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Bis[(3-fluorobenzyl)triphenylphosphonium] bis(1,2-dicyanoethene-1,2-dithiolato-κ^2S,S')nickel(II)

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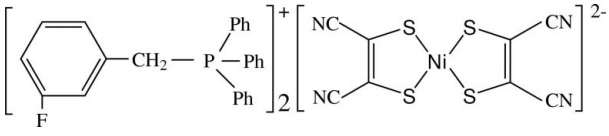
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.106; data-to-parameter ratio = 15.7.

In the title salt, $(C_{25}H_{21}FP)_2[Ni(C_4N_2S_2)_2]$, the Ni^{II} ion lies on an inversion centre and the $[Ni(mnt)_2]^{2-}$ anion (mnt is maleonitriledithiolate) exhibits a square-planar coordination geometry. The (3-fluorobenzyl)triphenylphosphonium cation adopts a conformation in which the four aromatic rings are twisted with respect to the plane including the P atom and the two C atoms linking it to the 3-fluorobenzyl ring. A weak C—H···N hydrogen bond and a C—H···π interaction stabilize the crystal structure.

Related literature

For details of other $[Ni(mnt)_2]^{2-}$ complexes, see: Robertson & Cronin (2002); Ni *et al.* (2004, 2005); Liu & Ni (2006). For closely related $[Ni(mnt)_2]^{2-}$ complexes with square-planar geometry and a substituted triphenylphosphinium counterion, see: Yang & Ni (2006); Zhou *et al.* (2007).



Experimental

Crystal data

$(C_{25}H_{21}FP)_2[Ni(C_4N_2S_2)_2]$
M_r = 1081.85
Monoclinic, $P2_1/n$
a = 9.429 (1) Å
b = 14.625 (1) Å
c = 18.912 (1) Å
β = 98.73 (1)°
V = 2577.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 291 (2) K
0.51 × 0.41 × 0.30 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.730, T_{max} = 0.825
14690 measured reflections
5065 independent reflections
4084 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.106
S = 1.00
5065 reflections
322 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C24–C29 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···N1^{i}	0.93	2.61	3.495 (3)	160
C13—H13···Cg^{ii}	0.93	3.16	3.705 (2)	130

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2383).

References

Bruker (2000). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SMART* (Version 5.62) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, M.-G. & Ni, C.-L. (2006). *Acta Cryst.* E**62**, m2851–m2852.
Ni, C. L., Dang, D. B., Song, Y., Gao, S., Li, Y. Z., Ni, Z. P., Tian, Z. F., Wen, L. L. & Meng, Q. J. (2004). *Chem. Phys. Lett.* **396**, 353–358.
Ni, C. L., Li, Y. Z. & Meng, Q. J. (2005). *J. Coord. Chem.* **58**, 759–766.
Robertson, N. & Cronin, L. (2002). *Coord. Chem. Rev.* **227**, 93–127.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
Yang, S.-B. & Ni, C.-L. (2006). *Acta Cryst.* E**62**, m483–m485.
Zhou, J.-R., Ni, C.-L. & Yu, L.-L. (2007). *Acta Cryst.* E**63**, m1427–m1429.

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supplementary materials

Acta Cryst. (2007). E**63**, m2858 [**doi:10.1107/S160053680705297X**]

Bis[(3-fluorobenzyl)triphenylphosphonium] bis(1,2-dicyanoethene-1,2-dithiolato-κ^2S,S')nickel(II)

Q.-B. Liao, M.-G. Liu and C.-L. Ni

Comment

The unusual physical properties of complexes containing the $Ni(mnt)_2^{2-}$ anion are partly attributed to intermolecular interactions between $Ni(mnt)_2^{2-}$ anions and a variety of multifunctional cations (Robertson & Cronin, 2002; Ni *et al.*, 2004). In recent years, we have introduced other substituted benzyltriphenylphosphinium cations into the $Ni(mnt)_2^{2-}$ system and obtained some $Ni(mnt)_2^{2-}$-based molecular solids (Ni *et al.*, 2005; Yang & Ni, 2006; Liu & Ni, 2006; Zhou *et al.*, 2007). As shown in Fig.1, the title compound is isostructural with $(BzTPP)_2^+$ $[Ni(mnt)_2]^{2-}$ Zhou *et al.*, 2007). The asymmetric unit of (I) consists of one $[mFBzTPP]^+$ cation and one-half of a $Ni(mnt)_2^{2-}$ anion as the Ni atom lies on an inversion centre. The nickel(II) ion is coordinated by four S atoms from two mnt^{2-} ligands and the $Ni(mnt)_2^{2-}$ anion is in a square planar configuration. The two N atoms of the CN groups deviate from the Ni1/S1/S2 plane by 0.392 (2) Å for N1 and 0.451 (2) Å for N2.

The $[mFBzTPP]^+$ cation adopts a conformation where four phenyl rings are twisted with respect to the P1—C11—C10 plane with dihedral angles of 91.2 (2) for the C5/C6/C7/C8/C9/C10 ring, 81.7 (2)° for the C12/C13/C14/C15/C16/C17 ring, 20.6 (2)° for the C18/C19/C20/C21/C22/C23 ring, and 86.9 (2)° for the C24/C25/C26/C27/C28/C29 ring. The deviation of the F atom from the C5/C6/C7/C8/C9/C10 phenyl ring plane is −0.041 (2) Å.

The crystal structure is stabilized by a C9—H9···N1 hydrogen bond, Table 1, and a C13—H13···π interaction with the $C24^i$···$C29^i$ ring [symmetry code: (i) $1-x, -y, 1-z$]. The distance between C13 and the centroid of the $C24^i$···$C29^i$ ring is 3.705 (2) Å, Fig 2.

Experimental

The title compound was prepared by the direct reaction of $NiCl_2{\cdot}6H_2O$, Na_2mnt and (mFBzTPP)Br in methanol. Red block-shaped single crystals were obtained by slow evaporation of a CH_3CN solution at room temperature over two weeks.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, $U_{iso} = 1.2U_{eq}$(C) for aromatic and 0.97 Å, $U_{iso} = 1.2U_{eq}$(C) for CH_2 atoms.

Figures

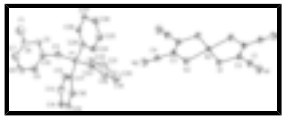

Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

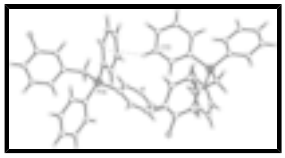

Fig. 2. The C—H···π hydrogen bond between cations.

Bis[(3-fluorobenzyl)triphenylphosphonium] bis(1,2-dicyanoethene-1,2-dithiolato-κ^2S,S')nickel(II)

Crystal data

$(C_{25}H_{21}FP)_2[Ni(C_4N_2S_2)_2]$	F_{000} = 1116
M_r = 1081.85	D_x = 1.394 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 6299 reflections
a = 9.429 (1) Å	θ = 2.3–27.3º
b = 14.625 (1) Å	μ = 0.65 mm^{-1}
c = 18.912 (1) Å	T = 291 (2) K
β = 98.73 (1)º	Block, red
V = 2577.7 (4) Å^3	0.51 × 0.41 × 0.30 mm
Z = 2	

Data collection

Bruker SMART APEX CCD diffractometer	5065 independent reflections
Radiation source: fine-focus sealed tube	4084 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
T = 291(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −11→11
T_{min} = 0.730, T_{max} = 0.825	k = −13→18
14690 measured reflections	l = −23→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.034	H-atom parameters constrained
$wR(F^2)$ = 0.106	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
5065 reflections	$\Delta\rho_{max}$ = 0.61 e Å^{-3}
322 parameters	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
1 restraint	Extinction correction: none

Primary atom site location: structure-invariant direct methods

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.5000	0.0000	0.04385 (12)
P1	0.78361 (5)	0.64448 (4)	0.83224 (3)	0.04648 (15)
S1	0.67420 (5)	0.40712 (4)	0.03967 (3)	0.05430 (16)
S2	0.59246 (6)	0.59631 (4)	0.08152 (3)	0.05951 (17)
N1	0.8175 (2)	0.17840 (17)	−0.00067 (13)	0.0870 (7)
N2	0.5246 (2)	0.83161 (15)	0.14742 (11)	0.0734 (6)
F1	0.4030 (2)	0.92911 (15)	0.89371 (15)	0.1436 (9)
C1	0.7381 (2)	0.23857 (17)	−0.00796 (11)	0.0603 (6)
C2	0.6407 (2)	0.31418 (15)	−0.01694 (10)	0.0497 (5)
C3	0.4754 (2)	0.68785 (14)	0.06882 (10)	0.0482 (5)
C4	0.5041 (2)	0.76731 (16)	0.11311 (11)	0.0558 (5)
C5	0.5660 (2)	0.80705 (17)	0.90768 (14)	0.0678 (6)
H5	0.4917	0.7668	0.8916	0.081*
C6	0.5389 (3)	0.89860 (19)	0.91348 (16)	0.0789 (7)
C7	0.6417 (3)	0.9608 (2)	0.93787 (14)	0.0791 (7)
H7	0.6196	1.0223	0.9425	0.095*
C8	0.7797 (3)	0.9290 (2)	0.95544 (15)	0.0874 (8)
H8	0.8531	0.9700	0.9714	0.105*
C9	0.8112 (3)	0.8374 (2)	0.94982 (13)	0.0761 (7)
H9	0.9052	0.8172	0.9622	0.091*
C10	0.7038 (2)	0.77539 (16)	0.92591 (10)	0.0562 (5)
C11	0.7404 (2)	0.67552 (16)	0.91959 (11)	0.0605 (6)
H11A	0.6597	0.6389	0.9292	0.073*
H11B	0.8217	0.6609	0.9557	0.073*
C12	0.8433 (2)	0.80663 (14)	0.76758 (12)	0.0565 (5)
H12	0.7450	0.8115	0.7526	0.068*
C13	0.9331 (3)	0.87451 (16)	0.75220 (14)	0.0664 (6)
H13	0.8957	0.9257	0.7268	0.080*
C14	1.0780 (3)	0.86767 (17)	0.77401 (14)	0.0690 (6)
H14	1.1387	0.9139	0.7629	0.083*
C15	1.1338 (2)	0.79326 (17)	0.81201 (13)	0.0656 (6)
H15	1.2322	0.7893	0.8270	0.079*
C16	1.0452 (2)	0.72424 (15)	0.82816 (11)	0.0558 (5)
H16	1.0833	0.6736	0.8541	0.067*
C17	0.89864 (19)	0.73057 (13)	0.80547 (10)	0.0452 (4)
C18	0.9536 (3)	0.51284 (16)	0.78456 (14)	0.0657 (6)
H18	0.9538	0.5507	0.7451	0.079*
C19	1.0288 (3)	0.43144 (18)	0.78898 (18)	0.0805 (8)
H19	1.0810	0.4150	0.7530	0.097*
C20	1.0259 (3)	0.37512 (19)	0.8466 (2)	0.0928 (10)
H20	1.0770	0.3205	0.8500	0.111*
C21	0.9487 (3)	0.3988 (2)	0.89900 (19)	0.0920 (10)
H21	0.9458	0.3594	0.9373	0.110*

C22	0.8753 (3)	0.47950 (18)	0.89629 (15)	0.0751 (7)
H22	0.8238	0.4952	0.9327	0.090*
C23	0.8783 (2)	0.53805 (15)	0.83866 (11)	0.0524 (5)
C24	0.6370 (2)	0.63541 (16)	0.69513 (11)	0.0569 (5)
H24	0.7260	0.6447	0.6808	0.068*
C25	0.5170 (2)	0.62204 (17)	0.64484 (13)	0.0674 (6)
H25	0.5261	0.6209	0.5966	0.081*
C26	0.3853 (3)	0.61046 (16)	0.66474 (15)	0.0694 (6)
H26	0.3048	0.6029	0.6302	0.083*
C27	0.3719 (2)	0.60994 (15)	0.73614 (15)	0.0655 (6)
H27	0.2819	0.6022	0.7497	0.079*
C28	0.4904 (2)	0.62075 (14)	0.78769 (12)	0.0549 (5)
H28	0.4808	0.6186	0.8359	0.066*
C29	0.6246 (2)	0.63497 (13)	0.76764 (10)	0.0464 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0420 (2)	0.0564 (2)	0.03404 (19)	0.00268 (15)	0.00871 (14)	−0.00133 (14)
P1	0.0459 (3)	0.0522 (3)	0.0420 (3)	−0.0005 (2)	0.0087 (2)	0.0077 (2)
S1	0.0499 (3)	0.0656 (4)	0.0452 (3)	0.0081 (2)	0.0001 (2)	−0.0077 (2)
S2	0.0557 (3)	0.0685 (4)	0.0502 (3)	0.0104 (3)	−0.0050 (2)	−0.0119 (3)
N1	0.0793 (15)	0.0901 (16)	0.0855 (16)	0.0270 (13)	−0.0068 (12)	−0.0113 (13)
N2	0.0780 (14)	0.0693 (13)	0.0709 (13)	−0.0023 (11)	0.0047 (11)	−0.0146 (11)
F1	0.0827 (12)	0.1171 (15)	0.228 (3)	0.0133 (11)	0.0136 (13)	−0.0575 (16)
C1	0.0591 (13)	0.0697 (15)	0.0502 (12)	0.0076 (12)	0.0019 (10)	−0.0074 (11)
C2	0.0494 (11)	0.0578 (12)	0.0429 (11)	0.0046 (9)	0.0102 (9)	−0.0015 (9)
C3	0.0485 (11)	0.0552 (12)	0.0416 (10)	0.0024 (9)	0.0091 (8)	−0.0023 (9)
C4	0.0536 (12)	0.0650 (14)	0.0487 (12)	0.0022 (10)	0.0070 (9)	−0.0034 (11)
C5	0.0548 (13)	0.0735 (16)	0.0790 (16)	−0.0137 (12)	0.0224 (11)	−0.0236 (13)
C6	0.0685 (14)	0.0797 (18)	0.0902 (19)	−0.0038 (13)	0.0178 (13)	−0.0230 (15)
C7	0.092 (2)	0.0690 (16)	0.0770 (17)	−0.0121 (15)	0.0159 (15)	−0.0146 (14)
C8	0.090 (2)	0.083 (2)	0.085 (2)	−0.0294 (16)	0.0008 (15)	−0.0191 (15)
C9	0.0634 (15)	0.095 (2)	0.0654 (15)	−0.0096 (14)	−0.0037 (12)	−0.0114 (14)
C10	0.0635 (13)	0.0701 (14)	0.0366 (10)	−0.0092 (11)	0.0128 (9)	−0.0052 (9)
C11	0.0682 (14)	0.0716 (15)	0.0426 (11)	−0.0004 (11)	0.0109 (10)	0.0064 (10)
C12	0.0474 (11)	0.0563 (13)	0.0661 (14)	0.0078 (10)	0.0091 (10)	0.0107 (11)
C13	0.0706 (15)	0.0461 (12)	0.0841 (17)	0.0029 (11)	0.0171 (13)	0.0161 (12)
C14	0.0657 (15)	0.0563 (14)	0.0871 (18)	−0.0149 (11)	0.0183 (13)	0.0013 (12)
C15	0.0478 (12)	0.0661 (15)	0.0803 (16)	−0.0101 (11)	0.0009 (11)	−0.0007 (12)
C16	0.0505 (11)	0.0558 (12)	0.0569 (13)	−0.0029 (10)	−0.0050 (9)	0.0054 (10)
C17	0.0453 (10)	0.0470 (11)	0.0435 (10)	−0.0011 (8)	0.0071 (8)	0.0033 (8)
C18	0.0644 (14)	0.0566 (14)	0.0774 (16)	0.0039 (11)	0.0154 (12)	0.0078 (11)
C19	0.0639 (15)	0.0595 (15)	0.119 (2)	0.0050 (12)	0.0168 (15)	−0.0017 (16)
C20	0.0581 (15)	0.0516 (15)	0.159 (3)	0.0008 (12)	−0.0140 (18)	0.0178 (18)
C21	0.0782 (19)	0.0719 (19)	0.121 (3)	−0.0015 (15)	−0.0026 (18)	0.0453 (18)
C22	0.0697 (16)	0.0733 (16)	0.0800 (17)	0.0006 (13)	0.0038 (13)	0.0307 (14)
C23	0.0460 (11)	0.0494 (11)	0.0610 (13)	−0.0031 (9)	0.0054 (9)	0.0107 (10)

C24	0.0511 (12)	0.0700 (14)	0.0506 (12)	−0.0007 (10)	0.0106 (9)	0.0038 (10)
C25	0.0680 (15)	0.0775 (16)	0.0537 (13)	0.0012 (12)	−0.0007 (11)	0.0026 (11)
C26	0.0578 (14)	0.0640 (15)	0.0807 (18)	0.0016 (11)	−0.0076 (12)	−0.0066 (13)
C27	0.0425 (12)	0.0584 (14)	0.0969 (19)	−0.0034 (10)	0.0147 (12)	−0.0143 (13)
C28	0.0527 (12)	0.0534 (12)	0.0623 (13)	−0.0030 (10)	0.0212 (10)	−0.0055 (10)
C29	0.0434 (10)	0.0472 (11)	0.0494 (11)	0.0012 (8)	0.0097 (8)	0.0006 (9)

Geometric parameters (Å, °)

Ni1—S2^{i}	2.1709 (5)	C12—H12	0.9300
Ni1—S2	2.1709 (5)	C13—C14	1.370 (3)
Ni1—S1^{i}	2.1753 (5)	C13—H13	0.9300
Ni1—S1	2.1753 (5)	C14—C15	1.365 (3)
P1—C17	1.7846 (19)	C14—H14	0.9300
P1—C23	1.790 (2)	C15—C16	1.374 (3)
P1—C29	1.790 (2)	C15—H15	0.9300
P1—C11	1.818 (2)	C16—C17	1.386 (2)
S1—C2	1.729 (2)	C16—H16	0.9300
S2—C3	1.729 (2)	C18—C23	1.381 (3)
N1—C1	1.150 (3)	C18—C19	1.381 (3)
N2—C4	1.142 (3)	C18—H18	0.9300
F1—C6	1.355 (3)	C19—C20	1.370 (4)
C1—C2	1.431 (3)	C19—H19	0.9300
C2—C3^{i}	1.354 (3)	C20—C21	1.360 (5)
C3—C2^{i}	1.354 (3)	C20—H20	0.9300
C3—C4	1.434 (3)	C21—C22	1.364 (4)
C5—C6	1.371 (4)	C21—H21	0.9300
C5—C10	1.374 (3)	C22—C23	1.390 (3)
C5—H5	0.9300	C22—H22	0.9300
C6—C7	1.358 (4)	C24—C25	1.377 (3)
C7—C8	1.374 (4)	C24—C29	1.394 (3)
C7—H7	0.9300	C24—H24	0.9300
C8—C9	1.380 (4)	C25—C26	1.362 (3)
C8—H8	0.9300	C25—H25	0.9300
C9—C10	1.383 (3)	C26—C27	1.375 (4)
C9—H9	0.9300	C26—H26	0.9300
C10—C11	1.510 (3)	C27—C28	1.376 (3)
C11—H11A	0.9700	C27—H27	0.9300
C11—H11B	0.9700	C28—C29	1.390 (3)
C12—C13	1.365 (3)	C28—H28	0.9300
C12—C17	1.382 (3)		
S2^{i}—Ni1—S2	180.00 (2)	C12—C13—H13	119.8
S2^{i}—Ni1—S1^{i}	87.67 (2)	C14—C13—H13	119.8
S2—Ni1—S1^{i}	92.33 (2)	C15—C14—C13	120.2 (2)
S2^{i}—Ni1—S1	92.33 (2)	C15—C14—H14	119.9
S2—Ni1—S1	87.67 (2)	C13—C14—H14	119.9
S1^{i}—Ni1—S1	180.00 (3)	C14—C15—C16	120.3 (2)

C17—P1—C23	108.32 (9)	C14—C15—H15	119.9
C17—P1—C29	110.09 (9)	C16—C15—H15	119.9
C23—P1—C29	109.66 (10)	C15—C16—C17	119.6 (2)
C17—P1—C11	108.13 (10)	C15—C16—H16	120.2
C23—P1—C11	109.50 (10)	C17—C16—H16	120.2
C29—P1—C11	111.08 (10)	C12—C17—C16	119.64 (19)
C2—S1—Ni1	102.69 (7)	C12—C17—P1	121.12 (15)
C3—S2—Ni1	102.98 (7)	C16—C17—P1	119.03 (15)
N1—C1—C2	179.3 (3)	C23—C18—C19	120.1 (2)
$C3^{i}$—C2—C1	120.16 (19)	C23—C18—H18	119.9
$C3^{i}$—C2—S1	121.15 (16)	C19—C18—H18	119.9
C1—C2—S1	118.69 (15)	C20—C19—C18	119.6 (3)
$C2^{i}$—C3—C4	120.07 (18)	C20—C19—H19	120.2
$C2^{i}$—C3—S2	120.82 (15)	C18—C19—H19	120.2
C4—C3—S2	119.10 (15)	C21—C20—C19	120.2 (3)
N2—C4—C3	178.5 (3)	C21—C20—H20	119.9
C6—C5—C10	119.3 (2)	C19—C20—H20	119.9
C6—C5—H5	120.3	C20—C21—C22	121.2 (3)
C10—C5—H5	120.3	C20—C21—H21	119.4
F1—C6—C7	118.0 (3)	C22—C21—H21	119.4
F1—C6—C5	118.6 (2)	C21—C22—C23	119.4 (3)
C7—C6—C5	123.4 (3)	C21—C22—H22	120.3
C6—C7—C8	117.1 (3)	C23—C22—H22	120.3
C6—C7—H7	121.4	C18—C23—C22	119.4 (2)
C8—C7—H7	121.4	C18—C23—P1	119.30 (16)
C7—C8—C9	121.1 (3)	C22—C23—P1	121.32 (19)
C7—C8—H8	119.4	C25—C24—C29	119.7 (2)
C9—C8—H8	119.4	C25—C24—H24	120.1
C8—C9—C10	120.4 (3)	C29—C24—H24	120.1
C8—C9—H9	119.8	C26—C25—C24	121.0 (2)
C10—C9—H9	119.8	C26—C25—H25	119.5
C5—C10—C9	118.6 (2)	C24—C25—H25	119.5
C5—C10—C11	121.7 (2)	C25—C26—C27	119.7 (2)
C9—C10—C11	119.7 (2)	C25—C26—H26	120.1
C10—C11—P1	113.51 (14)	C27—C26—H26	120.1
C10—C11—H11A	108.9	C26—C27—C28	120.6 (2)
P1—C11—H11A	108.9	C26—C27—H27	119.7
C10—C11—H11B	108.9	C28—C27—H27	119.7
P1—C11—H11B	108.9	C27—C28—C29	119.9 (2)
H11A—C11—H11B	107.7	C27—C28—H28	120.0
C13—C12—C17	119.88 (19)	C29—C28—H28	120.0
C13—C12—H12	120.1	C28—C29—C24	119.01 (19)
C17—C12—H12	120.1	C28—C29—P1	121.88 (16)
C12—C13—C14	120.4 (2)	C24—C29—P1	118.96 (15)

Symmetry codes: (i) $-x+1, -y+1, -z$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···N1^{ii}	0.93	2.61	3.495 (3)	160
C13—H13···Cg^{iii}	0.93	Missing	3.705 (2)	Missing

Symmetry codes: (ii) −*x*+2, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*, −*z*+1.

Fig. 1

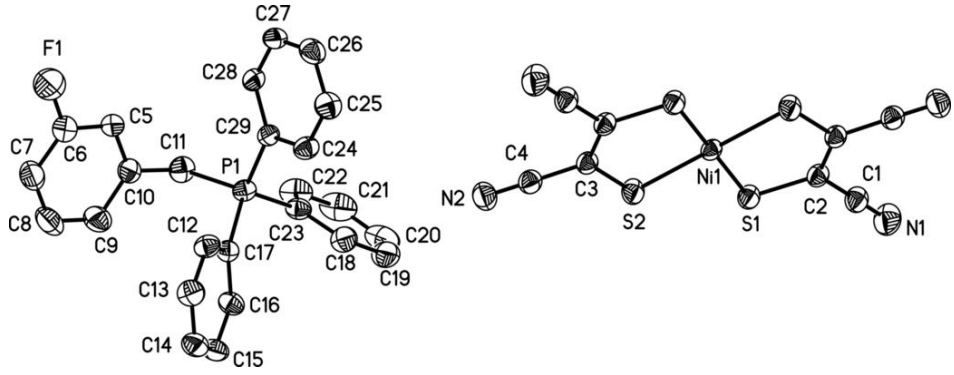
C27
C26
F1
C28
C25
C5
C29
C7
C6
C24
C11
P1
C22
C21
C10
N2
C4
C3
Ni1
C1
C8
C12
C23
C20
C9
C17
C18
C19
S2
S1
C2
N1
C13
C16
C14
C15

Fig. 2