Table 1. Crystal data and structure refinement for 1.

Identification code	FO1229
Empirical formula	$C_{48}H_{56}N_6Ni_2$
Formula weight	834.41
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 8.3999(3) Å alpha = 103.617(2)° b = 11.7368(5) Å beta = 107.802(2)° c = 13.0598(6) Å gamma = 108.26(2)°
Volume, Z	1083.18(8) Å^3, 1
Density (calculated)	1.279 Mg/m^3
Absorption coefficient	0.909 mm^{-1}
F(000)	442
Crystal size	0.19 x 0.12 x 0.10 mm
θ range for data collection	3.35 to 27.47°
Limiting indices	$-10 \le h \le 10$, $-15 \le k \le 13$, $-16 \le l \le 16$
Reflections collected	7206
Independent reflections	4774 (R_{int} = 0.0200)
Completeness to θ = 27.47°	96.4 %
Max. and min. transmission	0.9146 and 0.8463
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4774 / 0 / 223
Goodness-of-fit on F^2	1.012
Final R indices [I>2σ(I)]	R1 = 0.0505, wR2 = 0.1412
R indices (all data)	R1 = 0.0575, wR2 = 0.1474
Largest diff. peak and hole	0.836 and -0.534 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni	7230(1)	6964(1)	6971(1)	31(1)
N(1)	6958(3)	6407(2)	5411(2)	33(1)
N(2)	5059(3)	5408(2)	6423(2)	33(1)
N(3)	9233(3)	8460(2)	7166(2)	32(1)
C(1)	5558(3)	5294(2)	4700(2)	30(1)
C(2)	8258(4)	7272(3)	5112(2)	34(1)
C(3)	9531(4)	8450(2)	6200(2)	31(1)
C(4)	10912(4)	9478(3)	6193(3)	39(1)
C(5)	12012(4)	10571(3)	7195(3)	47(1)
C(6)	11706(5)	10596(3)	8184(3)	50(1)
C(7)	10339(4)	9540(3)	8145(2)	42(1)
C(8)	7609(5)	7488(3)	8590(2)	45(1)
C(9)	4005(3)	5028(2)	7062(2)	30(1)
C(10)	2566(4)	5404(3)	7025(2)	34(1)
C(11)	1567(4)	5047(3)	7661(3)	40(1)
C(12)	1995(4)	4355(3)	8361(2)	41(1)
C(13)	3473(4)	4031(3)	8412(2)	36(1)
C(14)	4481(4)	4345(2)	7766(2)	33(1)
C(15)	2127(5)	6201(3)	6310(3)	48(1)
C(16)	900(6)	3967(4)	9052(3)	64(1)
C(17)	6023(4)	3939(3)	7800(3)	46(1)
C(18)	15379(10)	10167(6)	9828(6)	74(2)
C(19)	15427(8)	10895(4)	10854(5)	57(2)
C(20)	14450(9)	10295(6)	11407(5)	77(2)
C(21)	13426(10)	8967(6)	10936(6)	88(4)
C(22)	13378(9)	8239(4)	9910(6)	84(3)
C(23)	14354(10)	8839(6)	9357(5)	78(3)
C(24)	16480(20)	10898(14)	9303(14)	105(5)
C(25)	6006(6)	10851(4)	5330(5)	64(2)
C(26)	4431(8)	10649(5)	4417(5)	56(2)
C(27)	2960(6)	9441(6)	3871(4)	71(2)
C(28)	3064(7)	8436(4)	4237(6)	92(3)
C(29)	4638(9)	8638(4)	5149(6)	74(2)
C(30)	6110(6)	9846(5)	5696(4)	55(2)
C(31)	7480(19)	12144(14)	5813(12)	110(4)

Table 3. Bond lengths [Å] and angles [°] for 1.

Ni-N(1)	1.905(2)	Ni-N(3)	1.912(2)
Ni-N(2)	1.916(2)	Ni-C(8)	1.950(3)
N(1)-C(1)	1.323(3)	N(1)-C(2)	1.459(3)
N(2)-C(1)#1	1.341(3)	N(2)-C(9)	1.435(3)
N(3)-C(3)	1.357(4)	N(3)-C(7)	1.370(3)
C(1)-N(2)#1	1.341(3)	C(1)-C(1)#1	1.506(5)
C(2)-C(3)	1.514(4)	C(3)-C(4)	1.392(4)
C(4)-C(5)	1.393(4)	C(5)-C(6)	1.388(5)
C(6)-C(7)	1.378(4)	C(9)-C(14)	1.405(4)
C(9)-C(10)	1.402(4)	C(10)-C(11)	1.392(4)
C(10)-C(15)	1.517(4)	C(11)-C(12)	1.398(4)
C(12)-C(13)	1.395(4)	C(12)-C(16)	1.519(4)
C(13)-C(14)	1.397(4)	C(14)-C(17)	1.506(4)
C(18)-C(19)	1.3900	C(18)-C(23)	1.3900
C(18)-C(24)	1.496(17)	C(19)-C(20)	1.3900
C(20)-C(21)	1.3900	C(21)-C(22)	1.3900
C(22)-C(23)	1.3900	C(25)-C(26)	1.3900
C(25)-C(30)	1.3900	C(25)-C(31)	1.458(15)
C(26)-C(27)	1.3900	C(27)-C(28)	1.3900
C(28)-C(29)	1.3900	C(29)-C(30)	1.3900

N(1)-Ni-N(3)	84.18(9)	N(1)-Ni-N(2)	83.83(9)
N(3)-Ni-N(2)	167.38(9)	N(1)-Ni-C(8)	176.66(12)
N(3)-Ni-C(8)	95.69(11)	N(2)-Ni-C(8)	96.50(11)
C(1)-N(1)-C(2)	126.8(2)	C(1)-N(1)-Ni	116.20(18)
C(2)-N(1)-Ni	116.95(17)	C(1)#1-N(2)-C(9)	119.8(2)
C(1)#1-N(2)-Ni	113.69(17)	C(9)-N(2)-Ni	126.26(17)
C(3)-N(3)-C(7)	117.2(2)	C(3)-N(3)-Ni	115.10(17)
C(7)-N(3)-Ni	127.7(2)	N(1)-C(1)-N(2)#1	133.7(2)
N(1)-C(1)-C(1)#1	111.9(3)	N(2)#1-C(1)-C(1)#1	114.3(3)
N(1)-C(2)-C(3)	106.9(2)	N(3)-C(3)-C(4)	122.1(2)
N(3)-C(3)-C(2)	116.8(2)	C(4)-C(3)-C(2)	121.0(2)
C(5)-C(4)-C(3)	119.8(3)	C(6)-C(5)-C(4)	118.5(3)
C(7)-C(6)-C(5)	119.1(3)	C(6)-C(7)-N(3)	123.2(3)
C(14)-C(9)-C(10)	120.5(2)	C(14)-C(9)-N(2)	119.9(2)
C(10)-C(9)-N(2)	119.5(2)	C(11)-C(10)-C(9)	119.1(3)
C(11)-C(10)-C(15)	120.8(3)	C(9)-C(10)-C(15)	120.1(3)
C(10)-C(11)-C(12)	121.7(3)	C(11)-C(12)-C(13)	118.0(3)
C(11)-C(12)-C(16)	121.5(3)	C(13)-C(12)-C(16)	120.5(3)
C(14)-C(13)-C(12)	122.1(3)	C(13)-C(14)-C(9)	118.6(2)
C(13)-C(14)-C(17)	121.1(3)	C(9)-C(14)-C(17)	120.3(3)
C(19)-C(18)-C(23)	120.0	C(19)-C(18)-C(24)	116.0(7)
C(23)-C(18)-C(24)	124.0(7)	C(18)-C(19)-C(20)	120.0
C(21)-C(20)-C(19)	120.0	C(20)-C(21)-C(22)	120.0
C(23)-C(22)-C(21)	120.0	C(22)-C(23)-C(18)	120.0
C(26)-C(25)-C(30)	120.0	C(26)-C(25)-C(31)	115.2(7)
C(30)-C(25)-C(31)	124.8(7)	C(27)-C(26)-C(25)	120.0
C(26)-C(27)-C(28)	120.0	C(27)-C(28)-C(29)	120.0
C(30)-C(29)-C(28)	120.0	C(29)-C(30)-C(25)	120.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

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	32(1)	26(1)	23(1)	6(1)	8(1)	4(1)
N(1)	34(1)	27(1)	27(1)	7(1)	11(1)	4(1)
N(2)	34(1)	29(1)	26(1)	7(1)	11(1)	5(1)
N(3)	33(1)	26(1)	28(1)	7(1)	7(1)	7(1)
C(1)	31(1)	27(1)	27(1)	9(1)	11(1)	9(1)
C(2)	35(1)	28(1)	29(1)	8(1)	12(1)	5(1)
C(3)	31(1)	27(1)	31(1)	10(1)	9(1)	9(1)
C(4)	38(1)	32(1)	38(2)	12(1)	13(1)	7(1)
C(5)	44(2)	30(1)	45(2)	12(1)	12(1)	0(1)
C(6)	54(2)	33(2)	35(2)	5(1)	6(1)	0(1)
C(7)	47(2)	30(1)	29(1)	6(1)	7(1)	3(1)
C(8)	47(2)	39(2)	27(1)	6(1)	11(1)	0(1)
C(9)	31(1)	26(1)	23(1)	5(1)	9(1)	6(1)
C(10)	36(1)	29(1)	28(1)	5(1)	8(1)	12(1)
C(11)	39(1)	42(2)	38(2)	7(1)	16(1)	19(1)
C(12)	43(2)	44(2)	33(1)	10(1)	20(1)	15(1)
C(13)	43(1)	34(1)	28(1)	12(1)	15(1)	12(1)
C(14)	33(1)	28(1)	30(1)	7(1)	11(1)	10(1)
C(15)	51(2)	46(2)	48(2)	22(1)	14(1)	25(2)
C(16)	66(2)	83(3)	56(2)	28(2)	43(2)	28(2)
C(17)	43(2)	48(2)	57(2)	24(2)	22(1)	25(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	7597	7522	4497	40
H(2B)	8969	6843	4831	40
H(4A)	11102	9435	5507	46
H(5A)	12952	11285	7201	56
H(6A)	12430	11330	8879	60
H(7A)	10154	9562	8830	50
H(8A)	8706	8302	9040	67
H(8B)	7776	6821	8886	67
H(8C)	6534	7604	8657	67
H(11A)	569	5279	7618	48
H(13A)	3805	3584	8902	43
H(15A)	2963	6359	5925	72
H(15B)	2279	7026	6816	72
H(15C)	855	5733	5728	72
H(16A)	-80	4271	8912	96
H(16B)	1717	4354	9877	96
H(16C)	356	3026	8812	96
H(17A)	6168	3477	8332	69
H(17B)	7169	4705	8066	69
H(17C)	5737	3373	7024	69
H(19A)	16127	11802	11176	68
H(20A)	14483	10793	12108	92
H(21A)	12758	8557	11314	106
H(22A)	12678	7332	9588	101
H(23A)	14322	8341	8656	94
H(24A)	17093	11817	9788	158
H(24B)	15669	10779	8529	158
H(24C)	17412	10578	9247	158
H(26A)	4361	11336	4167	68
H(27A)	1884	9303	3247	85
H(28A)	2058	7610	3863	110
H(29A)	4709	7951	5399	88
H(30A)	7186	9984	6319	66
H(31A)	7073	12681	5418	165
H(31B)	8565	12094	5707	165
H(31C)	7793	12526	6640	165

Table 1. Crystal data and structure refinement for 3.

Identification code	FO1308
Empirical formula	$C_{48}H_{44}N_6Ni_{22}*C_7H_8$
Formula weight	1006.58
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 16.7638(5) Å alpha = 90° b = 14.6380(3) Å beta = 90° c = 22.0254(7) Å gamma = 90°
Volume, Z	5404.8(3) $Å^3$, 4
Density (calculated)	1.237 Mg/m^3
Absorption coefficient	0.741 mm^{-1}
F(000)	2120
Crystal size	0.20 x 0.18 x 0.12 mm
θ range for data collection	2.95 to 27.49°
Limiting indices	$-21 \le h \le 21$, $-18 \le k \le 18$, $-28 \le l \le 28$
Reflections collected	11650
Independent reflections	6175 (R_{int} = 0.0752)
Completeness to θ = 27.49°	99.7 %
Max. and min. transmission	0.9164 and 0.8660
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6175 / 0 / 356
Goodness-of-fit on F^2	1.204
Final R indices [I>2σ(I)]	R1 = 0.1100, wR2 = 0.1490
R indices (all data)	R1 = 0.1648, wR2 = 0.1637
Largest diff. peak and hole	0.359 and -0.420 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 3. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni	727(1)	9904(1)	1048(1)	32(1)
N(1)	52(2)	10741(2)	634(2)	32(1)
N(2)	621(2)	9201(2)	343(2)	35(1)
N(3)	1384(2)	8930(2)	1321(2)	33(1)
C(1)	167(2)	9544(3)	-87(2)	29(1)
C(2)	1043(3)	8326(3)	332(2)	43(1)
C(3)	1494(2)	8252(3)	918(2)	37(1)
C(4)	1999(3)	7526(3)	1034(2)	49(1)
C(5)	2396(3)	7484(3)	1580(2)	53(1)
C(6)	2282(3)	8174(3)	1998(2)	49(1)
C(7)	1780(3)	8881(3)	1857(2)	41(1)
C(8)	-219(2)	11599(3)	868(2)	34(1)
C(9)	-919(3)	11619(3)	1210(2)	46(1)
C(10)	-1172(3)	12457(3)	1435(2)	53(1)
C(11)	-756(3)	13257(3)	1338(2)	47(1)
C(12)	-56(3)	13209(3)	1005(2)	44(1)
C(13)	221(3)	12386(3)	766(2)	37(1)
C(14)	-1378(3)	10746(4)	1331(3)	78(2)
C(15)	-1045(4)	14159(3)	1596(3)	72(2)
C(16)	976(3)	12344(3)	404(2)	52(1)
C(17)	849(2)	10635(2)	1753(2)	28(1)
C(18)	927(3)	11137(3)	2160(2)	43(1)
C(19)	994(3)	11802(3)	2655(2)	39(1)
C(20)	554(3)	12613(3)	2637(2)	53(1)
C(21)	615(3)	13240(4)	3101(3)	64(2)
C(22)	1104(4)	13090(4)	3589(2)	65(2)
C(23)	1551(3)	12279(4)	3614(2)	59(1)
C(24)	1487(3)	11654(3)	3151(2)	46(1)
C(25)	3867(9)	10553(11)	1444(5)	64(5)
C(26)	4516(6)	10911(10)	1131(6)	55(4)
C(27)	4535(8)	10877(9)	501(6)	60(5)
C(28)	3906(12)	10485(9)	183(5)	83(6)
C(29)	3258(10)	10127(12)	495(9)	109(9)
C(30)	3238(8)	10160(13)	1126(9)	80(8)
C(31)	3819(10)	10570(11)	2094(7)	105(6)
C(25A)	3532(9)	10243(10)	457(6)	63(5)
C(26A)	3235(8)	9996(12)	1023(7)	71(7)
C(27A)	3644(12)	10241(11)	1546(6)	85(6)
C(28A)	4352(10)	10733(9)	1505(9)	99(8)
C(29A)	4649(6)	10979(10)	939(12)	98(11)
C(30A)	4239(8)	10734(10)	415(9)	88(9)
C(31A)	3132(13)	9994(13)	-66(8)	128(8)

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

Ni-N(2)	1.872(3)	Ni-C(17)	1.897(4)
Ni-N(3)	1.900(3)	Ni-N(1)	1.901(3)
N(1)-C(1)#1	1.328(5)	N(1)-C(8)	1.431(5)
N(2)-C(1)	1.314(5)	N(2)-C(2)	1.463(5)
N(3)-C(3)	1.346(5)	N(3)-C(7)	1.355(5)
C(1)-N(1)#1	1.327(5)	C(1)-C(1)#1	1.497(7)
C(2)-C(3)	1.499(6)	C(3)-C(4)	1.382(6)
C(4)-C(5)	1.376(6)	C(5)-C(6)	1.380(7)
C(6)-C(7)	1.369(6)	C(8)-C(13)	1.385(6)
C(8)-C(9)	1.394(6)	C(9)-C(10)	1.390(6)
C(9)-C(14)	1.516(7)	C(10)-C(11)	1.379(7)
C(11)-C(12)	1.385(7)	C(11)-C(15)	1.517(6)
C(12)-C(13)	1.395(6)	C(13)-C(16)	1.498(6)
C(17)-C(18)	1.166(6)	C(18)-C(19)	1.465(6)
C(19)-C(24)	1.387(6)	C(19)-C(20)	1.398(6)
C(20)-C(21)	1.378(7)	C(21)-C(22)	1.369(8)
C(22)-C(23)	1.406(8)	C(23)-C(24)	1.373(6)
C(25)-C(26)	1.3900	C(25)-C(30)	1.3900
C(25)-C(31)	1.434(18)	C(26)-C(27)	1.3900
C(27)-C(28)	1.3900	C(28)-C(29)	1.3900
C(29)-C(30)	1.3900	C(25A)-C(31A)	1.38(2)
C(25A)-C(26A)	1.3900	C(25A)-C(30A)	1.3900
C(26A)-C(27A)	1.3900	C(27A)-C(28A)	1.3900
C(28A)-C(29A)	1.3900	C(29A)-C(30A)	1.3900

N(2)-Ni-C(17)	178.80(16)	N(2)-Ni-N(3)	84.56(14)
C(17)-Ni-N(3)	95.79(15)	N(2)-Ni-N(1)	84.29(14)
C(17)-Ni-N(1)	95.36(15)	N(3)-Ni-N(1)	168.85(15)
C(1)#1-N(1)-C(8)	121.0(3)	C(1)#1-N(1)-Ni	113.4(2)
C(8)-N(1)-Ni	125.6(3)	C(1)-N(2)-C(2)	127.1(3)
C(1)-N(2)-Ni	116.2(3)	C(2)-N(2)-Ni	116.7(3)
C(3)-N(3)-C(7)	117.9(4)	C(3)-N(3)-Ni	115.1(3)
C(7)-N(3)-Ni	126.9(3)	N(2)-C(1)-N(1)#1	133.9(4)
N(2)-C(1)-C(1)#1	112.0(4)	N(1)#1-C(1)-C(1)#1	114.1(4)
N(2)-C(2)-C(3)	107.1(3)	N(3)-C(3)-C(4)	121.9(4)
N(3)-C(3)-C(2)	116.5(3)	C(4)-C(3)-C(2)	121.6(4)
C(5)-C(4)-C(3)	119.5(4)	C(4)-C(5)-C(6)	118.9(4)
C(7)-C(6)-C(5)	119.2(4)	N(3)-C(7)-C(6)	122.6(4)
C(13)-C(8)-C(9)	121.1(4)	C(13)-C(8)-N(1)	120.2(4)
C(9)-C(8)-N(1)	118.7(4)	C(10)-C(9)-C(8)	118.0(4)
C(10)-C(9)-C(14)	121.8(4)	C(8)-C(9)-C(14)	120.3(4)
C(11)-C(10)-C(9)	122.6(4)	C(10)-C(11)-C(12)	117.9(4)
C(10)-C(11)-C(15)	121.3(5)	C(12)-C(11)-C(15)	120.8(5)
C(11)-C(12)-C(13)	121.7(4)	C(8)-C(13)-C(12)	118.7(4)
C(8)-C(13)-C(16)	120.1(4)	C(12)-C(13)-C(16)	121.2(4)
C(18)-C(17)-Ni	175.2(4)	C(17)-C(18)-C(19)	176.8(5)
C(24)-C(19)-C(20)	118.0(4)	C(24)-C(19)-C(18)	121.9(4)
C(20)-C(19)-C(18)	120.2(4)	C(21)-C(20)-C(19)	120.3(5)
C(22)-C(21)-C(20)	121.4(5)	C(21)-C(22)-C(23)	119.0(5)
C(24)-C(23)-C(22)	119.5(5)	C(23)-C(24)-C(19)	121.9(5)
C(26)-C(25)-C(30)	120.0	C(26)-C(25)-C(31)	122.1(15)
C(30)-C(25)-C(31)	117.9(15)	C(25)-C(26)-C(27)	120.0
C(28)-C(27)-C(26)	120.0	C(27)-C(28)-C(29)	120.0
C(30)-C(29)-C(28)	120.0	C(29)-C(30)-C(25)	120.0
C(31A)-C(25A)-C(26A)	120.3(14)	C(31A)-C(25A)-C(30A)	119.7(14)

C(26A)-C(25A)-C(30A)	120.0	C(27A)-C(26A)-C(25A)	120.0
C(26A)-C(27A)-C(28A)	120.0	C(29A)-C(28A)-C(27A)	120.0
C(28A)-C(29A)-C(30A)	120.0	C(29A)-C(30A)-C(25A)	120.0

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 3.

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	32(1)	29(1)	34(1)	-3(1)	-2(1)	4(1)
N(1)	33(2)	26(2)	38(2)	-5(2)	-2(2)	8(1)
N(2)	33(2)	30(2)	41(2)	-7(2)	-7(2)	8(2)
N(3)	28(2)	34(2)	36(2)	4(2)	0(2)	1(2)
C(1)	23(2)	27(2)	38(2)	-3(2)	0(2)	1(2)
C(2)	48(3)	29(2)	52(3)	-6(2)	-18(2)	12(2)
C(3)	33(2)	33(2)	45(3)	2(2)	-3(2)	3(2)
C(4)	44(3)	45(3)	59(3)	-8(2)	-14(3)	13(2)
C(5)	47(3)	48(3)	64(3)	3(3)	-8(3)	17(2)
C(6)	41(3)	59(3)	45(3)	13(2)	-6(2)	8(2)
C(7)	40(2)	47(3)	36(3)	6(2)	2(2)	2(2)
C(8)	36(2)	32(2)	34(2)	-4(2)	-6(2)	7(2)
C(9)	49(3)	36(2)	53(3)	1(2)	9(2)	6(2)
C(10)	59(3)	46(3)	54(3)	-1(2)	19(3)	17(3)
C(11)	73(3)	35(2)	33(2)	-3(2)	2(2)	16(3)
C(12)	67(3)	30(2)	36(2)	1(2)	-2(2)	-3(2)
C(13)	47(2)	35(2)	28(2)	-1(2)	-3(2)	4(2)
C(14)	59(4)	48(3)	127(6)	2(3)	40(4)	0(3)
C(15)	120(5)	42(3)	55(3)	-4(2)	22(3)	28(3)
C(16)	51(3)	52(3)	54(3)	-5(2)	10(2)	-8(2)
C(17)	29(2)	24(2)	29(2)	-4(2)	-4(2)	0(2)
C(18)	34(2)	50(3)	44(3)	10(2)	6(2)	-2(2)
C(19)	41(2)	42(2)	35(3)	-1(2)	8(2)	-5(2)
C(20)	59(3)	54(3)	46(3)	-7(2)	1(2)	8(3)
C(21)	78(4)	52(3)	61(4)	-11(3)	13(3)	10(3)
C(22)	91(4)	59(3)	44(3)	-14(3)	10(3)	-6(3)
C(23)	73(4)	62(3)	41(3)	0(3)	-8(3)	-15(3)
C(24)	51(3)	43(3)	42(3)	3(2)	-3(2)	-4(2)
C(25)	55(12)	50(9)	86(11)	9(7)	12(8)	-21(8)
C(26)	49(8)	52(8)	62(8)	29(7)	22(7)	-11(6)
C(27)	59(12)	61(9)	60(9)	5(7)	-1(7)	-3(8)
C(28)	114(16)	62(10)	73(10)	14(8)	27(11)	-27(10)
C(29)	160(20)	73(12)	100(20)	-6(12)	7(15)	-51(13)
C(30)	87(17)	81(12)	71(14)	18(10)	-16(11)	-60(12)
C(31)	124(14)	119(13)	71(11)	21(9)	-20(9)	-11(11)
C(25A)	86(10)	46(9)	57(12)	20(7)	11(8)	3(8)
C(26A)	78(15)	85(13)	50(13)	-10(10)	0(9)	-36(10)
C(27A)	66(11)	83(13)	105(16)	-10(11)	-8(11)	-38(9)
C(28A)	58(11)	66(10)	170(30)	-1(12)	-23(14)	-27(8)
C(29A)	69(11)	64(11)	160(30)	46(15)	33(15)	-17(9)
C(30A)	33(10)	41(9)	190(30)	17(12)	30(12)	-6(8)
C(31A)	180(20)	121(14)	79(13)	5(11)	-7(12)	5(14)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 3.

	x	y	z	U(eq)
H(2A)	1415	8303	-16	52
H(2B)	659	7816	294	52
H(4A)	2071	7059	739	59
H(5A)	2743	6988	1668	64
H(6A)	2549	8160	2378	58
H(7A)	1705	9355	2146	49
H(10A)	-1651	12480	1665	64
H(12A)	243	13751	938	53
H(14A)	-1850	10884	1577	117
H(14B)	-1036	10315	1550	117
H(14C)	-1544	10475	944	117
H(15A)	-1545	14062	1817	108
H(15B)	-1135	14592	1263	108
H(15C)	-641	14405	1873	108
H(16A)	1210	12957	377	79
H(16B)	859	12118	-5	79
H(16C)	1354	11931	603	79
H(20A)	211	12732	2303	64
H(21A)	312	13787	3082	76
H(22A)	1141	13528	3906	78
H(23A)	1895	12163	3948	70
H(24A)	1788	11106	3172	55
H(26A)	4946	11179	1348	65
H(27A)	4979	11122	287	72
H(28A)	3920	10462	-248	99
H(29A)	2828	9859	278	131
H(30A)	2794	9916	1339	96
H(31A)	4297	10863	2259	157
H(31B)	3782	9943	2248	157
H(31C)	3345	10915	2218	157
H(26B)	2751	9660	1051	85
H(27B)	3441	10072	1933	101
H(28B)	4632	10900	1863	119
H(29B)	5133	11315	910	118
H(30B)	4443	10903	28	105
H(31D)	2668	9619	40	192
H(31E)	3491	9641	-329	192
H(31F)	2955	10543	-281	192

Table 1. Crystal data and structure refinement for 5.

Identification code	FO1258
Empirical formula	$C_{16}H_{40}Li_4Ni_2O_2$
Formula weight	409.66
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 6.9022(3) Å alpha = 110.586(3)° b = 8.4718(5) Å beta = 97.200(3)° c = 10.1497(6) Å gamma = 97.684(3)°
Volume, Z	541.02(5) $Å^3$, 1
Density (calculated)	1.257 Mg/m^3
Absorption coefficient	1.742 mm^{-1}
F(000)	220
Crystal size	0.18 x 0.16 x 0.12 mm
θ range for data collection	3.03 to 27.47°
Limiting indices	$-8 \le h \le 8$, $-9 \le k \le 10$, $-12 \le l \le 13$
Reflections collected	3645
Independent reflections	2404 (R_{int} = 0.0226)
Completeness to θ = 27.47°	97.7 %
Max. and min. transmission	0.8182 and 0.7445
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2404 / 0 / 189
Goodness-of-fit on F^2	0.705
Final R indices [I>2σ(I)]	R1 = 0.0274, wR2 = 0.0829
R indices (all data)	R1 = 0.0312, wR2 = 0.0865
Largest diff. peak and hole	0.375 and -0.405 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 5. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni	4238(1)	10733(1)	3835(1)	22(1)
Li(1)	6374(5)	12428(4)	6376(4)	32(1)
Li(2)	7231(4)	9686(4)	4235(3)	28(1)
C(1)	3323(3)	12717(2)	5214(2)	30(1)
C(2)	1426(3)	9391(3)	3304(2)	29(1)
C(3)	5011(3)	8948(3)	2174(2)	30(1)
C(4)	6845(3)	12263(3)	4064(2)	29(1)
O(1)	7804(2)	14750(2)	7737(2)	39(1)
C(5)	9804(3)	15510(3)	7735(3)	47(1)
C(6)	10289(4)	17217(4)	8944(3)	59(1)
C(7)	8324(5)	17691(3)	9189(3)	54(1)
C(8)	6967(4)	16000(3)	8775(3)	50(1)

Table 3. Bond lengths [Å] and angles [°] for 5.

Ni-C(4)	2.0083(19)	Ni-C(1)	2.009(2)
Ni-C(3)	2.016(2)	Ni-C(2)	2.0166(19)
Ni-Li(2)	2.398(3)	Ni-Li(2)#1	2.426(3)
Ni-Li(1)#1	2.582(3)	Ni-Li(1)	2.601(3)
Li(1)-O(1)	1.995(3)	Li(1)-C(4)	2.367(4)
Li(1)-C(1)	2.368(4)	Li(1)-C(2)#1	2.375(4)
Li(1)-C(3)#1	2.388(4)	Li(1)-Ni#1	2.582(3)
Li(1)-Li(2)#1	2.725(4)	Li(1)-Li(2)	2.758(5)
Li(2)-C(3)	2.266(4)	Li(2)-C(1)#1	2.292(4)
Li(2)-C(4)	2.297(4)	Li(2)-C(2)#1	2.359(4)
Li(2)-Ni#1	2.426(3)	Li(2)-Li(1)#1	2.725(4)
C(1)-Li(2)#1	2.292(4)	C(2)-Li(2)#1	2.359(4)
C(2)-Li(1)#1	2.375(4)	C(3)-Li(1)#1	2.388(4)
O(1)-C(5)	1.443(3)	O(1)-C(8)	1.448(3)
C(5)-C(6)	1.493(3)	C(6)-C(7)	1.490(4)
C(7)-C(8)	1.492(3)		

C(4)-Ni-C(1)	90.00(9)	C(4)-Ni-C(3)	88.05(8)
C(1)-Ni-C(3)	168.88(9)	C(4)-Ni-C(2)	168.28(9)
C(1)-Ni-C(2)	88.92(8)	C(3)-Ni-C(2)	90.76(8)
C(4)-Ni-Li(2)	62.10(9)	C(1)-Ni-Li(2)	127.03(10)
C(3)-Ni-Li(2)	61.05(9)	C(2)-Ni-Li(2)	126.90(10)
C(4)-Ni-Li(2)#1	125.74(10)	C(1)-Ni-Li(2)#1	61.39(9)
C(3)-Ni-Li(2)#1	127.88(10)	C(2)-Ni-Li(2)#1	63.36(9)
Li(2)-Ni-Li(2)#1	97.92(9)	C(4)-Ni-Li(1)#1	127.93(9)
C(1)-Ni-Li(1)#1	127.60(10)	C(3)-Ni-Li(1)#1	61.12(10)
C(2)-Ni-Li(1)#1	60.71(9)	Li(2)-Ni-Li(1)#1	66.22(10)
Li(2)#1-Ni-Li(1)#1	66.76(11)	C(4)-Ni-Li(1)	60.20(10)
C(1)-Ni-Li(1)	60.20(9)	C(3)-Ni-Li(1)	127.28(9)
C(2)-Ni-Li(1)	128.41(10)	Li(2)-Ni-Li(1)	66.84(10)
Li(2)#1-Ni-Li(1)	65.55(10)	Li(1)#1-Ni-Li(1)	104.66(8)
O(1)-Li(1)-C(4)	106.46(16)	O(1)-Li(1)-C(1)	108.48(15)
C(4)-Li(1)-C(1)	73.72(12)	O(1)-Li(1)-C(2)#1	102.91(15)
C(4)-Li(1)-C(2)#1	97.98(14)	C(1)-Li(1)-C(2)#1	148.60(16)
O(1)-Li(1)-C(3)#1	105.42(17)	C(4)-Li(1)-C(3)#1	148.11(16)
C(1)-Li(1)-C(3)#1	96.78(14)	C(2)#1-Li(1)-C(3)#1	74.11(12)
O(1)-Li(1)-Ni#1	140.36(17)	C(4)-Li(1)-Ni#1	104.09(13)
C(1)-Li(1)-Ni#1	103.87(12)	C(2)#1-Li(1)-Ni#1	47.78(8)
C(3)#1-Li(1)-Ni#1	47.65(8)	O(1)-Li(1)-Ni	144.24(17)
C(4)-Li(1)-Ni	47.40(8)	C(1)-Li(1)-Ni	47.41(8)
C(2)#1-Li(1)-Ni	104.62(13)	C(3)#1-Li(1)-Ni	103.75(12)
Ni#1-Li(1)-Ni	75.34(8)	O(1)-Li(1)-Li(2)#1	139.57(17)
C(4)-Li(1)-Li(2)#1	101.52(14)	C(1)-Li(1)-Li(2)#1	52.93(10)
C(2)#1-Li(1)-Li(2)#1	101.41(14)	C(3)#1-Li(1)-Li(2)#1	52.10(10)
Ni#1-Li(1)-Li(2)#1	53.65(9)	Ni-Li(1)-Li(2)#1	54.13(9)
O(1)-Li(1)-Li(2)	137.23(17)	C(4)-Li(1)-Li(2)	52.58(11)
C(1)-Li(1)-Li(2)	100.48(14)	C(2)#1-Li(1)-Li(2)	54.09(10)
C(3)#1-Li(1)-Li(2)	101.55(14)	Ni#1-Li(1)-Li(2)	53.90(9)
Ni-Li(1)-Li(2)	53.07(9)	Li(2)#1-Li(1)-Li(2)	83.14(13)
C(3)-Li(2)-C(1)#1	102.56(15)	C(3)-Li(2)-C(4)	75.59(12)
C(1)#1-Li(2)-C(4)	159.93(16)	C(3)-Li(2)-C(2)#1	160.88(16)
C(1)#1-Li(2)-C(2)#1	74.62(12)	C(4)-Li(2)-C(2)#1	100.44(14)
C(3)-Li(2)-Ni	51.11(8)	C(1)#1-Li(2)-Ni	112.46(13)
C(4)-Li(2)-Ni	50.59(8)	C(2)#1-Li(2)-Ni	111.81(13)
C(3)-Li(2)-Ni#1	113.60(13)	C(1)#1-Li(2)-Ni#1	50.31(8)

C(4)-Li(2)-Ni#1	111.51(13)	C(2)#1-Li(2)-Ni#1	49.83(8)
Ni-Li(2)-Ni#1	82.08(9)	C(3)-Li(2)-Li(1)#1	56.27(11)
C(1)#1-Li(2)-Li(1)#1	55.52(11)	C(4)-Li(2)-Li(1)#1	110.44(14)
C(2)#1-Li(2)-Li(1)#1	109.81(15)	Ni-Li(2)-Li(1)#1	60.13(9)
Ni#1-Li(2)-Li(1)#1	60.32(10)	C(3)-Li(2)-Li(1)	110.77(14)
C(1)#1-Li(2)-Li(1)	109.26(15)	C(4)-Li(2)-Li(1)	54.93(11)
C(2)#1-Li(2)-Li(1)	54.63(11)	Ni-Li(2)-Li(1)	60.09(9)
Ni#1-Li(2)-Li(1)	59.33(10)	Li(1)#1-Li(2)-Li(1)	96.86(13)
Ni-C(1)-Li(2)#1	68.30(10)	Ni-C(1)-Li(1)	72.39(10)
Li(2)#1-C(1)-Li(1)	71.56(12)	Ni-C(2)-Li(2)#1	66.80(9)
Ni-C(2)-Li(1)#1	71.50(10)	Li(2)#1-C(2)-Li(1)#1	71.28(12)
Ni-C(3)-Li(2)	67.85(10)	Ni-C(3)-Li(1)#1	71.23(10)
Li(2)-C(3)-Li(1)#1	71.63(12)	Ni-C(4)-Li(2)	67.31(9)
Ni-C(4)-Li(1)	72.40(10)	Li(2)-C(4)-Li(1)	72.48(13)
C(5)-O(1)-C(8)	109.09(17)	C(5)-O(1)-Li(1)	124.43(16)
C(8)-O(1)-Li(1)	126.22(17)	O(1)-C(5)-C(6)	106.3(2)
C(7)-C(6)-C(5)	104.9(2)	C(6)-C(7)-C(8)	103.6(2)
O(1)-C(8)-C(7)	106.6(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 5.

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	19(1)	22(1)	25(1)	10(1)	5(1)	5(1)
Li(1)	29(2)	23(1)	38(2)	8(1)	5(1)	3(1)
Li(2)	25(1)	31(2)	30(2)	12(1)	8(1)	8(1)
C(1)	28(1)	23(1)	40(1)	11(1)	8(1)	10(1)
C(2)	22(1)	33(1)	31(1)	12(1)	4(1)	5(1)
C(3)	29(1)	35(1)	25(1)	10(1)	8(1)	6(1)
C(4)	25(1)	28(1)	35(1)	14(1)	10(1)	2(1)
O(1)	33(1)	28(1)	45(1)	-1(1)	13(1)	0(1)
C(5)	32(1)	35(1)	57(2)	0(1)	12(1)	-3(1)
C(6)	54(2)	48(2)	47(2)	-7(1)	10(1)	-16(1)
C(7)	70(2)	34(1)	46(1)	2(1)	20(1)	3(1)
C(8)	42(1)	36(1)	57(2)	-2(1)	20(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5.

	x	y	z	U(eq)
H(1A)	2160(50)	12630(40)	5670(30)	49(8)
H(1B)	4110(50)	13630(40)	5920(30)	51(8)
H(1C)	2900(40)	13130(40)	4590(30)	41(7)
H(2A)	680(50)	9280(40)	3950(40)	63(9)
H(2B)	950(40)	10010(40)	2840(30)	55(8)
H(2C)	1080(50)	8180(50)	2610(40)	63(9)
H(3A)	6380(40)	8730(40)	2060(30)	45(7)
H(3B)	4330(40)	7770(40)	1790(30)	42(7)
H(3C)	4650(40)	9460(40)	1500(30)	58(8)
H(4A)	7990(40)	11840(40)	3760(30)	49(8)
H(4B)	6410(50)	12560(40)	3270(30)	62(9)
H(4C)	7200(40)	13310(40)	4820(30)	52(8)
H(5A)	9890(60)	15680(50)	6810(40)	85(12)
H(5B)	10550(50)	14770(40)	7680(40)	67(9)
H(6A)	11130(80)	18020(70)	8790(60)	130(17)
H(6B)	10890(80)	17230(70)	9620(60)	130(20)
H(7A)	8380(50)	18440(40)	10110(40)	74(10)
H(7B)	7790(60)	18260(50)	8490(50)	111(15)
H(8A)	5630(50)	15840(40)	8440(30)	57(8)
H(8B)	7100(50)	15710(40)	9800(40)	78(10)

Table 1. Crystal data and structure refinement for 6.

Identification code	FO1330
Empirical formula	$C_{24}H_{56}Li_4Ni_2O_4$
Formula weight	553.87
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 8.5892(8) Å alpha = 111.184(6)° b = 8.9512(8) Å beta = 107.343(8)° c = 11.0999(9) Å gamma = 91.881(7)°
Volume, Z	750.0(1) $Å^3$, 1
Density (calculated)	1.226 Mg/m^3
Absorption coefficient	1.279 mm^{-1}
F(000)	300
Crystal size	0.20 x 0.18 x 0.12 mm
θ range for data collection	3.77 to 27.53°
Limiting indices	$-10 \le h \le 11$, $-10 \le k \le 11$, $-14 \le l \le 14$
Reflections collected	4990
Independent reflections	3311 (R_{int} = 0.0328)
Completeness to θ = 27.53°	95.6 %
Max. and min. transmission	0.8617 and 0.7840
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3311 / 0 / 202
Goodness-of-fit on F^2	1.188
Final R indices [I>2σ(I)]	R1 = 0.0865, wR2 = 0.1436
R indices (all data)	R1 = 0.1012, wR2 = 0.1488
Largest diff. peak and hole	0.706 and -0.730 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 6. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni	1110(1)	5591(1)	4311(1)	26(1)
Li(1)	-668(9)	2865(9)	3428(8)	35(2)
Li(2)	1891(9)	4137(9)	5937(8)	35(2)
O(1)	-1325(4)	665(4)	1803(3)	42(1)
O(2)	3831(4)	3186(4)	6885(3)	40(1)
C(1)	2124(6)	3570(6)	3775(5)	38(1)
C(2)	3083(6)	6601(6)	6014(5)	36(1)
C(3)	438(6)	7777(6)	4644(5)	36(1)
C(4)	-565(6)	4766(6)	2415(5)	36(1)
C(5)	-2692(8)	287(7)	599(6)	63(2)
C(6)	-2946(8)	-1474(7)	-233(6)	69(2)
C(7)	-1467(9)	-2062(7)	417(7)	76(2)
C(8)	-527(8)	-729(6)	1705(6)	62(2)
C(9)	4201(7)	1598(6)	6290(7)	65(2)
C(10)	5665(8)	1396(8)	7253(7)	76(2)
C(11)	6364(8)	3014(8)	8351(8)	82(2)
C(12)	5244(8)	4119(7)	8027(6)	64(2)

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

Ni-C(3)	1.994(5)	Ni-C(2)	2.005(5)
Ni-C(1)	2.005(5)	Ni-C(4)	2.011(5)
Ni-Li(1)	2.526(7)	Ni-Li(2)#1	2.539(7)
Ni-Li(1)#1	2.540(8)	Ni-Li(2)	2.537(8)
Li(1)-O(1)	2.050(8)	Li(1)-C(1)	2.339(9)
Li(1)-C(2)#1	2.353(9)	Li(1)-C(4)	2.367(9)
Li(1)-C(3)#1	2.364(9)	Li(1)-Ni#1	2.540(8)
Li(1)-Li(2)	2.789(10)	Li(1)-Li(2)#1	2.839(11)
Li(2)-O(2)	2.075(8)	Li(2)-C(1)	2.339(9)
Li(2)-C(3)#1	2.358(9)	Li(2)-C(2)	2.363(9)
Li(2)-C(4)#1	2.372(9)	Li(2)-Ni#1	2.539(7)
Li(2)-Li(1)#1	2.839(11)	O(1)-C(5)	1.412(6)
O(1)-C(8)	1.428(6)	O(2)-C(12)	1.424(6)
O(2)-C(9)	1.426(6)	C(2)-Li(1)#1	2.353(9)
C(3)-Li(2)#1	2.358(9)	C(3)-Li(1)#1	2.364(9)
C(4)-Li(2)#1	2.372(9)	C(5)-C(6)	1.480(8)
C(6)-C(7)	1.477(9)	C(7)-C(8)	1.462(8)
C(9)-C(10)	1.453(8)	C(10)-C(11)	1.475(9)
C(11)-C(12)	1.464(8)		

C(3)-Ni-C(2)	88.9(2)	C(3)-Ni-C(1)	166.6(2)
C(2)-Ni-C(1)	89.5(2)	C(3)-Ni-C(4)	89.0(2)
C(2)-Ni-C(4)	167.4(2)	C(1)-Ni-C(4)	89.6(2)
C(3)-Ni-Li(1)	129.2(2)	C(2)-Ni-Li(1)	128.1(2)
C(1)-Ni-Li(1)	60.9(2)	C(4)-Ni-Li(1)	61.7(2)
C(3)-Ni-Li(2)#1	61.3(2)	C(2)-Ni-Li(2)#1	127.4(2)
C(1)-Ni-Li(2)#1	128.9(2)	C(4)-Ni-Li(2)#1	61.6(2)
Li(1)-Ni-Li(2)#1	68.2(2)	C(3)-Ni-Li(1)#1	61.5(2)
C(2)-Ni-Li(1)#1	61.0(2)	C(1)-Ni-Li(1)#1	128.5(2)
C(4)-Ni-Li(1)#1	128.0(2)	Li(1)-Ni-Li(1)#1	103.3(2)
Li(2)#1-Ni-Li(1)#1	66.6(2)	C(3)-Ni-Li(2)	129.2(2)
C(2)-Ni-Li(2)	61.4(2)	C(1)-Ni-Li(2)	60.6(2)
C(4)-Ni-Li(2)	128.3(2)	Li(1)-Ni-Li(2)	66.8(2)
Li(2)#1-Ni-Li(2)	103.5(2)	Li(1)#1-Ni-Li(2)	68.0(2)
O(1)-Li(1)-C(1)	103.1(4)	O(1)-Li(1)-C(2)#1	105.3(3)
C(1)-Li(1)-C(2)#1	151.6(4)	O(1)-Li(1)-C(4)	103.9(3)
C(1)-Li(1)-C(4)	73.9(3)	C(2)#1-Li(1)-C(4)	98.8(3)
O(1)-Li(1)-C(3)#1	104.6(3)	C(1)-Li(1)-C(3)#1	100.3(3)
C(2)#1-Li(1)-C(3)#1	72.8(3)	C(4)-Li(1)-C(3)#1	151.5(4)
O(1)-Li(1)-Ni	140.9(4)	C(1)-Li(1)-Ni	48.49(19)
C(2)#1-Li(1)-Ni	106.1(3)	C(4)-Li(1)-Ni	48.41(19)
C(3)#1-Li(1)-Ni	106.6(3)	O(1)-Li(1)-Ni#1	142.5(4)
C(1)-Li(1)-Ni#1	106.5(3)	C(2)#1-Li(1)-Ni#1	48.19(19)
C(4)-Li(1)-Ni#1	106.1(3)	C(3)#1-Li(1)-Ni#1	47.82(19)
Ni-Li(1)-Ni#1	76.7(2)	O(1)-Li(1)-Li(2)	134.0(4)
C(1)-Li(1)-Li(2)	53.4(3)	C(2)#1-Li(1)-Li(2)	104.7(3)
C(4)-Li(1)-Li(2)	105.0(3)	C(3)#1-Li(1)-Li(2)	53.7(3)
Ni-Li(1)-Li(2)	56.8(2)	Ni#1-Li(1)-Li(2)	56.7(2)
O(1)-Li(1)-Li(2)#1	135.8(4)	C(1)-Li(1)-Li(2)#1	104.5(3)
C(2)#1-Li(1)-Li(2)#1	53.1(3)	C(4)-Li(1)-Li(2)#1	53.3(3)
C(3)#1-Li(1)-Li(2)#1	103.6(3)	Ni-Li(1)-Li(2)#1	56.1(2)
Ni#1-Li(1)-Li(2)#1	55.9(2)	Li(2)-Li(1)-Li(2)#1	90.2(3)
O(2)-Li(2)-C(1)	103.6(3)	O(2)-Li(2)-C(3)#1	103.2(3)
C(1)-Li(2)-C(3)#1	100.5(3)	O(2)-Li(2)-C(2)	106.0(3)
C(1)-Li(2)-C(2)	73.8(3)	C(3)#1-Li(2)-C(2)	150.8(4)

O(2)-Li(2)-C(4)#1	104.8(3)	C(1)-Li(2)-C(4)#1	151.6(4)
C(3)#1-Li(2)-C(4)#1	72.8(3)	C(2)-Li(2)-C(4)#1	98.4(3)
O(2)-Li(2)-Ni#1	141.2(4)	C(1)-Li(2)-Ni#1	106.6(3)
C(3)#1-Li(2)-Ni#1	47.88(19)	C(2)-Li(2)-Ni#1	105.3(3)
C(4)#1-Li(2)-Ni#1	48.20(19)	O(2)-Li(2)-Ni	142.2(4)
C(1)-Li(2)-Ni	48.35(19)	C(3)#1-Li(2)-Ni	106.4(3)
C(2)-Li(2)-Ni	48.14(19)	C(4)#1-Li(2)-Ni	106.0(3)
Ni#1-Li(2)-Ni	76.5(2)	O(2)-Li(2)-Li(1)	133.4(4)
C(1)-Li(2)-Li(1)	53.4(3)	C(3)#1-Li(2)-Li(1)	53.9(2)
C(2)-Li(2)-Li(1)	104.4(3)	C(4)#1-Li(2)-Li(1)	104.8(3)
Ni#1-Li(2)-Li(1)	56.7(2)	Ni-Li(2)-Li(1)	56.4(2)
O(2)-Li(2)-Li(1)#1	136.8(4)	C(1)-Li(2)-Li(1)#1	104.3(3)
C(3)#1-Li(2)-Li(1)#1	103.4(3)	C(2)-Li(2)-Li(1)#1	52.8(3)
C(4)#1-Li(2)-Li(1)#1	53.1(2)	Ni#1-Li(2)-Li(1)#1	55.7(2)
Ni-Li(2)-Li(1)#1	56.0(2)	Li(1)-Li(2)-Li(1)#1	89.8(3)
C(5)-O(1)-C(8)	109.1(4)	C(5)-O(1)-Li(1)	124.3(4)
C(8)-O(1)-Li(1)	126.6(4)	C(12)-O(2)-C(9)	107.8(4)
C(12)-O(2)-Li(2)	125.0(4)	C(9)-O(2)-Li(2)	125.0(4)
Ni-C(1)-Li(1)	70.6(2)	Ni-C(1)-Li(2)	71.0(2)
Li(1)-C(1)-Li(2)	73.2(3)	Ni-C(2)-Li(1)#1	70.8(2)
Ni-C(2)-Li(2)	70.5(2)	Li(1)#1-C(2)-Li(2)	74.1(3)
Ni-C(3)-Li(2)#1	70.8(2)	Ni-C(3)-Li(1)#1	70.7(2)
Li(2)#1-C(3)-Li(1)#1	72.4(3)	Ni-C(4)-Li(1)	69.9(2)
Ni-C(4)-Li(2)#1	70.2(2)	Li(1)-C(4)-Li(2)#1	73.6(3)
O(1)-C(5)-C(6)	108.9(4)	C(5)-C(6)-C(7)	105.4(5)
C(8)-C(7)-C(6)	107.2(5)	O(1)-C(8)-C(7)	108.4(5)
O(2)-C(9)-C(10)	108.7(5)	C(9)-C(10)-C(11)	106.5(5)
C(12)-C(11)-C(10)	106.4(5)	O(2)-C(12)-C(11)	108.4(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1

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

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	26(1)	25(1)	28(1)	11(1)	11(1)	3(1)
Li(1)	33(4)	31(4)	35(4)	10(3)	7(3)	2(3)
Li(2)	33(4)	34(4)	34(4)	11(3)	10(3)	8(3)
O(1)	45(2)	31(2)	36(2)	7(1)	-1(2)	11(1)
O(2)	35(2)	29(2)	39(2)	5(1)	1(1)	6(1)
C(1)	36(2)	44(3)	39(3)	16(2)	19(2)	13(2)
C(2)	25(2)	35(3)	44(3)	14(2)	8(2)	0(2)
C(3)	43(3)	27(2)	41(3)	17(2)	13(2)	1(2)
C(4)	40(3)	40(3)	29(2)	14(2)	13(2)	9(2)
C(5)	60(3)	41(3)	54(3)	5(3)	-12(3)	10(3)
C(6)	72(4)	48(3)	51(3)	-4(3)	-1(3)	13(3)
C(7)	89(5)	38(3)	69(4)	2(3)	3(4)	24(3)
C(8)	88(4)	39(3)	50(3)	15(2)	8(3)	29(3)
C(9)	57(3)	31(3)	72(4)	5(3)	-10(3)	16(2)
C(10)	74(4)	55(4)	72(4)	12(3)	0(4)	35(3)
C(11)	62(4)	53(4)	84(5)	17(3)	-30(4)	7(3)
C(12)	67(4)	34(3)	55(3)	7(3)	-14(3)	2(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 6.

	x	y	z	U(eq)
H(1A)	2870(70)	3850(70)	3310(60)	58(16)
H(1B)	2890(80)	3300(70)	4390(60)	63(18)
H(1C)	1470(90)	2520(90)	3010(70)	80(20)
H(2A)	3700(70)	6030(70)	6420(60)	49(16)
H(2B)	3090(70)	7620(80)	6730(70)	67(18)
H(2C)	3820(90)	6910(80)	5680(70)	80(20)
H(3A)	-730(70)	7920(60)	4110(60)	54(15)
H(3B)	680(70)	8590(70)	5550(60)	51(15)
H(3C)	1160(70)	8160(60)	4200(50)	51(15)
H(4A)	-1550(60)	5260(60)	2250(50)	41(13)
H(4B)	110(70)	5120(60)	2000(60)	50(15)
H(4C)	-910(70)	3570(80)	1800(60)	64(17)
H(5A)	-2487	910	69	75
H(5B)	-3693	584	839	75
H(6A)	-3049	-1672	-1192	83
H(6B)	-3957	-2029	-226	83
H(7A)	-1796	-3013	593	91
H(7B)	-790	-2388	-190	91
H(8A)	-481	-1032	2488	75
H(8B)	617	-488	1728	75
H(9A)	4400	1455	5424	78
H(9B)	3258	773	6082	78
H(10A)	6476	970	6793	91
H(10B)	5371	627	7635	91
H(11A)	6437	2994	9251	99
H(11B)	7484	3366	8380	99
H(12A)	4906	4721	8826	76
H(12B)	5808	4914	7803	76