metal-organic compounds

Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

Bis[1-(3-cyanobenzyl)triphenylphosphonium] bis(1,2-dicyanoethene-1,2dithiolato- $\kappa^2 S, S'$)nickelate(II)

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Received 28 October 2007; accepted 30 October 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ (C–C) = 0.006 Å; R factor = 0.061; wR factor = 0.139; data-to-parameter ratio = 14.2.

The title complex, $(C_{26}H_{21}NP)_2[Ni(C_4N_2S_2)_2]$, is a salt of the mCNBzTPP⁺cation and the [Ni(mnt)₂]²⁻ anion [mCNBzTPP⁺ is the 1-(3-cyanobenzyltriphenylphosphonium) cation and mnt²⁻ is the maleonitriledithiolate anion] and was prepared by the direct reaction of NiCl₂, Na₂mnt and $(mCNBzTPP)^+ \cdot Br^-$ in ethanol. The asymmetric unit consists of two unique mCNBzTPP⁺cations and half each of two [Ni(mnt)₂]²⁻ anions with each Ni atom lying on an inversion centre. The Ni^{II} ions adopt a square-planar coordination geometry, binding to the S atoms of two mnt²⁻ ligands. Both [mCNBzTPP]⁺ cations adopt conformations in which their four aromatic rings are twisted with respect to the planes that include the P atoms and the two C atoms linking them to the 3cvanobenzyl rings. Three weak $C-H \cdots N$ hydrogen bonds play an important role in stabilizing the crystal structure.

Related literature

For details of other square-planar $M(\text{dithiolene})_2$ complexes, see: Robertson & Cronin (2002); Ni *et al.* (2004); Nishijo *et al.* (2003); Canadell (1999). For the structures of related Ni(mnt)₂²⁻ complexes with square-planar geometry and a substituted triphenylphosphonium counter-ion, see: Ni *et al.* (2005); Yang & Ni (2006); Liu & Ni, 2006; Zhou *et al.* (2007).



Experimental

Crystal data	
$(C_{26}H_{21}NP)_2[Ni(C_4N_2S_2)_2]$	a = 19.158 (4) A
$M_r = 1095.89$ Monoclinic. $P2_1/n$	b = 14.956 (3) A c = 19.598 (4) A
, 1,	

$\beta = 108.785 \ (4)^{\circ}$
$V = 5316.3 (19) \text{ Å}^3$
Z = 4
Mo $K\alpha$ radiation

Data collection

Bruker SMART APEX CCD
diffractometer
Absorption correction: multi-scan
(SADABS; Sheldrick, 2004)
$T_{\min} = 0.834, \ T_{\max} = 0.912$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.061$ 661 parameters $wR(F^2) = 0.139$ H-atom parameters constrainedS = 1.09 $\Delta \rho_{max} = 0.83$ e Å $^{-3}$ 9356 reflections $\Delta \rho_{min} = -0.74$ e Å $^{-3}$

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

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
C10 $-$ H10 \cdots N4 ⁱ C33 $-$ H33 \cdots N2 ⁱⁱ C36 $-$ H36 \cdots N2 ⁱ	0.93 0.93 0.93	2.57 2.62 2.47	3.479 (7) 3.452 (6) 3.250 (6)	165 149 141
		. 1 . 1	1	

 $\mu = 0.63 \text{ mm}^{-1}$ T = 298 (2) K

 $R_{\rm int} = 0.076$

 $0.34 \times 0.22 \times 0.15 \text{ mm}$

25624 measured reflections

9356 independent reflections 6235 reflections with $I > 2\sigma(I)$

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

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*.

The authors thank the Science and Technology Project (No. 2007B011000008) of Guangdong Science and Technology Department and the President's Science Foundation of South China Agricultural University (No. 2005K092) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2398).

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.
- Canadell, E. (1999). Coord. Chem. Rev. 185-186, 629-651.
- Liu, M.-G. & Ni, C.-L. (2006). Acta Cryst. E62, 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.
- Nishijo, J., Ogura, E., Yamaura, J., Miyazaki, A., Enoki, T., Takano, T., Kuwatani, Y. & Iyoda, M. (2003). Synth. Met. 133-134, 539-542.
- 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. E62, m483-m485.

Zhou, J.-R., Ni, C.-L. & Yu, L.-L. (2007). Acta Cryst. E63, m1427-m1429.

Acta Cryst. (2007). E63, m2904 [doi:10.1107/S160053680705430X]

Bis[1-(3-cyanobenzyl)triphenylphosphonium] $\kappa^2 S, S'$)nickelate(II)

bis(1,2-dicyanoethene-1,2-dithiolato-

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Comment

Much effort has been devoted to the study of square planar M(dithiolene)₂ complexes (Robertson & Cronin, 2002; Ni *et al.*, 2004; Nishijo *et al.*, 2003; Canadell, 1999). Recently, we have carried out a systematic investigation on the coordination chemistry of salts containing Ni(mnt)₂ anion and substituted benzyltriphenylphosphonium cations and obtained some Ni(mnt)₂^{2⁻}-based molecular solids (Ni *et al.*, 2005; Yang & Ni, 2006; Liu & Ni, 2006; Zhou *et al.*, 2007). In this paper, we report the structure of the title compound, Fig. 1. There are two halves of non-equivalent Ni(mnt)₂^{2⁻} anions and two (mCNBzTPP)⁺ cations in the asymmetric unit. For the two Ni(mnt)₂^{2⁻} anions. The Ni1 and Ni2 atoms are each coordinated to four sulfur atoms and exhibit square planar coordination geometry with the Ni atoms lying on inversion centres. The N atoms of the four unique CN groups deviate from the C1/C2/Ni1/S1/S2 or C5/C6/Ni2/S3/S4 planes by 0.029 (3) Å for N1, -0.077 (3) Å for N2, -0.216 (2) Å for N3 and -0.242 (2) Å for N4 respectively.

The two (mCNBzTPP)⁺ cations adopt a conformation where four phenyl rings are twisted with respect to the plane including the P atom and the two C atoms linking it to the 3-cyanobenzyl ring. For the cation containing P1, the dihedral angles are 88.7 (3) for the C9/C10/C11/C12/C13/C14 ring, 84.0 (2) ° for the C17/C18/C19/C20/C21/C22 ring, 24.4 (2) ° for the C23/C24/C25/C26/C27/C28 ring, and 87.7 (2) ° for the C29/C30/C31/C32/C33/C34 ring. For the cation containing P2, the dihedral angles are 90.6 (3) for the C35/C36/C37/C38/C39/C40 ring, 93.2 (2) ° for the C43/C44/C45/C46/C47/C48 ring, 23.0 (2) ° for the C49/C50/C51/C52/C53/C54 ring, and 82.1 (2) ° for the C55/C56/C57/C58/C59/C60 ring. The deviations of the N5 and N6 atoms from the C9/C10/C11/C12/C13/C14 and C35/C36/C37/C38/C39/C40 phenyl ring planes are -0.052 (2)Å and 0.130 (2) Å respectively.

The crystal structure is stabilized by C10—H10···N4, C33—H33···N2 and C36—H36···N hydrogen bonds, Fig 2, Table 1.

Experimental

The title compound was prepared by the direct reaction of NiCl₂·6H₂O, Na₂mnt and (mCNBzTPP)⁺Br⁻ in methanol. Red block-shaped single crystals were obtained by slow evaporation of a CH₃CN 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 CH₂ atoms.

Figures





Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms. Labelled atoms are related to unlabelled atoms by the symmetry operations -x + 1, -y, -z + 2 and -x + 2, -y, -z + 2.

Fig. 2. Crystal packing of (I) showing the C—H…N hydrogen bonds between the anions and cations drawn as dashed lines.

Bis[1-(3-cyanobenzyl)triphenylphosphonium] bis(1,2-dicyanoethene-1,2- dithiolato- $\kappa^2 S$,S')nickelate(II)

Crystal data

$(C_{26}H_{21}NP)_2[Ni(C_4N_2S_2)_2]$	$F_{000} = 2264$
$M_r = 1095.89$	$D_{\rm x} = 1.369 {\rm Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 957 reflections
a = 19.158 (4) Å	$\theta = 2.6 - 22.9^{\circ}$
<i>b</i> = 14.956 (3) Å	$\mu = 0.63 \text{ mm}^{-1}$
c = 19.598 (4) Å	T = 298 (2) K
$\beta = 108.785 \ (4)^{\circ}$	Block, red
$V = 5316.3 (19) \text{ Å}^3$	$0.34 \times 0.22 \times 0.15 \text{ mm}$
Z = 4	

Data collection

Bruker Smart Apex CCD diffractometer	9356 independent reflections
Radiation source: fine-focus sealed tube	6235 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.076$
T = 298(2) K	$\theta_{\rm max} = 25.0^{\circ}$
ϕ and ω scans	$\theta_{\min} = 2.2^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -22 \rightarrow 22$
$T_{\min} = 0.834, T_{\max} = 0.912$	$k = -17 \rightarrow 8$
25624 measured reflections	<i>l</i> = −23→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.061$	H-atom parameters constrained
$wR(F^2) = 0.139$	$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
<i>S</i> = 1.09	$(\Delta/\sigma)_{\rm max} = 0.015$
9356 reflections	$\Delta \rho_{max} = 0.83 \text{ e} \text{ Å}^{-3}$
661 parameters	$\Delta \rho_{min} = -0.73 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct	

Primary atom site location: structure-invariant direct methods Extinction correction: none

	x	У	Ζ	$U_{\rm iso}$ */ $U_{\rm eq}$
Ni1	0.5000	0.0000	1.0000	0.05280 (19)
Ni2	1.0000	0.0000	1.0000	0.05428 (19)
C1	0.42984 (18)	0.1858 (2)	0.98368 (18)	0.0558 (9)
C2	0.45351 (18)	0.1800 (2)	0.92638 (19)	0.0589 (9)
C3	0.4419 (2)	0.2543 (3)	0.8777 (2)	0.0668 (10)
C4	0.3917 (2)	0.2625 (3)	0.9953 (2)	0.0682 (11)
C5	0.9070 (2)	0.1704 (2)	0.97231 (18)	0.0587 (9)
C6	0.96210 (19)	0.1926 (2)	0.94730 (18)	0.0568 (9)
C7	0.9619 (2)	0.2757 (3)	0.9121 (2)	0.0655 (10)
C8	0.8462 (2)	0.2295 (3)	0.9644 (2)	0.0664 (10)
C9	0.6312 (2)	0.2789 (3)	0.07367 (19)	0.0657 (10)
C10	0.6713 (3)	0.3359 (4)	0.0437 (2)	0.0982 (16)
H10	0.7084	0.3127	0.0279	0.118*
C11	0.6563 (3)	0.4260 (4)	0.0376 (3)	0.122 (2)
H11	0.6835	0.4630	0.0174	0.146*
C12	0.6027 (3)	0.4618 (3)	0.0604 (3)	0.1008 (16)
H12	0.5934	0.5229	0.0566	0.121*
C13	0.5623 (3)	0.4066 (3)	0.0892 (2)	0.0733 (11)
C14	0.5765 (2)	0.3156 (3)	0.09584 (18)	0.0617 (10)
H14	0.5486	0.2790	0.1155	0.074*
C15	0.6486 (2)	0.1806 (3)	0.08122 (17)	0.0658 (10)
H15A	0.6652	0.1617	0.0416	0.079*
H15B	0.6040	0.1477	0.0778	0.079*
C16	0.5037 (3)	0.4444 (3)	0.1115 (2)	0.0886 (14)
C17	0.78815 (18)	0.2373 (2)	0.18514 (17)	0.0524 (9)
C18	0.8438 (2)	0.2316 (3)	0.1540 (2)	0.0670 (10)
H18	0.8475	0.1814	0.1274	0.080*
C19	0.8927 (2)	0.2998 (3)	0.1626 (2)	0.0858 (13)
H19	0.9298	0.2958	0.1417	0.103*
C20	0.8882 (3)	0.3739 (3)	0.2014 (3)	0.0920 (14)

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

H20	0.9223	0.4199	0.2070	0.110*
C21	0.8336 (3)	0.3806 (3)	0.2323 (2)	0.0834 (13)
H21	0.8307	0.4311	0.2590	0.100*
C22	0.7827 (2)	0.3126 (3)	0.22363 (19)	0.0653 (10)
H22	0.7450	0.3176	0.2437	0.078*
C23	0.76030 (19)	0.0478 (2)	0.15672 (18)	0.0527 (9)
C24	0.7239 (2)	-0.0135 (3)	0.1050 (2)	0.0703 (11)
H24	0.6769	-0.0011	0.0738	0.084*
C25	0.7578 (3)	-0.0931 (3)	0.1001 (2)	0.0819 (13)
H25	0.7337	-0.1341	0.0647	0.098*
C26	0.8260 (3)	-0.1129 (3)	0.1461 (3)	0.0789 (12)
H26	0.8481	-0.1672	0.1422	0.095*
C27	0.8621 (2)	-0.0529 (3)	0.1983 (2)	0.0777 (12)
H27	0.9088	-0.0663	0.2298	0.093*
C28	0.8297 (2)	0.0267 (3)	0.2043 (2)	0.0661 (10)
H28	0.8540	0.0670	0.2403	0.079*
C29	0.68050 (19)	0.1447 (2)	0.23794 (18)	0.0498 (8)
C30	0.60572 (19)	0.1288 (2)	0.2250 (2)	0.0593 (9)
H30	0.5734	0.1263	0.1781	0.071*
C31	0.5804 (2)	0.1170 (3)	0.2823 (2)	0.0721 (11)
H31	0.5302	0.1083	0.2736	0.087*
C32	0.6266 (3)	0.1177 (3)	0.3513 (2)	0.0750 (12)
H32	0.6084	0.1089	0.3894	0.090*
C33	0.7008 (2)	0.1317 (3)	0.3643 (2)	0.0729 (11)
H33	0.7330	0.1313	0.4114	0.088*
C34	0.7278 (2)	0.1462 (2)	0.30799 (19)	0.0638 (10)
H34	0 7778	0 1570	0 3172	0.077*
C35	0.1902 (2)	0.3078 (3)	0.07543 (17)	0.0595 (9)
C36	0.2387 (2)	0.3790 (3)	0.0796 (2)	0.0723 (11)
H36	0.2871	0.3675	0.0818	0.087*
C37	0 2153 (3)	0 4658 (3)	0 0803 (2)	0.0841 (13)
H37	0.2482	0.5123	0.0829	0.101*
C38	0.1447(3)	0.4850 (3)	0.0772 (2)	0.0800 (13)
H38	0 1294	0 5439	0 0779	0.096*
C39	0.0969(2)	0.4154 (3)	0.0731(2)	0.0683 (11)
C40	0.0303(2)	0.3278 (3)	0.0731(2)	0.0623 (10)
H40	0.0851	0.2818	0.0680	0.0025 (10)
C41	0.0051 0.2163(2)	0.2010 0.2123(2)	0.07693 (17)	0.0617 (10)
H41A	0.2541	0.2090	0.0539	0.074*
H41B	0.1754	0.1749	0.0498	0.074*
C42	0.1731	0.4321(3)	0.0721(2)	0.0849(13)
C43	0.0227(5) 0.32015(19)	0.4521(5) 0.2503(2)	0.0721(2) 0.21637(18)	0.0049(13)
C44	0.32013(1))	0.2303(2) 0.2469(3)	0.21057(10) 0.20863(19)	0.0550(9)
H44	0.4022	0.1993	0.1845	0.0042 (10)
C45	0.4392(2)	0.1775	0.2365 (2)	0.077 0.0781 (12)
H45	0.4858	0.3114	0.2315	0.094*
C46	0.4205 (3)	0.3839 (3)	0.2313 0.2717(2)	0.024
H46	0.4545	0.4291	0.2905	0.0021(13)
C47	0.3521 (3)	0.7291	0.2798 (2)	0.0799 (12)
U r/	0.5521 (5)	0.000 (0)	0.2770 (2)	0.0777 (14)

H47	0.3399	0.4361	0.3042	0.096*
C48	0.3014 (2)	0.3214 (3)	0.25145 (19)	0.0669 (10)
H48	0.2546	0.3244	0.2561	0.080*
C49	0.2971 (2)	0.0648 (2)	0.1677 (2)	0.0581 (9)
C50	0.2752 (2)	0.0107 (3)	0.1084 (2)	0.0779 (12)
H50	0.2386	0.0297	0.0669	0.094*
C51	0.3071 (3)	-0.0713 (3)	0.1102 (3)	0.0985 (16)
H51	0.2919	-0.1078	0.0697	0.118*
C52	0.3601 (3)	-0.1002 (3)	0.1694 (4)	0.0963 (16)
H52	0.3815	-0.1561	0.1697	0.116*
C53	0.3825 (3)	-0.0470 (3)	0.2295 (3)	0.0910 (14)
H53	0.4193	-0.0667	0.2705	0.109*
C54	0.3509 (2)	0.0355 (3)	0.2293 (2)	0.0768 (11)
H54	0.3656	0.0713	0.2702	0.092*
C55	0.18144 (19)	0.1573 (2)	0.20786 (18)	0.0534 (9)
C56	0.1109 (2)	0.1369 (2)	0.1647 (2)	0.0597 (9)
H56	0.1003	0.1313	0.1151	0.072*
C57	0.0561 (2)	0.1250 (3)	0.1953 (2)	0.0723 (11)
H57	0.0084	0.1118	0.1662	0.087*
C58	0.0715 (3)	0.1324 (3)	0.2675 (3)	0.0786 (12)
H58	0.0338	0.1257	0.2875	0.094*
C59	0.1418 (3)	0.1498 (3)	0.3114 (2)	0.0778 (12)
H59	0.1521	0.1529	0.3611	0.093*
C60	0.1974 (2)	0.1626 (2)	0.2818 (2)	0.0658 (10)
H60	0.2451	0.1747	0.3113	0.079*
N1	0.4317 (2)	0.3151 (3)	0.84045 (19)	0.0875 (11)
N2	0.3606 (2)	0.3238 (3)	1.0040 (2)	0.1000 (13)
N3	0.9608 (2)	0.3414 (2)	0.8829 (2)	0.0867 (11)
N4	0.7969 (2)	0.2761 (3)	0.9571 (2)	0.0936 (12)
N5	0.4584 (3)	0.4751 (3)	0.1290 (3)	0.1336 (19)
N6	-0.0351 (2)	0.4436 (3)	0.0736 (2)	0.1084 (14)
P1	0.71916 (5)	0.15259 (6)	0.16601 (5)	0.0517 (2)
P2	0.25325 (5)	0.17021 (6)	0.16846 (5)	0.0535 (3)
S1	0.44310 (5)	0.09780 (7)	1.04475 (5)	0.0612 (3)
S2	0.49732 (6)	0.08587 (7)	0.91018 (5)	0.0721 (3)
S3	0.90439 (5)	0.06748 (7)	1.01219 (6)	0.0694 (3)
S4	1.03274 (5)	0.11747 (7)	0.95286 (5)	0.0627 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nil	0.0455 (4)	0.0584 (4)	0.0527 (4)	0.0018 (3)	0.0133 (3)	0.0064 (3)
Ni2	0.0468 (4)	0.0560 (4)	0.0551 (4)	0.0025 (3)	0.0096 (3)	0.0013 (3)
C1	0.0410 (19)	0.061 (2)	0.063 (2)	0.0029 (18)	0.0134 (17)	0.0062 (19)
C2	0.051 (2)	0.062 (2)	0.063 (2)	0.0034 (19)	0.0166 (18)	0.009 (2)
C3	0.063 (3)	0.069 (3)	0.073 (3)	0.007 (2)	0.028 (2)	0.007 (2)
C4	0.066 (3)	0.069 (3)	0.073 (3)	0.004 (2)	0.027 (2)	0.003 (2)
C5	0.055 (2)	0.057 (2)	0.056 (2)	0.012 (2)	0.0077 (18)	0.0009 (18)

C6	0.054 (2)	0.058 (2)	0.056 (2)	0.0011 (19)	0.0143 (18)	0.0000 (19)
C7	0.070 (3)	0.065 (3)	0.063 (2)	0.006 (2)	0.025 (2)	0.001 (2)
C8	0.070 (3)	0.066 (3)	0.061 (2)	0.004 (2)	0.018 (2)	0.002 (2)
C9	0.059 (2)	0.078 (3)	0.054 (2)	0.012 (2)	0.0104 (19)	0.010(2)
C10	0.085 (3)	0.122 (5)	0.097 (3)	0.024 (3)	0.043 (3)	0.045 (3)
C11	0.123 (5)	0.116 (5)	0.142 (5)	0.015 (4)	0.064 (4)	0.070 (4)
C12	0.127 (5)	0.075 (3)	0.102 (4)	0.008 (3)	0.039 (3)	0.035 (3)
C13	0.096 (3)	0.061 (3)	0.058 (2)	0.007 (3)	0.019 (2)	0.012 (2)
C14	0.069 (3)	0.058 (3)	0.057 (2)	0.001 (2)	0.0195 (19)	0.0055 (19)
C15	0.058 (2)	0.080 (3)	0.058 (2)	0.005 (2)	0.0168 (19)	-0.009 (2)
C16	0.134 (5)	0.057 (3)	0.080 (3)	0.015 (3)	0.042 (3)	0.007 (2)
C17	0.050 (2)	0.053 (2)	0.055 (2)	0.0036 (17)	0.0169 (17)	0.0043 (18)
C18	0.079 (3)	0.056 (2)	0.076 (3)	-0.004 (2)	0.039 (2)	0.000 (2)
C19	0.092 (3)	0.068 (3)	0.121 (4)	-0.011 (3)	0.066 (3)	-0.001 (3)
C20	0.097 (4)	0.062 (3)	0.131 (4)	-0.026 (3)	0.056 (3)	-0.008 (3)
C21	0.102 (4)	0.048 (3)	0.108 (3)	-0.011 (3)	0.046 (3)	-0.016 (2)
C22	0.072 (3)	0.057 (2)	0.074 (2)	0.005 (2)	0.035 (2)	-0.004 (2)
C23	0.054 (2)	0.046 (2)	0.059 (2)	-0.0021 (18)	0.0206 (19)	-0.0077 (18)
C24	0.058 (2)	0.072 (3)	0.080 (3)	-0.002 (2)	0.021 (2)	-0.024 (2)
C25	0.087 (3)	0.068 (3)	0.099 (3)	-0.012 (3)	0.042 (3)	-0.031 (3)
C26	0.089 (3)	0.049 (3)	0.118 (4)	0.006 (2)	0.059 (3)	-0.006 (3)
C27	0.072 (3)	0.059 (3)	0.100 (3)	0.016 (2)	0.025 (2)	-0.003 (2)
C28	0.066 (3)	0.055 (2)	0.073 (2)	0.000 (2)	0.015 (2)	-0.008 (2)
C29	0.051 (2)	0.040 (2)	0.060 (2)	0.0013 (16)	0.0196 (18)	-0.0042 (17)
C30	0.047 (2)	0.056 (2)	0.071 (2)	0.0061 (18)	0.0144 (19)	0.0035 (19)
C31	0.058 (2)	0.065 (3)	0.106 (3)	0.006 (2)	0.043 (3)	0.011 (3)
C32	0.086 (3)	0.071 (3)	0.085 (3)	-0.001 (2)	0.051 (3)	0.003 (2)
C33	0.076 (3)	0.075 (3)	0.068 (2)	-0.002 (2)	0.024 (2)	-0.002 (2)
C34	0.060 (2)	0.069 (3)	0.064 (2)	-0.006 (2)	0.024 (2)	-0.005 (2)
C35	0.064 (2)	0.065 (3)	0.050 (2)	0.003 (2)	0.0187 (18)	0.0066 (19)
C36	0.070 (3)	0.078 (3)	0.081 (3)	-0.004 (2)	0.040 (2)	0.006 (2)
C37	0.099 (4)	0.065 (3)	0.098 (3)	-0.012 (3)	0.046 (3)	0.010 (3)
C38	0.093 (3)	0.061 (3)	0.098 (3)	0.006 (3)	0.048 (3)	0.019 (2)
C39	0.075 (3)	0.063 (3)	0.075 (3)	0.012 (2)	0.034 (2)	0.015 (2)
C40	0.059 (2)	0.067 (3)	0.060 (2)	-0.004 (2)	0.0176 (19)	0.007 (2)
C41	0.056 (2)	0.072 (3)	0.058 (2)	-0.001 (2)	0.0185 (18)	-0.0052 (19)
C42	0.095 (4)	0.068 (3)	0.101 (3)	0.019 (3)	0.045 (3)	0.031 (2)
C43	0.055 (2)	0.051 (2)	0.056 (2)	-0.0016 (18)	0.0136 (18)	-0.0009 (18)
C44	0.062 (2)	0.056 (2)	0.077 (3)	-0.005 (2)	0.026 (2)	-0.001 (2)
C45	0.065 (3)	0.064 (3)	0.106 (3)	-0.013 (2)	0.028 (2)	0.002 (3)
C46	0.083 (3)	0.063 (3)	0.090 (3)	-0.022 (3)	0.013 (3)	0.005 (2)
C47	0.108 (4)	0.052 (3)	0.075 (3)	-0.005 (3)	0.021 (3)	-0.009 (2)
C48	0.077 (3)	0.056 (2)	0.070 (2)	0.001 (2)	0.027 (2)	-0.007 (2)
C49	0.057 (2)	0.049 (2)	0.073 (2)	-0.0080 (19)	0.029 (2)	-0.010 (2)
C50	0.076 (3)	0.070 (3)	0.091 (3)	-0.002 (2)	0.031 (2)	-0.025 (2)
C51	0.112 (4)	0.070 (3)	0.132 (5)	-0.007 (3)	0.067 (4)	-0.032 (3)
C52	0.112 (4)	0.050 (3)	0.159 (5)	0.006 (3)	0.088 (4)	-0.001 (3)
C53	0.085 (3)	0.068 (3)	0.125 (4)	0.017 (3)	0.040 (3)	0.012 (3)
C54	0.083 (3)	0.059 (3)	0.089 (3)	0.006 (2)	0.028 (3)	-0.003 (2)

C55	0.053 (2)	0.047 (2)	0.061 (2)	0.0034 (18)	0.0197 (19)	-0.0019 (18)
C56	0.061 (2)	0.052 (2)	0.065 (2)	0.0040 (19)	0.017 (2)	0.0067 (19)
C57	0.062 (3)	0.065 (3)	0.093 (3)	0.002 (2)	0.031 (2)	0.010 (2)
C58	0.078 (3)	0.059 (3)	0.118 (4)	0.006 (2)	0.060 (3)	0.012 (3)
C59	0.104 (4)	0.069 (3)	0.075 (3)	0.006 (3)	0.050 (3)	0.004 (2)
C60	0.074 (3)	0.060 (3)	0.065 (2)	0.000 (2)	0.024 (2)	-0.001 (2)
N1	0.095 (3)	0.079 (3)	0.090 (3)	0.008 (2)	0.032 (2)	0.023 (2)
N2	0.107 (3)	0.089 (3)	0.117 (3)	0.029 (3)	0.056 (3)	0.002 (2)
N3	0.104 (3)	0.066 (2)	0.099 (3)	0.012 (2)	0.045 (2)	0.013 (2)
N4	0.082 (3)	0.097 (3)	0.102 (3)	0.032 (2)	0.031 (2)	0.006 (2)
N5	0.211 (6)	0.083 (3)	0.142 (4)	0.051 (3)	0.106 (4)	0.015 (3)
N6	0.104 (3)	0.093 (3)	0.147 (4)	0.027 (3)	0.068 (3)	0.046 (3)
P1	0.0482 (5)	0.0511 (6)	0.0556 (5)	0.0023 (4)	0.0166 (4)	-0.0061 (5)
P2	0.0509 (6)	0.0529 (6)	0.0574 (5)	-0.0007 (5)	0.0182 (4)	-0.0080 (5)
S1	0.0583 (6)	0.0668 (6)	0.0607 (6)	0.0045 (5)	0.0221 (5)	0.0076 (5)
S2	0.0835 (7)	0.0727 (7)	0.0708 (6)	0.0205 (6)	0.0397 (6)	0.0171 (5)
S3	0.0596 (6)	0.0699 (7)	0.0816 (7)	0.0097 (5)	0.0268 (5)	0.0137 (6)
S4	0.0561 (6)	0.0621 (6)	0.0705 (6)	0.0069 (5)	0.0215 (5)	0.0061 (5)

Geometric parameters (Å, °)

Ni1—S2 ⁱ	2.1661 (10)	C29—C30	1.392 (4)
Ni1—S2	2.1661 (10)	C29—P1	1.795 (3)
Ni1—S1	2.1709 (10)	C30—C31	1.370 (5)
Ni1—S1 ⁱ	2.1709 (10)	С30—Н30	0.9300
Ni2—S4 ⁱⁱ	2.1695 (10)	C31—C32	1.357 (5)
Ni2—S4	2.1695 (10)	С31—Н31	0.9300
Ni2—S3	2.1709 (10)	C32—C33	1.377 (5)
Ni2—S3 ⁱⁱ	2.1709 (10)	С32—Н32	0.9300
C1—C2	1.342 (4)	C33—C34	1.378 (5)
C1—C4	1.416 (5)	С33—Н33	0.9300
C1—S1	1.742 (4)	C34—H34	0.9300
C2—C3	1.434 (5)	C35—C40	1.379 (5)
C2—S2	1.720 (4)	C35—C36	1.398 (5)
C3—N1	1.143 (5)	C35—C41	1.510 (5)
C4—N2	1.137 (5)	C36—C37	1.375 (5)
C5—C6	1.341 (5)	С36—Н36	0.9300
C5—C8	1.430 (5)	C37—C38	1.365 (6)
C5—S3	1.735 (4)	С37—Н37	0.9300
C6—C7	1.421 (5)	C38—C39	1.371 (5)
C6—S4	1.735 (4)	С38—Н38	0.9300
C7—N3	1.135 (4)	C39—C40	1.379 (5)
C8—N4	1.145 (5)	C39—C42	1.437 (6)
C9—C14	1.372 (5)	C40—H40	0.9300
C9—C10	1.397 (6)	C41—P2	1.816 (3)
C9—C15	1.505 (5)	C41—H41A	0.9700
C10—C11	1.375 (7)	C41—H41B	0.9700
С10—Н10	0.9300	C42—N6	1.130 (5)

C11-III10.9300C43-C441.386 (5)C12-U120.9300C44-C451.367 (5)C13-C141.387 (5)C44-U451.365 (5)C13-C161.445 (6)C45-C461.365 (5)C14-H140.9300C45-H450.9300C15-P11.821 (3)C46-C471.371 (6)C15-H15A0.9700C46-H460.9300C15-H15A0.9700C46-H460.9300C17-C121.378 (5)C48-H480.9300C17-C121.378 (5)C48-H480.9300C17-C131.392 (5)C49-C501.366 (5)C18-C191.357 (5)C49-C501.366 (5)C18-C191.357 (5)C49-C511.381 (5)C18-C191.357 (5)C49-C521.383 (5)C18-C191.357 (5)C49-C521.346 (7)C19-C201.363 (6)C50-C511.347 (6)C20-C211.371 (5)C51-C521.344 (7)C20-C211.371 (5)C51-L510.9300C21-C220.9300C52-C561.378 (6)C22-C241.377 (5)C54-H540.9300C23-C281.352 (5)C55-C661.378 (5)C23-C241.375 (5)C55-C181.371 (5)C23-C241.370 (6)C55-C561.378 (5)C24-C251.375 (5)C55-U21.390 (6)C23-C241.370 (6)C55-C561.378 (5)C24-C251.351 (6)C55-U21.390 (6)C25-C251.361 (6)C55-U21.390 (6) <th>C11—C12</th> <th>1.357 (7)</th> <th>C43—C48</th> <th>1.376 (5)</th>	C11—C12	1.357 (7)	C43—C48	1.376 (5)
C12—C131370 (6)C43—P21.784 (4)C12—H120.9300C44—C451.367 (5)C13—C141.387 (5)C44—H440.9300C13—C161.445 (6)C45—C461.365 (5)C14—H140.9300C45—H450.9300C15—P11.821 (3)C46—C471.371 (6)C15—H15A0.9700C46—H460.9300C15—H15B0.9700C47—C481.381 (5)C16—N51.128 (6)C47—I1470.9300C17—C121.378 (5)C49—C501.366 (5)C17—C181.392 (5)C49—C541.383 (5)C18—C191.357 (5)C49—C541.383 (5)C19—C201.363 (6)C50—C511.367 (6)C19—C201.363 (6)C50—H1500.9300C19—L190.9300C51—C521.370 (6)C20—C211.381 (5)C52—C531.370 (6)C21—U210.9300C53—C541.374 (6)C21—U210.9300C53—C541.374 (6)C21—U210.9300C55—C561.378 (5)C23—C241.377 (5)C55—C561.378 (5)C24—C251.357 (5)C55—C561.378 (5)C24—C241.361 (6)C56—C571.377 (5)C25—C261.361 (6)C56—C571.377 (5)C25—C261.361 (6)C56—C571.378 (5)C25—C261.361 (6)C56—C571.378 (5)C25—C261.360 (7)C57—C581.356 (5)C26—C271.370 (6)C57—L1331.98<	C11—H11	0.9300	C43—C44	1.386 (5)
C12-H120.9300C44-C451.367 (5)C13-C141.387 (5)C44-H440.9300C13-C161.445 (6)C45-C461.355 (5)C14-H140.9300C45-H450.9300C15-P11.821 (3)C46-C471.317 (6)C15-H15A0.9700C47-C481.381 (5)C16-N51.128 (6)C47-H470.9300C17-C121.378 (5)C49-C501.366 (5)C17-C181.392 (5)C49-C501.366 (5)C17-C181.392 (5)C49-C511.383 (5)C18-C191.57 (5)C49-C521.384 (4)C18-C191.357 (5)C49-C521.344 (7)C20-C211.363 (6)C50-C511.367 (6)C19-H190.9300C51-C521.344 (7)C20-C211.371 (5)C51-H510.9300C21-H210.9300C52-C531.370 (6)C21-H220.9300C53-C541.374 (6)C23-C241.377 (5)C54-H540.9300C3-H250.9300C55-C601.383 (5)C3-C241.370 (6)C57-H570.9300C3-H250.9300C57-C581.355 (5)C24-C251.356 (5)C58-H580.9300C3-H260.9300C59-C601.381 (5)C3-C271.370 (6)C57-H570.9300C3-H270.9300C59-C581.355 (5)C4-H260.9300C59-C581.355 (5)C24-C271.380 (4)C60-H600.9300C3-H280.93	C12—C13	1.370 (6)	C43—P2	1.784 (4)
C13-C141.387 (5)C44-H440.9300C13-C161.445 (6)C45-H450.9300C15-H11.821 (3)C45-H450.9300C15-H11.821 (3)C46-C471.371 (6)C15-H15B0.9700C47-C481.381 (5)C16-M5S1.128 (6)C47-H470.9300C17-C121.378 (5)C48-H480.9300C17-C181.325 (5)C49-C501.366 (5)C17-P11.781 (3)C49-C541.383 (5)C18-C191.357 (5)C49-C511.367 (6)C19-C201.363 (6)C50-H500.9300C19-C211.371 (5)C51-H510.9300C20-C211.371 (5)C51-H510.9300C21-H210.9300C52-C531.370 (6)C21-H220.9300C52-H520.9300C21-H210.9300C53-C541.374 (6)C23-C241.375 (5)C55-C601.383 (5)C3-C241.375 (5)C55-C561.378 (5)C24-C251.375 (5)C55-C561.378 (5)C24-C251.361 (6)C56-H550.9300C3-C241.361 (6)C56-H550.9300C25-H250.9300C59-L571.378 (5)C25-C261.361 (6)C56-H560.9300C27-H271.370 (6)C59-H570.9300C26-H260.9300C59-H570.9300C27-H270.9300C59-H590.9300C27-H280.9300C59-H570.9300C26-H260.9300 <td>C12—H12</td> <td>0.9300</td> <td>C44—C45</td> <td>1.367 (5)</td>	C12—H12	0.9300	C44—C45	1.367 (5)
C13—C161.445 (6)C45—C461.365 (5)C14—H140.9300C45—H450.9300C15—H11.821 (3)C46—C471.371 (6)C15—H15A0.9700C46—H460.9300C15—H15A0.9700C47—C481.381 (5)C16—N51.128 (6)C47—H470.9300C17—C121.378 (5)C48—H480.9300C17—C181.392 (5)C49—C501.366 (5)C17—C191.781 (3)C49—C541.383 (5)C18—C191.357 (5)C49—P21.788 (4)C18—H180.9300C50—C511.367 (6)C19—C201.361 (6)C50—H500.9300C19—C211.371 (5)C51—H510.9300C20—H200.9300C52—C531.370 (6)C21—C221.381 (5)C52—H520.9300C21—C221.381 (5)C52—H520.9300C21—H210.9300C53—C541.374 (6)C23—C241.377 (5)C54—H540.9300C23—C281.325 (5)C55—C601.383 (5)C24—C251.351 (5)C55—C561.378 (5)C24—C251.351 (6)C56—H560.9300C25—H220.9300C57—C581.357 (5)C26—C271.370 (6)C57—H570.9300C25—H250.9300C59—C601.381 (5)C25—C261.356 (5)C58—H580.9300C25—H250.9300C59—H590.9300C25—H250.9300C59—H590.9300C25—H260.9300<	C13—C14	1.387 (5)	C44—H44	0.9300
C14—H140 9300C45—H450 9300C15—H15A0 9700C46—H460 9300C15—H15B0 9700C47—C481.381 (5)C16—K51.128 (6)C47—L480 9300C17—C221.378 (5)C48—H480 9300C17—C181.392 (5)C49—C501.366 (5)C18—C191.357 (5)C49—C511.337 (6)C18—C191.357 (5)C49—C511.367 (6)C19—C201.363 (6)C50—H500 9300C19—C121.331 (5)C51—H510 9300C20—C211.331 (5)C51—H510 9300C20—H200 9300C51—C521.344 (7)C20—C211.331 (5)C54—H340 9300C21—H210 9300C53—C541.374 (6)C22—H220 9300C53—C541.374 (6)C23—C241.377 (5)C54—H340 9300C23—C241.375 (5)C55—C601.383 (5)C24—H240 9300C55—C561.378 (5)C24—H240 9300C57—C581.377 (5)C24—H240 9300C57—C581.357 (5)C25—C261.361 (6)C56—H560 9300C25—H250 9300C57—C581.369 (6)C25—H260 9300C57—C581.369 (6)C25—H260 9300C57—H570 9300C25—H260 9300C57—C581.369 (6)C25—H260 9300C57—C581.369 (6)C25—H260 9300C58—H580 9300C25—H370 9300 <td< td=""><td>C13—C16</td><td>1.445 (6)</td><td>C45—C46</td><td>1.365 (5)</td></td<>	C13—C16	1.445 (6)	C45—C46	1.365 (5)
C15=P11 k21 (a)C46—C471 371 (b)C15=H15A0.9700C46—H460.9300C15=H15B0.9700C47—C481.381 (s)C16—N51.128 (c)C47—H470.9300C17—C221.378 (c)C48—H480.9300C17—C181.392 (c)C49—C501.366 (c)C17—C181.929 (c)C49—C541.383 (s)C18—C191.357 (c)C49—C511.376 (c)C18—C190.9300C50—C511.376 (c)C19—C201.363 (c)C50—H500.9300C19—C100.9300C51—C521.344 (7)C20—C211.371 (s)C51—H510.9300C20—H200.9300C53—C531.370 (c)C21—H210.9300C53—H530.9300C22—H220.9300C53—H530.9300C23—C241.377 (s)C54—H540.9300C23—C241.375 (s)C55—C601.378 (s)C24—C251.375 (s)C55—P21.378 (s)C24—C251.375 (s)C56—C571.377 (s)C25—C261.361 (6)C50—H560.9300C25—H250.9300C59—C591.369 (6)C27—C281.365 (s)C58—H580.9300C25—H211.380 (4)C60—H600.9300C25—H221.380 (4)C60—H600.9300C25—H230.9300C59—C591.381 (s)C25—C261.361 (6)C59—H590.9300C25—H250.9300C59—C591.381 (s)C25—H261.38	C14—H14	0.9300	C45—H45	0.9300
C15—H15A0.9700C46—H460.9300C15—H15B0.9700C47—C481.381 (5)C16—N51.128 (6)C47—H470.9300C17—C221.378 (5)C48—H480.9300C17—C181.392 (5)C49—C501.366 (5)C17—P11.781 (3)C49—C541.333 (5)C18—C191.357 (5)C49—P21.788 (4)C18—C191.357 (5)C49—P21.788 (4)C19—C201.363 (6)C50—L510.9300C19—H190.9300C51—C521.344 (7)C20—C211.331 (5)C51—H510.9300C21—L200.9300C53—C531.370 (6)C21—L210.9300C53—C541.374 (6)C22—L220.9300C53—H530.9300C23—C241.377 (5)C55—C601.383 (5)C23—C241.377 (5)C55—C601.383 (5)C24—L251.361 (6)C56—H560.9300C23—C241.361 (6)C56—H560.9300C24—H240.9300C56—C571.375 (5)C25—C261.361 (6)C56—H560.9300C25—L250.9300C59—C591.369 (6)C26—L271.370 (6)C57—H570.9300C26—L260.9300C59—C601.381 (5)C28—L280.9300C59—C601.381 (5)C26—L261.361 (6)C59—C601.381 (5)C26—L270.9300C59—C601.381 (5)C26—L261.360 (6)C59—C591.369 (6)C27—L28 <td< td=""><td>C15—P1</td><td>1.821 (3)</td><td>C46—C47</td><td>1.371 (6)</td></td<>	C15—P1	1.821 (3)	C46—C47	1.371 (6)
C15—H15B0.9700C47—C481.381 (5)C16—N51.128 (6)C47—H470.9300C17—C221.378 (5)C48—H480.9300C17—C181.392 (5)C49—C501.366 (5)C17—P11.781 (3)C49—C541.383 (5)C18—C191.357 (5)C49—P21.788 (4)C18—H180.9300C50—C511.367 (6)C19—C201.363 (6)C50—H500.9300C19—H190.9300C51—C521.344 (7)C20—C211.371 (5)C51—H510.9300C20—H200.9300C53—H520.9300C21—H210.9300C53—H530.9300C22—H220.9300C53—H540.9300C23—C241.377 (5)C54—H540.9300C23—C241.375 (5)C55—P21.378 (5)C24—C251.375 (5)C55—P21.792 (3)C24—H240.9300C55—C561.338 (5)C24—C251.361 (6)C56—H560.9300C25—C261.361 (6)C56—H571.377 (5)C25—C250.9300C57—C581.355 (5)C26—C271.370 (6)C57—H570.9300C27—H270.9300C59—H590.9300C27—H270.9300C59—H590.9300C27—H270.9300C59—H590.9300C27—H270.9300C59—H590.9300C27—H270.9300C59—H590.9300C27—H280.9300C59—H590.9300C27—H290.9300C59—H59<	C15—H15A	0.9700	C46—H46	0.9300
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C15—H15B	0.9700	C47—C48	1.381 (5)
C17—C121.37k (5)C48—H480.9300C17—C181.392 (5)C49—C501.366 (5)C17—P11.781 (3)C49—C541.383 (5)C18—C191.357 (5)C49—P21.788 (4)C18—C191.357 (5)C49—P21.788 (4)C19—C201.363 (6)C50—H500.9300C19—H190.9300C51—C521.344 (7)C20—C211.371 (5)C51—H510.9300C20—H200.9300C53—C531.370 (6)C21—H210.9300C53—C541.374 (6)C22—H220.9300C53—H530.9300C23—C241.377 (5)C54—H540.9300C23—C281.392 (5)C55—C601.383 (5)C23—P11.790 (3)C55—C561.378 (5)C24—C251.375 (5)C55—P21.777 (5)C25—C261.361 (6)C56—H560.9300C25—H250.9300C57—C581.355 (5)C25—C261.361 (6)C56—H560.9300C25—H250.9300C58—C591.369 (6)C27—C281.365 (5)C58—H580.9300C27—C281.365 (5)C58—H580.9300C27—H270.9300C59—H590.9300C27—H270.9300C59—H590.9300C27—H270.9300C59—H590.9300C27—H270.9300C59—H590.9300C27—H270.9300C59—H590.9300C29—H280.9300C59—H590.9300C29—H291.380 (4)C6	C16—N5	1.128 (6)	C47—H47	0.9300
C17—C181.392 (5)C49—C501.366 (5)C17—P11.781 (3)C49—C541.383 (5)C18—C191.357 (5)C49—P21.788 (4)C18—H180.9300C50—C511.367 (6)C19—C201.363 (6)C50—H500.9300C19—H190.9300C51—C521.344 (7)C20—C211.371 (5)C51—H510.9300C20—H200.9300C52—C531.370 (6)C21—C221.381 (5)C52—H520.9300C23—C241.377 (5)C54—H540.9300C23—C241.377 (5)C54—H540.9300C24—H210.9300C55—C601.383 (5)C24—C251.375 (5)C55—C601.378 (5)C24—C251.375 (5)C55—C601.378 (5)C24—C251.370 (6)C56—C571.377 (5)C24—H240.9300C56—C571.375 (5)C25—C261.361 (6)C56—H560.9300C25—H250.9300C57—C581.355 (5)C26—H250.9300C59—C601.381 (5)C26—H260.9300C59—C601.381 (5)C26—H260.9300C59—C601.381 (5)C29—C341.380 (4)C60—H600.9300C29—C341.380 (4)C60—H600.9300C29—N1—S19.2.59 (4)C32—C33—H33119.8S2 ¹ —N1—S18.7.41 (4)C29—C34—H34120.1S1—N1—S18.7.41 (4)C29—C34—H34120.1S1—N1—S18.7.69 (4)C40—C35—C44120.6 (4)	C17—C22	1.378 (5)	C48—H48	0.9300
$C17=P1$ 1.781 $C49=C54$ 1.383 (5) $C18=C19$ 1.357 (5) $C49=P2$ 1.788 (4) $C19=C20$ 1.363 (6) $C50-C51$ 1.367 (6) $C19=C20$ 1.363 (6) $C50-C51$ 1.376 (6) $C20=C11$ 1.371 (5) $C51-C52$ 1.344 (7) $C20=H20$ 9.9300 $C52-C53$ 1.370 (6) $C21-C22$ 1.381 (5) $C52-H52$ 0.9300 $C21-H21$ 0.9300 $C53-H53$ 0.9300 $C22-H22$ 0.9300 $C53-H53$ 0.9300 $C23-C24$ 1.377 (5) $C54-H54$ 0.9300 $C23-C28$ 1.392 (5) $C55-C60$ 1.383 (5) $C24-H24$ 0.9300 $C56-C57$ 1.378 (5) $C24-H24$ 0.9300 $C56-C57$ 1.377 (5) $C24-H24$ 0.9300 $C56-C57$ 1.377 (5) $C25-C26$ 1.361 (6) $C56-H56$ 0.9300 $C25-H25$ 0.9300 $C57-C58$ 1.355 (5) $C26-H26$ 0.9300 $C58-H58$ 0.9300 $C27-C28$ 1.365 (5) $C58-H58$ 0.9300 $C27-H27$ 0.9300 $C59-C60$ 1.381 (5) $C28-H28$ 0.9300 $C59-H59$ 0.9300 $C29-C34$ 1.380 (4) $C60-H50$ 0.9300 $C29-C34$ 1.380 (4) $C32-C33-C34$ 1204 (4) $S2^1-Ni1-S1$ 87.41 (4) $C29-C34-C33$ 119.8 $S2^1-Ni1-S1$ 87.41 (4) $C29-C34-C33$ 119.9 (4) $S2^1-Ni1-S1^1$ 87.69 (4) </td <td>C17—C18</td> <td>1.392 (5)</td> <td>C49—C50</td> <td>1.366 (5)</td>	C17—C18	1.392 (5)	C49—C50	1.366 (5)
C18—C191.357 (5)C49—221.788 (4)C18—C190.9300C50—C511.367 (6)C19—C201.363 (6)C50—H500.9300C19—C100.9300C51—C521.344 (7)C20—C211.371 (5)C51—H510.9300C20—H200.9300C52—C531.370 (6)C21—H210.9300C53—H530.9300C23—C241.377 (5)C54—H540.9300C23—C241.377 (5)C54—H540.9300C23—C241.377 (5)C55—C601.378 (5)C24—C251.375 (5)C55—C661.378 (5)C24—C251.375 (5)C55—C661.378 (5)C24—H240.9300C56—C571.377 (5)C24—H240.9300C56—C571.375 (5)C24—H240.9300C57—C581.355 (5)C25—C261.361 (6)C56—H560.9300C26—H250.9300C58—C591.369 (6)C27—C281.365 (5)C58—C591.361 (5)C28—H280.9300C59—C601.381 (5)C28—H280.9300C59—C601.381 (5)C28—H280.9300C59—C601.381 (5)C28—H291.380 (4)C60—H600.9300C28—H211.380 (4)C60—H600.9300C28—H221.380 (4)C32—C33—H33119.8S2—Ni1—S187.41 (4)C32—C33—H33119.8S2—Ni1—S187.41 (4)C32—C34—H34120.1S1—Ni1—S187.49 (4)C34—C35—C41120.6 (4) <t< td=""><td>C17—P1</td><td>1.781 (3)</td><td>C49—C54</td><td>1.383 (5)</td></t<>	C17—P1	1.781 (3)	C49—C54	1.383 (5)
C18—H180.9300C50—C511.367 (6)C19—C201.363 (6)C50—H500.9300C19—H190.9300C51—C521.344 (7)C20—C211.371 (5)C51—H510.9300C20—H200.9300C52—C531.370 (6)C21—C221.381 (5)C52—H520.9300C21—H210.9300C53—C541.374 (6)C22—H220.9300C53—H530.9300C23—C241.377 (5)C54—H540.9300C23—C281.392 (5)C55—C561.383 (5)C24—C251.375 (5)C55—C561.378 (5)C24—C251.375 (5)C55—C561.378 (5)C25—C261.361 (6)C56—C571.377 (5)C25—C261.361 (6)C56—C571.375 (5)C25—C261.361 (6)C58—C591.369 (6)C27—C281.365 (5)C58—C591.369 (6)C27—C281.365 (5)C58—C591.361 (6)C29—C341.380 (4)C60—H600.9300C29—C341.380 (4)C60—H600.9300C29—N1I—S187.41 (4)C32—C33—H33119.8S2 ¹ —N1I—S1 ¹ 80.00 (1)C33—C34—H34120.1S1 ² —N1I—S1 ¹ 87.49 (4)C34—C35—C36117.9 (4)S4 ¹ —N12—S387.69 (4)C40—C35—C41120.6 (4)S4 ¹ —N12—S3 ¹¹ 87.69 (4)C40—C35—C41120.6 (4)S4 ¹ —N12—S3 ¹¹ 87.69 (4)C37—C36—C35120.4 (4)S4 ¹ —N12—S3 ¹¹ 87.69 (4)C37—C36—C35120.4 (4)	C18—C19	1.357 (5)	C49—P2	1.788 (4)
C19-C201.363 (6)C50-H500.9300C19-H190.9300C51-C521.344 (7)C20-C211.371 (5)C51-H510.9300C20-H200.9300C52-C531.370 (6)C21-C221.381 (5)C52-H520.9300C21-H210.9300C53-C541.374 (6)C22-H220.9300C53-H530.9300C23-C241.377 (5)C54-H540.9300C23-C281.392 (5)C55-C601.383 (5)C24-C251.375 (5)C55-C561.378 (5)C24-C251.375 (5)C56-C571.377 (5)C24-C251.351 (6)C56-H560.9300C25-C261.361 (6)C56-H560.9300C26-C271.370 (6)C57-C581.355 (5)C26-C271.370 (6)C57-C581.359 (6)C27-C281.365 (5)C58-H580.9300C27-H270.9300C59-C601.381 (5)C28-H280.9300C59-C601.381 (5)C28-H280.9300C59-C601.381 (5)C28-H280.9300C59-C601.381 (5)C28-H280.9300C59-C601.381 (5)C28-H291.380 (4)C60-H600.9300C29-C341.380 (4)C29-C33-C34120.4 (4)S2 ¹ -Ni1-S187.41 (4)C29-C33-C34120.4 (4)S2 ¹ -Ni1-S187.41 (4)C29-C34-C33119.9 (4)S2 ¹ -Ni1-S1180.000 (1)C33-C34-H34120.1S4 ¹ -Ni2-S387.69 (4)C40-C35-C41 </td <td>C18—H18</td> <td>0.9300</td> <td>C50—C51</td> <td>1.367 (6)</td>	C18—H18	0.9300	C50—C51	1.367 (6)
C19—H190.9300C51—C521.344 (7)C20—C211.371 (5)C51—H510.9300C20—H200.9300C52—C531.370 (6)C21—C221.381 (5)C52—H520.9300C21—H210.9300C53—C541.374 (6)C22—H220.9300C53—H530.9300C23—C241.377 (5)C54—H540.9300C23—C281.392 (5)C55—C601.383 (5)C24—C251.375 (5)C55—C561.378 (5)C24—C251.375 (5)C55—C561.377 (5)C24—C251.376 (6)C56—H560.9300C25—C261.361 (6)C56—H560.9300C25—H250.9300C57—C581.355 (5)C26—H260.9300C58—C591.369 (6)C27—C281.365 (5)C58—H580.9300C29—C341.380 (4)C60—H600.9300C29—C341.380 (4)C60—H600.9300C29—C341.380 (4)C32—C33—C34120.4 (4)S2 ¹ —Ni1—S187.41 (4)C32—C33—C34119.8S2 ¹ —Ni1—S1 ¹ 180.000 (1)C33—C34—H34120.1S4 ¹ —Ni1—S1 ¹ 180.000 (1)C33—C34—H34120.1<	C19—C20	1.363 (6)	С50—Н50	0.9300
C20—C211.371 (5)C51—H510.9300C20—H200.9300C52—C531.370 (6)C21—C221.381 (5)C52—H520.9300C21—H210.9300C53—C541.374 (6)C22—H220.9300C53—H530.9300C23—C241.377 (5)C54—H540.9300C23—C281.392 (5)C55—C601.383 (5)C24—C251.375 (5)C55—P21.792 (3)C24—C251.375 (5)C55—P21.377 (5)C24—H240.9300C56—C571.377 (5)C25—C261.361 (6)C56—H560.9300C25—H250.9300C57—C581.355 (5)C26—H260.9300C58—C591.369 (6)C27—C281.365 (5)C58—H580.9300C27—H270.9300C59—C601.381 (5)C28—H280.9300C59—H590.9300C29—C341.380 (4)C60—H600.9300C24—H140.92-C33—C33119.8S2 ¹ —N1I—S187.41 (4)C32—C33—H33119.8S2 ¹ —N1I—S1 ¹ 180.00C34—C33—H33119.8S2 ¹ —N1I—S1 ¹ 180.00C34—C33—H33119.9S2 ¹ —N1I—S1 ¹ 180.00C34—C33—H34120.1S4 ¹ ¬N1I—S1 ¹ 180.00C34—C33—H34120.1S4 ¹ ¬N1I—S1 ¹ 180.00C34—C33—H34119.8S2 ¹ —N1I—S1 ¹ 180.00C34—C33—H34119.4S2-N1I—S1 ¹ 180.00C34—C34—H34120.1S4 ¹ ¬N1I—S1 ¹ 180.00C34—C35—C36 <t< td=""><td>С19—Н19</td><td>0.9300</td><td>C51—C52</td><td>1.344 (7)</td></t<>	С19—Н19	0.9300	C51—C52	1.344 (7)
C20—H200.9300C52—C531.370 (6)C21—C221.381 (5)C52—H520.9300C21—H210.9300C53—C541.374 (6)C22—H220.9300C53—H530.9300C23—C241.377 (5)C54—H540.9300C23—C281.392 (5)C55—C601.383 (5)C24—C251.375 (5)C55—C561.378 (5)C24—C251.375 (5)C55—P21.772 (3)C24—H240.9300C56—C571.377 (5)C25—C261.361 (6)C56—H560.9300C25—H250.9300C57—C581.355 (5)C26—C271.370 (6)C57—H570.9300C26—H260.9300C58—C591.369 (6)C27—C281.365 (5)C58—H580.9300C28—H280.9300C59—H590.9300C29—C341.380 (4)C60—H600.9300S2 ¹ —N11—S187.41 (4)C32—C33—C34120.4 (4)S2 ¹ —N11—S1 ¹ 92.59 (4)C34—C33—H33119.8S2 ¹ —N11—S1 ¹ 87.41 (4)C29—C34—C33119.9 (4)S2 ¹ —N11—S1 ¹ 180.00 (1)C33—C34—H34120.1S4 ¹¹ —N12—S387.69 (4)C40—C35—C41121.5 (4)S4 ¹¹ —N12—S3 ¹¹ 87.69 (4)C40—C35—C41120.6 (4)S4 ¹¹ —N12—S3 ¹¹ 87.69 (4)C37—C36—C35120.4 (4)S4 ¹¹ —N12—S3 ¹¹ 87.69 (4)C37—C36—C35120.4 (4)S4 ¹¹ —N12—S3 ¹¹ 87.69 (4)C37—C36—C35120.4 (4)	C20—C21	1.371 (5)	С51—Н51	0.9300
C21-C221.381 (5)C52-H520.9300C21-H210.9300C53-C541.374 (6)C22-H220.9300C53-H530.9300C23-C241.377 (5)C54-H540.9300C23-C281.392 (5)C55-C601.383 (5)C24-C251.375 (5)C55-C561.378 (5)C24-H240.9300C56-C571.377 (5)C25-C261.361 (6)C56-H560.9300C25-H250.9300C57-C581.355 (5)C26-C271.370 (6)C57-H570.9300C26-H260.9300C58-C591.369 (6)C27-C281.365 (5)C58-H580.9300C27-C281.365 (5)C58-H580.9300C27-H270.9300C59-H590.9300C29-C341.380 (4)C60-H600.9300S2 ¹ -N11-S187.41 (4)C32-C33-C34120.4 (4)S2 ² -N11-S187.41 (4)C34-C33-H33119.8S2 ¹ -N11-S1 ¹ 92.59 (4)C34-C33-H33119.9 (4)S2-N11-S187.41 (4)C29-C34-C33119.9 (4)S2 ¹ -N11-S1 ¹ 180.00 (1)C33-C34-H34120.1S4 ¹¹ -N12-S387.69 (4)C40-C35-C41121.5 (4)S4 ¹¹ -N12-S392.31 (4)C36-C35-C41120.6 (4)S4 ¹¹ -N12-S3 ¹¹ 87.69 (4)C37-C36-C35120.4 (4)S4 ¹¹ -N12-S3 ¹¹ 87.69 (4)C37-C36-C35120.4 (4)S4 ¹¹ -N12-S3 ¹¹ 87.69 (4)C37-C36-C35120.4 (4)	С20—Н20	0.9300	C52—C53	1.370 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C21—C22	1.381 (5)	С52—Н52	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C21—H21	0.9300	C53—C54	1.374 (6)
C23-C241.377 (5)C54-H540.9300C23-C281.392 (5)C55-C601.383 (5)C23-P11.790 (3)C55-C561.378 (5)C24-C251.375 (5)C55-P21.792 (3)C24-H240.9300C56-C571.377 (5)C25-C261.361 (6)C56-H560.9300C25-H250.9300C57-C581.355 (5)C26-C271.370 (6)C57-H570.9300C26-H260.9300C58-C591.369 (6)C27-C281.365 (5)C58-H580.9300C27-H270.9300C59-C601.381 (5)C28-H280.9300C59-H590.9300C29-C341.380 (4)C60-H600.9300S2 ⁱ -Ni1-S187.41 (4)C32-C33-C34120.4 (4)S2 ⁱ -Ni1-S192.59 (4)C34-C33-H33119.8S2 ⁱ -Ni1-S187.41 (4)C29-C34-C33119.9 (4)S2 ⁱ -Ni1-S187.41 (4)C29-C34-C33119.9 (4)S2 ⁱ -Ni1-S187.41 (4)C29-C34-C33119.9 (4)S2 ⁱ -Ni1-S1 ⁱ 180.000 (1)C33-C34-H34120.1S4 ⁱⁱ -Ni2-S387.69 (4)C40-C35-C41121.5 (4)S4 ⁱⁱ -Ni2-S392.31 (4)C36-C35-C41120.6 (4)S4 ⁱⁱ -Ni2-S3 ⁱⁱ 92.31 (4)C37-C36-H36119.8	С22—Н22	0.9300	С53—Н53	0.9300
$C23-C28$ 1.392 (5) $C55-C60$ 1.383 (5) $C23-P1$ 1.790 (3) $C55-C56$ 1.378 (5) $C24-C25$ 1.375 (5) $C55-P2$ 1.792 (3) $C24-H24$ 0.9300 $C56-C57$ 1.377 (5) $C25-C26$ 1.361 (6) $C56-H56$ 0.9300 $C25-H25$ 0.9300 $C57-C58$ 1.355 (5) $C26-H26$ 0.9300 $C57-H57$ 0.9300 $C26-H26$ 0.9300 $C58-C59$ 1.369 (6) $C27-C28$ 1.365 (5) $C58-H58$ 0.9300 $C27-H27$ 0.9300 $C59-C60$ 1.381 (5) $C28-H28$ 0.9300 $C59-H59$ 0.9300 $C29-C34$ 1.380 (4) $C60-H60$ 0.9300 $C29-C34$ 1.380 (4) $C32-C33-H33$ 119.8 $S2^1-Ni1-S1$ 87.41 (4) $C32-C33-H33$ 119.8 $S2^1-Ni1-S1^i$ 92.59 (4) $C34-C33-H33$ 119.9 (4) $S2-Ni1-S1^i$ 87.41 (4) $C29-C34-H34$ 120.1 $S1-Ni1-S1^i$ 180.00 (1) $C33-C34-H34$ 120.1 $S4^{ii}-Ni2-S3$ 87.69 (4) $C40-C35-C41$ 121.5 (4) $S4^{ii}-Ni2-S3$ 92.31 (4) $C36-C35-C41$ 120.6 (4) $S4^{-Ni2}-S3^{ii}$ 92.31 (4) $C37-C36-C35$ 120.4 (4) $S4^{-Ni2}-S3^{ii}$ 92.31 (4) $C37-C36-C35$ 120.4 (4) $S4^{-Ni2}-S3^{ii}$ 92.31 (4) $C37-C36-C35$ 120.4 (4)	C23—C24	1.377 (5)	C54—H54	0.9300
C23—P11.790 (3)C55—C561.378 (5)C24—C251.375 (5)C55—P21.792 (3)C24—H240.9300C56—C571.377 (5)C25—C261.361 (6)C56—H560.9300C25—H250.9300C57—C581.355 (5)C26—C271.370 (6)C57—H570.9300C26—H260.9300C58—C591.369 (6)C27—C281.365 (5)C58—H580.9300C29—C341.380 (4)C60—H600.9300C29—C341.380 (4)C60—H600.9300S2 ¹ —N1—S187.41 (4)C32—C33—C34120.4 (4)S2 ¹ —N1—S192.59 (4)C34—C33—H33119.8S2 ¹ —N1—S192.59 (4)C34—C33—H33119.9 (4)S2-N11—S192.59 (4)C34—C33—H34120.1S4 ¹¹ —N12—S4180.00 (1)C33—C34—H34120.1S4 ¹¹ —N12—S387.69 (4)C40—C35—C36117.9 (4)S4 ¹¹ —N12—S392.31 (4)C36—C35—C41120.6 (4)S4 ¹¹ —N12—S3 ¹¹ 92.31 (4)C37—C36—C35120.4 (4)S4 ¹¹ —N12—S3 ¹¹ 87.69 (4)C37—C36—C35120.4 (4)S4 ¹¹ —N12—S3 ¹¹ 92.31 (4)C37—C36—C35120.4 (4)S4 ¹¹ —N12—S3 ¹¹ 87.69 (4)C37—C36—C35	C23—C28	1.392 (5)	C55—C60	1.383 (5)
C24-C251.375 (5)C55-P21.792 (3)C24-H240.9300C56-C571.377 (5)C25-C261.361 (6)C56-H560.9300C25-H250.9300C57-C581.355 (5)C26-C271.370 (6)C57-H570.9300C26-H260.9300C58-C591.369 (6)C27-C281.365 (5)C58-H580.9300C27-H270.9300C59-C601.381 (5)C28-H280.9300C59-H590.9300C29-C341.380 (4)C60-H600.9300S2 ⁱ -Ni1-S187.41 (4)C32-C33-C34120.4 (4)S2 ⁱ -Ni1-S192.59 (4)C34-C33-H33119.8S2 ⁱ -Ni1-S192.59 (4)C34-C33-H33119.9 (4)S2 ⁱ -Ni1-S1 ⁱ 87.41 (4)C29-C34-H34120.1S1-Ni1-S1 ⁱ 180.000 (1)C33-C34-H34120.1S4 ⁱⁱ -Ni2-S387.69 (4)C40-C35-C41121.5 (4)S4 ⁱⁱ -Ni2-S3 ⁱⁱ 92.31 (4)C36-C35-C41120.6 (4)S4 ⁱⁱ -Ni2-S3 ⁱⁱⁱ 87.69 (4)C37-C36-C35120.4 (4)S4-Ni2-S3 ⁱⁱⁱ 87.69 (4)C37-C36-C35120.4 (4)	C23—P1	1.790 (3)	C55—C56	1.378 (5)
C24—H240.9300C56—C571.377 (5)C25—C261.361 (6)C56—H560.9300C25—H250.9300C57—C581.355 (5)C26—C271.370 (6)C57—H570.9300C26—H260.9300C58—C591.369 (6)C27—C281.365 (5)C58—H580.9300C27—H270.9300C59—C601.381 (5)C28—H280.9300C59—H590.9300C29—C341.380 (4)C60—H600.9300S2 ⁱ —Ni1—S187.41 (4)C32—C33—C34120.4 (4)S2 ⁱ —Ni1—S192.59 (4)C34—C33—H33119.8S2 ⁱ —Ni1—S1 ⁱ 92.59 (4)C34—C33—H33119.9 (4)S2 ⁱ —Ni1—S1 ⁱ 87.41 (4)C29—C34—H34120.1S1—Ni1—S1 ⁱ 87.41 (4)C29—C34—H34120.1S4 ⁱⁱ —Ni2—S4180.00 (1)C33—C34—H34120.1S4 ⁱⁱ —Ni2—S387.69 (4)C40—C35—C41121.5 (4)S4 ⁱⁱ —Ni2—S3 ⁱⁱ 92.31 (4)C36—C35120.4 (4)S4 ⁱⁱ —Ni2—S3 ⁱⁱⁱ 87.69 (4)C37—C36—H36119.8	C24—C25	1.375 (5)	C55—P2	1.792 (3)
C25—C261.361 (6)C36—H360.9300C25—H250.9300C57—C581.355 (5)C26—C271.370 (6)C57—H570.9300C26—H260.9300C58—C591.369 (6)C27—C281.365 (5)C58—H580.9300C29—C341.380 (4)C60—H600.9300C29—C341.380 (4)C60—H600.9300S2 ⁱ —Ni1—S2180.0C32—C33—C34120.4 (4)S2 ⁱ —Ni1—S192.59 (4)C34—C33—H33119.8S2 ⁱ —Ni1—S1 ⁱ 92.59 (4)C29—C34—C33119.9 (4)S2 ⁱ —Ni1—S1 ⁱ 87.41 (4)C29—C34—H34120.1S1—Ni1—S1 ⁱ 87.41 (4)C29—C34—H34120.1S4 ⁱⁱ —Ni2—S387.69 (4)C40—C35—C41121.5 (4)S4 ⁱⁱ —Ni2—S392.31 (4)C36—C35—C41120.6 (4)S4 ⁱⁱ —Ni2—S3 ⁱⁱ 92.31 (4)C37—C36—H36119.8	C24—H24	0.9300	C56—C57	1.377 (5)
C25-H25 0.9300 C57-C58 1.355 (5)C26-C27 1.370 (6)C57-H57 0.9300 C26-H26 0.9300 C58-C59 1.369 (6)C27-C28 1.365 (5)C58-H58 0.9300 C27-H27 0.9300 C59-C60 1.381 (5)C28-H28 0.9300 C59-H59 0.9300 C29-C34 1.380 (4)C60-H60 0.9300 S2 ⁱ -Ni1-S2180.0C32-C33-C34120.4 (4)S2 ⁱ -Ni1-S187.41 (4)C32-C33-H33119.8S2-Ni1-S192.59 (4)C34-C33-H33119.8S2 ⁱ -Ni1-S1 ⁱ 87.41 (4)C29-C34-C33119.9 (4)S2-Ni1-S1 ⁱ 87.41 (4)C29-C34-H34120.1S1-Ni1-S1 ⁱ 87.41 (4)C29-C34-H34120.1S4 ⁱⁱ -Ni2-S387.69 (4)C40-C35-C41121.5 (4)S4 ⁱⁱ -Ni2-S392.31 (4)C36-C35-C41120.6 (4)S4 ⁱⁱ -Ni2-S3 ⁱⁱ 92.31 (4)C37-C36-C35120.4 (4)S4-Ni2-S3 ⁱⁱ 87.69 (4)C37-C36-H36119.8	C25—C26	1.361 (6)	C56—H56	0.9300
C26-C271.370 (6)C57-H570.9300C26-H260.9300C58-C591.369 (6)C27-C281.365 (5)C58-H580.9300C27-H270.9300C59-C601.381 (5)C28-H280.9300C59-H590.9300C29-C341.380 (4)C60-H600.9300S2 ⁱ -Ni1-S2180.0C32-C33-C34120.4 (4)S2 ⁱ -Ni1-S187.41 (4)C32-C33-H33119.8S2-Ni1-S192.59 (4)C34-C33-H33119.8S2 ⁱ -Ni1-S1 ⁱ 92.59 (4)C29-C34-C33119.9 (4)S2-Ni1-S1 ⁱ 87.41 (4)C29-C34-H34120.1S1-Ni1-S1 ⁱ 180.000 (1)C33-C34-H34120.1S4 ⁱⁱ -Ni2-S387.69 (4)C40-C35-C41121.5 (4)S4 ⁱⁱ -Ni2-S3 ⁱⁱ 92.31 (4)C37-C36-C35120.4 (4)S4-Ni2-S3 ⁱⁱⁱ 87.69 (4)C37-C36-C35120.4 (4)	C25—H25	0.9300	C57—C58	1.355 (5)
C26—H26 0.9300 C38—C59 1.369 (6)C27—C28 1.365 (5)C58—H58 0.9300 C27—H27 0.9300 C59—C60 1.381 (5)C28—H28 0.9300 C59—H59 0.9300 C29—C34 1.380 (4)C60—H60 0.9300 S2 ⁱ —Ni1—S2180.0C32—C33—C34120.4 (4)S2 ⁱ —Ni1—S187.41 (4)C32—C33—H33119.8S2—Ni1—S192.59 (4)C34—C33—H33119.8S2 ⁱ —Ni1—S1 ⁱ 92.59 (4)C29—C34—C33119.9 (4)S2—Ni1—S1 ⁱ 87.41 (4)C29—C34—H34120.1S1—Ni1—S1 ⁱ 87.41 (4)C29—C34—H34120.1S4 ⁱⁱ —Ni2—S4180.0C40—C35—C36117.9 (4)S4 ⁱⁱ —Ni2—S387.69 (4)C40—C35—C41121.5 (4)S4 ⁱⁱ —Ni2—S3 ⁱⁱ 92.31 (4)C37—C36—C35120.4 (4)S4—Ni2—S3 ⁱⁱ 87.69 (4)C37—C36—H36119.8	C26—C27	1.370 (6)	C57—H57	0.9300
$C27-L28$ 1.365 (5) $C58-H58$ 0.9300 $C27-H27$ 0.9300 $C59-C60$ $1.381 (5)$ $C28-H28$ 0.9300 $C59-H59$ 0.9300 $C29-C34$ $1.380 (4)$ $C60-H60$ 0.9300 $S2^{i}-Ni1-S2$ 180.0 $C32-C33-C34$ $120.4 (4)$ $S2^{i}-Ni1-S1$ $87.41 (4)$ $C32-C33-H33$ 119.8 $S2-Ni1-S1$ $92.59 (4)$ $C34-C33-H33$ 119.8 $S2^{i}-Ni1-S1^{i}$ $92.59 (4)$ $C29-C34-C33$ $119.9 (4)$ $S2-Ni1-S1^{i}$ $87.41 (4)$ $C29-C34-C33$ $119.9 (4)$ $S2-Ni1-S1^{i}$ $87.41 (4)$ $C29-C34-H34$ 120.1 $S1-Ni1-S1^{i}$ $87.41 (4)$ $C29-C34-H34$ 120.1 $S1-Ni1-S1^{i}$ $87.41 (4)$ $C29-C34-H34$ 120.1 $S4^{ii}-Ni2-S4$ $180.000 (1)$ $C33-C34-H34$ 120.1 $S4^{ii}-Ni2-S3$ $87.69 (4)$ $C40-C35-C41$ $121.5 (4)$ $S4-Ni2-S3^{ii}$ $92.31 (4)$ $C37-C36-C35$ $120.4 (4)$ $S4-Ni2-S3^{ii}$ $87.69 (4)$ $C37-C36-C35$ $120.4 (4)$	C26—H26	0.9300	C58—C59	1.369 (6)
$C27-H27$ 0.9300 $C59-C60$ $1.381(5)$ $C28-H28$ 0.9300 $C59-H59$ 0.9300 $C29-C34$ $1.380(4)$ $C60-H60$ 0.9300 $S2^{i}-Ni1-S2$ 180.0 $C32-C33-C34$ $120.4(4)$ $S2^{i}-Ni1-S1$ $87.41(4)$ $C32-C33-H33$ 119.8 $S2-Ni1-S1$ $92.59(4)$ $C34-C33-H33$ 119.8 $S2^{i}-Ni1-S1^{i}$ $92.59(4)$ $C29-C34-C33$ $119.9(4)$ $S2-Ni1-S1^{i}$ $87.41(4)$ $C29-C34-H34$ 120.1 $S1-Ni1-S1^{i}$ $87.41(4)$ $C29-C34-H34$ 120.1 $S1-Ni1-S1^{i}$ $87.41(4)$ $C29-C34-H34$ 120.1 $S4^{ii}-Ni2-S4$ $180.00(1)$ $C33-C34-H34$ 120.1 $S4^{ii}-Ni2-S3$ $87.69(4)$ $C40-C35-C36$ $117.9(4)$ $S4^{ii}-Ni2-S3$ $92.31(4)$ $C36-C35-C41$ $120.6(4)$ $S4^{ii}-Ni2-S3^{ii}$ $92.31(4)$ $C37-C36-C35$ $120.4(4)$ $S4-Ni2-S3^{ii}$ $87.69(4)$ $C37-C36-H36$ 119.8	C27—C28	1.365 (5)	C58—H58	0.9300
C28—H28 0.9300 $C39$ —H39 0.9300 C29—C34 1.380 (4)C60—H60 0.9300 S2 ⁱ —Ni1—S2 180.0 C32—C33—C34 120.4 (4)S2 ⁱ —Ni1—S1 87.41 (4)C32—C33—H33 119.8 S2—Ni1—S1 92.59 (4)C34—C33—H33 119.8 S2 ⁱ —Ni1—S1 ⁱ 92.59 (4)C29—C34—C33 119.9 (4)S2—Ni1—S1 ⁱ 87.41 (4)C29—C34—H34 120.1 S1—Ni1—S1 ⁱ 87.41 (4)C29—C34—H34 120.1 S4 ⁱⁱ —Ni2—S4 180.000 (1)C33—C34—H34 120.1 S4 ⁱⁱ —Ni2—S3 87.69 (4)C40—C35—C36 117.9 (4)S4 Ni2—S3 92.31 (4)C36—C35—C41 120.6 (4)S4 ⁻ⁱⁱ —Ni2—S3 ⁱⁱ 92.31 (4)C37—C36—C35 120.4 (4)S4—Ni2—S3 ⁱⁱ 87.69 (4)C37—C36—H36 119.8	C27—H27	0.9300	C59—C60	1.381 (5)
$C29-C34$ 1.380 (4) $C80-H60$ 0.9500 $S2^{i}-Ni1-S2$ 180.0 $C32-C33-C34$ 120.4 (4) $S2^{i}-Ni1-S1$ 87.41 (4) $C32-C33-H33$ 119.8 $S2-Ni1-S1$ 92.59 (4) $C34-C33-H33$ 119.8 $S2^{i}-Ni1-S1^{i}$ 92.59 (4) $C29-C34-C33$ 119.9 (4) $S2-Ni1-S1^{i}$ 87.41 (4) $C29-C34-H34$ 120.1 $S1-Ni1-S1^{i}$ 87.41 (4) $C29-C34-H34$ 120.1 $S1-Ni1-S1^{i}$ 180.000 (1) $C33-C34-H34$ 120.1 $S4^{ii}-Ni2-S4$ 180.0 $C40-C35-C36$ 117.9 (4) $S4^{ii}-Ni2-S3$ 92.31 (4) $C36-C35-C41$ 121.5 (4) $S4^{ii}-Ni2-S3^{ii}$ 92.31 (4) $C37-C36-C35$ 120.4 (4) $S4^{ii}-Ni2-S3^{ii}$ 87.69 (4) $C37-C36-H36$ 119.8	C28—H28	0.9300	C(0, 1)(0	0.9300
$S2^{i}$ —Ni1—S2180.0 $C32$ —C33—C34120.4 (4) $S2^{i}$ —Ni1—S1 87.41 (4) $C32$ —C33—H33119.8 $S2$ —Ni1—S1 92.59 (4) $C34$ —C33—H33119.8 $S2^{i}$ —Ni1—S1 92.59 (4) $C29$ —C34—C33119.9 (4) $S2$ —Ni1—S1 ⁱ 87.41 (4) $C29$ —C34—H34120.1 $S1$ —Ni1—S1 ⁱ 87.41 (4) $C33$ —C34—H34120.1 $S1$ —Ni1—S1 ⁱ 180.000 (1) $C33$ —C34—H34120.1 $S4^{ii}$ —Ni2—S4 180.0 $C40$ —C35—C36117.9 (4) $S4^{ii}$ —Ni2—S3 92.31 (4) $C36$ —C35—C41121.5 (4) $S4^{ii}$ —Ni2—S3 ⁱⁱ 92.31 (4) $C37$ —C36—C35120.4 (4) $S4$ —Ni2—S3 ⁱⁱ 87.69 (4) $C37$ —C36—H36119.8		1.380 (4)	C60—H60	0.9300
$S2^{i}$ —Ni1—S1 87.41 (4) $C32$ —C33—H33 119.8 $S2$ —Ni1—S1 92.59 (4) $C34$ —C33—H33 119.8 $S2^{i}$ —Ni1—S1 ⁱ 92.59 (4) $C29$ —C34—C33 119.9 (4) $S2$ —Ni1—S1 ⁱ 87.41 (4) $C29$ —C34—H34 120.1 $S1$ —Ni1—S1 ⁱ 180.000 (1) $C33$ —C34—H34 120.1 $S4^{ii}$ —Ni2—S4 180.0 $C40$ —C35—C36 117.9 (4) $S4^{ii}$ —Ni2—S3 87.69 (4) $C40$ —C35—C41 121.5 (4) $S4^{ii}$ —Ni2—S3 92.31 (4) $C36$ —C35—C41 120.6 (4) $S4^{ii}$ —Ni2—S3 ⁱⁱ 92.31 (4) $C37$ —C36—C35 120.4 (4) $S4$ —Ni2—S3 ⁱⁱ 87.69 (4) $C37$ —C36—H36 119.8	S2 ¹ —Ni1—S2	180.0	C32—C33—C34	120.4 (4)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	S2 ¹ —Ni1—S1	87.41 (4)	С32—С33—Н33	119.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S2—Ni1—S1	92.59 (4)	С34—С33—Н33	119.8
S2—Ni1—S1 ⁱ 87.41 (4)C29—C34—H34120.1S1—Ni1—S1 ⁱ 180.000 (1)C33—C34—H34120.1S4 ⁱⁱ —Ni2—S4180.0C40—C35—C36117.9 (4)S4 ⁱⁱ —Ni2—S387.69 (4)C40—C35—C41121.5 (4)S4—Ni2—S392.31 (4)C36—C35—C41120.6 (4)S4 ⁱⁱ —Ni2—S3 ⁱⁱ 92.31 (4)C37—C36—C35120.4 (4)S4—Ni2—S3 ⁱⁱ 87.69 (4)C37—C36—H36119.8	$S2^{i}$ —Ni1— $S1^{i}$	92.59 (4)	C29—C34—C33	119.9 (4)
$S1-Ni1-S1^{i}$ 180.000 (1) $C33-C34-H34$ 120.1 $S4^{ii}-Ni2-S4$ 180.0 $C40-C35-C36$ 117.9 (4) $S4^{ii}-Ni2-S3$ 87.69 (4) $C40-C35-C41$ 121.5 (4) $S4-Ni2-S3$ 92.31 (4) $C36-C35-C41$ 120.6 (4) $S4^{ii}-Ni2-S3^{ii}$ 92.31 (4) $C37-C36-C35$ 120.4 (4) $S4-Ni2-S3^{ii}$ 87.69 (4) $C37-C36-H36$ 119.8	S2—Ni1—S1 ⁱ	87.41 (4)	C29—C34—H34	120.1
$S4^{ii}$ —Ni2—S4180.0C40—C35—C36117.9 (4) $S4^{ii}$ —Ni2—S387.69 (4)C40—C35—C41121.5 (4) $S4$ —Ni2—S392.31 (4)C36—C35—C41120.6 (4) $S4^{ii}$ —Ni2—S3 ⁱⁱ 92.31 (4)C37—C36—C35120.4 (4) $S4$ —Ni2—S3 ⁱⁱ 87.69 (4)C37—C36—H36119.8	S1—Ni1—S1 ⁱ	180.000 (1)	C33—C34—H34	120.1
$S4^{ii}$ —Ni2—S3 87.69 (4) $C40$ —C35—C41 121.5 (4) $S4$ —Ni2—S3 92.31 (4) $C36$ —C35—C41 120.6 (4) $S4^{ii}$ —Ni2—S3^{ii} 92.31 (4) $C37$ —C36—C35 120.4 (4) $S4$ —Ni2—S3^{ii} 87.69 (4) $C37$ —C36—H36 119.8	S4 ⁱⁱ —Ni2—S4	180.0	C40—C35—C36	117.9 (4)
S4—Ni2—S392.31 (4)C36—C35—C41120.6 (4)S4 ⁱⁱ —Ni2—S3 ⁱⁱ 92.31 (4)C37—C36—C35120.4 (4)S4—Ni2—S3 ⁱⁱ 87.69 (4)C37—C36—H36119.8	S4 ⁱⁱ —Ni2—S3	87.69 (4)	C40—C35—C41	121.5 (4)
S4 ⁱⁱ —Ni2—S3 ⁱⁱ 92.31 (4)C37—C36—C35120.4 (4)S4—Ni2—S3 ⁱⁱ 87.69 (4)C37—C36—H36119.8	S4—Ni2—S3	92.31 (4)	C36—C35—C41	120.6 (4)
S4—Ni2—S3 ⁱⁱ 87.69 (4) C37—C36—H36 119.8	S4 ⁱⁱ —Ni2—S3 ⁱⁱ	92.31 (4)	C37—C36—C35	120.4 (4)
	S4—Ni2—S3 ⁱⁱ	87.69 (4)	С37—С36—Н36	119.8

83—Ni2—83 ⁱⁱ	180.00 (5)	С35—С36—Н36	119.8
C2—C1—C4	121.2 (3)	C38—C37—C36	121.4 (4)
C2—C1—S1	120.8 (3)	С38—С37—Н37	119.3
C4—C1—S1	118.0 (3)	С36—С37—Н37	119.3
C1—C2—C3	118.9 (3)	C37—C38—C39	118.4 (4)
C1—C2—S2	121.6 (3)	С37—С38—Н38	120.8
C3—C2—S2	119.4 (3)	С39—С38—Н38	120.8
N1—C3—C2	177.7 (4)	C40—C39—C38	121.4 (4)
N2	179.4 (5)	C40—C39—C42	118.1 (4)
C6—C5—C8	121.1 (3)	C38—C39—C42	120.5 (4)
C6—C5—S3	121.6 (3)	C39—C40—C35	120.5 (4)
C8—C5—S3	117.2 (3)	С39—С40—Н40	119.7
C5—C6—C7	120.9 (3)	C35—C40—H40	119.7
C5—C6—S4	120.4 (3)	C35—C41—P2	111.6 (2)
C7—C6—S4	118.5 (3)	C35—C41—H41A	109.3
N3—C7—C6	178.7 (5)	P2—C41—H41A	109.3
N4—C8—C5	179.0 (5)	C35—C41—H41B	109.3
C14—C9—C10	118.0 (4)	P2—C41—H41B	109.3
C14—C9—C15	121.8 (4)	H41A—C41—H41B	108.0
C10—C9—C15	120.2 (4)	N6—C42—C39	177.6 (5)
C11—C10—C9	120.5 (5)	C48—C43—C44	119.8 (3)
C11—C10—H10	119.7	C48—C43—P2	121.5 (3)
С9—С10—Н10	119.7	C44—C43—P2	118.0 (3)
C12—C11—C10	121.1 (5)	C45—C44—C43	119.9 (4)
C12—C11—H11	119.5	C45—C44—H44	120.1
C10—C11—H11	119.5	C43—C44—H44	120.0
C11—C12—C13	119.1 (5)	C44—C45—C46	120.1 (4)
C11—C12—H12	120.5	C44—C45—H45	120.0
C13—C12—H12	120.5	C46—C45—H45	120.0
C14—C13—C12	120.7 (4)	C47—C46—C45	120.8 (4)
C14—C13—C16	120.2 (4)	C47—C46—H46	119.6
C12—C13—C16	119.0 (4)	C45—C46—H46	119.6
C9—C14—C13	120.6 (4)	C46—C47—C48	119.5 (4)
C9—C14—H14	119.7	C46—C47—H47	120.2
C13—C14—H14	119.7	C48—C47—H47	120.2
C9—C15—P1	113.0 (2)	C43—C48—C47	119.9 (4)
C9—C15—H15A	109.0	C43—C48—H48	120.1
P1—C15—H15A	109.0	C47—C48—H48	120.1
C9—C15—H15B	109.0	C50—C49—C54	119.6 (4)
Р1—С15—Н15В	109.0	C50—C49—P2	120.9 (3)
H15A—C15—H15B	107.8	C54—C49—P2	119.5 (3)
N5-C16-C13	179.0 (6)	C51—C50—C49	119.8 (5)
C22—C17—C18	119.6 (3)	С51—С50—Н50	120.1
C22—C17—P1	121.0 (3)	C49—C50—H50	120.1
C18—C17—P1	119.1 (3)	C52—C51—C50	121.2 (5)
C19—C18—C17	119.7 (4)	C52—C51—H51	119.4
C19—C18—H18	120.1	C50—C51—H51	119.4
C17—C18—H18	120.1	C51—C52—C53	119.7 (5)
C18—C19—C20	121.0 (4)	C51—C52—H52	120.1

С18—С19—Н19	119.5	С53—С52—Н52	120.1
С20—С19—Н19	119.5	C54—C53—C52	120.2 (5)
C19—C20—C21	120.0 (4)	С54—С53—Н53	119.9
С19—С20—Н20	120.0	С52—С53—Н53	119.9
C21—C20—H20	120.0	C53—C54—C49	119.4 (4)
C20—C21—C22	120.1 (4)	С53—С54—Н54	120.3
C20—C21—H21	120.0	C49—C54—H54	120.3
C22—C21—H21	120.0	C60—C55—C56	119.8 (3)
C17—C22—C21	119.6 (4)	C60—C55—P2	120.3 (3)
С17—С22—Н22	120.2	C56—C55—P2	119.8 (3)
C21—C22—H22	120.2	C55—C56—C57	119.7 (4)
C24—C23—C28	119.4 (3)	С55—С56—Н56	120.2
C24—C23—P1	121.5 (3)	С57—С56—Н56	120.2
C28—C23—P1	119.1 (3)	C58—C57—C56	120.3 (4)
C25—C24—C23	119.3 (4)	С58—С57—Н57	119.8
C25—C24—H24	120.3	С56—С57—Н57	119.8
C23—C24—H24	120.3	C57—C58—C59	120.7 (4)
C26—C25—C24	121.1 (4)	C57—C58—H58	119.7
С26—С25—Н25	119.4	C59—C58—H58	119.7
C24—C25—H25	119.4	C58—C59—C60	119.9 (4)
C25—C26—C27	119.9 (4)	С58—С59—Н59	120.1
С25—С26—Н26	120.1	C60—C59—H59	120.1
С27—С26—Н26	120.1	C55—C60—C59	119.5 (4)
C28—C27—C26	120.1 (4)	С55—С60—Н60	120.2
С28—С27—Н27	119.9	С59—С60—Н60	120.2
С26—С27—Н27	119.9	C17—P1—C23	108.84 (16)
C27—C28—C23	120.1 (4)	C17—P1—C29	110.34 (16)
С27—С28—Н28	119.9	C23—P1—C29	109.18 (15)
С23—С28—Н28	119.9	C17—P1—C15	108.13 (17)
C34—C29—C30	119.4 (3)	C23—P1—C15	109.27 (16)
C34—C29—P1	118.4 (3)	C29—P1—C15	111.05 (17)
C30—C29—P1	121.9 (3)	C43—P2—C49	109.69 (17)
C31—C30—C29	119.2 (3)	C43—P2—C55	111.52 (17)
С31—С30—Н30	120.4	C49—P2—C55	109.65 (16)
С29—С30—Н30	120.4	C43—P2—C41	105.81 (17)
C32—C31—C30	121.7 (4)	C49—P2—C41	109.37 (17)
С32—С31—Н31	119.2	C55—P2—C41	110.73 (16)
С30—С31—Н31	119.2	C1—S1—Ni1	102.29 (13)
C31—C32—C33	119.3 (4)	C2—S2—Ni1	102.74 (12)
C31—C32—H32	120.3	C5—S3—Ni2	102.43(13)
С33—С32—Н32	120.3	C6—S4—Ni2	102.97 (13)
Symmetry codes: (i) $-x+1$, $-v$, $-v$	z+2; (ii) $-x+2$, $-v$, $-z+2$.		

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	$D\!\!-\!\!\mathrm{H}^{\dots}\!A$
C10—H10···N4 ⁱⁱⁱ	0.93	2.57	3.479 (7)	165
C33—H33····N2 ^{iv}	0.93	2.62	3.452 (6)	149

C36—H36…N2 ⁱⁱⁱ	0.93	2.47	3.250 (6)	141
Symmetry codes: (iii) $x, y, z-1$; (iv) $x+1/2, -y+1/2$	2, <i>z</i> -1/2.			

Fig. 1





