Boča, Jóna, Kabešová, Macašková, Šima, Pelikán & Valach, 1982) where Ni—N(pip) > Ni—N(py).

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Structure of a Dinuclear Nickel Compound, $Ni_2(PPh_3)_2(SC_3H_6S)_2$

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Abstract. Bis(1,2-propanedithiolato-1:2$\kappa^2S',2\kappa S^2$)bis-(triphenylphosphine)dinickel, $[Ni_2(C_3H_6S_2)_2\{(C_6H_5)_3P\}_2]$, $M_r = 854.43$, monoclinic, $C2/c$, $a = 26.499$ (13), $b = 9.037$ (6), $c = 17.419$ (7) Å, $\beta = 107.33$ (3)°, $V = 3982.1$ Å^3, $Z = 4$, $D_x = 1.43$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 12.6$ cm^{-1}, $F(000) = 1776$, $T = 296$ K, $R = 0.053$ and $wR = 0.059$ for 2575 reflections with $I > 3\sigma(I)$. The complex is a dimer, where each Ni atom is four-coordinated by one P and three S atoms with square-planar geometry. The average Ni—S and Ni—P bond lengths are 2.190 and 2.193 Å, respectively.

Experimental. The title complex was prepared by reaction of Na, H_2pdt, PPh_3 and $NiCl_2.6H_2O$ in MeOH solution and a crystal suitable for the X-ray analysis was grown in a solution of 1,2-$C_2H_4Cl_2$/MeOH.

A crystal of dimensions 0.8 × 0.5 × 0.2 mm was used for the X-ray analysis. Cell parameters were obtained from least-squares refinement of 20 strong reflections within the 2θ range 12–14°, measured on a Rigaku AFC-5*R* four-circle diffractometer with Mo $K\alpha$ radiation. Integrated intensities were measured at room temperature in the 2θ range within 50° ($0 < h < 31$, $0 < k < 10$, $-20 < l < 20$) by the $\theta/2\theta$ scan mode. Among 3852 reflections, 2575 with $I > 3\sigma(I)$ were used for structure determination. The data were corrected for anisotropic decay (between 0.966 and 1.034), Lp effects, and empirical absorption based on a series of ψ scans (between 0.608 and 1.000). An empirical absorption correction was made by the program *DIFABS* (Walker & Stuart, 1983) after structure refinement with isotropic thermal parameters; the maximum and minimum absorption corrections were 1.054 and 0.705, respectively.

All calculations were performed on a VAX 785 computer with the *SDP* program package (Frenz, 1978). The coordinates of all metal atoms were determined by direct methods and the remaining non-H atoms were located from successive difference Fourier maps. H atoms were not included. Full-matrix least-squares refinement with anisotropic temperature factors for all non-H atoms led to convergence with $R = 0.053$ and $wR = 0.059$. The function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w = 1/[\sigma^2(F) + 0.0001F^2 + 1.0]$ (Killean & Lawrence, 1969). Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The final cycle of refinement included 226 variable parameters. The goodness of fit (S) was 2.45. The largest Δ/σ was 0.80 while the extreme peaks in the difference electron density map were 1.01 and −0.62 e Å^{-3}. Final positional parameters are given in Table 1 and selected bond distances and angles are listed in Table 2.* The structure of the molecule is depicted in Fig. 1.

Related literature. The structures of $[Ni(PPh_3)(SCH_2CH_2SCH_2CH_2S)]$ (Cao, Lei, Huang, Hong &

* Lists of anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55048 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0501]

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Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

	x	y	z	B_{eq}
Ni	0.44444 (3)	0.18004 (9)	0.20866 (4)	2.73 (1)
S(1)	0.51054 (6)	0.0752 (2)	0.17695 (8)	3.41 (3)
S(2)	0.42082 (6)	0.2947 (2)	0.09404 (9)	4.32 (4)
P	0.37384 (6)	0.2690 (2)	0.23326 (8)	2.73 (3)
C(1)	0.5109 (3)	0.1706 (9)	0.0837 (3)	5.3 (2)
C(2)	0.4580 (3)	0.2010 (10)	0.0364 (4)	7.4 (2)
C(3)	0.4547 (3)	0.2910 (10)	−0.0411 (4)	7.1 (2)
C(11)	0.3103 (2)	0.2016 (7)	0.1686 (3)	3.1 (1)
C(12)	0.3075 (3)	0.1256 (7)	0.0985 (4)	4.0 (2)
C(13)	0.2572 (3)	0.0795 (9)	0.0480 (4)	5.6 (2)
C(14)	0.2119 (3)	0.1110 (10)	0.0689 (4)	6.1 (2)
C(15)	0.2150 (3)	0.1840 (10)	0.1406 (4)	6.1 (2)
C(16)	0.2642 (2)	0.2293 (8)	0.1919 (4)	4.8 (2)
C(21)	0.3665 (2)	0.2343 (6)	0.3327 (3)	2.9 (1)
C(22)	0.3556 (2)	0.0901 (7)	0.3501 (4)	4.0 (1)
C(23)	0.3527 (3)	0.0530 (8)	0.4280 (4)	4.8 (2)
C(24)	0.3624 (3)	0.1620 (8)	0.4870 (4)	5.5 (2)
C(25)	0.3738 (3)	0.3073 (8)	0.4694 (4)	5.5 (2)
C(26)	0.3749 (3)	0.3435 (7)	0.3914 (3)	4.3 (2)
C(31)	0.3721 (2)	0.4703 (7)	0.2220 (3)	3.3 (1)
C(32)	0.3252 (3)	0.5459 (8)	0.1813 (4)	5.0 (2)
C(33)	0.3277 (3)	0.7040 (8)	0.1727 (4)	6.2 (2)
C(34)	0.3757 (4)	0.7757 (8)	0.2045 (4)	6.6 (2)
C(35)	0.4212 (3)	0.7003 (8)	0.2446 (4)	6.0 (2)
C(36)	0.4198 (3)	0.5440 (8)	0.2529 (4)	5.0 (2)

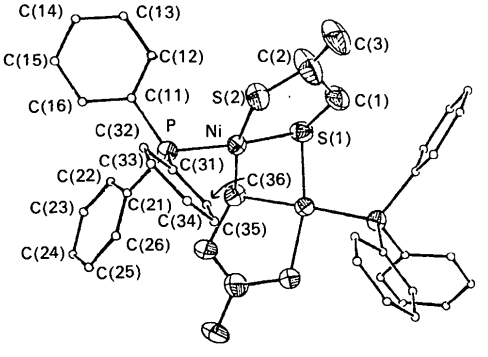

Fig. 1. The molecular structure of the title compound.

Table 2. *Selected bond distances* (Å) *and bond angles* (°)

Ni—S(1)	2.201 (1)	P—C(11)	1.829 (4)
Ni—S(1′)	2.209 (2)	P—C(21)	1.827 (4)
Ni—S(2)	2.170 (1)	P—C(31)	1.828 (5)
Ni—P	2.193 (1)	C(1)—C(2)	1.424 (6)
S(1)—C(1)	1.841 (4)	C(2)—C(3)	1.559 (6)
S(2)—C(2)	1.812 (5)		

S(1)—Ni—S(1′)	77.61 (5)	C(11)—P—C(21)	100.9 (2)
S(1)—Ni—S(2)	90.44 (4)	C(11)—P—C(31)	106.0 (2)
S(1)—Ni—P	174.71 (4)	C(21)—P—C(31)	105.5 (2)
S(1′)—Ni—S(2)	164.93 (5)	S(1)—C(1)—C(2)	109.8 (4)
S(1′)—Ni—P	104.13 (4)	S(2)—C(2)—C(1)	111.9 (4)
S(2)—Ni—P	88.61 (4)	S(2)—C(2)—C(3)	109.7 (4)
Ni—S(1)—Ni′	81.11 (4)	C(1)—C(2)—C(3)	113.2 (5)
Ni—S(1)—C(1)	103.5 (2)	P—C(11)—C(12)	120.4 (3)
Ni—S(1′)—C(1′)	116.9 (2)	P—C(11)—C(16)	118.5 (4)
Ni—S(2)—C(2)	103.4 (2)	P—C(21)—C(22)	117.2 (3)
Ni—P—C(11)	116.1 (1)	P—C(21)—C(26)	122.4 (4)
Ni—P—C(21)	117.4 (1)	P—C(31)—C(32)	121.7 (3)
Ni—P—C(31)	109.8 (1)	P—C(31)—C(36)	116.4 (3)

Liu, 1992) and $[Ni_2(PPh_3)_2(SCH_2CH_2S)_2]$ (Cao, Huang, Lei, Hong & Liu, 1992) have been reported.

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Structure of the Condensation Product Formed by Pyrrolidine, Acetonitrile and Copper(I) Iodide

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Abstract. Bis[1-aza-2-(1-pyrrolidinyl)propenyl]copper(I) iodide, $[Cu(C_6H_{12}N_2)_2]I$, $M_r = 414.80$, monoclinic, $A2/a$, $a = 16.149$ (1), $b = 7.205$ (5), $c = 15.358$ (5) Å, $\beta = 115.09$ (5)°, $V = 1618.4$ (2) Å^3, $Z = 4$, $D_x = 1.702$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 32.32$ cm^{-1}, $F(000) = 824$, $T = 294$ K, $R = 4.7\%$ for

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