

θ -Grenzen für Datensammlung	2.92 bis 30.99°.
Indexbereich	$-15 \leq h \leq 15$, $-20 \leq k \leq 20$, $-34 \leq l \leq 34$
Aufgenommene Reflexe	50077
Unabhängige Reflexe	11796 [$R_{\text{int}} = 0.0720$]
Reflexe mit $I > 2\sigma(I)$	10146
Vollständigkeit für $\theta = 30.99^\circ$	99.8 %
Absorptionskorrektur	Gaussian
Max. and min. Transmission	0.96 und 0.91
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2
Daten / Einschränkungen / Parameter	11796 / 0 / 388
Goodness-of-fit auf F^2	0.847
R [$I > 2\sigma(I)$]	$R_1 = 0.0406$ $w R^2 = 0.1086$
R-Werte (sämtliche Daten)	$R_1 = 0.0550$ $w R^2 = 0.1200$
Restelektronendichte	0.554 und $-0.471 \text{ e} \cdot \text{\AA}^{-3}$

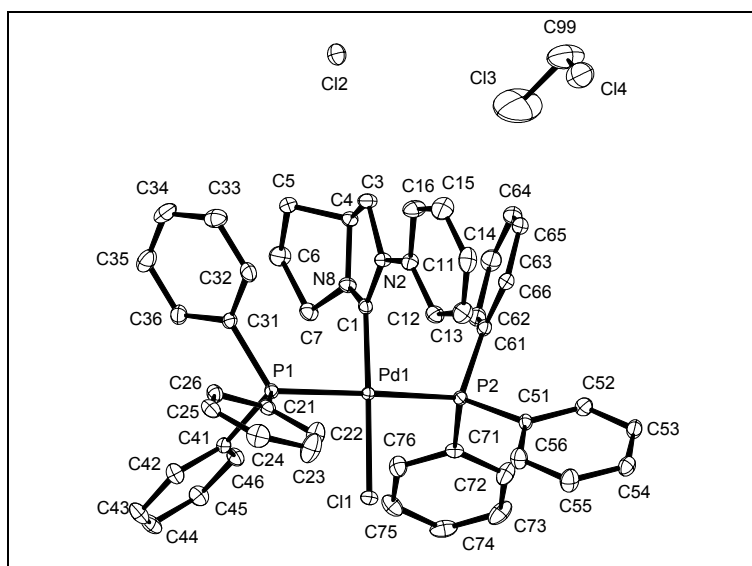
Bindungslängen [\AA] and -winkel [$^\circ$]

N(1)-C(1)	1.348(4)	N(1)-C(8)	1.458(4)
N(1)-C(2)	1.483(4)	N(2)-C(1)	1.345(4)
N(2)-C(14)	1.456(4)	N(2)-C(7)	1.476(4)
C(1)-Pd(1)	1.971(3)	C(2)-C(3)	1.512(5)
C(2)-C(7)	1.515(4)	C(3)-C(4)	1.548(5)
C(4)-C(5)	1.539(5)	C(5)-C(6)	1.550(5)
C(6)-C(7)	1.507(4)	C(8)-C(9)	1.526(4)
C(9)-C(10)	1.545(4)	C(10)-C(13)	1.515(6)
C(10)-C(12)	1.528(5)	C(10)-C(11)	1.541(5)
C(14)-C(15)	1.532(4)	C(15)-C(16)	1.539(4)
C(16)-C(18)	1.526(6)	C(16)-C(19)	1.530(5)
C(16)-C(17)	1.534(5)	C(21)-C(22)	1.386(4)
C(21)-C(26)	1.402(4)	C(21)-P(1)	1.822(3)
C(22)-C(23)	1.403(4)	C(23)-C(24)	1.379(5)
C(24)-C(25)	1.391(6)	C(25)-C(26)	1.405(5)
C(31)-C(32)	1.399(4)	C(31)-C(36)	1.407(4)
C(31)-P(1)	1.821(3)	C(32)-C(33)	1.394(5)

C(33)-C(34)	1.373(5)	C(34)-C(35)	1.388(5)
CC(35)-C(36)	1.389(4)	C(41)-C(46)	1.392(4)
C(41)-C(42)	1.401(4)	C(41)-P(1)	1.820(3)
C(42)-C(43)	1.384(4)	C(43)-C(44)	1.400(5)
C(44)-C(45)	1.383(5)	C(45)-C(46)	1.396(4)
P(1)-Pd(1)	2.2526(8)	Cl(1)-Pd(1)	2.3428(9)
Cl(2)-Pd(1)	2.3541(8)		
C(1)-N(1)-C(8)	125.0(3)	C(1)-N(1)-C(2)	109.5(3)
C(8)-N(1)-C(2)	122.6(3)	C(1)-N(2)-C(14)	124.9(3)
C(1)-N(2)-C(7)	109.0(2)	C(14)-N(2)-C(7)	122.1(3)
N(2)-C(1)-N(1)	109.0(3)	N(2)-C(1)-Pd(1)	124.7(2)
N(1)-C(1)-Pd(1)	126.3(2)	N(1)-C(2)-C(3)	119.9(3)
N(1)-C(2)-C(7)	99.8(2)	C(3)-C(2)-C(7)	111.0(3)
C(2)-C(3)-C(4)	106.6(3)	C(5)-C(4)-C(3)	113.2(3)
C(4)-C(5)-C(6)	113.0(3)	C(7)-C(6)-C(5)	104.8(3)
N(2)-C(7)-C(6)	122.7(3)	N(2)-C(7)-C(2)	100.1(3)
C(6)-C(7)-C(2)	111.2(3)	N(1)-C(8)-C(9)	111.3(2)
C(8)-C(9)-C(10)	115.5(3)	C(13)-C(10)-C(12)	109.6(3)
C(13)-C(10)-C(11)	109.4(4)	C(12)-C(10)-C(11)	109.3(3)
C(13)-C(10)-C(9)	110.5(3)	C(12)-C(10)-C(9)	111.0(3)
C(11)-C(10)-C(9)	107.0(3)	N(2)-C(14)-C(15)	111.4(2)
C(14)-C(15)-C(16)	115.6(3)	C(18)-C(16)-C(19)	110.8(3)
C(18)-C(16)-C(17)	108.5(3)	C(19)-C(16)-C(17)	109.1(3)
C(18)-C(16)-C(15)	109.8(3)	C(19)-C(16)-C(15)	110.6(3)
C(17)-C(16)-C(15)	108.0(3)	C(22)-C(21)-C(26)	119.7(3)
C(22)-C(21)-P(1)	119.3(2)	C(26)-C(21)-P(1)	121.0(2)
C(21)-C(22)-C(23)	120.4(3)	C(24)-C(23)-C(22)	120.0(3)
C(23)-C(24)-C(25)	120.4(3)	C(24)-C(25)-C(26)	119.9(3)
C(21)-C(26)-C(25)	119.6(3)	C(32)-C(31)-C(36)	118.5(3)
C(32)-C(31)-P(1)	121.4(2)	C(36)-C(31)-P(1)	119.7(2)
C(33)-C(32)-C(31)	120.5(3)	C(34)-C(33)-C(32)	120.5(3)
C(33)-C(34)-C(35)	119.7(3)	C(34)-C(35)-C(36)	120.8(3)
C(35)-C(36)-C(31)	119.9(3)	C(46)-C(41)-C(42)	119.3(3)

C(46)-C(41)-P(1)	123.6(2)	C(42)-C(41)-P(1)	117.0(2)
C(43)-C(42)-C(41)	120.5(3)	C(42)-C(43)-C(44)	120.2(3)
C(45)-C(44)-C(43)	119.1(3)	C(44)-C(45)-C(46)	121.2(3)
C(41)-C(46)-C(45)	119.6(3)	C(41)-P(1)-C(31)	102.85(14)
C(41)-P(1)-C(21)	107.30(14)	C(31)-P(1)-C(21)	104.79(15)
C(41)-P(1)-Pd(1)	111.65(10)	C(31)-P(1)-Pd(1)	116.18(11)
C(21)-P(1)-Pd(1)	113.16(11)	C(1)-Pd(1)-P(1)	91.65(8)
C(1)-Pd(1)-Cl(1)	89.06(8)	P(1)-Pd(1)-Cl(1)	178.33(3)
C(1)-Pd(1)-Cl(2)	177.25(9)	P(1)-Pd(1)-Cl(2)	87.28(3)
Cl(1)-Pd(1)-Cl(2)	92.08(3)		

Kristallographische Daten der Verbindung 87



Kristalldaten

Summenformel	$\text{C}_{49}\text{H}_{46}\text{Cl}_4\text{N}_2\text{P}_2\text{Pd}$	
Farbe	farblos	
Molmasse	$973.02 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Orthorhombisch	
Raumgruppe	$\text{P2}_1 \text{2}_1 \text{2}_1$, (no. 19)	
Gitterkonstanten	$a = 14.99730(10) \text{ \AA}$	$\alpha = 90^\circ$.
	$b = 15.29630(10) \text{ \AA}$	$\beta = 90^\circ$.
	$c = 19.02290(10) \text{ \AA}$	$\gamma = 90^\circ$.
Volumen	$4363.91(5) \text{ \AA}^3$	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	$1.481 \text{ mg} \cdot \text{m}^{-1}$	
Absorptionskoeffizient	0.781 mm^{-1}	
$F(000)$	1992 e	
Kristallgröße	$0.15 \times 0.10 \times 0.06 \text{ mm}^3$	
θ -Grenzen für Datensammlung	2.92 bis 31.50° .	
Indexgrenzen	$-22 \leq h \leq 22$, $-22 \leq k \leq 20$, $-27 \leq l \leq 27$	
Gemessene Reflexe	63808	
Unabhängige Reflexe	14486 [$R_{\text{int}} = 0.0570$]	

Reflexe mit $I > 2\sigma(I)$	12438	
Vollständigkeit für $\theta = 31.50^\circ$	99.8 %	
Absorptionskorrektur	Psi-scan	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	14486 / 0 / 523	
Goodness-of-fit auf F^2	1.012	
R [$I > 2\sigma(I)$]	$R_1 = 0.0366$	$wR^2 = 0.0722$
R-Werte (sämtliche Daten)	$R_1 = 0.0496$	$wR^2 = 0.0769$
Absolute Struktur Parameter	-0.016(16)	
Größte Differenz Peak und Loch	1.375 und -0.785 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

Pd(1)-C(1)	1.975(2)	Pd(1)-P(1)	2.3383(6)
Pd(1)-Cl(1)	2.3461(5)	Pd(1)-P(2)	2.3584(6)
Cl(3)-C(99)	1.710(4)	Cl(4)-C(99)	1.756(4)
P(1)-C(21)	1.825(3)	P(1)-C(41)	1.826(3)
P(1)-C(31)	1.826(3)	P(2)-C(51)	1.818(3)
P(2)-C(71)	1.821(2)	P(2)-C(61)	1.825(3)
C(1)-N(8)	1.322(3)	C(1)-N(2)	1.359(3)
N(2)-C(11)	1.414(3)	N(2)-C(3)	1.495(3)
C(3)-C(4)	1.526(3)	C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900	C(4)-N(8)	1.471(3)
C(4)-C(5)	1.515(3)	C(4)-H(4)	1.0000
C(5)-C(6)	1.536(3)	C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900	C(6)-C(7)	1.544(3)
C(6)-H(6A)	0.9900	C(6)-H(6B)	0.9900
C(7)-N(8)	1.466(3)	C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900	C(11)-C(16)	1.394(3)
C(11)-C(12)	1.401(3)	C(12)-C(13)	1.377(3)
C(12)-H(12)	0.9500	C(13)-C(14)	1.383(3)
C(13)-H(13)	0.9500	C(14)-C(15)	1.378(4)
C(14)-H(14)	0.9500	C(15)-C(16)	1.385(3)
C(15)-H(15)	0.9500	C(16)-H(16)	0.9500

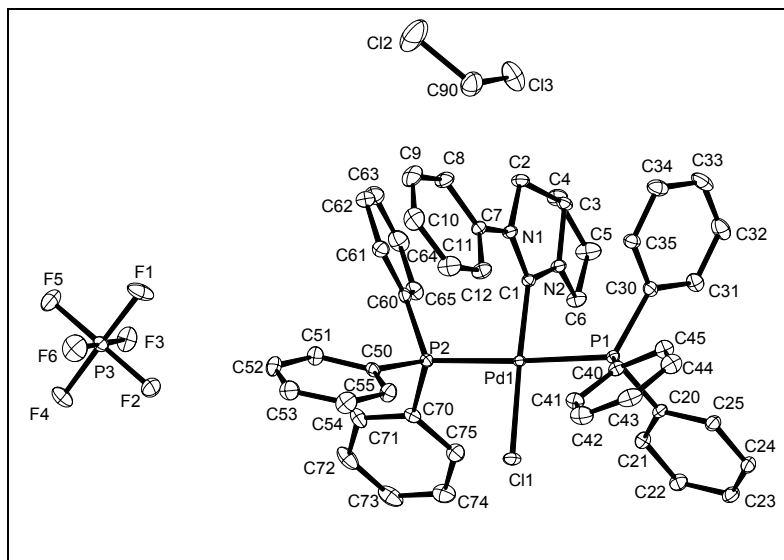
C(21)-C(22)	1.389(4)	C(21)-C(26)	1.408(4)
C(22)-C(23)	1.398(4)	C(22)-H(22)	0.9500
C(23)-C(24)	1.391(4)	C(23)-H(23)	0.9500
C(24)-C(25)	1.376(4)	C(24)-H(24)	0.9500
C(25)-C(26)	1.380(4)	C(25)-H(25)	0.9500
C(26)-H(26)	0.9500	C(31)-C(36)	1.392(4)
C(31)-C(32)	1.399(4)	C(32)-C(33)	1.398(4)
C(32)-H(32)	0.9500	C(33)-C(34)	1.379(4)
C(33)-H(33)	0.9500	C(34)-C(35)	1.383(5)
C(34)-H(34)	0.9500	C(35)-C(36)	1.398(4)
C(35)-H(35)	0.9500	C(36)-H(36)	0.9500
C(41)-C(46)	1.391(3)	C(41)-C(42)	1.397(3)
C(42)-C(43)	1.396(4)	C(42)-H(42)	0.9500
C(43)-C(44)	1.383(4)	C(43)-H(43)	0.9500
C(44)-C(45)	1.382(4)	C(44)-H(44)	0.9500
C(45)-C(46)	1.394(4)	C(45)-H(45)	0.9500
C(46)-H(46)	0.9500	C(51)-C(56)	1.395(4)
C(51)-C(52)	1.401(3)	C(52)-C(53)	1.399(4)
C(52)-H(52)	0.9500	C(53)-C(54)	1.380(4)
C(53)-H(53)	0.9500	C(54)-C(55)	1.385(4)
C(54)-H(54)	0.9500	C(55)-C(56)	1.393(4)
C(55)-H(55)	0.9500	C(56)-H(56)	0.9500
C(61)-C(62)	1.391(4)	C(61)-C(66)	1.407(4)
C(62)-C(63)	1.396(4)	C(62)-H(62)	0.9500
C(63)-C(64)	1.387(4)	C(63)-H(63)	0.9500
C(64)-C(65)	1.376(4)	C(64)-H(64)	0.9500
C(65)-C(66)	1.383(4)	C(65)-H(65)	0.9500
C(66)-H(66)	0.9500	C(71)-C(76)	1.383(4)
C(71)-C(72)	1.394(3)	C(72)-C(73)	1.394(4)
C(72)-H(72)	0.9500	C(73)-C(74)	1.378(4)
C(73)-H(73)	0.9500	C(74)-C(75)	1.385(4)
C(74)-H(74)	0.9500	C(75)-C(76)	1.391(4)
C(75)-H(75)	0.9500	C(76)-H(76)	0.9500
C(99)-H(99A)	0.9900	C(99)-H(99B)	0.9900

C(1)-Pd(1)-P(1)	91.34(7)	C(1)-Pd(1)-Cl(1)	177.68(6)
P(1)-Pd(1)-Cl(1)	88.57(2)	C(1)-Pd(1)-P(2)	88.62(7)
P(1)-Pd(1)-P(2)	173.99(2)	Cl(1)-Pd(1)-P(2)	91.23(2)
C(21)-P(1)-C(41)	107.39(12)	C(21)-P(1)-C(31)	101.92(12)
C(41)-P(1)-C(31)	104.10(12)	C(21)-P(1)-Pd(1)	115.52(9)
C(41)-P(1)-Pd(1)	109.25(7)	C(31)-P(1)-Pd(1)	117.61(8)
C(51)-P(2)-C(71)	105.69(12)	C(51)-P(2)-C(61)	103.91(11)
C(71)-P(2)-C(61)	104.61(12)	C(51)-P(2)-Pd(1)	116.69(8)
C(71)-P(2)-Pd(1)	109.81(8)	C(61)-P(2)-Pd(1)	115.06(8)
N(8)-C(1)-N(2)	108.65(18)	N(8)-C(1)-Pd(1)	121.85(15)
N(2)-C(1)-Pd(1)	129.42(15)	C(1)-N(2)-C(11)	128.30(17)
C(1)-N(2)-C(3)	110.99(17)	C(11)-N(2)-C(3)	120.66(16)
N(2)-C(3)-C(4)	102.81(17)	N(2)-C(3)-H(3A)	111.2
C(4)-C(3)-H(3A)	111.2	N(2)-C(3)-H(3B)	111.2
C(4)-C(3)-H(3B)	111.2	H(3A)-C(3)-H(3B)	109.1
N(8)-C(4)-C(5)	101.53(18)	N(8)-C(4)-C(3)	102.04(17)
C(5)-C(4)-C(3)	121.8(2)	N(8)-C(4)-H(4)	110.1
C(5)-C(4)-H(4)	110.1	C(3)-C(4)-H(4)	110.1
C(4)-C(5)-C(6)	101.8(2)	C(4)-C(5)-H(5A)	111.4
C(6)-C(5)-H(5A)	111.4	C(4)-C(5)-H(5B)	111.4
C(6)-C(5)-H(5B)	111.4	H(5A)-C(5)-H(5B)	109.3
C(5)-C(6)-C(7)	105.04(18)	C(5)-C(6)-H(6A)	110.7
C(7)-C(6)-H(6A)	110.7	C(5)-C(6)-H(6B)	110.7
C(7)-C(6)-H(6B)	110.7	H(6A)-C(6)-H(6B)	108.8
N(8)-C(7)-C(6)	102.61(17)	N(8)-C(7)-H(7A)	111.2
C(6)-C(7)-H(7A)	111.2	N(8)-C(7)-H(7B)	111.2
C(6)-C(7)-H(7B)	111.2	H(7A)-C(7)-H(7B)	109.2
C(1)-N(8)-C(7)	130.36(19)	C(1)-N(8)-C(4)	114.25(18)
C(7)-N(8)-C(4)	112.16(18)	C(16)-C(11)-C(12)	118.1(2)
C(16)-C(11)-N(2)	118.75(19)	C(12)-C(11)-N(2)	123.08(19)
C(13)-C(12)-C(11)	120.2(2)	C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9	C(12)-C(13)-C(14)	121.6(2)
C(12)-C(13)-H(13)	119.2	C(14)-C(13)-H(13)	119.2

C(15)-C(14)-C(13)	118.3(2)	C(15)-C(14)-H(14)	120.8
C(13)-C(14)-H(14)	120.8	C(14)-C(15)-C(16)	121.2(2)
C(14)-C(15)-H(15)	119.4	C(16)-C(15)-H(15)	119.4
C(15)-C(16)-C(11)	120.6(2)	C(15)-C(16)-H(16)	119.7
C(11)-C(16)-H(16)	119.7	C(22)-C(21)-C(26)	119.3(2)
C(22)-C(21)-P(1)	120.5(2)	C(26)-C(21)-P(1)	120.1(2)
C(21)-C(22)-C(23)	119.7(3)	C(21)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.2	C(24)-C(23)-C(22)	120.6(3)
C(24)-C(23)-H(23)	119.7	C(22)-C(23)-H(23)	119.7
C(25)-C(24)-C(23)	119.3(3)	C(25)-C(24)-H(24)	120.3
C(23)-C(24)-H(24)	120.3	C(24)-C(25)-C(26)	121.2(2)
C(24)-C(25)-H(25)	119.4	C(26)-C(25)-H(25)	119.4
C(25)-C(26)-C(21)	119.9(2)	C(25)-C(26)-H(26)	120.1
C(21)-C(26)-H(26)	120.1	C(36)-C(31)-C(32)	119.5(2)
C(36)-C(31)-P(1)	122.0(2)	C(32)-C(31)-P(1)	118.4(2)
C(33)-C(32)-C(31)	120.0(3)	C(33)-C(32)-H(32)	120.0
C(31)-C(32)-H(32)	120.0	C(34)-C(33)-C(32)	120.0(3)
C(34)-C(33)-H(33)	120.0	C(32)-C(33)-H(33)	120.0
C(33)-C(34)-C(35)	120.3(3)	C(33)-C(34)-H(34)	119.8
C(35)-C(34)-H(34)	119.8	C(34)-C(35)-C(36)	120.3(3)
C(34)-C(35)-H(35)	119.9	C(36)-C(35)-H(35)	119.9
C(31)-C(36)-C(35)	119.8(3)	C(31)-C(36)-H(36)	120.1
C(35)-C(36)-H(36)	120.1	C(46)-C(41)-C(42)	119.4(2)
C(46)-C(41)-P(1)	117.99(18)	C(42)-C(41)-P(1)	122.56(19)
C(43)-C(42)-C(41)	119.5(2)	C(43)-C(42)-H(42)	120.2
C(41)-C(42)-H(42)	120.2	C(44)-C(43)-C(42)	120.3(3)
C(44)-C(43)-H(43)	119.9	C(42)-C(43)-H(43)	119.9
C(45)-C(44)-C(43)	120.8(3)	C(45)-C(44)-H(44)	119.6
C(43)-C(44)-H(44)	119.6	C(44)-C(45)-C(46)	119.1(3)
C(44)-C(45)-H(45)	120.4	C(46)-C(45)-H(45)	120.4
C(41)-C(46)-C(45)	120.9(2)	C(41)-C(46)-H(46)	119.5
C(45)-C(46)-H(46)	119.5	C(56)-C(51)-C(52)	118.7(2)
C(56)-C(51)-P(2)	120.7(2)	C(52)-C(51)-P(2)	120.52(19)
C(53)-C(52)-C(51)	120.5(2)	C(53)-C(52)-H(52)	119.7

C(51)-C(52)-H(52)	119.7	C(54)-C(53)-C(52)	120.0(2)
C(54)-C(53)-H(53)	120.0	C(52)-C(53)-H(53)	120.0
C(53)-C(54)-C(55)	119.9(2)	C(53)-C(54)-H(54)	120.1
C(55)-C(54)-H(54)	120.1	C(54)-C(55)-C(56)	120.5(3)
C(54)-C(55)-H(55)	119.7	C(56)-C(55)-H(55)	119.7
C(55)-C(56)-C(51)	120.3(2)	C(55)-C(56)-H(56)	119.8
C(51)-C(56)-H(56)	119.8	C(62)-C(61)-C(66)	119.0(2)
C(62)-C(61)-P(2)	121.8(2)	C(66)-C(61)-P(2)	119.0(2)
C(61)-C(62)-C(63)	120.4(3)	C(61)-C(62)-H(62)	119.8
C(63)-C(62)-H(62)	119.8	C(64)-C(63)-C(62)	119.7(3)
C(64)-C(63)-H(63)	120.2	C(62)-C(63)-H(63)	120.2
C(65)-C(64)-C(63)	120.4(3)	C(65)-C(64)-H(64)	119.8
C(63)-C(64)-H(64)	119.8	C(64)-C(65)-C(66)	120.5(3)
C(64)-C(65)-H(65)	119.8	C(66)-C(65)-H(65)	119.8
C(65)-C(66)-C(61)	120.1(3)	C(65)-C(66)-H(66)	120.0
C(61)-C(66)-H(66)	120.0	C(76)-C(71)-C(72)	119.4(2)
C(76)-C(71)-P(2)	119.45(19)	C(72)-C(71)-P(2)	121.2(2)
C(73)-C(72)-C(71)	120.2(3)	C(73)-C(72)-H(72)	119.9
C(71)-C(72)-H(72)	119.9	C(74)-C(73)-C(72)	119.7(3)
C(74)-C(73)-H(73)	120.1	C(72)-C(73)-H(73)	120.1
C(73)-C(74)-C(75)	120.6(3)	C(73)-C(74)-H(74)	119.7
C(75)-C(74)-H(74)	119.7	C(74)-C(75)-C(76)	119.5(3)
C(74)-C(75)-H(75)	120.2	C(76)-C(75)-H(75)	120.2
C(71)-C(76)-C(75)	120.6(2)	C(71)-C(76)-H(76)	119.7
C(75)-C(76)-H(76)	119.7	Cl(3)-C(99)-Cl(4)	113.8(2)
Cl(3)-C(99)-H(99A)	108.8	Cl(4)-C(99)-H(99A)	108.8
Cl(3)-C(99)-H(99B)	108.8	Cl(4)-C(99)-H(99B)	108.8
H(99A)-C(99)-H(99B)	107.7		

Kristallographische Daten der Verbindung 110



Kristalldaten

Summenformel	$\text{C}_{49}\text{H}_{46}\text{Cl}_3\text{F}_6\text{N}_2\text{P}_3\text{Pd}$	
Farbe	farblos	
Molmasse	1082.54 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Orthorhombisch	
Raumgruppe	P2₁ 2₁ 2₁, (no. 19)	
Gitterkonstanten	$a = 14.80630(10)$ Å	$\alpha = 90^\circ$.
	$b = 16.43080(10)$ Å	$\beta = 90^\circ$.
	$c = 19.2805(2)$ Å	$\gamma = 90^\circ$.
Volume	4690.55(6) Å ³	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	1.533 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.730 mm^{-1}	
F(000)	2200 e	
Kristallgröße	0.28 x 0.20 x 0.05 mm ³	
θ -Grenzen für Datensammlung	4.11 bis 31.07°.	
Indexbereich	$-21 \leq h \leq 21$, $-23 \leq k \leq 23$, $-27 \leq l \leq 27$	
Aufgenommene Reflexe	70574	
Unabhängige Reflexe	14999 [$R_{\text{int}} = 0.0618$]	

Reflexe mit $I > 2\sigma(I)$	14084	
Vollständigkeit für $\theta = 27.50^\circ$	99.5 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.96 und 0.82	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameters	14999 / 0 / 577	
Goodness-of-fit auf F^2	1.015	
R [$I > 2\sigma(I)$]	$R_1 = 0.0295$	$wR^2 = 0.0664$
R-Werte (sämtliche Werte)	$R_1 = 0.0336$	$wR^2 = 0.0683$
Absolute Struktur Parameter	-0.016(11)	
Größte Differenz Peak und Loch	0.468 und -0.413 e·Å ⁻³	

Bindungslängen [Å] und -winkel [°]

Pd(1)-C(1)	1.9687(17)	Pd(1)-P(2)	2.3357(5)
Pd(1)-Cl(1)	2.3484(4)	Pd(1)-P(1)	2.3553(5)
P(1)-C(40)	1.8191(19)	P(1)-C(20)	1.8154(18)
P(1)-C(30)	1.821(2)	F(1)-P(3)	1.5994(14)
N(1)-C(1)	1.352(2)	N(1)-C(7)	1.409(2)
N(1)-C(2)	1.491(2)	C(1)-N(2)	1.316(2)
P(2)-C(60)	1.818(2)	P(2)-C(50)	1.8241(19)
P(2)-C(70)	1.8267(18)	F(2)-P(3)	1.5995(14)
N(2)-C(6)	1.464(2)	N(2)-C(3)	1.471(2)
C(2)-C(3)	1.525(3)	C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900	Cl(2)-C(90)	1.758(3)
P(3)-F(4)	1.5918(14)	P(3)-F(6)	1.5970(14)
P(3)-F(5)	1.6028(14)	P(3)-F(3)	1.6071(13)
C(3)-C(4)	1.517(3)	C(3)-H(3)	1.0000
Cl(3)-C(90)	1.752(3)	C(4)-C(5)	1.540(3)
C(4)-H(4A)	0.9900	C(4)-H(4B)	0.9900
C(5)-C(6)	1.546(3)	C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900	C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900	C(7)-C(12)	1.395(3)
C(7)-C(8)	1.400(3)	C(8)-C(9)	1.393(3)

C(8)-H(8)	0.9500	C(9)-C(10)	1.372(3)
C(9)-H(9)	0.9500	C(10)-C(11)	1.385(3)
C(10)-H(10)	0.9500	C(11)-C(12)	1.387(3)
C(11)-H(11)	0.9500	C(12)-H(12)	0.9500
C(20)-C(21)	1.391(3)	C(20)-C(25)	1.397(2)
C(21)-C(22)	1.398(3)	C(21)-H(21)	0.9500
C(22)-C(23)	1.384(3)	C(22)-H(22)	0.9500
C(23)-C(24)	1.390(3)	C(23)-H(23)	0.9500
C(24)-C(25)	1.385(2)	C(24)-H(24)	0.9500
C(25)-H(25)	0.9500	C(30)-C(31)	1.393(3)
C(30)-C(35)	1.397(3)	C(31)-C(32)	1.392(3)
C(31)-H(31)	0.9500	C(32)-C(33)	1.382(3)
C(32)-H(32)	0.9500	C(33)-C(34)	1.391(3)
C(33)-H(33)	0.9500	C(34)-C(35)	1.390(3)
C(34)-H(34)	0.9500	C(35)-H(35)	0.9500
C(40)-C(41)	1.388(3)	C(40)-C(45)	1.401(3)
C(41)-C(42)	1.401(3)	C(41)-H(41)	0.9500
C(42)-C(43)	1.379(3)	C(42)-H(42)	0.9500
C(43)-C(44)	1.390(3)	C(43)-H(43)	0.9500
C(44)-C(45)	1.386(3)	C(44)-H(44)	0.9500
C(45)-H(45)	0.9500	C(50)-C(55)	1.394(3)
C(50)-C(51)	1.400(3)	C(51)-C(52)	1.385(3)
C(51)-H(51)	0.9500	C(52)-C(53)	1.390(3)
C(52)-H(52)	0.9500	C(53)-C(54)	1.379(3)
C(53)-H(53)	0.9500	C(54)-C(55)	1.394(3)
C(54)-H(54)	0.9500	C(55)-H(55)	0.9500
C(60)-C(61)	1.397(3)	C(60)-C(65)	1.405(3)
C(61)-C(62)	1.393(3)	C(61)-H(61)	0.9500
C(62)-C(63)	1.395(3)	C(62)-H(62)	0.9500
C(63)-C(64)	1.373(3)	C(63)-H(63)	0.9500
C(64)-C(65)	1.390(3)	C(64)-H(64)	0.9500
C(65)-H(65)	0.9500	C(70)-C(75)	1.389(3)
C(70)-C(71)	1.397(3)	C(71)-C(72)	1.389(3)
C(71)-H(71)	0.9500	C(72)-C(73)	1.387(3)

C(72)-H(72)	0.9500	C(73)-C(74)	1.375(3)
C(73)-H(73)	0.9500	C(74)-C(75)	1.399(3)
C(74)-H(74)	0.9500	C(75)-H(75)	0.9500
C(90)-H(90A)	0.9900	C(90)-H(90B)	0.9900
C(1)-Pd(1)-P(2)	89.63(5)	C(1)-Pd(1)-Cl(1)	176.91(5)
P(2)-Pd(1)-Cl(1)	91.456(17)	C(1)-Pd(1)-P(1)	87.80(5)
P(2)-Pd(1)-P(1)	177.222(18)	Cl(1)-Pd(1)-P(1)	91.164(16)
C(40)-P(1)-C(20)	104.82(8)	C(40)-P(1)-C(30)	103.16(9)
C(20)-P(1)-C(30)	105.58(9)	C(40)-P(1)-Pd(1)	114.22(7)
C(20)-P(1)-Pd(1)	112.24(6)	C(30)-P(1)-Pd(1)	115.72(6)
C(1)-N(1)-C(7)	127.09(16)	C(1)-N(1)-C(2)	110.70(14)
C(7)-N(1)-C(2)	121.86(14)	N(2)-C(1)-N(1)	108.95(15)
N(2)-C(1)-Pd(1)	121.25(12)	N(1)-C(1)-Pd(1)	129.75(13)
C(60)-P(2)-C(50)	104.48(9)	C(60)-P(2)-C(70)	101.83(9)
C(50)-P(2)-C(70)	106.61(9)	C(60)-P(2)-Pd(1)	116.23(6)
C(50)-P(2)-Pd(1)	111.65(7)	C(70)-P(2)-Pd(1)	114.92(6)
C(1)-N(2)-C(6)	132.01(15)	C(1)-N(2)-C(3)	113.52(14)
C(6)-N(2)-C(3)	113.11(14)	N(1)-C(2)-C(3)	101.94(13)
N(1)-C(2)-H(2A)	111.4	C(3)-C(2)-H(2A)	111.4
N(1)-C(2)-H(2B)	111.4	C(3)-C(2)-H(2B)	111.4
H(2A)-C(2)-H(2B)	109.2	F(4)-P(3)-F(6)	90.56(9)
F(4)-P(3)-F(1)	178.75(9)	F(6)-P(3)-F(1)	90.26(8)
F(4)-P(3)-F(2)	89.68(8)	F(6)-P(3)-F(2)	90.21(8)
F(1)-P(3)-F(2)	89.37(8)	F(4)-P(3)-F(5)	90.57(8)
F(6)-P(3)-F(5)	90.56(8)	F(1)-P(3)-F(5)	90.37(8)
F(2)-P(3)-F(5)	179.19(8)	F(4)-P(3)-F(3)	89.95(8)
F(6)-P(3)-F(3)	179.48(9)	F(1)-P(3)-F(3)	89.23(8)
F(2)-P(3)-F(3)	89.85(7)	F(5)-P(3)-F(3)	89.38(8)
N(2)-C(3)-C(4)	101.79(15)	N(2)-C(3)-C(2)	101.61(14)
C(4)-C(3)-C(2)	122.42(18)	N(2)-C(3)-H(3)	110.0
C(4)-C(3)-H(3)	110.0	C(2)-C(3)-H(3)	110.0
C(3)-C(4)-C(5)	102.15(16)	C(3)-C(4)-H(4A)	111.3
C(5)-C(4)-H(4A)	111.3	C(3)-C(4)-H(4B)	111.3

C(5)-C(4)-H(4B)	111.3	H(4A)-C(4)-H(4B)	109.2
C(4)-C(5)-C(6)	105.72(16)	C(4)-C(5)-H(5A)	110.6
C(6)-C(5)-H(5A)	110.6	C(4)-C(5)-H(5B)	110.6
C(6)-C(5)-H(5B)	110.6	H(5A)-C(5)-H(5B)	108.7
N(2)-C(6)-C(5)	102.20(15)	N(2)-C(6)-H(6A)	111.3
C(5)-C(6)-H(6A)	111.3	N(2)-C(6)-H(6B)	111.3
C(5)-C(6)-H(6B)	111.3	H(6A)-C(6)-H(6B)	109.2
C(12)-C(7)-C(8)	118.84(17)	C(12)-C(7)-N(1)	122.02(16)
C(8)-C(7)-N(1)	119.14(17)	C(9)-C(8)-C(7)	119.7(2)
C(9)-C(8)-H(8)	120.2	C(7)-C(8)-H(8)	120.2
C(10)-C(9)-C(8)	121.2(2)	C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4	C(9)-C(10)-C(11)	119.3(2)
C(9)-C(10)-H(10)	120.4	C(11)-C(10)-H(10)	120.4
C(12)-C(11)-C(10)	120.6(2)	C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7	C(11)-C(12)-C(7)	120.37(18)
C(11)-C(12)-H(12)	119.8	C(7)-C(12)-H(12)	119.8
C(21)-C(20)-C(25)	119.60(16)	C(21)-C(20)-P(1)	119.55(13)
C(25)-C(20)-P(1)	120.85(13)	C(20)-C(21)-C(22)	119.87(18)
C(20)-C(21)-H(21)	120.1	C(22)-C(21)-H(21)	120.1
C(23)-C(22)-C(21)	120.17(18)	C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9	C(22)-C(23)-C(24)	120.00(17)
C(22)-C(23)-H(23)	120.0	C(24)-C(23)-H(23)	120.0
C(25)-C(24)-C(23)	120.16(17)	C(25)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9	C(24)-C(25)-C(20)	120.20(17)
C(24)-C(25)-H(25)	119.9	C(20)-C(25)-H(25)	119.9
C(31)-C(30)-C(35)	119.12(18)	C(31)-C(30)-P(1)	122.06(15)
C(35)-C(30)-P(1)	118.76(15)	C(32)-C(31)-C(30)	120.2(2)
C(32)-C(31)-H(31)	119.9	C(30)-C(31)-H(31)	119.9
C(33)-C(32)-C(31)	120.4(2)	C(33)-C(32)-H(32)	119.8
C(31)-C(32)-H(32)	119.8	C(32)-C(33)-C(34)	119.8(2)
C(32)-C(33)-H(33)	120.1	C(34)-C(33)-H(33)	120.1
C(35)-C(34)-C(33)	120.0(2)	C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0	C(34)-C(35)-C(30)	120.4(2)
C(34)-C(35)-H(35)	119.8	C(30)-C(35)-H(35)	119.8

C(41)-C(40)-C(45)	119.12(18)	C(41)-C(40)-P(1)	120.62(15)
C(45)-C(40)-P(1)	120.02(15)	C(40)-C(41)-C(42)	120.04(19)
C(40)-C(41)-H(41)	120.0	C(42)-C(41)-H(41)	120.0
C(43)-C(42)-C(41)	120.1(2)	C(43)-C(42)-H(42)	120.0
C(41)-C(42)-H(42)	120.0	C(42)-C(43)-C(44)	120.5(2)
C(42)-C(43)-H(43)	119.7	C(44)-C(43)-H(43)	119.8
C(45)-C(44)-C(43)	119.4(2)	C(45)-C(44)-H(44)	120.3
C(43)-C(44)-H(44)	120.3	C(44)-C(45)-C(40)	120.8(2)
C(44)-C(45)-H(45)	119.6	C(40)-C(45)-H(45)	119.6
C(55)-C(50)-C(51)	119.00(18)	C(55)-C(50)-P(2)	120.32(15)
C(51)-C(50)-P(2)	120.64(15)	C(52)-C(51)-C(50)	120.73(19)
C(52)-C(51)-H(51)	119.6	C(50)-C(51)-H(51)	119.6
C(51)-C(52)-C(53)	119.6(2)	C(51)-C(52)-H(52)	120.2
C(53)-C(52)-H(52)	120.2	C(54)-C(53)-C(52)	120.3(2)
C(54)-C(53)-H(53)	119.9	C(52)-C(53)-H(53)	119.9
C(53)-C(54)-C(55)	120.3(2)	C(53)-C(54)-H(54)	119.8
C(55)-C(54)-H(54)	119.8	C(50)-C(55)-C(54)	119.99(19)
C(50)-C(55)-H(55)	120.0	C(54)-C(55)-H(55)	120.0
C(61)-C(60)-C(65)	118.78(19)	C(61)-C(60)-P(2)	121.68(15)
C(65)-C(60)-P(2)	119.50(15)	C(62)-C(61)-C(60)	120.3(2)
C(62)-C(61)-H(61)	119.8	C(60)-C(61)-H(61)	119.8
C(61)-C(62)-C(63)	120.3(2)	C(61)-C(62)-H(62)	119.8
C(63)-C(62)-H(62)	119.8	C(64)-C(63)-C(62)	119.5(2)
C(64)-C(63)-H(63)	120.3	C(62)-C(63)-H(63)	120.3
C(63)-C(64)-C(65)	121.1(2)	C(63)-C(64)-H(64)	119.4
C(65)-C(64)-H(64)	119.4	C(64)-C(65)-C(60)	120.01(19)
C(64)-C(65)-H(65)	120.0	C(60)-C(65)-H(65)	120.0
C(75)-C(70)-C(71)	119.63(18)	C(75)-C(70)-P(2)	120.80(15)
C(71)-C(70)-P(2)	119.49(15)	C(72)-C(71)-C(70)	120.2(2)
C(72)-C(71)-H(71)	119.9	C(70)-C(71)-H(71)	119.9
C(71)-C(72)-C(73)	119.8(2)	C(71)-C(72)-H(72)	120.1
C(73)-C(72)-H(72)	120.1	C(74)-C(73)-C(72)	120.3(2)
C(74)-C(73)-H(73)	119.8	C(72)-C(73)-H(73)	119.8
C(73)-C(74)-C(75)	120.3(2)	C(73)-C(74)-H(74)	119.8

C(75)-C(74)-H(74)	119.8	C(70)-C(75)-C(74)	119.7(2)
C(70)-C(75)-H(75)	120.2	C(74)-C(75)-H(75)	120.2
Cl(3)-C(90)-Cl(2)	111.42(14)	Cl(3)-C(90)-H(90A)	109.3
Cl(2)-C(90)-H(90A)	109.3	Cl(3)-C(90)-H(90B)	109.3
Cl(2)-C(90)-H(90B)	109.3	H(90A)-C(90)-H(90B)	108.0

Reflexe mit $I > 2\sigma(I)$	9814	
Vollständigkeit für $\theta = 33.15^\circ$	99.5 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.96 and 0.94	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	11978 / 0 / 372	
Goodness-of-fit auf F^2	1.001	
R [$I > 2\sigma(I)$]	$R_1 = 0.0404$	$wR^2 = 0.0668$
R-Werte (alle Daten)	$R_1 = 0.0609$	$wR^2 = 0.0726$
Absolute Struktur Parameter	-0.021(17)	
Größte Differenz Peak und Loch	0.462 und -0.592 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

Pd(1)-C(1)	1.981(2)	Pd(1)-P(1)	2.2460(6)
Pd(1)-Cl(1)	2.3562(6)	Pd(1)-Cl(2)	2.3612(6)
P(1)-C(31)	1.818(3)	P(1)-C(51)	1.824(2)
P(1)-C(41)	1.821(2)	C(1)-N(5)	1.333(3)
C(1)-N(2)	1.350(3)	N(2)-C(2)	1.457(3)
N(2)-C(3)	1.477(3)	C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800	C(2)-H(2C)	0.9800
C(3)-C(11)	1.509(3)	C(3)-C(4)	1.550(3)
C(3)-H(3)	1.0000	C(4)-N(5)	1.484(3)
C(4)-C(21)	1.510(3)	C(4)-H(4)	1.0000
N(5)-C(5)	1.451(3)	C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800	C(5)-H(5C)	0.9800
C(11)-C(12)	1.389(4)	C(11)-C(16)	1.395(4)
C(12)-C(13)	1.392(4)	C(12)-H(12)	0.9500
C(13)-C(14)	1.385(4)	C(13)-H(13)	0.9500
C(14)-C(15)	1.373(4)	C(14)-H(14)	0.9500
C(15)-C(16)	1.389(4)	C(15)-H(15)	0.9500
C(16)-H(16)	0.9500	C(21)-C(22)	1.386(3)
C(21)-C(26)	1.397(3)	C(22)-C(23)	1.393(3)
C(22)-H(22)	0.9500	C(23)-C(24)	1.390(4)

C(23)-H(23)	0.9500	C(24)-C(25)	1.382(4)
C(24)-H(24)	0.9500	C(25)-C(26)	1.388(3)
C(25)-H(25)	0.9500	C(26)-H(26)	0.9500
C(31)-C(32)	1.385(3)	C(31)-C(36)	1.403(3)
C(32)-C(33)	1.389(3)	C(32)-H(32)	0.9500
C(33)-C(34)	1.387(4)	C(33)-H(33)	0.9500
C(34)-C(35)	1.386(4)	C(34)-H(34)	0.9500
C(35)-C(36)	1.390(3)	C(35)-H(35)	0.9500
C(36)-H(36)	0.9500	C(41)-C(46)	1.388(3)
C(41)-C(42)	1.392(3)	C(42)-C(43)	1.382(4)
C(42)-H(42)	0.9500	C(43)-C(44)	1.391(4)
C(43)-H(43)	0.9500	C(44)-C(45)	1.374(4)
C(44)-H(44)	0.9500	C(45)-C(46)	1.388(3)
C(45)-H(45)	0.9500	C(46)-H(46)	0.9500
C(51)-C(56)	1.387(4)	C(51)-C(52)	1.396(4)
C(52)-C(53)	1.389(4)	C(52)-H(52)	0.9500
C(53)-C(54)	1.374(5)	C(53)-H(53)	0.9500
C(54)-C(55)	1.378(5)	C(54)-H(54)	0.9500
C(55)-C(56)	1.388(4)	C(55)-H(55)	0.9500
C(56)-H(56)	0.9500	C(1)-Pd(1)-P(1)	97.01(7)
C(1)-Pd(1)-Cl(1)	174.34(7)	P(1)-Pd(1)-Cl(1)	88.22(2)
C(1)-Pd(1)-Cl(2)	81.60(7)	P(1)-Pd(1)-Cl(2)	178.54(2)
Cl(1)-Pd(1)-Cl(2)	93.14(2)	C(31)-P(1)-C(51)	102.97(11)
C(31)-P(1)-C(41)	105.73(11)	C(51)-P(1)-C(41)	105.61(11)
C(31)-P(1)-Pd(1)	116.06(8)	C(51)-P(1)-Pd(1)	114.44(8)
C(41)-P(1)-Pd(1)	111.05(8)	N(5)-C(1)-N(2)	109.1(2)
N(5)-C(1)-Pd(1)	124.35(17)	N(2)-C(1)-Pd(1)	125.43(17)
C(1)-N(2)-C(2)	123.8(2)	C(1)-N(2)-C(3)	110.50(19)
C(2)-N(2)-C(3)	118.15(19)	N(2)-C(2)-H(2A)	109.5
N(2)-C(2)-H(2B)	109.5	H(2A)-C(2)-H(2B)	109.5
N(2)-C(2)-H(2C)	109.5	H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5	N(2)-C(3)-C(11)	115.2(2)
N(2)-C(3)-C(4)	102.23(18)	C(11)-C(3)-C(4)	115.3(2)
N(2)-C(3)-H(3)	107.9	C(11)-C(3)-H(3)	107.9

C(4)-C(3)-H(3)	107.9	N(5)-C(4)-C(21)	111.65(19)
N(5)-C(4)-C(3)	100.54(17)	C(21)-C(4)-C(3)	113.38(19)
N(5)-C(4)-H(4)	110.3	C(21)-C(4)-H(4)	110.3
C(3)-C(4)-H(4)	110.3	C(1)-N(5)-C(5)	127.0(2)
C(1)-N(5)-C(4)	113.02(19)	C(5)-N(5)-C(4)	119.46(19)
N(5)-C(5)-H(5A)	109.5	N(5)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5	N(5)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5	H(5B)-C(5)-H(5C)	109.5
C(12)-C(11)-C(16)	118.8(2)	C(12)-C(11)-C(3)	122.7(2)
C(16)-C(11)-C(3)	118.5(2)	C(13)-C(12)-C(11)	120.9(2)
C(13)-C(12)-H(12)	119.5	C(11)-C(12)-H(12)	119.5
C(14)-C(13)-C(12)	119.6(3)	C(14)-C(13)-H(13)	120.2
C(12)-C(13)-H(13)	120.2	C(15)-C(14)-C(13)	120.0(3)
C(15)-C(14)-H(14)	120.0	C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(16)	120.8(3)	C(14)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6	C(15)-C(16)-C(11)	119.9(2)
C(15)-C(16)-H(16)	120.0	C(11)-C(16)-H(16)	120.0
C(22)-C(21)-C(26)	119.4(2)	C(22)-C(21)-C(4)	121.0(2)
C(26)-C(21)-C(4)	119.6(2)	C(21)-C(22)-C(23)	120.2(2)
C(21)-C(22)-H(22)	119.9	C(23)-C(22)-H(22)	119.9
C(24)-C(23)-C(22)	120.1(2)	C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9	C(25)-C(24)-C(23)	119.9(2)
C(25)-C(24)-H(24)	120.1	C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	120.2(2)	C(24)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9	C(25)-C(26)-C(21)	120.2(2)
C(25)-C(26)-H(26)	119.9	C(21)-C(26)-H(26)	119.9
C(32)-C(31)-C(36)	119.4(2)	C(32)-C(31)-P(1)	122.73(19)
C(36)-C(31)-P(1)	117.90(18)	C(31)-C(32)-C(33)	120.3(2)
C(31)-C(32)-H(32)	119.9	C(33)-C(32)-H(32)	119.9
C(34)-C(33)-C(32)	120.5(2)	C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7	C(35)-C(34)-C(33)	119.5(2)
C(35)-C(34)-H(34)	120.2	C(33)-C(34)-H(34)	120.2
C(34)-C(35)-C(36)	120.4(3)	C(34)-C(35)-H(35)	119.8
C(36)-C(35)-H(35)	119.8	C(35)-C(36)-C(31)	119.9(2)

C(35)-C(36)-H(36)	120.0	C(31)-C(36)-H(36)	120.0
C(46)-C(41)-C(42)	118.5(2)	C(46)-C(41)-P(1)	122.47(19)
C(42)-C(41)-P(1)	119.00(18)	C(43)-C(42)-C(41)	121.2(2)
C(43)-C(42)-H(42)	119.4	C(41)-C(42)-H(42)	119.4
C(42)-C(43)-C(44)	119.4(2)	C(42)-C(43)-H(43)	120.3
C(44)-C(43)-H(43)	120.3	C(45)-C(44)-C(43)	120.0(2)
C(45)-C(44)-H(44)	120.0	C(43)-C(44)-H(44)	120.0
C(44)-C(45)-C(46)	120.3(2)	C(44)-C(45)-H(45)	119.8
C(46)-C(45)-H(45)	119.8	C(41)-C(46)-C(45)	120.5(2)
C(41)-C(46)-H(46)	119.8	C(45)-C(46)-H(46)	119.8
C(56)-C(51)-C(52)	119.2(2)	C(56)-C(51)-P(1)	120.0(2)
C(52)-C(51)-P(1)	120.76(19)	C(53)-C(52)-C(51)	119.8(3)
C(53)-C(52)-H(52)	120.1	C(51)-C(52)-H(52)	120.1
C(54)-C(53)-C(52)	120.4(3)	C(54)-C(53)-H(53)	119.8
C(52)-C(53)-H(53)	119.8	C(53)-C(54)-C(55)	120.0(3)
C(53)-C(54)-H(54)	120.0	C(55)-C(54)-H(54)	120.0
C(54)-C(55)-C(56)	120.2(3)	C(54)-C(55)-H(55)	119.9
C(56)-C(55)-H(55)	119.9	C(51)-C(56)-C(55)	120.2(3)
C(51)-C(56)-H(56)	119.9	C(55)-C(56)-H(56)	119.9

Reflexe mit $I > 2\sigma(I)$	16740	
Vollständigkeit für $\theta = 33.21^\circ$	99.0 %	
Absorptionskorrektur	Psi-scan (Scalepack)	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	18690 / 3 / 649	
Goodness-of-fit auf F^2	0.929	
R [$I > 2\sigma(I)$]	$R_1 = 0.0492$	$wR^2 = 0.1284$
R-Werte (sämtliche Daten)	$R_1 = 0.0611$	$wR^2 = 0.1474$
Absolute Struktur Parameter	-0.014(18)	
Größte Differenz Peak und Loch	1.257 und -1.079 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

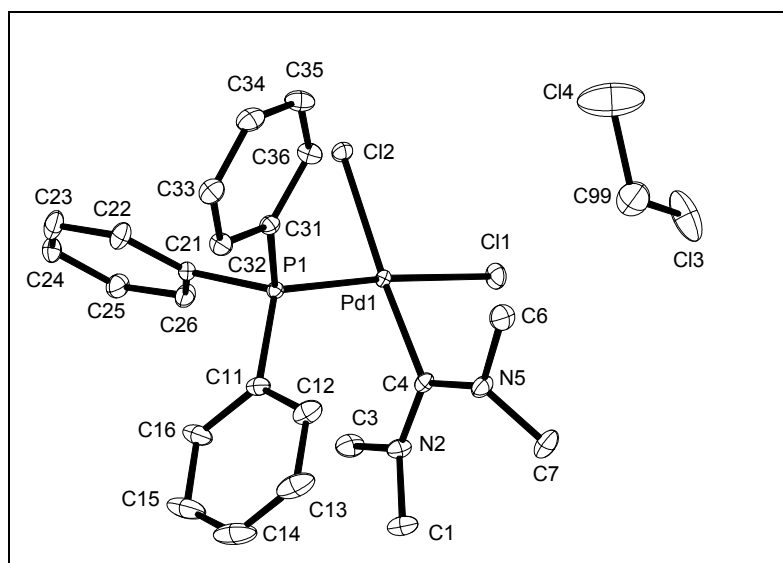
C(1)-N(2)	1.324(5)	C(1)-N(1)	1.353(5)
C(1)-Pd(1)	1.986(4)	C(2)-N(1)	1.474(5)
C(2)-C(11)	1.510(5)	C(2)-C(3)	1.542(5)
C(3)-N(2)	1.489(4)	C(3)-C(21)	1.510(5)
C(4)-N(1)	1.452(5)	C(5)-N(2)	1.460(5)
C(11)-C(16)	1.394(5)	C(11)-C(12)	1.394(5)
C(12)-C(13)	1.393(6)	C(13)-C(14)	1.387(8)
C(14)-C(15)	1.391(7)	C(15)-C(16)	1.385(5)
C(21)-C(22)	1.390(5)	C(21)-C(26)	1.393(5)
C(22)-C(23)	1.390(5)	C(23)-C(24)	1.396(6)
C(24)-C(25)	1.376(6)	C(25)-C(26)	1.384(6)
C(31)-C(32)	1.400(6)	C(31)-C(36)	1.409(5)
C(31)-P(1)	1.817(4)	C(32)-C(33)	1.381(6)
C(33)-C(34)	1.384(7)	C(34)-C(35)	1.399(7)
C(35)-C(36)	1.390(6)	C(41)-C(42)	1.396(5)
C(41)-C(46)	1.397(5)	C(41)-P(1)	1.811(3)
C(42)-C(43)	1.394(5)	C(43)-C(44)	1.376(6)
C(44)-C(45)	1.385(7)	C(45)-C(46)	1.403(6)
C(51)-C(52)	1.397(6)	C(51)-C(56)	1.401(6)
C(51)-P(1)	1.833(4)	C(52)-C(53)	1.389(6)
C(53)-C(54)	1.374(8)	C(54)-C(55)	1.398(8)

C(55)-C(56)	1.394(6)	C(61)-C(66)	1.388(6)
C(61)-C(62)	1.405(5)	C(61)-P(2)	1.816(4)
C(62)-C(63)	1.393(6)	C(63)-C(64)	1.390(8)
C(64)-C(65)	1.384(7)	C(65)-C(66)	1.404(5)
C(71)-C(72)	1.402(5)	C(71)-C(76)	1.410(5)
C(71)-P(2)	1.808(4)	C(72)-C(73)	1.392(6)
C(73)-C(74)	1.389(7)	C(74)-C(75)	1.388(7)
C(75)-C(76)	1.396(6)	C(81)-C(86)	1.392(6)
C(81)-C(82)	1.402(5)	C(81)-P(2)	1.823(4)
C(82)-C(83)	1.371(5)	C(83)-C(84)	1.372(7)
C(84)-C(85)	1.384(7)	C(85)-C(86)	1.388(6)
C(98)-Cl(2)	1.762(5)	C(98)-Cl(3)	1.768(6)
C(99)-Cl(5)	1.745(7)	C(99)-Cl(4)	1.785(7)
F(1)-P(3)	1.595(4)	F(2)-P(3)	1.593(3)
F(3)-P(3)	1.606(4)	F(4)-P(3)	1.604(3)
F(5)-P(3)	1.592(4)	F(6)-P(3)	1.594(4)
P(1)-Pd(1)	2.3338(10)	P(2)-Pd(1)	2.3221(10)
Cl(1)-Pd(1)	2.3414(9)		
N(2)-C(1)-N(1)	109.6(3)	N(2)-C(1)-Pd(1)	125.7(3)
N(1)-C(1)-Pd(1)	124.6(3)	N(1)-C(2)-C(11)	116.4(3)
N(1)-C(2)-C(3)	100.3(3)	C(11)-C(2)-C(3)	114.8(3)
N(2)-C(3)-C(21)	113.5(3)	N(2)-C(3)-C(2)	100.2(3)
C(21)-C(3)-C(2)	118.4(3)	C(16)-C(11)-C(12)	118.8(3)
C(16)-C(11)-C(2)	122.5(3)	C(12)-C(11)-C(2)	118.7(3)
C(13)-C(12)-C(11)	120.3(4)	C(14)-C(13)-C(12)	120.1(4)
C(13)-C(14)-C(15)	120.0(4)	C(16)-C(15)-C(14)	119.6(4)
C(15)-C(16)-C(11)	121.2(4)	C(22)-C(21)-C(26)	118.2(3)
C(22)-C(21)-C(3)	117.8(3)	C(26)-C(21)-C(3)	124.0(3)
C(23)-C(22)-C(21)	121.0(4)	C(22)-C(23)-C(24)	119.6(4)
C(25)-C(24)-C(23)	119.8(4)	C(24)-C(25)-C(26)	120.2(4)
C(25)-C(26)-C(21)	121.2(4)	C(32)-C(31)-C(36)	119.0(4)
C(32)-C(31)-P(1)	118.7(3)	C(36)-C(31)-P(1)	122.2(3)
C(33)-C(32)-C(31)	121.3(4)	C(32)-C(33)-C(34)	119.3(4)

C(33)-C(34)-C(35)	120.8(4)	C(36)-C(35)-C(34)	119.9(4)
C(35)-C(36)-C(31)	119.7(4)	C(42)-C(41)-C(46)	119.5(3)
C(42)-C(41)-P(1)	120.9(3)	C(46)-C(41)-P(1)	119.3(3)
C(43)-C(42)-C(41)	120.1(4)	C(44)-C(43)-C(42)	120.0(4)
C(43)-C(44)-C(45)	120.8(4)	C(44)-C(45)-C(46)	119.6(4)
C(41)-C(46)-C(45)	119.9(4)	C(52)-C(51)-C(56)	119.3(4)
C(52)-C(51)-P(1)	122.0(3)	C(56)-C(51)-P(1)	118.6(3)
C(53)-C(52)-C(51)	120.2(5)	C(54)-C(53)-C(52)	120.5(4)
C(53)-C(54)-C(55)	120.2(4)	C(56)-C(55)-C(54)	119.8(5)
C(55)-C(56)-C(51)	120.0(4)	C(66)-C(61)-C(62)	120.0(4)
C(66)-C(61)-P(2)	120.4(3)	C(62)-C(61)-P(2)	119.6(3)
C(63)-C(62)-C(61)	120.3(4)	C(64)-C(63)-C(62)	119.1(4)
C(65)-C(64)-C(63)	121.0(4)	C(64)-C(65)-C(66)	120.0(4)
C(61)-C(66)-C(65)	119.5(4)	C(72)-C(71)-C(76)	118.9(4)
C(72)-C(71)-P(2)	119.7(3)	C(76)-C(71)-P(2)	121.3(3)
C(73)-C(72)-C(71)	120.1(4)	C(74)-C(73)-C(72)	120.8(4)
C(75)-C(74)-C(73)	119.7(4)	C(74)-C(75)-C(76)	120.3(4)
C(75)-C(76)-C(71)	120.2(4)	C(86)-C(81)-C(82)	118.6(4)
C(86)-C(81)-P(2)	123.5(3)	C(82)-C(81)-P(2)	117.8(3)
C(83)-C(82)-C(81)	121.2(4)	C(82)-C(83)-C(84)	120.1(4)
C(83)-C(84)-C(85)	119.8(4)	C(84)-C(85)-C(86)	120.9(4)
C(85)-C(86)-C(81)	119.5(4)	Cl(2)-C(98)-Cl(3)	111.1(3)
Cl(5)-C(99)-Cl(4)	112.4(3)	C(1)-N(1)-C(4)	124.3(3)
C(1)-N(1)-C(2)	110.1(3)	C(4)-N(1)-C(2)	120.9(3)
C(1)-N(2)-C(5)	124.9(3)	C(1)-N(2)-C(3)	110.7(3)
C(5)-N(2)-C(3)	123.1(3)	C(41)-P(1)-C(31)	107.66(17)
C(41)-P(1)-C(51)	101.20(17)	C(31)-P(1)-C(51)	107.27(18)
C(41)-P(1)-Pd(1)	113.66(12)	C(31)-P(1)-Pd(1)	109.57(13)
C(51)-P(1)-Pd(1)	116.82(12)	C(71)-P(2)-C(61)	106.31(17)
C(71)-P(2)-C(81)	106.62(18)	C(61)-P(2)-C(81)	102.98(17)
C(71)-P(2)-Pd(1)	110.26(12)	C(61)-P(2)-Pd(1)	113.20(13)
C(81)-P(2)-Pd(1)	116.69(12)	F(5)-P(3)-F(2)	91.0(2)
F(5)-P(3)-F(6)	90.0(3)	F(2)-P(3)-F(6)	90.0(3)
F(5)-P(3)-F(1)	91.9(3)	F(2)-P(3)-F(1)	90.7(2)

F(6)-P(3)-F(1)	178.0(3)	F(5)-P(3)-F(4)	90.0(2)
F(2)-P(3)-F(4)	179.0(3)	F(6)-P(3)-F(4)	89.9(3)
F(1)-P(3)-F(4)	89.3(2)	F(5)-P(3)-F(3)	178.8(2)
F(2)-P(3)-F(3)	90.2(2)	F(6)-P(3)-F(3)	89.9(3)
F(1)-P(3)-F(3)	88.2(2)	F(4)-P(3)-F(3)	88.8(2)
C(1)-Pd(1)-P(2)	92.85(11)	C(1)-Pd(1)-P(1)	89.34(11)
P(2)-Pd(1)-P(1)	177.75(4)	C(1)-Pd(1)-Cl(1)	176.13(12)
P(2)-Pd(1)-Cl(1)	87.08(4)	P(1)-Pd(1)-Cl(1)	90.77(4)

Kristallographische Daten der Verbindung 150



Kristalldaten

Summenformel	$\text{C}_{24}\text{H}_{29}\text{Cl}_4\text{N}_2\text{PPd}$	
Farbe	farblos	
Molmasse	$624.66 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Triklin	
Raumgruppe	$\text{P}\bar{1}$, (no. 2)	
Gitterkonstanten	$a = 10.83190(10) \text{ \AA}$	$\alpha = 100.76^\circ$
	$b = 10.86860(10) \text{ \AA}$	$\beta = 91.15^\circ$
	$c = 11.44660(10) \text{ \AA}$	$\gamma = 90.98^\circ$
Volumen	$1323.30(2) \text{ \AA}^3$	
Teilchen pro Elementarzelle	2	
Berechnete Dichte	$1.568 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	1.181 mm^{-1}	
$F(000)$	632 e	
Kristallgröße	$0.20 \times 0.17 \times 0.10 \text{ mm}^3$	
θ -Grenzen für Datensammlung	4.12 bis 33.17°	
Indexbereich	$-16 \leq h \leq 16, -16 \leq k \leq 16, -17 \leq l \leq 17$	
Aufgenommene Reflexe	42141	
Unabhängige Reflexe	10085 [$R_{\text{int}} = 0.0300$]	

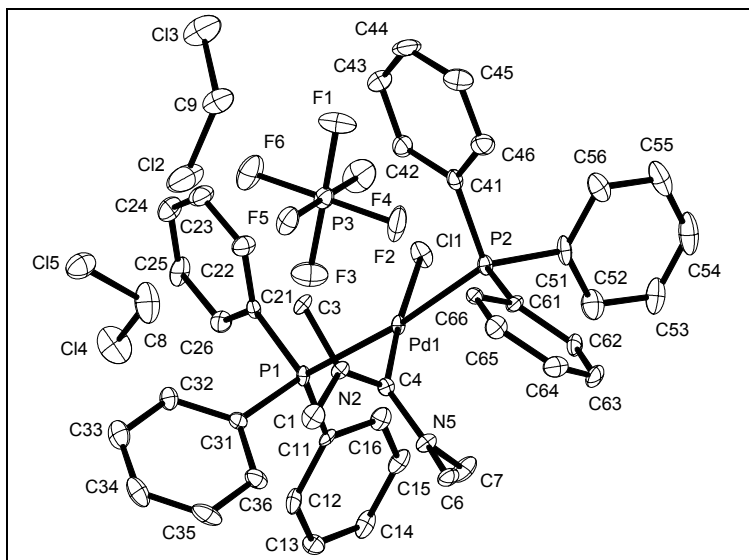
Reflexe mit $I > 2\sigma(I)$	9236	
Vollständigkeit für $\theta = 27.75^\circ$	99.7 %	
Absorptionskorrektur	Psi-scan (Scalepack)	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	10085 / 0 / 293	
Goodness-of-fit auf F^2	0.994	
R [$I > 2\sigma(I)$]	$R_1 = 0.0258$	$wR^2 = 0.0715$
R-Werte (sämtliche Daten)	$R_1 = 0.0298$	$wR^2 = 0.0740$
Größte Differenz Peak und Loch	1.693 und -1.450 e · Å ⁻³	

Bindungswinkel [Å] und -längen [°]

Pd(1)-C(4)	1.9825(13)	Pd(1)-P(1)	2.2543(3)
Pd(1)-Cl(1)	2.3568(3)	Pd(1)-Cl(2)	2.3754(3)
Cl(3)-C(99)	1.758(2)	Cl(4)-C(99)	1.747(2)
P(1)-C(21)	1.8193(13)	P(1)-C(31)	1.8257(13)
P(1)-C(11)	1.8266(14)	C(1)-N(2)	1.4623(19)
N(2)-C(4)	1.3386(18)	N(2)-C(3)	1.4620(19)
C(4)-N(5)	1.3375(17)	N(5)-C(6)	1.467(2)
N(5)-C(7)	1.471(2)	C(11)-C(16)	1.393(2)
C(11)-C(12)	1.401(2)	C(12)-C(13)	1.391(2)
CC(13)-C(14)	1.389(3)	C(14)-C(15)	1.377(3)
C(15)-C(16)	1.395(2)	C(21)-C(22)	1.3973(19)
C(21)-C(26)	1.398(2)	C(22)-C(23)	1.394(2)
C(23)-C(24)	1.384(2)	C(24)-C(25)	1.389(2)
C(25)-C(26)	1.393(2)	C(31)-C(36)	1.3955(19)
C(31)-C(32)	1.4034(19)	C(32)-C(33)	1.395(2)
C(33)-C(34)	1.391(2)	C(34)-C(35)	1.390(2)
C(35)-C(36)	1.394(2)		
C(4)-Pd(1)-P(1)	93.19(4)	C(4)-Pd(1)-Cl(1)	83.46(4)
P(1)-Pd(1)-Cl(1)	175.896(12)	C(4)-Pd(1)-Cl(2)	176.31(4)
P(1)-Pd(1)-Cl(2)	90.438(12)	Cl(1)-Pd(1)-Cl(2)	92.945(12)
C(21)-P(1)-C(31)	105.67(6)	C(21)-P(1)-C(11)	104.11(6)

C(31)-P(1)-C(11)	102.65(6)	C(21)-P(1)-Pd(1)	111.02(5)
C(31)-P(1)-Pd(1)	116.05(5)	C(11)-P(1)-Pd(1)	116.10(5)
C(4)-N(2)-C(1)	123.53(12)	C(4)-N(2)-C(3)	120.75(12)
C(1)-N(2)-C(3)	114.33(12)	N(5)-C(4)-N(2)	119.20(12)
N(5)-C(4)-Pd(1)	119.02(10)	N(2)-C(4)-Pd(1)	121.62(10)
C(4)-N(5)-C(6)	120.03(12)	C(4)-N(5)-C(7)	122.81(13)
C(6)-N(5)-C(7)	113.28(12)	C(16)-C(11)-C(12)	118.97(14)
C(16)-C(11)-P(1)	121.84(12)	C(12)-C(11)-P(1)	119.19(11)
C(13)-C(12)-C(11)	120.03(17)	C(14)-C(13)-C(12)	120.57(17)
C(15)-C(14)-C(13)	119.56(16)	C(14)-C(15)-C(16)	120.54(18)
C(11)-C(16)-C(15)	120.33(17)	C(22)-C(21)-C(26)	119.32(13)
C(22)-C(21)-P(1)	122.50(11)	C(26)-C(21)-P(1)	118.14(10)
C(23)-C(22)-C(21)	119.72(14)	C(24)-C(23)-C(22)	120.83(14)
C(23)-C(24)-C(25)	119.68(14)	C(24)-C(25)-C(26)	120.10(14)
C(25)-C(26)-C(21)	120.34(13)	C(36)-C(31)-C(32)	119.45(13)
C(36)-C(31)-P(1)	120.57(10)	C(32)-C(31)-P(1)	119.86(10)
C(33)-C(32)-C(31)	119.92(13)	C(34)-C(33)-C(32)	120.37(14)
C(33)-C(34)-C(35)	119.72(13)	C(34)-C(35)-C(36)	120.41(14)
C(35)-C(36)-C(31)	120.11(14)	Cl(4)-C(99)-Cl(3)	112.83(11)

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Kristalldaten

Summenformel	$\text{C}_{41}\text{H}_{42}\text{ClN}_2\text{P}_2\text{PdPF}_6 \cdot 2 \text{CH}_2\text{Cl}_2$	
Farbe	weiß	
Molmasse	1081.38 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Monoklin	
Raumgruppe	P2₁/c, (no. 14)	
Gitterkonstanten	$a = 11.5234(2)$ Å	$\alpha = 90^\circ$.
	$b = 27.8267(6)$ Å	$\beta = 110.2350(10)^\circ$.
	$c = 15.3671(3)$ Å	$\gamma = 90^\circ$.
Volumen	4623.46(16) Å ³	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	1.554 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.852 mm^{-1}	
F(000)	2192 e	
Kristallgröße	0.19 x 0.17 x 0.02 mm ³	
θ -Bereich für Datensammlung	4.12 bis 30.45°.	
Indexbereich	$-11 \leq h \leq 15, -12 \leq k \leq 39, -21 \leq l \leq 15$	
Aufgenommene Reflexe	15643	
Unabhängige Reflexe	11335 [$R_{\text{int}} = 0.0582$]	

Reflexe mit $I > 2\sigma(I)$	7624	
Vollständigkeit für $\theta = 30.45^\circ$	80.7 %	
Absorptionskorrektur	Psi-scan	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	11335 / 0 / 541	
Goodness-of-fit auf F^2	1.084	
R [$I > 2\sigma(I)$]	$R_1 = 0.0726$	$wR^2 = 0.1379$
R-Werte (sämtliche Werte)	$R_1 = 0.1225$	$wR^2 = 0.1571$
Größte Differenz Peak und Loch	1.404 und -1.002 e · Å ⁻³	

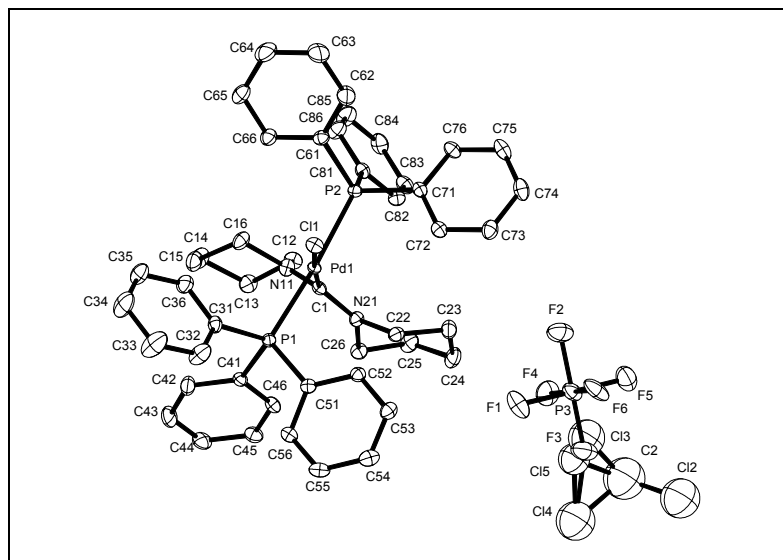
Bindungslängen [Å] und -winkel [°]

C(1)-N(2)	1.470(7)	C(3)-N(2)	1.462(7)
C(4)-N(5)	1.335(7)	C(4)-N(2)	1.339(6)
C(4)-Pd(1)	2.003(5)	C(6)-N(5)	1.472(7)
CC(7)-N(5)	1.457(7)	C(8)-Cl(4)	1.756(7)
C(8)-Cl(5)	1.769(7)	C(9)-Cl(2)	1.743(7)
C(9)-Cl(3)	1.767(7)	C(11)-C(12)	1.399(9)
C(11)-C(16)	1.401(8)	C(11)-P(1)	1.821(5)
C(12)-C(13)	1.392(8)	C(13)-C(14)	1.385(9)
C(14)-C(15)	1.387(9)	C(15)-C(16)	1.379(8)
C(21)-C(22)	1.388(8)	C(21)-C(26)	1.395(7)
C(21)-P(1)	1.813(5)	C(22)-C(23)	1.392(8)
C(23)-C(24)	1.397(9)	C(24)-C(25)	1.372(9)
C(25)-C(26)	1.386(8)	C(31)-C(36)	1.386(8)
C(31)-C(32)	1.397(7)	C(31)-P(1)	1.823(6)
C(32)-C(33)	1.396(8)	C(33)-C(34)	1.373(9)
C(34)-C(35)	1.392(9)	C(35)-C(36)	1.388(8)
C(41)-C(46)	1.401(8)	C(41)-C(42)	1.408(8)
C(41)-P(2)	1.815(6)	C(42)-C(43)	1.374(8)
C(43)-C(44)	1.381(9)	C(44)-C(45)	1.387(9)
C(45)-C(46)	1.383(9)	C(51)-C(56)	1.386(9)
C(51)-C(52)	1.395(9)	C(51)-P(2)	1.824(6)
C(52)-C(53)	1.386(9)	C(53)-C(54)	1.366(11)

C(54)-C(55)	1.378(11)	C(55)-C(56)	1.386(9)
C(61)-C(66)	1.405(7)	C(61)-C(62)	1.406(7)
C(61)-P(2)	1.821(5)	C(62)-C(63)	1.393(8)
C(63)-C(64)	1.387(8)	C(64)-C(65)	1.378(8)
C(65)-C(66)	1.391(8)	F(1)-P(3)	1.587(4)
F(2)-P(3)	1.598(4)	F(3)-P(3)	1.613(4)
F(4)-P(3)	1.593(4)	F(5)-P(3)	1.609(4)
F(6)-P(3)	1.608(4)	P(1)-Pd(1)	2.3482(15)
P(2)-Pd(1)	2.3419(14)	Cl(1)-Pd(1)	2.3610(14)
N(5)-C(4)-N(2)	121.6(5)	N(5)-C(4)-Pd(1)	118.3(4)
N(2)-C(4)-Pd(1)	120.0(4)	Cl(4)-C(8)-Cl(5)	112.4(4)
Cl(2)-C(9)-Cl(3)	111.4(4)	C(12)-C(11)-C(16)	119.0(5)
C(12)-C(11)-P(1)	123.2(4)	C(16)-C(11)-P(1)	117.7(4)
C(13)-C(12)-C(11)	119.7(6)	C(14)-C(13)-C(12)	120.5(6)
C(13)-C(14)-C(15)	120.0(6)	C(16)-C(15)-C(14)	120.0(6)
C(15)-C(16)-C(11)	120.7(6)	C(22)-C(21)-C(26)	119.6(5)
C(22)-C(21)-P(1)	119.1(4)	C(26)-C(21)-P(1)	121.1(4)
C(21)-C(22)-C(23)	120.0(5)	C(22)-C(23)-C(24)	119.7(6)
C(25)-C(24)-C(23)	120.2(5)	C(24)-C(25)-C(26)	120.2(5)
C(25)-C(26)-C(21)	120.2(6)	C(36)-C(31)-C(32)	119.0(5)
C(36)-C(31)-P(1)	120.2(4)	C(32)-C(31)-P(1)	120.8(4)
C(31)-C(32)-C(33)	120.4(6)	C(34)-C(33)-C(32)	119.6(6)
C(33)-C(34)-C(35)	120.7(6)	C(36)-C(35)-C(34)	119.4(6)
C(31)-C(36)-C(35)	120.8(6)	C(46)-C(41)-C(42)	117.9(6)
C(46)-C(41)-P(2)	121.6(4)	C(42)-C(41)-P(2)	120.5(4)
C(43)-C(42)-C(41)	120.9(6)	C(42)-C(43)-C(44)	120.5(6)
C(43)-C(44)-C(45)	119.7(6)	C(46)-C(45)-C(44)	120.3(6)
C(45)-C(46)-C(41)	120.7(6)	C(56)-C(51)-C(52)	118.8(6)
C(56)-C(51)-P(2)	121.9(5)	C(52)-C(51)-P(2)	119.3(5)
C(53)-C(52)-C(51)	120.2(7)	C(54)-C(53)-C(52)	120.2(7)
C(53)-C(54)-C(55)	120.4(6)	C(54)-C(55)-C(56)	119.9(7)
C(51)-C(56)-C(55)	120.5(7)	C(66)-C(61)-C(62)	118.7(5)
C(66)-C(61)-P(2)	119.8(4)	C(62)-C(61)-P(2)	121.4(4)

C(63)-C(62)-C(61)	120.5(5)	C(64)-C(63)-C(62)	120.0(5)
C(65)-C(64)-C(63)	119.8(5)	C(64)-C(65)-C(66)	121.3(6)
C(65)-C(66)-C(61)	119.7(5)	C(4)-N(2)-C(3)	120.6(4)
C(4)-N(2)-C(1)	126.4(5)	C(3)-N(2)-C(1)	112.2(4)
C(4)-N(5)-C(7)	120.7(5)	C(4)-N(5)-C(6)	126.6(5)
C(7)-N(5)-C(6)	111.8(4)	C(21)-P(1)-C(11)	105.7(2)
C(21)-P(1)-C(31)	103.5(2)	C(11)-P(1)-C(31)	104.9(3)
C(21)-P(1)-Pd(1)	109.22(19)	C(11)-P(1)-Pd(1)	113.51(18)
C(31)-P(1)-Pd(1)	118.85(18)	C(41)-P(2)-C(61)	104.2(2)
C(41)-P(2)-C(51)	105.6(3)	C(61)-P(2)-C(51)	104.8(3)
C(41)-P(2)-Pd(1)	110.52(18)	C(61)-P(2)-Pd(1)	116.07(19)
C(51)-P(2)-Pd(1)	114.6(2)	F(1)-P(3)-F(4)	91.0(2)
F(1)-P(3)-F(2)	90.3(2)	F(4)-P(3)-F(2)	90.7(2)
F(1)-P(3)-F(6)	89.9(2)	F(4)-P(3)-F(6)	89.9(2)
F(2)-P(3)-F(6)	179.3(2)	F(1)-P(3)-F(5)	89.8(2)
F(4)-P(3)-F(5)	179.2(2)	F(2)-P(3)-F(5)	89.6(2)
F(6)-P(3)-F(5)	89.7(2)	F(1)-P(3)-F(3)	179.2(3)
F(4)-P(3)-F(3)	89.8(2)	F(2)-P(3)-F(3)	90.0(2)
F(6)-P(3)-F(3)	89.8(2)	F(5)-P(3)-F(3)	89.5(2)
C(4)-Pd(1)-P(2)	89.35(15)	C(4)-Pd(1)-P(1)	91.53(15)
P(2)-Pd(1)-P(1)	173.79(5)	C(4)-Pd(1)-Cl(1)	175.71(15)
P(2)-Pd(1)-Cl(1)	88.12(5)	P(1)-Pd(1)-Cl(1)	91.36(5)

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Kristalldaten

Summenformel	$\text{C}_{48}\text{H}_{52}\text{ClF}_6\text{N}_2\text{P}_3\text{Pd}_3$	
Farbe	farblos	
Molmasse	1218.48 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Monoklin	
Raumgruppe	$\text{P2}_1/\text{n}$, (no. 14)	
Gitterkonstanten	$a = 16.00390(10)$ Å	$\alpha = 90^\circ$.
	$b = 11.25450(10)$ Å	$\beta = 92.96^\circ$.
	$c = 26.6487(2)$ Å	$\gamma = 90^\circ$.
Volumen	4793.43(6) Å ³	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	1.688 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	1.329 mm^{-1}	
F(000)	2432 e	
Kristallgröße	0.25 x 0.10 x 0.05 mm ³	
θ -Grenzen für Datensammlung	4.16 bis 30.57°.	
Index ranges	$-22 \leq h \leq 22$, $-16 \leq k \leq 16$, $-38 \leq l \leq 38$	
Aufgenommene Reflexe	98616	
Unabhängige Reflexe	14635 [$R_{\text{int}} = 0.0716$]	

Reflexe mit $I > 2\sigma(I)$	12245	
Vollständigkeit für $\theta = 27.50^\circ$	99.6 %	
Absorptionskorrektur	Psi-scan	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	14635 / 10 / 565	
Goodness-of-fit auf F^2	1.085	
R [$I > 2\sigma(I)$]	$R_1 = 0.0633$	$wR^2 = 0.1532$
R-Werte (sämtliche Daten)	$R_1 = 0.0792$	$wR^2 = 0.1612$
Größte Differenz Peak und Loch	2.535 und -1.599 e · Å ⁻³	

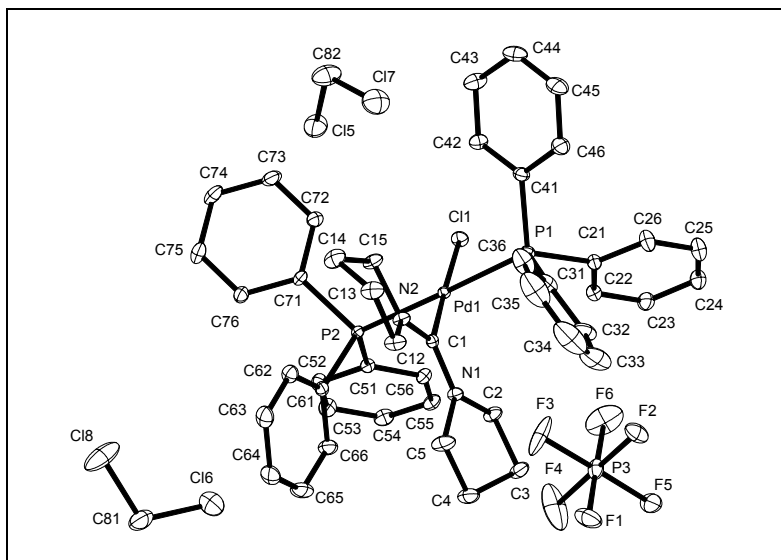
Bindungslängen [Å] und -winkel [°]

Pd(1)-C(1)	2.023(3)	Pd(1)-P(2)	2.3356(9)
Pd(1)-P(1)	2.3415(9)	Pd(1)-Cl(1)	2.3570(8)
P(1)-C(31)	1.813(3)	P(1)-C(51)	1.819(3)
P(1)-C(41)	1.826(3)	P(2)-C(71)	1.813(3)
P(2)-C(61)	1.814(3)	P(2)-C(81)	1.829(3)
F(1)-P(3)	1.605(3)	F(2)-P(3)	1.599(3)
P(3)-F(3)	1.592(3)	P(3)-F(4)	1.598(3)
P(3)-F(6)	1.612(3)	P(3)-F(5)	1.606(3)
C(2)-Cl(2)	1.838(12)	C(2)-Cl(4)	1.814(15)
C(2)-Cl(5)	1.847(14)	C(2)-Cl(3)	1.879(13)
C(1)-N(11)	1.334(4)	C(1)-N(21)	1.340(4)
N(11)-C(16)	1.472(5)	N(11)-C(12)	1.481(4)
C(12)-C(13)	1.522(5)	C(13)-C(14)	1.513(6)
C(14)-C(15)	1.530(6)	C(15)-C(16)	1.517(5)
N(21)-C(22)	1.469(4)	N(21)-C(26)	1.481(4)
C(22)-C(23)	1.528(5)	C(23)-C(24)	1.521(6)
C(24)-C(25)	1.529(6)	C(25)-C(26)	1.528(5)
C(31)-C(36)	1.390(5)	C(31)-C(32)	1.390(5)
C(32)-C(33)	1.386(6)	C(33)-C(34)	1.387(7)
C(34)-C(35)	1.383(7)	C(35)-C(36)	1.392(5)
C(41)-C(42)	1.397(5)	C(41)-C(46)	1.398(5)
C(42)-C(43)	1.387(5)	C(43)-C(44)	1.380(6)

C(44)-C(45)	1.383(5)	C(45)-C(46)	1.387(5)
C(51)-C(52)	1.389(5)	C(51)-C(56)	1.408(5)
C(52)-C(53)	1.394(5)	C(53)-C(54)	1.384(5)
C(54)-C(55)	1.385(6)	C(55)-C(56)	1.385(5)
C(61)-C(66)	1.388(5)	C(61)-C(62)	1.394(5)
C(62)-C(63)	1.386(6)	C(63)-C(64)	1.390(7)
C(64)-C(65)	1.376(6)	C(65)-C(66)	1.395(5)
C(71)-C(72)	1.396(5)	C(71)-C(76)	1.406(5)
C(72)-C(73)	1.394(5)	C(73)-C(74)	1.388(6)
C(74)-C(75)	1.381(6)	C(75)-C(76)	1.384(5)
C(81)-C(86)	1.387(5)	C(81)-C(82)	1.402(5)
C(82)-C(83)	1.379(5)	C(83)-C(84)	1.387(6)
C(84)-C(85)	1.380(6)	C(85)-C(86)	1.391(5)
C(1)-Pd(1)-P(2)	91.12(9)	C(1)-Pd(1)-P(1)	94.12(9)
P(2)-Pd(1)-P(1)	173.95(3)	C(1)-Pd(1)-Cl(1)	175.94(10)
P(2)-Pd(1)-Cl(1)	87.85(3)	P(1)-Pd(1)-Cl(1)	87.14(3)
C(31)-P(1)-C(51)	108.66(16)	C(31)-P(1)-C(41)	102.53(16)
C(51)-P(1)-C(41)	101.64(15)	C(31)-P(1)-Pd(1)	111.44(12)
C(51)-P(1)-Pd(1)	112.41(11)	C(41)-P(1)-Pd(1)	119.14(11)
C(71)-P(2)-C(61)	108.72(16)	C(71)-P(2)-C(81)	101.51(16)
C(61)-P(2)-C(81)	102.70(16)	C(71)-P(2)-Pd(1)	112.75(11)
C(61)-P(2)-Pd(1)	111.50(12)	C(81)-P(2)-Pd(1)	118.64(11)
F(3)-P(3)-F(4)	89.81(16)	F(3)-P(3)-F(2)	179.30(19)
F(4)-P(3)-F(2)	90.68(16)	F(3)-P(3)-F(1)	89.82(18)
F(4)-P(3)-F(1)	90.61(16)	F(2)-P(3)-F(1)	89.68(18)
F(3)-P(3)-F(6)	90.80(16)	F(4)-P(3)-F(6)	179.05(18)
F(2)-P(3)-F(6)	88.70(16)	F(1)-P(3)-F(6)	88.67(16)
F(3)-P(3)-F(5)	90.70(18)	F(4)-P(3)-F(5)	89.70(17)
F(2)-P(3)-F(5)	89.80(17)	F(1)-P(3)-F(5)	179.39(18)
F(6)-P(3)-F(5)	91.01(16)	Cl(2)-C(2)-Cl(4)	102.1(9)
Cl(2)-C(2)-Cl(5)	108.6(9)	Cl(4)-C(2)-Cl(5)	55.9(9)
Cl(2)-C(2)-Cl(3)	104.8(8)	Cl(4)-C(2)-Cl(3)	75.9(8)
Cl(5)-C(2)-Cl(3)	20.1(4)	N(11)-C(1)-N(21)	122.3(3)

N(11)-C(1)-Pd(1)	118.9(2)	N(21)-C(1)-Pd(1)	118.7(2)
C(1)-N(11)-C(16)	120.8(3)	C(1)-N(11)-C(12)	128.6(3)
C(16)-N(11)-C(12)	109.9(3)	N(11)-C(12)-C(13)	109.9(3)
C(12)-C(13)-C(14)	109.5(3)	C(15)-C(14)-C(13)	110.8(3)
C(16)-C(15)-C(14)	110.5(3)	C(1)-N(21)-C(22)	120.8(3)
C(1)-N(21)-C(26)	127.9(3)	C(22)-N(21)-C(26)	110.0(3)
N(21)-C(22)-C(23)	111.4(3)	C(24)-C(23)-C(22)	112.0(3)
C(23)-C(24)-C(25)	110.9(3)	C(24)-C(25)-C(26)	109.2(3)
N(21)-C(26)-C(25)	110.1(3)	C(36)-C(31)-C(32)	119.5(3)
C(36)-C(31)-P(1)	117.2(3)	C(32)-C(31)-P(1)	122.9(3)
C(33)-C(32)-C(31)	119.9(4)	C(32)-C(33)-C(34)	120.5(4)
C(33)-C(34)-C(35)	119.9(4)	C(34)-C(35)-C(36)	119.8(4)
C(31)-C(36)-C(35)	120.4(4)	C(42)-C(41)-C(46)	118.9(3)
C(42)-C(41)-P(1)	123.7(3)	C(46)-C(41)-P(1)	117.4(2)
C(43)-C(42)-C(41)	119.9(4)	C(44)-C(43)-C(42)	120.7(4)
C(43)-C(44)-C(45)	120.1(4)	C(44)-C(45)-C(46)	119.7(3)
C(45)-C(46)-C(41)	120.7(3)	C(52)-C(51)-C(56)	119.1(3)
C(52)-C(51)-P(1)	120.8(3)	C(56)-C(51)-P(1)	120.1(3)
C(51)-C(52)-C(53)	120.4(3)	C(54)-C(53)-C(52)	119.8(3)
C(55)-C(54)-C(53)	120.3(3)	C(54)-C(55)-C(56)	120.1(3)
C(55)-C(56)-C(51)	120.1(3)	C(66)-C(61)-C(62)	119.2(3)
C(66)-C(61)-P(2)	117.9(3)	C(62)-C(61)-P(2)	122.4(3)
C(63)-C(62)-C(61)	119.7(4)	C(62)-C(63)-C(64)	121.0(4)
C(65)-C(64)-C(63)	119.4(4)	C(64)-C(65)-C(66)	120.2(4)
C(61)-C(66)-C(65)	120.5(4)	C(72)-C(71)-C(76)	118.7(3)
C(72)-C(71)-P(2)	120.7(3)	C(76)-C(71)-P(2)	120.5(3)
C(71)-C(72)-C(73)	120.3(3)	C(74)-C(73)-C(72)	120.0(4)
C(75)-C(74)-C(73)	120.1(4)	C(74)-C(75)-C(76)	120.4(3)
C(75)-C(76)-C(71)	120.4(3)	C(86)-C(81)-C(82)	118.8(3)
C(86)-C(81)-P(2)	123.8(3)	C(82)-C(81)-P(2)	117.4(3)
C(83)-C(82)-C(81)	120.6(3)	C(82)-C(83)-C(84)	120.2(3)
C(85)-C(84)-C(83)	119.5(3)	C(86)-C(85)-C(84)	120.8(4)
C(85)-C(86)-C(81)	120.0(4)		

Kristallographische Daten der Verbindung 154



Kristalldaten

Summenformel	$\text{C}_{47}\text{H}_{50}\text{Cl}_5\text{F}_6\text{N}_2\text{P}_3\text{Pd}$	
Farbe	farblos	
Molmasse	1139.45 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Monoklin	
Raumgruppe	P2₁/c, (no. 14)	
Gitterkonstanten	$a = 16.2585(2)$ Å	$\alpha = 90^\circ$.
	$b = 14.8371(2)$ Å	$\beta = 92.5550(10)^\circ$.
	$c = 20.0057(3)$ Å	$\gamma = 90^\circ$.
Volumen	4821.16(11) Å ³	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	1.562 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.821 mm^{-1}	
F(000)	2304 e	
Kristallgröße	0.30 x 0.25 x 0.18 mm ³	
θ -Grenzen für Datensammlung	2.93 bis 31.51°.	
Indexbereich	$-23 \leq h \leq 23, -21 \leq k \leq 21, -29 \leq l \leq 29$	
Aufgenommene Reflexe	70728	
Unabhängige Reflexe	16021 [$R_{\text{int}} = 0.0854$]	

Reflexe mit $I > 2\sigma(I)$	13932	
Vollständigkeit für $\theta = 31.51^\circ$	99.8 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.90 und 0.82	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	16021 / 0 / 577	
Goodness-of-fit auf F^2	1.186	
R [$I > 2\sigma(I)$]	$R_1 = 0.0464$	$wR^2 = 0.1342$
R-Werte (sämtliche Werte)	$R_1 = 0.0600$	$wR^2 = 0.1538$
Größte Differenz Peak und Loch	1.010 und -1.640 e · Å ⁻³	

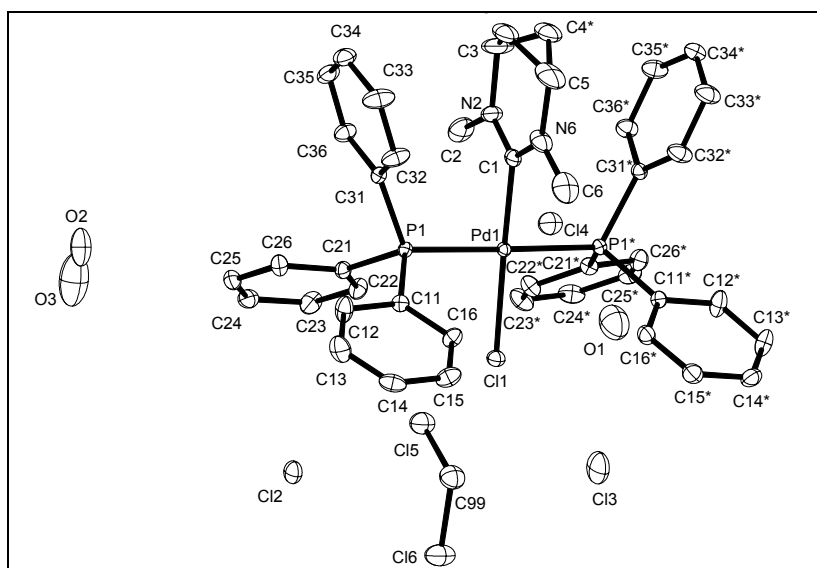
Bindungslängen [Å] und -winkel [°]

C(1)-N(1)	1.330(3)	C(1)-N(2)	1.335(3)
C(1)-Pd(1)	2.003(3)	C(2)-N(1)	1.483(3)
C(2)-C(3)	1.517(4)	C(3)-C(4)	1.521(4)
C(4)-C(5)	1.525(4)	C(5)-N(1)	1.489(4)
C(12)-N(2)	1.487(4)	C(12)-C(13)	1.528(4)
C(13)-C(14)	1.523(5)	C(14)-C(15)	1.529(4)
C(15)-N(2)	1.482(4)	C(21)-C(22)	1.386(4)
C(21)-C(26)	1.404(4)	C(21)-P(1)	1.824(3)
C(22)-C(23)	1.401(4)	C(23)-C(24)	1.381(4)
C(24)-C(25)	1.394(5)	C(25)-C(26)	1.385(5)
C(31)-C(36)	1.389(5)	C(31)-C(32)	1.401(5)
C(31)-P(1)	1.828(3)	C(32)-C(33)	1.395(5)
C(33)-C(34)	1.385(9)	C(34)-C(35)	1.372(9)
C(35)-C(36)	1.391(5)	C(41)-C(42)	1.395(4)
C(41)-C(46)	1.406(4)	C(41)-P(1)	1.829(3)
C(42)-C(43)	1.396(4)	C(43)-C(44)	1.393(5)
C(44)-C(45)	1.387(5)	C(45)-C(46)	1.391(4)
C(51)-C(56)	1.398(4)	C(51)-C(52)	1.407(4)
C(51)-P(2)	1.827(3)	C(52)-C(53)	1.391(4)
C(53)-C(54)	1.396(4)	C(54)-C(55)	1.392(4)
C(55)-C(56)	1.391(4)	C(61)-C(66)	1.393(4)

C(61)-C(62)	1.399(4)	C(61)-P(2)	1.831(3)
C(62)-C(63)	1.389(4)	C(63)-C(64)	1.384(5)
C(64)-C(65)	1.390(5)	C(65)-C(66)	1.395(4)
C(71)-C(72)	1.399(4)	C(71)-C(76)	1.406(4)
C(71)-P(2)	1.829(3)	C(72)-C(73)	1.394(4)
C(73)-C(74)	1.392(5)	C(74)-C(75)	1.392(5)
C(75)-C(76)	1.396(4)	C(81)-Cl(8)	1.762(4)
C(81)-Cl(6)	1.770(4)	C(82)-Cl(7)	1.762(4)
C(82)-Cl(5)	1.766(4)	F(1)-P(3)	1.619(3)
F(2)-P(3)	1.593(2)	F(3)-P(3)	1.599(2)
F(4)-P(3)	1.600(2)	F(5)-P(3)	1.591(2)
F(6)-P(3)	1.603(3)	P(1)-Pd(1)	2.3522(7)
P(2)-Pd(1)	2.3524(7)	Cl(1)-Pd(1)	2.3674(6)
N(1)-C(1)-N(2)	123.9(2)	N(1)-C(1)-Pd(1)	117.56(19)
N(2)-C(1)-Pd(1)	118.57(19)	N(1)-C(2)-C(3)	103.3(2)
C(2)-C(3)-C(4)	101.9(2)	C(3)-C(4)-C(5)	103.2(2)
N(1)-C(5)-C(4)	103.4(2)	N(2)-C(12)-C(13)	103.1(2)
C(14)-C(13)-C(12)	102.8(2)	C(13)-C(14)-C(15)	102.0(3)
N(2)-C(15)-C(14)	103.3(2)	C(22)-C(21)-C(26)	119.3(3)
C(22)-C(21)-P(1)	121.2(2)	C(26)-C(21)-P(1)	119.4(2)
C(21)-C(22)-C(23)	120.1(3)	C(24)-C(23)-C(22)	120.4(3)
C(23)-C(24)-C(25)	119.6(3)	C(26)-C(25)-C(24)	120.3(3)
C(25)-C(26)-C(21)	120.3(3)	C(36)-C(31)-C(32)	119.3(3)
C(36)-C(31)-P(1)	121.2(3)	C(32)-C(31)-P(1)	119.4(3)
C(33)-C(32)-C(31)	119.6(4)	C(34)-C(33)-C(32)	120.5(5)
C(35)-C(34)-C(33)	119.7(4)	C(34)-C(35)-C(36)	120.7(5)
C(31)-C(36)-C(35)	120.2(4)	C(42)-C(41)-C(46)	119.4(3)
C(42)-C(41)-P(1)	119.8(2)	C(46)-C(41)-P(1)	120.7(2)
C(41)-C(42)-C(43)	119.9(3)	C(44)-C(43)-C(42)	120.5(3)
C(45)-C(44)-C(43)	119.7(3)	C(44)-C(45)-C(46)	120.4(3)
C(45)-C(46)-C(41)	120.2(3)	C(56)-C(51)-C(52)	119.8(2)
C(56)-C(51)-P(2)	119.6(2)	C(52)-C(51)-P(2)	120.5(2)
C(53)-C(52)-C(51)	119.8(3)	C(52)-C(53)-C(54)	120.1(3)

C(55)-C(54)-C(53)	120.2(3)	C(56)-C(55)-C(54)	120.1(3)
C(55)-C(56)-C(51)	120.0(3)	C(66)-C(61)-C(62)	119.2(3)
C(66)-C(61)-P(2)	120.6(2)	C(62)-C(61)-P(2)	120.1(2)
C(63)-C(62)-C(61)	120.5(3)	C(64)-C(63)-C(62)	120.0(3)
C(63)-C(64)-C(65)	120.0(3)	C(64)-C(65)-C(66)	120.3(3)
C(61)-C(66)-C(65)	119.9(3)	C(72)-C(71)-C(76)	119.3(2)
C(72)-C(71)-P(2)	119.7(2)	C(76)-C(71)-P(2)	120.9(2)
C(73)-C(72)-C(71)	120.2(3)	C(74)-C(73)-C(72)	120.5(3)
C(75)-C(74)-C(73)	119.6(3)	C(74)-C(75)-C(76)	120.4(3)
C(75)-C(76)-C(71)	120.0(3)	Cl(8)-C(81)-Cl(6)	111.7(2)
Cl(7)-C(82)-Cl(5)	111.9(2)	C(1)-N(1)-C(2)	120.9(2)
C(1)-N(1)-C(5)	128.7(2)	C(2)-N(1)-C(5)	110.0(2)
C(1)-N(2)-C(15)	121.4(2)	C(1)-N(2)-C(12)	127.8(2)
C(15)-N(2)-C(12)	110.5(2)	C(21)-P(1)-C(31)	102.50(14)
C(21)-P(1)-C(41)	106.66(13)	C(31)-P(1)-C(41)	103.76(14)
C(21)-P(1)-Pd(1)	114.17(9)	C(31)-P(1)-Pd(1)	115.28(9)
C(41)-P(1)-Pd(1)	113.29(9)	C(51)-P(2)-C(71)	105.46(12)
C(51)-P(2)-C(61)	103.88(12)	C(71)-P(2)-C(61)	103.20(12)
C(51)-P(2)-Pd(1)	113.03(9)	C(71)-P(2)-Pd(1)	113.06(9)
C(61)-P(2)-Pd(1)	116.98(9)	F(5)-P(3)-F(2)	90.50(13)
F(5)-P(3)-F(3)	178.96(17)	F(2)-P(3)-F(3)	89.64(14)
F(5)-P(3)-F(4)	89.56(16)	F(2)-P(3)-F(4)	178.17(18)
F(3)-P(3)-F(4)	90.28(17)	F(5)-P(3)-F(6)	89.88(15)
F(2)-P(3)-F(6)	89.90(14)	F(3)-P(3)-F(6)	91.15(17)
F(4)-P(3)-F(6)	91.93(19)	F(5)-P(3)-F(1)	89.74(13)
F(2)-P(3)-F(1)	89.04(12)	F(3)-P(3)-F(1)	89.24(16)
F(4)-P(3)-F(1)	89.13(18)	F(6)-P(3)-F(1)	178.87(16)
C(1)-Pd(1)-P(1)	89.11(7)	C(1)-Pd(1)-P(2)	88.45(7)
P(1)-Pd(1)-P(2)	176.66(2)	C(1)-Pd(1)-Cl(1)	177.21(8)
P(1)-Pd(1)-Cl(1)	91.53(2)	P(2)-Pd(1)-Cl(1)	91.02(2)

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Kristalldaten

Summenformel	$\text{C}_{43}\text{H}_{48}\text{Cl}_4\text{N}_2\text{O}_2\text{P}_2\text{Pd}$	
Farbe	farblos	
Molmasse	$934.97 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Hexagonal	
Raumgruppe	P6₃/m, (no. 176)	
Gitterkonstanten	$a = 22.24080(10) \text{ \AA}$	$\alpha = 90^\circ$.
	$b = 22.24080(10) \text{ \AA}$	$\beta = 90^\circ$.
	$c = 14.698 \text{ \AA}$	$\gamma = 120^\circ$.
Volumen	$6296.45(4) \text{ \AA}^3$	
Teilchen pro Elementarzelle	6	
Berechnete Dichte	$1.479 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.812 mm^{-1}	
F(000)	2880 e	
Kristallgröße	$0.22 \times 0.16 \times 0.12 \text{ mm}^3$	
θ -Grenzen für Datensammlung	4.21 bis 32.03° .	
Indexbereich	$-33 \leq h \leq 30, -33 \leq k \leq 31, -21 \leq l \leq 21$	
Aufgenommene Reflexe	130892	
Unabhängige Reflexe	7538 [$R_{\text{int}} = 0.0604$]	

Reflexe mit $I > 2\sigma(I)$	6382	
Vollständigkeit für $\theta = 27.75^\circ$	99.5 %	
Absorptionskorrektur	Psi-scan	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	7538 / 0 / 278	
Goodness-of-fit auf F^2	1.099	
R [$I > 2\sigma(I)$]	$R_1 = 0.0318$	$wR^2 = 0.0841$
R-Werte (sämtliche Daten)	$R_1 = 0.0420$	$wR^2 = 0.0886$
Größte Differenz Peak und Loch	1.623 und -1.092 e · Å ⁻³	

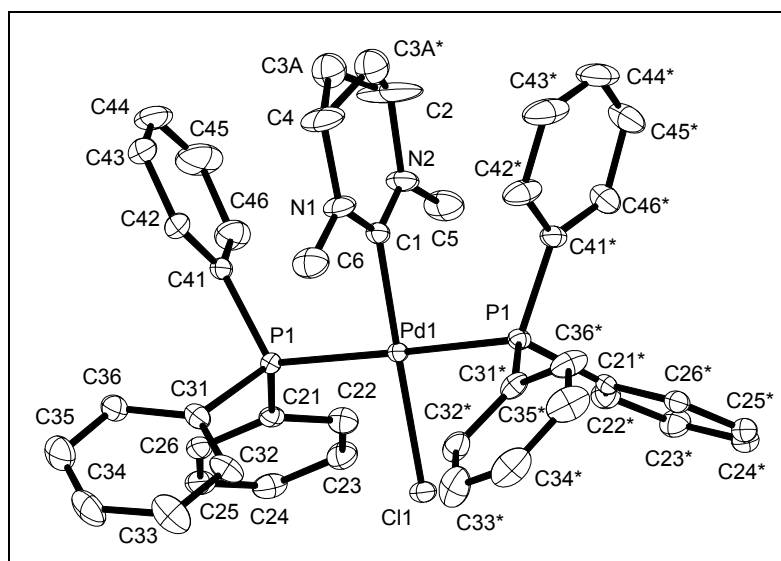
Bindungslängen [Å] und -winkel [°]

Pd(1)-C(1)	2.005(2)	Pd(1)-P(1)*	2.3424(4)
Pd(1)-P(1)	2.3424(4)	Pd(1)-Cl(1)	2.3608(6)
P(1)-C(31)	1.8226(16)	P(1)-C(21)	1.8260(16)
P(1)-C(11)	1.8280(16)	C(1)-N(2)	1.331(3)
C(1)-N(6)	1.338(3)	N(2)-C(2)	1.450(4)
N(2)-C(3)	1.477(4)	C(3)-C(4)	1.465(7)
C(4)-C(5)	1.481(6)	C(5)-N(6)	1.464(4)
N(6)-C(6)	1.464(4)	C(11)-C(16)	1.394(2)
C(11)-C(12)	1.398(2)	C(12)-C(13)	1.390(3)
C(13)-C(14)	1.387(3)	C(14)-C(15)	1.383(3)
C(15)-C(16)	1.395(2)	C(21)-C(22)	1.397(2)
C(21)-C(26)	1.404(2)	C(22)-C(23)	1.395(2)
C(23)-C(24)	1.390(3)	C(24)-C(25)	1.391(3)
C(25)-C(26)	1.392(2)	C(31)-C(36)	1.393(2)
C(31)-C(32)	1.395(2)	C(32)-C(33)	1.395(2)
C(33)-C(34)	1.388(3)	C(34)-C(35)	1.380(3)
C(35)-C(36)	1.394(2)	C(99)-Cl(5)	1.762(3)
C(99)-Cl(6)	1.764(3)	OO(2)-O(3)	0.771(11)
C(1)-Pd(1)-P(1)*	89.848(11)	C(1)-Pd(1)-P(1)	89.850(10)
P(1)*-Pd(1)-P(1)	176.12(2)	C(1)-Pd(1)-Cl(1)	177.04(8)
P(1)*-Pd(1)-Cl(1)	90.252(10)	P(1)-Pd(1)-Cl(1)	90.249(10)

C(31)-P(1)-C(21)	103.01(7)	C(31)-P(1)-C(11)	103.65(7)
C(21)-P(1)-C(11)	108.27(7)	C(31)-P(1)-Pd(1)	116.14(5)
C(21)-P(1)-Pd(1)	111.64(5)	C(11)-P(1)-Pd(1)	113.26(5)
N(2)-C(1)-N(6)	120.1(2)	N(2)-C(1)-Pd(1)	121.38(19)
N(6)-C(1)-Pd(1)	118.52(19)	C(1)-N(2)-C(2)	122.0(2)
C(1)-N(2)-C(3)	122.7(3)	C(2)-N(2)-C(3)	115.3(3)
C(4)-C(3)-N(2)	112.2(3)	C(3)-C(4)-C(5)	113.8(3)
N(6)-C(5)-C(4)	111.9(3)	C(1)-N(6)-C(6)	122.1(2)
C(1)-N(6)-C(5)	123.2(3)	C(6)-N(6)-C(5)	114.7(3)
C(16)-C(11)-C(12)	118.70(15)	C(16)-C(11)-P(1)	121.01(12)
C(12)-C(11)-P(1)	120.26(13)	C(13)-C(12)-C(11)	120.53(17)
C(14)-C(13)-C(12)	120.33(17)	C(15)-C(14)-C(13)	119.62(16)
C(14)-C(15)-C(16)	120.37(17)	C(11)-C(16)-C(15)	120.44(16)
C(22)-C(21)-C(26)	118.64(15)	C(22)-C(21)-P(1)	120.17(12)
C(26)-C(21)-P(1)	121.17(12)	C(23)-C(22)-C(21)	120.75(16)
C(24)-C(23)-C(22)	119.99(17)	C(23)-C(24)-C(25)	119.95(16)
C(24)-C(25)-C(26)	120.09(17)	C(25)-C(26)-C(21)	120.57(16)
C(36)-C(31)-C(32)	118.68(15)	C(36)-C(31)-P(1)	121.00(12)
C(32)-C(31)-P(1)	120.17(12)	C(31)-C(32)-C(33)	120.55(16)
C(34)-C(33)-C(32)	120.26(17)	C(35)-C(34)-C(33)	119.41(16)
C(34)-C(35)-C(36)	120.66(16)	C(31)-C(36)-C(35)	120.43(16)
Cl(5)-C(99)-Cl(6)	110.96(16)		

Symmetrieumformung, die benutzt wurde um äquivalente Atome zu erzeugen: * x,y,-z+1/2

Kristallographische Daten der Verbindung 170



Kristalldaten

Summenformel	$\text{C}_{43}\text{H}_{44}\text{Cl}_3\text{F}_6\text{N}_2\text{P}_3\text{Pd}$	
Farbe	weiß-gelblich	
Molmasse	1008.46 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Monoklin	
Raumgruppe	P2₁/m, (no. 11)	
Gitterkonstanten	$a = 9.57680(10)$ Å	$\alpha = 90^\circ$.
	$b = 22.7126(2)$ Å	$\beta = 93.62^\circ$.
	$c = 19.9983(2)$ Å	$\gamma = 90^\circ$.
Volumen	4341.22(7) Å ³	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	1.543 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.783 mm^{-1}	
F(000)	2048 e	
Kristallgröße	0.46 x 0.14 x 0.14 mm ³	
θ -Grenzen für Datensammlung	3.73 bis 30.53°.	
Indexbereich	$-13 \leq h \leq 13, -32 \leq k \leq 32, -28 \leq l \leq 28$	
Aufgenommene Reflexe	61540	
Unabhängige Reflexe	13550 [$R_{\text{int}} = 0.0458$]	

Reflexe mit $I > 2\sigma(I)$	12027	
Vollständigkeit für $\theta = 27.75^\circ$	99.6 %	
Absorptionskorrektur	Psi-scan	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	13550 / 222 / 649	
Goodness-of-fit auf F^2	1.144	
R [$I > 2\sigma(I)$]	$R_1 = 0.0471$	$wR^2 = 0.1107$
R-Werte (sämtliche Werte)	$R_1 = 0.0550$	$wR^2 = 0.1144$
Größte Differenz Peak und Loch	1.344 und -1.041 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

C(1)-N(1)	1.331(5)	C(1)-N(2)	1.334(5)
C(1)-Pd(1)	2.005(4)	C(2)-C(3)*	1.415(10)
C(2)-C(3)	1.415(10)	C(2)-N(2)	1.476(6)
C(3)-C(3)*	0.787(14)	C(3)-C(4)	1.504(9)
C(4)-N(1)	1.487(5)	C(4)-C(3)*	1.504(9)
C(5)-N(2)	1.444(6)	C(6)-N(1)	1.462(6)
C(11)-N(4)	1.328(5)	C(11)-N(3)	1.337(5)
C(11)-Pd(2)	1.999(4)	C(12)-C(13)	1.364(8)
C(12)-C(13)*	1.364(8)	C(12)-N(3)	1.469(6)
C(13)-C(13)*	0.798(11)	C(13)-C(14)	1.521(7)
C(14)-N(4)	1.480(5)	C(14)-C(13)*	1.521(7)
C(15)-N(3)	1.456(6)	C(16)-N(4)	1.462(5)
C(21)-C(22)	1.395(4)	C(21)-C(26)	1.402(4)
C(21)-P(1)	1.820(3)	C(22)-C(23)	1.394(4)
C(23)-C(24)	1.385(5)	C(24)-C(25)	1.387(4)
C(25)-C(26)	1.385(4)	C(31)-C(32)	1.398(4)
C(31)-C(36)	1.401(4)	C(31)-P(1)	1.819(3)
C(32)-C(33)	1.398(4)	C(33)-C(34)	1.386(6)
C(34)-C(35)	1.389(6)	C(35)-C(36)	1.389(4)
C(41)-C(42)	1.390(4)	C(41)-C(46)	1.392(5)
C(41)-P(1)	1.821(3)	C(42)-C(43)	1.399(5)
C(43)-C(44)	1.370(7)	C(44)-C(45)	1.388(7)

C(45)-C(46)	1.391(5)	C(51)-C(56)	1.395(4)
C(51)-C(52)	1.400(4)	C(51)-P(3)	1.816(3)
C(52)-C(53)	1.392(4)	C(53)-C(54)	1.389(4)
C(54)-C(55)	1.381(5)	C(55)-C(56)	1.396(4)
C(61)-C(66)	1.394(4)	C(61)-C(62)	1.399(4)
C(61)-P(3)	1.823(3)	C(62)-C(63)	1.390(4)
C(63)-C(64)	1.391(4)	C(64)-C(65)	1.387(4)
C(65)-C(66)	1.389(4)	C(71)-C(76)	1.393(4)
C(71)-C(72)	1.396(4)	C(71)-P(3)	1.821(3)
C(72)-C(73)	1.390(4)	C(73)-C(74)	1.384(5)
C(74)-C(75)	1.387(4)	C(75)-C(76)	1.397(4)
P(1)-Pd(1)	2.3323(7)	P(3)-Pd(2)	2.3348(6)
Cl(1)-Pd(1)	2.3630(9)	Cl(2)-Pd(2)	2.3730(9)
Pd(1)-P(1)*	2.3322(7)	Pd(2)-P(3)*	2.3349(6)
P(2)-Cl(6)	1.575(5)	P(2)-F(6)	1.575(6)
P(2)-F(4)	1.581(5)	P(2)-F(3)	1.586(6)
P(2)-F(1)	1.592(5)	P(2)-F(5)	1.599(7)
P(2)-F(2)	1.594(6)	P(2)-Cl(5)	1.863(4)
C(99)-Cl(6)	1.770(15)	C(99)-Cl(5)	1.779(14)
P(4)-Cl(4)	1.432(4)	P(4)-F(71)	1.452(7)
P(4)-F(41)	1.510(6)	P(4)-F(51)	1.521(8)
P(4)-F(61)	1.525(7)	P(4)-F(81)	1.538(8)
P(4)-F(31)	1.534(6)	P(4)-Cl(3)	1.824(4)
C(98)-Cl(4)	1.761(12)	C(98)-Cl(3)	1.761(14)
N(1)-C(1)-N(2)	119.6(4)	N(1)-C(1)-Pd(1)	120.8(3)
N(2)-C(1)-Pd(1)	119.6(3)	C(3)*-C(2)-C(3)	32.3(6)
C(3)*-C(2)-N(2)	114.9(5)	C(3)-C(2)-N(2)	114.9(5)
C(3)*-C(3)-C(2)	73.9(3)	C(3)*-C(3)-C(4)	74.8(3)
C(2)-C(3)-C(4)	117.2(5)	N(1)-C(4)-C(3)	111.1(4)
N(1)-C(4)-C(3)*	111.1(4)	C(3)-C(4)-C(3)*	30.3(5)
N(4)-C(11)-N(3)	119.3(3)	N(4)-C(11)-Pd(2)	121.7(3)
N(3)-C(11)-Pd(2)	118.9(3)	C(13)-C(12)-C(13)*	34.0(5)
C(13)-C(12)-N(3)	116.4(5)	C(13)*-C(12)-N(3)	116.4(5)

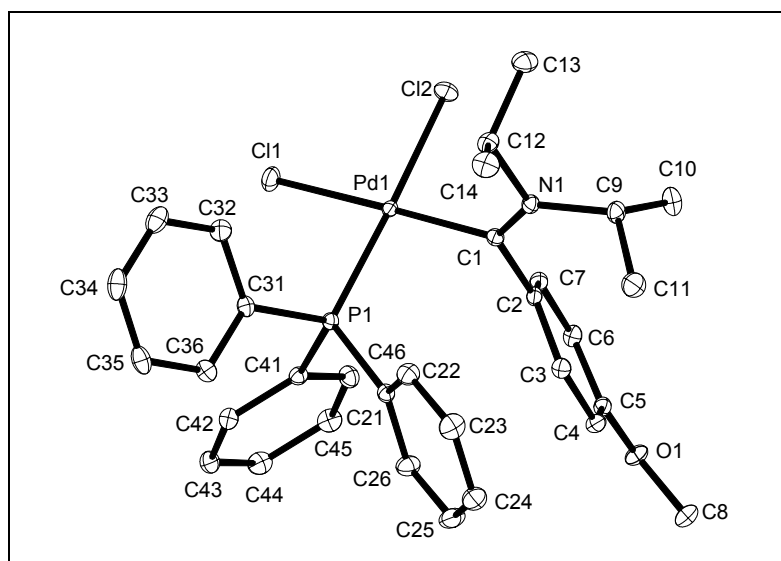
C(13)*-C(13)-C(12)	73.0(2)	C(13)*-C(13)-C(14)	74.8(2)
C(12)-C(13)-C(14)	116.7(4)	N(4)-C(14)-C(13)*	110.6(3)
N(4)-C(14)-C(13)	110.6(3)	C(13)*-C(14)-C(13)	30.4(4)
C(22)-C(21)-C(26)	119.2(3)	C(22)-C(21)-P(1)	120.1(2)
C(26)-C(21)-P(1)	120.5(2)	C(21)-C(22)-C(23)	120.2(3)
C(24)-C(23)-C(22)	120.0(3)	C(23)-C(24)-C(25)	120.1(3)
C(26)-C(25)-C(24)	120.3(3)	C(25)-C(26)-C(21)	120.2(3)
C(32)-C(31)-C(36)	119.4(3)	C(32)-C(31)-P(1)	119.2(2)
C(36)-C(31)-P(1)	121.3(2)	C(33)-C(32)-C(31)	120.0(3)
C(34)-C(33)-C(32)	120.1(3)	C(33)-C(34)-C(35)	120.1(3)
C(36)-C(35)-C(34)	120.3(3)	C(35)-C(36)-C(31)	120.1(3)
C(42)-C(41)-C(46)	119.6(3)	C(42)-C(41)-P(1)	120.8(2)
C(46)-C(41)-P(1)	119.5(2)	C(41)-C(42)-C(43)	120.1(4)
C(44)-C(43)-C(42)	119.9(4)	C(43)-C(44)-C(45)	120.6(3)
C(46)-C(45)-C(44)	119.9(4)	C(45)-C(46)-C(41)	120.0(4)
C(56)-C(51)-C(52)	119.4(2)	C(56)-C(51)-P(3)	119.9(2)
C(52)-C(51)-P(3)	120.6(2)	C(53)-C(52)-C(51)	120.3(3)
C(54)-C(53)-C(52)	119.8(3)	C(55)-C(54)-C(53)	120.3(3)
C(54)-C(55)-C(56)	120.3(3)	C(51)-C(56)-C(55)	119.8(3)
C(66)-C(61)-C(62)	118.9(2)	C(66)-C(61)-P(3)	119.6(2)
C(62)-C(61)-P(3)	121.44(19)	C(63)-C(62)-C(61)	120.3(2)
C(64)-C(63)-C(62)	120.2(3)	C(65)-C(64)-C(63)	119.8(3)
C(64)-C(65)-C(66)	120.1(3)	C(65)-C(66)-C(61)	120.7(3)
C(76)-C(71)-C(72)	118.8(2)	C(76)-C(71)-P(3)	121.0(2)
C(72)-C(71)-P(3)	120.1(2)	C(73)-C(72)-C(71)	120.7(3)
C(74)-C(73)-C(72)	120.2(3)	C(73)-C(74)-C(75)	119.8(3)
C(74)-C(75)-C(76)	120.2(3)	C(71)-C(76)-C(75)	120.4(3)
C(1)-N(1)-C(6)	122.0(3)	C(1)-N(1)-C(4)	124.8(4)
C(6)-N(1)-C(4)	113.3(4)	C(1)-N(2)-C(5)	122.5(4)
C(1)-N(2)-C(2)	122.9(4)	C(5)-N(2)-C(2)	114.6(4)
C(11)-N(3)-C(15)	122.6(3)	C(11)-N(3)-C(12)	122.0(4)
C(15)-N(3)-C(12)	115.4(4)	C(11)-N(4)-C(16)	121.2(3)
C(11)-N(4)-C(14)	124.7(3)	C(16)-N(4)-C(14)	114.1(3)
C(31)-P(1)-C(41)	104.32(13)	C(31)-P(1)-C(21)	106.36(12)

C(41)-P(1)-C(21)	102.60(13)	C(31)-P(1)-Pd(1)	112.25(10)
C(41)-P(1)-Pd(1)	116.02(9)	C(21)-P(1)-Pd(1)	114.20(9)
C(51)-P(3)-C(71)	103.43(12)	C(51)-P(3)-C(61)	107.18(12)
C(71)-P(3)-C(61)	104.43(12)	C(51)-P(3)-Pd(2)	114.05(9)
C(71)-P(3)-Pd(2)	116.77(9)	C(61)-P(3)-Pd(2)	110.11(8)
C(1)-Pd(1)-P(1)*	89.014(18)	C(1)-Pd(1)-P(1)	89.013(18)
P(1)*-Pd(1)-P(1)	175.07(4)	C(1)-Pd(1)-Cl(1)	178.60(12)
P(1)*-Pd(1)-Cl(1)	91.041(17)	P(1)-Pd(1)-Cl(1)	91.042(17)
C(11)-Pd(2)-P(3)	89.055(19)	C(11)-Pd(2)-P(3)*	89.053(19)
P(3)-Pd(2)-P(3)*	170.49(3)	C(11)-Pd(2)-Cl(2)	175.37(11)
P(3)-Pd(2)-Cl(2)	91.318(17)	P(3)*-Pd(2)-Cl(2)	91.320(17)
Cl(6)-P(2)-F(6)	53.3(3)	Cl(6)-P(2)-F(4)	40.1(2)
F(6)-P(2)-F(4)	90.7(3)	Cl(6)-P(2)-F(3)	79.0(3)
F(6)-P(2)-F(3)	91.6(5)	F(4)-P(2)-F(3)	90.3(4)
Cl(6)-P(2)-F(1)	139.5(4)	F(6)-P(2)-F(1)	88.9(3)
F(4)-P(2)-F(1)	179.6(5)	F(3)-P(2)-F(1)	89.6(3)
Cl(6)-P(2)-F(5)	103.7(3)	F(6)-P(2)-F(5)	90.9(4)
F(4)-P(2)-F(5)	91.2(4)	F(3)-P(2)-F(5)	177.0(5)
F(1)-P(2)-F(5)	89.0(3)	Cl(6)-P(2)-F(2)	127.6(3)
F(6)-P(2)-F(2)	178.9(5)	F(4)-P(2)-F(2)	90.0(3)
F(3)-P(2)-F(2)	89.1(4)	F(1)-P(2)-F(2)	90.4(3)
F(5)-P(2)-F(2)	88.2(4)	Cl(6)-P(2)-Cl(5)	116.2(3)
F(6)-P(2)-Cl(5)	128.7(4)	F(4)-P(2)-Cl(5)	106.1(3)
F(3)-P(2)-Cl(5)	41.8(3)	F(1)-P(2)-Cl(5)	74.1(2)
F(5)-P(2)-Cl(5)	135.2(4)	F(2)-P(2)-Cl(5)	51.8(3)
Cl(6)-C(99)-Cl(5)	110.9(10)	C(99)-Cl(5)-P(2)	6.8(8)
P(2)-Cl(6)-C(99)	4.3(9)	Cl(4)-P(4)-F(71)	57.8(4)
Cl(4)-P(4)-F(41)	63.9(4)	F(71)-P(4)-F(41)	93.8(5)
Cl(4)-P(4)-F(51)	123.9(4)	F(71)-P(4)-F(51)	178.1(5)
F(41)-P(4)-F(51)	87.8(5)	Cl(4)-P(4)-F(61)	47.4(5)
F(71)-P(4)-F(61)	94.2(6)	F(41)-P(4)-F(61)	87.5(5)
F(51)-P(4)-F(61)	86.8(5)	Cl(4)-P(4)-F(81)	116.8(5)
F(71)-P(4)-F(81)	88.6(6)	F(41)-P(4)-F(81)	177.4(6)
F(51)-P(4)-F(81)	89.8(6)	F(61)-P(4)-F(81)	91.4(5)

Cl(4)-P(4)-F(31)	139.3(5)	F(71)-P(4)-F(31)	91.6(5)
F(41)-P(4)-F(31)	95.5(5)	F(51)-P(4)-F(31)	87.3(5)
F(61)-P(4)-F(31)	173.3(7)	F(81)-P(4)-F(31)	85.3(5)
Cl(4)-P(4)-Cl(3)	125.0(2)	F(71)-P(4)-Cl(3)	95.2(5)
F(41)-P(4)-Cl(3)	170.0(5)	F(51)-P(4)-Cl(3)	83.1(4)
F(61)-P(4)-Cl(3)	96.2(4)	F(81)-P(4)-Cl(3)	8.5(5)
F(31)-P(4)-Cl(3)	79.9(3)	Cl(4)-C(98)-Cl(3)	110.6(9)
C(98)-Cl(3)-P(4)	11.8(5)	P(4)-Cl(4)-C(98)	6.4(7)

Symmetrieumformung, die benutzt wurde um äquivalente Atome zu erzeugen: * x,-y+1/2,z

Kristallographische Daten der Verbindung 198



Kristalldaten

Summenformel	$\text{C}_{32}\text{H}_{36}\text{Cl}_2\text{NOPPd}$	
Farbe	weiß-gelblich	
Molmasse	$658.89 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Monoklin	
Raumgruppe	$P 2_1/n$, (no. 14)	
Gitterkonstanten	$a = 10.49190(10) \text{ \AA}$	$\alpha = 90^\circ$.
	$b = 17.3034(2) \text{ \AA}$	$\beta = 94.22^\circ$.
	$c = 16.0856(2) \text{ \AA}$	$\gamma = 90^\circ$.
Volumen	$2912.36(6) \text{ \AA}^3$	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	$1.503 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.902 mm^{-1}	
$F(000)$	1352 e	
Kristallgröße	$0.24 \times 0.24 \times 0.08 \text{ mm}^3$	
θ -Grenzen für Datensammlung	3.06 bis 30.99° .	
Indexbereich	$-15 \leq h \leq 14, -25 \leq k \leq 25, -23 \leq l \leq 23$	
Aufgenommene Reflexe	49601	
Unabhängige Reflexe	9247 [$R_{\text{int}} = 0.0441$]	

Reflexe mit $I > 2\sigma(I)$	8441	
Vollständigkeit für $\theta = 30.99^\circ$	99.7 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.95 und 0.88	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	9247 / 0 / 487	
Goodness-of-fit auf F^2	1.006	
R [$I > 2\sigma(I)$]	$R_1 = 0.0234$	$wR^2 = 0.0566$
R-Werte (sämtliche Daten)	$R_1 = 0.0274$	$wR^2 = 0.0585$
Größte Differenz Peak und Loch	0.459 und -0.599 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

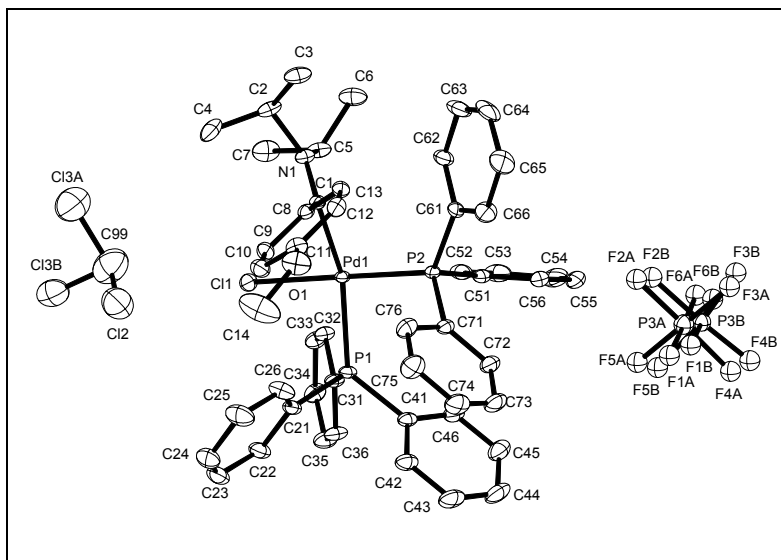
C(1)-N(1)	1.3026(16)	C(1)-C(2)	1.4811(17)
C(1)-Pd(1)	1.9937(12)	C(2)-C(3)	1.3965(18)
C(2)-C(7)	1.4089(17)	C(3)-C(4)	1.3963(18)
C(3)-H(3)	0.956(17)	C(4)-C(5)	1.3929(18)
C(4)-H(4)	0.96(2)	C(5)-O(1)	1.3622(15)
C(5)-C(6)	1.4014(18)	C(6)-C(7)	1.3822(17)
C(6)-H(6)	0.961(19)	C(7)-H(7)	0.968(17)
C(8)-O(1)	1.4331(17)	C(8)-H(8A)	0.95(2)
C(8)-H(8B)	0.976(19)	C(8)-H(8C)	0.953(18)
C(9)-N(1)	1.5178(17)	C(9)-C(10)	1.5261(19)
C(9)-C(11)	1.527(2)	C(9)-H(9)	0.953(18)
C(10)-H(10A)	0.93(2)	C(10)-H(10B)	0.962(19)
C(10)-H(10C)	0.97(2)	C(11)-H(11A)	0.99(2)
C(11)-H(11B)	0.98(2)	C(11)-H(11C)	0.95(2)
C(12)-N(1)	1.5017(16)	C(12)-C(14)	1.5228(19)
C(12)-C(13)	1.528(2)	C(12)-H(12)	0.961(18)
C(13)-H(13A)	0.96(2)	C(13)-H(13B)	0.919(19)
C(13)-H(13C)	0.95(2)	C(14)-H(14A)	0.97(2)
C(14)-H(14B)	0.95(2)	C(14)-H(14C)	0.96(2)
C(21)-C(26)	1.3931(18)	C(21)-C(22)	1.4030(18)
C(21)-P(1)	1.8249(13)	C(22)-C(23)	1.388(2)

C(22)-H(22)	0.93(2)	C(23)-C(24)	1.394(2)
C(23)-H(23)	0.96(2)	C(24)-C(25)	1.384(2)
C(24)-H(24)	0.93(2)	C(25)-C(26)	1.394(2)
C(25)-H(25)	0.91(2)	C(26)-H(26)	0.92(2)
C(31)-C(32)	1.3960(18)	C(31)-C(36)	1.4041(18)
C(31)-P(1)	1.8248(13)	C(32)-C(33)	1.3920(19)
C(32)-H(32)	0.93(2)	C(33)-C(34)	1.391(2)
C(33)-H(33)	0.95(2)	C(34)-C(35)	1.392(2)
C(34)-H(34)	0.93(2)	C(35)-C(36)	1.3905(19)
C(35)-H(35)	0.928(19)	C(36)-H(36)	0.935(19)
C(41)-C(42)	1.3966(18)	C(41)-C(46)	1.4014(17)
C(41)-P(1)	1.8285(13)	C(42)-C(43)	1.3932(18)
C(42)-H(42)	0.922(18)	C(43)-C(44)	1.3932(19)
C(43)-H(43)	0.926(19)	C(44)-C(45)	1.392(2)
C(44)-H(44)	0.953(19)	C(45)-C(46)	1.3945(18)
C(45)-H(45)	0.948(19)	C(46)-H(46)	0.955(18)
P(1)-Pd(1)	2.2690(3)	Cl(1)-Pd(1)	2.3780(3)
Cl(2)-Pd(1)	2.3561(3)		
N(1)-C(1)-C(2)	122.44(11)	N(1)-C(1)-Pd(1)	126.01(9)
C(2)-C(1)-Pd(1)	111.24(8)	C(3)-C(2)-C(7)	118.45(11)
C(3)-C(2)-C(1)	123.07(11)	C(7)-C(2)-C(1)	118.28(11)
C(4)-C(3)-C(2)	121.42(12)	C(4)-C(3)-H(3)	117.5(10)
C(2)-C(3)-H(3)	121.0(10)	C(5)-C(4)-C(3)	119.16(12)
C(5)-C(4)-H(4)	120.9(12)	C(3)-C(4)-H(4)	119.9(12)
O(1)-C(5)-C(4)	124.32(12)	O(1)-C(5)-C(6)	115.57(11)
C(4)-C(5)-C(6)	120.11(12)	C(7)-C(6)-C(5)	120.26(12)
C(7)-C(6)-H(6)	121.1(11)	C(5)-C(6)-H(6)	118.6(11)
C(6)-C(7)-C(2)	120.49(12)	C(6)-C(7)-H(7)	120.0(10)
C(2)-C(7)-H(7)	119.5(10)	O(1)-C(8)-H(8A)	113.6(12)
O(1)-C(8)-H(8B)	111.9(11)	H(8A)-C(8)-H(8B)	109.2(16)
O(1)-C(8)-H(8C)	104.6(11)	H(8A)-C(8)-H(8C)	107.6(16)
H(8B)-C(8)-H(8C)	109.8(15)	N(1)-C(9)-C(10)	112.70(11)
N(1)-C(9)-C(11)	113.82(11)	C(10)-C(9)-C(11)	113.86(12)

N(1)-C(9)-H(9)	103.8(10)	C(10)-C(9)-H(9)	104.8(11)
C(11)-C(9)-H(9)	106.7(11)	C(9)-C(10)-H(10A)	113.4(12)
C(9)-C(10)-H(10B)	112.0(11)	H(10A)-C(10)-H(10B)	106.5(16)
C(9)-C(10)-H(10C)	107.2(13)	H(10A)-C(10)-H(10C)	107.4(17)
H(10B)-C(10)-H(10C)	110.1(16)	C(9)-C(11)-H(11A)	111.3(13)
C(9)-C(11)-H(11B)	110.5(13)	H(11A)-C(11)-H(11B)	111.5(17)
C(9)-C(11)-H(11C)	109.0(13)	H(11A)-C(11)-H(11C)	108.2(18)
H(11B)-C(11)-H(11C)	106.1(18)	N(1)-C(12)-C(14)	111.27(11)
N(1)-C(12)-C(13)	110.57(11)	C(14)-C(12)-C(13)	112.13(11)
N(1)-C(12)-H(12)	103.2(11)	C(14)-C(12)-H(12)	110.1(10)
C(13)-C(12)-H(12)	109.1(10)	C(12)-C(13)-H(13A)	107.9(12)
C(12)-C(13)-H(13B)	111.8(12)	H(13A)-C(13)-H(13B)	107.7(16)
C(12)-C(13)-H(13C)	109.8(13)	H(13A)-C(13)-H(13C)	111.0(17)
H(13B)-C(13)-H(13C)	108.7(17)	C(12)-C(14)-H(14A)	112.3(12)
C(12)-C(14)-H(14B)	111.3(12)	H(14A)-C(14)-H(14B)	106.9(17)
C(12)-C(14)-H(14C)	107.6(13)	H(14A)-C(14)-H(14C)	109.3(17)
H(14B)-C(14)-H(14C)	109.4(17)	C(26)-C(21)-C(22)	118.79(12)
C(26)-C(21)-P(1)	122.67(10)	C(22)-C(21)-P(1)	118.53(10)
C(23)-C(22)-C(21)	120.41(13)	C(23)-C(22)-H(22)	122.1(13)
C(21)-C(22)-H(22)	117.5(13)	C(22)-C(23)-C(24)	120.27(13)
C(22)-C(23)-H(23)	119.9(12)	C(24)-C(23)-H(23)	119.8(12)
C(25)-C(24)-C(23)	119.62(13)	C(25)-C(24)-H(24)	118.4(12)
C(23)-C(24)-H(24)	122.0(12)	C(24)-C(25)-C(26)	120.32(13)
C(24)-C(25)-H(25)	120.2(14)	C(26)-C(25)-H(25)	119.5(14)
C(21)-C(26)-C(25)	120.57(13)	C(21)-C(26)-H(26)	119.3(12)
C(25)-C(26)-H(26)	120.1(12)	C(32)-C(31)-C(36)	119.31(12)
C(32)-C(31)-P(1)	120.55(10)	C(36)-C(31)-P(1)	120.12(10)
C(33)-C(32)-C(31)	120.06(13)	C(33)-C(32)-H(32)	120.3(13)
C(31)-C(32)-H(32)	119.6(13)	C(34)-C(33)-C(32)	120.23(13)
C(34)-C(33)-H(33)	119.6(12)	C(32)-C(33)-H(33)	120.2(12)
C(33)-C(34)-C(35)	120.20(13)	C(33)-C(34)-H(34)	120.2(13)
C(35)-C(34)-H(34)	119.6(13)	C(36)-C(35)-C(34)	119.72(13)
C(36)-C(35)-H(35)	120.1(12)	C(34)-C(35)-H(35)	120.1(12)
C(35)-C(36)-C(31)	120.42(13)	C(35)-C(36)-H(36)	119.8(12)

C(31)-C(36)-H(36)	119.7(12)	C(42)-C(41)-C(46)	119.21(12)
C(42)-C(41)-P(1)	123.31(10)	C(46)-C(41)-P(1)	117.42(10)
C(43)-C(42)-C(41)	120.12(12)	C(43)-C(42)-H(42)	119.2(11)
C(41)-C(42)-H(42)	120.7(11)	C(44)-C(43)-C(42)	120.72(13)
C(44)-C(43)-H(43)	120.0(12)	C(42)-C(43)-H(43)	119.3(12)
C(45)-C(44)-C(43)	119.26(13)	C(45)-C(44)-H(44)	121.7(11)
C(43)-C(44)-H(44)	119.1(11)	C(44)-C(45)-C(46)	120.45(13)
C(44)-C(45)-H(45)	121.3(12)	C(46)-C(45)-H(45)	118.3(12)
C(45)-C(46)-C(41)	120.24(12)	C(45)-C(46)-H(46)	119.9(11)
C(41)-C(46)-H(46)	119.8(11)	C(1)-N(1)-C(12)	119.71(11)
C(1)-N(1)-C(9)	127.23(11)	C(12)-N(1)-C(9)	112.60(10)
C(5)-O(1)-C(8)	117.10(10)	C(31)-P(1)-C(21)	100.84(6)
C(31)-P(1)-C(41)	108.45(6)	C(21)-P(1)-C(41)	103.70(6)
C(31)-P(1)-Pd(1)	114.33(4)	C(21)-P(1)-Pd(1)	119.66(4)
C(41)-P(1)-Pd(1)	108.89(4)	C(1)-Pd(1)-P(1)	95.16(4)
C(1)-Pd(1)-Cl(2)	87.80(4)	P(1)-Pd(1)-Cl(2)	176.530(12)
C(1)-Pd(1)-Cl(1)	172.41(4)	P(1)-Pd(1)-Cl(1)	86.677(12)
Cl(2)-Pd(1)-Cl(1)	90.155(12)		

Kristallographische Daten der Verbindung 199



Kristalldaten

Summenformel	$\text{C}_{51}\text{H}_{53}\text{Cl}_3\text{F}_6\text{NOP}_3\text{Pd}$	
Farbe	gelb	
Molmasse	1115.60 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Triklin	
Raumgruppe	$\text{P}\bar{1}$, (no. 2)	
Gitterkonstanten	$a = 10.95160(10)$ Å	$\alpha = 84.09^\circ$.
	$b = 14.63970(10)$ Å	$\beta = 87.9010(10)^\circ$.
	$c = 16.5360(2)$ Å	$\gamma = 71.4710(10)^\circ$.
Volumen	$2500.36(4)$ Å ³	
Teilchen pro Elementarzelle	2	
Berechnete Dichte	1.482 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.688 mm^{-1}	
F(000)	1140 e	
Kristallgröße	0.25 x 0.19 x 0.07 mm ³	
θ -Grenzen für Datensammlung	2.95 bis 30.99° .	
Indexbereich	$-15 \leq h \leq 15$, $-21 \leq k \leq 21$, $-23 \leq l \leq 23$	
Aufgenommene Reflexe	60449	
Unabhängige Reflexe	15859 [$R_{\text{int}} = 0.0473$]	

Reflexe mit $I > 2\sigma(I)$	14246	
Vollständigkeit für $\theta = 30.99^\circ$	99.6 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.96 und 0.84	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrat auf F^2	
Daten/ Einschränkungen/ Parameter	15859 / 0 / 597	
Goodness-of-fit auf F^2	1.060	
R [$I > 2\sigma(I)$]	$R_1 = 0.0558$	$wR^2 = 0.1569$
R-Werte (sämtliche Daten)	$R_1 = 0.0625$	$wR^2 = 0.1616$
Größte Differenz Peak und Loch	1.120 und -2.750 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

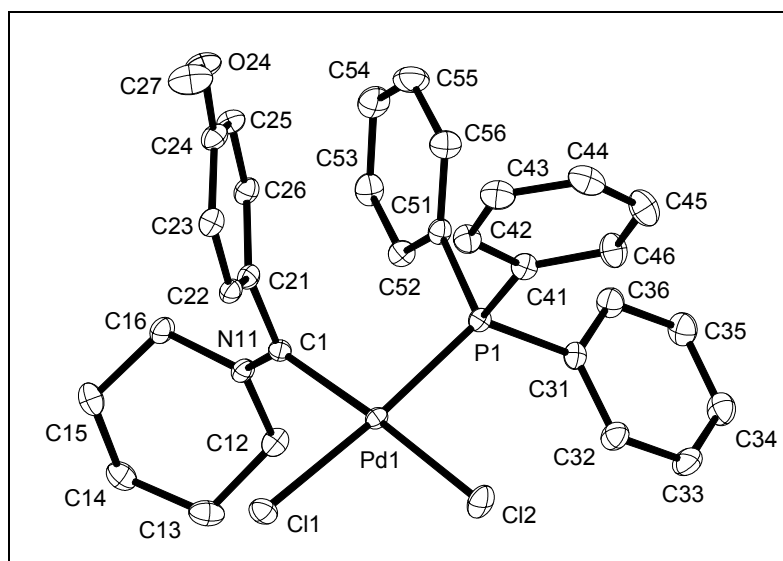
C(1)-N(1)	1.301(4)	C(1)-C(8)	1.493(4)
C(1)-Pd(1)	2.047(3)	C(2)-C(3)	1.518(5)
C(2)-N(1)	1.518(4)	C(2)-C(4)	1.523(5)
C(5)-N(1)	1.507(4)	C(5)-C(7)	1.528(5)
C(5)-C(6)	1.533(5)	C(8)-C(13)	1.405(4)
C(8)-C(9)	1.405(4)	C(9)-C(10)	1.389(4)
C(9)-C(10)-C(11)	1.398(4)	C(11)-O(1)	1.362(4)
C(11)-C(12)	1.395(4)	C(12)-C(13)	1.388(4)
C(14)-O(1)	1.437(5)	C(21)-C(22)	1.390(4)
C(21)-C(26)	1.395(5)	C(21)-P(1)	1.829(3)
C(22)-C(23)	1.392(5)	C(23)-C(24)	1.371(6)
C(24)-C(25)	1.388(6)	C(25)-C(26)	1.391(5)
C(31)-C(32)	1.394(4)	C(31)-C(36)	1.401(4)
C(31)-P(1)	1.827(3)	C(32)-C(33)	1.394(4)
C(33)-C(34)	1.387(4)	C(34)-C(35)	1.392(4)
C(35)-C(36)	1.387(4)	C(41)-C(42)	1.394(4)
C(41)-C(46)	1.403(4)	C(41)-P(1)	1.831(3)
C(42)-C(43)	1.395(5)	C(43)-C(44)	1.375(6)
C(44)-C(45)	1.400(6)	C(45)-C(46)	1.392(4)
C(51)-C(52)	1.401(5)	C(51)-C(56)	1.404(4)
C(51)-P(2)	1.818(3)	C(52)-C(53)	1.392(5)

C(53)-C(54)	1.389(6)	C(54)-C(55)	1.369(7)
C(55)-C(56)	1.403(5)	C(61)-C(66)	1.390(5)
C(61)-C(62)	1.398(5)	C(61)-P(2)	1.819(3)
C(62)-C(63)	1.387(4)	C(63)-C(64)	1.370(7)
C(64)-C(65)	1.382(7)	C(65)-C(66)	1.400(5)
C(71)-C(72)	1.392(4)	C(71)-C(76)	1.401(5)
C(71)-P(2)	1.816(3)	C(72)-C(73)	1.392(5)
C(73)-C(74)	1.380(6)	C(74)-C(75)	1.390(5)
C(75)-C(76)	1.385(5)	C(99)-Cl(3B)	1.772(17)
C(99)-Cl(2)	1.757(7)	C(99)-Cl(3A)	1.741(7)
F(1A)-P(3A)	1.617(4)	F(2A)-P(3A)	1.595(4)
F(3A)-P(3A)	1.617(4)	F(4A)-P(3A)	1.614(4)
F(5A)-P(3A)	1.604(4)	F(6A)-P(3A)	1.628(5)
F(1B)-P(3B)	1.618(11)	F(2B)-P(3B)	1.611(13)
F(3B)-P(3B)	1.497(13)	F(4B)-P(3B)	1.492(12)
F(5B)-P(3B)	1.624(12)	F(6B)-P(3B)	1.409(15)
P(1)-Pd(1)	2.3931(7)	P(2)-Pd(1)	2.2686(7)
Cl(1)-Pd(1)	2.3554(7)		
N(1)-C(1)-C(8)	124.0(2)	N(1)-C(1)-Pd(1)	127.2(2)
C(8)-C(1)-Pd(1)	107.97(18)	C(3)-C(2)-N(1)	114.0(3)
C(3)-C(2)-C(4)	114.7(3)	N(1)-C(2)-C(4)	110.2(3)
N(1)-C(5)-C(7)	111.1(3)	N(1)-C(5)-C(6)	111.5(3)
C(7)-C(5)-C(6)	110.7(3)	C(13)-C(8)-C(9)	118.1(3)
C(13)-C(8)-C(1)	121.8(2)	C(9)-C(8)-C(1)	119.2(2)
C(10)-C(9)-C(8)	121.1(3)	C(9)-C(10)-C(11)	119.9(3)
O(1)-C(11)-C(12)	116.0(3)	O(1)-C(11)-C(10)	124.4(3)
C(12)-C(11)-C(10)	119.7(3)	C(13)-C(12)-C(11)	120.2(3)
C(12)-C(13)-C(8)	121.0(3)	C(22)-C(21)-C(26)	118.7(3)
C(22)-C(21)-P(1)	123.5(3)	C(26)-C(21)-P(1)	117.9(2)
C(21)-C(22)-C(23)	120.0(3)	C(24)-C(23)-C(22)	121.0(3)
C(23)-C(24)-C(25)	119.7(3)	C(24)-C(25)-C(26)	119.7(4)
C(25)-C(26)-C(21)	120.9(3)	C(32)-C(31)-C(36)	119.1(3)
C(32)-C(31)-P(1)	120.2(2)	C(36)-C(31)-P(1)	120.6(2)

C(33)-C(32)-C(31)	120.3(3)	C(34)-C(33)-C(32)	120.1(3)
C(33)-C(34)-C(35)	120.0(3)	C(36)-C(35)-C(34)	119.9(3)
C(35)-C(36)-C(31)	120.5(3)	C(42)-C(41)-C(46)	119.1(3)
C(42)-C(41)-P(1)	121.7(2)	C(46)-C(41)-P(1)	119.2(2)
C(41)-C(42)-C(43)	120.0(3)	C(44)-C(43)-C(42)	120.7(3)
C(43)-C(44)-C(45)	120.1(3)	C(46)-C(45)-C(44)	119.4(4)
C(45)-C(46)-C(41)	120.6(3)	C(52)-C(51)-C(56)	119.7(3)
C(52)-C(51)-P(2)	119.0(2)	C(56)-C(51)-P(2)	121.1(3)
C(53)-C(52)-C(51)	120.3(3)	C(54)-C(53)-C(52)	119.7(4)
C(55)-C(54)-C(53)	120.4(3)	C(54)-C(55)-C(56)	121.2(3)
C(55)-C(56)-C(51)	118.7(4)	C(66)-C(61)-C(62)	119.7(3)
C(66)-C(61)-P(2)	122.6(3)	C(62)-C(61)-P(2)	117.7(3)
C(63)-C(62)-C(61)	120.2(4)	C(64)-C(63)-C(62)	120.2(4)
C(63)-C(64)-C(65)	120.1(3)	C(64)-C(65)-C(66)	120.8(4)
C(61)-C(66)-C(65)	119.0(4)	C(72)-C(71)-C(76)	119.8(3)
C(72)-C(71)-P(2)	125.9(3)	C(76)-C(71)-P(2)	114.3(2)
C(71)-C(72)-C(73)	119.4(3)	C(74)-C(73)-C(72)	120.7(3)
C(73)-C(74)-C(75)	120.1(3)	C(76)-C(75)-C(74)	119.7(4)
C(75)-C(76)-C(71)	120.3(3)	Cl(3B)-C(99)-Cl(2)	109.4(6)
Cl(3B)-C(99)-Cl(3A)	87.2(5)	Cl(2)-C(99)-Cl(3A)	113.9(4)
C(1)-N(1)-C(5)	120.4(2)	C(1)-N(1)-C(2)	125.5(3)
C(5)-N(1)-C(2)	113.6(2)	C(11)-O(1)-C(14)	116.6(3)
C(31)-P(1)-C(21)	108.44(14)	C(31)-P(1)-C(41)	100.75(13)
C(21)-P(1)-C(41)	102.57(14)	C(31)-P(1)-Pd(1)	112.69(9)
C(21)-P(1)-Pd(1)	104.62(10)	C(41)-P(1)-Pd(1)	126.54(9)
C(71)-P(2)-C(51)	111.50(14)	C(71)-P(2)-C(61)	102.46(14)
C(51)-P(2)-C(61)	102.56(14)	C(71)-P(2)-Pd(1)	108.99(10)
C(51)-P(2)-Pd(1)	112.29(11)	C(61)-P(2)-Pd(1)	118.56(10)
F(2A)-P(3A)-F(5A)	88.90(19)	F(2A)-P(3A)-F(4A)	178.8(2)
F(5A)-P(3A)-F(4A)	90.0(2)	F(2A)-P(3A)-F(3A)	90.25(19)
F(5A)-P(3A)-F(3A)	177.8(2)	F(4A)-P(3A)-F(3A)	90.8(2)
F(2A)-P(3A)-F(1A)	89.62(18)	F(5A)-P(3A)-F(1A)	88.63(18)
F(4A)-P(3A)-F(1A)	89.88(19)	F(3A)-P(3A)-F(1A)	89.4(2)
F(2A)-P(3A)-F(6A)	90.2(2)	F(5A)-P(3A)-F(6A)	88.5(2)

F(4A)-P(3A)-F(6A)	90.2(2)	F(3A)-P(3A)-F(6A)	93.5(2)
F(1A)-P(3A)-F(6A)	177.1(2)	F(6B)-P(3B)-F(4B)	88.1(8)
F(6B)-P(3B)-F(3B)	80.7(8)	F(4B)-P(3B)-F(3B)	96.1(7)
F(6B)-P(3B)-F(2B)	89.1(8)	F(4B)-P(3B)-F(2B)	176.3(8)
F(3B)-P(3B)-F(2B)	81.1(7)	F(6B)-P(3B)-F(1B)	176.4(8)
F(4B)-P(3B)-F(1B)	92.8(6)	F(3B)-P(3B)-F(1B)	95.7(7)
F(2B)-P(3B)-F(1B)	89.8(6)	F(6B)-P(3B)-F(5B)	93.6(8)
F(4B)-P(3B)-F(5B)	91.9(7)	F(3B)-P(3B)-F(5B)	170.1(7)
F(2B)-P(3B)-F(5B)	90.7(7)	F(1B)-P(3B)-F(5B)	89.9(6)
C(1)-Pd(1)-P(2)	96.56(8)	C(1)-Pd(1)-Cl(1)	83.75(8)
P(2)-Pd(1)-Cl(1)	179.50(3)	C(1)-Pd(1)-P(1)	164.40(8)
P(2)-Pd(1)-P(1)	94.93(3)	Cl(1)-Pd(1)-P(1)	84.70(2)

Kristallographische Daten der Verbindung 203



Kristalldaten

Summenformel	$\text{C}_{31.5}\text{H}_{32}\text{Cl}_{3.25}\text{NOPPd}$	
Farbe	farblos	
Molmasse	$693.16 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Orthorhombisch	
Raumgruppe	Pbcn, (no. 60)	
Gitterkonstanten	$a = 21.6007(2) \text{ \AA}$	$\alpha = 90^\circ$
	$b = 16.6871(2) \text{ \AA}$	$\beta = 90^\circ$
	$c = 16.9748(2) \text{ \AA}$	$\gamma = 90^\circ$
Volumen	$6118.62(12) \text{ \AA}^3$	
Teilchen pro Elementarzelle	8	
Berechnete Dichte	$1.505 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.969 mm^{-1}	
F(000)	2818 e	
Kristallgröße	$0.08 \times 0.05 \times 0.04 \text{ mm}^3$	
θ -Grenzen für Datensammlung	3.05 bis 31.50°	
Indexbereich	$-31 \leq h \leq 31, -24 \leq k \leq 22, -22 \leq l \leq 24$	
Aufgenommene Reflexe	90112	
Unabhängige Reflexe	10168 [$R_{\text{int}} = 0.0642$]	

Reflexe mit $I > 2\sigma(I)$	8229	
Vollständigkeit für $\theta = 27.75^\circ$	99.9 %	
Absorptionskorrektur	Keine	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	10168 / 0 / 389	
Goodness-of-fit auf F^2	1.032	
R [$I > 2\sigma(I)$]	$R_1 = 0.0384$	$wR^2 = 0.1301$
R-Werte (sämtliche Daten)	$R_1 = 0.0545$	$wR^2 = 0.1406$
Größte Differenz Peak und Loch	1.059 und -1.217 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

Pd(1)-C(1)	1.975(2)	Pd(1)-P(1)	2.2831(6)
Pd(1)-Cl(1)	2.3631(6)	Pd(1)-Cl(2)	2.3675(6)
Cl(3)-Cl(5)	0.812(6)	Cl(3)-C(99)	1.047(19)
Cl(3)-C(99) ¹	1.678(18)	Cl(4)-Cl(7)	0.718(8)
Cl(4)-Cl(4) ²	1.241(18)	Cl(4)-C(98)	1.355(15)
Cl(4)-C(98) ²	1.760(16)	Cl(4)-Cl(5) ³	2.364(12)
Cl(5)-C(99)	1.68(2)	Cl(5)-C(99) ¹	1.828(19)
Cl(5)-Cl(4) ⁴	2.364(12)	Cl(6)-Cl(6) ²	0.660(11)
Cl(6)-C(98)	1.632(18)	Cl(6)-C(98) ²	1.807(18)
Cl(7)-Cl(4) ²	0.718(8)	Cl(7)-C(98) ²	1.784(18)
Cl(7)-C(98)	1.784(18)	Cl(8)-Cl(6) ²	0.43(3)
Cl(8)-C(98)	1.44(3)	Cl(8)-C(98) ²	1.44(3)
C(98)-C(98) ²	1.06(3)	C(98)-Cl(4) ²	1.760(16)
C(98)-Cl(6) ²	1.807(18)	C(99)-C(99) ¹	1.17(3)
C(99)-Cl(3) ¹	1.678(18)	C(99)-Cl(5) ¹	1.828(19)
P(1)-C(51)	1.817(2)	P(1)-C(41)	1.828(2)
P(1)-C(31)	1.828(2)	C(1)-N(11)	1.300(3)
C(1)-C(21)	1.484(3)	N(11)-C(12)	1.481(3)
N(11)-C(16)	1.488(3)	C(12)-C(13)	1.520(4)
C(13)-C(14)	1.532(4)	C(14)-C(15)	1.525(4)
C(15)-C(16)	1.525(4)	C(21)-C(26)	1.404(3)
C(21)-C(22)	1.406(3)	C(22)-C(23)	1.388(3)

C(23)-C(24)	1.397(3)	O(24)-C(24)	1.361(3)
O(24)-C(27)	1.436(3)	C(24)-C(25)	1.392(3)
C(25)-C(26)	1.388(3)	C(31)-C(36)	1.399(3)
C(31)-C(32)	1.403(3)	C(32)-C(33)	1.386(4)
C(33)-C(34)	1.393(4)	C(34)-C(35)	1.386(4)
C(35)-C(36)	1.388(4)	C(41)-C(42)	1.394(3)
C(41)-C(46)	1.395(3)	C(42)-C(43)	1.397(3)
C(43)-C(44)	1.389(4)	C(44)-C(45)	1.381(4)
C(45)-C(46)	1.396(4)	C(51)-C(56)	1.385(4)
C(51)-C(52)	1.410(3)	C(52)-C(53)	1.385(3)
C(53)-C(54)	1.402(4)	C(54)-C(55)	1.382(4)
C(55)-C(56)	1.406(4)		
C(1)-Pd(1)-P(1)	93.56(7)	C(1)-Pd(1)-Cl(1)	83.48(7)
P(1)-Pd(1)-Cl(1)	175.93(2)	C(1)-Pd(1)-Cl(2)	172.60(7)
P(1)-Pd(1)-Cl(2)	91.68(2)	Cl(1)-Pd(1)-Cl(2)	91.02(2)
Cl(5)-Cl(3)-C(99)	129.2(12)	Cl(5)-Cl(3)-C(99) ¹	87.2(8)
C(99)-Cl(3)-C(99) ¹	43.5(14)	Cl(7)-Cl(4)-Cl(4) ²	30.2(17)
Cl(7)-Cl(4)-C(98)	115(2)	Cl(4) ² -Cl(4)-C(98)	85.3(7)
Cl(7)-Cl(4)-C(98) ²	80.2(18)	Cl(4) ² -Cl(4)-C(98) ²	50.1(5)
C(98)-Cl(4)-C(98) ²	37.1(10)	Cl(7)-Cl(4)-Cl(5) ³	121.9(18)
Cl(4) ² -Cl(4)-Cl(5) ³	151.8(2)	C(98)-Cl(4)-Cl(5) ³	122.8(8)
C(98) ² -Cl(4)-Cl(5) ³	155.3(6)	Cl(3)-Cl(5)-C(99)	28.9(8)
Cl(3)-Cl(5)-C(99) ¹	66.5(8)	C(99)-Cl(5)-C(99) ¹	38.6(10)
Cl(3)-Cl(5)-Cl(4) ⁴	131.8(7)	C(99)-Cl(5)-Cl(4) ⁴	148.2(7)
C(99) ¹ -Cl(5)-Cl(4) ⁴	131.4(6)	Cl(6) ² -Cl(6)-C(98)	94.5(6)
Cl(6) ² -Cl(6)-C(98) ²	64.2(5)	C(98)-Cl(6)-C(98) ²	35.6(9)
Cl(4)-Cl(7)-Cl(4) ²	120(3)	Cl(4)-Cl(7)-C(98) ²	76.5(19)
Cl(4) ² -Cl(7)-C(98) ²	43.4(16)	Cl(4)-Cl(7)-C(98)	43.4(16)
Cl(4) ² -Cl(7)-C(98)	76.5(19)	C(98) ² -Cl(7)-C(98)	34.7(9)
Cl(6) ² -Cl(8)-C(98)	147(5)	Cl(6) ² -Cl(8)-C(98) ²	110(4)
C(98)-Cl(8)-C(98) ²	43.5(14)	C(98) ² -C(98)-Cl(4)	92.6(7)
C(98) ² -C(98)-Cl(8)	68.3(7)	Cl(4)-C(98)-Cl(8)	159.4(12)
C(98) ² -C(98)-Cl(6)	81.2(6)	Cl(4)-C(98)-Cl(6)	165.0(12)

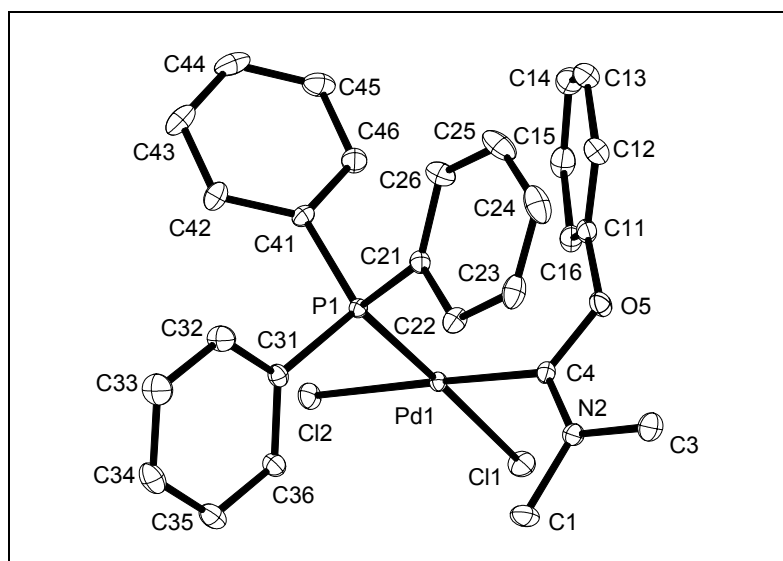
Cl(8)-C(98)-Cl(6)	14.2(5)	C(98) ² -C(98)-Cl(4) ²	50.3(5)
Cl(4)-C(98)-Cl(4) ²	44.7(7)	Cl(8)-C(98)-Cl(4) ²	118.1(10)
Cl(6)-C(98)-Cl(4) ²	131.5(9)	C(98) ² -C(98)-Cl(7)	72.6(4)
Cl(4)-C(98)-Cl(7)	21.4(5)	Cl(8)-C(98)-Cl(7)	140.9(10)
Cl(6)-C(98)-Cl(7)	153.2(9)	Cl(4) ² -C(98)-Cl(7)	23.4(3)
C(98) ² -C(98)-Cl(6) ²	63.2(5)	Cl(4)-C(98)-Cl(6) ²	155.7(11)
Cl(8)-C(98)-Cl(6) ²	7.5(5)	Cl(6)-C(98)-Cl(6) ²	21.4(4)
Cl(4) ² -C(98)-Cl(6) ²	112.2(8)	Cl(7)-C(98)-Cl(6) ²	135.5(8)
Cl(3)-C(99)-C(99) ¹	98(2)	Cl(3)-C(99)-Cl(3) ¹	136.5(14)
C(99) ¹ -C(99)-Cl(3) ¹	38.1(14)	Cl(3)-C(99)-Cl(5)	22.0(6)
C(99) ¹ -C(99)-Cl(5)	77.5(18)	Cl(3) ¹ -C(99)-Cl(5)	115.3(10)
Cl(3)-C(99)-Cl(5) ¹	161.2(14)	C(99) ¹ -C(99)-Cl(5) ¹	63.9(17)
Cl(3) ¹ -C(99)-Cl(5) ¹	26.3(3)	Cl(5)-C(99)-Cl(5) ¹	141.4(10)
C(51)-P(1)-C(41)	104.45(11)	C(51)-P(1)-C(31)	101.48(11)
C(41)-P(1)-C(31)	104.99(11)	C(51)-P(1)-Pd(1)	114.87(8)
C(41)-P(1)-Pd(1)	109.10(8)	C(31)-P(1)-Pd(1)	120.42(8)
N(11)-C(1)-C(21)	121.8(2)	N(11)-C(1)-Pd(1)	123.20(17)
C(21)-C(1)-Pd(1)	114.90(16)	C(1)-N(11)-C(12)	122.2(2)
C(1)-N(11)-C(16)	125.7(2)	C(12)-N(11)-C(16)	111.93(19)
N(11)-C(12)-C(13)	110.6(2)	C(15)-C(14)-C(13)	110.1(2)
C(14)-C(15)-C(16)	111.9(2)	N(11)-C(16)-C(15)	110.1(2)
C(26)-C(21)-C(22)	118.3(2)	C(26)-C(21)-C(1)	122.1(2)
C(22)-C(21)-C(1)	119.2(2)	C(23)-C(22)-C(21)	121.1(2)
C(22)-C(23)-C(24)	119.7(2)	C(24)-O(24)-C(27)	117.2(2)
O(24)-C(24)-C(25)	116.5(2)	O(24)-C(24)-C(23)	123.7(2)
C(25)-C(24)-C(23)	119.8(2)	C(26)-C(25)-C(24)	120.4(2)
C(25)-C(26)-C(21)	120.6(2)	C(36)-C(31)-C(32)	118.5(2)
C(36)-C(31)-P(1)	120.51(19)	C(32)-C(31)-P(1)	120.98(18)
C(33)-C(32)-C(31)	120.1(2)	C(32)-C(33)-C(34)	121.1(3)
C(35)-C(34)-C(33)	119.0(2)	C(34)-C(35)-C(36)	120.4(2)
C(35)-C(36)-C(31)	120.9(2)	C(42)-C(41)-C(46)	119.0(2)
C(42)-C(41)-P(1)	118.79(18)	C(46)-C(41)-P(1)	122.16(19)
C(41)-C(42)-C(43)	120.9(2)	C(44)-C(43)-C(42)	119.3(3)
C(45)-C(44)-C(43)	120.3(2)	C(44)-C(45)-C(46)	120.4(3)

C(41)-C(46)-C(45)	120.0(2)	C(56)-C(51)-C(52)	119.3(2)
C(56)-C(51)-P(1)	123.34(18)	C(52)-C(51)-P(1)	117.39(18)
C(53)-C(52)-C(51)	120.9(2)	C(52)-C(53)-C(54)	119.2(2)
C(55)-C(54)-C(53)	120.6(2)	C(54)-C(55)-C(56)	120.0(3)
C(51)-C(56)-C(55)	120.1(2)		

Symmetrienumformungen, die benutzt wurden um äquivalente Atome zu erzeugen:

$$^1 -x+2, -y, -z \quad ^2 -x+1, y, -z+1/2 \quad ^3 x-1/2, -y+1/2, -z \quad ^4 x+1/2, -y+1/2, -z$$

Kristallographische Daten der Verbindung 237



Kristalldaten

Summenformel	$C_{27}H_{26}Cl_2NOPPd$	
Farbe	farblos	
Molmasse	$588.76 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Monoklin	
Raumgruppe	$P2_1/n$, (no. 14)	
Gitterkonstanten	$a = 9.6858(1) \text{ \AA}$	$\alpha = 90^\circ$.
	$b = 16.8205(1) \text{ \AA}$	$\beta = 91.30^\circ$.
	$c = 15.2823(1) \text{ \AA}$	$\gamma = 90^\circ$.
Volumen	$2489.15(3) \text{ \AA}^3$	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	$1.571 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	1.045 mm^{-1}	
$F(000)$	1192 e	
Kristallgröße	$0.33 \times 0.22 \times 0.07 \text{ mm}^3$	
θ -Grenzen für Datensammlung	3.21 bis 31.51° .	
Indexbereich	$-14 \leq h \leq 14$, $-24 \leq k \leq 24$, $-22 \leq l \leq 22$	
Aufgenommene Reflexe	65806	
Unabhängige Reflexe	8279 [$R_{\text{int}} = 0.0310$]	

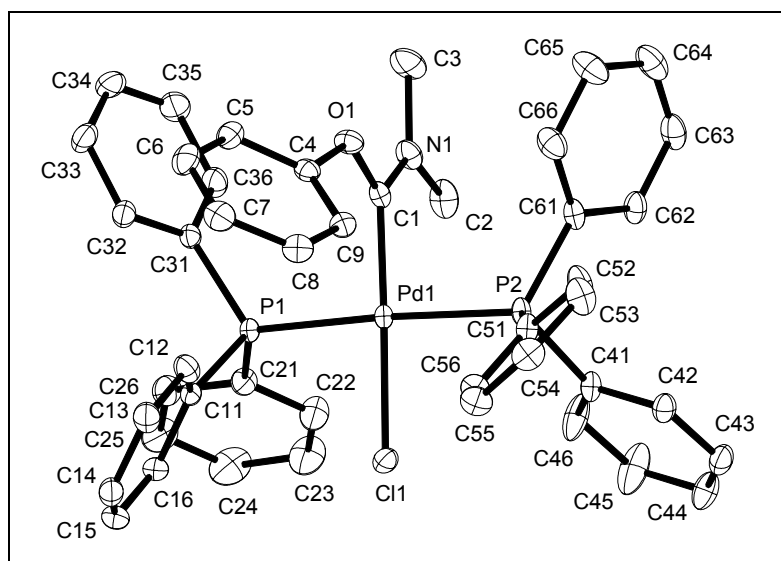
Reflexe mit $I > 2\sigma(I)$	7930	
Vollständigkeit für $\theta = 27.75^\circ$	99.6 %	
Absorptionskorrektur	Semi-empirical from equivalents	
Max. and min. Transmission	1.00 und 0.8921	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	8279 / 0 / 300	
Goodness-of-fit auf F^2	1.088	
R [$I > 2\sigma(I)$]	$R_1 = 0.0200$	$wR^2 = 0.0487$
R-Werte (sämtliche Daten)	$R_1 = 0.0216$	$wR^2 = 0.0493$
Größte Differenz Peak und Loch	0.629 und -0.684 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

Pd(1)-C(4)	1.9791(11)	Pd(1)-P(1)	2.2611(3)
Pd(1)-Cl(2)	2.3500(3)	Pd(1)-Cl(1)	2.3731(3)
P(1)-C(31)	1.8159(11)	P(1)-C(41)	1.8183(11)
P(1)-C(21)	1.8253(11)	C(1)-N(2)	1.4638(15)
N(2)-C(4)	1.3125(14)	N(2)-C(3)	1.4709(15)
C(4)-O(5)	1.3448(13)	O(5)-C(11)	1.4100(14)
C(11)-C(12)	1.3866(17)	C(11)-C(16)	1.3923(17)
C(12)-C(13)	1.3987(18)	C(13)-C(14)	1.385(2)
C(14)-C(15)	1.391(2)	C(15)-C(16)	1.3975(17)
C(21)-C(26)	1.3965(16)	C(21)-C(22)	1.4061(16)
C(22)-C(23)	1.3892(16)	C(23)-C(24)	1.389(2)
C(24)-C(25)	1.386(2)	C(25)-C(26)	1.3999(18)
C(31)-C(36)	1.3959(16)	C(31)-C(32)	1.4035(16)
C(32)-C(33)	1.3902(17)	C(33)-C(34)	1.3930(19)
C(34)-C(35)	1.3890(18)	C(35)-C(36)	1.3964(16)
C(41)-C(42)	1.3942(16)	C(41)-C(46)	1.3990(16)
C(42)-C(43)	1.3959(17)	C(43)-C(44)	1.387(2)
C(44)-C(45)	1.387(2)	C(45)-C(46)	1.3928(17)
C(4)-Pd(1)-P(1)	93.17(3)	C(4)-Pd(1)-Cl(2)	178.48(3)
P(1)-Pd(1)-Cl(2)	86.929(10)	C(4)-Pd(1)-Cl(1)	86.43(3)

P(1)-Pd(1)-Cl(1)	177.668(11)	Cl(2)-Pd(1)-Cl(1)	93.412(11)
C(31)-P(1)-C(41)	108.86(5)	C(31)-P(1)-C(21)	102.92(5)
C(41)-P(1)-C(21)	104.72(5)	C(31)-P(1)-Pd(1)	113.31(4)
C(41)-P(1)-Pd(1)	111.30(4)	C(21)-P(1)-Pd(1)	115.03(4)
C(4)-N(2)-C(1)	121.13(10)	C(4)-N(2)-C(3)	123.83(10)
C(1)-N(2)-C(3)	114.93(10)	N(2)-C(4)-O(5)	111.63(9)
N(2)-C(4)-Pd(1)	123.02(8)	O(5)-C(4)-Pd(1)	125.35(8)
C(4)-O(5)-C(11)	121.88(9)	C(12)-C(11)-C(16)	122.28(11)
C(12)-C(11)-O(5)	115.36(10)	C(16)-C(11)-O(5)	122.14(11)
C(11)-C(12)-C(13)	118.53(12)	C(14)-C(13)-C(12)	120.33(12)
C(13)-C(14)-C(15)	120.08(12)	C(14)-C(15)-C(16)	120.75(12)
C(11)-C(16)-C(15)	117.94(11)	C(26)-C(21)-C(22)	119.15(11)
C(26)-C(21)-P(1)	123.36(9)	C(22)-C(21)-P(1)	117.19(8)
C(23)-C(22)-C(21)	120.37(11)	C(22)-C(23)-C(24)	119.93(12)
C(25)-C(24)-C(23)	120.23(12)	C(24)-C(25)-C(26)	120.16(12)
C(21)-C(26)-C(25)	119.95(12)	C(36)-C(31)-C(32)	119.27(10)
C(36)-C(31)-P(1)	120.61(9)	C(32)-C(31)-P(1)	120.09(9)
C(33)-C(32)-C(31)	120.07(12)	C(32)-C(33)-C(34)	120.25(12)
C(35)-C(34)-C(33)	119.84(11)	C(34)-C(35)-C(36)	120.14(12)
C(31)-C(36)-C(35)	120.18(11)	C(42)-C(41)-C(46)	119.30(11)
C(42)-C(41)-P(1)	124.00(9)	C(46)-C(41)-P(1)	116.65(9)
C(41)-C(42)-C(43)	120.07(12)	C(44)-C(43)-C(42)	120.24(12)
C(45)-C(44)-C(43)	119.99(11)	C(44)-C(45)-C(46)	120.09(12)
C(45)-C(46)-C(41)	120.25(11)		

Kristallographische Daten der Verbindung 238



Kristalldaten

Summenformel	$\text{C}_{45}\text{H}_{41}\text{ClF}_6\text{NOP}_3\text{Pd}$	
Farbe	farblos	
Molmasse	960.55 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Monoklin	
Raumgruppe	P2₁/n, (no. 14)	
Gitterkonstanten	$a = 13.41710(10)$ Å	$\alpha = 90^\circ$.
	$b = 17.81360(10)$ Å	$\beta = 91.63^\circ$.
	$c = 19.37510(10)$ Å	$\gamma = 90^\circ$.
Volumen	4628.90(5) Å ³	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	1.378 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.620 mm^{-1}	
F(000)	1952 e	
Kristallgröße	0.22 x 0.14 x 0.04 mm ³	
θ -Grenzen für Datensammlung	2.92 bis 31.04°.	
Indexbereich	$-19 \leq h \leq 19, -25 \leq k \leq 25, -28 \leq l \leq 28$	
Aufgenommene Reflexe	127351	
Unabhängige Reflexe	14761 [$R_{\text{int}} = 0.0324$]	

Reflexe mit $I > 2\sigma(I)$	13666	
Vollständigkeit für $\theta = 31.04^\circ$	99.7 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.98 und 0.88	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	14761 / 0 / 523	
Goodness-of-fit auf F^2	1.080	
R [$I > 2\sigma(I)$]	$R_1 = 0.0296$	$wR^2 = 0.1193$
R-Werte (sämtliche Daten)	$R_1 = 0.0325$	$wR^2 = 0.1232$
Größte Differenz Peak und Loch	0.777 und -0.811 e · Å ⁻³	

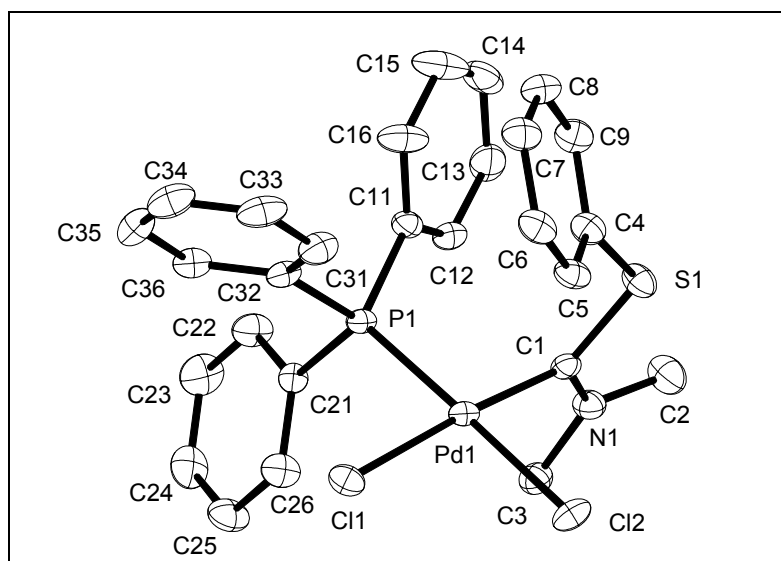
Bindungslängen [Å] und -winkel [°]

C(1)-N(1)	1.3152(17)	C(1)-O(1)	1.3463(17)
C(1)-Pd(1)	1.9907(14)	C(2)-N(1)	1.470(2)
C(3)-N(1)	1.475(2)	C(4)-C(5)	1.387(2)
C(4)-C(9)	1.3877(19)	C(4)-O(1)	1.4075(17)
C(5)-C(6)	1.396(2)	C(6)-C(7)	1.391(2)
C(7)-C(8)	1.389(2)	C(8)-C(9)	1.3969(19)
C(11)-C(16)	1.3949(18)	C(11)-C(12)	1.398(2)
C(11)-P(1)	1.8169(13)	C(12)-C(13)	1.3970(19)
C(13)-C(14)	1.392(2)	C(14)-C(15)	1.379(2)
C(15)-C(16)	1.402(2)	C(21)-C(22)	1.393(2)
C(21)-C(26)	1.4017(19)	C(21)-P(1)	1.8100(14)
C(22)-C(23)	1.400(2)	C(23)-C(24)	1.382(3)
C(24)-C(25)	1.383(3)	C(25)-C(26)	1.393(2)
C(31)-C(32)	1.3979(19)	C(31)-C(36)	1.4036(19)
C(31)-P(1)	1.8232(14)	C(32)-C(33)	1.401(2)
C(33)-C(34)	1.386(2)	C(34)-C(35)	1.387(3)
C(35)-C(36)	1.395(2)	C(41)-C(46)	1.387(2)
C(41)-C(42)	1.4011(18)	C(41)-P(2)	1.8141(14)
C(42)-C(43)	1.390(2)	C(43)-C(44)	1.384(2)
C(44)-C(45)	1.380(2)	C(45)-C(46)	1.391(2)
C(51)-C(52)	1.3967(19)	C(51)-C(56)	1.4048(19)

C(51)-P(2)	1.8253(13)	C(52)-C(53)	1.3927(19)
C(53)-C(54)	1.386(2)	C(54)-C(55)	1.387(2)
C(55)-C(56)	1.3941(19)	C(61)-C(66)	1.395(2)
C(61)-C(62)	1.4012(18)	C(61)-P(2)	1.8239(14)
C(62)-C(63)	1.397(2)	C(63)-C(64)	1.382(3)
C(64)-C(65)	1.389(2)	C(65)-C(66)	1.396(2)
F(1)-P(3)	1.5963(15)	F(2)-P(3)	1.5999(15)
F(3)-P(3)	1.5961(12)	F(4)-P(3)	1.5845(14)
F(5)-P(3)	1.5975(13)	F(6)-P(3)	1.5899(14)
P(1)-Pd(1)	2.3409(3)	P(2)-Pd(1)	2.3701(3)
Cl(1)-Pd(1)	2.3368(3)		
N(1)-C(1)-O(1)	111.08(12)	N(1)-C(1)-Pd(1)	123.63(10)
O(1)-C(1)-Pd(1)	125.28(9)	C(5)-C(4)-C(9)	121.78(13)
C(5)-C(4)-O(1)	115.66(12)	C(9)-C(4)-O(1)	122.41(12)
C(4)-C(5)-C(6)	118.61(14)	C(7)-C(6)-C(5)	120.48(14)
C(6)-C(7)-C(8)	119.98(14)	C(7)-C(8)-C(9)	120.23(13)
C(4)-C(9)-C(8)	118.84(13)	C(16)-C(11)-C(12)	119.72(13)
C(16)-C(11)-P(1)	122.44(11)	C(12)-C(11)-P(1)	117.67(10)
C(13)-C(12)-C(11)	120.44(13)	C(14)-C(13)-C(12)	119.55(15)
C(15)-C(14)-C(13)	120.16(13)	C(14)-C(15)-C(16)	120.81(14)
C(11)-C(16)-C(15)	119.31(14)	C(22)-C(21)-C(26)	119.60(13)
C(22)-C(21)-P(1)	121.34(11)	C(26)-C(21)-P(1)	119.05(11)
C(21)-C(22)-C(23)	119.80(15)	C(24)-C(23)-C(22)	119.57(17)
C(25)-C(24)-C(23)	121.52(15)	C(24)-C(25)-C(26)	119.00(16)
C(25)-C(26)-C(21)	120.42(15)	C(32)-C(31)-C(36)	119.01(13)
C(32)-C(31)-P(1)	122.55(10)	C(36)-C(31)-P(1)	118.38(11)
C(31)-C(32)-C(33)	120.12(13)	C(34)-C(33)-C(32)	120.05(15)
C(35)-C(34)-C(33)	120.46(14)	C(34)-C(35)-C(36)	119.77(14)
C(35)-C(36)-C(31)	120.56(14)	C(46)-C(41)-C(42)	119.48(13)
C(46)-C(41)-P(2)	120.24(11)	C(42)-C(41)-P(2)	120.02(10)
C(43)-C(42)-C(41)	120.10(13)	C(42)-C(43)-C(44)	119.96(13)
C(45)-C(44)-C(43)	120.02(14)	C(44)-C(45)-C(46)	120.57(15)
C(41)-C(46)-C(45)	119.87(14)	C(52)-C(51)-C(56)	118.88(12)

C(52)-C(51)-P(2)	122.36(10)	C(56)-C(51)-P(2)	118.74(10)
C(53)-C(52)-C(51)	120.68(14)	C(54)-C(53)-C(52)	119.88(14)
C(53)-C(54)-C(55)	120.28(13)	C(54)-C(55)-C(56)	120.14(14)
C(55)-C(56)-C(51)	120.12(13)	C(66)-C(61)-C(62)	118.70(13)
C(66)-C(61)-P(2)	120.60(10)	C(62)-C(61)-P(2)	120.62(11)
C(63)-C(62)-C(61)	120.32(15)	C(64)-C(63)-C(62)	120.27(14)
C(63)-C(64)-C(65)	120.04(15)	C(66)-C(65)-C(64)	119.87(17)
C(61)-C(66)-C(65)	120.78(14)	C(1)-N(1)-C(2)	121.34(13)
C(1)-N(1)-C(3)	122.34(13)	C(2)-N(1)-C(3)	116.32(12)
C(1)-O(1)-C(4)	121.75(11)	C(21)-P(1)-C(11)	106.06(6)
C(21)-P(1)-C(31)	103.48(6)	C(11)-P(1)-C(31)	106.73(6)
C(21)-P(1)-Pd(1)	114.15(5)	C(11)-P(1)-Pd(1)	108.20(4)
C(31)-P(1)-Pd(1)	117.44(4)	C(41)-P(2)-C(61)	102.91(6)
C(41)-P(2)-C(51)	105.29(6)	C(61)-P(2)-C(51)	105.26(6)
C(41)-P(2)-Pd(1)	114.98(4)	C(61)-P(2)-Pd(1)	114.75(4)
C(51)-P(2)-Pd(1)	112.55(4)	F(4)-P(3)-F(5)	88.85(9)
F(4)-P(3)-F(6)	178.63(10)	F(5)-P(3)-F(6)	90.40(9)
F(4)-P(3)-F(3)	91.17(8)	F(5)-P(3)-F(3)	179.89(10)
F(6)-P(3)-F(3)	89.58(8)	F(4)-P(3)-F(2)	90.28(10)
F(5)-P(3)-F(2)	91.26(9)	F(6)-P(3)-F(2)	90.87(10)
F(3)-P(3)-F(2)	88.85(7)	F(4)-P(3)-F(1)	89.09(9)
F(5)-P(3)-F(1)	89.88(9)	F(6)-P(3)-F(1)	89.77(10)
F(3)-P(3)-F(1)	90.01(8)	F(2)-P(3)-F(1)	178.69(10)
C(1)-Pd(1)-Cl(1)	178.74(4)	C(1)-Pd(1)-P(1)	91.75(4)
Cl(1)-Pd(1)-P(1)	86.998(12)	C(1)-Pd(1)-P(2)	91.58(4)
Cl(1)-Pd(1)-P(2)	89.676(12)	P(1)-Pd(1)-P(2)	176.416(12)

Kristallographische Daten der Verbindung 242



Kristalldaten

Summenformel	$\text{C}_{28}\text{H}_{28}\text{Cl}_4\text{NPPdS}$	
Farbe	farblos	
Molmasse	$689.74 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	triklin	
Raumgruppe	$\text{P}\bar{1}$, (no. 2)	
Gitterkonstanten	$a = 9.5008(3) \text{ \AA}$	$\alpha = 65.3260(10)^\circ$
	$b = 13.3533(5) \text{ \AA}$	$\beta = 83.911(2)^\circ$
	$c = 14.6947(6) \text{ \AA}$	$\gamma = 69.611(2)^\circ$
Volumen	$1586.23(10) \text{ \AA}^3$	
Teilchen pro Elementarzelle	2	
Berechnete Dichte	$1.444 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	1.056 mm^{-1}	
$F(000)$	696 e	
Kristallgröße	$0.06 \times 0.03 \times 0.02 \text{ mm}^3$	
θ -Grenzen für Datensammlung	2.29 bis 25.00°	
Indexbereich	$-11 \leq h \leq 11$, $-15 \leq k \leq 15$, $-17 \leq l \leq 17$	
Aufgenommene Reflexe	22092	
Unabhängige Reflexe	5575 [$R_{\text{int}} = 0.0508$]	

Reflexe mit $I > 2\sigma(I)$	4803	
Vollständigkeit für $\theta = 25.00^\circ$	99.9 %	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	5575 / 0 / 348	
Goodness-of-fit auf F^2	1.066	
R [$I > 2\sigma(I)$]	$R_1 = 0.0433$	$wR^2 = 0.1226$
R-Werte (sämtliche Daten)	$R_1 = 0.0530$	$wR^2 = 0.1285$
Größte Differenz Peak und Loch	1.607 und -0.998 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

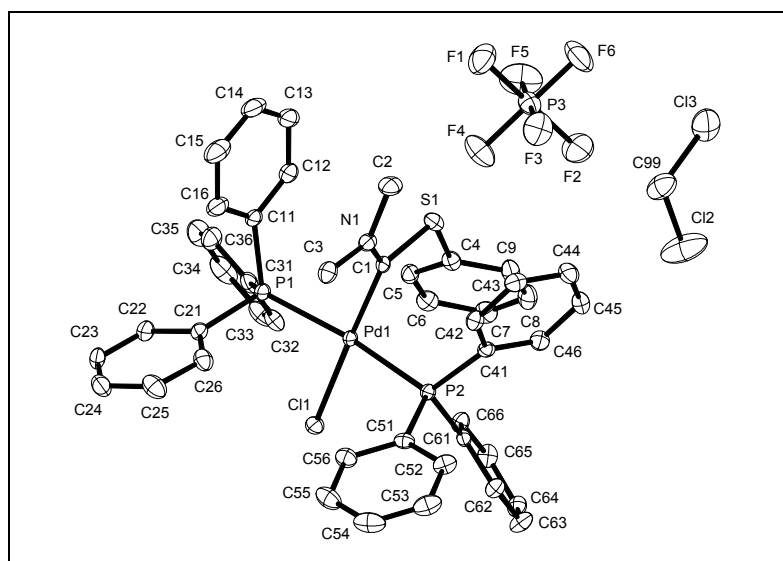
C(1)-N(1)	1.310(6)	C(1)-S(1)	1.747(5)
C(1)-Pd(1)	1.985(5)	C(2)-N(1)	1.464(7)
C(3)-N(1)	1.469(6)	C(4)-C(9)	1.389(7)
C(4)-C(5)	1.390(7)	C(4)-S(1)	1.777(5)
C(5)-C(6)	1.382(7)	C(6)-C(7)	1.393(7)
C(7)-C(8)	1.378(7)	C(8)-C(9)	1.378(7)
C(11)-C(12)	1.387(7)	C(11)-C(16)	1.385(7)
C(11)-P(1)	1.819(5)	C(12)-C(13)	1.385(7)
C(13)-C(14)	1.386(8)	C(14)-C(15)	1.361(9)
C(15)-C(16)	1.390(8)	C(21)-C(26)	1.379(7)
C(21)-C(22)	1.395(7)	C(21)-P(1)	1.820(4)
C(22)-C(23)	1.379(7)	C(23)-C(24)	1.383(8)
C(24)-C(25)	1.369(8)	C(25)-C(26)	1.394(7)
C(31)-C(36)	1.386(7)	C(31)-C(32)	1.395(7)
C(31)-P(1)	1.821(5)	C(32)-C(33)	1.378(8)
C(33)-C(34)	1.373(8)	C(34)-C(35)	1.394(8)
C(35)-C(36)	1.382(7)	C(99)-Cl(3)	1.712(8)
C(99)-Cl(4)	1.727(8)	P(1)-Pd(1)	2.2590(12)
Cl(1)-Pd(1)	2.3415(12)	Cl(2)-Pd(1)	2.3757(12)
C(100)-C(104)	1.25(2)	C(100)-C(104)*	1.25(2)
C(100)-C(105)	1.60(3)	C(100)-C(105)*	1.60(3)
C(100)-C(103)*	1.805(12)	C(100)-C(103)	1.805(12)
C(101)-C(105)	1.56(4)	C(102)-C(105)	1.51(4)

C(103)-C(104)	0.84(2)	C(103)-C(105)	1.59(3)
C(104)-C(105)	1.74(4)		
N(1)-C(1)-S(1)	113.8(3)	N(1)-C(1)-Pd(1)	121.4(3)
S(1)-C(1)-Pd(1)	124.6(3)	C(9)-C(4)-C(5)	120.5(4)
C(9)-C(4)-S(1)	116.0(4)	C(5)-C(4)-S(1)	123.1(4)
C(6)-C(5)-C(4)	119.3(5)	C(5)-C(6)-C(7)	120.1(5)
C(8)-C(7)-C(6)	120.1(5)	C(9)-C(8)-C(7)	120.2(5)
C(8)-C(9)-C(4)	119.7(5)	C(12)-C(11)-C(16)	119.1(5)
C(12)-C(11)-P(1)	120.2(4)	C(16)-C(11)-P(1)	120.7(4)
C(11)-C(12)-C(13)	120.3(5)	C(14)-C(13)-C(12)	119.7(6)
C(15)-C(14)-C(13)	120.6(5)	C(14)-C(15)-C(16)	119.9(5)
C(11)-C(16)-C(15)	120.5(6)	C(26)-C(21)-C(22)	118.8(4)
C(26)-C(21)-P(1)	120.0(3)	C(22)-C(21)-P(1)	121.2(4)
C(23)-C(22)-C(21)	120.3(5)	C(22)-C(23)-C(24)	120.3(5)
C(25)-C(24)-C(23)	120.0(5)	C(24)-C(25)-C(26)	119.9(5)
C(21)-C(26)-C(25)	120.7(5)	C(36)-C(31)-C(32)	119.5(5)
C(36)-C(31)-P(1)	122.1(4)	C(32)-C(31)-P(1)	118.4(4)
C(33)-C(32)-C(31)	120.2(5)	C(34)-C(33)-C(32)	120.3(5)
C(33)-C(34)-C(35)	119.9(5)	C(36)-C(35)-C(34)	120.0(5)
C(35)-C(36)-C(31)	120.0(5)	Cl(3)-C(99)-Cl(4)	113.9(4)
C(1)-N(1)-C(2)	122.9(4)	C(1)-N(1)-C(3)	121.6(4)
C(2)-N(1)-C(3)	115.5(4)	C(21)-P(1)-C(11)	103.6(2)
C(21)-P(1)-C(31)	107.3(2)	C(11)-P(1)-C(31)	105.2(2)
C(21)-P(1)-Pd(1)	112.76(15)	C(11)-P(1)-Pd(1)	115.63(16)
C(31)-P(1)-Pd(1)	111.70(15)	C(1)-S(1)-C(4)	106.5(2)
C(1)-Pd(1)-P(1)	93.78(13)	C(1)-Pd(1)-Cl(1)	175.70(13)
P(1)-Pd(1)-Cl(1)	88.70(4)	C(1)-Pd(1)-Cl(2)	85.89(13)
P(1)-Pd(1)-Cl(2)	177.69(4)	Cl(1)-Pd(1)-Cl(2)	91.49(4)
C(104)-C(100)-C(104)*	179.997(6)	C(104)-C(100)-C(105)	74.0(15)
C(104)*-C(100)-C(105)	106.0(15)	C(104)-C(100)-C(105)*	106.0(15)
C(104)*-C(100)-C(105)*	74.0(15)	C(105)-C(100)-C(105)*	180(2)
C(104)-C(100)-C(103)*	156.0(11)	C(104)*-C(100)-C(103)*	24.0(11)
C(105)-C(100)-C(103)*	124.5(12)	C(105)*-C(100)-C(103)*	55.5(12)

C(104)-C(100)-C(103)	24.0(11)	C(104)*-C(100)-C(103)	156.0(11)
C(105)-C(100)-C(103)	55.5(12)	C(105)*-C(100)-C(103)	124.5(12)
C(103)*-C(100)-C(103)	180.0(4)	C(104)-C(103)-C(105)	85(2)
C(104)-C(103)-C(100)	37.6(17)	C(105)-C(103)-C(100)	55.6(12)
C(103)-C(104)-C(100)	118(2)	C(103)-C(104)-C(105)	66(2)
C(100)-C(104)-C(105)	62.2(14)	C(102)-C(105)-C(101)	12.9(9)
C(102)-C(105)-C(100)	103(2)	C(101)-C(105)-C(100)	115(2)
C(102)-C(105)-C(103)	125(2)	C(101)-C(105)-C(103)	124(2)
C(100)-C(105)-C(103)	68.9(14)	C(102)-C(105)-C(104)	133(2)
C(101)-C(105)-C(104)	139(2)	C(100)-C(105)-C(104)	43.8(11)
C(103)-C(105)-C(104)	28.7(9)		

Symmetrienumformung, die benutzt wurde um äquivalente Atome zu erzeugen: * -x+3,-y,-z+2

Kristallographische Daten der Verbindung 243



Kristalldaten

Summenformel	$\text{C}_{46}\text{H}_{43}\text{Cl}_3\text{F}_6\text{NP}_3\text{PdS}$	
Farbe	farblos	
Molmasse	$1061.53 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Monoklin	
Raumgruppe	P 2₁/c, (no. 14)	
Gitterkonstanten	$a = 19.2454(4) \text{ \AA}$	$\alpha = 90^\circ$.
	$b = 13.9966(3) \text{ \AA}$	$\beta = 97.2090(10)^\circ$.
	$c = 17.0816(2) \text{ \AA}$	$\gamma = 90^\circ$.
Volumen	$4564.90(15) \text{ \AA}^3$	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	$1.545 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.792 mm^{-1}	
F(000)	2152 e	
Kristallgröße	$0.06 \times 0.04 \times 0.04 \text{ mm}^3$	
θ -Grenzen für Datensammlung	2.91 bis 30.98° .	
Indexbereich	$-27 \leq h \leq 27, -20 \leq k \leq 20, -24 \leq l \leq 24$	
Aufgenommene Reflexe	77600	
Unabhängige Reflexe	14509 [$R_{\text{int}} = 0.0940$]	

Reflexe mit $I > 2\sigma(I)$	10033	
Vollständigkeit für $\theta = 30.98^\circ$	99.8 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.98 und 0.96	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	14509 / 0 / 552	
Goodness-of-fit auf F^2	1.000	
R [$I > 2\sigma(I)$]	$R_1 = 0.0491$	$wR^2 = 0.0915$
R-Werte (sämtliche Daten)	$R_1 = 0.0885$	$wR^2 = 0.1053$
Größte Differenz Peak und Loch	1.338 und -1.368 e · Å ⁻³	

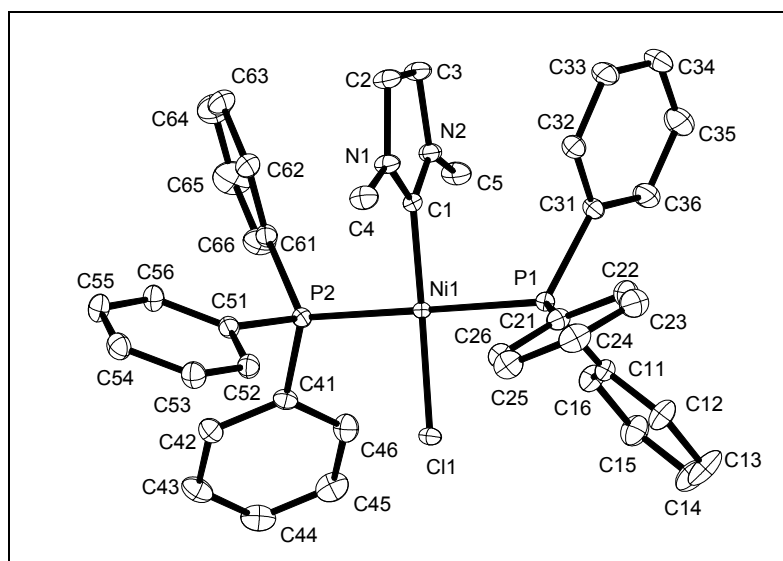
Bindungslängen [Å] und -winkel [°]

C(1)-N(1)	1.313(4)	C(1)-S(1)	1.741(3)
C(1)-Pd(1)	1.998(3)	C(2)-N(1)	1.477(4)
C(3)-N(1)	1.463(4)	C(4)-C(9)	1.393(4)
C(4)-C(5)	1.395(4)	C(4)-S(1)	1.775(3)
C(5)-C(6)	1.382(4)	C(6)-C(7)	1.380(4)
C(7)-C(8)	1.392(5)	C(8)-C(9)	1.387(4)
C(11)-C(16)	1.386(4)	C(11)-C(12)	1.396(4)
C(11)-P(1)	1.828(3)	C(12)-C(13)	1.391(5)
C(13)-C(14)	1.383(6)	C(14)-C(15)	1.382(6)
C(15)-C(16)	1.397(4)	C(21)-C(26)	1.387(4)
C(21)-C(22)	1.402(4)	C(21)-P(1)	1.819(3)
C(22)-C(23)	1.384(4)	C(23)-C(24)	1.376(5)
C(24)-C(25)	1.390(5)	C(25)-C(26)	1.392(4)
C(31)-C(32)	1.393(4)	C(31)-C(36)	1.399(4)
C(31)-P(1)	1.827(3)	C(32)-C(33)	1.395(4)
C(33)-C(34)	1.394(5)	C(34)-C(35)	1.364(5)
C(35)-C(36)	1.381(5)	C(41)-C(46)	1.385(4)
C(41)-C(42)	1.404(4)	C(41)-P(2)	1.821(3)
C(42)-C(43)	1.383(4)	C(43)-C(44)	1.394(4)
C(44)-C(45)	1.377(4)	C(45)-C(46)	1.390(4)
C(51)-C(56)	1.390(4)	C(51)-C(52)	1.396(4)

C(51)-P(2)	1.824(3)	C(52)-C(53)	1.390(4)
C(53)-C(54)	1.383(5)	C(54)-C(55)	1.384(5)
C(55)-C(56)	1.393(4)	C(61)-C(66)	1.391(4)
C(61)-C(62)	1.392(4)	C(61)-P(2)	1.823(3)
C(62)-C(63)	1.393(4)	C(63)-C(64)	1.385(4)
C(64)-C(65)	1.386(4)	C(65)-C(66)	1.392(4)
C(99)-Cl(2)	1.747(4)	C(99)-Cl(3)	1.761(4)
F(1)-P(3)	1.583(2)	F(2)-P(3)	1.594(2)
F(3)-P(3)	1.604(2)	F(4)-P(3)	1.593(2)
F(5)-P(3)	1.580(3)	F(6)-P(3)	1.580(2)
P(1)-Pd(1)	2.3714(7)	P(2)-Pd(1)	2.3451(7)
Cl(1)-Pd(1)	2.3436(7)		
N(1)-C(1)-S(1)	113.5(2)	N(1)-C(1)-Pd(1)	123.7(2)
S(1)-C(1)-Pd(1)	122.78(16)	C(9)-C(4)-C(5)	120.4(3)
C(9)-C(4)-S(1)	116.3(2)	C(5)-C(4)-S(1)	122.8(2)
C(6)-C(5)-C(4)	119.7(3)	C(7)-C(6)-C(5)	120.3(3)
C(6)-C(7)-C(8)	119.9(3)	C(9)-C(8)-C(7)	120.5(3)
C(8)-C(9)-C(4)	119.0(3)	C(16)-C(11)-C(12)	119.2(3)
C(16)-C(11)-P(1)	121.6(2)	C(12)-C(11)-P(1)	118.9(2)
C(13)-C(12)-C(11)	120.4(3)	C(14)-C(13)-C(12)	119.9(3)
C(15)-C(14)-C(13)	120.2(3)	C(14)-C(15)-C(16)	120.0(4)
C(11)-C(16)-C(15)	120.3(3)	C(26)-C(21)-C(22)	119.2(3)
C(26)-C(21)-P(1)	119.2(2)	C(22)-C(21)-P(1)	121.5(2)
C(23)-C(22)-C(21)	119.7(3)	C(24)-C(23)-C(22)	121.0(3)
C(23)-C(24)-C(25)	119.8(3)	C(24)-C(25)-C(26)	119.7(3)
C(21)-C(26)-C(25)	120.6(3)	C(32)-C(31)-C(36)	119.2(3)
C(32)-C(31)-P(1)	120.9(2)	C(36)-C(31)-P(1)	119.8(2)
C(31)-C(32)-C(33)	119.8(3)	C(34)-C(33)-C(32)	119.7(3)
C(35)-C(34)-C(33)	120.4(3)	C(34)-C(35)-C(36)	120.5(3)
C(35)-C(36)-C(31)	120.3(3)	C(46)-C(41)-C(42)	118.9(3)
C(46)-C(41)-P(2)	122.1(2)	C(42)-C(41)-P(2)	118.8(2)
C(43)-C(42)-C(41)	120.6(3)	C(42)-C(43)-C(44)	119.6(3)
C(45)-C(44)-C(43)	120.1(3)	C(44)-C(45)-C(46)	120.4(3)

C(41)-C(46)-C(45)	120.4(3)	C(56)-C(51)-C(52)	119.0(3)
C(56)-C(51)-P(2)	120.4(2)	C(52)-C(51)-P(2)	120.5(2)
C(53)-C(52)-C(51)	120.3(3)	C(54)-C(53)-C(52)	120.2(3)
C(53)-C(54)-C(55)	120.0(3)	C(54)-C(55)-C(56)	120.1(3)
C(51)-C(56)-C(55)	120.4(3)	C(66)-C(61)-C(62)	119.6(3)
C(66)-C(61)-P(2)	118.5(2)	C(62)-C(61)-P(2)	121.9(2)
C(61)-C(62)-C(63)	119.6(3)	C(64)-C(63)-C(62)	120.4(3)
C(63)-C(64)-C(65)	120.2(3)	C(64)-C(65)-C(66)	119.5(3)
C(61)-C(66)-C(65)	120.6(3)	Cl(2)-C(99)-Cl(3)	112.4(2)
C(1)-N(1)-C(3)	122.7(2)	C(1)-N(1)-C(2)	122.7(2)
C(3)-N(1)-C(2)	114.6(2)	C(21)-P(1)-C(31)	105.59(13)
C(21)-P(1)-C(11)	104.36(13)	C(31)-P(1)-C(11)	103.54(14)
C(21)-P(1)-Pd(1)	110.38(10)	C(31)-P(1)-Pd(1)	118.03(10)
C(11)-P(1)-Pd(1)	113.73(9)	C(41)-P(2)-C(61)	105.49(12)
C(41)-P(2)-C(51)	103.58(13)	C(61)-P(2)-C(51)	106.08(12)
C(41)-P(2)-Pd(1)	116.15(9)	C(61)-P(2)-Pd(1)	112.39(9)
C(51)-P(2)-Pd(1)	112.24(10)	F(5)-P(3)-F(6)	90.51(15)
F(5)-P(3)-F(1)	91.03(15)	F(6)-P(3)-F(1)	89.78(13)
F(5)-P(3)-F(4)	90.26(14)	F(6)-P(3)-F(4)	179.23(16)
F(1)-P(3)-F(4)	90.15(13)	F(5)-P(3)-F(2)	90.11(15)
F(6)-P(3)-F(2)	89.85(14)	F(1)-P(3)-F(2)	178.80(16)
F(4)-P(3)-F(2)	90.21(14)	F(5)-P(3)-F(3)	178.96(14)
F(6)-P(3)-F(3)	90.46(14)	F(1)-P(3)-F(3)	89.36(13)
F(4)-P(3)-F(3)	88.77(13)	F(2)-P(3)-F(3)	89.50(14)
C(1)-S(1)-C(4)	106.34(13)	C(1)-Pd(1)-Cl(1)	177.78(8)
C(1)-Pd(1)-P(2)	90.83(8)	Cl(1)-Pd(1)-P(2)	88.56(2)
C(1)-Pd(1)-P(1)	92.42(8)	Cl(1)-Pd(1)-P(1)	88.50(2)
P(2)-Pd(1)-P(1)	171.21(3)		

Kristallographische Daten der Verbindung 258



Kristalldaten

Summenformel	$\text{C}_{42}\text{H}_{42}\text{Cl}_3\text{F}_6\text{N}_2\text{NiP}_3$	
Farbe	gelb	
Molmasse	$946.75 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Triklin	
Raumgruppe	$\text{P}\bar{1}$, (no. 2)	
Gitterkonstanten	$a = 12.58330(10) \text{ \AA}$	$\alpha = 108.14^\circ$
	$b = 18.08800(10) \text{ \AA}$	$\beta = 96.15^\circ$
	$c = 20.55670(10) \text{ \AA}$	$\gamma = 100.60^\circ$
Volumen	$4302.09(5) \text{ \AA}^3$	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	$1.462 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.808 mm^{-1}	
$F(000)$	1944 e	
Kristallgröße	$0.20 \times 0.19 \times 0.05 \text{ mm}^3$	
θ -Grenzen für Datensammlung	4.10 bis 33.11°	
Indexbereich	$-19 \leq h \leq 19, -27 \leq k \leq 27, -31 \leq l \leq 31$	
Aufgenommene Reflexe	135076	
Unabhängige Reflexe	32612 [$R_{\text{int}} = 0.0529$]	

Reflexe mit $I > 2\sigma(I)$	26339	
Vollständigkeit für $\theta = 27.50^\circ$	99.6 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.96 und 0.86	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrat auf F^2	
Daten/ Einschränkungen/ Parameter	32612 / 0 / 1031	
Goodness-of-fit auf F^2	1.063	
R [$I > 2\sigma(I)$]	$R_1 = 0.0488$	$wR^2 = 0.1282$
R-Werte (sämtliche Daten)	$R_1 = 0.0648$	$wR^2 = 0.1355$
Größte Peak und Loch	0.960 und -0.898 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

Cl(1A)-Ni(2)	2.1893(5)	P(1A)-C(21A)	1.818(2)
P(1A)-C(11A)	1.826(2)	P(1A)-C(31A)	1.8294(19)
P(1A)-Ni(2)	2.2322(5)	N(1A)-C(1A)	1.332(2)
N(1A)-C(4A)	1.450(3)	N(1A)-C(2A)	1.473(3)
C(1A)-N(2A)	1.327(2)	C(1A)-Ni(2)	1.8660(18)
Ni(1)-C(1)	1.8650(18)	Ni(1)-Cl(1)	2.1863(5)
Ni(1)-P(1)	2.2333(6)	Ni(1)-P(2)	2.2417(6)
P(1)-C(11)	1.819(2)	P(1)-C(21)	1.826(2)
P(1)-C(31)	1.826(2)	N(1)-C(1)	1.341(2)
N(1)-C(4)	1.449(3)	N(1)-C(2)	1.477(3)
C(1)-N(2)	1.327(2)	F(1)-P(3)	1.6020(19)
F(1A)-P(4)	1.5978(18)	Ni(2)-P(2A)	2.2401(5)
P(2A)-C(41A)	1.822(2)	P(2A)-C(51A)	1.823(2)
P(2A)-C(61A)	1.830(2)	N(2A)-C(5A)	1.448(3)
N(2A)-C(3A)	1.469(2)	C(2A)-C(3A)	1.535(3)
P(2)-C(41)	1.826(2)	P(2)-C(51)	1.827(2)
P(2)-C(61)	1.834(2)	N(2)-C(5)	1.446(3)
N(2)-C(3)	1.472(3)	C(2)-C(3)	1.538(3)
F(2)-P(3)	1.5988(19)	Cl(2)-C(67)	1.774(3)
F(2A)-P(4)	1.6065(17)	Cl(3)-C(67)	1.763(3)
P(3)-F(5)	1.593(2)	P(3)-F(6)	1.5974(16)

P(3)-F(3)	1.601(2)	P(3)-F(4)	1.6057(19)
F(3A)-P(4)	1.5913(19)	P(4)-F(6A)	1.587(2)
P(4)-F(4A)	1.5974(18)	P(4)-F(5A)	1.6049(16)
Cl(3A)-C(67A)	1.753(3)	Cl(2A)-C(67A)	1.785(3)
C(11A)-C(16A)	1.398(3)	C(11A)-C(12A)	1.402(3)
C(11)-C(12)	1.392(3)	C(11)-C(16)	1.398(3)
C(12A)-C(13A)	1.395(3)	C(12)-C(13)	1.398(3)
C(13A)-C(14A)	1.388(4)	C(13)-C(14)	1.386(4)
C(14A)-C(15A)	1.387(4)	C(14)-C(15)	1.391(4)
C(15A)-C(16A)	1.394(3)	C(15)-C(16)	1.389(3)
C(21A)-C(26A)	1.399(3)	C(21A)-C(22A)	1.403(3)
C(21)-C(26)	1.396(3)	C(21)-C(22)	1.407(3)
C(22A)-C(23A)	1.385(3)	C(22A)-H(22A)	0.9500
C(22)-C(23)	1.399(3)	C(22)-H(22)	0.9500
C(23A)-C(24A)	1.385(3)	C(23A)-H(23A)	0.9500
C(23)-C(24)	1.392(4)	C(23)-H(23)	0.9500
C(24A)-C(25A)	1.388(3)	C(24A)-H(24A)	0.9500
C(24)-C(25)	1.386(4)	C(25A)-C(26A)	1.392(3)
C(25)-C(26)	1.389(3)	C(31A)-C(36A)	1.394(3)
C(31A)-C(32A)	1.401(3)	C(31)-C(36)	1.391(3)
C(31)-C(32)	1.400(3)	C(32A)-C(33A)	1.399(3)
C(32)-C(33)	1.385(3)	C(33A)-C(34A)	1.387(4)
C(33)-C(34)	1.390(4)	C(34A)-C(35A)	1.382(4)
C(34)-C(35)	1.384(4)	C(35A)-C(36A)	1.398(3)
C(35)-C(36)	1.402(3)	C(41A)-C(42A)	1.402(3)
C(41A)-C(46A)	1.404(3)	C(41)-C(46)	1.397(3)
C(41)-C(42)	1.399(3)	C(42A)-C(43A)	1.395(3)
C(42)-C(43)	1.394(3)	C(43A)-C(44A)	1.387(3)
C(43)-C(44)	1.388(4)	C(44A)-C(45A)	1.386(4)
C(44)-C(45)	1.385(4)	C(45A)-C(46A)	1.395(3)
C(45)-C(46)	1.393(3)	C(51A)-C(52A)	1.397(3)
C(51A)-C(56A)	1.397(3)	C(51)-C(56)	1.399(3)
C(51)-C(52)	1.403(3)	C(52A)-C(53A)	1.399(3)
C(52)-C(53)	1.392(3)	C(53A)-C(54A)	1.387(4)

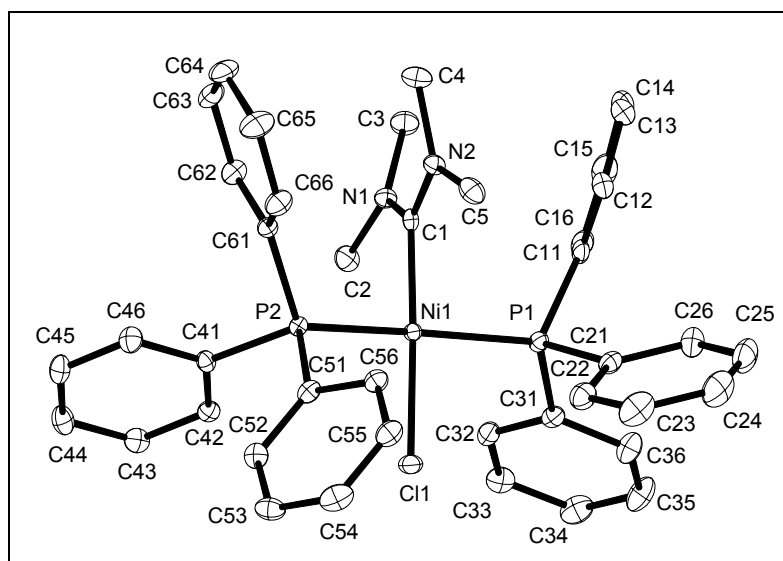
C(53)-C(54)	1.391(3)	C(54A)-C(55A)	1.382(4)
C(54)-C(55)	1.389(3)	C(55A)-C(56A)	1.392(3)
C(55)-C(56)	1.389(3)	C(61A)-C(62A)	1.397(3)
C(61A)-C(66A)	1.398(3)	C(61)-C(62)	1.397(3)
C(61)-C(66)	1.400(3)	C(62A)-C(63A)	1.393(3)
C(62)-C(63)	1.398(3)	C(63A)-C(64A)	1.390(4)
C(63)-C(64)	1.388(4)	C(64A)-C(65A)	1.385(4)
C(64)-C(65)	1.384(4)	C(65A)-C(66A)	1.395(3)
C(65)-C(66)	1.398(3)		
C(21A)-P(1A)-C(11A)	106.11(9)	C(21A)-P(1A)-C(31A)	104.95(9)
C(11A)-P(1A)-C(31A)	103.09(9)	C(21A)-P(1A)-Ni(2)	111.04(6)
C(11A)-P(1A)-Ni(2)	114.99(6)	C(31A)-P(1A)-Ni(2)	115.67(7)
C(1A)-N(1A)-C(4A)	126.86(16)	C(1A)-N(1A)-C(2A)	112.43(16)
C(4A)-N(1A)-C(2A)	120.71(16)	N(2A)-C(1A)-N(1A)	109.95(16)
N(2A)-C(1A)-Ni(2)	126.12(14)	N(1A)-C(1A)-Ni(2)	123.93(14)
C(1)-Ni(1)-Cl(1)	172.02(6)	C(1)-Ni(1)-P(1)	90.07(6)
Cl(1)-Ni(1)-P(1)	88.55(2)	C(1)-Ni(1)-P(2)	89.73(6)
Cl(1)-Ni(1)-P(2)	92.33(2)	P(1)-Ni(1)-P(2)	175.05(2)
C(11)-P(1)-C(21)	108.39(9)	C(11)-P(1)-C(31)	104.23(9)
C(21)-P(1)-C(31)	102.75(10)	C(11)-P(1)-Ni(1)	110.05(7)
C(21)-P(1)-Ni(1)	113.74(7)	C(31)-P(1)-Ni(1)	116.92(7)
C(1)-N(1)-C(4)	126.52(17)	C(1)-N(1)-C(2)	112.01(16)
C(4)-N(1)-C(2)	121.45(16)	N(2)-C(1)-N(1)	109.90(16)
N(2)-C(1)-Ni(1)	126.42(14)	N(1)-C(1)-Ni(1)	123.68(14)
C(1A)-Ni(2)-Cl(1A)	174.26(6)	C(1A)-Ni(2)-P(1A)	87.25(6)
Cl(1A)-Ni(2)-P(1A)	91.899(19)	C(1A)-Ni(2)-P(2A)	89.03(6)
Cl(1A)-Ni(2)-P(2A)	91.832(19)	P(1A)-Ni(2)-P(2A)	176.27(2)
C(41A)-P(2A)-C(51A)	104.85(9)	C(41A)-P(2A)-C(61A)	105.33(10)
C(51A)-P(2A)-C(61A)	103.26(10)	C(41A)-P(2A)-Ni(2)	112.01(7)
C(51A)-P(2A)-Ni(2)	114.30(7)	C(61A)-P(2A)-Ni(2)	115.98(7)
C(1A)-N(2A)-C(5A)	125.75(16)	C(1A)-N(2A)-C(3A)	112.40(16)
C(5A)-N(2A)-C(3A)	121.85(16)	N(1A)-C(2A)-C(3A)	102.33(15)
C(41)-P(2)-C(51)	105.61(9)	C(41)-P(2)-C(61)	102.03(10)

C(51)-P(2)-C(61)	103.59(9)	C(41)-P(2)-Ni(1)	115.02(7)
C(51)-P(2)-Ni(1)	111.21(7)	C(61)-P(2)-Ni(1)	117.98(7)
C(1)-N(2)-C(5)	125.44(17)	C(1)-N(2)-C(3)	112.80(16)
C(5)-N(2)-C(3)	121.73(16)	N(1)-C(2)-C(3)	102.74(16)
N(2A)-C(3A)-C(2A)	102.88(15)	F(5)-P(3)-F(6)	89.76(11)
F(5)-P(3)-F(2)	90.58(13)	F(6)-P(3)-F(2)	178.78(12)
F(5)-P(3)-F(3)	90.55(12)	F(6)-P(3)-F(3)	90.26(10)
F(2)-P(3)-F(3)	90.91(12)	F(5)-P(3)-F(1)	178.92(12)
F(6)-P(3)-F(1)	89.40(10)	F(2)-P(3)-F(1)	90.25(13)
F(3)-P(3)-F(1)	90.13(12)	F(5)-P(3)-F(4)	89.86(11)
F(6)-P(3)-F(4)	89.67(10)	F(2)-P(3)-F(4)	89.16(12)
F(3)-P(3)-F(4)	179.58(12)	F(1)-P(3)-F(4)	89.46(11)
N(2)-C(3)-C(2)	102.55(16)	F(6A)-P(4)-F(3A)	179.42(16)
F(6A)-P(4)-F(4A)	90.53(14)	F(3A)-P(4)-F(4A)	88.92(12)
F(6A)-P(4)-F(1A)	90.15(14)	F(3A)-P(4)-F(1A)	90.39(12)
F(4A)-P(4)-F(1A)	179.30(14)	F(6A)-P(4)-F(5A)	89.77(10)
F(3A)-P(4)-F(5A)	90.41(11)	F(4A)-P(4)-F(5A)	88.99(10)
F(1A)-P(4)-F(5A)	90.88(9)	F(6A)-P(4)-F(2A)	90.21(11)
F(3A)-P(4)-F(2A)	89.61(12)	F(4A)-P(4)-F(2A)	90.83(10)
F(1A)-P(4)-F(2A)	89.30(10)	F(5A)-P(4)-F(2A)	179.82(13)
C(16A)-C(11A)-C(12A)	119.62(19)	C(16A)-C(11A)-P(1A)	119.51(15)
C(12A)-C(11A)-P(1A)	120.85(15)	C(12)-C(11)-C(16)	119.75(19)
C(12)-C(11)-P(1)	122.43(17)	C(16)-C(11)-P(1)	117.82(15)
C(13A)-C(12A)-C(11A)	119.7(2)	C(11)-C(12)-C(13)	119.3(2)
C(14A)-C(13A)-C(12A)	120.3(2)	C(14)-C(13)-C(12)	120.9(2)
C(15A)-C(14A)-C(13A)	120.0(2)	C(13)-C(14)-C(15)	119.8(2)
C(14A)-C(15A)-C(16A)	120.3(2)	C(16)-C(15)-C(14)	119.7(2)
C(15A)-C(16A)-C(11A)	119.9(2)	C(15)-C(16)-C(11)	120.5(2)
C(26A)-C(21A)-C(22A)	118.83(18)	C(26A)-C(21A)-P(1A)	119.66(15)
C(22A)-C(21A)-P(1A)	121.50(15)	C(26)-C(21)-C(22)	119.33(19)
C(26)-C(21)-P(1)	120.61(16)	C(22)-C(21)-P(1)	120.01(16)
C(23A)-C(22A)-C(21A)	120.29(19)	C(23)-C(22)-C(21)	119.8(2)
C(24A)-C(23A)-C(22A)	120.3(2)	C(24)-C(23)-C(22)	120.1(2)
C(23A)-C(24A)-C(25A)	120.2(2)	C(25)-C(24)-C(23)	120.1(2)

C(24A)-C(25A)-C(26A)	119.8(2)	C(24)-C(25)-C(26)	120.4(2)
C(25A)-C(26A)-C(21A)	120.55(19)	C(25)-C(26)-C(21)	120.4(2)
C(36A)-C(31A)-C(32A)	119.15(19)	C(36A)-C(31A)-P(1A)	118.54(15)
C(32A)-C(31A)-P(1A)	122.14(16)	C(36)-C(31)-C(32)	118.95(19)
C(36)-C(31)-P(1)	122.61(16)	C(32)-C(31)-P(1)	118.39(16)
C(33A)-C(32A)-C(31A)	119.7(2)	C(33)-C(32)-C(31)	120.6(2)
C(34A)-C(33A)-C(32A)	120.5(2)	C(32)-C(33)-C(34)	120.4(2)
C(35A)-C(34A)-C(33A)	120.1(2)	C(35)-C(34)-C(33)	119.5(2)
C(34A)-C(35A)-C(36A)	119.8(2)	C(34)-C(35)-C(36)	120.5(2)
C(31A)-C(36A)-C(35A)	120.7(2)	C(31)-C(36)-C(35)	120.1(2)
C(42A)-C(41A)-C(46A)	119.08(19)	C(42A)-C(41A)-P(2A)	118.76(15)
C(46A)-C(41A)-P(2A)	122.00(17)	C(46)-C(41)-C(42)	119.23(19)
C(46)-C(41)-P(2)	120.28(16)	C(42)-C(41)-P(2)	120.33(16)
C(43A)-C(42A)-C(41A)	120.3(2)	C(43)-C(42)-C(41)	120.3(2)
C(44A)-C(43A)-C(42A)	120.0(2)	C(44)-C(43)-C(42)	119.9(2)
C(45A)-C(44A)-C(43A)	120.4(2)	C(45)-C(44)-C(43)	120.1(2)
C(44A)-C(45A)-C(46A)	120.1(2)	C(44)-C(45)-C(46)	120.3(2)
C(45A)-C(46A)-C(41A)	120.1(2)	C(45)-C(46)-C(41)	120.1(2)
C(52A)-C(51A)-C(56A)	119.6(2)	C(52A)-C(51A)-P(2A)	119.39(16)
C(56A)-C(51A)-P(2A)	121.00(17)	C(56)-C(51)-C(52)	119.07(19)
C(56)-C(51)-P(2)	121.81(15)	C(52)-C(51)-P(2)	119.11(15)
C(51A)-C(52A)-C(53A)	119.9(2)	C(53)-C(52)-C(51)	120.20(19)
C(54A)-C(53A)-C(52A)	120.1(2)	C(54)-C(53)-C(52)	120.2(2)
C(55A)-C(54A)-C(53A)	120.0(2)	C(55)-C(54)-C(53)	119.9(2)
C(54A)-C(55A)-C(56A)	120.6(2)	C(54)-C(55)-C(56)	120.2(2)
C(55A)-C(56A)-C(51A)	119.8(2)	C(55)-C(56)-C(51)	120.4(2)
C(62A)-C(61A)-C(66A)	119.2(2)	C(62A)-C(61A)-P(2A)	120.56(17)
C(66A)-C(61A)-P(2A)	119.85(17)	C(62)-C(61)-C(66)	119.1(2)
C(62)-C(61)-P(2)	119.87(17)	C(66)-C(61)-P(2)	121.03(17)
C(63A)-C(62A)-C(61A)	120.7(2)	C(61)-C(62)-C(63)	120.4(2)
C(64A)-C(63A)-C(62A)	119.7(3)	C(64)-C(63)-C(62)	120.1(2)
C(65A)-C(64A)-C(63A)	120.0(2)	C(65)-C(64)-C(63)	119.8(2)
C(64A)-C(65A)-C(66A)	120.6(3)	C(64)-C(65)-C(66)	120.5(3)
C(65A)-C(66A)-C(61A)	119.7(2)	C(65)-C(66)-C(61)	120.0(2)

Cl(3)-C(67)-Cl(2)	110.57(14)	Cl(3A)-C(67A)-Cl(2A)	111.90(13)
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Kristallographische Daten der Verbindung 259



Kristalldaten

Summenformel	$\text{C}_{42}\text{H}_{44}\text{Cl}_3\text{F}_6\text{N}_2\text{NiP}_3$	
Farbe	gelb-orange	
Molmasse	948.76 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Triklin	
Raumgruppe	$\text{P}\bar{1}$, (no. 2)	
Gitterkonstanten	$a = 12.18140(10)$ Å	$\alpha = 71.21^\circ$
	$b = 17.50240(10)$ Å	$\beta = 82.00^\circ$
	$c = 21.3701(2)$ Å	$\gamma = 89.91^\circ$
Volumen	4266.78(6) Å ³	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	1.477 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.815 mm^{-1}	
F(000)	1952 e	
Kristallgröße	0.12 x 0.09 x 0.04 mm ³	
θ -Grenzen für Datensammlung	2.92 bis 27.50°	
Indexbereich	$-15 \leq h \leq 15$, $-22 \leq k \leq 22$, $-27 \leq l \leq 27$	
Aufgenommene Reflexe	95991	
Unabhängige Reflexe	19569 [$R_{\text{int}} = 0.0727$]	

Reflexe mit $I > 2\sigma(I)$	15204	
Vollständigkeit für $\theta = 27.50^\circ$	99.9 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.98 und 0.91	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	19569 / 0 / 1037	
Goodness-of-fit auf F^2	1.013	
R [$I > 2\sigma(I)$]	$R_1 = 0.0521$	$wR^2 = 0.1176$
R-Werte (sämtliche Daten)	$R_1 = 0.0737$	$wR^2 = 0.1290$
Größte Differenz Peak und Loch	2.198 und -1.151 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

C(1)-N(2)	1.341(4)	C(1)-N(1)	1.344(4)
C(1)-Ni(1)	1.894(3)	C(2)-N(1)	1.470(4)
C(3)-N(1)	1.470(4)	C(4)-N(2)	1.472(4)
C(5)-N(2)	1.459(4)	C(11)-C(12)	1.392(4)
C(11)-C(16)	1.405(4)	C(11)-P(1)	1.828(3)
C(12)-C(13)	1.390(5)	C(13)-C(14)	1.383(5)
C(14)-C(15)	1.378(5)	C(15)-C(16)	1.385(5)
C(21)-C(26)	1.402(4)	C(21)-C(22)	1.404(4)
C(21)-P(1)	1.828(3)	C(22)-C(23)	1.391(5)
C(23)-C(24)	1.387(5)	C(24)-C(25)	1.382(5)
C(25)-C(26)	1.389(5)	C(31)-C(36)	1.391(4)
C(31)-C(32)	1.398(4)	C(31)-P(1)	1.825(3)
C(32)-C(33)	1.395(4)	C(33)-C(34)	1.382(5)
C(34)-C(35)	1.383(5)	C(35)-C(36)	1.393(5)
C(41)-C(42)	1.390(4)	C(41)-C(46)	1.405(4)
C(41)-P(2)	1.826(3)	C(42)-C(43)	1.399(4)
C(43)-C(44)	1.384(4)	C(44)-C(45)	1.390(4)
C(45)-C(46)	1.388(4)	C(51)-C(52)	1.393(4)
C(51)-C(56)	1.405(4)	C(51)-P(2)	1.826(3)
C(52)-C(53)	1.403(4)	C(53)-C(54)	1.382(5)
C(54)-C(55)	1.391(5)	C(55)-C(56)	1.386(4)

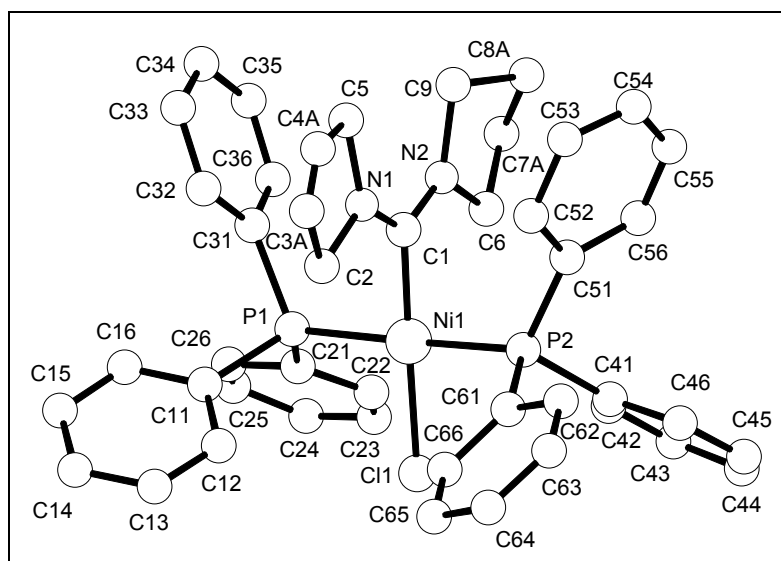
C(61)-C(62)	1.396(4)	C(61)-C(66)	1.403(4)
C(61)-P(2)	1.824(3)	C(62)-C(63)	1.396(4)
C(63)-C(64)	1.379(5)	C(64)-C(65)	1.387(5)
C(65)-C(66)	1.387(4)	C(71)-N(3)	1.339(4)
C(71)-N(4)	1.345(4)	C(71)-Ni(2)	1.892(3)
C(72)-N(3)	1.462(4)	C(73)-N(3)	1.468(4)
C(74)-N(4)	1.464(4)	C(75)-N(4)	1.473(4)
C(81)-C(82)	1.397(5)	C(81)-C(86)	1.404(4)
C(81)-P(3)	1.832(3)	C(82)-C(83)	1.383(5)
C(83)-C(84)	1.393(6)	C(84)-C(85)	1.375(6)
C(85)-C(86)	1.379(5)	C(91)-C(96)	1.391(4)
C(91)-C(92)	1.398(4)	C(91)-P(3)	1.823(3)
C(92)-C(93)	1.393(4)	C(93)-C(94)	1.384(5)
C(94)-C(95)	1.375(5)	C(95)-C(96)	1.402(5)
C(101)-C(102)	1.392(4)	C(101)-C(106)	1.399(4)
C(101)-P(3)	1.831(3)	C(102)-C(103)	1.392(5)
C(103)-C(104)	1.391(5)	C(104)-C(105)	1.381(5)
C(105)-C(106)	1.399(5)	C(111)-C(112)	1.391(4)
C(111)-C(116)	1.399(4)	C(111)-P(4)	1.834(3)
C(112)-C(113)	1.398(4)	C(113)-C(114)	1.384(5)
C(114)-C(115)	1.393(5)	C(115)-C(116)	1.390(4)
C(121)-C(122)	1.387(4)	C(121)-C(126)	1.408(4)
C(121)-P(4)	1.823(3)	C(122)-C(123)	1.399(4)
C(123)-C(124)	1.388(4)	C(124)-C(125)	1.384(5)
C(125)-C(126)	1.383(4)	C(131)-C(136)	1.394(4)
C(131)-C(132)	1.402(4)	C(131)-P(4)	1.825(3)
C(132)-C(133)	1.382(4)	C(133)-C(134)	1.392(5)
C(134)-C(135)	1.381(5)	C(135)-C(136)	1.397(4)
C(201)-Cl(6)	1.737(4)	C(201)-Cl(5)	1.766(4)
C(301)-Cl(4B)	1.468(9)	C(301)-Cl(4A)	1.717(6)
C(301)-Cl(3)	1.763(5)	F(1)-P(5)	1.593(2)
F(2)-P(5)	1.592(2)	F(3)-P(5)	1.607(2)
F(4)-P(5)	1.591(2)	F(5)-P(5)	1.600(2)
F(6)-P(5)	1.611(3)	F(7)-P(6)	1.594(2)

F(8)-P(6)	1.587(3)	F(9)-P(6)	1.586(2)
F(10)-P(6)	1.609(2)	F(11)-P(6)	1.603(2)
F(12)-P(6)	1.604(3)	P(1)-Ni(1)	2.2410(8)
P(2)-Ni(1)	2.2390(8)	P(3)-Ni(2)	2.2369(8)
P(4)-Ni(2)	2.2341(8)	Cl(1)-Ni(1)	2.1936(8)
Cl(2)-Ni(2)	2.1862(8)		
N(2)-C(1)-N(1)	121.3(3)	N(2)-C(1)-Ni(1)	121.9(2)
N(1)-C(1)-Ni(1)	116.8(2)	C(12)-C(11)-C(16)	118.8(3)
C(12)-C(11)-P(1)	119.7(2)	C(16)-C(11)-P(1)	121.1(2)
C(13)-C(12)-C(11)	120.6(3)	C(14)-C(13)-C(12)	119.9(3)
C(15)-C(14)-C(13)	120.0(3)	C(14)-C(15)-C(16)	120.7(3)
C(15)-C(16)-C(11)	119.9(3)	C(26)-C(21)-C(22)	118.9(3)
C(26)-C(21)-P(1)	121.0(2)	C(22)-C(21)-P(1)	120.0(2)
C(23)-C(22)-C(21)	120.1(3)	C(24)-C(23)-C(22)	120.5(3)
C(25)-C(24)-C(23)	119.5(3)	C(24)-C(25)-C(26)	121.0(3)
C(25)-C(26)-C(21)	119.9(3)	C(36)-C(31)-C(32)	119.1(3)
C(36)-C(31)-P(1)	121.6(2)	C(32)-C(31)-P(1)	118.6(2)
C(33)-C(32)-C(31)	120.5(3)	C(34)-C(33)-C(32)	119.8(3)
C(33)-C(34)-C(35)	120.1(3)	C(34)-C(35)-C(36)	120.5(3)
C(31)-C(36)-C(35)	120.0(3)	C(42)-C(41)-C(46)	119.7(3)
C(42)-C(41)-P(2)	121.3(2)	C(46)-C(41)-P(2)	118.9(2)
C(41)-C(42)-C(43)	119.8(3)	C(44)-C(43)-C(42)	120.2(3)
C(43)-C(44)-C(45)	120.2(3)	C(46)-C(45)-C(44)	120.1(3)
C(45)-C(46)-C(41)	120.0(3)	C(52)-C(51)-C(56)	119.3(3)
C(52)-C(51)-P(2)	121.6(2)	C(56)-C(51)-P(2)	118.8(2)
C(51)-C(52)-C(53)	120.0(3)	C(54)-C(53)-C(52)	120.0(3)
C(53)-C(54)-C(55)	120.3(3)	C(56)-C(55)-C(54)	120.1(3)
C(55)-C(56)-C(51)	120.3(3)	C(62)-C(61)-C(66)	118.5(3)
C(62)-C(61)-P(2)	123.2(2)	C(66)-C(61)-P(2)	118.2(2)
C(61)-C(62)-C(63)	119.9(3)	C(64)-C(63)-C(62)	121.0(3)
C(63)-C(64)-C(65)	119.8(3)	C(64)-C(65)-C(66)	119.8(3)
C(65)-C(66)-C(61)	121.1(3)	N(3)-C(71)-N(4)	120.8(3)
N(3)-C(71)-Ni(2)	122.1(2)	N(4)-C(71)-Ni(2)	117.1(2)

C(82)-C(81)-C(86)	118.5(3)	C(82)-C(81)-P(3)	120.0(2)
C(86)-C(81)-P(3)	121.5(3)	C(83)-C(82)-C(81)	120.6(3)
C(82)-C(83)-C(84)	120.1(4)	C(85)-C(84)-C(83)	119.6(3)
C(84)-C(85)-C(86)	120.9(3)	C(85)-C(86)-C(81)	120.2(3)
C(96)-C(91)-C(92)	119.2(3)	C(96)-C(91)-P(3)	122.2(3)
C(92)-C(91)-P(3)	118.5(2)	C(93)-C(92)-C(91)	120.3(3)
C(94)-C(93)-C(92)	119.8(3)	C(95)-C(94)-C(93)	120.5(3)
C(94)-C(95)-C(96)	120.0(3)	C(91)-C(96)-C(95)	120.0(3)
C(102)-C(101)-C(106)	119.4(3)	C(102)-C(101)-P(3)	120.4(2)
C(106)-C(101)-P(3)	120.2(2)	C(101)-C(102)-C(103)	120.3(3)
C(104)-C(103)-C(102)	120.3(3)	C(105)-C(104)-C(103)	119.6(3)
C(104)-C(105)-C(106)	120.6(3)	C(101)-C(106)-C(105)	119.8(3)
C(112)-C(111)-C(116)	119.5(3)	C(112)-C(111)-P(4)	121.5(2)
C(116)-C(111)-P(4)	118.8(2)	C(111)-C(112)-C(113)	120.2(3)
C(114)-C(113)-C(112)	119.9(3)	C(113)-C(114)-C(115)	120.3(3)
C(116)-C(115)-C(114)	119.9(3)	C(115)-C(116)-C(111)	120.2(3)
C(122)-C(121)-C(126)	119.4(3)	C(122)-C(121)-P(4)	121.5(2)
C(126)-C(121)-P(4)	119.1(2)	C(121)-C(122)-C(123)	120.1(3)
C(124)-C(123)-C(122)	119.7(3)	C(125)-C(124)-C(123)	120.6(3)
C(126)-C(125)-C(124)	119.9(3)	C(125)-C(126)-C(121)	120.2(3)
C(136)-C(131)-C(132)	118.7(3)	C(136)-C(131)-P(4)	123.2(2)
C(132)-C(131)-P(4)	118.0(2)	C(133)-C(132)-C(131)	121.0(3)
C(132)-C(133)-C(134)	120.2(3)	C(135)-C(134)-C(133)	119.2(3)
C(134)-C(135)-C(136)	121.2(3)	C(131)-C(136)-C(135)	119.8(3)
Cl(6)-C(201)-Cl(5)	112.2(2)	Cl(4B)-C(301)-Cl(4A)	85.4(4)
Cl(4B)-C(301)-Cl(3)	125.3(5)	Cl(4A)-C(301)-Cl(3)	111.9(3)
C(1)-N(1)-C(2)	119.3(2)	C(1)-N(1)-C(3)	127.7(3)
C(2)-N(1)-C(3)	112.0(2)	C(1)-N(2)-C(5)	119.7(3)
C(1)-N(2)-C(4)	126.8(3)	C(5)-N(2)-C(4)	112.9(2)
C(71)-N(3)-C(72)	119.5(3)	C(71)-N(3)-C(73)	127.1(3)
C(72)-N(3)-C(73)	112.8(3)	C(71)-N(4)-C(74)	119.6(2)
C(71)-N(4)-C(75)	127.4(3)	C(74)-N(4)-C(75)	111.9(2)
C(31)-P(1)-C(11)	101.15(14)	C(31)-P(1)-C(21)	108.76(14)
C(11)-P(1)-C(21)	103.17(14)	C(31)-P(1)-Ni(1)	115.59(10)

C(11)-P(1)-Ni(1)	116.65(10)	C(21)-P(1)-Ni(1)	110.42(10)
C(61)-P(2)-C(51)	106.56(13)	C(61)-P(2)-C(41)	101.73(13)
C(51)-P(2)-C(41)	104.49(13)	C(61)-P(2)-Ni(1)	117.13(10)
C(51)-P(2)-Ni(1)	108.77(9)	C(41)-P(2)-Ni(1)	117.00(10)
C(91)-P(3)-C(101)	107.53(15)	C(91)-P(3)-C(81)	102.62(14)
C(101)-P(3)-C(81)	102.98(14)	C(91)-P(3)-Ni(2)	115.43(10)
C(101)-P(3)-Ni(2)	109.87(10)	C(81)-P(3)-Ni(2)	117.28(10)
C(121)-P(4)-C(131)	101.93(13)	C(121)-P(4)-C(111)	104.41(14)
C(131)-P(4)-C(111)	106.40(13)	C(121)-P(4)-Ni(2)	116.04(10)
C(131)-P(4)-Ni(2)	117.48(10)	C(111)-P(4)-Ni(2)	109.39(10)
F(4)-P(5)-F(2)	91.40(17)	F(4)-P(5)-F(1)	89.70(13)
F(2)-P(5)-F(1)	178.77(16)	F(4)-P(5)-F(5)	89.93(14)
F(2)-P(5)-F(5)	90.45(13)	F(1)-P(5)-F(5)	90.10(12)
F(4)-P(5)-F(3)	90.26(13)	F(2)-P(5)-F(3)	89.64(13)
F(1)-P(5)-F(3)	89.81(11)	F(5)-P(5)-F(3)	179.80(17)
F(4)-P(5)-F(6)	178.01(15)	F(2)-P(5)-F(6)	90.49(17)
F(1)-P(5)-F(6)	88.40(14)	F(5)-P(5)-F(6)	90.68(14)
F(3)-P(5)-F(6)	89.14(13)	F(9)-P(6)-F(8)	91.40(19)
F(9)-P(6)-F(7)	89.49(13)	F(8)-P(6)-F(7)	178.97(18)
F(9)-P(6)-F(11)	90.23(14)	F(8)-P(6)-F(11)	90.52(13)
F(7)-P(6)-F(11)	90.00(12)	F(9)-P(6)-F(12)	177.77(18)
F(8)-P(6)-F(12)	90.8(2)	F(7)-P(6)-F(12)	88.33(16)
F(11)-P(6)-F(12)	90.23(15)	F(9)-P(6)-F(10)	90.17(13)
F(8)-P(6)-F(10)	89.75(13)	F(7)-P(6)-F(10)	89.72(12)
F(11)-P(6)-F(10)	179.51(15)	F(12)-P(6)-F(10)	89.36(14)
C(1)-Ni(1)-Cl(1)	172.57(9)	C(1)-Ni(1)-P(2)	92.83(9)
Cl(1)-Ni(1)-P(2)	89.26(3)	C(1)-Ni(1)-P(1)	90.95(8)
Cl(1)-Ni(1)-P(1)	88.33(3)	P(2)-Ni(1)-P(1)	168.80(3)
C(71)-Ni(2)-Cl(2)	172.67(9)	C(71)-Ni(2)-P(4)	94.21(9)
Cl(2)-Ni(2)-P(4)	88.06(3)	C(71)-Ni(2)-P(3)	91.12(9)
Cl(2)-Ni(2)-P(3)	87.89(3)	P(4)-Ni(2)-P(3)	168.65(3)

Kristallographische Daten der Verbindung 261



Kristalldaten

Summenformel	$\text{C}_{45.5}\text{H}_{49}\text{ClF}_6\text{N}_2\text{NiP}_6$	
Farbe	farblos	
Molmasse	$1017.85 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Monoklin	
Raumgruppe	P 2₁/c, (no. 14)	
Gitterkonstanten	$a = 15.9359(8) \text{ \AA}$	$\alpha = 90^\circ$.
	$b = 14.7996(6) \text{ \AA}$	$\beta = 91.925(2)^\circ$.
	$c = 20.0188(9) \text{ \AA}$	$\gamma = 90^\circ$.
Volumen	$4718.7(4) \text{ \AA}^3$	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	$1.433 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.730 mm^{-1}	
F(000)	2100 e	
Kristallgröße	$0.09 \times 0.06 \times 0.02 \text{ mm}^3$	
θ -Grenzen für Datensammlung	2.12 bis 22.50° .	
Indexbereich	$-17 \leq h \leq 17, -15 \leq k \leq 14, -21 \leq l \leq 21$	
Aufgenommene Reflexe	30193	
Unabhängige Reflexe	6157 [$R_{\text{int}} = 0.0477$]	

Reflexe mit $I > 2\sigma(I)$	5472	
Vollständigkeit für $\theta = 22.50^\circ$	99.9 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.96 und 0.99	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrat auf F^2	
Daten/ Einschränkungen/ Parameter	6157 / 0 / 568	
Goodness-of-fit auf F^2	3.128	
R [$I > 2\sigma(I)$]	$R_1 = 0.1241$	$wR^2 = 0.3792$
R-Werte (sämtliche Daten)	$R_1 = 0.1343$	$wR^2 = 0.3820$
Größte Differenz Peak und Loch	1.646 und -1.494 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

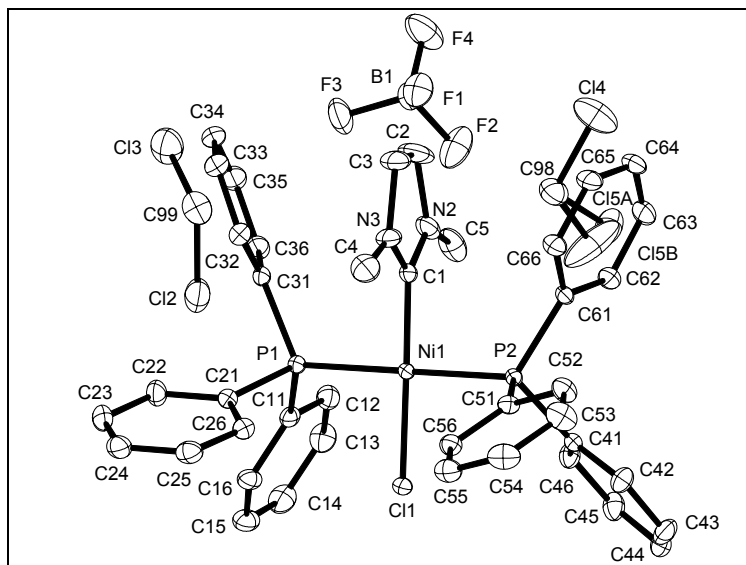
C(1)-N(1)	1.297(15)	C(1)-N(2)	1.369(15)
C(1)-Ni(1)	1.868(11)	C(2)-C(3B)	1.48(3)
C(2)-N(1)	1.507(15)	C(2)-C(3A)	1.55(3)
C(3A)-C(4A)	1.03(3)	C(4A)-C(5)	1.71(3)
C(7A)-C(6)	1.54(2)	C(7A)-C(8A)	1.54(3)
C(8A)-C(9)	1.59(2)	C(3B)-C(4B)	1.53(3)
C(4B)-C(5)	1.49(2)	C(7B)-C(8B)	1.38(4)
C(7B)-C(6)	1.59(3)	C(8B)-C(9)	1.57(4)
C(5)-N(1)	1.478(15)	C(6)-N(2)	1.469(14)
C(9)-N(2)	1.523(15)	C(11)-C(16)	1.385(17)
C(11)-C(12)	1.386(16)	C(11)-P(1)	1.849(12)
C(12)-C(13)	1.353(16)	C(13)-C(14)	1.375(17)
C(14)-C(15)	1.375(18)	C(15)-C(16)	1.374(18)
C(21)-C(22)	1.383(17)	C(21)-C(26)	1.388(18)
C(21)-P(1)	1.835(13)	C(22)-C(23)	1.402(18)
C(23)-C(24)	1.346(19)	C(24)-C(25)	1.392(19)
C(25)-C(26)	1.342(18)	C(31)-C(32)	1.390(17)
C(31)-C(36)	1.390(18)	C(31)-P(1)	1.828(11)
C(32)-C(33)	1.383(19)	C(33)-C(34)	1.39(3)
C(34)-C(35)	1.42(2)	C(35)-C(36)	1.352(19)
C(41)-C(42)	1.336(17)	C(41)-C(46)	1.407(17)

C(41)-P(2)	1.867(12)	C(42)-C(43)	1.389(17)
C(43)-C(44)	1.396(18)	C(44)-C(45)	1.390(19)
C(45)-C(46)	1.345(17)	C(51)-C(52)	1.386(17)
C(51)-C(56)	1.452(17)	C(51)-P(2)	1.791(12)
C(52)-C(53)	1.431(17)	C(53)-C(54)	1.355(19)
C(54)-C(55)	1.373(19)	C(55)-C(56)	1.363(18)
C(61)-C(62)	1.373(17)	C(61)-C(66)	1.427(17)
C(61)-P(2)	1.842(11)	C(62)-C(63)	1.390(17)
C(63)-C(64)	1.355(18)	C(64)-C(65)	1.41(2)
C(65)-C(66)	1.345(18)	C(98)-Cl(5)	1.74(5)
C(98)-Cl(4)	1.94(7)	C(99)-Cl(2)	1.754(14)
C(99)-Cl(3)	1.768(18)	F(1)-P(3)	1.624(8)
F(2)-P(3)	1.565(9)	F(3)-P(3)	1.572(8)
F(4)-P(3)	1.572(7)	F(5)-P(3)	1.593(8)
F(6)-P(3)	1.610(8)	P(1)-Ni(1)	2.245(3)
P(2)-Ni(1)	2.251(3)	Cl(1)-Ni(1)	2.208(3)
N(1)-C(1)-N(2)	122.9(10)	N(1)-C(1)-Ni(1)	120.8(8)
N(2)-C(1)-Ni(1)	116.2(9)	C(3B)-C(2)-N(1)	106.4(13)
C(3B)-C(2)-C(3A)	25.2(12)	N(1)-C(2)-C(3A)	100.1(12)
C(4A)-C(3A)-C(2)	117(3)	C(3A)-C(4A)-C(5)	114(3)
C(6)-C(7A)-C(8A)	95.7(15)	C(7A)-C(8A)-C(9)	103.5(14)
C(2)-C(3B)-C(4B)	107.1(18)	C(5)-C(4B)-C(3B)	107.4(16)
C(8B)-C(7B)-C(6)	104(2)	C(7B)-C(8B)-C(9)	98(3)
N(1)-C(5)-C(4B)	105.1(11)	N(1)-C(5)-C(4A)	95.2(13)
C(4B)-C(5)-C(4A)	35.6(12)	N(2)-C(6)-C(7A)	105.4(10)
N(2)-C(6)-C(7B)	97.6(12)	C(7A)-C(6)-C(7B)	28.3(10)
N(2)-C(9)-C(8B)	98.4(16)	N(2)-C(9)-C(8A)	97.7(11)
C(8B)-C(9)-C(8A)	34.7(13)	C(16)-C(11)-C(12)	118.6(11)
C(16)-C(11)-P(1)	120.8(9)	C(12)-C(11)-P(1)	120.5(8)
C(13)-C(12)-C(11)	120.2(11)	C(12)-C(13)-C(14)	121.3(12)
C(15)-C(14)-C(13)	119.4(11)	C(16)-C(15)-C(14)	119.7(12)
C(15)-C(16)-C(11)	120.8(13)	C(22)-C(21)-C(26)	118.2(12)
C(22)-C(21)-P(1)	121.2(10)	C(26)-C(21)-P(1)	120.4(10)

C(21)-C(22)-C(23)	119.7(12)	C(24)-C(23)-C(22)	121.0(13)
C(23)-C(24)-C(25)	118.6(13)	C(26)-C(25)-C(24)	121.3(12)
C(25)-C(26)-C(21)	121.0(12)	C(32)-C(31)-C(36)	118.1(11)
C(32)-C(31)-P(1)	120.8(9)	C(36)-C(31)-P(1)	121.0(10)
C(31)-C(32)-C(33)	120.3(13)	C(32)-C(33)-C(34)	119.6(16)
C(33)-C(34)-C(35)	121.2(14)	C(36)-C(35)-C(34)	116.4(15)
C(35)-C(36)-C(31)	124.2(15)	C(42)-C(41)-C(46)	120.7(11)
C(42)-C(41)-P(2)	120.9(9)	C(46)-C(41)-P(2)	118.3(10)
C(41)-C(42)-C(43)	121.4(11)	C(42)-C(43)-C(44)	118.3(12)
C(45)-C(44)-C(43)	119.3(12)	C(46)-C(45)-C(44)	121.5(12)
C(45)-C(46)-C(41)	118.6(12)	C(52)-C(51)-C(56)	116.7(11)
C(52)-C(51)-P(2)	121.1(9)	C(56)-C(51)-P(2)	122.1(10)
C(51)-C(52)-C(53)	119.4(11)	C(54)-C(53)-C(52)	122.4(13)
C(55)-C(54)-C(53)	118.4(14)	C(54)-C(55)-C(56)	122.1(13)
C(55)-C(56)-C(51)	120.9(12)	C(62)-C(61)-C(66)	118.4(11)
C(62)-C(61)-P(2)	121.4(9)	C(66)-C(61)-P(2)	120.0(9)
C(63)-C(62)-C(61)	118.9(12)	C(64)-C(63)-C(62)	122.8(12)
C(63)-C(64)-C(65)	118.8(11)	C(66)-C(65)-C(64)	119.2(12)
C(65)-C(66)-C(61)	121.8(12)	Cl(5)-C(98)-Cl(4)	105(4)
Cl(2)-C(99)-Cl(3)	110.6(8)	C(1)-N(1)-C(5)	129.8(9)
C(1)-N(1)-C(2)	120.3(9)	C(5)-N(1)-C(2)	109.9(9)
C(1)-N(2)-C(6)	120.7(9)	C(1)-N(2)-C(9)	128.5(10)
C(6)-N(2)-C(9)	110.5(9)	C(21)-P(1)-C(31)	101.7(6)
C(21)-P(1)-C(11)	105.7(6)	C(31)-P(1)-C(11)	103.4(5)
C(21)-P(1)-Ni(1)	115.2(4)	C(31)-P(1)-Ni(1)	116.7(4)
C(11)-P(1)-Ni(1)	112.6(4)	C(51)-P(2)-C(61)	101.0(5)
C(51)-P(2)-C(41)	103.8(5)	C(61)-P(2)-C(41)	106.8(5)
C(51)-P(2)-Ni(1)	118.7(4)	C(61)-P(2)-Ni(1)	113.0(4)
C(41)-P(2)-Ni(1)	112.2(4)	F(2)-P(3)-F(3)	90.1(5)
F(2)-P(3)-F(4)	90.3(4)	F(3)-P(3)-F(4)	91.4(5)
F(2)-P(3)-F(5)	91.0(5)	F(3)-P(3)-F(5)	178.3(5)
F(4)-P(3)-F(5)	89.9(5)	F(2)-P(3)-F(6)	90.9(5)
F(3)-P(3)-F(6)	88.8(5)	F(4)-P(3)-F(6)	178.8(5)
F(5)-P(3)-F(6)	89.9(5)	F(2)-P(3)-F(1)	179.0(5)

F(3)-P(3)-F(1)	89.6(4)	F(4)-P(3)-F(1)	90.7(4)
F(5)-P(3)-F(1)	89.3(4)	F(6)-P(3)-F(1)	88.1(4)
C(1)-Ni(1)-Cl(1)	178.9(3)	C(1)-Ni(1)-P(1)	89.8(3)
Cl(1)-Ni(1)-P(1)	91.32(11)	C(1)-Ni(1)-P(2)	88.2(3)
Cl(1)-Ni(1)-P(2)	90.66(11)	P(1)-Ni(1)-P(2)	177.47(13)

Kristallographische Daten der Verbindung 263



Kristalldaten

Summenformel	$\text{C}_{43}\text{H}_{44}\text{BCl}_5\text{F}_4\text{N}_2\text{NiP}_2$	
Farbe	gelb	
Molmasse	$973.51 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Monoklin	
Raumgruppe	P 2₁, (no. 4)	
Gitterkonstanten	$a = 9.18310(10) \text{ Å}$	$\alpha = 90^\circ$.
	$b = 20.86120(10) \text{ Å}$	$\beta = 91.75^\circ$.
	$c = 11.61080(10) \text{ Å}$	$\gamma = 90^\circ$.
Volumen	$2223.24(3) \text{ Å}^3$	
Teilchen pro Elementarzelle	2	
Berechnete Dichte	$1.454 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.859 mm^{-1}	
F(000)	1000 e	
Kristallgröße	0.22 x 0.18 x 0.08 mm ³	
θ -Grenzen für Datensammlung	2.95 bis 31.03°.	
Indexbereich	$-13 \leq h \leq 13, -30 \leq k \leq 30, -16 \leq l \leq 16$	
Aufgenommene Reflexe	57225	
Unabhängige Reflexe	14113 [$R_{\text{int}} = 0.0361$]	

Reflexe mit $I > 2\sigma(I)$	13455	
Vollständigkeit für $\theta = 27.75^\circ$	99.5 %	
Absorptionskorrektur	Semi-empirical from equivalents	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	14113 / 1 / 535	
Goodness-of-fit auf F^2	1.004	
R [$I > 2\sigma(I)$]	$R_1 = 0.0268$	$wR^2 = 0.0644$
R-Werte (sämtliche Daten)	$R_1 = 0.0290$	$wR^2 = 0.0655$
Absolute Strukturparameter	0.009(5)	
Größte Differenz Peak und Loch	0.539 und -0.378 e · Å ⁻³	

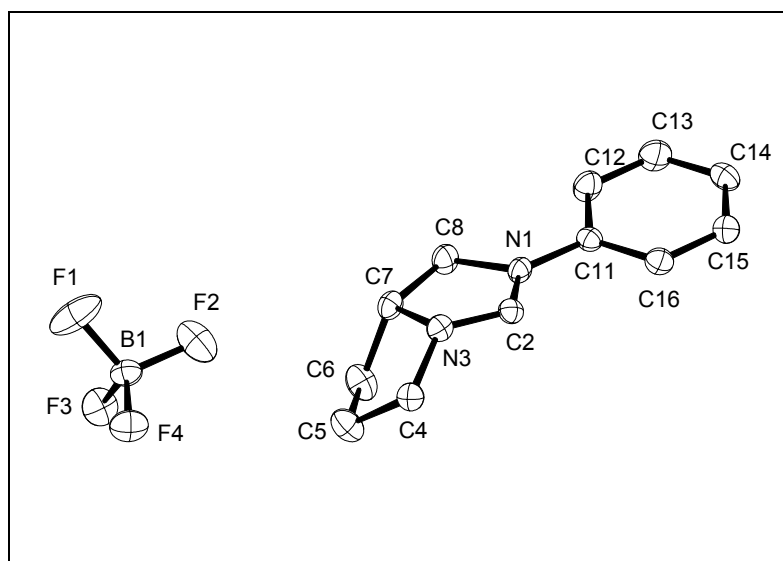
Bindungslängen [Å] und -winkel [°]

Ni(1)-C(1)	1.8626(14)	Ni(1)-Cl(1)	2.1793(3)
Ni(1)-P(2)	2.2366(3)	Ni(1)-P(1)	2.2473(3)
Cl(2)-C(99)	1.769(2)	Cl(3)-C(99)	1.779(2)
Cl(4)-C(98)	1.7489(18)	Cl(5A)-C(98)	1.820(3)
Cl(5B)-C(98)	1.634(7)	P(1)-C(11)	1.8232(15)
P(1)-C(21)	1.8263(15)	P(1)-C(31)	1.8349(13)
P(2)-C(51)	1.8210(14)	P(2)-C(61)	1.8243(12)
P(2)-C(41)	1.8278(14)	F(1)-B(1)	1.396(2)
F(2)-B(1)	1.393(2)	F(3)-B(1)	1.382(2)
F(4)-B(1)	1.378(2)	C(1)-N(2)	1.3202(19)
C(1)-N(3)	1.339(2)	N(2)-C(5)	1.438(2)
N(2)-C(2)	1.485(2)	C(2)-C(3)	1.499(3)
N(3)-C(4)	1.446(2)	N(3)-C(3)	1.470(2)
C(11)-C(12)	1.399(2)	C(11)-C(16)	1.404(2)
C(12)-C(13)	1.390(2)	C(13)-C(14)	1.386(3)
C(14)-C(15)	1.392(3)	C(15)-C(16)	1.388(2)
C(21)-C(26)	1.391(2)	C(21)-C(22)	1.402(2)
C(22)-C(23)	1.393(2)	C(23)-C(24)	1.395(3)
C(24)-C(25)	1.386(3)	C(25)-C(26)	1.397(2)
C(31)-C(36)	1.399(2)	C(31)-C(32)	1.403(2)
C(32)-C(33)	1.388(2)	C(33)-C(34)	1.393(2)

C(34)-C(35)	1.381(3)	C(35)-C(36)	1.398(2)
C(41)-C(42)	1.396(2)	C(41)-C(46)	1.399(2)
C(42)-C(43)	1.394(2)	C(43)-C(44)	1.379(2)
C(44)-C(45)	1.393(2)	C(45)-C(46)	1.392(2)
C(51)-C(56)	1.3980(19)	C(51)-C(52)	1.406(2)
C(52)-C(53)	1.391(2)	C(53)-C(54)	1.385(2)
C(54)-C(55)	1.389(2)	C(55)-C(56)	1.399(2)
C(61)-C(62)	1.396(2)	C(61)-C(66)	1.400(2)
C(62)-C(63)	1.396(2)	C(63)-C(64)	1.388(3)
C(64)-C(65)	1.382(3)	C(65)-C(66)	1.391(2)
C(1)-Ni(1)-Cl(1)	179.17(5)	C(1)-Ni(1)-P(2)	89.28(4)
Cl(1)-Ni(1)-P(2)	91.344(13)	C(1)-Ni(1)-P(1)	90.30(4)
Cl(1)-Ni(1)-P(1)	89.052(13)	P(2)-Ni(1)-P(1)	178.158(16)
C(11)-P(1)-C(21)	105.46(7)	C(11)-P(1)-C(31)	106.82(7)
C(21)-P(1)-C(31)	100.99(6)	C(11)-P(1)-Ni(1)	111.21(5)
C(21)-P(1)-Ni(1)	113.54(5)	C(31)-P(1)-Ni(1)	117.69(4)
C(51)-P(2)-C(61)	104.77(7)	C(51)-P(2)-C(41)	104.13(7)
C(61)-P(2)-C(41)	104.79(6)	C(51)-P(2)-Ni(1)	111.56(5)
C(61)-P(2)-Ni(1)	115.96(4)	C(41)-P(2)-Ni(1)	114.49(5)
F(4)-B(1)-F(3)	109.60(15)	F(4)-B(1)-F(2)	109.43(16)
F(3)-B(1)-F(2)	109.57(15)	F(4)-B(1)-F(1)	109.06(15)
F(3)-B(1)-F(1)	110.64(15)	F(2)-B(1)-F(1)	108.52(15)
N(2)-C(1)-N(3)	109.85(13)	N(2)-C(1)-Ni(1)	124.89(12)
N(3)-C(1)-Ni(1)	125.26(11)	C(1)-N(2)-C(5)	126.59(15)
C(1)-N(2)-C(2)	110.83(15)	C(5)-N(2)-C(2)	122.38(15)
N(2)-C(2)-C(3)	104.05(13)	C(1)-N(3)-C(4)	126.96(13)
C(1)-N(3)-C(3)	112.47(15)	C(4)-N(3)-C(3)	120.54(15)
N(3)-C(3)-C(2)	102.11(14)	C(12)-C(11)-C(16)	118.85(13)
C(12)-C(11)-P(1)	120.49(11)	C(16)-C(11)-P(1)	120.57(11)
C(13)-C(12)-C(11)	120.31(15)	C(12)-C(13)-C(14)	120.34(16)
C(13)-C(14)-C(15)	119.92(15)	C(16)-C(15)-C(14)	120.08(15)
C(15)-C(16)-C(11)	120.44(15)	C(26)-C(21)-C(22)	119.26(13)
C(26)-C(21)-P(1)	121.91(11)	C(22)-C(21)-P(1)	118.82(11)

C(23)-C(22)-C(21)	120.27(15)	C(22)-C(23)-C(24)	119.80(15)
C(25)-C(24)-C(23)	120.24(14)	C(24)-C(25)-C(26)	119.88(15)
C(21)-C(26)-C(25)	120.53(14)	C(36)-C(31)-C(32)	118.80(13)
C(36)-C(31)-P(1)	124.16(11)	C(32)-C(31)-P(1)	117.00(11)
C(33)-C(32)-C(31)	120.66(14)	C(32)-C(33)-C(34)	120.05(15)
C(35)-C(34)-C(33)	119.86(14)	C(34)-C(35)-C(36)	120.57(15)
C(35)-C(36)-C(31)	120.06(15)	C(42)-C(41)-C(46)	119.05(13)
C(42)-C(41)-P(2)	120.78(11)	C(46)-C(41)-P(2)	120.16(11)
C(43)-C(42)-C(41)	120.46(14)	C(44)-C(43)-C(42)	120.14(14)
C(43)-C(44)-C(45)	119.99(14)	C(44)-C(45)-C(46)	120.17(14)
C(45)-C(46)-C(41)	120.14(14)	C(56)-C(51)-C(52)	119.19(13)
C(56)-C(51)-P(2)	119.52(11)	C(52)-C(51)-P(2)	121.16(11)
C(53)-C(52)-C(51)	119.90(14)	C(54)-C(53)-C(52)	120.44(15)
C(53)-C(54)-C(55)	120.37(15)	C(54)-C(55)-C(56)	119.67(14)
C(51)-C(56)-C(55)	120.42(14)	C(62)-C(61)-C(66)	119.12(12)
C(62)-C(61)-P(2)	119.88(12)	C(66)-C(61)-P(2)	120.77(12)
C(63)-C(62)-C(61)	120.01(16)	C(64)-C(63)-C(62)	120.32(16)
C(65)-C(64)-C(63)	119.93(13)	C(66)-C(65)-C(64)	120.25(16)
C(65)-C(66)-C(61)	120.38(16)	Cl(5B)-C(98)-Cl(4)	122.0(10)
Cl(5B)-C(98)-Cl(5A)	16.3(9)	Cl(4)-C(98)-Cl(5A)	107.28(12)
Cl(2)-C(99)-Cl(3)	111.05(10)		

Kristallographische Daten der Verbindung 292



Kristalldaten

Summenformel	$\text{C}_{12}\text{H}_{15}\text{BF}_4\text{N}_2$	
Farbe	farblos	
Molmasse	274.07 $\text{g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 Å	
Kristallsystem	Orthorhombisch	
Raumgruppe	P2₁ 2₁ 2₁, (no. 19)	
Gitterkonstanten	$a = 8.18180(10)$ Å	$\alpha = 90^\circ$.
	$b = 15.7298(3)$ Å	$\beta = 90^\circ$.
	$c = 19.7459(4)$ Å	$\gamma = 90^\circ$.
Volumen	2541.26(8) Å ³	
Teilchen pro Elementarzelle	8	
Berechnete Dichte	1.433 $\text{mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.126 mm^{-1}	
F(000)	1136 e	
Kristallgröße	0.23 x 0.18 x 0.06 mm ³	
θ -Grenzen für Datensammlung	2.99 bis 33.14°.	
Indexbereich	$-12 \leq h \leq 12$, $-23 \leq k \leq 24$, $-14 \leq l \leq 30$	
Aufgenommene Reflexe	29150	
Unabhängige Reflexe	9672 [$R_{\text{int}} = 0.1170$]	

Reflexe mit $I > 2\sigma(I)$	5596	
Vollständigkeit für $\theta = 27.50^\circ$	99.5 %	
Absorptionskorrektur	keine	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	9672 / 0 / 371	
Goodness-of-fit auf F^2	1.024	
R [$I > 2\sigma(I)$]	$R_1 = 0.0802$	$wR^2 = 0.1640$
R-Werte (sämtliche Daten)	$R_1 = 0.1492$	$wR^2 = 0.1955$
Absolute Strukturparameter	0.6(7)	
Größte Differenz Peak und Loch	0.492 und -0.369 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

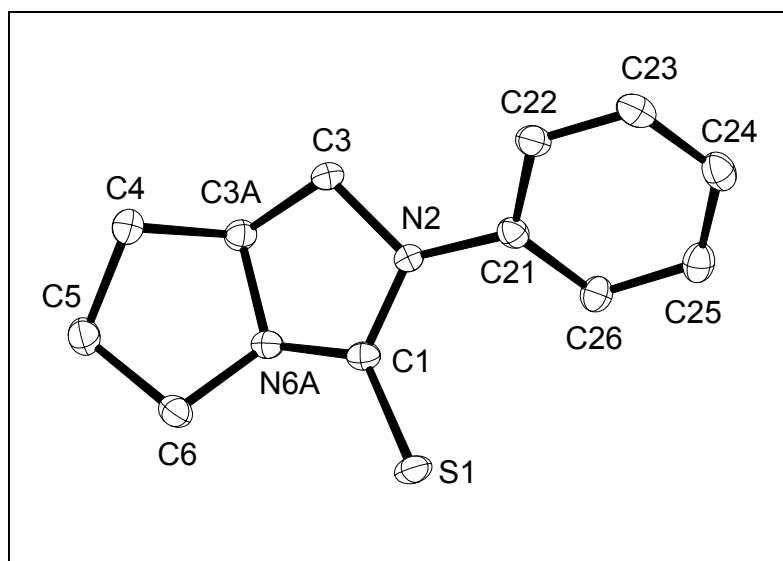
C(2)-N(3)	1.307(3)	C(2)-N(1)	1.311(3)
C(2)-H(2)	0.9500	C(2B)-N(3B)	1.297(4)
C(2B)-N(1B)	1.325(4)	C(2B)-H(2B)	0.9500
C(4)-N(3)	1.477(3)	C(4)-C(5)	1.544(4)
C(4)-H(4A)	0.9900	C(4)-H(4B)	0.9900
C(4B)-N(3B)	1.483(3)	C(4B)-C(5B)	1.529(4)
C(4B)-H(4B1)	0.9900	C(4B)-H(4B2)	0.9900
C(5)-C(6)	1.544(4)	C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900	C(5B)-C(6B)	1.537(4)
C(5B)-H(5B1)	0.9900	C(5B)-H(5B2)	0.9900
C(6)-C(7)	1.518(4)	C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900	C(6B)-C(7B)	1.528(4)
C(6B)-H(6B1)	0.9900	C(6B)-H(6B2)	0.9900
C(7)-N(3)	1.483(3)	C(7)-C(8)	1.541(4)
C(7)-H(7)	1.0000	C(7B)-N(3B)	1.481(3)
C(7B)-C(8B)	1.546(4)	C(7B)-H(7B)	1.0000
C(8)-N(1)	1.484(3)	C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900	C(8B)-N(1B)	1.485(3)
C(8B)-H(8B1)	0.9900	C(8B)-H(8B2)	0.9900
C(11)-C(16)	1.388(4)	C(11)-C(12)	1.392(4)
C(11)-N(1)	1.422(3)	C(11B)-C(16B)	1.384(4)

C(11B)-C(12B)	1.400(4)	C(11B)-N(1B)	1.425(3)
C(12)-C(13)	1.382(4)	C(12)-H(12)	0.9500
C(12B)-C(13B)	1.382(4)	C(12B)-H(12B)	0.9500
C(13)-C(14)	1.388(4)	C(13)-H(13)	0.9500
C(13B)-C(14B)	1.389(5)	C(13B)-H(13B)	0.9500
C(14)-C(15)	1.381(4)	C(14)-H(14)	0.9500
C(14B)-C(15B)	1.389(5)	C(14B)-H(14B)	0.9500
C(15)-C(16)	1.389(4)	C(15)-H(15)	0.9500
C(15B)-C(16B)	1.391(4)	C(15B)-H(15B)	0.9500
C(16)-H(16)	0.9500	C(16B)-H(16B)	0.9500
B(1)-F(4)	1.371(4)	B(1)-F(2)	1.377(4)
B(1)-F(1)	1.394(4)	B(1)-F(3)	1.405(4)
B(1B)-F(6B)	1.249(10)	B(1B)-F(5B)	1.304(10)
B(1B)-F(7B)	1.347(13)	B(1B)-F(4B)	1.362(6)
B(1B)-F(2B)	1.373(6)	B(1B)-F(1B)	1.382(4)
B(1B)-F(3B)	1.418(6)		
N(3)-C(2)-N(1)	114.1(2)	N(3)-C(2)-H(2)	122.9
N(1)-C(2)-H(2)	122.9	N(3B)-C(2B)-N(1B)	113.2(2)
N(3B)-C(2B)-H(2B)	123.4	N(1B)-C(2B)-H(2B)	123.4
N(3)-C(4)-C(5)	103.2(2)	N(3)-C(4)-H(4A)	111.1
C(5)-C(4)-H(4A)	111.1	N(3)-C(4)-H(4B)	111.1
C(5)-C(4)-H(4B)	111.1	H(4A)-C(4)-H(4B)	109.1
N(3B)-C(4B)-C(5B)	102.6(2)	N(3B)-C(4B)-H(4B1)	111.2
C(5B)-C(4B)-H(4B1)	111.2	N(3B)-C(4B)-H(4B2)	111.2
C(5B)-C(4B)-H(4B2)	111.2	H(4B1)-C(4B)-H(4B2)	109.2
C(6)-C(5)-C(4)	105.0(2)	C(6)-C(5)-H(5A)	110.7
C(4)-C(5)-H(5A)	110.7	C(6)-C(5)-H(5B)	110.7
C(4)-C(5)-H(5B)	110.7	H(5A)-C(5)-H(5B)	108.8
C(4B)-C(5B)-C(6B)	106.6(2)	C(4B)-C(5B)-H(5B1)	110.4
C(6B)-C(5B)-H(5B1)	110.4	C(4B)-C(5B)-H(5B2)	110.4
C(6B)-C(5B)-H(5B2)	110.4	H(5B1)-C(5B)-H(5B2)	108.6
C(7)-C(6)-C(5)	103.1(2)	C(7)-C(6)-H(6A)	111.2
C(5)-C(6)-H(6A)	111.2	C(7)-C(6)-H(6B)	111.2

C(5)-C(6)-H(6B)	111.2	H(6A)-C(6)-H(6B)	109.1
C(7B)-C(6B)-C(5B)	102.8(2)	C(7B)-C(6B)-H(6B1)	111.2
C(5B)-C(6B)-H(6B1)	111.2	C(7B)-C(6B)-H(6B2)	111.2
C(5B)-C(6B)-H(6B2)	111.2	H(6B1)-C(6B)-H(6B2)	109.1
N(3)-C(7)-C(6)	100.9(2)	N(3)-C(7)-C(8)	102.6(2)
C(6)-C(7)-C(8)	120.2(2)	N(3)-C(7)-H(7)	110.7
C(6)-C(7)-H(7)	110.7	C(8)-C(7)-H(7)	110.7
N(3B)-C(7B)-C(6B)	101.1(2)	N(3B)-C(7B)-C(8B)	102.5(2)
C(6B)-C(7B)-C(8B)	120.2(2)	N(3B)-C(7B)-H(7B)	110.7
C(6B)-C(7B)-H(7B)	110.7	C(8B)-C(7B)-H(7B)	110.7
N(1)-C(8)-C(7)	102.8(2)	N(1)-C(8)-H(8A)	111.2
C(7)-C(8)-H(8A)	111.2	N(1)-C(8)-H(8B)	111.2
C(7)-C(8)-H(8B)	111.2	H(8A)-C(8)-H(8B)	109.1
N(1B)-C(8B)-C(7B)	102.5(2)	N(1B)-C(8B)-H(8B1)	111.3
C(7B)-C(8B)-H(8B1)	111.3	N(1B)-C(8B)-H(8B2)	111.3
C(7B)-C(8B)-H(8B2)	111.3	H(8B1)-C(8B)-H(8B2)	109.2
C(16)-C(11)-C(12)	119.9(2)	C(16)-C(11)-N(1)	120.8(2)
C(12)-C(11)-N(1)	119.2(2)	C(16B)-C(11B)-C(12B)	120.3(3)
C(16B)-C(11B)-N(1B)	119.2(2)	C(12B)-C(11B)-N(1B)	120.5(3)
C(13)-C(12)-C(11)	119.7(3)	C(13)-C(12)-H(12)	120.2
C(11)-C(12)-H(12)	120.2	C(13B)-C(12B)-C(11B)	119.4(3)
C(13B)-C(12B)-H(12B)	120.3	C(11B)-C(12B)-H(12B)	120.3
C(12)-C(13)-C(14)	120.9(3)	C(12)-C(13)-H(13)	119.6
C(14)-C(13)-H(13)	119.6	C(12B)-C(13B)-C(14B)	120.5(3)
C(12B)-C(13B)-H(13B)	119.7	C(14B)-C(13B)-H(13B)	119.7
C(15)-C(14)-C(13)	119.1(3)	C(15)-C(14)-H(14)	120.4
C(13)-C(14)-H(14)	120.4	C(13B)-C(14B)-C(15B)	119.7(3)
C(13B)-C(14B)-H(14B)	120.1	C(15B)-C(14B)-H(14B)	120.1
C(14)-C(15)-C(16)	120.8(3)	C(14)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6	C(14B)-C(15B)-C(16B)	120.2(3)
C(14B)-C(15B)-H(15B)	119.9	C(16B)-C(15B)-H(15B)	119.9
C(11)-C(16)-C(15)	119.6(3)	C(11)-C(16)-H(16)	120.2
C(15)-C(16)-H(16)	120.2	C(11B)-C(16B)-C(15B)	119.8(3)
C(11B)-C(16B)-H(16B)	120.1	C(15B)-C(16B)-H(16B)	120.1

F(4)-B(1)-F(2)	111.8(3)	F(4)-B(1)-F(1)	109.7(2)
F(2)-B(1)-F(1)	108.9(3)	F(4)-B(1)-F(3)	110.1(3)
F(2)-B(1)-F(3)	108.3(2)	F(1)-B(1)-F(3)	108.0(3)
F(6B)-B(1B)-F(5B)	116.9(10)	F(6B)-B(1B)-F(7B)	108.0(10)
F(5B)-B(1B)-F(7B)	101.5(10)	F(6B)-B(1B)-F(4B)	121.9(8)
F(5B)-B(1B)-F(4B)	77.3(10)	F(7B)-B(1B)-F(4B)	24.3(9)
F(6B)-B(1B)-F(2B)	87.8(9)	F(5B)-B(1B)-F(2B)	36.4(9)
F(7B)-B(1B)-F(2B)	134.3(8)	F(4B)-B(1B)-F(2B)	111.6(5)
F(6B)-B(1B)-F(1B)	112.0(6)	F(5B)-B(1B)-F(1B)	112.2(5)
F(7B)-B(1B)-F(1B)	104.9(6)	F(4B)-B(1B)-F(1B)	112.2(4)
F(2B)-B(1B)-F(1B)	108.1(3)	F(6B)-B(1B)-F(3B)	19.2(9)
F(5B)-B(1B)-F(3B)	129.2(6)	F(7B)-B(1B)-F(3B)	90.0(7)
F(4B)-B(1B)-F(3B)	107.2(4)	F(2B)-B(1B)-F(3B)	105.5(4)
F(1B)-B(1B)-F(3B)	112.1(4)	C(2)-N(1)-C(11)	126.6(2)
C(2)-N(1)-C(8)	109.9(2)	C(11)-N(1)-C(8)	123.5(2)
C(2B)-N(1B)-C(11B)	126.5(2)	C(2B)-N(1B)-C(8B)	110.0(2)
C(11B)-N(1B)-C(8B)	123.4(2)	C(2)-N(3)-C(4)	127.8(2)
C(2)-N(3)-C(7)	109.9(2)	C(4)-N(3)-C(7)	111.7(2)
C(2B)-N(3B)-C(7B)	111.2(2)	C(2B)-N(3B)-C(4B)	128.8(2)
C(7B)-N(3B)-C(4B)	112.4(2)		

Kristallographische Daten der Verbindung 85



Kristalldaten

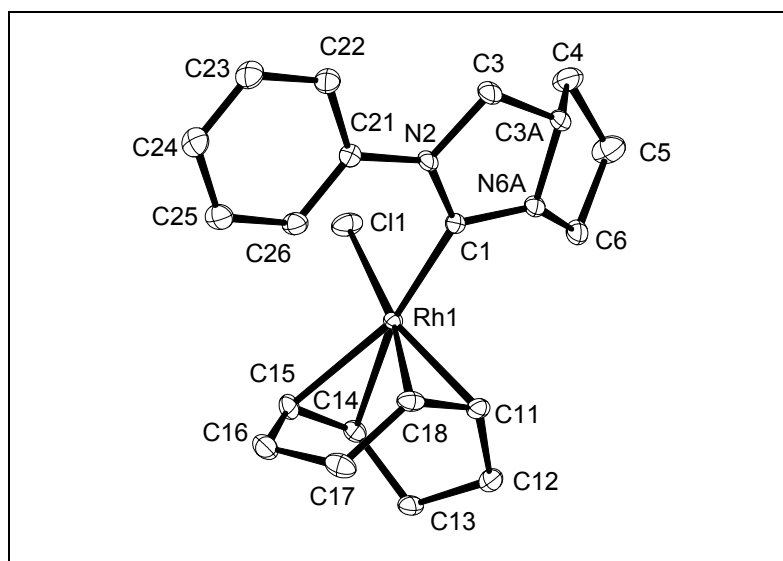
Summenformel	$\text{C}_{12}\text{H}_{14}\text{N}_2\text{S}$	
Farbe	farblos	
Molmasse	$218.31 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Monoklin	
Raumgruppe	P2₁, (no. 4)	
Gitterkonstanten	$a = 5.30140(10) \text{ \AA}$	$\alpha = 90^\circ$.
	$b = 12.9538(3) \text{ \AA}$	$\beta = 107.7120(10)^\circ$.
	$c = 8.2297(2) \text{ \AA}$	$\gamma = 90^\circ$.
Volumen	$538.37(2) \text{ \AA}^3$	
Teilchen pro Elementarzelle	2	
Berechnete Dichte	$1.347 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	0.267 mm^{-1}	
F(000)	232 e	
Kristallgröße	$0.18 \times 0.13 \times 0.10 \text{ mm}^3$	
θ -Grenzen für Datensammlung	2.60 bis 30.97° .	
Indexbereich	$-7 \leq h \leq 7, -18 \leq k \leq 18, -11 \leq l \leq 11$	
Aufgenommene Reflexe	14969	
Unabhängige Reflexe	3421 [$R_{\text{int}} = 0.0426$]	

Reflexe mit $I > 2\sigma(I)$	3224	
Vollständigkeit für $\theta = 30.97^\circ$	99.9 %	
Absorptionskorrektur	keine	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	3421 / 1 / 192	
Goodness-of-fit auf F^2	1.036	
R [$I > 2\sigma(I)$]	$R_1 = 0.0286$	$wR^2 = 0.0700$
R-Werte (sämtliche Daten)	$R_1 = 0.0321$	$wR^2 = 0.0717$
Absolute Strukturparameter	-0.01(5)	
Größte Differenz Peak und Loch	0.261 und -0.157 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

C(1)-N(6A)	1.3423(15)	C(1)-N(2)	1.3814(15)
C(1)-S(1)	1.6745(12)	C(3)-N(2)	1.4828(14)
C(3)-C(3A)	1.5268(17)	C(3A)-N(6A)	1.4736(14)
C(3A)-C(4)	1.5256(16)	C(4)-C(5)	1.5454(18)
C(5)-C(6)	1.5416(18)	C(6)-N(6A)	1.4657(15)
C(21)-C(26)	1.3984(16)	C(21)-C(22)	1.3976(16)
C(21)-N(2)	1.4144(14)	C(22)-C(23)	1.3959(18)
C(23)-C(24)	1.3931(18)	C(24)-C(25)	1.3882(19)
C(25)-C(26)	1.3910(17)		
N(6A)-C(1)-N(2)	107.39(10)	N(6A)-C(1)-S(1)	124.33(9)
N(2)-C(1)-S(1)	128.24(9)	N(2)-C(3)-C(3A)	101.71(9)
N(6A)-C(3A)-C(3)	101.96(9)	N(6A)-C(3A)-C(4)	102.95(9)
C(3)-C(3A)-C(4)	120.10(10)	C(3A)-C(4)-C(5)	102.30(10)
C(6)-C(5)-C(4)	104.62(10)	N(6A)-C(6)-C(5)	102.60(10)
C(26)-C(21)-C(22)	119.64(11)	C(26)-C(21)-N(2)	121.22(10)
C(22)-C(21)-N(2)	119.01(11)	C(23)-C(22)-C(21)	120.13(12)
C(22)-C(23)-C(24)	120.17(11)	C(25)-C(24)-C(23)	119.42(11)
C(24)-C(25)-C(26)	121.04(12)	C(25)-C(26)-C(21)	119.59(11)
C(1)-N(2)-C(21)	127.78(10)	C(1)-N(2)-C(3)	110.19(9)
C(21)-N(2)-C(3)	121.35(10)	C(1)-N(6A)-C(6)	128.25(10)
C(1)-N(6A)-C(3A)	113.10(9)	C(6)-N(6A)-C(3A)	113.27(9)

Kristallographische Daten der Verbindung 294



Kristalldaten

Summenformel	$\text{C}_{20}\text{H}_{26}\text{ClN}_2\text{Rh}$	
Farbe	gelb	
Molmasse	$432.79 \text{ g} \cdot \text{mol}^{-1}$	
Temperatur	100 K	
Wellenlänge	0.71073 \AA	
Kristallsystem	Orthorhombisch	
Raumgruppe	$\text{P2}_1\text{2}_1\text{2}_1$, (no. 19)	
Gitterkonstanten	$a = 10.09290(10) \text{ \AA}$	$\alpha = 90^\circ$.
	$b = 11.35430(10) \text{ \AA}$	$\beta = 90^\circ$.
	$c = 15.2804(2) \text{ \AA}$	$\gamma = 90^\circ$.
Volumen	$1751.10(3) \text{ \AA}^3$	
Teilchen pro Elementarzelle	4	
Berechnete Dichte	$1.642 \text{ mg} \cdot \text{m}^{-3}$	
Absorptionskoeffizient	1.131 mm^{-1}	
$F(000)$	888 e	
Kristallgröße	$0.45 \times 0.05 \times 0.04 \text{ mm}^3$	
θ -Grenzen für Datensammlung	4.62 bis 33.25° .	
Indexbereich	$-15 \leq h \leq 14$, $-17 \leq k \leq 13$, $-23 \leq l \leq 23$	
Aufgenommene Reflexe	23570	
Unabhängige Reflexe	6713 [$R_{\text{int}} = 0.0468$]	

Reflexe mit $I > 2\sigma(I)$	6155	
Vollständigkeit für $\theta = 27.50^\circ$	99.2 %	
Absorptionskorrektur	Gaussian	
Max. and min. Transmission	0.96 und 0.75	
Verfeinerungsmethode	Vollmatrix, kleinste Fehlerquadrate auf F^2	
Daten/ Einschränkungen/ Parameter	6713 / 0 / 217	
Goodness-of-fit auf F^2	1.039	
R [$I > 2\sigma(I)$]	$R_1 = 0.0274$	$wR^2 = 0.0571$
R-Werte (sämtliche Daten)	$R_1 = 0.0325$	$wR^2 = 0.0587$
Absolute Strukturparameter	-0.03(2)	
Größte Differenz Peak und Loch	0.539 und -0.707 e · Å ⁻³	

Bindungslängen [Å] und -winkel [°]

Rh(1)-C(1)	2.0068(17)	Rh(1)-C(11)	2.0956(17)
Rh(1)-C(18)	2.1166(18)	Rh(1)-C(15)	2.192(2)
Rh(1)-C(14)	2.236(2)	Rh(1)-Cl(1)	2.3681(5)
C(1)-N(6A)	1.335(3)	C(1)-N(2)	1.357(2)
N(2)-C(21)	1.410(2)	N(2)-C(3)	1.474(3)
C(3)-C(3A)	1.526(3)	C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900	C(3A)-N(6A)	1.473(3)
C(3A)-C(4)	1.512(3)	C(3A)-H(3C)	1.0000
C(4)-C(5)	1.539(3)	C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900	C(5)-C(6)	1.539(3)
C(5)-H(5A)	0.9900	C(5)-H(5B)	0.9900
C(6)-N(6A)	1.465(2)	C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900	C(11)-C(18)	1.403(3)
C(11)-C(12)	1.512(3)	C(11)-H(11)	1.0000
C(12)-C(13)	1.533(3)	C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900	C(13)-C(14)	1.504(3)
C(13)-H(13A)	0.9900	C(13)-H(13B)	0.9900
C(14)-C(15)	1.381(3)	C(14)-H(14)	1.0000
C(15)-C(16)	1.511(3)	C(15)-H(15)	1.0000
C(16)-C(17)	1.538(3)	C(16)-H(16A)	0.9900

C(16)-H(16B)	0.9900	C(17)-C(18)	1.529(3)
C(17)-H(17A)	0.9900	C(17)-H(17B)	0.9900
C(18)-H(18)	1.0000	C(21)-C(26)	1.397(3)
C(21)-C(22)	1.396(3)	C(22)-C(23)	1.395(3)
C(22)-H(22)	0.9500	C(23)-C(24)	1.380(3)
C(23)-H(23)	0.9500	C(24)-C(25)	1.388(3)
C(24)-H(24)	0.9500	C(25)-C(26)	1.374(3)
C(25)-H(25)	0.9500	C(26)-H(26)	0.9500
C(1)-Rh(1)-C(11)	93.05(8)	C(1)-Rh(1)-C(18)	95.36(7)
C(11)-Rh(1)-C(18)	38.90(7)	C(1)-Rh(1)-C(15)	159.17(9)
C(11)-Rh(1)-C(15)	97.99(8)	C(18)-Rh(1)-C(15)	82.56(8)
C(1)-Rh(1)-C(14)	164.33(9)	C(11)-Rh(1)-C(14)	81.35(8)
C(18)-Rh(1)-C(14)	89.44(7)	C(15)-Rh(1)-C(14)	36.34(8)
C(1)-Rh(1)-Cl(1)	85.85(5)	C(11)-Rh(1)-Cl(1)	152.60(5)
C(18)-Rh(1)-Cl(1)	168.46(6)	C(15)-Rh(1)-Cl(1)	92.21(6)
C(14)-Rh(1)-Cl(1)	92.42(6)	N(6A)-C(1)-N(2)	107.66(15)
N(6A)-C(1)-Rh(1)	121.94(14)	N(2)-C(1)-Rh(1)	130.13(14)
C(1)-N(2)-C(21)	127.51(16)	C(1)-N(2)-C(3)	112.59(16)
C(21)-N(2)-C(3)	119.91(16)	N(2)-C(3)-C(3A)	102.73(15)
N(2)-C(3)-H(3A)	111.2	C(3A)-C(3)-H(3A)	111.2
N(2)-C(3)-H(3B)	111.2	C(3A)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.1	N(6A)-C(3A)-C(4)	101.72(17)
N(6A)-C(3A)-C(3)	102.14(15)	C(4)-C(3A)-C(3)	119.20(18)
N(6A)-C(3A)-H(3C)	110.9	C(4)-C(3A)-H(3C)	110.9
C(3)-C(3A)-H(3C)	110.9	C(3A)-C(4)-C(5)	102.42(17)
C(3A)-C(4)-H(4A)	111.3	C(5)-C(4)-H(4A)	111.3
C(3A)-C(4)-H(4B)	111.3	C(5)-C(4)-H(4B)	111.3
H(4A)-C(4)-H(4B)	109.2	C(4)-C(5)-C(6)	105.27(18)
C(4)-C(5)-H(5A)	110.7	C(6)-C(5)-H(5A)	110.7
C(4)-C(5)-H(5B)	110.7	C(6)-C(5)-H(5B)	110.7
H(5A)-C(5)-H(5B)	108.8	N(6A)-C(6)-C(5)	104.11(16)
N(6A)-C(6)-H(6A)	110.9	C(5)-C(6)-H(6A)	110.9
N(6A)-C(6)-H(6B)	110.9	C(5)-C(6)-H(6B)	110.9

H(6A)-C(6)-H(6B)	109.0	C(1)-N(6A)-C(6)	125.92(16)
C(1)-N(6A)-C(3A)	113.16(16)	C(6)-N(6A)-C(3A)	109.77(15)
C(18)-C(11)-C(12)	125.21(19)	C(18)-C(11)-Rh(1)	71.36(11)
C(12)-C(11)-Rh(1)	110.90(13)	C(18)-C(11)-H(11)	113.9
C(12)-C(11)-H(11)	113.9	Rh(1)-C(11)-H(11)	113.9
C(11)-C(12)-C(13)	113.43(17)	C(11)-C(12)-H(12A)	108.9
C(13)-C(12)-H(12A)	108.9	C(11)-C(12)-H(12B)	108.9
C(13)-C(12)-H(12B)	108.9	H(12A)-C(12)-H(12B)	107.7
C(14)-C(13)-C(12)	112.25(16)	C(14)-C(13)-H(13A)	109.2
C(12)-C(13)-H(13A)	109.2	C(14)-C(13)-H(13B)	109.2
C(12)-C(13)-H(13B)	109.2	H(13A)-C(13)-H(13B)	107.9
C(15)-C(14)-C(13)	124.01(19)	C(15)-C(14)-Rh(1)	70.12(11)
C(13)-C(14)-Rh(1)	110.80(13)	C(15)-C(14)-H(14)	114.5
C(13)-C(14)-H(14)	114.5	Rh(1)-C(14)-H(14)	114.5
C(14)-C(15)-C(16)	125.7(2)	C(14)-C(15)-Rh(1)	73.55(11)
C(16)-C(15)-Rh(1)	106.76(13)	C(14)-C(15)-H(15)	114.2
C(16)-C(15)-H(15)	114.2	Rh(1)-C(15)-H(15)	114.2
C(15)-C(16)-C(17)	114.04(17)	C(15)-C(16)-H(16A)	108.7
C(17)-C(16)-H(16A)	108.7	C(15)-C(16)-H(16B)	108.7
C(17)-C(16)-H(16B)	108.7	H(16A)-C(16)-H(16B)	107.6
C(18)-C(17)-C(16)	112.34(17)	C(18)-C(17)-H(17A)	109.1
C(16)-C(17)-H(17A)	109.1	C(18)-C(17)-H(17B)	109.1
C(16)-C(17)-H(17B)	109.1	H(17A)-C(17)-H(17B)	107.9
C(11)-C(18)-C(17)	124.84(18)	C(11)-C(18)-Rh(1)	69.74(10)
C(17)-C(18)-Rh(1)	112.94(13)	C(11)-C(18)-H(18)	113.8
C(17)-C(18)-H(18)	113.8	Rh(1)-C(18)-H(18)	113.8
C(26)-C(21)-C(22)	118.54(18)	C(26)-C(21)-N(2)	121.70(17)
C(22)-C(21)-N(2)	119.77(17)	C(21)-C(22)-C(23)	120.1(2)
C(21)-C(22)-H(22)	120.0	C(23)-C(22)-H(22)	120.0
C(24)-C(23)-C(22)	120.8(2)	C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6	C(23)-C(24)-C(25)	118.9(2)
C(23)-C(24)-H(24)	120.6	C(25)-C(24)-H(24)	120.6
C(26)-C(25)-C(24)	121.0(2)	C(26)-C(25)-H(25)	119.5
C(24)-C(25)-H(25)	119.5	C(25)-C(26)-C(21)	120.67(19)

C(25)-C(26)-H(26)	119.7	C(21)-C(26)-H(26)	119.7
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