Electronic Supplementary Material (ESI) for Dalton Transactions.

Mechanism of proton transfer to coordinated thiolates: encapsulation of acid stabilizes precursor intermediate

Ahmed Alwaaly, William Clegg, Ross W. Harrington, Athinoula L. Petrou and Richard A. Henderson

SUPPLEMENTARY INFORMATION

Supplementary Information: Contents

1. Preparation and Characterization of Compounds

Preparation of [lutH]BPh_4.
The acid [lutH]BPh_4 was prepared by the method described in the literature.[3] The identity and purity of [lutH]BPh_4 was confirmed by comparison to the previously reported ^{1}H NMR spectrum: δ 15.93–14.46, (broad N*H*), 8.32 (t, *para-H*, *J* = 7.9 Hz, 1H), 7.69 (d, *meta-H*, *J* = 7.9 Hz, 2H), 7.25–6.73 (m, B*Ph*, 20H), 2.66 (s, CH_3, 6H).

Preparation of thiolate salts.
The thiolate salts were prepared by the method reported in the literature.[4] The identity and purity of the product was confirmed by ^{1}H NMR spectroscopy in D_2O. NaSEt: δ 0.06 (t, CH_3, *J* = 7.4 Hz, 3H), 1.23 (q, CH_2, *J* = 7.4 Hz, 2H); $NaSBu^t$: δ 1.25–1.15 (s, CH_3, 9H); NaSCy: δ 2.60 (t of t, *J* = 11.0, 3.8 Hz, 1H), 1.99–1.76 (m, 4H), 1.76–1.50 (m, 4H), 1.36–1.06 (m, 2H).

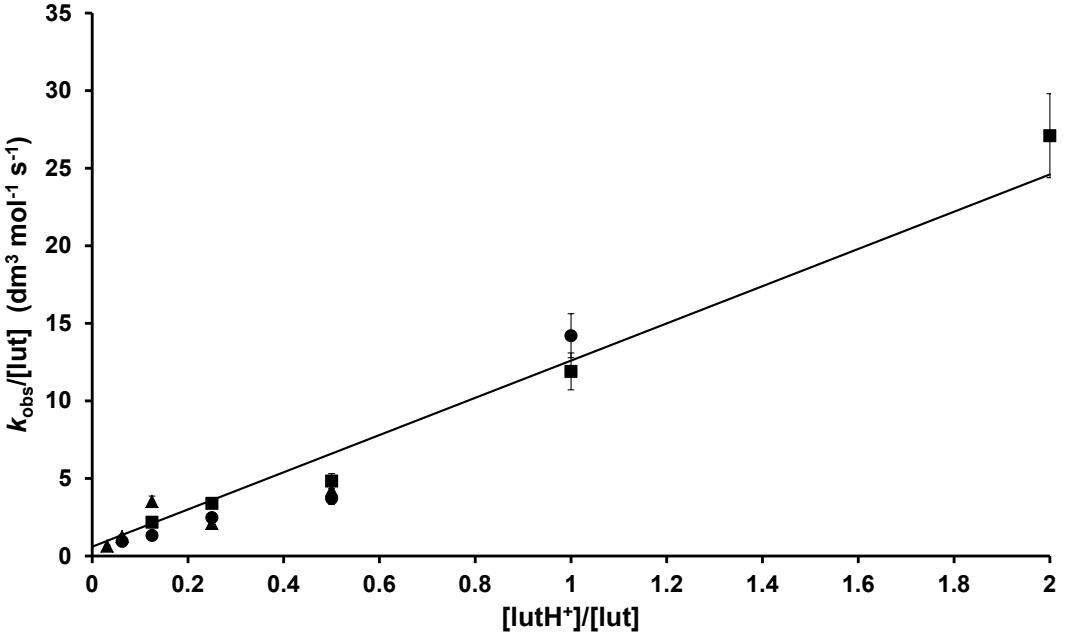
[NiCl(triphos)]BPh_4.
The complex was prepared by the method described in the literature.[5] The identity and purity of the product was confirmed by NMR spectroscopy. δ 8.24–7.39 (m, P*Ph*, 25H), 7.33–6.75 (m, B*Ph*, 20H), 3.2–2.4 (m, CH_2, 8H). $^{31}P\{^1H\}$ NMR: 111.5 (t, J_{PP} = 31.0 Hz, *P*Ph), 47.5 (d, J_{PP} = 31.1 Hz, *P*Ph_2).

(references 3, 4 and 5 in main text)

2. Kinetic Data

Table S1. Kinetic data for the reaction between [Ni(SEt)(triphos)]BPh_4 (0.1 mmol dm^{-3}) and mixtures of $lutH^+$ and lut in MeCN at 25.0°C (λ = 350 nm)

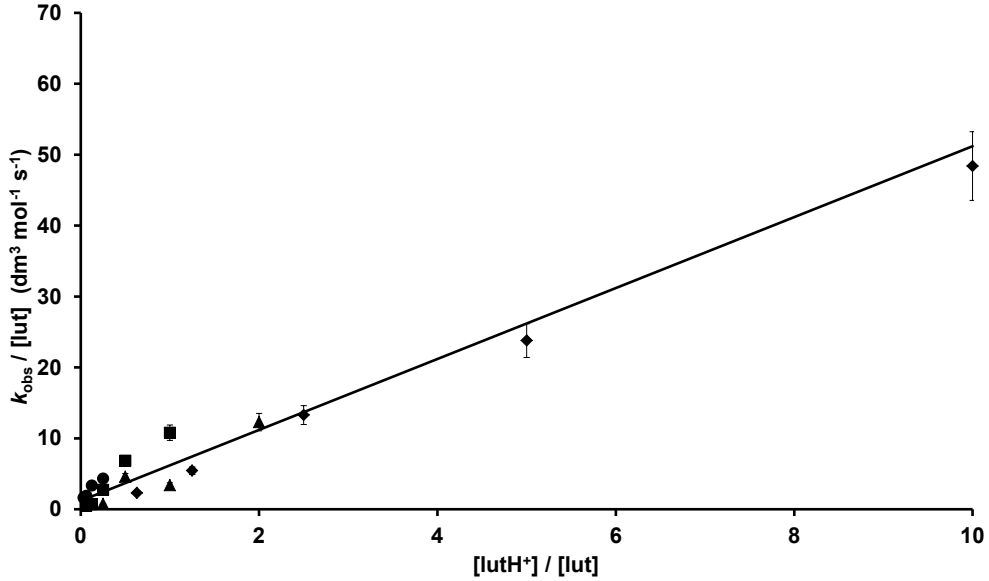
[$lutH^+$] / mmol dm^{-3}	[lut] / mmol dm^{-3}	k_{obs} / s^{-1}
1.25	2.5	0.011
	5.0	0.011
	10.0	0.015
	20.0	0.025
	40.0	0.025
2.50	2.5	0.036
	5.0	0.019
	10.0	0.025
	20.0	0.027
	40.0	0.038
5.0	2.5	0.068
	5.0	0.060
	10.0	0.048
	20.0	0.068
	40.0	0.087



Plot of k_{obs}/[lut] on [$lutH^+$]/[lut] for the reaction of [Ni(SEt)(triphos)]$^+$ with mixtures of $lutH^+$ and lut in MeCN at 25.0°C. Data points correspond to: [$lutH^+$] = 1.25 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (▲); [$lutH^+$] = 2.5 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (●); [$lutH^+$] = 5.0 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (■). The line is that defined by Equation (2) and the parameters shown in Table 3. Error bars correspond to ± 10 %.

Table S2. Kinetic data for the reaction between [Ni(SCy)(triphos)]BPh_4 (0.1 mmol dm^{-3}) and mixtures of $lutH^+$ and lut in MeCN at 25.0°C (λ = 320 nm)

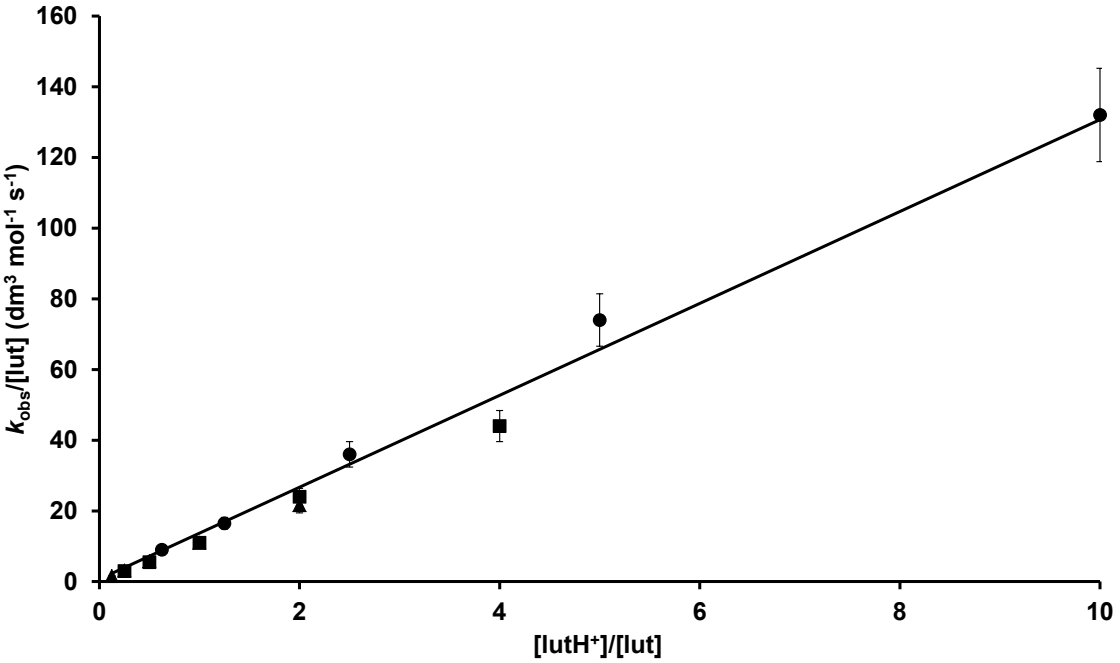
[$lutH^+$] / mmol dm^{-3}	[lut] / mmol dm^{-3}	k_{obs} / s^{-1}
1.25	2.5	0.048
	5.0	0.022
	10.0	0.034
	20.0	0.038
	40.0	0.066
2.50	2.5	0.027
	5.0	0.034
	10.0	0.028
	20.0	0.015
	40.0	0.022
5.0	2.5	0.031
	5.0	0.017
	10.0	0.046
	20.0	0.015
	40.0	0.038
25.0	2.5	0.12
	5.0	0.12
	10.0	0.13
	20.0	0.11
	40.0	0.09



Plot of k_{obs}/[lut] on [$lutH^+$]/[lut] for the reaction of [Ni(SCy)(triphos)]$^+$ with mixtures of $lutH^+$ and lut in MeCN at 25.0°C. Data points correspond to: [$lutH^+$] = 1.25 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (●); [$lutH^+$] = 2.5 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (■); [$lutH^+$] = 5.0 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (▲); [$lutH^+$] = 25.0 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (♦); The line is that defined by Equation (2) and the parameters shown in Table 3. Error bars correspond to ± 10 %.

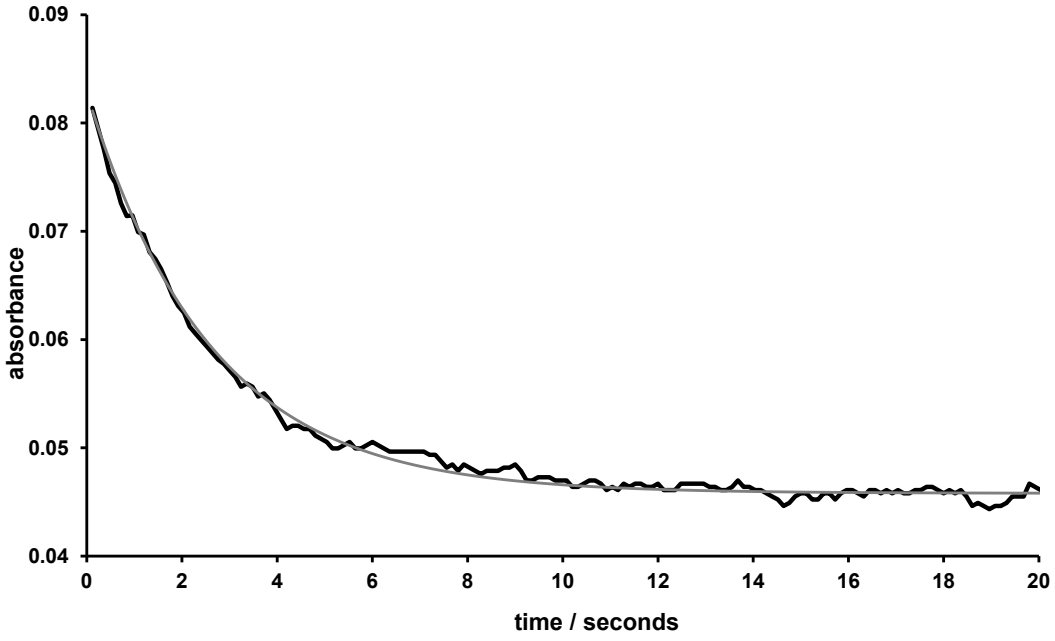
Table S3. Kinetic data for the reaction between [Ni(SBu^t)(triphos)]BPh_4 (0.1 mmol dm^{-3}) and mixtures of lutH$^+$ and lut in MeCN at 25.0°C (λ = 350 nm)

[lutH$^+$] / mmol dm^{-3}	[lut] / mmol dm^{-3}	k_{obs} / s^{-1}
5.0	2.5	0.054
	5.0	0.055
	10.0	0.057
	20.0	0.062
	40.0	0.062
10.0	2.5	0.036
	5.0	0.019
	10.0	0.025
	20.0	0.027
	40.0	0.038
25.0	2.5	0.33
	5.0	0.37
	10.0	0.36
	20.0	0.33
	40.0	0.23



Plot of k_{obs}/[lut] on [lutH$^+$]/[lut] for the reaction of [Ni(SBu^t)(triphos)]$^+$ with mixtures of lutH$^+$ and lut in MeCN at 25.0°C. Data points correspond to: [lutH$^+$] = 5.0 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (▲); [lutH$^+$] = 10.0 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (■); [lutH$^+$] = 25.0 mmol dm^{-3}, [lut] = 2.5–40 mmol dm^{-3} (●). The line is that defined by Equation (2) and the parameters shown in Table 3. Error bars correspond to ± 10 %.

Figure S1 Typical stopped-flow absorbance-time curve for the reaction of $[Ni(SBu^t)(triphos)]^+$ (0.1 mmol dm^{-3}) with $lutH^+$ (25.0 mmol dm^{-3}) and lut (5.0 mmol dm^{-3}) in MeCN at 25.0°C (λ = 350 nm). The experimental trace is shown in black and the exponential curve fit is shown in grey. The curve fit is that defined by the equation $A_t = 0.0458 + 0.037.\exp(-0.37t)$.



3. X-Ray Crystallography

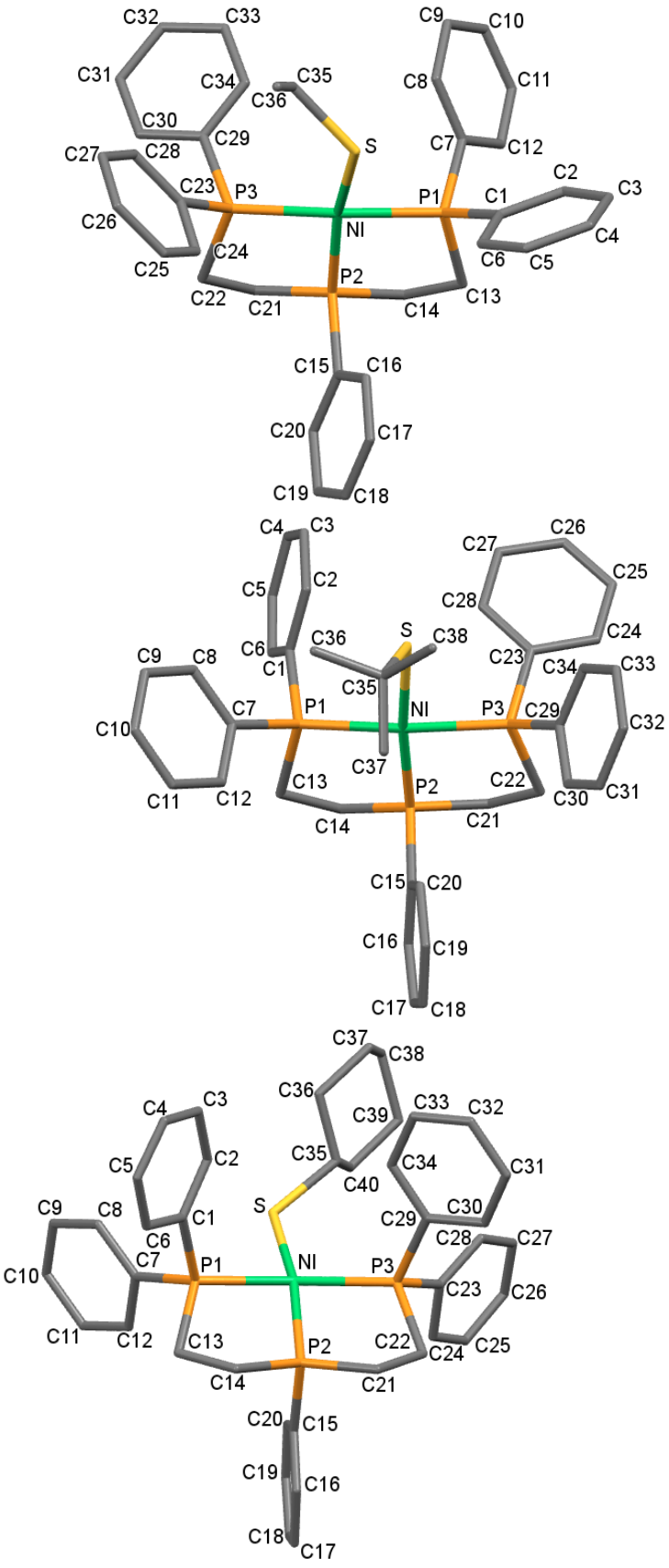


Fig S2 Structures of the cations in [Ni(SEt)(triphos)]BPh_4, [Ni(SBu^t)(triphos)]BPh_4, and [Ni(SCy)(triphos)]BPh_4.

Table S4 Results for the crystal structure of [Ni(SEt)(triphos)]BPh_4

Crystal data and structure refinement.

Identification code	rah200	
Chemical formula (moiety)	$C_{36}H_{38}NiP_3S^+ \cdot C_{24}H_{20}B^-$	
Chemical formula (total)	$C_{60}H_{58}BNiP_3S$	
Formula weight	973.55	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 11.4239(7) Å	α = 96.983(4)°
	b = 14.8484(7) Å	β = 106.192(5)°
	c = 16.8232(8) Å	γ = 110.902(5)°
Cell volume	2481.2(2) $Å^3$	
Z	2	
Calculated density	1.303 g/cm^3	
Absorption coefficient μ	0.569 mm^{-1}	
F(000)	1024	
Crystal colour and size	red, 0.300 × 0.200 × 0.050 mm^3	
Reflections for cell refinement	7075 (θ range 3.0 to 28.6°)	
Data collection method	Oxford Diffraction Gemini A Ultra diffractomer ω scans	
θ range for data collection	3.0 to 28.6°	
Index ranges	h –13 to 15, k –19 to 19, l –21 to 22	
Completeness to θ = 25.2°	99.6 %	
Reflections collected	25830	
Independent reflections	10547 (R_{int} = 0.0369)	
Reflections with $F^2>2\sigma$	8298	
Absorption correction	multi-scan	
Min. and max. transmission	0.85 and 0.97	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0257, 1.1373	
Data / restraints / parameters	10547 / 1168 / 779	
Final R indices [$F^2>2\sigma$]	R1 = 0.0381, wR2 = 0.0747	
R indices (all data)	R1 = 0.0578, wR2 = 0.0834	
Goodness-of-fit on F^2	1.033	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.37 and –0.39 e $Å^{-3}$	

Atomic coordinates and equivalent isotropic displacement parameters (Å^2). U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ni	0.49639(2)	0.72374(2)	0.18105(2)	0.02005(7)
P1	0.36441(5)	0.61272(3)	0.22803(3)	0.02042(11)
P2	0.65533(5)	0.70933(4)	0.27375(3)	0.02131(12)
P3	0.65219(5)	0.85923(4)	0.17609(3)	0.03005(14)
C1	0.2277(9)	0.5050(7)	0.1453(6)	0.020(2)
C2	0.1133(4)	0.4503(3)	0.1628(3)	0.0276(10)
C3	0.0142(4)	0.3643(3)	0.1042(3)	0.0371(12)
C4	0.0252(11)	0.3329(8)	0.0278(7)	0.031(2)
C5	0.1360(4)	0.3858(3)	0.0090(3)	0.0314(11)
C6	0.2366(4)	0.4702(3)	0.0672(2)	0.0263(10)
C1'	0.2277(9)	0.5024(7)	0.1566(6)	0.018(2)
C2'	0.1135(4)	0.5121(3)	0.1111(3)	0.0259(10)
C3'	0.0157(4)	0.4355(3)	0.0433(3)	0.0333(11)
C4'	0.0319(10)	0.3493(8)	0.0211(7)	0.034(2)
C5'	0.1441(4)	0.3382(3)	0.0684(3)	0.0325(11)
C6'	0.2444(4)	0.4155(3)	0.1354(3)	0.0257(10)
C7	0.29348(18)	0.67342(13)	0.29002(12)	0.0214(4)
C8	0.2456(2)	0.74127(15)	0.26046(15)	0.0313(5)
C9	0.1979(2)	0.79165(16)	0.30920(17)	0.0402(6)
C10	0.1980(2)	0.77537(16)	0.38774(16)	0.0382(6)
C11	0.2434(2)	0.70735(18)	0.41729(14)	0.0376(6)
C12	0.2916(2)	0.65705(16)	0.36938(13)	0.0296(5)
C13	0.4648(2)	0.56622(14)	0.30302(14)	0.0275(5)
C14	0.6000(2)	0.65239(14)	0.35375(13)	0.0251(4)
C15	0.7108(12)	0.6179(7)	0.2303(5)	0.0188(19)
C16	0.6234(5)	0.5471(4)	0.1544(3)	0.0259(12)
C17	0.6626(5)	0.4785(4)	0.1186(3)	0.0360(15)
C18	0.7877(6)	0.4817(5)	0.1564(4)	0.0421(14)
C19	0.8743(12)	0.5519(8)	0.2308(6)	0.043(2)
C20	0.8379(12)	0.6209(12)	0.2678(8)	0.029(2)
C15'	0.7128(12)	0.6357(8)	0.2143(5)	0.019(2)
C16'	0.6452(5)	0.5854(4)	0.1293(3)	0.0275(13)
C17'	0.6938(5)	0.5294(4)	0.0872(3)	0.0384(17)
C18'	0.8121(5)	0.5246(5)	0.1283(4)	0.0388(15)
C19'	0.8817(11)	0.5739(8)	0.2141(6)	0.043(3)
C20'	0.8289(14)	0.6263(13)	0.2566(9)	0.042(3)
C21	0.80091(19)	0.82751(14)	0.31882(12)	0.0254(4)
C22	0.8167(2)	0.86834(16)	0.24173(13)	0.0325(5)
C23	0.6519(7)	0.8804(5)	0.0711(4)	0.0174(13)
C24	0.6505(7)	0.7995(4)	0.0187(3)	0.0254(13)
C25	0.6474(7)	0.8022(3)	–0.0644(3)	0.0306(15)
C26	0.6462(7)	0.8838(3)	–0.0940(3)	0.0308(15)
C27	0.6462(8)	0.9630(5)	–0.0430(4)	0.0333(15)
C28	0.6486(9)	0.9618(5)	0.0399(4)	0.0235(14)
C23'	0.6793(8)	0.8577(6)	0.0733(5)	0.0183(14)
C24'	0.7016(7)	0.7834(4)	0.0311(3)	0.0237(13)
C25'	0.7177(7)	0.7876(4)	–0.0472(3)	0.0304(16)

C26'	0.7101(7)	0.8645(4)	–0.0829(3)	0.0303(15)
C27'	0.6842(8)	0.9376(5)	–0.0428(4)	0.0319(16)
C28'	0.6701(9)	0.9351(6)	0.0374(5)	0.0249(15)
C29	0.6433(2)	0.97111(15)	0.22428(12)	0.0315(5)
C30	0.7540(3)	1.06276(17)	0.24969(14)	0.0418(6)
C31	0.7481(3)	1.14753(18)	0.28864(15)	0.0517(8)
C32	0.6337(3)	1.14204(19)	0.30317(16)	0.0534(8)
C33	0.5234(3)	1.05225(19)	0.27856(16)	0.0486(7)
C34	0.5285(2)	0.96672(17)	0.23920(13)	0.0371(6)
S	0.32740(5)	0.70218(4)	0.07131(3)	0.02892(13)
C35	0.3217(6)	0.8115(4)	0.0277(4)	0.0334(15)
C36	0.2827(7)	0.7889(3)	–0.0686(3)	0.051(2)
C35'	0.3523(6)	0.7916(4)	0.0086(3)	0.0285(14)
C36'	0.3593(5)	0.7516(4)	–0.0757(3)	0.0327(15)
B	0.7607(2)	0.78609(16)	0.63319(14)	0.0219(5)
C37	0.84107(19)	0.72057(14)	0.60849(13)	0.0266(5)
C38	0.8558(2)	0.64828(16)	0.65199(16)	0.0395(6)
C39	0.9271(3)	0.59347(17)	0.6354(2)	0.0554(8)
C40	0.9834(3)	0.6066(2)	0.5729(2)	0.0592(9)
C41	0.9667(2)	0.6734(2)	0.52717(17)	0.0507(7)
C42	0.8979(2)	0.72964(16)	0.54471(14)	0.0333(5)
C43	0.8464(2)	0.86472(14)	0.72850(12)	0.0243(4)
C44	0.9315(2)	0.84759(17)	0.79644(13)	0.0349(5)
C45	0.9991(2)	0.91424(19)	0.87620(14)	0.0473(7)
C46	0.9849(3)	1.00216(18)	0.89084(14)	0.0497(7)
C47	0.9010(3)	1.02217(16)	0.82636(14)	0.0416(6)
C48	0.8332(2)	0.95458(15)	0.74659(12)	0.0284(5)
C49	0.73808(19)	0.85492(13)	0.56604(11)	0.0207(4)
C50	0.8493(2)	0.93060(14)	0.55936(12)	0.0240(4)
C51	0.8374(2)	0.99592(15)	0.50873(12)	0.0284(5)
C52	0.7127(2)	0.98898(15)	0.46216(13)	0.0309(5)
C53	0.6008(2)	0.91638(15)	0.46716(13)	0.0317(5)
C54	0.6142(2)	0.85112(14)	0.51836(12)	0.0246(4)
C55	0.61645(19)	0.70669(13)	0.63318(12)	0.0216(4)
C56	0.5267(2)	0.62922(15)	0.56143(12)	0.0282(5)
C57	0.4012(2)	0.56470(16)	0.55727(14)	0.0338(5)
C58	0.3600(2)	0.57376(15)	0.62600(15)	0.0332(5)
C59	0.4464(2)	0.64623(16)	0.69885(15)	0.0371(6)
C60	0.5715(2)	0.71090(15)	0.70158(14)	0.0310(5)

Bond lengths [Å] and angles [°].

Ni–P1	2.1962(6)	Ni–P2	2.1339(6)
Ni–P3	2.1888(6)	Ni–S	2.1600(6)
P1–C1	1.844(7)	P1–C1'	1.793(8)
P1–C7	1.8223(19)	P1–C13	1.831(2)
P2–C14	1.815(2)	P2–C15	1.847(11)
P2–C15'	1.800(11)	P2–C21	1.8196(19)
P3–C22	1.842(2)	P3–C23	1.831(7)
P3–C23'	1.839(7)	P3–C29	1.807(2)
C1–C2	1.404(10)	C1–C6	1.397(10)
C2–H2	0.950	C2–C3	1.387(5)
C3–H3	0.950	C3–C4	1.367(10)
C4–H4	0.950	C4–C5	1.375(11)
C5–H5	0.950	C5–C6	1.377(5)
C6–H6	0.950	C1'–C2'	1.383(10)
C1'–C6'	1.389(10)	C2'–H2'	0.950
C2'–C3'	1.382(5)	C3'–H3'	0.950
C3'–C4'	1.379(10)	C4'–H4'	0.950
C4'–C5'	1.384(10)	C5'–H5'	0.950
C5'–C6'	1.389(5)	C6'–H6'	0.950
C7–C8	1.387(3)	C7–C12	1.390(3)
C8–H8	0.950	C8–C9	1.385(3)
C9–H9	0.950	C9–C10	1.372(3)
C10–H10	0.950	C10–C11	1.374(3)
C11–H11	0.950	C11–C12	1.380(3)
C12–H12	0.950	C13–H13A	0.990
C13–H13B	0.990	C13–C14	1.530(3)
C14–H14A	0.990	C14–H14B	0.990
C15–C16	1.395(8)	C15–C20	1.394(9)
C16–H16	0.950	C16–C17	1.388(6)
C17–H17	0.950	C17–C18	1.374(6)
C18–H18	0.950	C18–C19	1.374(9)
C19–H19	0.950	C19–C20	1.379(10)
C20–H20	0.950	C15'–C16'	1.383(8)
C15'–C20'	1.383(10)	C16'–H16'	0.950
C16'–C17'	1.382(6)	C17'–H17'	0.950
C17'–C18'	1.367(6)	C18'–H18'	0.950
C18'–C19'	1.392(8)	C19'–H19'	0.950
C19'–C20'	1.387(10)	C20'–H20'	0.950
C21–H21A	0.990	C21–H21B	0.990
C21–C22	1.525(3)	C22–H22A	0.990
C22–H22B	0.990	C23–C24	1.393(6)
C23–C28	1.383(7)	C24–H24	0.950
C24–C25	1.394(6)	C25–H25	0.950
C25–C26	1.369(6)	C26–H26	0.950
C26–C27	1.368(6)	C27–H27	0.950
C27–C28	1.390(7)	C28–H28	0.950
C23'–C24'	1.377(7)	C23'–C28'	1.384(7)
C24'–H24'	0.950	C24'–C25'	1.385(6)
C25'–H25'	0.950	C25'–C26'	1.372(7)
C26'–H26'	0.950	C26'–C27'	1.372(7)

C27'–H27'	0.950	C27'–C28'	1.407(8)
C28'–H28'	0.950	C29–C30	1.401(3)
C29–C34	1.384(3)	C30–H30	0.950
C30–C31	1.379(4)	C31–H31	0.950
C31–C32	1.372(4)	C32–H32	0.950
C32–C33	1.383(4)	C33–H33	0.950
C33–C34	1.387(3)	C34–H34	0.950
S–C35	1.875(5)	S–C35'	1.788(5)
C35–H35A	0.990	C35–H35B	0.990
C35–C36	1.515(6)	C36–H36A	0.980
C36–H36B	0.980	C36–H36C	0.980
C35'–H35C	0.990	C35'–H35D	0.990
C35'–C36'	1.504(6)	C36'–H36D	0.980
C36'–H36E	0.980	C36'–H36F	0.980
B–C37	1.648(3)	B–C43	1.657(3)
B–C49	1.641(3)	B–C55	1.649(3)
C37–C38	1.403(3)	C37–C42	1.397(3)
C38–H38	0.950	C38–C39	1.396(3)
C39–H39	0.950	C39–C40	1.377(4)
C40–H40	0.950	C40–C41	1.359(4)
C41–H41	0.950	C41–C42	1.393(3)
C42–H42	0.950	C43–C44	1.394(3)
C43–C48	1.402(3)	C44–H44	0.950
C44–C45	1.389(3)	C45–H45	0.950
C45–C46	1.373(4)	C46–H46	0.950
C46–C47	1.373(4)	C47–H47	0.950
C47–C48	1.395(3)	C48–H48	0.950
C49–C50	1.408(3)	C49–C54	1.396(3)
C50–H50	0.950	C50–C51	1.384(3)
C51–H51	0.950	C51–C52	1.381(3)
C52–H52	0.950	C52–C53	1.379(3)
C53–H53	0.950	C53–C54	1.393(3)
C54–H54	0.950	C55–C56	1.401(3)
C55–C60	1.388(3)	C56–H56	0.950
C56–C57	1.388(3)	C57–H57	0.950
C57–C58	1.374(3)	C58–H58	0.950
C58–C59	1.372(3)	C59–H59	0.950
C59–C60	1.393(3)	C60–H60	0.950

P1–Ni–P2	85.24(2)	P1–Ni–P3	162.10(2)
P1–Ni–S	90.22(2)	P2–Ni–P3	85.23(2)
P2–Ni–S	165.83(2)	P3–Ni–S	102.43(2)
Ni–P1–C1	115.5(4)	Ni–P1–C1'	121.6(4)
Ni–P1–C7	109.08(6)	Ni–P1–C13	108.95(7)
C1–P1–C7	109.0(3)	C1–P1–C13	108.1(4)
C1'–P1–C7	106.2(3)	C1'–P1–C13	104.2(4)
C7–P1–C13	105.71(10)	Ni–P2–C14	111.52(7)
Ni–P2–C15	113.4(3)	Ni–P2–C15'	105.5(3)
Ni–P2–C21	111.09(7)	C14–P2–C15	99.8(3)
C14–P2–C15'	112.1(3)	C14–P2–C21	113.49(9)
C15–P2–C21	107.1(4)	C15'–P2–C21	102.5(4)
Ni–P3–C22	109.06(7)	Ni–P3–C23	118.1(2)

Ni–P3–C23'	115.5(2)	Ni–P3–C29	112.70(7)
C22–P3–C23	111.0(2)	C22–P3–C23'	98.3(3)
C22–P3–C29	104.06(10)	C23–P3–C29	100.8(2)
C23'–P3–C29	115.4(2)	P1–C1–C2	119.5(6)
P1–C1–C6	122.7(6)	C2–C1–C6	117.6(6)
C1–C2–H2	119.8	C1–C2–C3	120.4(5)
H2–C2–C3	119.8	C2–C3–H3	119.8
C2–C3–C4	120.5(6)	H3–C3–C4	119.8
C3–C4–H4	120.0	C3–C4–C5	120.1(8)
H4–C4–C5	120.0	C4–C5–H5	119.9
C4–C5–C6	120.2(6)	H5–C5–C6	119.9
C1–C6–C5	121.1(5)	C1–C6–H6	119.4
C5–C6–H6	119.4	P1–C1'–C2'	117.3(7)
P1–C1'–C6'	121.0(6)	C2'–C1'–C6'	120.5(6)
C1'–C2'–H2'	120.0	C1'–C2'–C3'	119.9(5)
H2'–C2'–C3'	120.0	C2'–C3'–H3'	120.0
C2'–C3'–C4'	120.1(6)	H3'–C3'–C4'	120.0
C3'–C4'–H4'	120.0	C3'–C4'–C5'	120.0(8)
H4'–C4'–C5'	120.0	C4'–C5'–H5'	119.8
C4'–C5'–C6'	120.5(5)	H5'–C5'–C6'	119.8
C1'–C6'–C5'	118.9(5)	C1'–C6'–H6'	120.5
C5'–C6'–H6'	120.5	P1–C7–C8	120.24(15)
P1–C7–C12	121.39(15)	C8–C7–C12	118.30(18)
C7–C8–H8	119.7	C7–C8–C9	120.6(2)
H8–C8–C9	119.7	C8–C9–H9	119.8
C8–C9–C10	120.3(2)	H9–C9–C10	119.8
C9–C10–H10	120.2	C9–C10–C11	119.6(2)
H10–C10–C11	120.2	C10–C11–H11	119.8
C10–C11–C12	120.5(2)	H11–C11–C12	119.8
C7–C12–C11	120.6(2)	C7–C12–H12	119.7
C11–C12–H12	119.7	P1–C13–H13A	110.0
P1–C13–H13B	110.0	P1–C13–C14	108.33(14)
H13A–C13–H13B	108.4	H13A–C13–C14	110.0
H13B–C13–C14	110.0	P2–C14–C13	104.72(14)
P2–C14–H14A	110.8	P2–C14–H14B	110.8
C13–C14–H14A	110.8	C13–C14–H14B	110.8
H14A–C14–H14B	108.9	P2–C15–C16	117.7(7)
P2–C15–C20	122.5(7)	C16–C15–C20	119.6(8)
C15–C16–H16	120.2	C15–C16–C17	119.5(6)
H16–C16–C17	120.2	C16–C17–H17	119.8
C16–C17–C18	120.3(4)	H17–C17–C18	119.8
C17–C18–H18	119.9	C17–C18–C19	120.2(6)
H18–C18–C19	119.9	C18–C19–H19	119.6
C18–C19–C20	120.7(9)	H19–C19–C20	119.6
C15–C20–C19	119.6(10)	C15–C20–H20	120.2
C19–C20–H20	120.2	P2–C15'–C16'	123.6(8)
P2–C15'–C20'	118.3(7)	C16'–C15'–C20'	118.1(9)
C15'–C16'–H16'	119.5	C15'–C16'–C17'	121.0(6)
H16'–C16'–C17'	119.5	C16'–C17'–H17'	119.7
C16'–C17'–C18'	120.5(4)	H17'–C17'–C18'	119.7
C17'–C18'–H18'	120.2	C17'–C18'–C19'	119.7(6)
H18'–C18'–C19'	120.2	C18'–C19'–H19'	120.4

C18'–C19'–C20'	119.2(9)	H19'–C19'–C20'	120.4
C15'–C20'–C19'	121.4(10)	C15'–C20'–H20'	119.3
C19'–C20'–H20'	119.3	P2–C21–H21A	110.9
P2–C21–H21B	110.9	P2–C21–C22	104.43(13)
H21A–C21–H21B	108.9	H21A–C21–C22	110.9
H21B–C21–C22	110.9	P3–C22–C21	107.89(14)
P3–C22–H22A	110.1	P3–C22–H22B	110.1
C21–C22–H22A	110.1	C21–C22–H22B	110.1
H22A–C22–H22B	108.4	P3–C23–C24	111.8(5)
P3–C23–C28	128.4(4)	C24–C23–C28	119.8(6)
C23–C24–H24	120.3	C23–C24–C25	119.4(5)
H24–C24–C25	120.3	C24–C25–H25	119.9
C24–C25–C26	120.2(4)	H25–C25–C26	119.9
C25–C26–H26	119.7	C25–C26–C27	120.5(4)
H26–C26–C27	119.7	C26–C27–H27	119.8
C26–C27–C28	120.3(5)	H27–C27–C28	119.8
C23–C28–C27	119.8(5)	C23–C28–H28	120.1
C27–C28–H28	120.1	P3–C23'–C24'	123.8(5)
P3–C23'–C28'	115.6(5)	C24'–C23'–C28'	120.6(6)
C23'–C24'–H24'	120.3	C23'–C24'–C25'	119.5(5)
H24'–C24'–C25'	120.3	C24'–C25'–H25'	119.8
C24'–C25'–C26'	120.4(5)	H25'–C25'–C26'	119.8
C25'–C26'–H26'	119.6	C25'–C26'–C27'	120.9(5)
H26'–C26'–C27'	119.6	C26'–C27'–H27'	120.4
C26'–C27'–C28'	119.2(5)	H27'–C27'–C28'	120.4
C23'–C28'–C27'	119.4(5)	C23'–C28'–H28'	120.3
C27'–C28'–H28'	120.3	P3–C29–C30	120.5(2)
P3–C29–C34	120.32(16)	C30–C29–C34	119.1(2)
C29–C30–H30	119.8	C29–C30–C31	120.3(3)
H30–C30–C31	119.8	C30–C31–H31	120.1
C30–C31–C32	119.9(2)	H31–C31–C32	120.1
C31–C32–H32	119.7	C31–C32–C33	120.6(3)
H32–C32–C33	119.7	C32–C33–H33	120.1
C32–C33–C34	119.8(3)	H33–C33–C34	120.1
C29–C34–C33	120.2(2)	C29–C34–H34	119.9
C33–C34–H34	119.9	Ni–S–C35	119.24(18)
Ni–S–C35'	117.1(2)	S–C35–H35A	109.1
S–C35–H35B	109.1	S–C35–C36	112.6(4)
H35A–C35–H35B	107.8	H35A–C35–C36	109.1
H35B–C35–C36	109.1	C35–C36–H36A	109.5
C35–C36–H36B	109.5	C35–C36–H36C	109.5
H36A–C36–H36B	109.5	H36A–C36–H36C	109.5
H36B–C36–H36C	109.5	S–C35'–H35C	109.0
S–C35'–H35D	109.0	S–C35'–C36'	112.8(4)
H35C–C35'–H35D	107.8	H35C–C35'–C36'	109.0
H35D–C35'–C36'	109.0	C35'–C36'–H36D	109.5
C35'–C36'–H36E	109.5	C35'–C36'–H36F	109.5
H36D–C36'–H36E	109.5	H36D–C36'–H36F	109.5
H36E–C36'–H36F	109.5	C37–B–C43	111.36(16)
C37–B–C49	111.91(16)	C37–B–C55	107.18(16)
C43–B–C49	105.69(15)	C43–B–C55	109.78(16)
C49–B–C55	110.97(16)	B–C37–C38	120.40(19)

B–C37–C42	125.06(19)	C38–C37–C42	114.5(2)
C37–C38–H38	118.8	C37–C38–C39	122.5(3)
H38–C38–C39	118.8	C38–C39–H39	119.7
C38–C39–C40	120.6(3)	H39–C39–C40	119.7
C39–C40–H40	120.8	C39–C40–C41	118.5(3)
H40–C40–C41	120.8	C40–C41–H41	119.5
C40–C41–C42	121.0(3)	H41–C41–C42	119.5
C37–C42–C41	122.8(2)	C37–C42–H42	118.6
C41–C42–H42	118.6	B–C43–C44	124.60(19)
B–C43–C48	120.41(18)	C44–C43–C48	114.96(18)
C43–C44–H44	118.5	C43–C44–C45	122.9(2)
H44–C44–C45	118.5	C44–C45–H45	119.9
C44–C45–C46	120.2(2)	H45–C45–C46	119.9
C45–C46–H46	120.4	C45–C46–C47	119.2(2)
H46–C46–C47	120.4	C46–C47–H47	119.9
C46–C47–C48	120.1(2)	H47–C47–C48	119.9
C43–C48–C47	122.5(2)	C43–C48–H48	118.7
C47–C48–H48	118.7	B–C49–C50	119.79(17)
B–C49–C54	124.96(17)	C50–C49–C54	115.00(18)
C49–C50–H50	118.6	C49–C50–C51	122.7(2)
H50–C50–C51	118.6	C50–C51–H51	119.9
C50–C51–C52	120.3(2)	H51–C51–C52	119.9
C51–C52–H52	120.5	C51–C52–C53	119.0(2)
H52–C52–C53	120.5	C52–C53–H53	119.9
C52–C53–C54	120.2(2)	H53–C53–C54	119.9
C49–C54–C53	122.80(19)	C49–C54–H54	118.6
C53–C54–H54	118.6	B–C55–C56	121.59(17)
B–C55–C60	124.21(17)	C56–C55–C60	114.19(18)
C55–C56–H56	118.4	C55–C56–C57	123.19(19)
H56–C56–C57	118.4	C56–C57–H57	119.8
C56–C57–C58	120.31(19)	H57–C57–C58	119.8
C57–C58–H58	120.7	C57–C58–C59	118.6(2)
H58–C58–C59	120.7	C58–C59–H59	119.8
C58–C59–C60	120.3(2)	H59–C59–C60	119.8
C55–C60–C59	123.37(19)	C55–C60–H60	118.3
C59–C60–H60	118.3		

Torsion angles [°].

Ni–P1–C1–C2	−157.2(7)	Ni–P1–C1–C6	27.7(10)
C7–P1–C1–C2	−34.0(10)	C7–P1–C1–C6	150.9(8)
C13–P1–C1–C2	80.5(8)	C13–P1–C1–C6	−94.6(9)
P1–C1–C2–C3	−174.7(5)	C6–C1–C2–C3	0.6(13)
C1–C2–C3–C4	−1.4(10)	C2–C3–C4–C5	0.9(12)
C3–C4–C5–C6	0.4(12)	C4–C5–C6–C1	−1.2(10)
P1–C1–C6–C5	175.8(6)	C2–C1–C6–C5	0.6(13)
Ni–P1–C1'–C2'	−77.6(8)	Ni–P1–C1'–C6'	90.3(9)
C7–P1–C1'–C2'	47.8(8)	C7–P1–C1'–C6'	−144.4(7)
C13–P1–C1'–C2'	159.1(7)	C13–P1–C1'–C6'	−33.0(9)
P1–C1'–C2'–C3'	167.1(5)	C6'–C1'–C2'–C3'	−0.8(12)
C1'–C2'–C3'–C4'	0.1(10)	C2'–C3'–C4'–C5'	2.1(12)
C3'–C4'–C5'–C6'	−3.6(13)	P1–C1'–C6'–C5'	−168.1(6)
C2'–C1'–C6'–C5'	−0.6(12)	C4'–C5'–C6'–C1'	2.9(10)
Ni–P1–C7–C8	43.81(17)	Ni–P1–C7–C12	−133.06(15)
C1–P1–C7–C8	−83.2(5)	C1–P1–C7–C12	100.0(5)
C1'–P1–C7–C8	−88.8(4)	C1'–P1–C7–C12	94.3(4)
C13–P1–C7–C8	160.82(16)	C13–P1–C7–C12	−16.05(18)
P1–C7–C8–C9	−176.60(17)	C12–C7–C8–C9	0.4(3)
C7–C8–C9–C10	0.3(3)	C8–C9–C10–C11	−1.2(3)
C9–C10–C11–C12	1.5(3)	C10–C11–C12–C7	−0.8(3)
P1–C7–C12–C11	176.83(16)	C8–C7–C12–C11	−0.1(3)
Ni–P1–C13–C14	35.90(15)	C1–P1–C13–C14	162.2(4)
C1'–P1–C13–C14	167.0(4)	C7–P1–C13–C14	−81.20(15)
P1–C13–C14–P2	−47.86(16)	Ni–P2–C14–C13	43.49(14)
C15–P2–C14–C13	−76.5(3)	C15'–P2–C14–C13	−74.6(4)
C21–P2–C14–C13	169.86(13)	Ni–P2–C15–C16	−19.7(8)
Ni–P2–C15–C20	156.7(10)	C14–P2–C15–C16	99.0(7)
C14–P2–C15–C20	−84.6(11)	C21–P2–C15–C16	−142.6(6)
C21–P2–C15–C20	33.8(11)	P2–C15–C16–C17	178.5(5)
C20–C15–C16–C17	2.0(13)	C15–C16–C17–C18	−1.5(9)
C16–C17–C18–C19	1.1(10)	C17–C18–C19–C20	−1.1(15)
C18–C19–C20–C15	2(2)	P2–C15–C20–C19	−178.3(10)
C16–C15–C20–C19	−2.0(19)	Ni–P2–C15'–C16'	−11.3(9)
Ni–P2–C15'–C20'	170.7(11)	C14–P2–C15'–C16'	110.3(7)
C14–P2–C15'–C20'	−67.7(12)	C21–P2–C15'–C16'	−127.7(8)
C21–P2–C15'–C20'	54.3(12)	P2–C15'–C16'–C17'	−179.5(6)
C20'–C15'–C16'–C17'	−1.5(15)	C15'–C16'–C17'–C18'	−1.8(10)
C16'–C17'–C18'–C19'	2.2(10)	C17'–C18'–C19'–C20'	0.6(16)
P2–C15'–C20'–C19'	−177.5(12)	C16'–C15'–C20'–C19'	4(2)
C18'–C19'–C20'–C15'	−4(2)	Ni–P2–C21–C22	−45.34(15)
C14–P2–C21–C22	−171.94(14)	C15–P2–C21–C22	78.9(3)
C15'–P2–C21–C22	66.9(3)	P2–C21–C22–P3	48.62(16)
Ni–P3–C22–C21	−35.64(15)	C23–P3–C22–C21	−167.5(3)
C23'–P3–C22–C21	−156.3(3)	C29–P3–C22–C21	84.86(15)
Ni–P3–C23–C24	−53.3(5)	Ni–P3–C23–C28	124.4(6)
C22–P3–C23–C24	73.7(5)	C22–P3–C23–C28	−108.6(7)

C29–P3–C23–C24	−176.5(4)	C29–P3–C23–C28	1.2(7)
P3–C23–C24–C25	178.7(4)	C28–C23–C24–C25	0.8(9)
C23–C24–C25–C26	0.2(8)	C24–C25–C26–C27	−0.9(8)
C25–C26–C27–C28	0.6(10)	P3–C23–C28–C27	−178.6(6)
C24–C23–C28–C27	−1.1(11)	C26–C27–C28–C23	0.4(11)
Ni–P3–C23'–C24'	−52.2(6)	Ni–P3–C23'–C28'	125.0(5)
C22–P3–C23'–C24'	63.6(6)	C22–P3–C23'–C28'	−119.2(6)
C29–P3–C23'–C24'	173.5(5)	C29–P3–C23'–C28'	−9.3(7)
P3–C23'–C24'–C25'	178.4(5)	C28'–C23'–C24'–C25'	1.4(10)
C23'–C24'–C25'–C26'	−0.7(8)	C24'–C25'–C26'–C27'	−1.1(8)
C25'–C26'–C27'–C28'	2.3(9)	P3–C23'–C28'–C27'	−177.5(6)
C24'–C23'–C28'–C27'	−0.2(11)	C26'–C27'–C28'–C23'	−1.6(11)
Ni–P3–C29–C30	161.16(15)	Ni–P3–C29–C34	−16.64(19)
C22–P3–C29–C30	43.15(19)	C22–P3–C29–C34	−134.65(17)
C23–P3–C29–C30	−72.0(3)	C23–P3–C29–C34	110.2(3)
C23'–P3–C29–C30	−63.3(3)	C23'–P3–C29–C34	118.9(3)
P3–C29–C30–C31	−178.17(17)	C34–C29–C30–C31	−0.3(3)
C29–C30–C31–C32	0.5(4)	C30–C31–C32–C33	−0.5(4)
C31–C32–C33–C34	0.3(4)	P3–C29–C34–C33	178.04(17)
C30–C29–C34–C33	0.2(3)	C32–C33–C34–C29	−0.2(4)
Ni–S–C35–C36	133.7(4)	Ni–S–C35'–C36'	106.8(4)
C43–B–C37–C38	69.7(2)	C43–B–C37–C42	−111.0(2)
C49–B–C37–C38	−172.28(17)	C49–B–C37–C42	7.1(3)
C55–B–C37–C38	−50.4(2)	C55–B–C37–C42	128.93(19)
B–C37–C38–C39	−177.6(2)	C42–C37–C38–C39	2.9(3)
C37–C38–C39–C40	−1.9(4)	C38–C39–C40–C41	−0.6(4)
C39–C40–C41–C42	1.9(4)	C40–C41–C42–C37	−0.8(3)
B–C37–C42–C41	179.01(19)	C38–C37–C42–C41	−1.6(3)
C37–B–C43–C44	−31.4(3)	C37–B–C43–C48	150.72(18)
C49–B–C43–C44	−153.08(19)	C49–B–C43–C48	29.0(2)
C55–B–C43–C44	87.2(2)	C55–B–C43–C48	−90.8(2)
B–C43–C44–C45	−178.3(2)	C48–C43–C44–C45	−0.2(3)
C43–C44–C45–C46	−0.7(4)	C44–C45–C46–C47	1.5(4)
C45–C46–C47–C48	−1.2(4)	C46–C47–C48–C43	0.2(3)
B–C43–C48–C47	178.61(19)	C44–C43–C48–C47	0.5(3)
C37–B–C49–C50	−63.2(2)	C37–B–C49–C54	122.86(19)
C43–B–C49–C50	58.2(2)	C43–B–C49–C54	−115.76(19)
C55–B–C49–C50	177.17(16)	C55–B–C49–C54	3.2(3)
B–C49–C50–C51	−175.19(17)	C54–C49–C50–C51	−0.6(3)
C49–C50–C51–C52	0.2(3)	C50–C51–C52–C53	0.2(3)
C51–C52–C53–C54	−0.2(3)	C52–C53–C54–C49	−0.3(3)
B–C49–C54–C53	174.89(18)	C50–C49–C54–C53	0.7(3)
C37–B–C55–C56	−56.1(2)	C37–B–C55–C60	125.3(2)
C43–B–C55–C56	−177.18(18)	C43–B–C55–C60	4.2(3)
C49–B–C55–C56	66.4(2)	C49–B–C55–C60	−112.2(2)
B–C55–C56–C57	−176.0(2)	C60–C55–C56–C57	2.7(3)
C55–C56–C57–C58	−1.1(3)	C56–C57–C58–C59	−1.4(3)
C57–C58–C59–C60	2.0(3)	B–C55–C60–C59	176.6(2)
C56–C55–C60–C59	−2.1(3)	C58–C59–C60–C55	−0.2(4)

Anisotropic displacement parameters ($Å^2$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	0.01456(12)	0.02167(13)	0.01744(12)	0.00068(10)	0.00562(10)	0.00150(10)
P1	0.0143(2)	0.0172(2)	0.0292(3)	0.0044(2)	0.0077(2)	0.0061(2)
P2	0.0141(2)	0.0219(3)	0.0226(3)	–0.0029(2)	0.0058(2)	0.0047(2)
P3	0.0227(3)	0.0333(3)	0.0161(2)	0.0018(2)	0.0062(2)	–0.0069(2)
C1	0.012(3)	0.013(3)	0.028(4)	0.005(3)	0.006(3)	–0.001(3)
C2	0.020(2)	0.030(2)	0.031(2)	0.0060(17)	0.0092(17)	0.0080(17)
C3	0.020(2)	0.035(2)	0.045(2)	0.007(2)	0.0079(18)	0.0012(19)
C4	0.022(4)	0.020(3)	0.041(4)	0.002(3)	0.003(3)	0.006(3)
C5	0.031(2)	0.025(2)	0.034(2)	–0.0016(18)	0.0073(18)	0.0132(19)
C6	0.024(2)	0.024(2)	0.031(2)	0.0066(16)	0.0109(17)	0.0084(17)
C1'	0.022(4)	0.022(4)	0.017(3)	0.011(2)	0.009(2)	0.013(3)
C2'	0.018(2)	0.021(2)	0.035(2)	0.0087(17)	0.0068(17)	0.0063(16)
C3'	0.015(2)	0.033(2)	0.040(2)	0.0042(19)	–0.0018(17)	0.0064(18)
C4'	0.019(4)	0.029(4)	0.034(4)	–0.003(3)	–0.003(3)	0.002(3)
C5'	0.029(2)	0.024(2)	0.036(2)	–0.0041(18)	0.0054(18)	0.0082(18)
C6'	0.0181(19)	0.025(2)	0.030(2)	0.0023(16)	0.0039(16)	0.0097(16)
C7	0.0156(9)	0.0179(9)	0.0283(10)	0.0046(8)	0.0080(8)	0.0042(8)
C8	0.0363(12)	0.0319(12)	0.0429(13)	0.0200(10)	0.0247(11)	0.0214(10)
C9	0.0405(14)	0.0298(12)	0.0654(17)	0.0169(12)	0.0297(13)	0.0210(11)
C10	0.0291(12)	0.0327(12)	0.0482(14)	–0.0061(11)	0.0196(11)	0.0080(10)
C11	0.0302(12)	0.0496(14)	0.0291(12)	0.0025(10)	0.0117(10)	0.0135(11)
C12	0.0251(11)	0.0353(12)	0.0284(11)	0.0082(9)	0.0071(9)	0.0141(10)
C13	0.0212(10)	0.0223(10)	0.0411(12)	0.0101(9)	0.0106(9)	0.0107(9)
C14	0.0219(10)	0.0230(10)	0.0308(11)	0.0065(9)	0.0081(9)	0.0105(9)
C15	0.023(3)	0.017(3)	0.020(3)	0.006(3)	0.011(3)	0.009(2)
C16	0.025(2)	0.026(3)	0.027(2)	0.0044(19)	0.0138(19)	0.008(2)
C17	0.047(3)	0.026(3)	0.038(3)	0.001(2)	0.025(2)	0.012(2)
C18	0.053(3)	0.034(3)	0.060(3)	0.014(2)	0.036(2)	0.028(3)
C19	0.037(3)	0.043(4)	0.061(4)	0.015(3)	0.023(3)	0.025(3)
C20	0.018(3)	0.035(4)	0.035(4)	0.009(3)	0.007(3)	0.014(3)
C15'	0.019(3)	0.020(4)	0.021(3)	0.008(3)	0.007(2)	0.010(3)
C16'	0.028(3)	0.029(3)	0.024(2)	0.004(2)	0.0056(19)	0.013(2)
C17'	0.051(3)	0.037(3)	0.030(3)	–0.001(2)	0.014(2)	0.023(3)
C18'	0.044(3)	0.031(3)	0.052(3)	0.008(2)	0.026(2)	0.021(2)
C19'	0.029(3)	0.043(5)	0.055(4)	–0.005(4)	0.009(3)	0.021(4)
C20'	0.037(5)	0.045(6)	0.036(4)	–0.014(4)	–0.002(3)	0.026(4)
C21	0.0181(10)	0.0261(11)	0.0211(10)	–0.0046(8)	0.0042(8)	0.0024(9)
C22	0.0209(10)	0.0362(12)	0.0256(11)	–0.0028(9)	0.0094(9)	–0.0024(10)
C23	0.016(3)	0.014(3)	0.018(2)	–0.002(2)	0.005(2)	0.0035(19)
C24	0.033(3)	0.020(2)	0.026(2)	0.0054(19)	0.010(2)	0.013(2)
C25	0.039(3)	0.030(2)	0.022(2)	–0.0005(17)	0.011(2)	0.015(2)
C26	0.045(4)	0.029(2)	0.019(2)	0.0046(19)	0.014(2)	0.013(2)
C27	0.051(4)	0.024(3)	0.024(2)	0.006(2)	0.017(2)	0.012(2)
C28	0.034(3)	0.018(3)	0.018(2)	0.005(2)	0.011(2)	0.009(2)
C23'	0.019(3)	0.014(3)	0.020(3)	0.006(2)	0.010(2)	0.003(2)
C24'	0.026(3)	0.023(2)	0.022(2)	0.0052(18)	0.011(2)	0.009(2)

C25'	0.028(3)	0.034(3)	0.022(2)	–0.0009(18)	0.011(2)	0.007(2)
C26'	0.028(3)	0.033(3)	0.018(2)	0.0022(18)	0.010(2)	0.000(2)
C27'	0.042(4)	0.022(3)	0.021(3)	0.007(2)	0.012(2)	–0.001(2)
C28'	0.029(3)	0.016(4)	0.024(2)	0.000(2)	0.007(2)	0.005(2)
C29	0.0348(12)	0.0291(11)	0.0158(10)	0.0079(9)	0.0033(9)	–0.0001(10)
C30	0.0438(14)	0.0337(13)	0.0269(11)	0.0112(10)	0.0055(10)	–0.0037(11)
C31	0.0643(19)	0.0282(13)	0.0322(13)	0.0100(11)	–0.0023(13)	–0.0013(13)
C32	0.074(2)	0.0342(14)	0.0337(14)	0.0074(11)	–0.0045(14)	0.0202(15)
C33	0.0522(16)	0.0515(16)	0.0372(14)	0.0086(12)	0.0055(12)	0.0242(14)
C34	0.0367(13)	0.0357(13)	0.0253(11)	0.0066(10)	0.0029(10)	0.0060(11)
S	0.0184(2)	0.0328(3)	0.0225(2)	0.0052(2)	0.0023(2)	0.0002(2)
C35	0.023(3)	0.050(3)	0.023(3)	0.017(2)	0.008(2)	0.007(2)
C36	0.079(5)	0.029(3)	0.032(3)	0.015(2)	0.007(3)	0.017(3)
C35'	0.015(3)	0.040(3)	0.023(3)	0.011(2)	0.0080(19)	0.001(2)
C36'	0.032(3)	0.039(3)	0.022(2)	0.0113(19)	0.0069(19)	0.011(2)
B	0.0186(11)	0.0246(12)	0.0189(11)	0.0050(9)	0.0034(9)	0.0073(10)
C37	0.0176(10)	0.0223(10)	0.0294(11)	–0.0012(8)	–0.0001(8)	0.0052(9)
C38	0.0293(12)	0.0274(12)	0.0512(15)	0.0069(11)	0.0020(11)	0.0099(10)
C39	0.0350(14)	0.0220(12)	0.087(2)	0.0018(13)	–0.0086(15)	0.0137(11)
C40	0.0324(14)	0.0450(16)	0.080(2)	–0.0241(15)	–0.0015(14)	0.0214(13)
C41	0.0289(13)	0.0581(17)	0.0497(16)	–0.0191(13)	0.0032(11)	0.0188(13)
C42	0.0220(11)	0.0365(12)	0.0327(12)	–0.0057(10)	0.0036(9)	0.0112(10)
C43	0.0213(10)	0.0253(10)	0.0197(10)	0.0050(8)	0.0066(8)	0.0027(9)
C44	0.0297(12)	0.0360(12)	0.0269(11)	0.0070(10)	0.0007(9)	0.0072(10)
C45	0.0355(14)	0.0531(16)	0.0256(12)	0.0112(11)	–0.0052(10)	–0.0010(12)
C46	0.0571(17)	0.0380(14)	0.0169(11)	–0.0008(10)	0.0035(11)	–0.0123(13)
C47	0.0614(17)	0.0244(11)	0.0269(12)	0.0019(9)	0.0196(12)	0.0023(11)
C48	0.0354(12)	0.0260(11)	0.0198(10)	0.0053(8)	0.0113(9)	0.0068(10)
C49	0.0238(10)	0.0207(10)	0.0145(9)	–0.0013(7)	0.0068(8)	0.0073(8)
C50	0.0238(10)	0.0272(11)	0.0167(9)	0.0025(8)	0.0066(8)	0.0070(9)
C51	0.0355(12)	0.0252(11)	0.0216(10)	0.0028(8)	0.0136(9)	0.0073(10)
C52	0.0463(14)	0.0242(11)	0.0218(10)	0.0072(9)	0.0100(10)	0.0150(10)
C53	0.0325(12)	0.0305(12)	0.0281(11)	0.0056(9)	0.0023(9)	0.0154(10)
C54	0.0223(10)	0.0231(10)	0.0241(10)	0.0036(8)	0.0047(8)	0.0077(9)
C55	0.0220(10)	0.0194(10)	0.0219(10)	0.0065(8)	0.0045(8)	0.0088(8)
C56	0.0299(11)	0.0276(11)	0.0196(10)	0.0077(9)	0.0053(9)	0.0051(9)
C57	0.0281(12)	0.0277(11)	0.0293(11)	0.0108(9)	–0.0028(9)	0.0020(10)
C58	0.0237(11)	0.0238(11)	0.0529(14)	0.0197(10)	0.0127(10)	0.0079(9)
C59	0.0439(14)	0.0277(12)	0.0475(14)	0.0108(10)	0.0300(12)	0.0121(11)
C60	0.0348(12)	0.0216(10)	0.0325(11)	0.0018(9)	0.0148(10)	0.0064(10)

Hydrogen coordinates and isotropic displacement parameters ($Å^2$).

	x	y	z	U
H2	0.1037	0.4722	0.2151	0.033
H3	–0.0619	0.3270	0.1172	0.044
H4	–0.0437	0.2744	–0.0123	0.037
H5	0.1431	0.3640	–0.0442	0.038
H6	0.3133	0.5054	0.0539	0.032
H2'	0.1022	0.5714	0.1265	0.031
H3'	–0.0627	0.4421	0.0120	0.040
H4'	–0.0339	0.2975	–0.0267	0.040
H5'	0.1525	0.2773	0.0550	0.039
H6'	0.3233	0.4091	0.1663	0.031
H8	0.2455	0.7533	0.2063	0.038
H9	0.1651	0.8377	0.2881	0.048
H10	0.1669	0.8109	0.4215	0.046
H11	0.2416	0.6948	0.4711	0.045
H12	0.3238	0.6108	0.3908	0.035
H13A	0.4186	0.5397	0.3423	0.033
H13B	0.4779	0.5119	0.2715	0.033
H14A	0.6643	0.6277	0.3855	0.030
H14B	0.5904	0.7006	0.3948	0.030
H16	0.5377	0.5458	0.1275	0.031
H17	0.6026	0.4292	0.0676	0.043
H18	0.8145	0.4353	0.1310	0.050
H19	0.9600	0.5529	0.2570	0.051
H20	0.8991	0.6702	0.3185	0.035
H16'	0.5641	0.5895	0.0994	0.033
H17'	0.6447	0.4939	0.0292	0.046
H18'	0.8467	0.4879	0.0985	0.047
H19'	0.9645	0.5716	0.2431	0.052
H20'	0.8733	0.6564	0.3160	0.050
H21A	0.7861	0.8733	0.3589	0.030
H21B	0.8812	0.8176	0.3495	0.030
H22A	0.8488	0.8293	0.2080	0.039
H22B	0.8825	0.9386	0.2607	0.039
H24	0.6516	0.7430	0.0395	0.030
H25	0.6462	0.7472	–0.1005	0.037
H26	0.6453	0.8855	–0.1504	0.037
H27	0.6445	1.0190	–0.0644	0.040
H28	0.6480	1.0167	0.0750	0.028
H24'	0.7059	0.7297	0.0555	0.028
H25'	0.7341	0.7370	–0.0762	0.036
H26'	0.7229	0.8672	–0.1361	0.036
H27'	0.6758	0.9893	–0.0689	0.038
H28'	0.6545	0.9860	0.0667	0.030
H30	0.8335	1.0666	0.2401	0.050
H31	0.8231	1.2096	0.3054	0.062
H32	0.6302	1.2005	0.3304	0.064
H33	0.4444	1.0492	0.2886	0.058

H34	0.4529	0.9050	0.2224	0.044
H35A	0.2566	0.8321	0.0442	0.040
H35B	0.4107	0.8678	0.0536	0.040
H36A	0.2811	0.8481	–0.0882	0.076
H36B	0.3478	0.7698	–0.0853	0.076
H36C	0.1938	0.7341	–0.0947	0.076
H35C	0.2780	0.8133	–0.0020	0.034
H35D	0.4363	0.8507	0.0412	0.034
H36D	0.3730	0.8033	–0.1075	0.049
H36E	0.4340	0.7314	–0.0657	0.049
H36F	0.2756	0.6940	–0.1089	0.049
H38	0.8157	0.6362	0.6943	0.047
H39	0.9370	0.5467	0.6676	0.066
H40	1.0327	0.5699	0.5619	0.071
H41	1.0025	0.6818	0.4826	0.061
H42	0.8893	0.7762	0.5119	0.040
H44	0.9439	0.7877	0.7878	0.042
H45	1.0552	0.8989	0.9208	0.057
H46	1.0326	1.0486	0.9449	0.060
H47	0.8890	1.0822	0.8361	0.050
H48	0.7759	0.9700	0.7028	0.034
H50	0.9363	0.9371	0.5909	0.029
H51	0.9153	1.0457	0.5060	0.034
H52	0.7041	1.0336	0.4272	0.037
H53	0.5144	0.9109	0.4356	0.038
H54	0.5356	0.8019	0.5210	0.030
H56	0.5531	0.6204	0.5133	0.034
H57	0.3436	0.5140	0.5067	0.041
H58	0.2735	0.5307	0.6231	0.040
H59	0.4209	0.6523	0.7477	0.045
H60	0.6290	0.7604	0.7529	0.037

Table S5 Results for the crystal structure of [Ni(SBu^t)(triphos)]BPh$_4$

Crystal data and structure refinement.

Identification code	rah213	
Chemical formula (moiety)	$C_{38}H_{42}NiP_3S^+ \cdot C_{24}H_{20}B^- \cdot 0.5CH_2Cl_2$	
Chemical formula (total)	$C_{62.5}H_{63}BClNiP_3S$	
Formula weight	1044.07	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 12.5663(6) Å	α = 72.371(4)°
	b = 13.8894(6) Å	β = 75.534(4)°
	c = 17.6784(8) Å	γ = 67.285(4)°
Cell volume	2681.4(2) Å^3	
Z	2	
Calculated density	1.293 g/cm^3	
Absorption coefficient μ	0.580 mm^{-1}	
F(000)	1098	
Crystal colour and size	purple, 0.400 × 0.150 × 0.100 mm^3	
Reflections for cell refinement	6673 (θ range 3.0 to 28.5°)	
Data collection method	Oxford Diffraction Gemini A Ultra ω scans	
θ range for data collection	3.0 to 26.4°	
Index ranges	h –12 to 15, k –17 to 17, l –21 to 21	
Completeness to θ = 25.2°	99.8 %	
Reflections collected	27976	
Independent reflections	10556 (R_{int} = 0.0430)	
Reflections with $F^2>2\sigma$	7732	
Absorption correction	multi-scan	
Min. and max. transmission	0.80 and 0.95	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0538, 2.1060	
Data / restraints / parameters	10556 / 43 / 653	
Final R indices [$F^2>2\sigma$]	R1 = 0.0506, wR2 = 0.1120	
R indices (all data)	R1 = 0.0785, wR2 = 0.1278	
Goodness-of-fit on F^2	1.021	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.77 and –0.70 e Å^{-3}	

Atomic coordinates and equivalent isotropic displacement parameters (Å^2). U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ni	0.23758(3)	0.25542(3)	0.80976(2)	0.02353(11)
P1	0.41903(7)	0.25013(6)	0.76188(4)	0.02376(17)
P2	0.19327(7)	0.37824(6)	0.70405(4)	0.02325(17)
P3	0.06658(7)	0.24354(7)	0.81863(5)	0.03079(19)
C1	0.4921(3)	0.1269(2)	0.72721(17)	0.0317(7)
C2	0.4958(3)	0.0293(2)	0.78138(19)	0.0362(8)
C3	0.5440(4)	–0.0649(3)	0.7558(2)	0.0510(10)
C4	0.5844(5)	–0.0640(3)	0.6762(2)	0.0746(15)
C5	0.5796(5)	0.0319(3)	0.6223(2)	0.0837(18)
C6	0.5355(4)	0.1267(3)	0.6470(2)	0.0573(12)
C7	0.5128(3)	0.2587(3)	0.82076(17)	0.0309(7)
C8	0.6083(3)	0.1717(3)	0.8469(2)	0.0428(8)
C9	0.6739(3)	0.1823(4)	0.8949(2)	0.0589(11)
C10	0.6471(4)	0.2777(4)	0.9146(3)	0.0645(12)
C11	0.5539(4)	0.3642(4)	0.8878(2)	0.0553(10)
C12	0.4858(3)	0.3551(3)	0.84197(19)	0.0385(8)
C13	0.4188(3)	0.3601(2)	0.67184(17)	0.0275(7)
C14	0.3203(3)	0.3797(2)	0.62762(16)	0.0259(6)
C15	0.1313(2)	0.5083(2)	0.72865(17)	0.0257(6)
C16	0.1080(3)	0.6024(3)	0.6695(2)	0.0430(9)
C17	0.0533(4)	0.7000(3)	0.6901(3)	0.0595(11)
C18	0.0226(3)	0.7050(3)	0.7695(2)	0.0518(10)
C19	0.0464(3)	0.6131(3)	0.8282(2)	0.0498(10)
C20	0.1001(3)	0.5152(3)	0.8084(2)	0.0404(8)
C21	0.0771(3)	0.3667(2)	0.66633(17)	0.0303(7)
C22	–0.0128(3)	0.3481(3)	0.73981(18)	0.0348(7)
C23	0.0885(3)	0.1201(3)	0.79321(18)	0.0399(8)
C24	–0.0073(4)	0.0981(3)	0.7852(2)	0.0565(11)
C25	0.0100(6)	0.0056(5)	0.7624(3)	0.0808(17)
C26	0.1203(6)	–0.0626(4)	0.7462(2)	0.0825(19)
C27	0.2171(5)	–0.0432(3)	0.7540(2)	0.0667(13)
C28	0.2000(4)	0.0489(3)	0.77792(19)	0.0463(9)
C29	–0.0343(3)	0.2494(3)	0.91178(18)	0.0357(8)
C30	–0.0932(3)	0.3469(3)	0.9327(2)	0.0482(9)
C31	–0.1615(4)	0.3524(4)	1.0074(2)	0.0573(11)
C32	–0.1712(3)	0.2604(4)	1.0606(2)	0.0576(11)
C33	–0.1149(3)	0.1639(4)	1.0402(2)	0.0589(11)
C34	–0.0455(3)	0.1578(3)	0.9661(2)	0.0479(9)
S	0.26385(8)	0.12743(6)	0.92322(4)	0.0346(2)
C35	0.2642(3)	0.1834(3)	1.00602(18)	0.0374(8)
C36	0.3880(3)	0.1462(3)	1.0238(2)	0.0512(10)
C37	0.2149(3)	0.3056(3)	0.9855(2)	0.0472(9)
C38	0.1888(3)	0.1395(3)	1.0803(2)	0.0509(10)
B	0.3670(3)	0.3530(2)	0.37852(19)	0.0251(7)
C39	0.3832(3)	0.3542(2)	0.28238(17)	0.0265(6)
C40	0.2884(3)	0.3785(4)	0.2448(2)	0.0559(11)

C41	0.2970(4)	0.3823(4)	0.1643(2)	0.0590(11)
C42	0.4027(3)	0.3642(3)	0.11638(19)	0.0418(8)
C43	0.4972(3)	0.3423(3)	0.1500(2)	0.0526(10)
C44	0.4881(3)	0.3374(3)	0.23114(19)	0.0446(9)
C45	0.4937(3)	0.3208(2)	0.40637(16)	0.0243(6)
C46	0.5816(3)	0.2219(2)	0.39930(18)	0.0312(7)
C47	0.6873(3)	0.1882(2)	0.42569(18)	0.0344(7)
C48	0.7117(3)	0.2514(2)	0.46174(18)	0.0329(7)
C49	0.6283(3)	0.3488(2)	0.47025(17)	0.0295(7)
C50	0.5225(3)	0.3819(2)	0.44273(17)	0.0273(7)
C51	0.3012(3)	0.2673(2)	0.43747(17)	0.0291(7)
C52	0.3478(3)	0.1894(2)	0.50235(18)	0.0381(8)
C53	0.2906(4)	0.1205(3)	0.5552(2)	0.0519(10)
C54	0.1846(4)	0.1263(3)	0.5441(2)	0.0514(10)
C55	0.1351(3)	0.2010(3)	0.4808(2)	0.0503(10)
C57	0.2850(2)	0.4750(2)	0.38814(16)	0.0231(6)
C56	0.1925(3)	0.2701(3)	0.4293(2)	0.0456(9)
C58	0.1860(3)	0.4997(2)	0.44545(16)	0.0260(6)
C59	0.1189(3)	0.6040(2)	0.45173(17)	0.0292(7)
C60	0.1509(3)	0.6885(2)	0.40105(18)	0.0290(7)
C61	0.2494(3)	0.6682(2)	0.34398(18)	0.0302(7)
C62	0.3136(3)	0.5637(2)	0.33768(17)	0.0268(6)
C63	0.8425(8)	0.0111(7)	0.6109(5)	0.074(3)
Cl1	0.9668(3)	0.0017(2)	0.5576(2)	0.0995(9)
Cl2	0.8209(4)	–0.0565(5)	0.6982(3)	0.100(2)
Cl2'	0.7957(7)	0.0314(12)	0.6954(5)	0.080(4)

Bond lengths [Å] and angles [°].

Ni–P1	2.2056(9)	Ni–P2	2.1372(8)
Ni–P3	2.1816(9)	Ni–S	2.2384(8)
P1–C1	1.814(3)	P1–C7	1.812(3)
P1–C13	1.842(3)	P2–C14	1.818(3)
P2–C15	1.811(3)	P2–C21	1.825(3)
P3–C22	1.843(3)	P3–C23	1.804(3)
P3–C29	1.812(3)	C1–C2	1.394(4)
C1–C6	1.386(4)	C2–H2	0.950
C2–C3	1.376(4)	C3–H3	0.950
C3–C4	1.370(5)	C4–H4	0.950
C4–C5	1.372(6)	C5–H5	0.950
C5–C6	1.376(5)	C6–H6	0.950
C7–C8	1.390(4)	C7–C12	1.393(4)
C8–H8	0.950	C8–C9	1.392(5)
C9–H9	0.950	C9–C10	1.365(6)
C10–H10	0.950	C10–C11	1.373(6)
C11–H11	0.950	C11–C12	1.376(5)
C12–H12	0.950	C13–H13A	0.990
C13–H13B	0.990	C13–C14	1.520(4)
C14–H14A	0.990	C14–H14B	0.990
C15–C16	1.384(4)	C15–C20	1.388(4)
C16–H16	0.950	C16–C17	1.378(5)
C17–H17	0.950	C17–C18	1.375(5)
C18–H18	0.950	C18–C19	1.361(5)
C19–H19	0.950	C19–C20	1.375(5)
C20–H20	0.950	C21–H21A	0.990
C21–H21B	0.990	C21–C22	1.523(4)
C22–H22A	0.990	C22–H22B	0.990
C23–C24	1.399(5)	C23–C28	1.385(5)
C24–H24	0.950	C24–C25	1.383(6)
C25–H25	0.950	C25–C26	1.362(8)
C26–H26	0.950	C26–C27	1.390(7)
C27–H27	0.950	C27–C28	1.390(5)
C28–H28	0.950	C29–C30	1.382(5)
C29–C34	1.376(5)	C30–H30	0.950
C30–C31	1.391(5)	C31–H31	0.950
C31–C32	1.366(6)	C32–H32	0.950
C32–C33	1.365(6)	C33–H33	0.950
C33–C34	1.387(5)	C34–H34	0.950
S–C35	1.855(3)	C35–C36	1.520(5)
C35–C37	1.525(5)	C35–C38	1.528(5)
C36–H36A	0.980	C36–H36B	0.980
C36–H36C	0.980	C37–H37A	0.980
C37–H37B	0.980	C37–H37C	0.980
C38–H38A	0.980	C38–H38B	0.980
C38–H38C	0.980	B–C39	1.656(4)
B–C45	1.639(4)	B–C51	1.662(4)
B–C57	1.644(4)	C39–C40	1.387(5)
C39–C44	1.381(4)	C40–H40	0.950
C40–C41	1.387(5)	C41–H41	0.950

C41–C42	1.361(5)	C42–H42	0.950
C42–C43	1.349(5)	C43–H43	0.950
C43–C44	1.394(5)	C44–H44	0.950
C45–C46	1.409(4)	C45–C50	1.396(4)
C46–H46	0.950	C46–C47	1.378(4)
C47–H47	0.950	C47–C48	1.383(4)
C48–H48	0.950	C48–C49	1.379(4)
C49–H49	0.950	C49–C50	1.390(4)
C50–H50	0.950	C51–C52	1.387(4)
C51–C56	1.393(5)	C52–H52	0.950
C52–C53	1.400(5)	C53–H53	0.950
C53–C54	1.363(6)	C54–H54	0.950
C54–C55	1.365(5)	C55–H55	0.950
C55–C56	1.395(5)	C57–C58	1.394(4)
C57–C62	1.399(4)	C56–H56	0.950
C58–H58	0.950	C58–C59	1.390(4)
C59–H59	0.950	C59–C60	1.374(4)
C60–H60	0.950	C60–C61	1.382(4)
C61–H61	0.950	C61–C62	1.385(4)
C62–H62	0.950	C63–H63A	0.990
C63–H63B	0.990	C63–H63C	0.990
C63–H63D	0.990	C63–Cl1	1.590(8)
C63–Cl2	1.564(8)	C63–Cl2'	1.531(10)

P1–Ni–P2	85.59(3)	P1–Ni–P3	160.01(3)
P1–Ni–S	100.57(3)	P2–Ni–P3	85.10(3)
P2–Ni–S	173.78(4)	P3–Ni–S	88.78(3)
Ni–P1–C1	106.18(11)	Ni–P1–C7	122.70(10)
Ni–P1–C13	108.84(10)	C1–P1–C7	107.70(15)
C1–P1–C13	106.01(14)	C7–P1–C13	104.38(14)
Ni–P2–C14	111.93(9)	Ni–P2–C15	109.73(10)
Ni–P2–C21	110.70(10)	C14–P2–C15	107.42(13)
C14–P2–C21	112.21(14)	C15–P2–C21	104.51(14)
Ni–P3–C22	110.25(11)	Ni–P3–C23	108.05(13)
Ni–P3–C29	119.88(10)	C22–P3–C23	103.58(15)
C22–P3–C29	106.23(15)	C23–P3–C29	107.65(15)
P1–C1–C2	119.2(2)	P1–C1–C6	122.2(2)
C2–C1–C6	118.4(3)	C1–C2–H2	119.7
C1–C2–C3	120.5(3)	H2–C2–C3	119.7
C2–C3–H3	119.7	C2–C3–C4	120.6(3)
H3–C3–C4	119.7	C3–C4–H4	120.4
C3–C4–C5	119.2(3)	H4–C4–C5	120.4
C4–C5–H5	119.4	C4–C5–C6	121.2(4)
H5–C5–C6	119.4	C1–C6–C5	120.1(3)
C1–C6–H6	119.9	C5–C6–H6	119.9
P1–C7–C8	122.2(3)	P1–C7–C12	118.4(2)
C8–C7–C12	119.4(3)	C7–C8–H8	120.4
C7–C8–C9	119.3(4)	H8–C8–C9	120.4
C8–C9–H9	119.6	C8–C9–C10	120.7(4)
H9–C9–C10	119.6	C9–C10–H10	119.9
C9–C10–C11	120.1(4)	H10–C10–C11	119.9
C10–C11–H11	119.8	C10–C11–C12	120.3(4)

H11–C11–C12	119.8	C7–C12–C11	120.1(3)
C7–C12–H12	119.9	C11–C12–H12	119.9
P1–C13–H13A	109.8	P1–C13–H13B	109.8
P1–C13–C14	109.47(19)	H13A–C13–H13B	108.2
H13A–C13–C14	109.8	H13B–C13–C14	109.8
P2–C14–C13	106.10(18)	P2–C14–H14A	110.5
P2–C14–H14B	110.5	C13–C14–H14A	110.5
C13–C14–H14B	110.5	H14A–C14–H14B	108.7
P2–C15–C16	121.5(2)	P2–C15–C20	120.0(2)
C16–C15–C20	118.4(3)	C15–C16–H16	119.9
C15–C16–C17	120.3(3)	H16–C16–C17	119.9
C16–C17–H17	119.8	C16–C17–C18	120.3(4)
H17–C17–C18	119.8	C17–C18–H18	120.0
C17–C18–C19	120.0(3)	H18–C18–C19	120.0
C18–C19–H19	119.9	C18–C19–C20	120.2(3)
H19–C19–C20	119.9	C15–C20–C19	120.8(3)
C15–C20–H20	119.6	C19–C20–H20	119.6
P2–C21–H21A	110.6	P2–C21–H21B	110.6
P2–C21–C22	105.5(2)	H21A–C21–H21B	108.8
H21A–C21–C22	110.6	H21B–C21–C22	110.6
P3–C22–C21	107.5(2)	P3–C22–H22A	110.2
P3–C22–H22B	110.2	C21–C22–H22A	110.2
C21–C22–H22B	110.2	H22A–C22–H22B	108.5
P3–C23–C24	120.0(3)	P3–C23–C28	120.5(3)
C24–C23–C28	119.5(3)	C23–C24–H24	120.0
C23–C24–C25	120.0(5)	H24–C24–C25	120.0
C24–C25–H25	120.1	C24–C25–C26	119.9(5)
H25–C25–C26	120.1	C25–C26–H26	119.3
C25–C26–C27	121.4(4)	H26–C26–C27	119.3
C26–C27–H27	120.6	C26–C27–C28	118.8(5)
H27–C27–C28	120.6	C23–C28–C27	120.4(4)
C23–C28–H28	119.8	C27–C28–H28	119.8
P3–C29–C30	119.5(3)	P3–C29–C34	121.5(3)
C30–C29–C34	118.7(3)	C29–C30–H30	119.6
C29–C30–C31	120.7(4)	H30–C30–C31	119.6
C30–C31–H31	120.2	C30–C31–C32	119.6(4)
H31–C31–C32	120.2	C31–C32–H32	119.9
C31–C32–C33	120.1(4)	H32–C32–C33	119.9
C32–C33–H33	119.8	C32–C33–C34	120.5(4)
H33–C33–C34	119.8	C29–C34–C33	120.2(4)
C29–C34–H34	119.9	C33–C34–H34	119.9
Ni–S–C35	110.57(11)	S–C35–C36	109.6(2)
S–C35–C37	111.6(2)	S–C35–C38	107.5(3)
C36–C35–C37	109.8(3)	C36–C35–C38	108.9(3)
C37–C35–C38	109.4(3)	C35–C36–H36A	109.5
C35–C36–H36B	109.5	C35–C36–H36C	109.5
H36A–C36–H36B	109.5	H36A–C36–H36C	109.5
H36B–C36–H36C	109.5	C35–C37–H37A	109.5
C35–C37–H37B	109.5	C35–C37–H37C	109.5
H37A–C37–H37B	109.5	H37A–C37–H37C	109.5
H37B–C37–H37C	109.5	C35–C38–H38A	109.5
C35–C38–H38B	109.5	C35–C38–H38C	109.5

H38A–C38–H38B	109.5	H38A–C38–H38C	109.5
H38B–C38–H38C	109.5	C39–B–C45	110.8(2)
C39–B–C51	112.2(2)	C39–B–C57	106.4(2)
C45–B–C51	108.5(2)	C45–B–C57	110.0(2)
C51–B–C57	108.9(2)	B–C39–C40	121.7(3)
B–C39–C44	124.8(3)	C40–C39–C44	113.5(3)
C39–C40–H40	118.0	C39–C40–C41	123.9(3)
H40–C40–C41	118.0	C40–C41–H41	119.9
C40–C41–C42	120.3(4)	H41–C41–C42	119.9
C41–C42–H42	121.1	C41–C42–C43	117.9(3)
H42–C42–C43	121.1	C42–C43–H43	119.2
C42–C43–C44	121.6(3)	H43–C43–C44	119.2
C39–C44–C43	122.8(3)	C39–C44–H44	118.6
C43–C44–H44	118.6	B–C45–C46	120.6(3)
B–C45–C50	125.0(2)	C46–C45–C50	114.3(3)
C45–C46–H46	118.5	C45–C46–C47	123.1(3)
H46–C46–C47	118.5	C46–C47–H47	119.7
C46–C47–C48	120.6(3)	H47–C47–C48	119.7
C47–C48–H48	120.7	C47–C48–C49	118.6(3)
H48–C48–C49	120.7	C48–C49–H49	120.0
C48–C49–C50	120.1(3)	H49–C49–C50	120.0
C45–C50–C49	123.4(3)	C45–C50–H50	118.3
C49–C50–H50	118.3	B–C51–C52	122.4(3)
B–C51–C56	123.7(3)	C52–C51–C56	113.8(3)
C51–C52–H52	118.4	C51–C52–C53	123.1(4)
H52–C52–C53	118.4	C52–C53–H53	119.7
C52–C53–C54	120.6(4)	H53–C53–C54	119.7
C53–C54–H54	120.7	C53–C54–C55	118.7(3)
H54–C54–C55	120.7	C54–C55–H55	120.0
C54–C55–C56	120.0(4)	H55–C55–C56	120.0
B–C57–C58	124.8(2)	B–C57–C62	120.3(2)
C58–C57–C62	114.9(2)	C51–C56–C55	123.8(3)
C51–C56–H56	118.1	C55–C56–H56	118.1
C57–C58–H58	118.4	C57–C58–C59	123.1(3)
H58–C58–C59	118.4	C58–C59–H59	120.1
C58–C59–C60	119.9(3)	H59–C59–C60	120.1
C59–C60–H60	120.4	C59–C60–C61	119.2(3)
H60–C60–C61	120.4	C60–C61–H61	120.0
C60–C61–C62	119.9(3)	H61–C61–C62	120.0
C57–C62–C61	123.0(3)	C57–C62–H62	118.5
C61–C62–H62	118.5	H63A–C63–H63B	106.3
H63A–C63–Cl1	106.0	H63A–C63–Cl2	106.0
H63B–C63–Cl1	106.0	H63B–C63–Cl2	106.0
H63C–C63–H63D	105.7	H63C–C63–Cl1	104.6
H63C–C63–Cl2'	104.6	H63D–C63–Cl1	104.6
H63D–C63–Cl2'	104.6	Cl1–C63–Cl2	125.2(7)
Cl1–C63–Cl2'	130.5(8)		

Torsion angles [°].

Ni–P1–C1–C2	−58.3(3)	Ni–P1–C1–C6	115.8(3)
C7–P1–C1–C2	74.8(3)	C7–P1–C1–C6	−111.1(3)
C13–P1–C1–C2	−173.9(3)	C13–P1–C1–C6	0.2(4)
P1–C1–C2–C3	175.9(3)	C6–C1–C2–C3	1.5(5)
C1–C2–C3–C4	−3.0(6)	C2–C3–C4–C5	2.0(8)
C3–C4–C5–C6	0.3(8)	C4–C5–C6–C1	−1.7(8)
P1–C1–C6–C5	−173.4(4)	C2–C1–C6–C5	0.8(6)
Ni–P1–C7–C8	110.4(3)	Ni–P1–C7–C12	−67.9(3)
C1–P1–C7–C8	−13.1(3)	C1–P1–C7–C12	168.6(2)
C13–P1–C7–C8	−125.5(3)	C13–P1–C7–C12	56.2(3)
P1–C7–C8–C9	−177.3(3)	C12–C7–C8–C9	1.0(5)
C7–C8–C9–C10	−1.7(6)	C8–C9–C10–C11	0.8(7)
C9–C10–C11–C12	0.9(6)	C10–C11–C12–C7	−1.5(6)
P1–C7–C12–C11	178.9(3)	C8–C7–C12–C11	0.6(5)
Ni–P1–C13–C14	−33.2(2)	C1–P1–C13–C14	80.6(2)
C7–P1–C13–C14	−165.8(2)	P1–C13–C14–P2	44.6(2)
Ni–P2–C14–C13	−40.4(2)	C15–P2–C14–C13	80.1(2)
C21–P2–C14–C13	−165.54(18)	Ni–P2–C15–C16	172.2(2)
Ni–P2–C15–C20	−11.5(3)	C14–P2–C15–C16	50.3(3)
C14–P2–C15–C20	−133.4(3)	C21–P2–C15–C16	−69.1(3)
C21–P2–C15–C20	107.3(3)	P2–C15–C16–C17	175.4(3)
C20–C15–C16–C17	−1.0(5)	C15–C16–C17–C18	0.8(6)
C16–C17–C18–C19	0.1(6)	C17–C18–C19–C20	−0.6(6)
C18–C19–C20–C15	0.4(6)	P2–C15–C20–C19	−176.0(3)
C16–C15–C20–C19	0.5(5)	Ni–P2–C21–C22	45.1(2)
C14–P2–C21–C22	170.9(2)	C15–P2–C21–C22	−73.0(2)
P2–C21–C22–P3	−46.8(2)	Ni–P3–C22–C21	33.2(2)
C23–P3–C22–C21	−82.2(2)	C29–P3–C22–C21	164.6(2)
Ni–P3–C23–C24	−172.8(2)	Ni–P3–C23–C28	4.3(3)
C22–P3–C23–C24	−55.8(3)	C22–P3–C23–C28	121.2(3)
C29–P3–C23–C24	56.4(3)	C29–P3–C23–C28	−126.5(3)
P3–C23–C24–C25	177.3(3)	C28–C23–C24–C25	0.2(5)
C23–C24–C25–C26	−1.4(6)	C24–C25–C26–C27	1.8(7)
C25–C26–C27–C28	−0.9(6)	P3–C23–C28–C27	−176.4(2)
C24–C23–C28–C27	0.7(5)	C26–C27–C28–C23	−0.3(5)
Ni–P3–C29–C30	75.4(3)	Ni–P3–C29–C34	−98.3(3)
C22–P3–C29–C30	−50.3(3)	C22–P3–C29–C34	136.1(3)
C23–P3–C29–C30	−160.7(3)	C23–P3–C29–C34	25.6(3)
P3–C29–C30–C31	−173.2(3)	C34–C29–C30–C31	0.7(5)
C29–C30–C31–C32	−0.4(6)	C30–C31–C32–C33	−0.6(6)
C31–C32–C33–C34	1.3(6)	P3–C29–C34–C33	173.8(3)
C30–C29–C34–C33	0.0(5)	C32–C33–C34–C29	−1.0(6)
Ni–S–C35–C36	−106.4(2)	Ni–S–C35–C37	15.4(3)
Ni–S–C35–C38	135.4(2)	C45–B–C39–C40	179.5(3)
C45–B–C39–C44	−3.9(4)	C51–B–C39–C40	58.1(4)
C51–B–C39–C44	−125.3(3)	C57–B–C39–C40	−60.9(4)
C57–B–C39–C44	115.7(3)	B–C39–C40–C41	179.0(4)

C44–C39–C40–C41	2.0(6)	C39–C40–C41–C42	−1.6(7)
C40–C41–C42–C43	0.3(6)	C41–C42–C43–C44	0.5(6)
B–C39–C44–C43	−178.1(3)	C40–C39–C44–C43	−1.3(5)
C42–C43–C44–C39	0.1(6)	C39–B–C45–C46	−59.1(3)
C39–B–C45–C50	125.1(3)	C51–B–C45–C46	64.4(3)
C51–B–C45–C50	−111.3(3)	C57–B–C45–C46	−176.5(2)
C57–B–C45–C50	7.8(4)	B–C45–C46–C47	−176.4(3)
C50–C45–C46–C47	−0.2(4)	C45–C46–C47–C48	0.5(5)
C46–C47–C48–C49	−0.3(5)	C47–C48–C49–C50	−0.1(4)
C48–C49–C50–C45	0.5(4)	B–C45–C50–C49	175.7(3)
C46–C45–C50–C49	−0.3(4)	C39–B–C51–C52	127.5(3)
C39–B–C51–C56	−55.9(4)	C45–B–C51–C52	4.8(4)
C45–B–C51–C56	−178.6(3)	C57–B–C51–C52	−115.0(3)
C57–B–C51–C56	61.6(4)	B–C51–C52–C53	176.4(3)
C56–C51–C52–C53	−0.5(4)	C51–C52–C53–C54	0.9(5)
C52–C53–C54–C55	−0.3(5)	C53–C54–C55–C56	−0.6(5)
C39–B–C57–C58	130.1(3)	C39–B–C57–C62	−51.1(3)
C45–B–C57–C58	−109.9(3)	C45–B–C57–C62	68.9(3)
C51–B–C57–C58	9.0(4)	C51–B–C57–C62	−172.2(2)
B–C51–C56–C55	−177.3(3)	C52–C51–C56–C55	−0.4(5)
C54–C55–C56–C51	1.0(6)	B–C57–C58–C59	179.9(3)
C62–C57–C58–C59	1.1(4)	C57–C58–C59–C60	−1.5(4)
C58–C59–C60–C61	0.4(4)	C59–C60–C61–C62	0.9(4)
C60–C61–C62–C57	−1.3(5)	B–C57–C62–C61	−178.6(3)
C58–C57–C62–C61	0.3(4)		

Anisotropic displacement parameters ($Å^2$) for rah213. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	0.0284(2)	0.0263(2)	0.01682(19)	–0.00299(14)	–0.00241(15)	–0.01228(16)
P1	0.0269(4)	0.0236(4)	0.0192(4)	–0.0046(3)	–0.0015(3)	–0.0083(3)
P2	0.0279(4)	0.0250(4)	0.0177(4)	–0.0042(3)	–0.0032(3)	–0.0106(3)
P3	0.0360(5)	0.0417(5)	0.0209(4)	–0.0039(3)	–0.0017(3)	–0.0238(4)
C1	0.0393(18)	0.0264(15)	0.0232(15)	–0.0068(12)	–0.0054(13)	–0.0033(13)
C2	0.045(2)	0.0291(16)	0.0270(16)	–0.0050(13)	–0.0078(14)	–0.0043(14)
C3	0.077(3)	0.0253(17)	0.042(2)	–0.0059(15)	–0.0156(19)	–0.0049(17)
C4	0.130(4)	0.031(2)	0.039(2)	–0.0145(17)	–0.016(2)	0.006(2)
C5	0.142(5)	0.041(2)	0.026(2)	–0.0117(17)	–0.005(2)	0.011(3)
C6	0.089(3)	0.0283(18)	0.0251(18)	–0.0061(14)	0.0014(18)	0.0053(18)
C7	0.0283(17)	0.0448(18)	0.0218(15)	–0.0072(13)	0.0021(13)	–0.0187(14)
C8	0.0289(18)	0.059(2)	0.0397(19)	–0.0147(17)	–0.0053(15)	–0.0112(16)
C9	0.036(2)	0.085(3)	0.059(3)	–0.016(2)	–0.0164(19)	–0.017(2)
C10	0.055(3)	0.102(4)	0.061(3)	–0.024(3)	–0.017(2)	–0.043(3)
C11	0.074(3)	0.073(3)	0.043(2)	–0.0205(19)	–0.005(2)	–0.046(2)
C12	0.047(2)	0.046(2)	0.0296(17)	–0.0106(15)	–0.0018(15)	–0.0232(16)
C13	0.0294(16)	0.0257(15)	0.0234(15)	–0.0022(12)	0.0032(12)	–0.0119(13)
C14	0.0327(17)	0.0220(14)	0.0174(14)	–0.0034(11)	–0.0002(12)	–0.0063(12)
C15	0.0239(15)	0.0309(15)	0.0256(15)	–0.0110(12)	0.0008(12)	–0.0121(12)
C16	0.057(2)	0.0338(18)	0.0322(18)	–0.0116(14)	0.0021(16)	–0.0114(16)
C17	0.078(3)	0.0310(19)	0.059(3)	–0.0156(18)	0.009(2)	–0.0146(19)
C18	0.057(2)	0.041(2)	0.061(3)	–0.0317(19)	0.0224(19)	–0.0242(18)
C19	0.061(3)	0.060(2)	0.040(2)	–0.0315(18)	0.0133(18)	–0.029(2)
C20	0.050(2)	0.045(2)	0.0322(18)	–0.0140(15)	–0.0025(16)	–0.0204(17)
C21	0.0370(18)	0.0342(16)	0.0238(15)	–0.0036(12)	–0.0087(13)	–0.0163(14)
C22	0.0362(19)	0.0467(19)	0.0288(17)	–0.0046(14)	–0.0120(14)	–0.0206(15)
C23	0.066(3)	0.048(2)	0.0198(16)	–0.0031(14)	0.0022(15)	–0.0429(19)
C24	0.087(3)	0.070(3)	0.032(2)	0.0027(18)	–0.009(2)	–0.059(2)
C25	0.149(5)	0.101(4)	0.036(2)	–0.008(2)	–0.001(3)	–0.102(4)
C26	0.178(6)	0.082(3)	0.026(2)	–0.018(2)	0.019(3)	–0.102(4)
C27	0.119(4)	0.055(2)	0.029(2)	–0.0162(17)	0.025(2)	–0.051(3)
C28	0.075(3)	0.047(2)	0.0254(17)	–0.0127(15)	0.0128(17)	–0.039(2)
C29	0.0292(17)	0.063(2)	0.0218(16)	–0.0094(15)	–0.0010(13)	–0.0250(16)
C30	0.050(2)	0.070(3)	0.038(2)	–0.0213(18)	0.0060(17)	–0.036(2)
C31	0.052(2)	0.086(3)	0.042(2)	–0.029(2)	0.0057(18)	–0.029(2)
C32	0.035(2)	0.104(4)	0.030(2)	–0.017(2)	0.0023(16)	–0.022(2)
C33	0.045(2)	0.087(3)	0.029(2)	0.005(2)	0.0025(17)	–0.024(2)
C34	0.044(2)	0.062(2)	0.0269(18)	0.0010(16)	0.0001(16)	–0.0176(18)
S	0.0484(5)	0.0313(4)	0.0186(4)	–0.0018(3)	–0.0034(3)	–0.0117(4)
C35	0.0358(19)	0.048(2)	0.0213(16)	–0.0092(14)	–0.0051(14)	–0.0056(15)
C36	0.041(2)	0.069(3)	0.037(2)	–0.0136(18)	–0.0102(16)	–0.0086(19)
C37	0.051(2)	0.050(2)	0.038(2)	–0.0140(16)	–0.0117(17)	–0.0075(17)
C38	0.046(2)	0.068(3)	0.0276(18)	–0.0066(17)	0.0021(16)	–0.0163(19)
B	0.0305(19)	0.0187(15)	0.0225(17)	–0.0051(12)	–0.0011(14)	–0.0060(14)

C39	0.0313(17)	0.0179(14)	0.0263(15)	–0.0063(11)	–0.0030(13)	–0.0040(12)
C40	0.035(2)	0.097(3)	0.036(2)	–0.027(2)	–0.0030(16)	–0.015(2)
C41	0.054(3)	0.091(3)	0.035(2)	–0.016(2)	–0.0160(19)	–0.021(2)
C42	0.060(2)	0.0369(18)	0.0246(17)	–0.0086(14)	–0.0059(16)	–0.0109(17)
C43	0.042(2)	0.075(3)	0.0287(19)	–0.0126(18)	0.0074(16)	–0.0145(19)
C44	0.0323(19)	0.066(2)	0.0271(18)	–0.0050(16)	–0.0025(15)	–0.0131(17)
C45	0.0292(16)	0.0203(14)	0.0167(14)	–0.0027(11)	0.0012(12)	–0.0053(12)
C46	0.0335(18)	0.0288(16)	0.0303(16)	–0.0118(13)	–0.0057(14)	–0.0050(13)
C47	0.0336(18)	0.0278(16)	0.0326(17)	–0.0102(13)	–0.0057(14)	0.0025(13)
C48	0.0281(17)	0.0344(17)	0.0330(17)	–0.0051(13)	–0.0070(13)	–0.0077(14)
C49	0.0361(18)	0.0276(15)	0.0261(16)	–0.0042(12)	–0.0033(13)	–0.0144(13)
C50	0.0325(17)	0.0196(14)	0.0240(15)	–0.0035(11)	–0.0015(13)	–0.0054(12)
C51	0.0367(18)	0.0188(14)	0.0274(16)	–0.0103(12)	0.0053(13)	–0.0070(13)
C52	0.053(2)	0.0317(17)	0.0264(17)	–0.0072(13)	0.0036(15)	–0.0167(16)
C53	0.077(3)	0.037(2)	0.0320(19)	–0.0020(15)	0.0072(19)	–0.0225(19)
C54	0.063(3)	0.0326(19)	0.052(2)	–0.0194(17)	0.028(2)	–0.0240(18)
C55	0.041(2)	0.0345(19)	0.072(3)	–0.0173(19)	0.0111(19)	–0.0172(16)
C57	0.0247(15)	0.0232(14)	0.0198(14)	–0.0052(11)	–0.0047(12)	–0.0055(12)
C56	0.038(2)	0.0333(18)	0.060(2)	–0.0053(16)	–0.0039(17)	–0.0128(15)
C58	0.0302(16)	0.0254(15)	0.0206(14)	–0.0025(11)	–0.0064(12)	–0.0081(12)
C59	0.0291(17)	0.0319(16)	0.0259(16)	–0.0124(13)	–0.0057(13)	–0.0041(13)
C60	0.0308(17)	0.0229(15)	0.0338(17)	–0.0105(12)	–0.0133(14)	–0.0014(12)
C61	0.0317(17)	0.0229(15)	0.0372(17)	–0.0027(13)	–0.0107(14)	–0.0103(13)
C62	0.0255(16)	0.0266(15)	0.0256(15)	–0.0045(12)	–0.0017(12)	–0.0084(12)
C63	0.075(5)	0.059(5)	0.061(5)	–0.003(4)	0.016(4)	–0.017(4)
Cl1	0.088(2)	0.0881(19)	0.119(2)	–0.0178(17)	–0.0123(17)	–0.0336(16)
Cl2	0.107(3)	0.105(4)	0.096(3)	0.017(3)	–0.063(2)	–0.047(3)
Cl2'	0.048(4)	0.122(9)	0.081(5)	–0.057(5)	–0.007(4)	–0.018(5)

Hydrogen coordinates and isotropic displacement parameters ($Å^2$).

	x	y	z	U
H2	0.4647	0.0279	0.8364	0.043
H3	0.5494	–0.1312	0.7937	0.061
H4	0.6154	–0.1289	0.6584	0.090
H5	0.6072	0.0329	0.5670	0.100
H6	0.5349	0.1920	0.6091	0.069
H8	0.6285	0.1057	0.8323	0.051
H9	0.7379	0.1226	0.9141	0.071
H10	0.6931	0.2842	0.9468	0.077
H11	0.5362	0.4307	0.9010	0.066
H12	0.4203	0.4148	0.8248	0.046
H13A	0.4081	0.4262	0.6877	0.033
H13B	0.4945	0.3410	0.6361	0.033
H14A	0.3407	0.3227	0.5986	0.031
H14B	0.3048	0.4499	0.5884	0.031
H16	0.1298	0.5997	0.6146	0.052
H17	0.0367	0.7643	0.6493	0.071
H18	–0.0151	0.7725	0.7834	0.062
H19	0.0259	0.6167	0.8830	0.060
H20	0.1159	0.4515	0.8498	0.049
H21A	0.0421	0.4333	0.6271	0.036
H21B	0.1078	0.3058	0.6399	0.036
H22A	–0.0694	0.3245	0.7265	0.042
H22B	–0.0560	0.4152	0.7585	0.042
H24	–0.0841	0.1466	0.7954	0.068
H25	–0.0551	–0.0102	0.7581	0.097
H26	0.1313	–0.1249	0.7291	0.099
H27	0.2935	–0.0920	0.7432	0.080
H28	0.2653	0.0631	0.7838	0.056
H30	–0.0869	0.4109	0.8955	0.058
H31	–0.2013	0.4197	1.0214	0.069
H32	–0.2172	0.2637	1.1120	0.069
H33	–0.1232	0.1004	1.0771	0.071
H34	–0.0057	0.0900	0.9528	0.058
H36A	0.3874	0.1726	1.0694	0.077
H36B	0.4369	0.1744	0.9765	0.077
H36C	0.4194	0.0676	1.0368	0.077
H37A	0.2148	0.3324	1.0308	0.071
H37B	0.1348	0.3292	0.9745	0.071
H37C	0.2633	0.3338	0.9378	0.071
H38A	0.1967	0.1586	1.1271	0.076
H38B	0.2142	0.0612	1.0895	0.076
H38C	0.1069	0.1705	1.0720	0.076
H40	0.2130	0.3934	0.2761	0.067
H41	0.2289	0.3976	0.1424	0.071
H42	0.4097	0.3668	0.0611	0.050
H43	0.5717	0.3299	0.1175	0.063
H44	0.5571	0.3218	0.2521	0.054

H46	0.5674	0.1764	0.3752	0.037
H47	0.7439	0.1211	0.4191	0.041
H48	0.7844	0.2281	0.4802	0.039
H49	0.6432	0.3934	0.4949	0.035
H50	0.4668	0.4496	0.4490	0.033
H52	0.4222	0.1825	0.5114	0.046
H53	0.3260	0.0692	0.5991	0.062
H54	0.1459	0.0793	0.5798	0.062
H55	0.0616	0.2060	0.4717	0.060
H56	0.1554	0.3220	0.3862	0.055
H58	0.1633	0.4424	0.4819	0.031
H59	0.0511	0.6170	0.4910	0.035
H60	0.1058	0.7600	0.4052	0.035
H61	0.2731	0.7258	0.3091	0.036
H62	0.3801	0.5517	0.2973	0.032
H63A	0.8051	0.0872	0.6140	0.089
H63B	0.7967	–0.0016	0.5790	0.089
H63C	0.7863	0.0682	0.5769	0.089
H63D	0.8307	–0.0565	0.6139	0.089

Table S6 Results for the crystal structure of [Ni(SCy)(triphos)]BPh_4

Crystal data and structure refinement for.

Identification code	rah209	
Chemical formula (moiety)	$C_{40}H_{34}NiP_3S^+ \cdot C_{24}H_{20}B^- \cdot C_4H_8O$	
Chemical formula (total)	$C_{68}H_{62}BNiOP_3S$	
Formula weight	1089.66	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 11.3585(4) Å	α = 79.270(3)°
	b = 14.9357(5) Å	β = 73.939(3)°
	c = 19.0458(8) Å	γ = 68.720(3)°
Cell volume	2879.9(2) $Å^3$	
Z	2	
Calculated density	1.257 g/cm^3	
Absorption coefficient μ	0.499 mm^{-1}	
F(000)	1144	
Crystal colour and size	red, 0.300 × 0.300 × 0.100 mm^3	
Reflections for cell refinement	15238 (θ range 2.8 to 29.3°)	
Data collection method	Oxford Diffraction Gemini A Ultra	
	ω scans	
θ range for data collection	2.8 to 26.4°	
Index ranges	h –13 to 14, k –18 to 18, l –23 to 23	
Completeness to θ = 25.2°	99.8 %	
Reflections collected	44424	
Independent reflections	11699 (R_{int} = 0.0335)	
Reflections with $F^2>2\sigma$	9626	
Absorption correction	multi-scan	
Min. and max. transmission	0.87 and 0.95	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0393, 1.7849	
Data / restraints / parameters	11699 / 0 / 631	
Final R indices [$F^2>2\sigma$]	R1 = 0.0377, wR2 = 0.0873	
R indices (all data)	R1 = 0.0505, wR2 = 0.0939	
Goodness-of-fit on F^2	1.021	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.92 and –0.57 e $Å^{-3}$	

Atomic coordinates and equivalent isotropic displacement parameters (Å^2). U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ni	0.74464(2)	0.28268(2)	0.77190(2)	0.02093(7)
P1	0.76740(5)	0.41561(4)	0.79022(3)	0.02466(12)
P2	0.92241(5)	0.26583(3)	0.69200(3)	0.02106(11)
P3	0.72910(5)	0.16926(3)	0.71960(3)	0.02008(11)
C1	0.65107(19)	0.51972(14)	0.75251(12)	0.0295(5)
C2	0.5246(2)	0.52238(18)	0.7639(2)	0.0664(9)
C3	0.4360(3)	0.6007(2)	0.7351(2)	0.0838(12)
C4	0.4734(3)	0.67644(19)	0.69330(18)	0.0580(8)
C5	0.5963(2)	0.67516(18)	0.68476(15)	0.0513(7)
C6	0.6856(2)	0.59673(16)	0.71375(14)	0.0420(6)
C7	0.7570(2)	0.43475(15)	0.88316(12)	0.0300(5)
C8	0.6552(2)	0.50624(17)	0.92049(13)	0.0390(5)
C9	0.6518(3)	0.51678(19)	0.99194(15)	0.0487(7)
C10	0.7484(3)	0.4581(2)	1.02525(14)	0.0496(6)
C11	0.8502(3)	0.38710(19)	0.98865(14)	0.0475(6)
C12	0.8537(2)	0.37443(17)	0.91808(13)	0.0396(5)
C13	0.92778(18)	0.42093(14)	0.73791(12)	0.0279(4)
C14	0.95828(19)	0.37846(14)	0.66557(11)	0.0274(4)
C15	1.05463(19)	0.18533(13)	0.73266(11)	0.0259(4)
C16	1.1816(2)	0.16300(17)	0.69166(14)	0.0384(5)
C17	1.2818(2)	0.0980(2)	0.72086(18)	0.0552(7)
C18	1.2557(3)	0.05518(19)	0.7908(2)	0.0635(9)
C19	1.1309(3)	0.07739(19)	0.83289(17)	0.0579(8)
C20	1.0294(2)	0.14313(16)	0.80389(13)	0.0378(5)
C21	0.93067(19)	0.20663(15)	0.61485(11)	0.0281(4)
C22	0.87933(18)	0.12383(14)	0.64975(11)	0.0270(4)
C23	0.7113(2)	0.05949(14)	0.77310(11)	0.0266(4)
C24	0.8117(3)	–0.00072(17)	0.80578(15)	0.0485(6)
C25	0.8035(3)	–0.08527(19)	0.84680(16)	0.0581(8)
C26	0.6965(3)	–0.11118(17)	0.85606(13)	0.0444(6)
C27	0.5983(2)	–0.05440(15)	0.82345(13)	0.0384(5)
C28	0.6059(2)	0.03095(14)	0.78154(12)	0.0324(5)
C29	0.60155(18)	0.21853(13)	0.66887(10)	0.0225(4)
C30	0.6068(2)	0.17566(15)	0.60891(12)	0.0307(5)
C31	0.5119(2)	0.21635(17)	0.56900(13)	0.0402(5)
C32	0.4108(2)	0.29943(16)	0.58925(14)	0.0408(6)
C33	0.4043(2)	0.34189(16)	0.64837(14)	0.0411(6)
C34	0.5003(2)	0.30237(14)	0.68797(12)	0.0315(5)
S	0.59398(5)	0.29251(4)	0.87185(3)	0.03205(13)
C35	0.47087(19)	0.23786(14)	0.87649(12)	0.0298(5)
C36	0.3394(2)	0.31673(15)	0.88280(14)	0.0386(5)
C37	0.2309(2)	0.27621(17)	0.88961(15)	0.0438(6)
C38	0.2265(2)	0.20110(17)	0.95470(14)	0.0438(6)
C39	0.3573(2)	0.12158(17)	0.94944(13)	0.0407(6)
C40	0.4676(2)	0.16075(16)	0.94140(12)	0.0362(5)
B	0.9842(2)	0.26845(15)	0.37473(12)	0.0218(4)
C41	1.12490(18)	0.21321(13)	0.39768(10)	0.0218(4)

C42	1.16231(19)	0.23512(15)	0.45458(11)	0.0281(4)
C43	1.2805(2)	0.18293(17)	0.47361(12)	0.0365(5)
C44	1.3675(2)	0.10712(16)	0.43526(13)	0.0365(5)
C45	1.3347(2)	0.08326(15)	0.37854(13)	0.0352(5)
C46	1.21578(19)	0.13417(14)	0.36109(12)	0.0281(4)
C47	0.88558(18)	0.34840(13)	0.43219(10)	0.0232(4)
C48	0.9198(2)	0.42554(14)	0.44246(12)	0.0293(4)
C49	0.8402(2)	0.49456(14)	0.49012(12)	0.0339(5)
C50	0.7199(2)	0.49036(15)	0.52911(12)	0.0367(5)
C51	0.6799(2)	0.41817(15)	0.51842(12)	0.0358(5)
C52	0.76173(19)	0.34837(14)	0.47131(11)	0.0283(4)
C53	0.99906(19)	0.32745(13)	0.29244(11)	0.0248(4)
C54	1.1115(2)	0.30936(15)	0.23671(12)	0.0328(5)
C55	1.1152(3)	0.35862(17)	0.16664(13)	0.0420(6)
C56	1.0055(3)	0.42792(16)	0.14998(13)	0.0424(6)
C57	0.8933(2)	0.44845(17)	0.20362(14)	0.0416(6)
C58	0.8908(2)	0.40001(15)	0.27299(12)	0.0334(5)
C59	0.92113(18)	0.18444(13)	0.37723(11)	0.0235(4)
C60	0.8726(2)	0.17217(14)	0.32175(13)	0.0328(5)
C61	0.8130(2)	0.10283(15)	0.32895(14)	0.0395(5)
C62	0.7995(2)	0.04352(14)	0.39314(14)	0.0353(5)
C63	0.8494(2)	0.05148(14)	0.44926(12)	0.0319(5)
C64	0.9095(2)	0.11988(14)	0.44073(11)	0.0275(4)

Bond lengths [Å] and angles [°].

Ni–P1	2.1934(5)	Ni–P2	2.1284(5)
Ni–P3	2.1990(5)	Ni–S	2.1663(6)
P1–C1	1.816(2)	P1–C7	1.810(2)
P1–C13	1.841(2)	P2–C14	1.8214(19)
P2–C15	1.8130(19)	P2–C21	1.816(2)
P3–C22	1.8390(19)	P3–C23	1.809(2)
P3–C29	1.8193(19)	C1–C2	1.378(3)
C1–C6	1.369(3)	C2–H2	0.950
C2–C3	1.376(4)	C3–H3	0.950
C3–C4	1.386(4)	C4–H4	0.950
C4–C5	1.353(4)	C5–H5	0.950
C5–C6	1.383(3)	C6–H6	0.950
C7–C8	1.383(3)	C7–C12	1.387(3)
C8–H8	0.950	C8–C9	1.387(4)
C9–H9	0.950	C9–C10	1.362(4)
C10–H10	0.950	C10–C11	1.374(4)
C11–H11	0.950	C11–C12	1.380(3)
C12–H12	0.950	C13–H13A	0.990
C13–H13B	0.990	C13–C14	1.524(3)
C14–H14A	0.990	C14–H14B	0.990
C15–C16	1.387(3)	C15–C20	1.385(3)
C16–H16	0.950	C16–C17	1.376(3)
C17–H17	0.950	C17–C18	1.369(4)
C18–H18	0.950	C18–C19	1.375(4)
C19–H19	0.950	C19–C20	1.389(3)
C20–H20	0.950	C21–H21A	0.990
C21–H21B	0.990	C21–C22	1.521(3)
C22–H22A	0.990	C22–H22B	0.990
C23–C24	1.391(3)	C23–C28	1.371(3)
C24–H24	0.950	C24–C25	1.375(3)
C25–H25	0.950	C25–C26	1.362(4)
C26–H26	0.950	C26–C27	1.360(3)
C27–H27	0.950	C27–C28	1.390(3)
C28–H28	0.950	C29–C30	1.387(3)
C29–C34	1.384(3)	C30–H30	0.950
C30–C31	1.384(3)	C31–H31	0.950
C31–C32	1.380(3)	C32–H32	0.950
C32–C33	1.364(4)	C33–H33	0.950
C33–C34	1.388(3)	C34–H34	0.950
S–C35	1.834(2)	C35–H35A	1.000
C35–C36	1.519(3)	C35–C40	1.527(3)
C36–H36A	0.990	C36–H36B	0.990
C36–C37	1.526(3)	C37–H37A	0.990
C37–H37B	0.990	C37–C38	1.512(3)
C38–H38A	0.990	C38–H38B	0.990
C38–C39	1.519(3)	C39–H39A	0.990
C39–H39B	0.990	C39–C40	1.527(3)
C40–H40A	0.990	C40–H40B	0.990
B–C41	1.650(3)	B–C47	1.648(3)
B–C53	1.646(3)	B–C59	1.643(3)

C41–C42	1.396(3)	C41–C46	1.403(3)
C42–H42	0.950	C42–C43	1.395(3)
C43–H43	0.950	C43–C44	1.374(3)
C44–H44	0.950	C44–C45	1.376(3)
C45–H45	0.950	C45–C46	1.387(3)
C46–H46	0.950	C47–C48	1.403(3)
C47–C52	1.398(3)	C48–H48	0.950
C48–C49	1.386(3)	C49–H49	0.950
C49–C50	1.381(3)	C50–H50	0.950
C50–C51	1.378(3)	C51–H51	0.950
C51–C52	1.392(3)	C52–H52	0.950
C53–C54	1.392(3)	C53–C58	1.400(3)
C54–H54	0.950	C54–C55	1.396(3)
C55–H55	0.950	C55–C56	1.374(3)
C56–H56	0.950	C56–C57	1.369(4)
C57–H57	0.950	C57–C58	1.381(3)
C58–H58	0.950	C59–C60	1.387(3)
C59–C64	1.407(3)	C60–H60	0.950
C60–C61	1.398(3)	C61–H61	0.950
C61–C62	1.376(3)	C62–H62	0.950
C62–C63	1.382(3)	C63–H63	0.950
C63–C64	1.385(3)	C64–H64	0.950

P1–Ni–P2	84.71(2)	P1–Ni–P3	162.86(2)
P1–Ni–S	90.27(2)	P2–Ni–P3	85.04(2)
P2–Ni–S	165.92(2)	P3–Ni–S	102.72(2)
Ni–P1–C1	109.74(7)	Ni–P1–C7	118.32(7)
Ni–P1–C13	109.43(7)	C1–P1–C7	108.14(10)
C1–P1–C13	105.18(10)	C7–P1–C13	105.19(10)
Ni–P2–C14	112.05(7)	Ni–P2–C15	108.79(7)
Ni–P2–C21	112.04(7)	C14–P2–C15	104.52(9)
C14–P2–C21	113.88(10)	C15–P2–C21	104.89(9)
Ni–P3–C22	108.87(7)	Ni–P3–C23	120.45(7)
Ni–P3–C29	110.94(6)	C22–P3–C23	102.52(9)
C22–P3–C29	104.84(9)	C23–P3–C29	107.87(9)
P1–C1–C2	119.63(18)	P1–C1–C6	121.40(16)
C2–C1–C6	119.0(2)	C1–C2–H2	120.0
C1–C2–C3	120.0(3)	H2–C2–C3	120.0
C2–C3–H3	119.7	C2–C3–C4	120.5(3)
H3–C3–C4	119.7	C3–C4–H4	120.4
C3–C4–C5	119.1(2)	H4–C4–C5	120.4
C4–C5–H5	119.8	C4–C5–C6	120.5(2)
H5–C5–C6	119.8	C1–C6–C5	120.8(2)
C1–C6–H6	119.6	C5–C6–H6	119.6
P1–C7–C8	122.22(18)	P1–C7–C12	118.47(16)
C8–C7–C12	119.3(2)	C7–C8–H8	120.2
C7–C8–C9	119.6(2)	H8–C8–C9	120.2
C8–C9–H9	119.7	C8–C9–C10	120.6(2)
H9–C9–C10	119.7	C9–C10–H10	119.8
C9–C10–C11	120.4(2)	H10–C10–C11	119.8
C10–C11–H11	120.1	C10–C11–C12	119.7(2)
H11–C11–C12	120.1	C7–C12–C11	120.4(2)

C7–C12–H12	119.8	C11–C12–H12	119.8
P1–C13–H13A	110.2	P1–C13–H13B	110.2
P1–C13–C14	107.66(13)	H13A–C13–H13B	108.5
H13A–C13–C14	110.2	H13B–C13–C14	110.2
P2–C14–C13	104.40(13)	P2–C14–H14A	110.9
P2–C14–H14B	110.9	C13–C14–H14A	110.9
C13–C14–H14B	110.9	H14A–C14–H14B	108.9
P2–C15–C16	120.12(16)	P2–C15–C20	120.30(16)
C16–C15–C20	119.5(2)	C15–C16–H16	119.8
C15–C16–C17	120.4(2)	H16–C16–C17	119.8
C16–C17–H17	120.2	C16–C17–C18	119.7(3)
H17–C17–C18	120.2	C17–C18–H18	119.5
C17–C18–C19	120.9(2)	H18–C18–C19	119.5
C18–C19–H19	120.1	C18–C19–C20	119.7(3)
H19–C19–C20	120.1	C15–C20–C19	119.7(2)
C15–C20–H20	120.2	C19–C20–H20	120.2
P2–C21–H21A	110.9	P2–C21–H21B	110.9
P2–C21–C22	104.48(13)	H21A–C21–H21B	108.9
H21A–C21–C22	110.9	H21B–C21–C22	110.9
P3–C22–C21	109.02(13)	P3–C22–H22A	109.9
P3–C22–H22B	109.9	C21–C22–H22A	109.9
C21–C22–H22B	109.9	H22A–C22–H22B	108.3
P3–C23–C24	118.27(17)	P3–C23–C28	123.60(16)
C24–C23–C28	118.11(19)	C23–C24–H24	119.6
C23–C24–C25	120.7(2)	H24–C24–C25	119.6
C24–C25–H25	119.9	C24–C25–C26	120.3(2)
H25–C25–C26	119.9	C25–C26–H26	120.0
C25–C26–C27	120.0(2)	H26–C26–C27	120.0
C26–C27–H27	119.9	C26–C27–C28	120.1(2)
H27–C27–C28	119.9	C23–C28–C27	120.7(2)
C23–C28–H28	119.7	C27–C28–H28	119.7
P3–C29–C30	120.96(15)	P3–C29–C34	119.95(15)
C30–C29–C34	119.04(18)	C29–C30–H30	119.9
C29–C30–C31	120.3(2)	H30–C30–C31	119.9
C30–C31–H31	120.0	C30–C31–C32	120.0(2)
H31–C31–C32	120.0	C31–C32–H32	119.9
C31–C32–C33	120.3(2)	H32–C32–C33	119.9
C32–C33–H33	119.9	C32–C33–C34	120.1(2)
H33–C33–C34	119.9	C29–C34–C33	120.3(2)
C29–C34–H34	119.8	C33–C34–H34	119.8
Ni–S–C35	117.08(7)	S–C35–H35A	108.8
S–C35–C36	108.83(14)	S–C35–C40	111.15(15)
H35A–C35–C36	108.8	H35A–C35–C40	108.8
C36–C35–C40	110.47(18)	C35–C36–H36A	109.2
C35–C36–H36B	109.2	C35–C36–C37	111.90(18)
H36A–C36–H36B	107.9	H36A–C36–C37	109.2
H36B–C36–C37	109.2	C36–C37–H37A	109.5
C36–C37–H37B	109.5	C36–C37–C38	110.9(2)
H37A–C37–H37B	108.1	H37A–C37–C38	109.5
H37B–C37–C38	109.5	C37–C38–H38A	109.5
C37–C38–H38B	109.5	C37–C38–C39	110.62(19)
H38A–C38–H38B	108.1	H38A–C38–C39	109.5

H38B–C38–C39	109.5	C38–C39–H39A	109.1
C38–C39–H39B	109.1	C38–C39–C40	112.36(19)
H39A–C39–H39B	107.9	H39A–C39–C40	109.1
H39B–C39–C40	109.1	C35–C40–C39	111.21(19)
C35–C40–H40A	109.4	C35–C40–H40B	109.4
C39–C40–H40A	109.4	C39–C40–H40B	109.4
H40A–C40–H40B	108.0	C41–B–C47	111.39(16)
C41–B–C53	112.57(16)	C41–B–C59	106.66(15)
C47–B–C53	106.48(15)	C47–B–C59	109.87(16)
C53–B–C59	109.89(16)	B–C41–C42	125.45(17)
B–C41–C46	119.88(17)	C42–C41–C46	114.60(17)
C41–C42–H42	118.6	C41–C42–C43	122.9(2)
H42–C42–C43	118.6	C42–C43–H43	119.8
C42–C43–C44	120.4(2)	H43–C43–C44	119.8
C43–C44–H44	120.7	C43–C44–C45	118.7(2)
H44–C44–C45	120.7	C44–C45–H45	119.7
C44–C45–C46	120.5(2)	H45–C45–C46	119.7
C41–C46–C45	122.9(2)	C41–C46–H46	118.5
C45–C46–H46	118.5	B–C47–C48	120.97(17)
B–C47–C52	124.05(17)	C48–C47–C52	114.92(18)
C47–C48–H48	118.4	C47–C48–C49	123.1(2)
H48–C48–C49	118.4	C48–C49–H49	120.0
C48–C49–C50	120.0(2)	H49–C49–C50	120.0
C49–C50–H50	120.6	C49–C50–C51	118.9(2)
H50–C50–C51	120.6	C50–C51–H51	119.8
C50–C51–C52	120.5(2)	H51–C51–C52	119.8
C47–C52–C51	122.53(19)	C47–C52–H52	118.7
C51–C52–H52	118.7	B–C53–C54	125.63(17)
B–C53–C58	119.66(18)	C54–C53–C58	114.65(18)
C53–C54–H54	118.7	C53–C54–C55	122.6(2)
H54–C54–C55	118.7	C54–C55–H55	119.8
C54–C55–C56	120.4(2)	H55–C55–C56	119.8
C55–C56–H56	120.7	C55–C56–C57	118.7(2)
H56–C56–C57	120.7	C56–C57–H57	119.8
C56–C57–C58	120.5(2)	H57–C57–C58	119.8
C53–C58–C57	123.2(2)	C53–C58–H58	118.4
C57–C58–H58	118.4	B–C59–C60	125.43(17)
B–C59–C64	119.55(17)	C60–C59–C64	114.99(18)
C59–C60–H60	118.7	C59–C60–C61	122.7(2)
H60–C60–C61	118.7	C60–C61–H61	119.8
C60–C61–C62	120.3(2)	H61–C61–C62	119.8
C61–C62–H62	120.5	C61–C62–C63	119.0(2)
H62–C62–C63	120.5	C62–C63–H63	120.1
C62–C63–C64	119.8(2)	H63–C63–C64	120.1
C59–C64–C63	123.2(2)	C59–C64–H64	118.4
C63–C64–H64	118.4		

Torsion angles [°].

Ni–P1–C1–C2	43.5(2)	Ni–P1–C1–C6	−137.46(18)
C7–P1–C1–C2	−86.9(2)	C7–P1–C1–C6	92.1(2)
C13–P1–C1–C2	161.1(2)	C13–P1–C1–C6	−19.8(2)
P1–C1–C2–C3	−179.5(3)	C6–C1–C2–C3	1.4(5)
C1–C2–C3–C4	1.3(6)	C2–C3–C4–C5	−3.9(6)
C3–C4–C5–C6	3.7(5)	P1–C1–C6–C5	179.4(2)
C2–C1–C6–C5	−1.6(4)	C4–C5–C6–C1	−1.0(4)
Ni–P1–C7–C8	−111.82(17)	Ni–P1–C7–C12	67.18(18)
C1–P1–C7–C8	13.7(2)	C1–P1–C7–C12	−167.34(17)
C13–P1–C7–C8	125.64(18)	C13–P1–C7–C12	−55.36(19)
P1–C7–C8–C9	179.33(18)	C12–C7–C8–C9	0.3(3)
C7–C8–C9–C10	0.7(4)	C8–C9–C10–C11	−0.5(4)
C9–C10–C11–C12	−0.8(4)	C10–C11–C12–C7	1.9(4)
P1–C7–C12–C11	179.32(19)	C8–C7–C12–C11	−1.6(3)
Ni–P1–C13–C14	36.54(15)	C1–P1–C13–C14	−81.28(15)
C7–P1–C13–C14	164.64(13)	P1–C13–C14–P2	−48.05(15)
Ni–P2–C14–C13	44.11(14)	C15–P2–C14–C13	−73.53(14)
C21–P2–C14–C13	172.59(12)	Ni–P2–C15–C16	−179.60(15)
Ni–P2–C15–C20	2.65(18)	C14–P2–C15–C16	−59.75(18)
C14–P2–C15–C20	122.49(17)	C21–P2–C15–C16	60.36(18)
C21–P2–C15–C20	−117.40(18)	P2–C15–C16–C17	−176.54(18)
C20–C15–C16–C17	1.2(3)	C15–C16–C17–C18	0.0(4)
C16–C17–C18–C19	−1.1(4)	C17–C18–C19–C20	0.9(4)
P2–C15–C20–C19	176.35(18)	C16–C15–C20–C19	−1.4(3)
C18–C19–C20–C15	0.4(4)	Ni–P2–C21–C22	−43.77(14)
C14–P2–C21–C22	−172.24(12)	C15–P2–C21–C22	74.09(14)
P2–C21–C22–P3	46.80(15)	Ni–P3–C22–C21	−34.24(15)
C23–P3–C22–C21	−162.89(14)	C29–P3–C22–C21	84.53(15)
Ni–P3–C23–C24	−63.1(2)	Ni–P3–C23–C28	118.76(17)
C22–P3–C23–C24	57.8(2)	C22–P3–C23–C28	−120.25(19)
C29–P3–C23–C24	168.16(18)	C29–P3–C23–C28	−9.9(2)
P3–C23–C24–C25	−179.7(2)	C28–C23–C24–C25	−1.5(4)
C23–C24–C25–C26	−0.1(5)	C24–C25–C26–C27	1.4(4)
C25–C26–C27–C28	−1.0(4)	P3–C23–C28–C27	179.98(17)
C24–C23–C28–C27	1.9(3)	C26–C27–C28–C23	−0.6(3)
Ni–P3–C29–C30	152.81(14)	Ni–P3–C29–C34	−24.34(17)
C22–P3–C29–C30	35.44(18)	C22–P3–C29–C34	−141.70(16)
C23–P3–C29–C30	−73.28(18)	C23–P3–C29–C34	109.57(17)
P3–C29–C30–C31	−177.27(16)	C34–C29–C30–C31	−0.1(3)
C29–C30–C31–C32	−0.6(3)	C30–C31–C32–C33	0.2(3)
C31–C32–C33–C34	0.8(4)	P3–C29–C34–C33	178.32(16)
C30–C29–C34–C33	1.1(3)	C32–C33–C34–C29	−1.5(3)
Ni–S–C35–C36	−116.55(14)	Ni–S–C35–C40	121.57(14)
S–C35–C36–C37	−178.03(17)	C40–C35–C36–C37	−55.7(3)
C35–C36–C37–C38	57.0(3)	C36–C37–C38–C39	−55.7(3)
C37–C38–C39–C40	55.2(3)	C38–C39–C40–C35	−54.5(3)
S–C35–C40–C39	174.91(15)	C36–C35–C40–C39	54.0(2)

C47–B–C41–C42	–4.8(3)	C47–B–C41–C46	171.91(16)
C53–B–C41–C42	114.7(2)	C53–B–C41–C46	–68.6(2)
C59–B–C41–C42	–124.71(19)	C59–B–C41–C46	52.0(2)
B–C41–C42–C43	177.00(18)	C46–C41–C42–C43	0.1(3)
C41–C42–C43–C44	1.1(3)	C42–C43–C44–C45	–0.8(3)
C43–C44–C45–C46	–0.7(3)	C44–C45–C46–C41	2.0(3)
B–C41–C46–C45	–178.69(18)	C42–C41–C46–C45	–1.6(3)
C41–B–C47–C48	59.4(2)	C41–B–C47–C52	–123.63(19)
C53–B–C47–C48	–63.6(2)	C53–B–C47–C52	113.30(19)
C59–B–C47–C48	177.40(17)	C59–B–C47–C52	–5.7(2)
B–C47–C48–C49	180.00(18)	C52–C47–C48–C49	2.8(3)
C47–C48–C49–C50	–1.3(3)	C48–C49–C50–C51	–1.4(3)
C49–C50–C51–C52	2.6(3)	C50–C51–C52–C47	–1.0(3)
B–C47–C52–C51	–178.76(18)	C48–C47–C52–C51	–1.7(3)
C41–B–C53–C54	21.8(3)	C41–B–C53–C58	–161.15(18)
C47–B–C53–C54	144.09(19)	C47–B–C53–C58	–38.8(2)
C59–B–C53–C54	–97.0(2)	C59–B–C53–C58	80.1(2)
B–C53–C54–C55	176.2(2)	C58–C53–C54–C55	–1.0(3)
C53–C54–C55–C56	–0.2(4)	C54–C55–C56–C57	0.9(4)
C55–C56–C57–C58	–0.2(4)	C56–C57–C58–C53	–1.1(4)
B–C53–C58–C57	–175.7(2)	C54–C53–C58–C57	1.7(3)
C41–B–C59–C60	–129.7(2)	C41–B–C59–C64	52.6(2)
C47–B–C59–C60	109.5(2)	C47–B–C59–C64	–68.3(2)
C53–B–C59–C60	–7.4(3)	C53–B–C59–C64	174.86(16)
B–C59–C60–C61	–176.1(2)	C64–C59–C60–C61	1.8(3)
C59–C60–C61–C62	0.5(3)	C60–C61–C62–C63	–2.1(3)
C61–C62–C63–C64	1.3(3)	C62–C63–C64–C59	1.1(3)
B–C59–C64–C63	175.38(18)	C60–C59–C64–C63	–2.6(3)

Anisotropic displacement parameters (Å^2). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	0.01806(13)	0.02345(13)	0.02248(14)	–0.00637(9)	0.00056(10)	–0.01005(10)
P1	0.0185(2)	0.0256(3)	0.0319(3)	–0.0091(2)	–0.0004(2)	–0.0104(2)
P2	0.0171(2)	0.0248(2)	0.0207(3)	–0.00335(19)	–0.00164(19)	–0.00756(19)
P3	0.0190(2)	0.0212(2)	0.0215(3)	–0.00346(18)	–0.00520(19)	–0.00710(19)
C1	0.0227(10)	0.0268(10)	0.0401(12)	–0.0117(9)	–0.0040(9)	–0.0076(8)
C2	0.0341(14)	0.0331(13)	0.139(3)	0.0039(15)	–0.0337(17)	–0.0146(11)
C3	0.0414(16)	0.0425(16)	0.179(4)	0.0048(19)	–0.053(2)	–0.0133(13)
C4	0.0410(15)	0.0418(15)	0.088(2)	–0.0027(14)	–0.0303(15)	–0.0006(12)
C5	0.0399(14)	0.0430(14)	0.0596(17)	0.0107(12)	–0.0066(12)	–0.0115(11)
C6	0.0282(12)	0.0414(13)	0.0551(16)	0.0063(11)	–0.0085(11)	–0.0160(10)
C7	0.0274(11)	0.0351(11)	0.0345(12)	–0.0127(9)	0.0006(9)	–0.0195(9)
C8	0.0310(12)	0.0449(13)	0.0437(14)	–0.0180(10)	–0.0003(10)	–0.0150(10)
C9	0.0421(14)	0.0593(16)	0.0494(16)	–0.0318(13)	0.0099(12)	–0.0245(12)
C10	0.0591(17)	0.0648(17)	0.0375(14)	–0.0174(12)	–0.0049(13)	–0.0333(14)
C11	0.0502(15)	0.0580(16)	0.0425(15)	–0.0118(12)	–0.0148(12)	–0.0208(13)
C12	0.0373(13)	0.0441(13)	0.0419(14)	–0.0139(10)	–0.0086(11)	–0.0141(10)
C13	0.0194(10)	0.0279(10)	0.0382(12)	–0.0056(8)	–0.0023(9)	–0.0118(8)
C14	0.0222(10)	0.0277(10)	0.0316(11)	0.0028(8)	–0.0034(8)	–0.0120(8)
C15	0.0259(10)	0.0243(10)	0.0325(11)	–0.0055(8)	–0.0126(9)	–0.0084(8)
C16	0.0248(11)	0.0466(13)	0.0476(14)	–0.0162(11)	–0.0106(10)	–0.0085(10)
C17	0.0311(13)	0.0589(17)	0.080(2)	–0.0241(15)	–0.0270(14)	–0.0014(12)
C18	0.0550(18)	0.0427(15)	0.109(3)	–0.0061(16)	–0.0601(19)	–0.0053(13)
C19	0.083(2)	0.0519(16)	0.0620(18)	0.0190(13)	–0.0516(17)	–0.0350(15)
C20	0.0438(13)	0.0420(13)	0.0373(13)	0.0045(10)	–0.0199(11)	–0.0215(11)
C21	0.0211(10)	0.0403(12)	0.0221(10)	–0.0076(8)	–0.0026(8)	–0.0087(9)
C22	0.0176(9)	0.0311(10)	0.0303(11)	–0.0131(8)	–0.0046(8)	–0.0015(8)
C23	0.0319(11)	0.0259(10)	0.0256(11)	–0.0032(8)	–0.0088(9)	–0.0116(8)
C24	0.0534(16)	0.0428(14)	0.0595(17)	0.0142(12)	–0.0324(13)	–0.0225(12)
C25	0.0682(19)	0.0464(15)	0.0651(19)	0.0214(13)	–0.0383(16)	–0.0211(14)
C26	0.0572(16)	0.0335(12)	0.0374(14)	0.0050(10)	–0.0075(12)	–0.0156(11)
C27	0.0342(12)	0.0319(11)	0.0457(14)	–0.0054(10)	0.0020(10)	–0.0143(10)
C28	0.0290(11)	0.0272(10)	0.0376(13)	–0.0027(9)	–0.0058(9)	–0.0069(9)
C29	0.0210(9)	0.0239(9)	0.0245(10)	0.0028(7)	–0.0061(8)	–0.0114(8)
C30	0.0283(11)	0.0335(11)	0.0343(12)	–0.0034(9)	–0.0108(9)	–0.0121(9)
C31	0.0431(14)	0.0490(14)	0.0412(14)	0.0004(10)	–0.0224(11)	–0.0229(11)
C32	0.0376(13)	0.0390(13)	0.0542(16)	0.0176(11)	–0.0290(12)	–0.0194(11)
C33	0.0308(12)	0.0306(12)	0.0559(16)	0.0070(10)	–0.0151(11)	–0.0045(9)
C34	0.0291(11)	0.0282(11)	0.0336(12)	–0.0007(9)	–0.0081(9)	–0.0058(9)
S	0.0309(3)	0.0389(3)	0.0307(3)	–0.0158(2)	0.0085(2)	–0.0220(2)
C35	0.0269(11)	0.0327(11)	0.0319(12)	–0.0088(9)	0.0001(9)	–0.0145(9)
C36	0.0325(12)	0.0308(11)	0.0477(14)	–0.0093(10)	0.0007(10)	–0.0094(9)
C37	0.0271(12)	0.0460(14)	0.0574(16)	–0.0096(11)	–0.0051(11)	–0.0120(10)
C38	0.0341(13)	0.0506(14)	0.0495(15)	–0.0123(11)	0.0064(11)	–0.0252(11)
C39	0.0460(14)	0.0431(13)	0.0350(13)	–0.0039(10)	0.0014(11)	–0.0250(11)

C40	0.0359(12)	0.0395(12)	0.0332(12)	–0.0045(9)	–0.0021(10)	–0.0164(10)
B	0.0203(10)	0.0235(10)	0.0244(11)	–0.0003(8)	–0.0079(9)	–0.0092(9)
C41	0.0224(10)	0.0233(9)	0.0219(10)	0.0033(7)	–0.0059(8)	–0.0120(8)
C42	0.0239(10)	0.0387(11)	0.0248(11)	–0.0032(8)	–0.0027(8)	–0.0158(9)
C43	0.0304(12)	0.0582(14)	0.0290(12)	0.0004(10)	–0.0116(9)	–0.0226(11)
C44	0.0244(11)	0.0460(13)	0.0388(13)	0.0131(10)	–0.0144(10)	–0.0142(10)
C45	0.0278(11)	0.0273(11)	0.0464(14)	0.0007(9)	–0.0099(10)	–0.0056(9)
C46	0.0285(11)	0.0250(10)	0.0327(11)	–0.0007(8)	–0.0121(9)	–0.0083(8)
C47	0.0230(10)	0.0233(9)	0.0237(10)	0.0021(7)	–0.0082(8)	–0.0082(8)
C48	0.0301(11)	0.0270(10)	0.0324(12)	–0.0008(8)	–0.0062(9)	–0.0130(9)
C49	0.0407(13)	0.0260(11)	0.0366(13)	–0.0040(9)	–0.0118(10)	–0.0102(9)
C50	0.0387(13)	0.0299(11)	0.0308(12)	–0.0056(9)	–0.0057(10)	0.0007(9)
C51	0.0258(11)	0.0329(11)	0.0378(13)	0.0030(9)	–0.0014(9)	–0.0047(9)
C52	0.0253(10)	0.0243(10)	0.0339(12)	0.0023(8)	–0.0077(9)	–0.0084(8)
C53	0.0292(10)	0.0238(9)	0.0280(11)	–0.0007(8)	–0.0113(9)	–0.0136(8)
C54	0.0367(12)	0.0303(11)	0.0291(12)	0.0010(8)	–0.0080(10)	–0.0097(9)
C55	0.0549(15)	0.0405(13)	0.0295(12)	–0.0012(10)	–0.0015(11)	–0.0215(12)
C56	0.0697(18)	0.0378(12)	0.0314(13)	0.0124(10)	–0.0254(13)	–0.0290(12)
C57	0.0460(14)	0.0400(13)	0.0473(15)	0.0123(10)	–0.0294(12)	–0.0183(11)
C58	0.0302(11)	0.0368(12)	0.0363(12)	0.0051(9)	–0.0144(10)	–0.0139(9)
C59	0.0173(9)	0.0217(9)	0.0309(11)	–0.0038(8)	–0.0049(8)	–0.0057(7)
C60	0.0355(12)	0.0286(11)	0.0403(13)	0.0025(9)	–0.0196(10)	–0.0121(9)
C61	0.0408(13)	0.0325(12)	0.0571(16)	–0.0048(10)	–0.0276(12)	–0.0135(10)
C62	0.0231(10)	0.0225(10)	0.0622(16)	–0.0082(10)	–0.0081(10)	–0.0088(8)
C63	0.0308(11)	0.0229(10)	0.0364(12)	–0.0050(8)	0.0035(9)	–0.0094(9)
C64	0.0307(11)	0.0265(10)	0.0265(11)	–0.0049(8)	–0.0044(9)	–0.0114(8)

Hydrogen coordinates and isotropic displacement parameters ($Å^2$).

	x	y	z	U
H2	0.4987	0.4701	0.7916	0.080
H3	0.3486	0.6028	0.7439	0.101
H4	0.4135	0.7286	0.6709	0.070
H5	0.6213	0.7285	0.6587	0.062
H6	0.7719	0.5963	0.7067	0.050
H8	0.5880	0.5478	0.8973	0.047
H9	0.5815	0.5654	1.0179	0.058
H10	0.7453	0.4663	1.0741	0.060
H11	0.9180	0.3469	1.0118	0.057
H12	0.9227	0.3241	0.8933	0.048
H13A	0.9268	0.4886	0.7285	0.033
H13B	0.9946	0.3834	0.7660	0.033
H14A	1.0506	0.3663	0.6402	0.033
H14B	0.9032	0.4225	0.6327	0.033
H16	1.1995	0.1928	0.6431	0.046
H17	1.3685	0.0829	0.6926	0.066
H18	1.3248	0.0095	0.8106	0.076
H19	1.1142	0.0479	0.8816	0.070
H20	0.9430	0.1591	0.8328	0.045
H21A	0.8762	0.2517	0.5821	0.034
H21B	1.0212	0.1821	0.5861	0.034
H22A	0.9449	0.0721	0.6727	0.032
H22B	0.8617	0.0965	0.6117	0.032
H24	0.8866	0.0168	0.7997	0.058
H25	0.8728	–0.1258	0.8688	0.070
H26	0.6904	–0.1689	0.8853	0.053
H27	0.5244	–0.0731	0.8293	0.046
H28	0.5373	0.0699	0.7585	0.039
H30	0.6759	0.1182	0.5952	0.037
H31	0.5162	0.1871	0.5277	0.048
H32	0.3456	0.3271	0.5619	0.049
H33	0.3340	0.3986	0.6625	0.049
H34	0.4964	0.3330	0.7284	0.038
H35A	0.4923	0.2071	0.8301	0.036
H36A	0.3421	0.3640	0.8389	0.046
H36B	0.3208	0.3511	0.9264	0.046
H37A	0.1466	0.3293	0.8955	0.053
H37B	0.2451	0.2468	0.8442	0.053
H38A	0.1591	0.1730	0.9563	0.053
H38B	0.2031	0.2320	1.0006	0.053
H39A	0.3752	0.0859	0.9067	0.049
H39B	0.3537	0.0756	0.9941	0.049
H40A	0.5513	0.1071	0.9342	0.043
H40B	0.4562	0.1888	0.9870	0.043
H42	1.1047	0.2879	0.4815	0.034
H43	1.3011	0.1999	0.5133	0.044
H44	1.4485	0.0719	0.4476	0.044
H45	1.3941	0.0315	0.3511	0.042

H46	1.1949	0.1147	0.3227	0.034
H48	1.0014	0.4307	0.4155	0.035
H49	0.8685	0.5447	0.4960	0.041
H50	0.6655	0.5365	0.5627	0.044
H51	0.5960	0.4160	0.5434	0.043
H52	0.7322	0.2988	0.4655	0.034
H54	1.1888	0.2616	0.2467	0.039
H55	1.1942	0.3441	0.1303	0.050
H56	1.0073	0.4610	0.1022	0.051
H57	0.8166	0.4964	0.1931	0.050
H58	0.8118	0.4167	0.3092	0.040
H60	0.8801	0.2125	0.2770	0.039
H61	0.7817	0.0966	0.2894	0.047
H62	0.7565	–0.0022	0.3988	0.042
H63	0.8425	0.0102	0.4935	0.038
H64	0.9445	0.1234	0.4796	0.033