
C(1)	833 (11)	3479 (5)	−1378 (4)	47 (2)*
C(11)	3139 (11)	2262 (5)	−1938 (5)	58 (3)*
C(12)	3219 (12)	1064 (6)	−1635 (5)	68 (3)*
C(13)	2705 (16)	979 (7)	−723 (5)	93 (4)*
C(14)	5338 (16)	656 (8)	−1590 (8)	122 (6)*
C(21)	−548 (11)	2313 (5)	−2570 (4)	54 (3)*
C(22)	−1125 (16)	2980 (8)	−3373 (5)	102 (4)*
C(23)	−2941 (16)	2454 (10)	−3942 (5)	115 (5)*
C(24)	477 (20)	3272 (12)	−3842 (8)	136 (6)*

* The equivalent isotropic U is defined as $\frac{1}{3}$ of the trace of the U_{ij} tensor.

Table 2. *Bond lengths* (Å) *and angles* (°) *for* Pd[Se$_2$CN(^{i}Bu)$_2$]$_2$

E.s.d.'s in the least-significant digits are given in parentheses.

Pd—Se(1)	2·437 (1)	Pd—Se(2)	2·429 (1)
Se(1)—C(1)	1·876 (6)	Se(2)—C(1)	1·888 (7)
N—C(1)	1·310 (8)	N—C(11)	1·453 (9)
N—C(21)	1·480 (8)	C(11)—C(12)	1·557 (10)
C(12)—C(13)	1·522 (12)	C(12)—C(14)	1·495 (13)
C(21)—C(22)	1·503 (11)	C(22)—C(23)	1·533 (14)
C(22)—C(24)	1·437 (17)		

Se(1)—Pd—Se(2)	78·0 (1)	Se(1)—Pd—Se(1')	180·0 (1)
Se(1)—Pd—Se(2')	102·0 (1)	Pd—Se(1)—C(1)	86·5 (2)
Pd—Se(2)—C(1)	86·4 (2)	C(1)—N—C(11)	122·0 (5)
C(1)—N—C(21)	120·4 (6)	C(11)—N—C(21)	117·5 (5)
Se(1)—C(1)—Se(2)	108·9 (3)	Se(1)—C(1)—N	126·1 (5)
Se(2)—C(1)—N	124·9 (5)	N—C(11)—C(12)	111·8 (6)
C(11)—C(12)—C(13)	110·5 (6)	C(11)—C(12)—C(14)	108·9 (7)
C(13)—C(12)—C(14)	106·6 (8)	N—C(21)—C(22)	115·7 (6)
C(21)—C(22)—C(23)	109·1 (8)	C(21)—C(22)—C(24)	116·9 (9)
C(23)—C(22)—C(24)	113·3 (8)		

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