Table 1. Crystal data and structure refinement for 2a.

Empirical formula	$C_{19}H_{18}F_6NiO$	
Formula weight	435.041 $g \cdot mol^{-1}$	
Temperature	199(2) K	
Wavelength	0.71073 Å	
Scanmodus	omega/theta	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.115(1) Å,	$\alpha = 90°$
	b = 9.311(1) Å	$\beta = 91.44(1)°$
	c = 15.057(1) Å	$\gamma = 90°$
Volume	1697.9(3) $Å^3$	
Z	4	
Density (calculated)	1.702 $Mg \cdot m^{-3}$	
Absorption coefficient	1.211 mm^{-1}	
F(000)	888	
Crystal size	0.1 × 0.15 × 0.5 mm	
θ-range for data collection	3.0 to 27.0°	
Index ranges	$-15 \le h \le 15$, $0 \le k \le 11$, $0 \le l \le 19$	
Reflections collected	3826	
Independent reflections	3682 (R_{int} = 0.0192)	
Observed reflections	2942	
Refinement method	Full-matrix Least-Squares on F^2	
Parameters	244	
Goodness-of Fit on F^2	1.069	
Final R indices [$F_0 > 4\sigma(F_0)$]	R1 = 0.0314, wR2 = 0.0794	
R indices (all data)	R1 = 0.0499, wR2 = 0.0871	
Largest diff. peak and hole	0.679, -0.419 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacment parameters [$Å^2 \cdot 10^3$] for 2a. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
C(1)	0.3419(2)	0.3934(2)	0.8585(2)	0.0250(5)
C(2)	0.2627(2)	0.2833(2)	0.8279(1)	0.0214(4)
C(3)	0.1472(2)	0.2728(2)	0.8480(1)	0.0221(4)
C(4)	0.0903(2)	0.3800(3)	0.9062(2)	0.0300(5)
C(5)	0.0720(2)	0.2113(3)	0.7767(2)	0.0282(5)
C(6)	0.4626(2)	0.3714(2)	0.8394(1)	0.0222(4)
C(7)	0.5030(2)	0.2632(2)	0.7849(1)	0.0261(5)
C(8)	0.6152(2)	0.2516(3)	0.7699(2)	0.0303(5)
C(9)	0.6888(2)	0.3468(3)	0.8103(2)	0.0327(5)
C(10)	0.6501(2)	0.4525(3)	0.8660(2)	0.0328(5)
C(11)	0.5380(2)	0.4657(3)	0.8797(2)	0.0280(5)
C(12)	0.3784(2)	0.1093(2)	0.9959(2)	0.0251(5)
C(13)	0.3748(2)	-0.0031(2)	0.9381(2)	0.0240(5)
C(14)	0.3371(2)	-0.1531(2)	0.9597(2)	0.0277(5)
C(15)	0.2134(2)	-0.1777(3)	0.9381(2)	0.0328(5)
C(16)	0.1423(2)	-0.0479(3)	0.9527(2)	0.0278(5)
C(17)	0.1497(2)	0.0429(3)	1.0233(2)	0.0279(5)
C(18)	0.2288(2)	0.0248(3)	1.1011(2)	0.0310(5)
C(19)	0.3373(2)	0.1081(3)	1.0896(2)	0.0316(5)
Ni(1)	0.23680(2)	0.13282(3)	0.91542(2)	0.01974(9)
O(1)	0.3155(2)	0.5004(2)	0.8991(2)	0.0441(5)
F(3)	0.0824(1)	0.5115(2)	0.8707(1)	0.0451(4)
F(2)	0.1410(1)	0.3957(2)	0.9858(1)	0.0385(4)
F(1)	-0.0130(1)	0.3390(2)	0.9230(1)	0.0504(5)
F(6)	-0.0122(1)	0.1346(2)	0.8073(1)	0.0379(3)
F(5)	0.1258(1)	0.1250(2)	0.7219(1)	0.0474(4)
F(4)	0.0249(1)	0.3139(2)	0.7249(1)	0.0471(4)

Table 3. Bond lengths [Å] and angles [°] for 2a.

C(1)-O(1)	1.216(3)	C(1)-C(2)	1.471(3)
C(1)-C(6)	1.510(3)	C(2)-C(3)	1.442(3)
C(2)-Ni(1)	1.955(2)	C(3)-C(5)	1.504(3)
C(3)-C(4)	1.507(3)	C(3)-Ni(1)	1.962(2)
C(4)-F(3)	1.338(3)	C(4)-F(1)	1.340(3)
C(4)-F(2)	1.341(3)	C(5)-F(5)	1.333(3)
C(5)-F(6)	1.338(3)	C(5)-F(4)	1.351(3)
C(6)-C(7)	1.395(3)	C(6)-C(11)	1.395(3)
C(7)-C(8)	1.388(3)	C(8)-C(9)	1.386(4)
C(9)-C(10)	1.383(4)	C(10)-C(11)	1.384(4)
C(12)-C(13)	1.360(3)	C(12)-C(19)	1.509(3)
C(12)-Ni(1)	2.087(2)	C(13)-C(14)	1.507(3)
C(13)-Ni(1)	2.118(2)	C(14)-C(15)	1.543(3)
C(15)-C(16)	1.503(4)	C(16)-C(17)	1.360(4)
C(16)-Ni(1)	2.119(2)	C(17)-C(18)	1.504(3)
C(17)-Ni(1)	2.131(2)	C(18)-C(19)	1.540(4)

O(1)-C(1)-C(2)	123.4(2)	O(1)-C(1)-C(6)	118.4(2)
C(2)-C(1)-C(6)	118.2(2)	C(3)-C(2)-C(1)	127.6(2)
C(3)-C(2)-Ni(1)	68.7(1)	C(1)-C(2)-Ni(1)	113.7(2)
C(2)-C(3)-C(5)	116.7(2)	C(2)-C(3)-C(4)	122.5(2)
C(5)-C(3)-C(4)	112.9(2)	C(2)-C(3)-Ni(1)	68.1(1)
C(5)-C(3)-Ni(1)	115.7(2)	C(4)-C(3)-Ni(1)	113.2(2)
F(3)-C(4)-F(1)	106.2(2)	F(3)-C(4)-F(2)	106.5(2)
F(1)-C(4)-F(2)	105.7(2)	F(3)-C(4)-C(3)	113.8(2)
F(1)-C(4)-C(3)	111.4(2)	F(2)-C(4)-C(3)	112.7(2)
F(5)-C(5)-F(6)	106.3(2)	F(5)-C(5)-F(4)	105.9(2)
F(6)-C(5)-F(4)	105.1(2)	F(5)-C(5)-C(3)	112.0(2)
F(6)-C(5)-C(3)	114.3(2)	F(4)-C(5)-C(3)	112.5(2)
C(7)-C(6)-C(11)	118.3(2)	C(7)-C(6)-C(1)	124.4(2)
C(11)-C(6)-C(1)	117.3(2)	C(8)-C(7)-C(6)	120.7(2)
C(9)-C(8)-C(7)	120.1(2)	C(10)-C(9)-C(8)	119.8(2)
C(9)-C(10)-C(11)	120.1(2)	C(10)-C(11)-C(6)	121.0(2)
C(13)-C(12)-C(19)	125.9(2)	C(13)-C(12)-Ni(1)	72.4(1)
C(19)-C(12)-Ni(1)	104.9(2)	C(12)-C(13)-C(14)	125.4(2)
C(12)-C(13)-Ni(1)	69.9(1)	C(14)-C(13)-Ni(1)	110.3(2)
C(13)-C(14)-C(15)	112.9(2)	C(16)-C(15)-C(14)	114.0(2)
C(17)-C(16)-C(15)	126.0(2)	C(17)-C(16)-Ni(1)	71.8(1)
C(15)-C(16)-Ni(1)	106.5(2)	C(16)-C(17)-C(18)	124.6(2)
C(16)-C(17)-Ni(1)	70.9(1)	C(18)-C(17)-Ni(1)	108.6(2)
C(17)-C(18)-C(19)	112.7(2)	C(12)-C(19)-C(18)	114.3(2)
C(2)-Ni(1)-C(3)	43.19(9)	C(2)-Ni(1)-C(12)	108.86(9)
C(3)-Ni(1)-C(12)	143.69(9)	C(2)-Ni(1)-C(13)	113.44(9)
C(3)-Ni(1)-C(13)	154.73(9)	C(12)-Ni(1)-C(13)	37.74(9)
C(2)-Ni(1)-C(16)	147.63(9)	C(3)-Ni(1)-C(16)	111.64(9)
C(12)-Ni(1)-C(16)	101.84(9)	C(13)-Ni(1)-C(16)	84.99(9)
C(2)-Ni(1)-C(17)	152.48(9)	C(3)-Ni(1)-C(17)	112.17(9)
C(12)-Ni(1)-C(17)	86.11(9)	C(13)-Ni(1)-C(17)	92.66(9)
C(16)-Ni(1)-C(17)	37.3(1)		

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 2a.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	28(1)	18(1)	29(1)	3(1)	-1(1)	-1(1)
C(2)	25(1)	16(1)	24(1)	2(1)	-2(1)	1(1)
C(3)	22(1)	19(1)	25(1)	2(1)	-3(1)	0(1)
C(4)	26(1)	25(1)	39(1)	-1(1)	-2(1)	4(1)
C(5)	26(1)	28(1)	30(1)	2(1)	-6(1)	-1(1)
C(6)	26(1)	18(1)	23(1)	6(1)	-1(1)	-3(1)
C(7)	32(1)	23(1)	23(1)	2(1)	-1(1)	-4(1)
C(8)	35(1)	29(1)	28(1)	3(1)	5(1)	2(1)
C(9)	24(1)	36(1)	38(1)	11(1)	2(1)	0(1)
C(10)	31(1)	29(1)	39(1)	4(1)	-3(1)	-9(1)
C(11)	33(1)	21(1)	30(1)	1(1)	-1(1)	-6(1)
C(12)	20(1)	24(1)	31(1)	5(1)	-6(1)	-1(1)
C(13)	19(1)	26(1)	27(1)	6(1)	1(1)	3(1)
C(14)	32(1)	20(1)	31(1)	1(1)	5(1)	6(1)
C(15)	39(1)	21(1)	39(1)	-1(1)	2(1)	-5(1)
C(16)	23(1)	26(1)	34(1)	9(1)	-1(1)	-6(1)
C(17)	23(1)	26(1)	35(1)	6(1)	8(1)	1(1)
C(18)	37(1)	31(1)	26(1)	0(1)	7(1)	4(1)
C(19)	36(1)	32(1)	27(1)	-2(1)	-5(1)	0(1)
Ni(1)	18(1)	17(1)	24(1)	3(1)	-2(1)	0(1)
O(1)	33(1)	25(1)	75(1)	-18(1)	8(1)	-3(1)
F(3)	51(1)	22(1)	61(1)	2(1)	-10(1)	14(1)
F(2)	46(1)	36(1)	33(1)	-10(1)	0(1)	4(1)
F(1)	28(1)	49(1)	76(1)	-21(1)	14(1)	-3(1)
F(6)	31(1)	38(1)	44(1)	4(1)	-7(1)	-12(1)
F(5)	35(1)	61(1)	46(1)	-28(1)	-6(1)	-3(1)
F(4)	48(1)	45(1)	47(1)	18(1)	-24(1)	-5(1)

Table 5. Hydrogen coordinates and isotropic displacement parameters [Å^2] for 2a.

	x/a	y/b	z/c	U(eq)
H(2)	0.2908(2)	0.2106(2)	0.7904(1)	0.026
H(7)	0.4531(2)	0.1968(2)	0.7577(1)	0.031
H(8)	0.6417(2)	0.1783(3)	0.7320(2)	0.036
H(9)	0.7656(2)	0.3394(3)	0.7997(2)	0.039
H(10)	0.7006(2)	0.5162(3)	0.8950(2)	0.039
H(11)	0.5121(2)	0.5400(3)	0.9170(2)	0.034
H(12)	0.4097(2)	0.1963(2)	0.9753(2)	0.030
H(13)	0.3979(2)	0.0144(2)	0.8793(2)	0.029
H(14A)	0.3515(2)	-0.1717(2)	1.0237(2)	0.033
H(14B)	0.3810(2)	-0.2227(2)	0.9257(2)	0.033
H(15A)	0.2048(2)	-0.2078(3)	0.8752(2)	0.039
H(15B)	0.1866(2)	-0.2572(3)	0.9754(2)	0.039
H(16)	0.0871(2)	-0.0274(3)	0.9085(2)	0.033
H(17)	0.1015(2)	0.1234(3)	1.0235(2)	0.033
H(18A)	0.2458(2)	-0.0785(3)	1.1088(2)	0.037
H(18B)	0.1929(2)	0.0587(3)	1.1556(2)	0.037
H(19A)	0.3263(2)	0.2085(3)	1.1090(2)	0.038
H(19B)	0.3949(2)	0.0651(3)	1.1291(2)	0.038

Table 1. Crystal data and structure refinement for 3d.

Empirical formula	$C_{25}H_{34}F_6N_2NiP_2$	
Formula weight	597.191 $g \cdot mol^{-1}$	
Temperature	199(2) K	
Wavelength	0.71073 Å	
Scanmodus	omega/theta	
Crystal system	orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	a = 19.754(2) Å,	$\alpha = 90°$
	b = 12.066(1) Å	$\beta = 90°$
	c = 12.019(1) Å	$\gamma = 90°$
Volume	2864.7(4) $Å^3$	
Z	4	
Density (calculated)	1.385 $Mg \cdot m^{-3}$	
Absorption coefficient	0.844 mm^{-1}	
F(000)	1240	
Crystal size	0.6 × 0.45 × 0.45 mm	
θ-range for data collection	3.0 to 27.0°	
Index ranges	$0 \le h \le 25$, $0 \le k \le 15$, $-15 \le l \le 15$	
Reflections collected	6192	
Independent reflections	6192	
Observed reflections	5741	
Refinement method	Full-matrix Least-Squares on F^2	
Restraints	1	
Parameters	335	
Goodness-of Fit on F^2	1.143	
Final R indices [$F_o > 4\sigma(F_o)$]	R1 = 0.0292, wR2 = 0.0894	
R indices (all data)	R1 = 0.0363, wR2 = 0.1068	
Flack-Parameter	-0.01(1)	
Extinction coefficient	0.0055(6)	
Largest diff. peak and hole	0.271, -0.188 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacment parameters [Å^2] for 3d. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
Ni(1)	0.94659(2)	0.00816(2)	0.06197(4)	0.0231(1)
P(1)	0.96809(4)	0.17906(6)	0.10713(7)	0.0305(2)
P(2)	0.83807(4)	0.01620(6)	0.02375(7)	0.0297(2)
F(31)	1.0148(1)	-0.1297(2)	0.2544(2)	0.0472(5)
F(32)	1.10500(9)	-0.1894(2)	0.1770(2)	0.0423(5)
F(33)	1.0973(1)	-0.0188(2)	0.2174(2)	0.0536(6)
F(41)	1.1251(1)	-0.1329(2)	-0.0420(2)	0.0488(5)
F(42)	1.1162(1)	0.0374(2)	0.0002(2)	0.0608(7)
F(43)	1.0496(1)	-0.0356(2)	-0.1207(2)	0.0508(5)
N(1)	0.8848(1)	-0.2419(2)	0.1078(2)	0.0266(4)
N(2)	0.9713(1)	-0.1376(2)	0.0323(2)	0.0238(4)
C(1)	0.9469(1)	-0.2352(2)	0.0768(2)	0.0234(5)
C(2)	1.0287(1)	-0.0798(2)	0.0671(2)	0.0236(4)
C(3)	1.0610(1)	-0.1041(2)	0.1781(3)	0.0308(6)
C(4)	1.0790(1)	-0.0532(2)	-0.0233(3)	0.0323(6)
C(11)	1.0445(2)	0.2085(3)	0.1875(4)	0.0483(9)
C(12)	0.9761(2)	0.2712(3)	-0.0119(3)	0.0493(8)
C(13)	0.9060(2)	0.2516(3)	0.1922(3)	0.0440(8)
C(21)	0.8060(2)	0.1408(3)	-0.0464(3)	0.0425(7)
C(22)	0.7841(2)	0.0053(3)	0.1452(4)	0.052(1)
C(23)	0.8045(2)	-0.0894(3)	-0.0688(3)	0.0448(8)
C(51)	0.9962(1)	-0.3298(2)	0.0780(2)	0.0262(5)
C(52)	1.0046(2)	-0.3949(2)	0.1722(3)	0.0323(6)
C(53)	1.0533(2)	-0.4778(3)	0.1737(4)	0.0433(8)
C(54)	1.0930(2)	-0.4963(2)	0.0794(4)	0.050(1)
C(55)	1.0842(2)	-0.4337(3)	-0.0141(4)	0.0464(8)
C(56)	1.0363(2)	-0.3495(3)	-0.0149(3)	0.0338(6)
C(61)	0.8528(1)	-0.3441(2)	0.1326(2)	0.0262(5)
C(62)	0.8295(1)	-0.3610(2)	0.2423(2)	0.0316(6)
C(63)	0.7931(2)	-0.4560(3)	0.2667(3)	0.0367(7)
C(64)	0.7771(2)	-0.5344(3)	0.1869(3)	0.0391(7)
C(65)	0.7997(2)	-0.5166(2)	0.0790(3)	0.0364(8)
C(66)	0.8379(1)	-0.4230(2)	0.0505(3)	0.0306(5)
C(67)	0.8442(2)	-0.2765(3)	0.3304(3)	0.0441(7)
C(68)	0.7362(2)	-0.6363(3)	0.2154(4)	0.054(1)
C(69)	0.8617(2)	-0.4084(3)	-0.0672(3)	0.0416(7)

Table 3. Bond lengths [A] and angles [°] for 3d.

Ni(1)-N(2)	1.859(2)	Ni(1)-C(2)	1.939(2)
Ni(1)-P(1)	2.1742(8)	Ni(1)-P(2)	2.1944(8)
P(1)-C(12)	1.819(4)	P(1)-C(13)	1.821(3)
P(1)-C(11)	1.827(3)	P(2)-C(22)	1.812(4)
P(2)-C(23)	1.817(4)	P(2)-C(21)	1.836(3)
F(31)-C(3)	1.331(4)	F(32)-C(3)	1.348(3)
F(33)-C(3)	1.340(3)	F(41)-C(4)	1.344(4)
F(42)-C(4)	1.347(4)	F(43)-C(4)	1.324(4)
N(1)-C(1)	1.285(3)	N(1)-C(61)	1.417(3)
N(2)-C(1)	1.380(3)	N(2)-C(2)	1.395(3)
C(1)-C(51)	1.501(3)	C(2)-C(4)	1.506(4)
C(2)-C(3)	1.507(4)	C(51)-C(52)	1.387(4)
C(51)-C(56)	1.389(4)	C(52)-C(53)	1.388(4)
C(53)-C(54)	1.396(7)	C(54)-C(55)	1.365(6)
C(55)-C(56)	1.389(4)	C(61)-C(66)	1.402(4)
C(61)-C(62)	1.412(4)	C(62)-C(63)	1.384(4)
C(62)-C(67)	1.499(5)	C(63)-C(64)	1.384(5)
C(64)-C(65)	1.388(5)	C(64)-C(68)	1.511(4)
C(65)-C(66)	1.401(4)	C(66)-C(69)	1.501(4)

N(2)-Ni(1)-C(2)	43.02(9)	N(2)-Ni(1)-P(1)	153.31(7)
C(2)-Ni(1)-P(1)	110.36(8)	N(2)-Ni(1)-P(2)	104.96(7)
C(2)-Ni(1)-P(2)	147.97(8)	P(1)-Ni(1)-P(2)	101.61(3)
C(12)-P(1)-C(13)	101.9(2)	C(12)-P(1)-C(11)	103.0(2)
C(13)-P(1)-C(11)	99.5(2)	C(12)-P(1)-Ni(1)	113.6(1)
C(13)-P(1)-Ni(1)	117.7(1)	C(11)-P(1)-Ni(1)	118.6(1)
C(22)-P(2)-C(23)	103.2(2)	C(22)-P(2)-C(21)	103.1(2)
C(23)-P(2)-C(21)	99.6(2)	C(22)-P(2)-Ni(1)	113.7(2)
C(23)-P(2)-Ni(1)	117.0(1)	C(21)-P(2)-Ni(1)	118.0(1)
C(1)-N(1)-C(61)	122.8(2)	C(1)-N(2)-C(2)	126.4(2)
C(1)-N(2)-Ni(1)	129.9(2)	C(2)-N(2)-Ni(1)	71.6(1)
N(1)-C(1)-N(2)	119.9(2)	N(1)-C(1)-C(51)	124.7(2)
N(2)-C(1)-C(51)	115.3(2)	N(2)-C(2)-C(4)	115.2(2)
N(2)-C(2)-C(3)	120.8(2)	C(4)-C(2)-C(3)	113.6(2)
N(2)-C(2)-Ni(1)	65.4(1)	C(4)-C(2)-Ni(1)	114.3(2)
C(3)-C(2)-Ni(1)	119.3(2)	F(31)-C(3)-F(33)	107.6(3)
F(31)-C(3)-F(32)	105.8(2)	F(33)-C(3)-F(32)	104.2(2)
F(31)-C(3)-C(2)	111.4(2)	F(33)-C(3)-C(2)	112.9(2)
F(32)-C(3)-C(2)	114.4(2)	F(43)-C(4)-F(41)	105.3(3)
F(43)-C(4)-F(42)	107.1(3)	F(41)-C(4)-F(42)	104.2(3)
F(43)-C(4)-C(2)	112.5(2)	F(41)-C(4)-C(2)	114.6(2)
F(42)-C(4)-C(2)	112.4(2)	C(52)-C(51)-C(56)	119.5(3)
C(52)-C(51)-C(1)	121.1(2)	C(56)-C(51)-C(1)	119.4(2)
C(51)-C(52)-C(53)	120.1(3)	C(52)-C(53)-C(54)	119.6(3)
C(55)-C(54)-C(53)	120.6(3)	C(54)-C(55)-C(56)	119.8(3)
C(55)-C(56)-C(51)	120.5(3)	C(66)-C(61)-C(62)	119.4(3)
C(66)-C(61)-N(1)	122.4(2)	C(62)-C(61)-N(1)	117.9(2)
C(63)-C(62)-C(61)	119.1(3)	C(63)-C(62)-C(67)	121.0(3)
C(61)-C(62)-C(67)	119.9(3)	C(64)-C(63)-C(62)	122.6(3)
C(63)-C(64)-C(65)	117.9(3)	C(63)-C(64)-C(68)	121.5(3)
C(65)-C(64)-C(68)	120.7(3)	C(64)-C(65)-C(66)	121.8(3)
C(65)-C(66)-C(61)	119.2(3)	C(65)-C(66)-C(69)	119.6(3)
C(61)-C(66)-C(69)	121.2(2)		

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 3d.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ni(1)	18(1)	20(1)	31(1)	1(1)	-1(1)	1(1)
P(1)	33(1)	22(1)	37(1)	-2(1)	-1(1)	2(1)
P(2)	19(1)	35(1)	35(1)	6(1)	0(1)	2(1)
F(31)	52(1)	64(1)	25(1)	4(1)	-2(1)	8(1)
F(32)	42(1)	35(1)	50(1)	-2(1)	-19(1)	14(1)
F(33)	64(1)	33(1)	65(1)	-7(1)	-35(1)	-3(1)
F(41)	34(1)	57(1)	55(1)	2(1)	14(1)	13(1)
F(42)	50(1)	51(1)	82(2)	-13(1)	23(1)	-28(1)
F(43)	40(1)	73(2)	39(1)	19(1)	7(1)	3(1)
N(1)	24(1)	26(1)	30(1)	0(1)	4(1)	0(1)
N(2)	22(1)	20(1)	29(1)	1(1)	-2(1)	2(1)
C(1)	27(1)	24(1)	19(1)	0(1)	-3(1)	0(1)
C(2)	19(1)	23(1)	29(1)	0(1)	0(1)	1(1)
C(3)	28(1)	28(1)	36(1)	-1(1)	-10(1)	1(1)
C(4)	24(1)	33(1)	40(2)	-1(1)	4(1)	-2(1)
C(11)	46(2)	31(2)	68(2)	-11(2)	-14(2)	-3(1)
C(12)	69(2)	36(2)	43(2)	5(1)	5(2)	-14(2)
C(13)	56(2)	42(2)	35(2)	-5(1)	-1(1)	17(2)
C(21)	36(2)	46(2)	46(2)	8(2)	-6(1)	11(1)
C(22)	37(2)	69(3)	49(2)	15(2)	11(2)	4(2)
C(23)	36(2)	45(2)	54(2)	4(2)	-12(1)	-6(1)
C(51)	25(1)	22(1)	32(2)	-1(1)	-3(1)	0(1)
C(52)	34(1)	26(1)	38(2)	3(1)	-3(1)	0(1)
C(53)	49(2)	24(1)	57(2)	5(1)	-19(2)	2(1)
C(54)	36(2)	30(1)	83(3)	-7(2)	-13(2)	9(1)
C(55)	37(2)	35(2)	67(2)	-11(2)	13(2)	5(1)
C(56)	33(1)	29(1)	40(2)	0(1)	5(1)	0(1)
C(61)	22(1)	26(1)	31(1)	3(1)	2(1)	2(1)
C(62)	25(1)	36(2)	34(2)	6(1)	3(1)	3(1)
C(63)	24(1)	43(2)	43(2)	15(1)	7(1)	6(1)
C(64)	23(1)	31(1)	63(2)	14(1)	6(1)	2(1)
C(65)	26(1)	30(1)	53(2)	-2(1)	0(1)	0(1)
C(66)	23(1)	32(1)	37(2)	0(1)	1(1)	0(1)
C(67)	42(2)	55(2)	36(2)	-4(1)	7(1)	0(2)
C(68)	35(2)	32(2)	96(3)	18(2)	15(2)	-3(1)
C(69)	41(2)	49(2)	35(2)	-8(1)	3(1)	-10(2)

Table 5. Hydrogen coordinates and isotropic displacement parameters [Å^2] for 3d.

	x/a	y/b	z/c	U(eq)
H(11A)	1.0421(7)	0.170(2)	0.259(1)	0.072
H(11B)	1.0481(9)	0.2886(4)	0.200(2)	0.072
H(11C)	1.0843(2)	0.183(2)	0.146(1)	0.072
H(12A)	0.9332(5)	0.273(2)	-0.052(2)	0.074
H(12B)	1.012(1)	0.244(1)	-0.060(1)	0.074
H(12C)	0.987(2)	0.3460(6)	0.0139(3)	0.074
H(13A)	0.903(1)	0.217(2)	0.2656(9)	0.066
H(13B)	0.8616(4)	0.248(2)	0.156(1)	0.066
H(13C)	0.9197(8)	0.3293(7)	0.201(2)	0.066
H(21A)	0.828(1)	0.148(1)	-0.119(1)	0.064
H(21B)	0.816(1)	0.2062(4)	0.000(1)	0.064
H(21C)	0.7569(3)	0.135(1)	-0.055(2)	0.064
H(22A)	0.7918(9)	0.069(1)	0.194(1)	0.078
H(22B)	0.7948(9)	-0.062(1)	0.186(1)	0.078
H(22C)	0.7366(2)	0.004(2)	0.1218(4)	0.078
H(23A)	0.8304(9)	-0.089(2)	-0.137(1)	0.067
H(23B)	0.7569(4)	-0.073(1)	-0.084(2)	0.067
H(23C)	0.808(1)	-0.1622(4)	-0.032(1)	0.067
H(52)	0.9769(2)	-0.3828(2)	0.2357(3)	0.039
H(53)	1.0596(2)	-0.5217(3)	0.2385(4)	0.052
H(54)	1.1264(2)	-0.5530(2)	0.0802(4)	0.059
H(55)	1.1107(2)	-0.4478(3)	-0.0785(4)	0.056
H(56)	1.0309(2)	-0.3049(3)	-0.0795(3)	0.041
H(63)	0.7787(2)	-0.4679(3)	0.3411(3)	0.044
H(65)	0.7890(2)	-0.5693(2)	0.0230(3)	0.044
H(67A)	0.830(1)	-0.2030(5)	0.3042(9)	0.066
H(67B)	0.8929(3)	-0.275(2)	0.347(2)	0.066
H(67C)	0.819(1)	-0.294(1)	0.3983(8)	0.066
H(68A)	0.732(1)	-0.683(1)	0.1495(8)	0.081
H(68B)	0.6909(6)	-0.6140(3)	0.240(3)	0.081
H(68C)	0.7587(9)	-0.676(2)	0.275(2)	0.081
H(69A)	0.9094(4)	-0.429(2)	-0.0727(6)	0.062
H(69B)	0.857(1)	-0.3306(5)	-0.0890(8)	0.062
H(69C)	0.835(1)	-0.454(2)	-0.1167(4)	0.062

Table 1. Crystal data and structure refinement for 4d.

Empirical formula	$C_{29}H_{34}F_6N_4Ni$	
Formula weight	611.311 $g \cdot mol^{-1}$	
Temperature	194(2) K	
Wavelength	0.71073 Å	
Scanmodus	omega	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.479(1) Å,	$\alpha = 90°$
	b = 18.482(1) Å	$\beta = 108.71(1)°$
	c = 15.128(1) Å	$\gamma = 90°$
Volume	3039.9(4) $Å^3$	
Z	4	
Density (calculated)	1.336 $Mg \cdot m^{-3}$	
Absorption coefficient	0.699 mm^{-1}	
F(000)	1272	
Crystal size	0.21 × 0.30 × 0.60 mm	
θ-range for data collection	3.0 to 26.0°	
Index ranges	$0 \le h \le 14$, $-22 \le k \le 0$, $-18 \le l \le 17$	
Reflections collected	5934	
Independent reflections	5934	
Observed reflections	4755	
Refinement method	Full-matrix Least-Squares on F^2	
Parameters	361	
Goodness-of Fit on F^2	1.044	
Final R indices [$F_o > 4\sigma(F_o)$]	R1 = 0.0353, wR2 = 0.0880	
R indices (all data)	R1 = 0.0550, wR2 = 0.0962	
Largest diff. peak and hole	0.663, -0.334 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacment parameters [Å^2] for 4d. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
Ni(1)	0.11951(2)	0.14971(1)	0.37412(2)	0.02646(9)
F(1)	0.3336(2)	0.12062(8)	0.2713(1)	0.0616(5)
F(2)	0.2412(2)	0.22306(9)	0.2398(1)	0.0589(4)
F(3)	0.4331(1)	0.21832(7)	0.3169(1)	0.0499(4)
F(4)	0.3869(2)	0.07037(7)	0.4469(1)	0.0646(5)
F(5)	0.3467(2)	0.1391(1)	0.5482(1)	0.0665(5)
F(6)	0.4951(1)	0.16437(8)	0.4970(1)	0.0563(4)
N(1)	0.0994(1)	0.24102(8)	0.4195(1)	0.0254(3)
N(2)	0.3032(2)	0.25904(9)	0.4304(1)	0.0293(4)
N(3)	-0.1339(2)	0.09433(9)	0.3599(1)	0.0364(4)
N(4)	0.1530(2)	0.00988(9)	0.2893(1)	0.0372(4)
C(1)	0.2037(2)	0.2818(1)	0.4439(1)	0.0251(4)
C(2)	0.2888(2)	0.1851(1)	0.3951(1)	0.0269(4)
C(3)	0.3244(2)	0.1862(1)	0.3071(2)	0.0380(5)
C(4)	0.3786(2)	0.1401(1)	0.4709(2)	0.0400(5)
C(5)	-0.0087(2)	0.2641(1)	0.4394(1)	0.0238(4)
C(6)	-0.1101(2)	0.2884(1)	0.3662(1)	0.0273(4)
C(7)	-0.2170(2)	0.3072(1)	0.3851(2)	0.0305(4)
C(8)	-0.2264(2)	0.3028(1)	0.4743(2)	0.0312(4)
C(9)	-0.1246(2)	0.2787(1)	0.5454(1)	0.0310(4)
C(10)	-0.0158(2)	0.2582(1)	0.5297(1)	0.0268(4)
C(11)	-0.1034(2)	0.2940(1)	0.2689(1)	0.0384(5)
C(12)	-0.3433(2)	0.3243(1)	0.4936(2)	0.0448(6)
C(13)	0.0903(2)	0.2295(1)	0.6080(2)	0.0377(5)
C(14)	0.2109(2)	0.3551(1)	0.4877(1)	0.0286(4)
C(15)	0.1257(2)	0.4094(1)	0.4508(2)	0.0400(5)
C(16)	0.1439(3)	0.4785(1)	0.4909(2)	0.0524(7)
C(17)	0.2440(3)	0.4920(1)	0.5682(2)	0.0571(8)
C(18)	0.3273(3)	0.4384(1)	0.6057(2)	0.0548(7)
C(19)	0.3126(2)	0.3704(1)	0.5651(2)	0.0397(5)
C(20)	-0.0392(2)	0.1178(1)	0.3653(2)	0.0329(4)
C(21)	-0.2552(2)	0.0668(1)	0.3550(2)	0.0447(6)
C(22)	-0.2686(3)	0.0789(2)	0.4504(2)	0.077(1)
C(23)	-0.3489(3)	0.1099(2)	0.2794(3)	0.0714(9)
C(24)	-0.2587(3)	-0.0126(1)	0.3303(2)	0.0617(8)
C(25)	0.1457(2)	0.0643(1)	0.3240(2)	0.0331(5)
C(26)	0.1643(2)	-0.0582(1)	0.2432(2)	0.0443(6)
C(27)	0.0769(3)	-0.1111(2)	0.2660(3)	0.0720(9)
C(28)	0.1262(3)	-0.0444(2)	0.1396(2)	0.0673(9)
C(29)	0.2978(3)	-0.0822(2)	0.2818(2)	0.0665(8)

Table 3. Bond lengths [Å] and angles [°] for 4d.

Ni(1)-C(25)	1.818(2)	Ni(1)-N(1)	1.864(2)
Ni(1)-C(20)	1.879(2)	Ni(1)-C(2)	1.978(2)
F(1)-C(3)	1.345(2)	F(2)-C(3)	1.338(3)
F(3)-C(3)	1.347(3)	F(4)-C(4)	1.350(3)
F(5)-C(4)	1.334(3)	F(6)-C(4)	1.344(3)
N(3)-C(20)	1.148(3)	N(3)-C(21)	1.462(3)
N(4)-C(25)	1.150(3)	N(4)-C(26)	1.465(3)
N(1)-C(1)	1.362(2)	N(1)-C(5)	1.433(2)
N(2)-C(1)	1.294(2)	N(2)-C(2)	1.457(2)
C(21)-C(24)	1.513(3)	C(21)-C(22)	1.516(4)
C(21)-C(23)	1.520(4)	C(26)-C(28)	1.508(4)
C(26)-C(27)	1.519(4)	C(26)-C(29)	1.520(4)
C(2)-C(3)	1.512(3)	C(2)-C(4)	1.520(3)
C(1)-C(14)	1.499(3)	C(5)-C(10)	1.398(3)
C(5)-C(6)	1.399(3)	C(6)-C(7)	1.390(3)
C(6)-C(11)	1.502(3)	C(7)-C(8)	1.390(3)
C(8)-C(9)	1.384(3)	C(8)-C(12)	1.516(3)
C(9)-C(10)	1.397(3)	C(10)-C(13)	1.497(3)
C(14)-C(15)	1.386(3)	C(14)-C(19)	1.391(3)
C(15)-C(16)	1.401(3)	C(16)-C(17)	1.374(4)
C(17)-C(18)	1.367(4)	C(18)-C(19)	1.386(3)

C(25)-Ni(1)-N(1)	175.26(8)	C(25)-Ni(1)-C(20)	89.08(9)
N(1)-Ni(1)-C(20)	94.52(8)	C(25)-Ni(1)-C(2)	93.93(8)
N(1)-Ni(1)-C(2)	82.70(7)	C(20)-Ni(1)-C(2)	174.96(9)
C(20)-N(3)-C(21)	177.9(2)	C(25)-N(4)-C(26)	178.1(2)
C(1)-N(1)-C(5)	121.6(2)	C(1)-N(1)-Ni(1)	113.5(1)
C(5)-N(1)-Ni(1)	124.4(1)	C(1)-N(2)-C(2)	111.2(2)
N(3)-C(20)-Ni(1)	176.1(2)	N(3)-C(21)-C(24)	107.4(2)
N(3)-C(21)-C(22)	106.6(2)	C(24)-C(21)-C(22)	112.1(2)
N(3)-C(21)-C(23)	106.8(2)	C(24)-C(21)-C(23)	111.5(3)
C(22)-C(21)-C(23)	112.1(3)	N(4)-C(25)-Ni(1)	175.0(2)
N(4)-C(26)-C(28)	108.0(2)	N(4)-C(26)-C(27)	106.2(2)
C(28)-C(26)-C(27)	110.7(3)	N(4)-C(26)-C(29)	107.5(2)
C(28)-C(26)-C(29)	111.7(2)	C(27)-C(26)-C(29)	112.5(3)
N(2)-C(2)-C(3)	106.2(2)	N(2)-C(2)-C(4)	105.5(2)
C(3)-C(2)-C(4)	111.2(2)	N(2)-C(2)-Ni(1)	111.0(1)
C(3)-C(2)-Ni(1)	113.1(1)	C(4)-C(2)-Ni(1)	109.5(1)
N(2)-C(1)-N(1)	121.4(2)	N(2)-C(1)-C(14)	116.0(2)
N(1)-C(1)-C(14)	122.6(2)	F(2)-C(3)-F(1)	106.4(2)
F(2)-C(3)-F(3)	105.6(2)	F(1)-C(3)-F(3)	104.6(2)
F(2)-C(3)-C(2)	110.5(2)	F(1)-C(3)-C(2)	114.9(2)
F(3)-C(3)-C(2)	114.3(2)	F(5)-C(4)-F(6)	105.9(2)
F(5)-C(4)-F(4)	106.5(2)	F(6)-C(4)-F(4)	104.4(2)
F(5)-C(4)-C(2)	111.0(2)	F(6)-C(4)-C(2)	114.1(2)
F(4)-C(4)-C(2)	114.2(2)	C(10)-C(5)-C(6)	120.3(2)
C(10)-C(5)-N(1)	120.5(2)	C(6)-C(5)-N(1)	119.0(2)
C(7)-C(6)-C(5)	118.8(2)	C(7)-C(6)-C(11)	120.7(2)
C(5)-C(6)-C(11)	120.5(2)	C(8)-C(7)-C(6)	122.3(2)
C(9)-C(8)-C(7)	117.7(2)	C(9)-C(8)-C(12)	120.8(2)
C(7)-C(8)-C(12)	121.5(2)	C(8)-C(9)-C(10)	122.2(2)
C(9)-C(10)-C(5)	118.7(2)	C(9)-C(10)-C(13)	120.4(2)
C(5)-C(10)-C(13)	120.9(2)	C(15)-C(14)-C(19)	119.1(2)
C(15)-C(14)-C(1)	122.9(2)	C(19)-C(14)-C(1)	117.8(2)
C(14)-C(15)-C(16)	119.8(2)	C(17)-C(16)-C(15)	120.1(3)
C(18)-C(17)-C(16)	120.3(2)	C(17)-C(18)-C(19)	120.3(3)
C(18)-C(19)-C(14)	120.4(2)		

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 4d.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Ni(1)	28(1)	20(1)	37(1)	-6(1)	17(1)	-3(1)
F(1)	88(1)	37(1)	91(1)	-24(1)	72(1)	-17(1)
F(2)	72(1)	69(1)	41(1)	12(1)	25(1)	4(1)
F(3)	56(1)	37(1)	78(1)	-5(1)	50(1)	-10(1)
F(4)	55(1)	27(1)	98(1)	6(1)	5(1)	9(1)
F(5)	70(1)	83(1)	47(1)	27(1)	20(1)	3(1)
F(6)	31(1)	47(1)	82(1)	7(1)	5(1)	-1(1)
N(3)	36(1)	26(1)	55(1)	-7(1)	26(1)	-5(1)
N(4)	39(1)	27(1)	53(1)	-12(1)	24(1)	-4(1)
N(1)	25(1)	22(1)	33(1)	-5(1)	15(1)	-1(1)
N(2)	30(1)	23(1)	40(1)	-5(1)	18(1)	-4(1)
C(20)	37(1)	22(1)	45(1)	-10(1)	21(1)	-3(1)
C(21)	39(1)	35(1)	72(2)	-7(1)	34(1)	-11(1)
C(25)	32(1)	28(1)	46(1)	-5(1)	20(1)	-5(1)
C(26)	50(1)	31(1)	58(2)	-20(1)	26(1)	2(1)
C(2)	26(1)	21(1)	38(1)	-2(1)	17(1)	-2(1)
C(1)	31(1)	20(1)	27(1)	-1(1)	13(1)	-2(1)
C(22)	89(2)	74(2)	97(2)	-22(2)	71(2)	-24(2)
C(23)	40(2)	66(2)	109(3)	2(2)	26(2)	4(1)
C(24)	68(2)	35(1)	96(2)	-11(1)	45(2)	-19(1)
C(27)	86(2)	33(1)	108(3)	-24(2)	47(2)	-17(1)
C(28)	62(2)	87(2)	58(2)	-26(2)	27(1)	16(2)
C(29)	62(2)	57(2)	81(2)	-16(2)	24(2)	21(1)
C(3)	48(1)	27(1)	51(1)	-5(1)	32(1)	-3(1)
C(4)	35(1)	30(1)	54(1)	5(1)	12(1)	0(1)
C(5)	26(1)	17(1)	30(1)	-4(1)	12(1)	-2(1)
C(6)	30(1)	22(1)	30(1)	-4(1)	11(1)	-2(1)
C(7)	27(1)	24(1)	37(1)	-1(1)	6(1)	2(1)
C(8)	29(1)	25(1)	44(1)	-5(1)	18(1)	-2(1)
C(9)	37(1)	27(1)	34(1)	-1(1)	20(1)	0(1)
C(10)	29(1)	22(1)	31(1)	-1(1)	12(1)	-2(1)
C(14)	36(1)	22(1)	36(1)	-4(1)	24(1)	-7(1)
C(15)	41(1)	25(1)	64(2)	-4(1)	30(1)	-3(1)
C(16)	62(2)	24(1)	91(2)	-4(1)	53(2)	-1(1)
C(17)	87(2)	31(1)	73(2)	-20(1)	53(2)	-22(1)
C(18)	80(2)	45(2)	45(1)	-16(1)	28(1)	-31(1)
C(19)	51(1)	34(1)	38(1)	-4(1)	19(1)	-16(1)
C(11)	42(1)	45(1)	28(1)	-1(1)	10(1)	2(1)
C(12)	36(1)	46(1)	61(2)	1(1)	26(1)	7(1)
C(13)	39(1)	42(1)	34(1)	6(1)	14(1)	3(1)

Table 5. Hydrogen coordinates and isotropic displacement parameters [Å^2] for 4d.

	x/a	y/b	z/c	U(eq)
H(22A)	-0.3509(3)	0.0637(2)	0.4493(2)	0.115
H(22B)	-0.2571(3)	0.1303(2)	0.4666(2)	0.115
H(22C)	-0.2065(3)	0.0504(2)	0.4970(2)	0.115
H(23A)	-0.4319(3)	0.0926(2)	0.2730(3)	0.107
H(23B)	-0.3328(3)	0.1038(2)	0.2200(3)	0.107
H(23C)	-0.3424(3)	0.1613(2)	0.2965(3)	0.107
H(24A)	-0.3388(3)	-0.0329(1)	0.3271(2)	0.093
H(24B)	-0.1935(3)	-0.0383(1)	0.3781(2)	0.093
H(24C)	-0.2459(3)	-0.0182(1)	0.2696(2)	0.093
H(27A)	0.0772(3)	-0.1570(2)	0.2336(3)	0.108
H(27B)	-0.0065(3)	-0.0909(2)	0.2458(3)	0.108
H(27C)	0.1034(3)	-0.1196(2)	0.3335(3)	0.108
H(28A)	0.1342(3)	-0.0891(2)	0.1072(2)	0.101
H(28B)	0.1791(3)	-0.0070(2)	0.1268(2)	0.101
H(28C)	0.0404(3)	-0.0281(2)	0.1174(2)	0.101
H(29A)	0.3079(3)	-0.1286(2)	0.2536(2)	0.100
H(29B)	0.3208(3)	-0.0879(2)	0.3496(2)	0.100
H(29C)	0.3507(3)	-0.0458(2)	0.2670(2)	0.100
H(7)	-0.2859(2)	0.3236(1)	0.3354(2)	0.037
H(9)	-0.1290(2)	0.2760(1)	0.6070(1)	0.037
H(15)	0.0551(2)	0.3997(1)	0.3986(2)	0.048
H(16)	0.0870(3)	0.5162(1)	0.4646(2)	0.063
H(17)	0.2553(3)	0.5387(1)	0.5958(2)	0.069
H(18)	0.3956(3)	0.4478(1)	0.6597(2)	0.066
H(19)	0.3723(2)	0.3339(1)	0.5902(2)	0.048
H(11A)	-0.1732(2)	0.3224(1)	0.2301(1)	0.058
H(11B)	-0.1062(2)	0.2454(1)	0.2423(1)	0.058
H(11C)	-0.0264(2)	0.3178(1)	0.2706(1)	0.058
H(12A)	-0.3485(2)	0.3772(1)	0.4955(2)	0.067
H(12B)	-0.3423(2)	0.3042(1)	0.5538(2)	0.067
H(12C)	-0.4146(2)	0.3055(1)	0.4441(2)	0.067
H(13A)	0.1604(2)	0.2625(1)	0.6196(2)	0.057
H(13B)	0.1134(2)	0.1816(1)	0.5911(2)	0.057
H(13C)	0.0665(2)	0.2254(1)	0.6645(2)	0.057

Table 1. Crystal data and structure refinement for 6a.

Empirical formula	$C_{32}H_{30}F_{12}N_2Ni_2O_2$	
Formula weight	820.001 $g \cdot mol^{-1}$	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Scanmodus	omega/theta	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 18.994(2) Å,	$\alpha = 90°$
	b = 11.377(1) Å	$\beta = 108.09(1)°$
	c = 18.074(1) Å	$\gamma = 90°$
Volume	3712.6(7) $Å^3$	
Z	4	
Density (calculated)	1.467 $Mg \cdot m^{-3}$	
Absorption coefficient	1.104 mm^{-1}	
F(000)	1664	
Crystal size	0.3 × 0.45 × 0.45 mm	
θ-range for data collection	3.0 to 26.0°	
Index ranges	$-23 \le h \le 22$, $0 \le k \le 14$, $0 \le l \le 22$	
Reflections collected	7475	
Independent reflections	7229 (R_{int} = 0.0246)	
Observed reflections	5343	
Refinement method	Full-matrix Least-Squares on F^2	
Parameters	451	
Goodness-of Fit on F^{2}	1.046	
Final R indices [$F_0 > 4\sigma(F_0)$]	R1 = 0.0402, wR2 = 0.0942	
R indices (all data)	R1 = 0.0724, wR2 = 0.1076	
Largest diff. peak and hole	0.729, -0.691 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacment parameters [Å^2] for 6a. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
Ni(1)	0.22850(2)	0.04961(3)	0.17242(2)	0.0323(1)
Ni(2)	0.31461(2)	-0.00727(3)	0.08576(2)	0.0308(1)
F(1)	0.1742(2)	-0.1017(2)	0.3534(2)	0.0872(9)
F(2)	0.1257(2)	0.0524(3)	0.2914(2)	0.010(1)
F(3)	0.2430(2)	0.0435(2)	0.3445(2)	0.0879(9)
F(4)	0.1120(2)	-0.2321(2)	0.2138(2)	0.0895(9)
F(5)	0.0650(1)	-0.0692(2)	0.1638(2)	0.107(1)
F(6)	0.1362(1)	-0.1660(2)	0.1140(2)	0.0755(7)
F(7)	0.2417(2)	-0.1222(2)	-0.0848(2)	0.105(1)
F(8)	0.2000(2)	0.0373(3)	-0.1436(1)	0.0933(9)
F(9)	0.1711(2)	-0.0122(3)	-0.0429(2)	0.096(1)
F(10)	0.3451(2)	0.1187(2)	-0.1170(1)	0.0794(8)
F(11)	0.3780(2)	-0.0493(2)	-0.0670(2)	0.095(1)
F(12)	0.4162(1)	0.1053(3)	-0.0002(2)	0.0863(8)
O(1)	0.3164(1)	-0.0339(2)	0.1918(1)	0.0311(4)
O(2)	0.2806(1)	0.1340(2)	0.1136(1)	0.0314(4)
N(1)	0.0931(2)	0.1958(3)	0.1368(2)	0.0619(9)
N(2)	0.3792(2)	-0.2332(2)	0.0564(2)	0.0441(7)
C(1)	0.3188(2)	-0.1340(3)	0.2342(2)	0.0315(6)
C(2)	0.2595(2)	-0.1568(3)	0.2562(2)	0.0405(8)
C(3)	0.1955(2)	-0.0702(3)	0.2314(2)	0.0428(8)
C(4)	0.1842(3)	-0.0184(4)	0.3047(3)	0.068(1)
C(5)	0.1275(2)	-0.1326(4)	0.1815(3)	0.064(1)
C(12)	0.1449(2)	0.1384(3)	0.1506(2)	0.0462(8)
C(13)	0.0262(2)	0.2663(5)	0.1216(5)	0.101(2)
C(14)	0.0166(5)	0.330(1)	0.0478(8)	0.248(7)
C(17)	0.2607(2)	0.2150(3)	0.0547(2)	0.0358(7)
C(18)	0.2686(2)	0.1817(3)	-0.0125(2)	0.0481(9)
C(19)	0.2919(2)	0.0564(3)	-0.0199(2)	0.0419(8)
C(20)	0.2274(3)	-0.0102(4)	-0.0726(2)	0.066(1)
C(21)	0.3572(3)	0.0564(4)	-0.0507(2)	0.057(1)
C(28)	0.3531(2)	-0.1458(3)	0.0665(2)	0.0394(7)
C(29)	0.4151(2)	-0.3401(3)	0.0414(2)	0.0465(9)
C(15)	0.0415(4)	0.3580(7)	0.1839(7)	0.199(6)
C(16)	-0.0351(3)	0.1900(6)	0.1198(7)	0.192(5)
C(32)	0.3938(7)	-0.3573(7)	-0.0411(3)	0.253(8)
C(31)	0.4945(4)	-0.3202(7)	0.0741(9)	0.274(9)
C(30)	0.3949(5)	-0.4369(4)	0.0818(5)	0.155(4)
C(6)	0.3902(2)	-0.1963(3)	0.2581(2)	0.0338(7)
C(11)	0.3963(2)	-0.3121(3)	0.2847(2)	0.0432(8)
C(10)	0.4647(2)	-0.3658(3)	0.3124(2)	0.0530(9)
C(9)	0.5276(2)	-0.3066(4)	0.3134(2)	0.060(1)
C(8)	0.5227(2)	-0.1922(4)	0.2868(3)	0.062(1)
C(7)	0.4544(2)	-0.1373(3)	0.2595(2)	0.0461(8)
C(22)	0.2043(2)	0.4147(4)	0.0208(2)	0.061(1)
C(27)	0.2396(2)	0.3320(3)	0.0767(2)	0.0402(7)
C(23)	0.1883(3)	0.5249(4)	0.0421(3)	0.076(1)
C(24)	0.2054(3)	0.5545(4)	0.1194(3)	0.075(1)
C(25)	0.2388(2)	0.4741(3)	0.1751(3)	0.060(1)
C(26)	0.2571(2)	0.3634(3)	0.1545(2)	0.0448(8)

Table 3. Bond lengths [Å] and angles [°] for 6a.

Ni(1)-C(12)	1.818(3)	Ni(1)-O(1)	1.856(2)
Ni(1)-O(2)	1.920(2)	Ni(1)-C(3)	1.950(3)
Ni(1)-Ni(2)	2.6718(6)	Ni(2)-C(28)	1.817(3)
Ni(2)-O(2)	1.859(2)	Ni(2)-O(1)	1.930(2)
Ni(2)-C(19)	1.962(3)	F(1)-C(4)	1.346(5)
F(2)-C(4)	1.332(5)	F(3)-C(4)	1.327(5)
F(4)-C(5)	1.348(5)	F(5)-C(5)	1.340(4)
F(6)-C(5)	1.337(5)	F(7)-C(20)	1.336(5)
F(8)-C(20)	1.340(5)	F(9)-C(20)	1.338(6)
F(10)-C(21)	1.349(4)	F(11)-C(21)	1.327(4)
F(12)-C(21)	1.327(5)	O(1)-C(1)	1.366(3)
O(2)-C(17)	1.368(4)	N(1)-C(12)	1.142(4)
N(1)-C(13)	1.456(5)	N(2)-C(28)	1.150(4)
N(2)-C(29)	1.460(4)	C(1)-C(2)	1.331(4)
C(1)-C(6)	1.472(4)	C(2)-C(3)	1.521(5)
C(3)-C(5)	1.504(5)	C(3)-C(4)	1.525(5)
C(13)-C(16)	1.445(8)	C(13)-C(15)	1.50(1)
C(13)-C(14)	1.48(1)	C(17)-C(18)	1.326(5)
C(17)-C(27)	1.480(4)	C(18)-C(19)	1.511(5)
C(19)-C(20)	1.503(5)	C(19)-C(21)	1.508(5)
C(29)-C(32)	1.433(7)	C(29)-C(30)	1.437(6)
C(29)-C(31)	1.457(8)	C(6)-C(7)	1.384(4)
C(6)-C(11)	1.394(4)	C(11)-C(10)	1.382(5)
C(10)-C(9)	1.367(6)	C(9)-C(8)	1.381(6)
C(8)-C(7)	1.384(5)	C(22)-C(23)	1.373(6)
C(22)-C(27)	1.391(5)	C(27)-C(26)	1.386(5)
C(23)-C(24)	1.375(7)	C(24)-C(25)	1.363(6)
C(25)-C(26)	1.388(5)		

C(12)-Ni(1)-O(1)	176.5(1)	C(12)-Ni(1)-O(2)	99.6(1)
O(1)-Ni(1)-O(2)	76.86(8)	C(12)-Ni(1)-C(3)	95.7(2)
O(1)-Ni(1)-C(3)	87.8(1)	O(2)-Ni(1)-C(3)	164.0(1)
C(12)-Ni(1)-Ni(2)	131.3(1)	O(1)-Ni(1)-Ni(2)	46.25(6)
O(2)-Ni(1)-Ni(2)	44.09(6)	C(3)-Ni(1)-Ni(2)	120.71(9)
C(28)-Ni(2)-O(2)	175.4(1)	C(28)-Ni(2)-O(1)	99.8(1)
O(2)-Ni(2)-O(1)	76.55(8)	C(28)-Ni(2)-C(19)	96.5(1)
O(2)-Ni(2)-C(19)	87.4(1)	O(1)-Ni(2)-C(19)	162.9(1)
C(28)-Ni(2)-Ni(1)	132.8(1)	O(2)-Ni(2)-Ni(1)	45.94(6)
O(1)-Ni(2)-Ni(1)	44.01(6)	C(19)-Ni(2)-Ni(1)	119.5(1)
C(1)-O(1)-Ni(1)	113.8(2)	C(1)-O(1)-Ni(2)	132.5(2)
Ni(1)-O(1)-Ni(2)	89.73(8)	C(17)-O(2)-Ni(2)	114.0(2)
C(17)-O(2)-Ni(1)	134.5(2)	Ni(2)-O(2)-Ni(1)	89.97(9)
C(12)-N(1)-C(13)	177.7(5)	C(28)-N(2)-C(29)	176.5(3)
C(2)-C(1)-O(1)	116.5(3)	C(2)-C(1)-C(6)	127.3(3)
O(1)-C(1)-C(6)	115.7(2)	C(1)-C(2)-C(3)	117.3(3)
C(5)-C(3)-C(2)	109.2(3)	C(5)-C(3)-C(4)	112.2(3)
C(2)-C(3)-C(4)	108.1(3)	C(5)-C(3)-Ni(1)	111.3(3)
C(2)-C(3)-Ni(1)	104.5(2)	C(4)-C(3)-Ni(1)	111.2(2)
F(3)-C(4)-F(2)	107.0(4)	F(3)-C(4)-F(1)	106.6(4)
F(2)-C(4)-F(1)	105.4(3)	F(3)-C(4)-C(3)	110.7(3)
F(2)-C(4)-C(3)	114.3(4)	F(1)-C(4)-C(3)	112.5(3)
F(6)-C(5)-F(5)	106.6(4)	F(6)-C(5)-F(4)	105.2(3)
F(5)-C(5)-F(4)	105.0(3)	F(6)-C(5)-C(3)	110.9(3)
F(5)-C(5)-C(3)	114.9(3)	F(4)-C(5)-C(3)	113.5(4)
N(1)-C(12)-Ni(1)	178.8(3)	C(16)-C(13)-N(1)	108.8(5)
C(16)-C(13)-C(15)	113.7(7)	N(1)-C(13)-C(15)	106.7(5)
C(16)-C(13)-C(14)	113.7(8)	N(1)-C(13)-C(14)	107.2(5)
C(15)-C(13)-C(14)	106.3(8)	C(18)-C(17)-O(2)	116.0(3)

C(18)-C(17)-C(27)	128.3(3)	O(2)-C(17)-C(27)	115.4(3)
C(17)-C(18)-C(19)	118.1(3)	C(20)-C(19)-C(21)	111.6(3)
C(20)-C(19)-C(18)	109.1(3)	C(21)-C(19)-C(18)	109.3(3)
C(20)-C(19)-Ni(2)	108.7(3)	C(21)-C(19)-Ni(2)	113.7(2)
C(18)-C(19)-Ni(2)	104.1(2)	F(7)-C(20)-F(9)	106.2(4)
F(7)-C(20)-F(8)	105.4(3)	F(9)-C(20)-F(8)	105.7(4)
F(7)-C(20)-C(19)	114.7(4)	F(9)-C(20)-C(19)	110.5(3)
F(8)-C(20)-C(19)	113.7(4)	F(12)-C(21)-F(11)	106.7(4)
F(12)-C(21)-F(10)	105.4(4)	F(11)-C(21)-F(10)	104.9(3)
F(12)-C(21)-C(19)	111.2(3)	F(11)-C(21)-C(19)	114.7(3)
F(10)-C(21)-C(19)	113.2(3)	N(2)-C(28)-Ni(2)	177.9(3)
C(32)-C(29)-C(30)	113.0(6)	C(32)-C(29)-C(31)	111.4(7)
C(30)-C(29)-C(31)	108.6(7)	C(32)-C(29)-N(2)	108.1(4)
C(30)-C(29)-N(2)	109.3(3)	C(31)-C(29)-N(2)	106.3(4)
C(7)-C(6)-C(11)	118.3(3)	C(7)-C(6)-C(1)	119.9(3)
C(11)-C(6)-C(1)	121.7(3)	C(10)-C(11)-C(6)	120.7(3)
C(9)-C(10)-C(11)	120.4(4)	C(10)-C(9)-C(8)	119.7(4)
C(9)-C(8)-C(7)	120.2(4)	C(8)-C(7)-C(6)	120.7(3)
C(23)-C(22)-C(27)	120.8(4)	C(26)-C(27)-C(22)	118.2(3)
C(26)-C(27)-C(17)	120.2(3)	C(22)-C(27)-C(17)	121.5(3)
C(24)-C(23)-C(22)	120.4(4)	C(25)-C(24)-C(23)	119.6(4)
C(24)-C(25)-C(26)	120.6(4)	C(27)-C(26)-C(25)	120.3(3)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 6a.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Ni(1)	29(1)	33(1)	39(1)	-3(1)	16(1)	3(1)
Ni(2)	34(1)	31(1)	30(1)	-1(1)	14(1)	5(1)
F(1)	122(2)	80(2)	95(2)	10(2)	86(2)	-2(2)
F(2)	127(2)	87(2)	128(2)	6(2)	102(2)	36(2)
F(3)	136(3)	79(2)	69(2)	-30(1)	62(2)	-32(2)
F(4)	75(2)	55(2)	154(3)	-3(2)	58(2)	-23(1)
F(5)	38(1)	60(2)	217(4)	-24(2)	33(2)	-2(1)
F(6)	69(2)	60(2)	83(2)	-18(1)	4(1)	-7(1)
F(7)	129(3)	65(2)	87(2)	-32(2)	-18(2)	-2(2)
F(8)	110(2)	108(2)	39(1)	-6(1)	-11(1)	10(2)
F(9)	63(2)	134(3)	81(2)	-7(2)	5(1)	-28(2)
F(10)	119(2)	85(2)	51(1)	17(1)	51(1)	13(2)
F(11)	155(3)	72(2)	98(2)	13(2)	99(2)	36(2)
F(12)	66(2)	133(3)	70(2)	2(2)	36(1)	-14(2)
O(1)	33(1)	33(1)	32(1)	3(1)	16(1)	4(1)
O(2)	34(1)	31(1)	30(1)	2(1)	13(1)	6(1)
N(1)	33(2)	59(2)	95(3)	-9(2)	22(2)	10(2)
N(2)	59(2)	37(2)	44(2)	0(1)	27(1)	9(1)
C(1)	37(2)	29(2)	29(1)	-1(1)	12(1)	2(1)
C(2)	47(2)	37(2)	44(2)	3(1)	24(2)	-2(2)
C(3)	42(2)	39(2)	59(2)	-5(2)	33(2)	-2(1)
C(4)	90(3)	61(3)	79(3)	-3(2)	65(3)	0(2)
C(5)	44(2)	44(2)	110(4)	-6(2)	31(2)	-3(2)
C(12)	35(2)	45(2)	63(2)	-10(2)	22(2)	0(2)
C(13)	40(2)	76(4)	186(7)	-6(4)	34(3)	24(2)
C(14)	81(6)	260(13)	390(17)	162(13)	53(8)	95(7)
C(17)	40(2)	35(2)	32(2)	4(1)	11(1)	8(1)
C(18)	68(2)	42(2)	35(2)	8(2)	17(2)	15(2)
C(19)	53(2)	43(2)	30(2)	-1(1)	14(1)	7(2)
C(20)	74(3)	68(3)	44(2)	-7(2)	3(2)	0(2)
C(21)	85(3)	55(2)	43(2)	3(2)	38(2)	11(2)
C(28)	45(2)	41(2)	38(2)	0(1)	21(2)	3(2)
C(29)	62(2)	34(2)	55(2)	-1(2)	34(2)	12(2)
C(15)	82(5)	133(6)	376(16)	-131(9)	63(7)	18(4)
C(16)	46(3)	93(5)	444(16)	-42(7)	84(6)	1(3)
C(32)	537(20)	159(7)	53(3)	7(4)	76(7)	226(11)
C(31)	85(5)	127(7)	629(25)	-176(11)	138(9)	-9(4)
C(30)	270(10)	43(3)	242(9)	31(4)	213(8)	42(4)
C(6)	41(2)	36(2)	24(1)	1(1)	11(1)	3(1)
C(11)	54(2)	40(2)	40(2)	7(2)	21(2)	4(2)
C(10)	68(3)	47(2)	45(2)	14(2)	18(2)	19(2)
C(9)	49(2)	66(3)	56(2)	4(2)	2(2)	22(2)
C(8)	36(2)	57(3)	84(3)	3(2)	8(2)	1(2)
C(7)	37(2)	39(2)	58(2)	5(2)	8(2)	1(2)
C(22)	75(3)	55(2)	52(2)	11(2)	21(2)	26(2)
C(27)	43(2)	38(2)	42(2)	6(2)	16(2)	10(1)
C(23)	95(4)	52(3)	87(3)	25(2)	35(3)	38(2)
C(24)	100(4)	47(2)	90(3)	-1(2)	47(3)	25(2)
C(25)	76(3)	47(2)	66(3)	-9(2)	34(2)	4(2)
C(26)	54(2)	35(2)	49(2)	-2(2)	21(2)	3(2)

Table 5. Hydrogen coordinates and isotropic displacement parameters [Å^2] for 6a.

	x/a	y/b	z/c	U(eq)
H(14A)	0.0616(2)	0.3669(3)	0.0446(2)	0.070
H(14B)	-0.0238(2)	0.3837(3)	0.0334(2)	0.070
H(14C)	0.0043(2)	0.2685(3)	0.0021(2)	0.070
H(15A)	0.0851(4)	0.4026(7)	0.1841(7)	0.298
H(15B)	0.0500(4)	0.3203(7)	0.2340(7)	0.298
H(15C)	-0.0007(4)	0.4104(7)	0.1739(7)	0.298
H(16A)	-0.0795(3)	0.2364(6)	0.1133(7)	0.288
H(16B)	-0.0233(3)	0.1470(6)	0.1685(7)	0.288
H(16C)	-0.0435(3)	0.1349(6)	0.0770(7)	0.288
H(32A)	0.3414(7)	-0.3757(7)	-0.0605(3)	0.380
H(32B)	0.4221(7)	-0.4218(7)	-0.0528(3)	0.380
H(32C)	0.4035(7)	-0.2862(7)	-0.0660(3)	0.380
H(31A)	0.5147(4)	-0.3730(7)	0.1177(9)	0.411
H(31B)	0.5034(4)	-0.2395(7)	0.0918(9)	0.411
H(31C)	0.5182(4)	-0.3351(7)	0.0346(9)	0.411
H(30A)	0.4049(5)	-0.4166(4)	0.1362(5)	0.232
H(30B)	0.4236(5)	-0.5057(4)	0.0776(5)	0.232
H(30C)	0.3426(5)	-0.4537(4)	0.0588(5)	0.232
H(11)	0.3533(2)	-0.3540(3)	0.2838(2)	0.052
H(10)	0.4680(2)	-0.4437(3)	0.3306(2)	0.064
H(9)	0.5740(2)	-0.3436(4)	0.3322(2)	0.072
H(8)	0.5658(2)	-0.1514(4)	0.2873(3)	0.074
H(7)	0.4516(2)	-0.0593(3)	0.2418(2)	0.055
H(22)	0.1909(2)	0.3945(3)	-0.0323(2)	0.048
H(23)	0.1655(3)	0.5804(4)	0.0036(3)	0.092
H(24)	0.1941(3)	0.6300(4)	0.1338(3)	0.090
H(25)	0.2496(2)	0.4937(3)	0.2280(3)	0.072
H(2)	0.2583(2)	-0.2169(3)	0.2935(2)	0.050
H(18)	0.2603(2)	0.2365(3)	-0.0522(2)	0.050
H(26)	0.2814(2)	0.3094(3)	0.1934(2)	0.060