Part I. Description of X-ray data collection and structural solutions

X-ray Structural Determination of (dippe)Ni(η^2-C,S-thiophene) (2). **2** was dissolved in cold CH_2Cl_2, layered with hexanes and kept at -30 °C overnight. A single crystal of dimensions 0.03 x 0.03 x 0.40 mm^3 was mounted on a glass fiber with oil. Data were collected at -80 °C on a Siemens SMART CCD area detector system employing a 3kW sealed tube X-ray source operating at 2.0 kW. 1.3 hemispheres of data were collected over 13 h, yielding 12790 total data after integration using SAINT. Laue symmetry revealed an rhomohedral crystal system, and cell parameters were determined from 2561 unique reflections.[1] The space group was assigned as *R3c* on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 18 there are 3 independent molecules within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0479$ and $wR_2 = 0.0652$.[2]

X-ray Structural Determination of (dippe)Ni(η^2-C,S-benzothiophene) (4). **4** was dissolved in cold CH_2Cl_2, layered with hexanes and kept at -30 °C overnight. A single crystal of dimensions 0.01 x 0.14 x 0.18 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 1.3 over 13 h, yielding 10280 total data after integration using SAINT. Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 2495 unique reflections. The space group was assigned as *C2/c* on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 12 there are 3 independent molecules within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with

hydrogens included in idealized locations. The structure refined with final residuals of R_1 = 0.1058 and wR_2 = 0.2465.

X-ray Structural Determination of (dippe)$_2$Ni$_2$(benzothiophene) (5). Crystals of **5** were obtained by slow evaporation of hexanes. A single crystal of dimensions 0.35 x 0.42 x 0.50 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 20055 total data after integration using SAINT. Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 6219 unique reflections. The space group was assigned as $P2_1/n$ on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a Z value of 4 there is one independent molecules within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of R_1 = 0.0336 and wR_2 = 0.0766.

X-ray Structural Determination of (dippe)Ni(2,2'-biphenyl) (7). Crystals of **7** were obtained by layering a THF solution of **7** with hexanes and cooling to -30 °C. A single crystal of dimensions 0.08 x 0.26 x 0.28 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 28192 total data after integration using SAINT. Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 7941 unique reflections. The space group was assigned as $P2_1/n$ on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a Z value of 4 there is one molecule within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of R_1 = 0.0497 and wR_2 = 0.0815.

X-ray Structural Determination of (dippe)$_2$Ni$_3$S$_2$(2,2'-biphenyl) (9). Crystals of **9** were obtained by standing a solution of **6** in benzene for 3 weeks. A single crystal of dimensions 0.20 x 0.20 x 0.40 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 28192 total data after integration using SAINT. Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 7941 unique reflections. The space group was assigned as *C2/c* on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 12 there is one and a half molecules within the asymmetric unit. Two molecules of benzene also crystallized on special positions in the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0504$ and $wR_2 = 0.1320$.

X-ray Structural Determination of dippe$_2$Ni (10). Crystals of **10** were obtained by slow evaporation of hexanes. A single crystal of dimensions 0.24 x 0.33 x 0.42 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 7983 total data after integration using SAINT. Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 2539 unique reflections. The space group was assigned as *C2/c* on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 4 there is one-half of a molecule within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0444$ and $wR_2 = 0.1148$.

X-ray Structural Determination of (dippe)Ni(SH)$_2$ (11). Crystals of **11** were obtained by layering a CH_2Cl_2 solution of **11** with hexanes and cooling to -30 °C. A single crystal of

dimensions 0.25 x 0.28 x 0.30 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 11979 total data after integration using SAINT. Laue symmetry revealed an tetragonal crystal system, and cell parameters were determined from 3973 unique reflections. The space group was assigned as *I*-4 on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 8 there is one molecule within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0379$ and $wR_2 = 0.0846$.

X-ray Structural Determination of (dippe)$_2$Ni$_2$(μ-S)(μ-H) (13). Crystals of **13** were obtained by cooling a pentane solution of **13** and **8** to -30 °C. A single crystal of dimensions 0.23 x 0.31 x 0.51 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 11136 total data after integration using SAINT. Laue symmetry revealed a triclinic crystal system, and cell parameters were determined from 6909 unique reflections. The space group was assigned as *P*1 on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 2 there is one molecule within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. A bridging hydride ligand, located in a difference Fourier map, was included and refined isotropically. The structure refined with final residuals of $R_1 = 0.0310$ and $wR_2 = 0.0673$.

X-ray Structural Determination of (dippe)$_2$Ni$_3$S$_2$(C$_{13}$H$_{10}$) (15). Crystals of **15** were obtained by standing a solution of **15** in benzene for 2 weeks. A single crystal of dimensions 0.20 x 0.25 x 0.35 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 30198 total data after integration using SAINT. Laue symmetry revealed an

triclinic crystal system, and cell parameters were determined from 12380 unique reflections. The space group was assigned as *P*-1 on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 6 there are three molecules within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0820$ and $wR_2 = 0.2202$.

X-ray Structural Determination of (dippe)Ni(η^2-C,S-1,9-dimethyldibenzothiophene) (19). Crystals of **19** were obtained by layering a THF solution of **19** with hexanes and cooling to -30 °C. A single crystal of dimensions 0.20 x 0.20 x 0.35 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 14 h, yielding 12550 total data after integration using SAINT. Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 3461 unique reflections. The space group was assigned as $P2_1/c$ on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 4 there is one molecule within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0824$ and $wR_2 = 0.2479$.

X-ray Structural Determination of (dippe)Ni(η^2-C,S-thioxanthene) (20). Crystals of **20** were obtained by layering a THF solution of **20** with hexanes and cooling to -30 °C. A single crystal of dimensions 0.20 x 0.20 x 0.30 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 15493 total data after integration using SAINT. Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 4686 unique reflections. The space group was assigned as $P2_1/c$ on the basis of systematic absences

using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 4 there is one molecule within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0632$ and $wR_2 = 0.1039$.

X-ray Structural Determination of (dippe)Ni(η^2-C,S-thianthrene) (21). Crystals of **21** were obtained by layering a THF solution of **21** with hexanes and cooling to -30 °C. A single crystal of dimensions 0.20 x 0.30 x 0.40 mm^3 was mounted on a glass fiber with oil. Data were collected as above over 7 h, yielding 15702 total data after integration using SAINT. Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 5124 unique reflections. The space group was assigned as $P2_1/c$ on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 4 there is one molecule within the asymmetric unit. In the final model, non-hydrogen atoms were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0519$ and $wR_2 = 0.1125$.

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(1) It has been noted that the integration program SAINT produces cell constant errors that are unreasonably small, since systematic error is not included. More reasonable errors might be estimated at 10x the listed values.((

(2) Using the SHELXTL 5.04 package, $R_1 = (\Sigma \| F_o | - | F_c \|) / \Sigma | F_o |$, $wR_2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2] \}^{½}$, where $w = 1/[\sigma^2(F_o^2) + (a \cdot P)^2 + b \cdot P]$ and $P = [f \cdot (\text{Maximum of 0 or } F_o^2) + (1-f) \cdot F_c^2]$.

Part II. ORTEP drawings of compounds with labeling scheme.

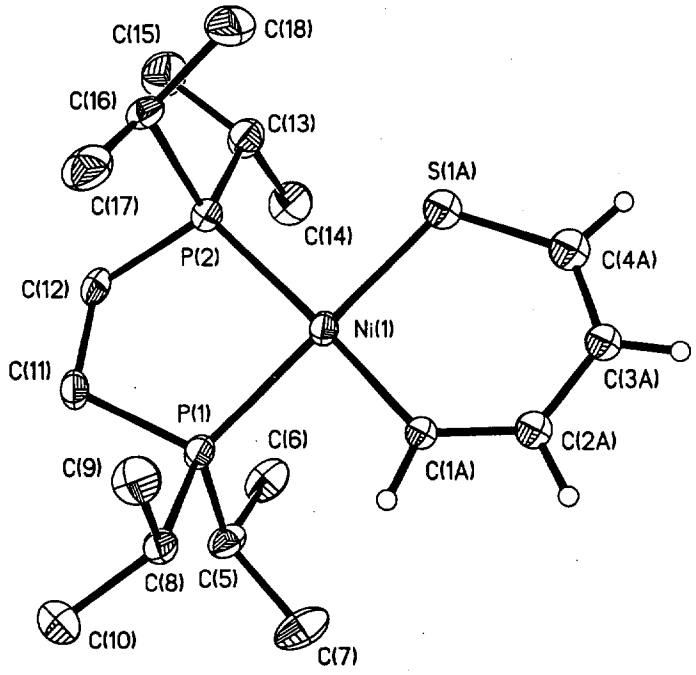

Figure 1. ORTEP drawing of (dippe)Ni(η^2-C,S-thiophene) **2**.

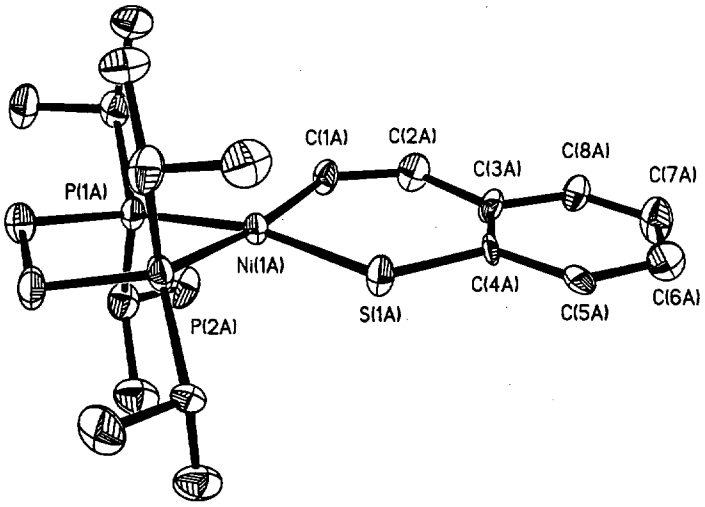

Figure 2. ORTEP drawing of (dippe)Ni(η^2-C,S-benzothiophene) **4**.

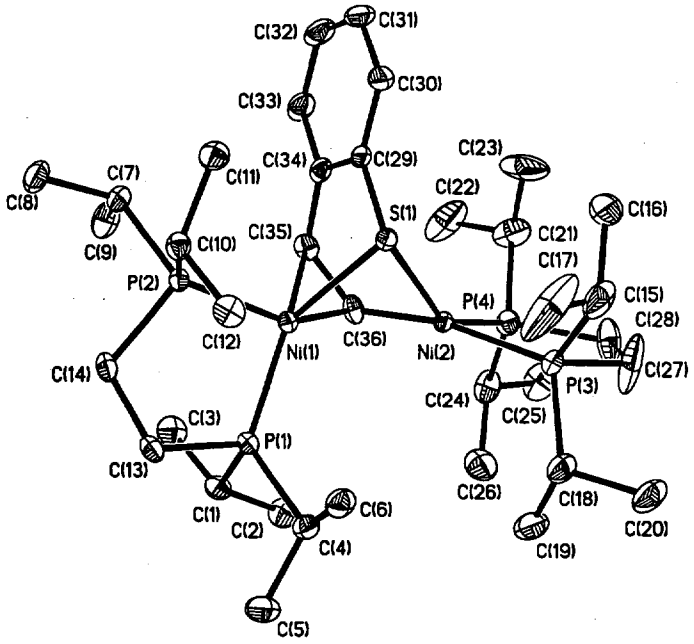

Figure 3. ORTEP drawing of $(dippe)_2Ni_2$(benzothiophene) **5**.

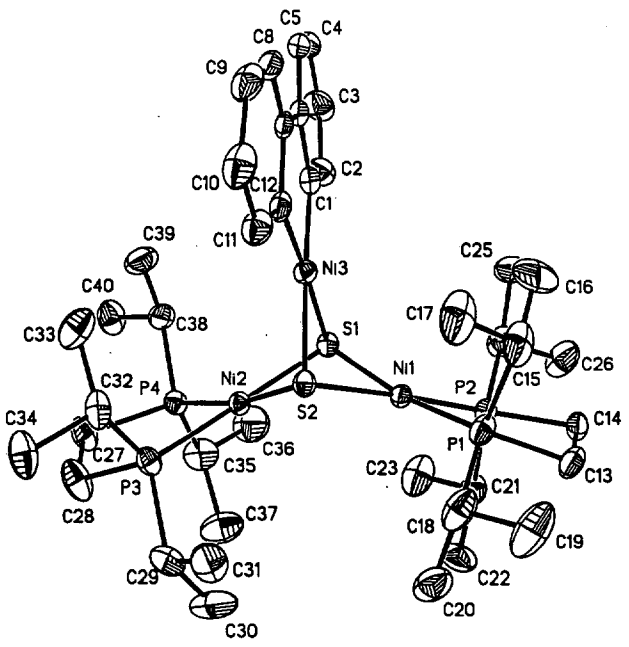

Figure 4. ORTEP drawing of $(dippe)_2Ni_3(\mu\text{-}S)_2(2,2'\text{-biphenyl})$ **9**.

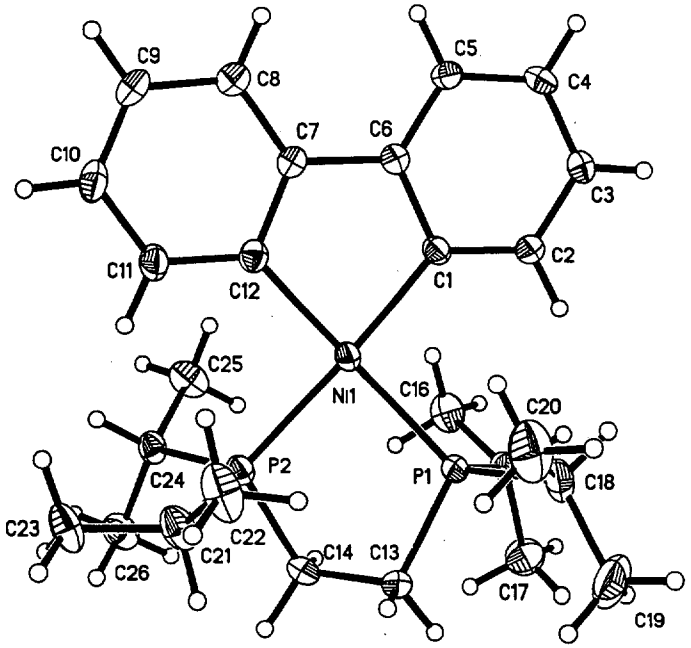

Figure 5. ORTEP drawing of (dippe)Ni_2(2,2'-biphenyl) **7**.

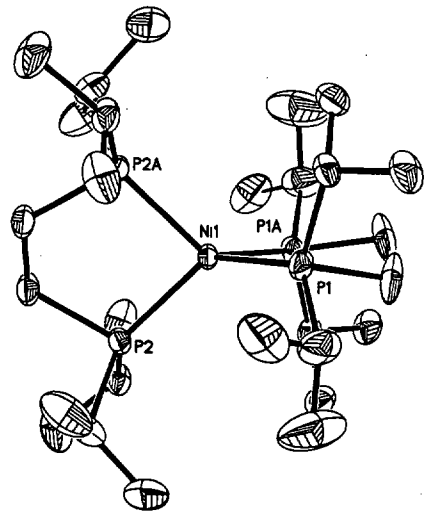

Figure 6. ORTEP drawing of $(dippe)_2Ni$ **10**.

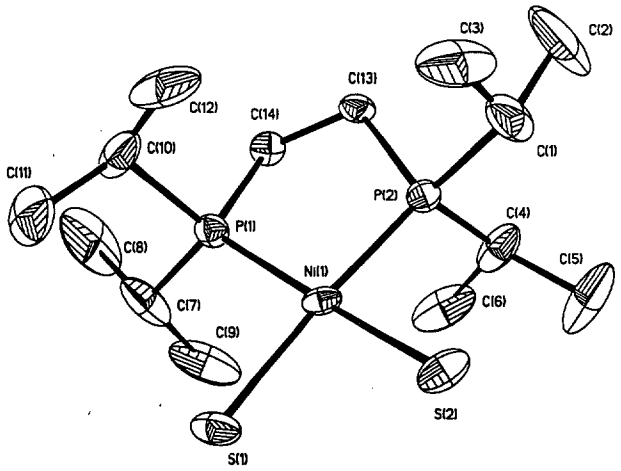

Figure 7. ORTEP drawing of (dippe)Ni(SH)$_2$ (**11**).

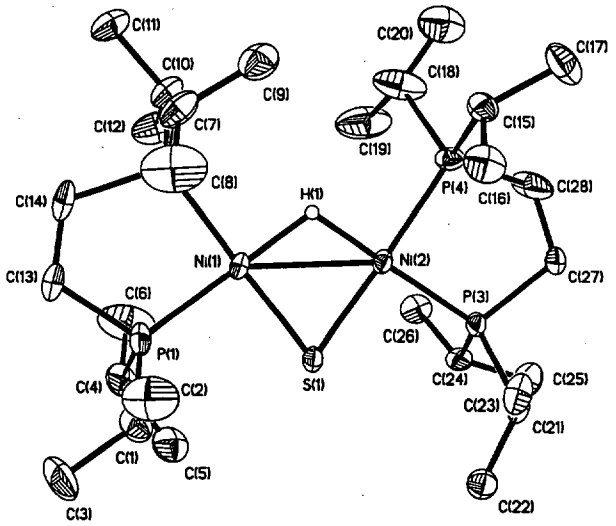

Figure 8 (a). ORTEP drawing of the cationic core of **12**. All hydrogen atoms except for the bridging hydride are omitted for clarity. The PF_6^- counterion is also omitted.

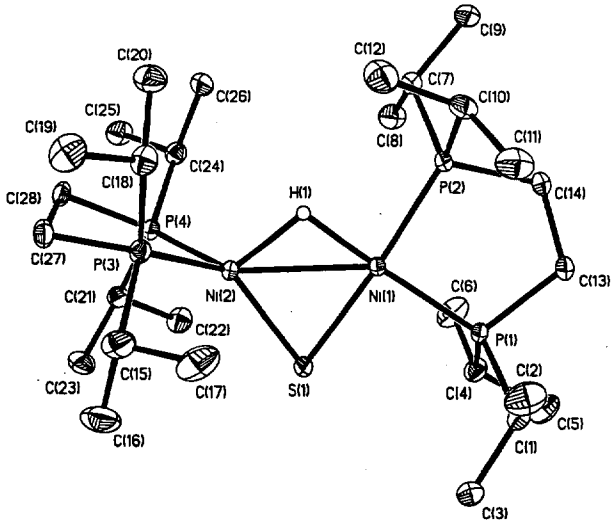

Figure 8 (b) ORTEP drawing of **13**. All hydrogen atoms except for the bridging hydride are omitted for clarity.

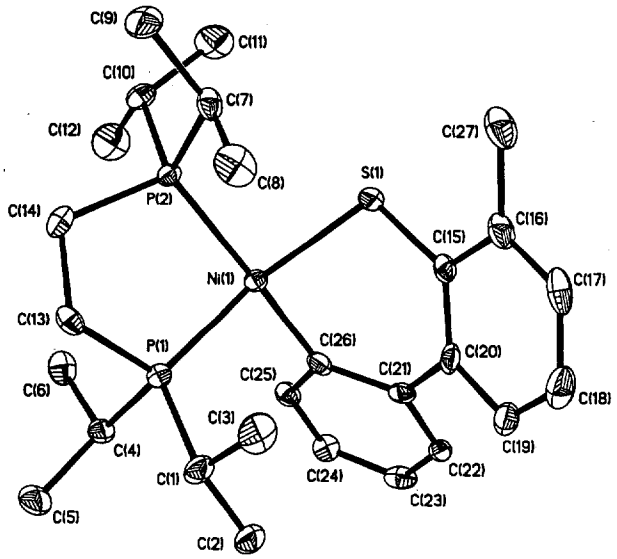

Figure 10. ORTEP drawing of (dippe)Ni(η^2-C,S-4-methyldibenzothiophene) **14**.

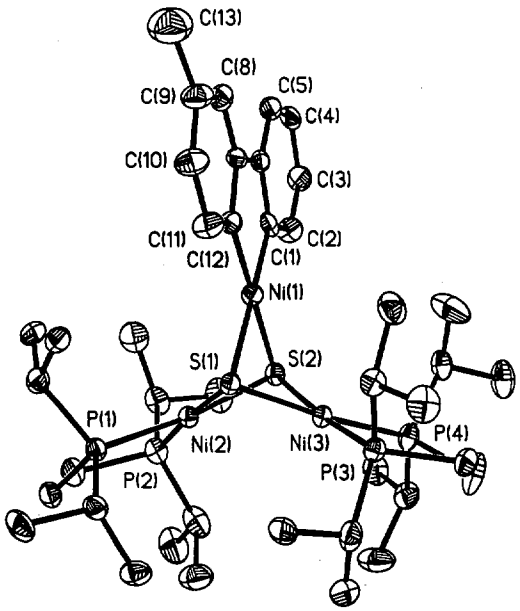

Figure 11. ORTEP drawing of rearranged product **15**.

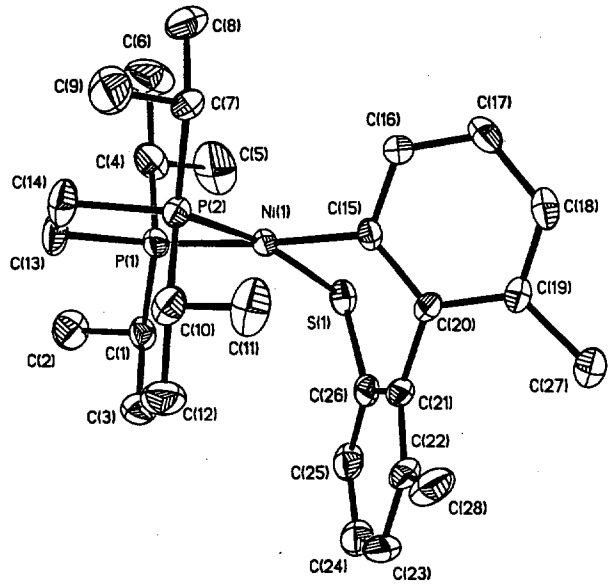

Figure 12. ORTEP drawing of (dippe)Ni(η^2-C,S-1,9-dimethyldibenzothiophene) **19**.

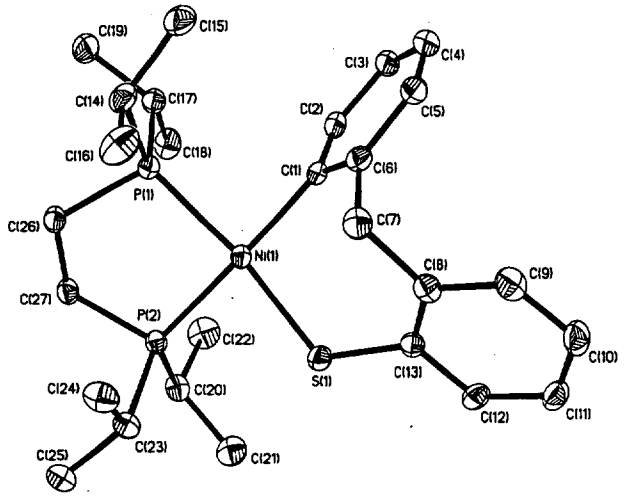

Figure 13. ORTEP drawing of (dippe)Ni(η^2-C,S-thioxanthene) **20**.

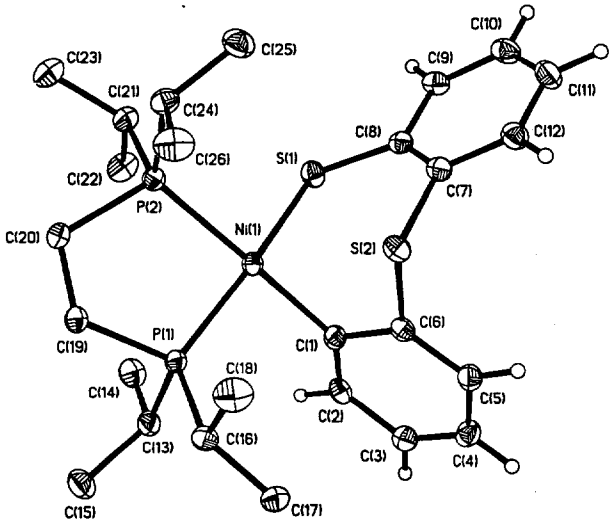

Figure 14. ORTEP drawing of (dippe)Ni(η^2-C,S-thianthrene) **21**.

Part III. Tables of Crystallographic Information:

Table S-1. Crystallographic data for compounds **2**, **4**, and **5**.

Crystal Parameters	**2**	**4**	**5**
chemical formula	$C_{18}H_{36}NiP_2S$	$C_{22}H_{38}NiP_2S$	$C_{28}H_{44}NiP_2S$
formula weight	405.18	455.24	776.28
cryst syst	rhombohedral	monoclinic	monoclinic
space group (No.)	*R*3*c*	*C*2/*c*	$P2_1/n$
Z	18	12	4
a, Å	26.9434(3)	26.8030 (20)	11.5365 (2)
b, Å	26.9434(3)	15.3487(13)	23.5981 (3)
c, Å	15.0018(3)	18.1040(14)	14.7722 (2)
β, deg	90	90	90.7210 (10)
vol., Å3	9431.5(2)	7407.9(10)	4021.26(10)
ρ_{calc}, g cm^{-3}	1.284	1.248	1.282
cryst dimens, mm^3	0.03 x 0.03 x 0.40	0.01 x 0.14 x 0.18	0.35 x 0.42 x 0.50
temp, °C	-70	-80	-80
Measurement of Intensity Data			
diffractometer	Siemens SMART	Siemens SMART	Siemens SMART
radiation	Mo, 0.71073 Å	Mo, 0.71073 Å	Mo, 0.71073 Å
frame range/time, deg/sec	0.3/30	0.3/30	0.3/10
2θ range, deg	3.02-46.56	3.06-40.00	3.30-46.50
data collected	$-29 \le h \le 29$, $-29 \le k \le 23$, $-16 \le l \le 16$	$-22 \le h$ 29, $-17 \le k \le 16$, $-20 \le l \le 18$	$-12 \le h \le 15$, $-31 \le k \le 27$, $-19 \le l \le 19$
no. of data collected	12790	10280	20055
no. of unique data	2974	3378	6997
no. of obs data ($F_o>4\sigma(F_o)$)	2561	2495	6219
agreement between equivalent data (R_{int})	0.0649	0.0802	0.0235
no. of params varied	190	362	404
μ, mm^{-1}	1.174	1.007	1.171
abs cor	empirical (SADABS)	empirical (SADABS)	empirical (SADABS)
range of trans. factors	0.928 - 0.814	0.928 - 0.805	0.928 - 0.817
$R_1(F_o)$, $wR_2(F_o^2)$, ($F_o>4\sigma(F_o)$)	0.0479, 0.0652	0.1058, 0.2465	0.0336, 0.0766
$R_1(F_o)$, $wR_2(F_o^2)$, (all data)	0.0612, 0.0679	0.1421, 0.2678	0.0400, 0.0797
goodness of fit	1.161	1.139	1.039

Table S-2. Crystallographic data for compounds **7**, **9**, and **10**.

Crystal Parameters	**7**	**9**·$(2C_6H_6)$	**10**
chemical formula	$C_{26}H_{40}NiP_2$	$C_{40}H_{72}Ni_3P_4S_2$	$C_{28}H_{64}NiP_4$
formula weight	473.23	917.09	583.38
cryst syst	monoclinic	monoclinic	monoclinic
space group (No.)	$P2_1/n$	$C2/c$	$C2/c$
Z	4	12	4
a, Å	8.3256 (3)	35.5706(1)	19.3695(2)
b, Å	15.3734(5)	20.9896(2)	9.8492(1)
c, Å	19.3875(6)	19.9602(2)	18.7555(2)
β, deg	95.3090(10)	98.7470(10)	113.0130(10)
vol., Å^3	2470.81(14)	14729.2(2)	3293.31(6)
ρ_{calc}, g cm^{-3}	1.272	1.273	1.177
cryst dimens, mm^3	0.08 x 0.26 x 0.28	0.20 x 0.20 x 0.40	0.24 x 0.33 x 0.42
temp, °C	-80	-80	-80
Measurement of Intensity Data			
diffractometer	Siemens SMART	Siemens SMART	Siemens SMART
radiation	Mo, 0.71073 Å	Mo, 0.71073 Å	Mo, 0.71073 Å
frame range/time, deg/sec	0.3/10	0.3/10	0.3/10
2θ range, deg	3.38-50.00	2.94-45.00	4.56-50.00
data collected	$-11 \le h \le 7$, $-17 \le k \le 20$, $-24 \le l \le 25$	$-47 \le h \le 37$, $-26 \le k \le 27$, $-24 \le l \le 26$	$-22 \le h \le 25$, $-13 \le k \le 12$, $-24 \le l \le 12$
no. of data collected	11659	28192	7983
no. of unique data	4238	9399	2846
no. of obs data ($F_o>4\sigma(F_o)$)	3438	7941	2539
agreement between equivalent data (R_{int})	0.0395	0.0330	0.0219
no. of params varied	270	687	150
μ, mm^{-1}	0.925	1.380	0.798
abs cor	empirical (SADABS)	empirical (SADABS)	empirical (SADABS)
range of trans. factors	0.928 - 0.774	0.928 - 0.784	0.928 - 0.832
$R_1(F_o)$, $wR_2(F_o^2)$, ($F_o>4\sigma(F_o)$)	0.0497, 0.0815	0.0504, 0.1320	0.0444, 0.1148
$R_1(F_o)$, $wR_2(F_o^2)$, (all data)	0.0697, 0.0878	0.0641, 0.1392	0.0512, 0.1190
goodness of fit	1.081	1.141	1.106

Table S-3. Crystallographic data for compounds **11**, **13**, and **15**.

Crystal Parameters	**11**	**13**	**15**
chemical formula	$C_{14}H_{32}P_2NiS$	$C_{28}H_{65}Ni_2P_4S$	$C_{41}H_{74}Ni_3P_4S_2$
formula weight	385.17	675.16	931.13
cryst syst	tetragonal	triclinic	triclinic
space group, Z	*I-4*,8	*P-1*,2	*P-1*,6
a, Å	14.62600(10)	9.0236(1)	20.4729(4)
b, Å	14.62600(10)	12.0684(2)	20.6412(4)
c, Å	18.450	18.4693(3)	20.9174(4)
β, deg	90	96.3630(10)	61.3710(10)
vol., Å^3	3946.74(4)	1786.73(5)	7564.3(3)
ρ_{calc}, g cm^{-3}	1.296	1.255	1.226
cryst dimens, mm^3	0.25 x 0.28 x 0.30	0.23 x 0.31 x 0.51	0.20 x 0.25 x 0.35
temp, °C	-80	-80	-80
Measurement of Intensity Data			
diffractometer	Siemens SMART	Siemens SMART	
radiation	Mo, 0.71073 Å	Mo, 0.71073 Å	Mo, 0.71073 Å
frame range/time, deg/sec	0.3/10	0.3/10	0.3/10
2θ range, deg	3.56 - 56056	3.78-56.62	2.76 - 46.50
data collected	$-19 \le h \le 18$, $-19 \le k \le 19$, $-24 \le l \le 19$	$-11 \le h \le 11$, $-6 \le k \le 16$, $-24 \le l \le 23$	$-27 \le h \le 21$, $-27 \le k \le 27$, $-27 \le l \le 25$
no. of data collected	11979	11136	30196
no. of unique data	4581	7841	19468
no. of obs data ($F_o>4\sigma(F_o)$)	3973	6909	12380
agreement between equivalent data (R_{int})	0.0228	0.0146	0.0423
no. of params varied	172	336	1397
μ, mm^{-1}	1.345	1.307	1.343
abs cor	empirical (SADABS)	empirical (SADABS)	empirical (SADABS)
range of trans. factors	0.928 - 0.825	0.928 - 0.778	0.928 - 0.827
$R_1(F_o)$, $wR_2(F_o^2)$, ($F_o>4\sigma(F_o)$)	0.0379, 0.0846	0.0310, 0.0673	0.0820, 0.2202
$R_1(F_o)$, $wR_2(F_o^2)$, (all data)	0.0474, 0.0895	0.0376, 0.0703	0.1249, 0.2442
goodness of fit	1.096	1.046	1.088

Table S-4. Crystallographic data for compounds **19**, **20**, and **21**.

Crystal Parameters	**19**	**20**	**21**
chemical formula	$C_{28}H_{44}NiP_2S$	$C_{27}H_{42}NiP_2S$	$C_{26}H_{40}NiP_2S_2$
formula weight	533.34	519.32	537.35
cryst syst	monoclinic	monoclinic	monoclinic
space group, Z	$P2_1/c$, 4	$P2_1/c$, 4	$P2_1/c$, 4
a, Å	9.4302(2)	11.4852(2)	10.3177(1)
b, Å	14.8247(1)	15.7422(3)	16.3507(2)
c, Å	22.2210(3)	14.9948(3)	15.9480(1)
β, deg	92.1920(10)	94.8800(10)	96.28
vol., Å^3	3104.22(8)	2701.27(9)	2674.33(4)
ρ_{calc}, g cm^{-3}	1.141	1.277	1.335
cryst dimens, mm^3	0.20 x 0.20 x 0.35	0.20 x 0.20 x 0.30	0.20 x 0.30 x 0.40
temp, °C	-80	-80	-80
Measurement of Intensity Data			
diffractometer	Siemens SMART	Siemens SMART	Siemens SMART
radiation	Mo, 0.71073 Å	Mo, 0.71073 Å	Mo, 0.71073 Å
frame range/time, deg/sec	0.3/30	0.3/10	0.3/10
2θ range, deg	3.30-46.50	3.56-56.6	3.58-56.66
data collected	$-10 \le h \le 12$, $-13 \le k \le 19$, $-24 \le l \le 28$	$-13 \le h \le 14$, $-11 \le k \le 20$, $-17 \le l \le 19$	$-13 \le h \le 5$, $-21 \le k \le 20$, $-21 \le l \le 21$
no. of data collected	12550	15493	15702
no. of unique data	4352	6198	6177
no. of obs data ($F_o>4\sigma(F_o)$)	3461	4686	5124
agreement between equivalent data (R_{int})	0.0428	0.0458	0.0513
no. of params varied	299	288	288
μ, mm^{-1}	0.808	0.927	1.014
abs cor	empirical (SADABS)	empirical (SADABS)	none
range of trans. factors	0.928 - 0.828	0.928 - 0.688	
$R_1(F_o)$, $wR_2(F_o^2)$, ($F_o>4\sigma(F_o)$)	0.0824, 0.2479	0.0632, 0.1039	0.0519, 0.1051
$R_1(F_o)$, $wR_2(F_o^2)$, (all data)	0.1035, 0.2622	0.0938, 0.1133	0.0677, 0.1125
goodness of fit	1.045	1.112	1.099

Table S-5A. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni(1)	4548(1)	5510(1)	1136(1)	30(1)
P(1)	4326(1)	4632(1)	802(1)	30(1)
P(2)	3811(1)	5379(1)	308(1)	33(1)
S(1A)	4805(1)	6406(1)	1186(1)	41(1)
C(4A)	5397(4)	6785(5)	1850(7)	45(3)
C(3A)	5681(4)	6593(4)	2344(7)	35(2)
C(2A)	5544(4)	6021(3)	2395(7)	35(2)
C(1A)	5109(4)	5560(4)	1975(7)	26(3)
S(1B)	5205(3)	5508(3)	1966(6)	41(1)
C(4B)	5624(12)	6180(9)	2384(20)	45(3)
C(3B)	5643(10)	6681(8)	2260(19)	35(2)
C(2B)	5254(10)	6754(10)	1725(17)	35(2)
C(1B)	4747(8)	6311(8)	1470(14)	26(3)
C(5)	4849(2)	4594(2)	37(3)	39(2)
C(6)	5031(2)	5048(3)	-684(4)	51(2)
C(7)	5372(2)	4655(3)	532(4)	62(2)
C(8)	4222(2)	4126(2)	1697(3)	31(1)
C(9)	3828(2)	4129(2)	2434(4)	48(2)
C(10)	3999(2)	3503(2)	1374(4)	50(2)
C(11)	3655(2)	4278(2)	152(3)	36(1)
C(12)	3549(2)	4715(2)	-347(4)	40(1)
C(13)	3917(2)	5926(2)	-533(4)	46(2)
C(14)	4431(3)	6066(3)	-1131(4)	59(2)
C(15)	3389(3)	5774(3)	-1108(4)	63(2)
C(16)	3169(2)	5273(2)	942(4)	39(1)
C(17)	2974(2)	4781(3)	1610(4)	60(2)
C(18)	3282(2)	5819(3)	1422(4)	60(2)

Table S-6A. Bond lengths [A] and angles [deg] for **2**.

Ni(1)-C(1B)	2.01(2)	S(1A)-Ni(1)-P(2)	87.70(7)
Ni(1)-C(1A)	1.923(10)	P(1)-Ni(1)-P(2)	87.72(5)
Ni(1)-S(1B)	2.168(8)	C(8)-P(1)-C(11)	104.9(2)
Ni(1)-S(1A)	2.152(2)	C(8)-P(1)-C(5)	104.4(2)
Ni(1)-P(1)	2.189(2)	C(11)-P(1)-C(5)	102.7(2)
Ni(1)-P(2)	2.215(2)	C(8)-P(1)-Ni(1)	119.7(2)
P(1)-C(8)	1.833(5)	C(11)-P(1)-Ni(1)	110.3(2)
P(1)-C(11)	1.845(5)	C(5)-P(1)-Ni(1)	113.3(2)
P(1)-C(5)	1.860(5)	C(12)-P(2)-C(13)	104.0(3)
P(2)-C(12)	1.845(5)	C(12)-P(2)-C(16)	104.3(2)
P(2)-C(13)	1.850(5)	C(13)-P(2)-C(16)	103.4(3)
P(2)-C(16)	1.867(5)	C(12)-P(2)-Ni(1)	109.4(2)
S(1A)-C(4A)	1.718(9)	C(13)-P(2)-Ni(1)	119.1(2)
C(4A)-C(3A)	1.339(13)	C(16)-P(2)-Ni(1)	115.3(2)
C(3A)-C(2A)	1.397(11)	C(4A)-S(1A)-Ni(1)	111.7(4)
C(2A)-C(1A)	1.363(12)	C(3A)-C(4A)-S(1A)	129.1(9)
S(1B)-C(4B)	1.70(2)	C(4A)-C(3A)-C(2A)	124.8(8)
C(4B)-C(3B)	1.34(3)	C(1A)-C(2A)-C(3A)	127.7(9)
C(3B)-C(2B)	1.41(2)	C(2A)-C(1A)-Ni(1)	130.9(7)
C(2B)-C(1B)	1.34(2)	C(4B)-S(1B)-Ni(1)	108.5(9)
C(5)-C(7)	1.527(7)	C(3B)-C(4B)-S(1B)	134(2)
C(5)-C(6)	1.519(7)	C(4B)-C(3B)-C(2B)	124(2)
C(8)-C(9)	1.536(6)	C(1B)-C(2B)-C(3B)	122(2)
C(8)-C(10)	1.549(6)	C(2B)-C(1B)-Ni(1)	129(2)
C(11)-C(12)	1.536(7)	C(7)-C(5)-C(6)	110.5(4)
C(13)-C(14)	1.531(7)	C(7)-C(5)-P(1)	112.3(4)
C(13)-C(15)	1.535(7)	C(6)-C(5)-P(1)	110.1(3)
C(16)-C(18)	1.527(7)	C(9)-C(8)-C(10)	109.7(4)
C(16)-C(17)	1.531(7)	C(9)-C(8)-P(1)	111.8(3)
		C(10)-C(8)-P(1)	114.2(4)
C(1B)-Ni(1)-S(1B)	94.6(5)	C(12)-C(11)-P(1)	111.8(3)
C(1A)-Ni(1)-S(1A)	95.6(3)	C(11)-C(12)-P(2)	110.9(3)
C(1B)-Ni(1)-P(1)	178.8(6)	C(14)-C(13)-C(15)	109.9(5)
C(1A)-Ni(1)-P(1)	90.2(3)	C(14)-C(13)-P(2)	110.8(4)
S(1B)-Ni(1)-P(1)	84.8(2)	C(15)-C(13)-P(2)	114.7(4)
S(1A)-Ni(1)-P(1)	168.56(8)	C(18)-C(16)-C(17)	110.1(5)
C(1B)-Ni(1)-P(2)	92.8(5)	C(18)-C(16)-P(2)	111.7(3)
C(1A)-Ni(1)-P(2)	172.1(3)	C(17)-C(16)-P(2)	110.9(4)
S(1B)-Ni(1)-P(2)	171.9(2)		

Table S-7A. Anisotropic displacement parameters (A^2 x 10^3) for **2**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni(1)	24(1)	28(1)	33(1)	-6(1)	-3(1)	10(1)
P(1)	24(1)	32(1)	34(1)	-4(1)	-3(1)	13(1)
P(2)	28(1)	32(1)	39(1)	-4(1)	-3(1)	15(1)
C(5)	33(3)	51(4)	41(3)	-9(3)	-3(3)	27(3)
C(6)	39(4)	79(5)	36(3)	5(3)	9(3)	29(3)
C(7)	46(4)	105(5)	54(4)	4(4)	9(3)	52(4)
C(8)	25(3)	31(3)	37(3)	-3(3)	2(3)	15(3)
C(9)	46(4)	50(4)	47(4)	15(3)	11(3)	22(3)
C(10)	53(4)	37(4)	59(4)	0(3)	-2(3)	22(3)
C(11)	27(3)	29(3)	46(4)	-9(3)	-2(3)	8(3)
C(12)	26(3)	41(4)	46(4)	-6(3)	-13(3)	12(3)
C(13)	39(4)	45(4)	53(4)	6(3)	-4(3)	18(3)
C(14)	58(4)	60(4)	57(4)	14(3)	5(4)	27(4)
C(15)	64(4)	68(5)	62(4)	11(4)	-14(4)	36(4)
C(16)	26(3)	46(4)	50(4)	-6(3)	1(3)	22(3)
C(17)	41(4)	67(5)	75(5)	10(4)	16(3)	30(4)
C(18)	53(4)	58(5)	78(5)	-3(4)	12(4)	34(4)

Table S-8A. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**.

	x	y	z	U(eq)
H(4AA)	5543(4)	7183(5)	1869(7)	54
H(3AA)	5994(4)	6863(4)	2681(7)	42
H(2AA)	5781(4)	5944(3)	2763(7)	42
H(1AA)	5079(4)	5206(4)	2121(7)	31
H(4BA)	5901(12)	6203(9)	2790(20)	54
H(3BA)	5936(10)	7006(8)	2548(19)	42
H(2BA)	5352(10)	7125(10)	1540(17)	42
H(1BA)	4442(8)	6386(8)	1444(14)	31
H(5A)	4655(2)	4214(2)	-255(3)	47
H(6A)	4694(2)	5005(3)	-988(4)	77
H(6B)	5277(2)	5003(3)	-1109(4)	77
H(6C)	5238(2)	5425(3)	-416(4)	77
H(7A)	5248(2)	4362(3)	989(4)	93
H(7B)	5578(2)	5030(3)	806(4)	93
H(7C)	5622(2)	4610(3)	114(4)	93
H(8A)	4601(2)	4258(2)	1972(3)	37
H(9A)	3969(2)	4519(2)	2636(4)	72
H(9B)	3823(2)	3895(2)	2929(4)	72
H(9C)	3442(2)	3975(2)	2201(4)	72
H(10A)	4249(2)	3502(2)	910(4)	75
H(10B)	3614(2)	3347(2)	1140(4)	75
H(10C)	3995(2)	3270(2)	1871(4)	75
H(11A)	3674(2)	4015(2)	-279(3)	44
H(11B)	3332(2)	4052(2)	554(3)	44
H(12A)	3137(2)	4548(2)	-460(4)	48
H(12B)	3746(2)	4804(2)	-923(4)	48
H(13A)	4010(2)	6281(2)	-204(4)	56
H(14A)	4762(3)	6159(3)	-763(4)	89
H(14B)	4512(3)	6390(3)	-1508(4)	89
H(14C)	4343(3)	5736(3)	-1500(4)	89
H(15A)	3064(3)	5684(3)	-726(4)	95
H(15B)	3301(3)	5444(3)	-1477(4)	95
H(15C)	3467(3)	6097(3)	-1487(4)	95
H(16A)	2853(2)	5169(2)	511(4)	47
H(17A)	2901(2)	4435(3)	1299(4)	90
H(17B)	2626(2)	4716(3)	1903(4)	90
H(17C)	3272(2)	4879(3)	2052(4)	90
H(18A)	3402(2)	6128(3)	992(4)	91
H(18B)	3582(2)	5922(3)	1862(4)	91
H(18C)	2934(2)	5755(3)	1716(4)	91

Table S-5B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni(1A)	2556(1)	2259(1)	2335(1)	28(1)
S(1A)	2048(2)	2836(3)	3023(2)	38(1)
C(1A)	2166(6)	2545(10)	1423(8)	34(4)
C(2A)	1731(6)	2970(11)	1280(8)	42(5)
C(3A)	1426(6)	3363(10)	1793(9)	35(4)
C(4A)	1511(5)	3327(10)	2561(8)	26(4)
C(5A)	1177(5)	3704(10)	2994(9)	35(4)
C(6A)	743(6)	4133(11)	2612(9)	49(5)
C(7A)	678(6)	4151(12)	1910(9)	54(5)
C(8A)	992(6)	3797(10)	1474(9)	41(5)
P(1A)	3174(2)	1855(3)	1745(2)	34(1)
P(2A)	2971(2)	1728(3)	3360(2)	32(1)
C(9A)	3553(6)	2774(11)	1448(9)	45(5)
C(10A)	3680(7)	3401(12)	2112(10)	60(6)
C(11A)	3311(7)	3262(11)	780(10)	55(5)
C(12A)	3059(6)	1169(11)	911(9)	40(5)
C(13A)	2699(7)	443(12)	1013(9)	55(5)
C(14A)	3545(7)	823(12)	629(9)	57(6)
C(15A)	2704(6)	698(11)	3677(9)	46(5)
C(16A)	2232(7)	858(12)	4064(10)	56(5)
C(17A)	2605(7)	61(11)	3039(10)	56(5)
C(18A)	3060(6)	2422(10)	4203(8)	35(4)
C(19A)	3374(7)	1967(12)	4854(9)	58(6)
C(20A)	3293(7)	3297(12)	4021(9)	56(5)
C(21A)	3628(6)	1184(11)	2350(8)	39(5)
C(22A)	3614(6)	1424(11)	3157(9)	46(5)
Ni(1B)	0	13(2)	2500	44(1)
S(1B)	24(3)	-1016(6)	1781(5)	39(2)
C(1B)	-11(5)	-603(17)	3398(14)	59(17)
C(2B)	15(15)	-1424(17)	3557(15)	101(21)
C(3B)	14(12)	-2114(12)	3036(12)	33(10)
C(4B)	28(12)	-2132(11)	2266(12)	27(10)
C(5B)	21(14)	-2927(15)	1947(13)	76(14)
C(6B)	0	-3737(14)	2500	68(8)
C(7B)	16(10)	-3603(14)	3138(12)	27(8)
C(8B)	23(11)	-2869(14)	3467(12)	41(9)
P(1B)	110(2)	1031(3)	1704(2)	41(1)
C(9B)	747(6)	1144(12)	1445(10)	50(5)
C(10B)	880(7)	477(14)	857(11)	76(7)
C(11B)	1120(7)	1071(14)	2159(11)	74(6)
C(12B)	-283(7)	1024(16)	786(11)	74(7)
C(13B)	-830(7)	870(17)	900(10)	90(8)
C(14B)	-234(10)	1849(21)	349(13)	139(13)
C(15B)	-26(9)	2080(12)	2112(9)	68(6)
O(1)	4614(4)	-536(7)	133(6)	50(3)

Table S-6B. Bond lengths [A] and angles [deg] for **4**.

Ni(1A)-C(1A)	1.910(14)	C(5B)-C(4B)#1	1.89(3)
Ni(1A)-S(1A)	2.131(4)	C(6B)-C(7B)	1.17(2)
Ni(1A)-P(1A)	2.152(4)	C(6B)-C(7B)#1	1.17(2)
Ni(1A)-P(2A)	2.219(4)	C(6B)-C(5B)#1	1.60(3)
S(1A)-C(4A)	1.758(14)	C(7B)-C(5B)#1	1.05(3)
C(1A)-C(2A)	1.34(2)	C(7B)-C(8B)	1.27(3)
C(2A)-C(3A)	1.43(2)	C(8B)-C(5B)#1	0.75(3)
C(3A)-C(4A)	1.39(2)	C(8B)-C(4B)#1	1.74(3)
C(3A)-C(8A)	1.41(2)	P(1B)-C(9B)	1.82(2)
C(4A)-C(5A)	1.38(2)	P(1B)-C(15B)	1.82(2)
C(5A)-C(6A)	1.45(2)	P(1B)-C(12B)	1.87(2)
C(6A)-C(7A)	1.27(2)	C(9B)-C(10B)	1.55(2)
C(7A)-C(8A)	1.33(2)	C(9B)-C(11B)	1.56(2)
P(1A)-C(12A)	1.84(2)	C(12B)-C(14B)	1.51(3)
P(1A)-C(9A)	1.85(2)	C(12B)-C(13B)	1.52(3)
P(1A)-C(21A)	1.86(2)	C(15B)-C(15B)#1	1.40(3)
P(2A)-C(15A)	1.85(2)		
P(2A)-C(18A)	1.86(2)	C(1A)-Ni(1A)-S(1A)	94.8(5)
P(2A)-C(22A)	1.86(2)	C(1A)-Ni(1A)-P(1A)	91.0(5)
C(9A)-C(11A)	1.51(2)	S(1A)-Ni(1A)-P(1A)	168.8(2)
C(9A)-C(10A)	1.55(2)	C(1A)-Ni(1A)-P(2A)	171.6(5)
C(12A)-C(13A)	1.50(2)	S(1A)-Ni(1A)-P(2A)	87.7(2)
C(12A)-C(14A)	1.54(2)	P(1A)-Ni(1A)-P(2A)	88.0(2)
C(15A)-C(17A)	1.52(2)	C(4A)-S(1A)-Ni(1A)	116.2(5)
C(15A)-C(16A)	1.53(2)	C(2A)-C(1A)-Ni(1A)	131.8(12)
C(18A)-C(20A)	1.53(2)	C(1A)-C(2A)-C(3A)	129(2)
C(18A)-C(19A)	1.54(2)	C(4A)-C(3A)-C(8A)	118.1(13)
C(21A)-C(22A)	1.51(2)	C(4A)-C(3A)-C(2A)	126.0(14)
Ni(1B)-C(1B)#1	1.88(2)	C(8A)-C(3A)-C(2A)	115.8(14)
Ni(1B)-C(1B)	1.88(2)	C(5A)-C(4A)-C(3A)	120.4(13)
Ni(1B)-S(1B)#1	2.052(9)	C(5A)-C(4A)-S(1A)	117.3(11)
Ni(1B)-S(1B)	2.052(9)	C(3A)-C(4A)-S(1A)	122.3(11)
Ni(1B)-P(1B)#1	2.167(5)	C(4A)-C(5A)-C(6A)	117.1(14)
Ni(1B)-P(1B)	2.167(5)	C(7A)-C(6A)-C(5A)	121(2)
S(1B)-C(1B)#1	0.71(3)	C(6A)-C(7A)-C(8A)	124(2)
S(1B)-C(2B)#1	0.87(3)	C(7A)-C(8A)-C(3A)	120(2)
S(1B)-C(3B)#1	1.72(2)	C(12A)-P(1A)-C(9A)	104.4(8)
S(1B)-C(4B)	1.92(2)	C(12A)-P(1A)-C(21A)	102.1(7)
C(1B)-S(1B)#1	0.71(3)	C(9A)-P(1A)-C(21A)	104.3(8)
C(1B)-C(2B)	1.29(3)	C(12A)-P(1A)-Ni(1A)	120.0(6)
C(2B)-S(1B)#1	0.87(3)	C(9A)-P(1A)-Ni(1A)	113.5(6)
C(2B)-C(3B)	1.42(3)	C(21A)-P(1A)-Ni(1A)	110.9(5)
C(2B)-C(4B)#1	1.84(3)	C(15A)-P(2A)-C(18A)	104.9(8)
C(3B)-C(4B)#1	0.55(3)	C(15A)-P(2A)-C(22A)	104.1(8)
C(3B)-C(5B)#1	1.25(3)	C(18A)-P(2A)-C(22A)	105.3(7)
C(3B)-C(8B)	1.40(3)	C(15A)-P(2A)-Ni(1A)	113.4(6)
C(3B)-C(4B)	1.40(3)	C(18A)-P(2A)-Ni(1A)	119.1(5)
C(3B)-S(1B)#1	1.72(2)	C(22A)-P(2A)-Ni(1A)	108.8(6)
C(3B)-C(3B)#1	1.94(4)	C(11A)-C(9A)-C(10A)	111(2)
C(4B)-C(3B)#1	0.55(3)	C(11A)-C(9A)-P(1A)	114.0(12)
C(4B)-C(4B)#1	0.88(4)	C(10A)-C(9A)-P(1A)	109.3(11)
C(4B)-C(5B)	1.35(3)	C(13A)-C(12A)-C(14A)	111(2)
C(4B)-C(8B)#1	1.74(3)	C(13A)-C(12A)-P(1A)	112.4(11)
C(4B)-C(2B)#1	1.84(3)	C(14A)-C(12A)-P(1A)	113.2(11)
C(4B)-C(5B)#1	1.89(3)	C(17A)-C(15A)-C(16A)	112(2)
C(5B)-C(8B)#1	0.75(3)	C(17A)-C(15A)-P(2A)	111.0(11)
C(5B)-C(7B)#1	1.05(3)	C(16A)-C(15A)-P(2A)	111.7(12)
C(5B)-C(3B)#1	1.25(3)	C(20A)-C(18A)-C(19A)	111.1(14)
C(5B)-C(6B)	1.60(3)	C(20A)-C(18A)-P(2A)	110.4(11)

C(19A)-C(18A)-P(2A)	112.4(11)	C(3B)#1-C(4B)-C(3B)	166(6)
C(22A)-C(21A)-P(1A)	110.8(11)	C(4B)#1-C(4B)-C(3B)	8(4)
C(21A)-C(22A)-P(2A)	111.6(11)	C(5B)-C(4B)-C(3B)	116(2)
C(1B)#1-Ni(1B)-C(1B)	120(2)	C(3B)#1-C(4B)-C(8B)#1	44(3)
C(1B)#1-Ni(1B)-S(1B)#1	99.5(9)	C(4B)#1-C(4B)-C(8B)#1	137(2)
C(1B)-Ni(1B)-S(1B)#1	20.2(8)	C(5B)-C(4B)-C(8B)#1	24.3(13)
C(1B)#1-Ni(1B)-S(1B)	20.2(8)	C(3B)-C(4B)-C(8B)#1	140(2)
C(1B)-Ni(1B)-S(1B)	99.5(9)	C(3B)#1-C(4B)-C(2B)#1	34(3)
S(1B)#1-Ni(1B)-S(1B)	79.4(5)	C(4B)#1-C(4B)-C(2B)#1	142(2)
C(1B)#1-Ni(1B)-P(1B)#1	162.1(8)	C(5B)-C(4B)-C(2B)#1	101(2)
C(1B)-Ni(1B)-P(1B)#1	76.9(8)	C(3B)-C(4B)-C(2B)#1	142(2)
S(1B)#1-Ni(1B)-P(1B)#1	96.8(3)	C(8B)#1-C(4B)-C(2B)#1	76.9(14)
S(1B)-Ni(1B)-P(1B)#1	172.9(3)	C(3B)#1-C(4B)-C(5B)#1	140(4)
C(1B)#1-Ni(1B)-P(1B)	76.8(8)	C(4B)#1-C(4B)-C(5B)#1	40.4(9)
C(1B)-Ni(1B)-P(1B)	162.1(8)	C(5B)-C(4B)-C(5B)#1	75(2)
S(1B)#1-Ni(1B)-P(1B)	172.9(3)	C(3B)-C(4B)-C(5B)#1	41.5(12)
S(1B)-Ni(1B)-P(1B)	96.8(3)	C(8B)#1-C(4B)-C(5B)#1	98.6(13)
P(1B)#1-Ni(1B)-P(1B)	87.7(3)	C(2B)#1-C(4B)-C(5B)#1	172(3)
C(1B)#1-S(1B)-C(2B)#1	109(3)	C(3B)#1-C(4B)-S(1B)	61(3)
C(1B)#1-S(1B)-C(3B)#1	164(3)	C(4B)#1-C(4B)-S(1B)	116.6(8)
C(2B)#1-S(1B)-C(3B)#1	55(2)	C(5B)-C(4B)-S(1B)	128(2)
C(1B)#1-S(1B)-C(4B)	177.6(14)	C(3B)-C(4B)-S(1B)	116.0(14)
C(2B)#1-S(1B)-C(4B)	71(2)	C(8B)#1-C(4B)-S(1B)	103.6(13)
C(3B)#1-S(1B)-C(4B)	16.1(11)	C(2B)#1-C(4B)-S(1B)	26.7(9)
C(1B)#1-S(1B)-Ni(1B)	66(2)	C(5B)#1-C(4B)-S(1B)	157.1(14)
C(2B)#1-S(1B)-Ni(1B)	170(3)	C(8B)#1-C(5B)-C(7B)#1	88(3)
C(3B)#1-S(1B)-Ni(1B)	128.7(9)	C(8B)#1-C(5B)-C(3B)#1	84(3)
C(4B)-S(1B)-Ni(1B)	113.2(7)	C(7B)#1-C(5B)-C(3B)#1	168(4)
S(1B)#1-C(1B)-C(2B)	40(2)	C(8B)#1-C(5B)-C(4B)	108(3)
S(1B)#1-C(1B)-Ni(1B)	93(3)	C(7B)#1-C(5B)-C(4B)	162(3)
C(2B)-C(1B)-Ni(1B)	133(2)	C(3B)#1-C(5B)-C(4B)	24(2)
S(1B)#1-C(2B)-C(1B)	31(2)	C(8B)#1-C(5B)-C(6B)	135(3)
S(1B)#1-C(2B)-C(3B)	94(2)	C(7B)#1-C(5B)-C(6B)	47(2)
C(1B)-C(2B)-C(3B)	126(2)	C(3B)#1-C(5B)-C(6B)	139(2)
S(1B)#1-C(2B)-C(4B)#1	82(2)	C(4B)-C(5B)-C(6B)	116(2)
C(1B)-C(2B)-C(4B)#1	114(2)	C(8B)#1-C(5B)-C(4B)#1	131(3)
C(3B)-C(2B)-C(4B)#1	12.5(12)	C(7B)#1-C(5B)-C(4B)#1	137(3)
C(4B)#1-C(3B)-C(5B)#1	88(3)	C(3B)#1-C(5B)-C(4B)#1	47.7(14)
C(4B)#1-C(3B)-C(8B)	120(3)	C(4B)-C(5B)-C(4B)#1	24.9(12)
C(5B)#1-C(3B)-C(8B)	32(2)	C(6B)-C(5B)-C(4B)#1	91.2(14)
C(4B)#1-C(3B)-C(4B)	13(6)	C(7B)-C(6B)-C(7B)#1	160(3)
C(5B)#1-C(3B)-C(4B)	91(2)	C(7B)-C(6B)-C(5B)#1	41.1(14)
C(8B)-C(3B)-C(4B)	123(2)	C(7B)#1-C(6B)-C(5B)#1	119(2)
C(4B)#1-C(3B)-C(2B)	133(4)	C(7B)-C(6B)-C(5B)	119(2)
C(5B)#1-C(3B)-C(2B)	136(2)	C(7B)#1-C(6B)-C(5B)	41.1(14)
C(8B)-C(3B)-C(2B)	104(2)	C(5B)#1-C(6B)-C(5B)	78(2)
C(4B)-C(3B)-C(2B)	133(2)	C(5B)#1-C(7B)-C(6B)	92(2)
C(4B)#1-C(3B)-S(1B)#1	103(3)	C(5B)#1-C(7B)-C(8B)	36(2)
C(5B)#1-C(3B)-S(1B)#1	165(3)	C(6B)-C(7B)-C(8B)	128(2)
C(8B)-C(3B)-S(1B)#1	135(2)	C(5B)#1-C(8B)-C(7B)	56(2)
C(4B)-C(3B)-S(1B)#1	103(2)	C(5B)#1-C(8B)-C(3B)	63(2)
C(2B)-C(3B)-S(1B)#1	30.4(12)	C(7B)-C(8B)-C(3B)	118(2)
C(4B)#1-C(3B)-C(3B)#1	10(4)	C(5B)#1-C(8B)-C(4B)#1	48(2)
C(5B)#1-C(3B)-C(3B)#1	92(2)	C(7B)-C(8B)-C(4B)#1	103(2)
C(8B)-C(3B)-C(3B)#1	123.9(12)	C(3B)-C(8B)-C(4B)#1	15.8(11)
C(4B)-C(3B)-C(3B)#1	4(2)	C(9B)-P(1B)-C(15B)	104.6(10)
C(2B)-C(3B)-C(3B)#1	131.6(13)	C(9B)-P(1B)-C(12B)	103.2(9)
S(1B)#1-C(3B)-C(3B)#1	101.3(8)	C(15B)-P(1B)-C(12B)	104.3(10)
C(3B)#1-C(4B)-C(4B)#1	158(9)	C(9B)-P(1B)-Ni(1B)	115.8(6)
C(3B)#1-C(4B)-C(5B)	68(3)	C(15B)-P(1B)-Ni(1B)	108.7(6)
C(4B)#1-C(4B)-C(5B)	114.7(13)	C(12B)-P(1B)-Ni(1B)	118.8(8)

C(10B)-C(9B)-C(11B)	110(2)	C(14B)-C(12B)-P(1B)	113(2)
C(10B)-C(9B)-P(1B)	113.8(12)	C(13B)-C(12B)-P(1B)	110.1(14)
C(11B)-C(9B)-P(1B)	108.6(12)	C(15B)#1-C(15B)-P(1B)	113.8(8)
C(14B)-C(12B)-C(13B)	110(2)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table S-7B. Anisotropic displacement parameters (A^2 x 10^3) for **4**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni(1A)	24(1)	32(1)	29(1)	1(1)	2(1)	6(1)
S(1A)	34(3)	48(3)	31(2)	0(2)	5(2)	15(2)
C(1A)	36(10)	36(11)	27(9)	2(8)	-5(8)	17(9)
C(2A)	50(12)	52(12)	23(10)	-1(9)	-2(9)	15(10)
C(3A)	35(11)	24(10)	46(12)	5(9)	8(9)	13(8)
C(4A)	1`(8)	36(10)	33(11)	-4(8)	6(8)	6(7)
C(5A)	22(10)	38(10)	48(11)	-6(9)	9(9)	-13(8)
C(7A)	47(12)	77(15)	37(11)	4(10)	-6(10)	28(11)
C(8A)	40(11)	33(11)	51(11)	3(9)	3(10)	15(9)
P(1A)	29(3)	39(3)	34(3)	-1(2)	4(2)	11(2)
P(2A)	25(3)	39(3)	31(3)	1(2)	-3(2)	9(2)
C(9A)	41(11)	44(11)	53(12)	8(10)	16(9)	2(9)
C(10A)	60(13)	69(15)	54(13)	-7(11)	16(11)	-20(11)
C(11A)	63(13)	40(12)	65(13)	17(10)	26(11)	8(10)
C(12A)	42(11)	48(12)	28(10)	2(9)	-5(8)	11(10)
C(13A)	66(13)	58(13)	38(11)	-23(10)	-12(10)	-5(11)
C(14A)	62(13)	68(14)	40(11)	-9(10)	-5(10)	32(11)
C(15A)	51(12)	41(12)	46(11)	18(10)	3(10)	14(9)
C(16A)	65(13)	58(13)	51(12)	-2(10)	24(11)	-7(11)
C(17A)	69(14)	44(12)	56(12)	-5(11)	1`(10)	-13(10)
C(18A)	33(10)	36(11)	33(10)	-9(8)	-8(8)	-2(8)
C(19A)	61(13)	77(15)	31(11)	3(10)	-17(10)	9(11)
C(20A)	64(13)	63(14)	40(11)	-18(10)	6(10)	-13(11)
C(21A)	39(11)	51(12)	27(10)	11(9)	3(8)	11(9)
C(22A)	32(10)	47(12)	59(13)	3(10)	4(9)	15(9)
Ni(1B)	38(2)	27(2)	68(2)	0	12(2)	0
S(1B)	57(7)	18(6)	44(6)	-3(6)	11(5)	-9(4)
P(1B)	51(3)	40(3)	30(3)	1(2)	-1(2)	3(2)
C(9B)	52(12)	40(12)	56(12)	1`(10)	-6(10)	-4(9)
C(10B)	62(14)	84(17)	87(16)	-6(14)	32(13)	-17(12)
C(11B)	55(14)	88(17)	78(15)	7(13)	8(12)	-26(12)
C(12B)	50(14)	118(19)	51(13)	3(13)	-7(11)	1`(12)
C(13B)	54(15)	174(25)	38(12)	7(14)	-1`(11)	6(15)
C(14B)	101(20)	241(35)	76(18)	103(22)	14(15)	35(21)
C(15B)	96(15)	45(13)	66(12)	2(9)	15(13)	12(12)

Table S-8B. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4**.

	x	y	z	U(eq)
H(1AA)	2307(6)	2349(10)	992(8)	40
H(2AA)	1607(6)	3018(11)	771(8)	51
H(5AA)	1228(5)	3683(10)	3521(9)	43
H(6AA)	506(6)	4404(11)	2891(9)	58
H(7AA)	387(6)	4434(12)	1681(9)	65
H(8AA)	925(6)	3836(10)	949(9)	50
H(9AA)	3876(6)	2528(11)	1310(9)	54
H(10A)	3883(36)	3092(24)	2511(26)	90
H(10B)	3369(7)	3605(58)	2294(41)	90
H(10C)	3869(37)	3900(38)	1950(18)	90
H(11A)	3288(37)	2879(24)	344(16)	82
H(11B)	3513(22)	3774(39)	688(37)	82
H(11C)	2973(17)	3448(62)	874(26)	82
H(12A)	2895(6)	1551(11)	510(9)	48
H(13A)	2388(16)	683(13)	1170(57)	83
H(13B)	2848(17)	40(38)	1392(43)	83
H(13C)	2624(32)	131(45)	542(18)	83
H(14A)	3770(18)	1312(14)	557(58)	86
H(14B)	3463(8)	519(63)	156(33)	86
H(14C)	3710(22)	418(56)	995(30)	86
H(15A)	2960(6)	429(11)	4049(9)	56
H(16A)	2315(11)	1232(58)	4498(36)	85
H(16B)	2101(24)	300(13)	4224(53)	85
H(16C)	1978(16)	1144(64)	3719(21)	85
H(17A)	2912(13)	-16(54)	2794(38)	84
H(17B)	2338(28)	288(35)	2681(30)	84
H(17C)	2503(39)	-502(23)	3230(12)	84
H(18A)	2721(6)	2544(10)	4363(8)	42
H(19A)	3225(24)	1399(33)	4945(40)	87
H(19B)	3378(35)	2328(36)	5301(18)	87
H(19C)	3718(13)	1885(66)	4729(26)	87
H(20A)	3089(23)	3569(34)	3603(40)	83
H(20B)	3634(16)	3201(14)	3888(58)	83
H(20C)	3305(38)	3680(28)	4456(22)	83
H(21A)	3544(6)	559(11)	2279(8)	47
H(21B)	3971(6)	1277(11)	2207(8)	47
H(22A)	3844(6)	1920(11)	3281(9)	55
H(22B)	3734(6)	925(11)	3473(9)	55
H(9BA)	780(6)	1741(12)	1234(10)	60
H(10D)	675(35)	588(54)	387(23)	114
H(10E)	815(47)	-114(15)	1029(34)	114
H(10F)	1236(14)	533(60)	783(54)	114
H(11D)	1050(32)	1533(53)	2508(31)	110
H(11E)	1464(8)	1134(86)	2029(14)	110
H(11F)	1082(35)	502(35)	2391(41)	110
H(12B)	-168(7)	528(16)	488(11)	89
H(13D)	-851(7)	475(79)	1321(55)	134
H(13E)	-1004(15)	610(92)	450(34)	134
H(13F)	-989(16)	1427(21)	1002(81)	134
H(14D)	116(18)	2044(82)	407(101)	208
H(14E)	-447(65)	2303(47)	532(82)	208
H(14F)	-339(79)	1739(42)	-178(21)	208
H(15B)	202(9)	2525(12)	1937(9)	82
H(15C)	-373(9)	2251(12)	1933(9)	82

Table S-5C. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni(1)	1692(1)	1066(1)	2433(1)	22(1)
Ni(2)	3076(1)	1733(1)	3470(1)	22(1)
S(1)	1541(1)	1244(1)	4002(1)	25(1)
P(1)	2769(1)	560(1)	1565(1)	24(1)
P(2)	249(1)	478(1)	2233(1)	23(1)
P(3)	4365(1)	1522(1)	4561(1)	31(1)
P(4)	3814(1)	2557(1)	3360(1)	34(1)
C(1)	3154(2)	836(1)	422(2)	33(1)
C(2)	4154(3)	1256(1)	460(2)	47(1)
C(3)	2096(3)	1112(1)	-29(2)	45(1)
C(4)	4165(2)	243(1)	1947(2)	31(1)
C(5)	4717(3)	-181(1)	1301(2)	47(1)
C(6)	4026(2)	-22(1)	2878(2)	40(1)
C(7)	-1205(2)	744(1)	1873(2)	34(1)
C(8)	-2123(3)	284(1)	1700(2)	47(1)
C(9)	-1118(3)	1125(1)	1045(2)	50(1)
C(10)	-134(2)	-34(1)	3141(2)	29(1)
C(11)	-831(2)	243(1)	3896(2)	37(1)
C(12)	954(2)	-312(1)	3533(2)	36(1)
C(13)	1944(2)	-88(1)	1242(2)	30(1)
C(14)	633(2)	-2(1)	1288(2)	31(1)
C(15)	3871(3)	1319(3)	5700(2)	86(2)
C(16)	2967(4)	1743(4)	6038(3)	178(4)
C(17)	3438(4)	715(3)	5716(3)	132(3)
C(18)	5540(2)	1008(1)	4370(2)	42(1)
C(19)	6124(3)	1115(2)	3473(2)	74(1)
C(20)	6457(3)	965(2)	5128(2)	57(1)
C(21)	2800(3)	3157(1)	3564(3)	72(1)
C(22)	2089(4)	3316(2)	2723(4)	100(2)
C(23)	2026(4)	3023(2)	4369(4)	112(2)
C(24)	4587(3)	2787(1)	2334(2)	45(1)
C(25)	5152(3)	3372(2)	2418(3)	64(1)
C(26)	5465(3)	2349(2)	2039(2)	61(1)
C(27)	5185(4)	2176(2)	4780(4)	101(2)
C(28)	4897(4)	2656(2)	4267(2)	66(1)
C(29)	382(2)	1719(1)	3881(2)	29(1)
C(30)	-362(2)	1830(1)	4598(2)	41(1)
C(31)	-1287(3)	2198(2)	4491(3)	56(1)
C(32)	-1485(3)	2453(2)	3668(3)	58(1)
C(33)	-756(3)	2348(1)	2951(2)	47(1)
C(34)	201(2)	1985(1)	3037(2)	33(1)
C(35)	1027(2)	1910(1)	2301(2)	31(1)
C(36)	2210(2)	1867(1)	2382(2)	29(1)

Table S-6C. Bond lengths [A] and angles [deg] for **5**.

Ni(1)-C(36)	1.985(2)	P(1)-Ni(1)-S(1)	137.01(3)
Ni(1)-C(35)	2.142(2)	P(2)-Ni(1)-S(1)	100.36(2)
Ni(1)-P(1)	2.1567(7)	C(36)-Ni(1)-Ni(2)	44.85(7)
Ni(1)-P(2)	2.1836(7)	C(35)-Ni(1)-Ni(2)	73.67(7)
Ni(1)-S(1)	2.3634(7)	P(1)-Ni(1)-Ni(2)	108.56(2)
Ni(1)-Ni(2)	2.7035(4)	P(2)-Ni(1)-Ni(2)	152.87(2)
Ni(2)-C(36)	1.908(2)	S(1)-Ni(1)-Ni(2)	52.53(2)
Ni(2)-P(4)	2.1296(7)	C(36)-Ni(2)-P(4)	89.38(7)
Ni(2)-P(3)	2.2355(7)	C(36)-Ni(2)-P(3)	168.78(9)
Ni(2)-S(1)	2.2630(7)	P(4)-Ni(2)-P(3)	89.70(3)
S(1)-C(29)	1.752(3)	C(36)-Ni(2)-S(1)	88.49(8)
P(1)-C(4)	1.857(3)	P(4)-Ni(2)-S(1)	143.86(3)
P(1)-C(13)	1.861(3)	P(3)-Ni(2)-S(1)	98.80(3)
P(1)-C(1)	1.868(3)	C(36)-Ni(2)-Ni(1)	47.21(7)
P(2)-C(14)	1.856(3)	P(4)-Ni(2)-Ni(1)	136.21(2)
P(2)-C(7)	1.862(3)	P(3)-Ni(2)-Ni(1)	131.47(2)
P(2)-C(10)	1.863(3)	S(1)-Ni(2)-Ni(1)	55.99(2)
P(3)-C(27)	1.836(4)	C(29)-S(1)-Ni(2)	103.76(9)
P(3)-C(18)	1.843(3)	C(29)-S(1)-Ni(1)	94.55(9)
P(3)-C(15)	1.846(4)	Ni(2)-S(1)-Ni(1)	71.48(2)
P(4)-C(28)	1.836(3)	C(4)-P(1)-C(13)	100.66(12)
P(4)-C(24)	1.849(3)	C(4)-P(1)-C(1)	101.51(12)
P(4)-C(21)	1.865(3)	C(13)-P(1)-C(1)	100.49(12)
C(1)-C(2)	1.521(4)	C(4)-P(1)-Ni(1)	123.08(9)
C(1)-C(3)	1.528(4)	C(13)-P(1)-Ni(1)	108.11(8)
C(4)-C(6)	1.522(4)	C(1)-P(1)-Ni(1)	119.34(9)
C(4)-C(5)	1.528(4)	C(14)-P(2)-C(7)	102.30(12)
C(7)-C(9)	1.523(4)	C(14)-P(2)-C(10)	101.91(12)
C(7)-C(8)	1.536(4)	C(7)-P(2)-C(10)	101.68(12)
C(10)-C(12)	1.525(4)	C(14)-P(2)-Ni(1)	107.51(8)
C(10)-C(11)	1.529(4)	C(7)-P(2)-Ni(1)	120.52(9)
C(13)-C(14)	1.529(4)	C(10)-P(2)-Ni(1)	120.14(8)
C(15)-C(17)	1.512(8)	C(27)-P(3)-C(18)	101.6(2)
C(15)-C(16)	1.532(7)	C(27)-P(3)-C(15)	102.8(3)
C(18)-C(19)	1.515(5)	C(18)-P(3)-C(15)	101.9(2)
C(18)-C(20)	1.534(4)	C(27)-P(3)-Ni(2)	106.08(12)
C(21)-C(22)	1.526(6)	C(18)-P(3)-Ni(2)	121.28(10)
C(21)-C(23)	1.530(6)	C(15)-P(3)-Ni(2)	120.28(11)
C(24)-C(26)	1.514(5)	C(28)-P(4)-C(24)	103.3(2)
C(24)-C(25)	1.532(4)	C(28)-P(4)-C(21)	102.0(2)
C(27)-C(28)	1.399(5)	C(24)-P(4)-C(21)	102.6(2)
C(29)-C(30)	1.396(4)	C(28)-P(4)-Ni(2)	109.24(11)
C(29)-C(34)	1.408(4)	C(24)-P(4)-Ni(2)	121.90(10)
C(30)-C(31)	1.384(4)	C(21)-P(4)-Ni(2)	115.44(11)
C(31)-C(32)	1.373(5)	C(2)-C(1)-C(3)	109.9(2)
C(32)-C(33)	1.383(5)	C(2)-C(1)-P(1)	112.5(2)
C(33)-C(34)	1.402(4)	C(3)-C(1)-P(1)	110.1(2)
C(34)-C(35)	1.466(4)	C(6)-C(4)-C(5)	110.1(2)
C(35)-C(36)	1.373(4)	C(6)-C(4)-P(1)	109.9(2)
		C(5)-C(4)-P(1)	116.2(2)
C(36)-Ni(1)-C(35)	38.62(10)	C(9)-C(7)-C(8)	109.6(2)
C(36)-Ni(1)-P(1)	109.16(8)	C(9)-C(7)-P(2)	111.1(2)
C(35)-Ni(1)-P(1)	131.94(8)	C(8)-C(7)-P(2)	115.3(2)
C(36)-Ni(1)-P(2)	146.01(8)	C(12)-C(10)-C(11)	110.1(2)
C(35)-Ni(1)-P(2)	107.83(8)	C(12)-C(10)-P(2)	110.6(2)
P(1)-Ni(1)-P(2)	90.70(3)	C(11)-C(10)-P(2)	112.3(2)
C(36)-Ni(1)-S(1)	83.93(7)	C(14)-C(13)-P(1)	112.4(2)
C(35)-Ni(1)-S(1)	83.88(7)	C(13)-C(14)-P(2)	111.1(2)

C(17)-C(15)-C(16)	112.6(4)	C(30)-C(29)-S(1)	121.2(2)
C(17)-C(15)-P(3)	111.4(3)	C(34)-C(29)-S(1)	118.7(2)
C(16)-C(15)-P(3)	110.3(4)	C(31)-C(30)-C(29)	120.8(3)
C(19)-C(18)-C(20)	109.9(3)	C(32)-C(31)-C(30)	119.7(3)
C(19)-C(18)-P(3)	111.2(2)	C(31)-C(32)-C(33)	120.2(3)
C(20)-C(18)-P(3)	115.7(2)	C(32)-C(33)-C(34)	121.8(3)
C(22)-C(21)-C(23)	111.7(4)	C(33)-C(34)-C(29)	117.4(3)
C(22)-C(21)-P(4)	112.8(3)	C(33)-C(34)-C(35)	121.7(3)
C(23)-C(21)-P(4)	109.9(3)	C(29)-C(34)-C(35)	120.8(2)
C(26)-C(24)-C(25)	110.7(3)	C(36)-C(35)-C(34)	126.8(2)
C(26)-C(24)-P(4)	111.5(2)	C(36)-C(35)-Ni(1)	64.52(14)
C(25)-C(24)-P(4)	114.0(2)	C(34)-C(35)-Ni(1)	106.3(2)
C(28)-C(27)-P(3)	117.8(2)	C(35)-C(36)-Ni(2)	126.5(2)
C(27)-C(28)-P(4)	116.6(2)	C(35)-C(36)-Ni(1)	76.9(2)
C(30)-C(29)-C(34)	120.1(3)	Ni(2)-C(36)-Ni(1)	87.94(10)

Table S-7C. Anisotropic displacement parameters (A^2 x 10^3) for **5**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni(1)	23(1)	21(1)	23(1)	-4(1)	0(1)	-1(1)
Ni(2)	19(1)	21(1)	26(1)	-3(1)	-2(1)	0(1)
S(1)	23(1)	29(1)	24(1)	-1(1)	-1(1)	-2(1)
P(1)	26(1)	22(1)	22(1)	-2(1)	2(1)	-1(1)
P(2)	24(1)	24(1)	21(1)	-2(1)	-2(1)	-3(1)
P(3)	23(1)	39(1)	31(1)	-4(1)	-6(1)	1(1)
P(4)	32(1)	24(1)	45(1)	-6(1)	-1(1)	-5(1)
C(1)	39(2)	34(1)	27(1)	1(1)	7(1)	0(1)
C(2)	48(2)	45(2)	48(2)	7(1)	11(1)	-8(1)
C(3)	53(2)	50(2)	31(2)	9(1)	1(1)	2(2)
C(4)	27(1)	32(1)	35(1)	0(1)	3(1)	0(1)
C(5)	42(2)	51(2)	48(2)	-3(2)	8(1)	15(2)
C(6)	36(2)	45(2)	38(2)	5(1)	-6(1)	7(1)
C(7)	25(1)	39(2)	37(2)	-3(1)	-6(1)	1(1)
C(8)	31(2)	60(2)	49(2)	-3(2)	-10(1)	-9(1)
C(9)	44(2)	52(2)	54(2)	14(2)	-22(2)	0(2)
C(10)	30(1)	29(1)	29(1)	1(1)	1(1)	-7(1)
C(11)	35(2)	47(2)	30(1)	5(1)	6(1)	-5(1)
C(12)	43(2)	32(2)	33(1)	6(1)	3(1)	1(1)
C(13)	37(2)	26(1)	27(1)	-7(1)	3(1)	-3(1)
C(14)	37(2)	30(1)	26(1)	-7(1)	-2(1)	-8(1)
C(15)	33(2)	199(6)	26(2)	7(2)	-6(1)	3(3)
C(16)	54(3)	417(13)	62(3)	-114(5)	-11(2)	48(5)
C(17)	46(2)	233(7)	115(4)	132(5)	-27(2)	-50(3)
C(18)	33(2)	46(2)	48(2)	1(1)	-1`(1)	8(1)
C(19)	41(2)	135(4)	46(2)	-15(2)	-3(2)	31(2)
C(20)	37(2)	79(3)	55(2)	14(2)	-12(2)	15(2)
C(21)	47(2)	29(2)	140(4)	-31(2)	14(2)	-7(2)
C(22)	51(2)	30(2)	217(6)	-8(3)	-31(3)	1`(2)
C(23)	76(3)	71(3)	189(6)	-84(3)	69(3)	-32(2)
C(24)	46(2)	39(2)	49(2)	12(1)	-8(1)	-14(1)
C(25)	62(2)	45(2)	87(3)	18(2)	-3(2)	-22(2)
C(26)	58(2)	68(2)	57(2)	-11(2)	21(2)	-21(2)
C(27)	107(4)	40(2)	154(5)	-6(2)	-102(4)	-8(2)
C(28)	85(3)	60(2)	52(2)	-1(2)	-18(2)	-45(2)
C(29)	20(1)	28(1)	40(2)	-13(1)	-1(1)	-3(1)
C(30)	30(2)	48(2)	47(2)	-18(1)	9(1)	-7(1)
C(31)	28(2)	58(2)	82(3)	-36(2)	16(2)	-3(1)
C(32)	27(2)	48(2)	100(3)	-26(2)	-2(2)	11(1)
C(33)	33(2)	37(2)	70(2)	-1`(2)	-11(2)	9(1)
C(34)	26(1)	24(1)	48(2)	-7(1)	-7(1)	0(1)
C(35)	41(2)	19(1)	33(1)	1(1)	-4(1)	4(1)
C(36)	43(2)	18(1)	25(1)	1(1)	-5(1)	-6(1)

Table S-8C. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5**.

	x	y	z	U(eq)
H(1A)	3395(2)	508(1)	41(2)	40
H(2A)	4300(13)	1402(7)	-149(3)	70
H(2B)	4851(5)	1066(3)	693(14)	70
H(2C)	3954(8)	1572(5)	861(12)	70
H(3A)	2300(6)	1243(8)	-636(6)	67
H(3B)	1843(11)	1435(6)	335(8)	67
H(3C)	1467(7)	834(3)	-76(13)	67
H(4A)	4727(2)	563(1)	2021(2)	37
H(5A)	5407(11)	-347(7)	1589(6)	71
H(5B)	4940(17)	14(2)	743(6)	71
H(5C)	4159(7)	-481(5)	1155(12)	71
H(6A)	4790(3)	-126(8)	3124(6)	59
H(6B)	3542(15)	-362(5)	2826(3)	59
H(6C)	3657(16)	250(3)	3283(4)	59
H(7A)	-1497(2)	985(1)	2378(2)	40
H(8A)	-2861(5)	463(2)	1529(14)	70
H(8B)	-2225(14)	59(6)	2251(5)	70
H(8C)	-1870(9)	36(6)	1208(10)	70
H(9A)	-1861(7)	1317(7)	941(9)	75
H(9B)	-929(20)	895(2)	514(4)	75
H(9C)	-509(14)	1408(6)	1147(7)	75
H(10A)	-625(2)	-338(1)	2862(2)	35
H(11A)	-1026(15)	-44(2)	4350(7)	56
H(11B)	-1545(8)	405(7)	3641(3)	56
H(11C)	-367(7)	543(6)	4181(9)	56
H(12A)	735(3)	-592(6)	3991(9)	54
H(12B)	1450(8)	-23(2)	3813(11)	54
H(12C)	1377(9)	-502(7)	3048(3)	54
H(13A)	2152(2)	-199(1)	618(2)	36
H(13B)	2172(2)	-402(1)	1652(2)	36
H(14A)	249(2)	-373(1)	1374(2)	38
H(14B)	347(2)	161(1)	709(2)	38
H(15A)	4556(3)	1342(3)	6119(2)	103
H(16A)	2731(46)	1637(18)	6650(20)	267
H(16B)	2289(27)	1738(23)	5631(28)	267
H(16C)	3303(21)	2124(6)	6048(46)	267
H(17A)	3231(42)	612(7)	6336(7)	197
H(17B)	4049(16)	461(4)	5503(33)	197
H(17C)	2754(27)	680(6)	5320(27)	197
H(18A)	5166(2)	627(1)	4323(2)	51
H(19A)	6562(21)	777(5)	3298(10)	111
H(19B)	6653(20)	1438(8)	3532(6)	111
H(19C)	5534(3)	1197(13)	3008(5)	111
H(20A)	7016(13)	667(7)	4979(8)	86
H(20B)	6079(4)	872(10)	5699(4)	86
H(20C)	6863(15)	1328(4)	5190(11)	86
H(21A)	3281(3)	3495(1)	3732(3)	87
H(22A)	1544(23)	3619(11)	2875(7)	149
H(22B)	1656(26)	2983(4)	2509(16)	149
H(22C)	2608(4)	3447(15)	2247(10)	149
H(23A)	1568(28)	3358(6)	4522(19)	168
H(23B)	2510(4)	2914(18)	4891(10)	168
H(23C)	1505(27)	2709(13)	4210(11)	168

H(24A)	3993(3)	2814(1)	1837(2)	54
H(25A)	5458(21)	3487(5)	1830(5)	97
H(25B)	5787(16)	3357(3)	2865(14)	97
H(25C)	4573(7)	3649(3)	2614(18)	97
H(26A)	5751(17)	2448(6)	1438(8)	91
H(26B)	5096(7)	1975(2)	2017(17)	91
H(26C)	6114(11)	2342(8)	2473(10)	91
H(27A)	5096(4)	2274(2)	5427(4)	121
H(27B)	6016(4)	2093(2)	4685(4)	121
H(28A)	5616(4)	2803(2)	3992(2)	79
H(28B)	4608(4)	2951(2)	4683(2)	79
H(30A)	-231(2)	1651(1)	5166(2)	50
H(31A)	-1783(3)	2274(2)	4985(3)	67
H(32A)	-2126(3)	2702(2)	3590(3)	70
H(33A)	-907(3)	2527(1)	2386(2)	56
H(35A)	729(2)	2012(1)	1684(2)	38
H(36A)	2667(2)	1979(1)	1839(2)	34

Table S-5D. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni(1)	1396(1)	1741(1)	2102(1)	28(1)
P(2)	3403(1)	2479(1)	2663(1)	30(1)
P(1)	1956(1)	2454(1)	1162(1)	32(1)
C(1)	-186(4)	957(2)	1619(2)	29(1)
C(2)	-603(4)	826(2)	917(2)	37(1)
C(3)	-1722(4)	206(2)	661(2)	40(1)
C(4)	-2485(4)	-302(2)	1106(2)	35(1)
C(5)	-2103(4)	-208(2)	1813(2)	32(1)
C(6)	-971(4)	404(2)	2068(2)	27(1)
C(7)	-452(4)	539(2)	2805(2)	27(1)
C(8)	-1070(4)	87(2)	3343(2)	34(1)
C(9)	-540(4)	267(2)	4029(2)	37(1)
C(10)	612(4)	900(3)	4167(2)	44(1)
C(11)	1221(4)	1346(3)	3630(2)	42(1)
C(12)	741(4)	1185(2)	2932(2)	32(1)
C(13)	3338(5)	3347(2)	1434(2)	49(1)
C(14)	4552(4)	2986(2)	2007(2)	46(1)
C(15)	3035(4)	1820(2)	528(2)	40(1)
C(16)	3805(5)	1002(3)	869(2)	51(1)
C(17)	4297(5)	2308(3)	153(2)	69(1)
C(18)	275(5)	3006(2)	633(2)	51(1)
C(19)	784(6)	3738(3)	170(2)	83(2)
C(20)	-972(5)	3319(3)	1106(2)	75(1)
C(21)	2905(5)	3461(2)	3171(2)	50(1)
C(22)	1127(5)	3677(3)	3064(2)	62(1)
C(23)	3527(5)	3496(3)	3923(2)	54(1)
C(24)	4957(4)	1845(2)	3194(2)	34(1)
C(25)	4986(4)	908(2)	2925(2)	50(1)
C(26)	6655(4)	2240(2)	3244(2)	47(1)

Table S-6D. Bond lengths [A] and angles [deg] for **7**.

Ni(1)-C(12)	1.944(3)	C(24)-P(2)-Ni(1)	117.29(11)
Ni(1)-C(1)	1.960(3)	C(21)-P(2)-Ni(1)	118.52(12)
Ni(1)-P(1)	2.2142(9)	C(13)-P(1)-C(18)	103.7(2)
Ni(1)-P(2)	2.2185(9)	C(13)-P(1)-C(15)	104.7(2)
P(2)-C(14)	1.834(4)	C(18)-P(1)-C(15)	105.0(2)
P(2)-C(24)	1.855(3)	C(13)-P(1)-Ni(1)	107.91(12)
P(2)-C(21)	1.870(4)	C(18)-P(1)-Ni(1)	118.28(14)
P(1)-C(13)	1.836(3)	C(15)-P(1)-Ni(1)	115.77(12)
P(1)-C(18)	1.861(4)	C(2)-C(1)-C(6)	115.3(3)
P(1)-C(15)	1.863(4)	C(2)-C(1)-Ni(1)	130.8(3)
C(1)-C(2)	1.388(4)	C(6)-C(1)-Ni(1)	113.7(2)
C(1)-C(6)	1.418(4)	C(1)-C(2)-C(3)	123.2(3)
C(2)-C(3)	1.391(4)	C(4)-C(3)-C(2)	120.1(3)
C(3)-C(4)	1.364(5)	C(3)-C(4)-C(5)	119.3(3)
C(4)-C(5)	1.384(4)	C(4)-C(5)-C(6)	120.6(3)
C(5)-C(6)	1.390(4)	C(5)-C(6)-C(1)	121.5(3)
C(6)-C(7)	1.468(4)	C(5)-C(6)-C(7)	124.8(3)
C(7)-C(8)	1.391(4)	C(1)-C(6)-C(7)	113.7(3)
C(7)-C(12)	1.411(4)	C(8)-C(7)-C(12)	121.6(3)
C(8)-C(9)	1.389(4)	C(8)-C(7)-C(6)	124.3(3)
C(9)-C(10)	1.375(5)	C(12)-C(7)-C(6)	114.1(3)
C(10)-C(11)	1.382(5)	C(9)-C(8)-C(7)	120.8(3)
C(11)-C(12)	1.396(4)	C(10)-C(9)-C(8)	118.8(3)
C(13)-C(14)	1.535(5)	C(9)-C(10)-C(11)	120.1(3)
C(15)-C(17)	1.529(5)	C(10)-C(11)-C(12)	123.4(3)
C(15)-C(16)	1.533(5)	C(11)-C(12)-C(7)	115.4(3)
C(18)-C(20)	1.525(6)	C(11)-C(12)-Ni(1)	130.3(3)
C(18)-C(19)	1.526(6)	C(7)-C(12)-Ni(1)	114.3(2)
C(21)-C(23)	1.502(5)	C(14)-C(13)-P(1)	106.9(2)
C(21)-C(22)	1.513(5)	C(13)-C(14)-P(2)	107.7(3)
C(24)-C(25)	1.533(5)	C(17)-C(15)-C(16)	109.2(3)
C(24)-C(26)	1.534(5)	C(17)-C(15)-P(1)	116.8(3)
		C(16)-C(15)-P(1)	110.6(2)
C(12)-Ni(1)-C(1)	84.12(13)	C(20)-C(18)-C(19)	111.3(4)
C(12)-Ni(1)-P(1)	174.86(10)	C(20)-C(18)-P(1)	109.4(3)
C(1)-Ni(1)-P(1)	95.43(10)	C(19)-C(18)-P(1)	115.1(3)
C(12)-Ni(1)-P(2)	94.32(10)	C(23)-C(21)-C(22)	111.7(3)
C(1)-Ni(1)-P(2)	172.45(10)	C(23)-C(21)-P(2)	117.8(3)
P(1)-Ni(1)-P(2)	86.78(3)	C(22)-C(21)-P(2)	111.5(2)
C(14)-P(2)-C(24)	103.1(2)	C(25)-C(24)-C(26)	110.5(3)
C(14)-P(2)-C(21)	100.2(2)	C(25)-C(24)-P(2)	109.7(2)
C(24)-P(2)-C(21)	108.0(2)	C(26)-C(24)-P(2)	114.7(2)
C(14)-P(2)-Ni(1)	107.17(11)		

Table S-7D. Anisotropic displacement parameters (A^2 x 10^3) for **7**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni(1)	30(1)	31(1)	23(1)	-3(1)	1(1)	-4(1)
P(2)	32(1)	26(1)	28(1)	-4(1)	-4(1)	0(1)
P(1)	40(1)	26(1)	28(1)	1(1)	-4(1)	-5(1)
C(1)	29(2)	31(2)	28(2)	-4(2)	2(1)	-4(2)
C(2)	41(2)	42(2)	29(2)	2(2)	3(2)	-12(2)
C(3)	45(2)	42(2)	30(2)	-3(2)	-5(2)	-9(2)
C(4)	31(2)	33(2)	41(2)	-6(2)	2(2)	-9(2)
C(5)	33(2)	31(2)	33(2)	2(2)	6(2)	-4(2)
C(6)	23(2)	26(2)	30(2)	-2(1)	2(1)	6(1)
C(7)	28(2)	25(2)	28(2)	0(1)	5(1)	9(1)
C(8)	39(2)	28(2)	36(2)	1(2)	7(2)	6(2)
C(9)	47(2)	36(2)	30(2)	8(2)	13(2)	12(2)
C(10)	45(2)	63(3)	24(2)	0(2)	3(2)	5(2)
C(11)	40(2)	60(2)	27(2)	-4(2)	3(2)	-9(2)
C(12)	30(2)	38(2)	28(2)	-1(2)	3(1)	3(2)
C(13)	73(3)	34(2)	36(2)	7(2)	-9(2)	-23(2)
C(14)	49(2)	42(2)	44(2)	1(2)	-7(2)	-20(2)
C(15)	41(2)	49(2)	28(2)	-6(2)	5(2)	-13(2)
C(16)	51(2)	54(2)	47(2)	-11(2)	6(2)	7(2)
C(17)	64(3)	96(4)	51(3)	6(2)	19(2)	-27(3)
C(18)	68(3)	38(2)	41(2)	-5(2)	-23(2)	8(2)
C(19)	126(5)	63(3)	56(3)	22(2)	-19(3)	14(3)
C(20)	68(3)	75(3)	77(3)	-8(3)	-16(3)	36(3)
C(21)	54(2)	41(2)	51(2)	-18(2)	-5(2)	8(2)
C(22)	57(3)	63(3)	63(3)	-27(2)	-14(2)	30(2)
C(23)	56(3)	57(3)	45(2)	-26(2)	-7(2)	7(2)
C(24)	33(2)	34(2)	34(2)	-1(2)	-5(2)	4(2)
C(25)	42(2)	36(2)	71(3)	-7(2)	-6(2)	1`(2)
C(26)	38(2)	43(2)	58(3)	-4(2)	-8(2)	3(2)

Table S-8D. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7**.

	x	y	z	U(eq)
H(2A)	-99(4)	1176(2)	595(2)	45
H(3A)	-1955(4)	136(2)	175(2)	47
H(4A)	-3270(4)	-715(2)	934(2)	42
H(5A)	-2620(4)	-565(2)	2125(2)	38
H(8A)	-1864(4)	-349(2)	3240(2)	41
H(9A)	-965(4)	-43(2)	4395(2)	44
H(10A)	989(4)	1031(3)	4633(2)	53
H(11A)	2006(4)	1785(3)	3741(2)	50
H(13A)	3905(5)	3553(2)	1038(2)	58
H(13B)	2733(5)	3840(2)	1611(2)	58
H(14A)	5233(4)	3462(2)	2217(2)	55
H(14B)	5262(4)	2551(2)	1812(2)	55
H(15A)	2194(4)	1614(2)	162(2)	48
H(16A)	4164(27)	616(8)	512(2)	76
H(16B)	3010(10)	699(9)	1125(10)	76
H(16C)	4733(18)	1169(3)	1190(10)	76
H(17A)	4670(26)	1936(7)	-211(10)	104
H(17B)	5213(17)	2461(17)	484(4)	104
H(17C)	3816(11)	2839(10)	-56(13)	104
H(18A)	-265(5)	2554(2)	321(2)	61
H(19A)	-158(10)	3948(15)	-124(12)	125
H(19B)	1595(30)	3521(6)	-123(12)	125
H(19C)	1242(37)	4217(9)	458(2)	125
H(20A)	-1927(16)	3534(19)	824(2)	112
H(20B)	-509(14)	3789(14)	1403(11)	112
H(20C)	-1280(28)	2835(6)	1395(11)	112
H(21A)	3455(5)	3954(2)	2952(2)	59
H(22A)	932(7)	4238(9)	3282(13)	93
H(22B)	507(5)	3222(10)	3274(13)	93
H(22C)	791(9)	3712(18)	2567(2)	93
H(23A)	3345(27)	4078(5)	4106(4)	80
H(23B)	4684(8)	3367(16)	3971(2)	80
H(23C)	2956(21)	3065(11)	4182(3)	80
H(24A)	4617(4)	1819(2)	3675(2)	41
H(25A)	5698(23)	555(4)	3244(7)	75
H(25B)	5387(28)	904(3)	2465(6)	75
H(25C)	3893(7)	666(6)	2893(12)	75
H(26A)	7377(8)	1896(9)	3565(10)	71
H(26B)	6615(6)	2839(6)	3413(12)	71
H(26C)	7059(12)	2237(14)	2785(3)	71

Table S-5E. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **9**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni(1)	2040(1)	293(1)	2456(1)	30(1)
Ni(2)	1603(1)	1501(1)	2326(1)	28(1)
Ni(3)	2389(1)	1500(1)	2481(1)	32(1)
Ni(4)	413(1)	4542(1)	7524(1)	26(1)
Ni(5)	0	5697(1)	7500	27(1)
S(2)	2004(1)	1089(1)	3155(1)	32(1)
S(1)	1970(1)	1038(1)	1677(1)	31(1)
S(3)	-50(1)	4886(1)	6758(1)	27(1)
P(3)	1272(1)	1953(1)	3017(1)	37(1)
P(2)	2042(1)	-476(1)	1738(1)	37(1)
P(1)	2216(1)	-378(1)	3262(1)	43(1)
P(4)	1282(1)	2026(1)	1498(1)	34(1)
P(5)	783(1)	4325(1)	6791(1)	31(1)
P(6)	859(1)	4258(1)	8320(1)	28(1)
C(1)	2727(2)	1821(3)	1899(3)	40(2)
C(2)	2696(2)	1783(3)	1194(3)	50(2)
C(3)	2962(2)	2072(3)	844(4)	61(2)
C(4)	3267(2)	2389(3)	1183(5)	60(2)
C(5)	3310(2)	2424(3)	1869(4)	51(2)
C(6)	3048(2)	2149(3)	2231(3)	41(2)
C(7)	3054(2)	2187(3)	2966(3)	40(2)
C(8)	3335(2)	2475(3)	3426(4)	53(2)
C(9)	3298(2)	2529(3)	4106(4)	65(2)
C(10)	2976(2)	2290(3)	4321(4)	63(2)
C(11)	2695(2)	1983(3)	3872(3)	50(2)
C(12)	2730(2)	1914(3)	3185(3)	40(2)
C(13)	2207(2)	-1192(3)	2917(3)	51(2)
C(14)	2259(2)	-1187(3)	2172(3)	47(2)
C(15)	2726(2)	-274(3)	3638(4)	71(2)
C(16)	2972(2)	-192(5)	3076(6)	104(3)
C(17)	2783(3)	277(4)	4120(5)	99(3)
C(18)	1961(2)	-438(3)	3989(3)	63(2)
C(19)	2135(3)	-941(4)	4520(4)	95(3)
C(20)	1537(2)	-547(4)	3761(4)	73(2)
C(21)	1565(2)	-746(3)	1339(3)	46(2)
C(22)	1308(2)	-849(4)	1874(4)	70(2)
C(23)	1388(2)	-285(3)	810(4)	77(3)
C(24)	2297(2)	-375(3)	1003(4)	61(2)
C(25)	2701(2)	-138(4)	1238(5)	87(3)
C(26)	2295(3)	-988(3)	574(4)	86(3)
C(27)	989(2)	2613(3)	1859(3)	56(2)
C(28)	906(2)	2449(4)	2531(3)	63(2)
C(29)	987(2)	1441(3)	3504(3)	56(2)
C(30)	782(2)	932(4)	3058(5)	91(3)
C(31)	1226(2)	1138(4)	4123(4)	70(2)
C(32)	1536(2)	2483(3)	3660(3)	52(2)
C(33)	1777(2)	2955(3)	3325(4)	77(2)
C(34)	1278(2)	2826(4)	4095(4)	70(2)
C(35)	947(2)	1617(4)	841(3)	63(2)
C(36)	1117(3)	1326(4)	299(4)	90(3)
C(37)	708(2)	1140(4)	1170(4)	83(3)
C(38)	1573(2)	2512(3)	998(3)	47(2)

C(39)	1881(2)	2871(3)	1447(4)	65(2)
C(40)	1346(2)	2959(3)	497(4)	66(2)
C(41)	-52(1)	6374(3)	6846(3)	30(1)
C(42)	-108(2)	6339(3)	6139(3)	38(1)
C(43)	-123(2)	6883(3)	5738(3)	45(2)
C(44)	-94(2)	7479(3)	6022(3)	46(2)
C(45)	-51(2)	7538(3)	6720(3)	40(2)
C(46)	-27(1)	6995(3)	7126(3)	31(1)
C(47)	1305(2)	4160(3)	7967(3)	32(1)
C(48)	1226(2)	3962(3)	7224(3)	33(1)
C(49)	943(2)	5042(3)	6377(3)	43(2)
C(50)	1046(2)	5567(3)	6896(4)	66(2)
C(51)	657(2)	5285(4)	5794(4)	69(2)
C(52)	624(2)	3779(3)	6079(3)	42(2)
C(53)	927(2)	3689(4)	5610(3)	59(2)
C(54)	501(2)	3142(3)	6336(3)	50(2)
C(55)	980(2)	4817(3)	9029(3)	32(1)
C(56)	1321(2)	4594(3)	9542(3)	46(2)
C(57)	1048(2)	5482(3)	8774(3)	45(2)
C(58)	794(2)	3485(3)	8739(3)	36(1)
C(59)	668(2)	2976(3)	8218(3)	49(2)
C(60)	502(2)	3539(3)	9230(3)	44(2)
C(1S)	0	-335(14)	2500	98(8)
C(2S)	331(5)	-652(9)	2493(10)	93(6)
C(3S)	338(6)	-1298(11)	2485(11)	115(7)
C(4S)	0	-1598(15)	2500	112(10)
C(5S)	4(10)	479(16)	-585(17)	174(12)
C(6S)	-236(7)	511(12)	5(14)	132(8)
C(7S)	-192(7)	25(13)	438(12)	117(7)