Crystal data and structure refinement for **2**.

Identification code	ass05	
Empirical formula	C22 H26 N2 Ni O4	
Formula weight	441.16	
Temperature	173(2) K	
Wavelength	0.71073 ≈	
Crystal system	Orthorhombic	
Space group	Pnma	
Unit cell dimensions	a = 7.5385(7) ≈	α= 90∞.
	b = 15.3049(15) ≈	β= 90∞.
	c = 17.806(2) ≈	γ = 90∞.
Volume	2054.4(4) ≈^{3}	
Z	4	
Density (calculated)	1.426 Mg/m^3	
Absorption coefficient	0.975 mm^{-1}	
F(000)	928	
Crystal size	0.15 x 0.10 x 0.02 mm^3	
Theta range for data collection	2.29 to 24.99∞.	
Index ranges	-8<=h<=8, -18<=k<=18, -20<=l<=21	
Reflections collected	3325	
Independent reflections	1865 [R(int) = 0.1308]	
Reflections [I>2sig.(I)]	911	
Completeness to theta = 24.99∞	99.2 %	
Max. and min. transmission	0.9808 and 0.8675	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1865 / 0 / 141	
Goodness-of-fit on F^2	0.917	
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.0977	
R indices (all data)	R1 = 0.1529, wR2 = 0.1268	
Largest diff. peak and hole	0.425 and -0.374 e.≈^{3}	

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Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for ass05. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	8080(2)	7500	5713(1)	33(1)
O(1)	11639(5)	8651(2)	5417(2)	44(1)
O(2)	10703(6)	9201(2)	4320(2)	52(1)
N(10)	7394(5)	8327(3)	6463(2)	32(1)
C(1)	9199(8)	7969(3)	4849(3)	31(1)
C(2)	10528(8)	8646(4)	4808(3)	36(2)
C(3)	12934(9)	9348(3)	5435(3)	56(2)
C(4)	8449(11)	7500	4166(4)	34(2)
C(5)	6477(12)	7500	3970(5)	46(2)
C(6)	6012(10)	8311(3)	3508(4)	71(2)
C(7)	5309(13)	7500	4660(5)	78(3)
C(8)	9675(13)	7500	3472(4)	49(2)
C(11)	6908(8)	7986(3)	7134(3)	33(1)
C(12)	6489(7)	8495(3)	7741(3)	42(2)
C(13)	6525(8)	9396(3)	7666(3)	45(2)
C(14)	7027(8)	9751(3)	6995(3)	42(2)
C(15)	7452(7)	9199(3)	6409(3)	36(2)

Bond lengths [≈] and angles [∞] for **2**.

Ni(1)-C(1)	1.897(5)
Ni(1)-C(1)#1	1.897(5)
Ni(1)-N(10)#1	1.911(4)
Ni(1)-N(10)	1.911(4)
O(1)-C(2)	1.370(6)
O(1)-C(3)	1.446(6)
O(2)-C(2)	1.223(5)
N(10)-C(15)	1.338(5)
N(10)-C(11)	1.354(6)
C(1)-C(1)#1	1.437(9)
C(1)-C(2)	1.443(7)
C(1)-C(4)	1.521(7)
C(4)-C(1)#1	1.521(7)
C(4)-C(5)	1.527(12)
C(4)-C(8)	1.543(10)
C(5)-C(6)#1	1.530(7)
C(5)-C(6)	1.530(7)
C(5)-C(7)	1.512(11)
C(11)-C(12)	1.370(6)
C(11)-C(11)#1	1.488(9)
C(12)-C(13)	1.386(6)
C(13)-C(14)	1.366(7)
C(14)-C(15)	1.381(6)
C(1)-Ni(1)-C(1)#1	44.5(3)
C(1)-Ni(1)-N(10)#1	159.77(19)
C(1)#1-Ni(1)-N(10)#1	115.90(18)
C(1)-Ni(1)-N(10)	115.90(19)
C(1)#1-Ni(1)-N(10)	159.77(19)
N(10)#1-Ni(1)-N(10)	82.9(2)
C(2)-O(1)-C(3)	115.8(4)
C(15)-N(10)-C(11)	117.2(4)
C(15)-N(10)-Ni(1)	126.9(4)
C(11)-N(10)-Ni(1)	115.8(3)

C(1)#1-C(1)-C(2)	135.9(3)
C(1)#1-C(1)-C(4)	61.8(2)
C(2)-C(1)-C(4)	123.9(4)
C(1)#1-C(1)-Ni(1)	67.75(14)
C(2)-C(1)-Ni(1)	128.4(3)
C(4)-C(1)-Ni(1)	107.7(4)
O(2)-C(2)-O(1)	119.5(5)
O(2)-C(2)-C(1)	127.5(5)
O(1)-C(2)-C(1)	112.9(4)
C(1)-C(4)-C(1)#1	56.4(4)
C(1)-C(4)-C(5)	123.0(6)
C(1)#1-C(4)-C(5)	123.0(6)
C(1)-C(4)-C(8)	114.7(6)
C(1)#1-C(4)-C(8)	114.7(6)
C(5)-C(4)-C(8)	113.6(6)
C(6)#1-C(5)-C(6)	108.4(7)
C(6)#1-C(5)-C(4)	110.2(5)
C(6)-C(5)-C(4)	110.2(5)
C(6)#1-C(5)-C(7)	107.7(5)
C(6)-C(5)-C(7)	107.7(5)
C(4)-C(5)-C(7)	112.5(7)
N(10)-C(11)-C(12)	122.7(4)
N(10)-C(11)-C(11)#1	112.7(2)
C(12)-C(11)-C(11)#1	124.6(3)
C(11)-C(12)-C(13)	119.0(5)
C(14)-C(13)-C(12)	119.1(5)
C(13)-C(14)-C(15)	118.8(5)
N(10)-C(15)-C(14)	123.2(5)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z

Anisotropic displacement parameters ($\approx^2$x 10^3) for for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2\, a^{*2}U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	35(1)	35(1)	31(1)	0	0(1)	0
O(1)	38(3)	52(2)	43(2)	0(2)	-5(2)	-11(2)
O(2)	57(3)	49(2)	51(2)	12(2)	-10(2)	-17(2)
N(10)	28(3)	35(2)	32(2)	-1(2)	-2(2)	2(2)
C(1)	29(4)	36(3)	29(3)	8(2)	0(3)	-5(3)
C(2)	33(4)	47(3)	29(3)	-3(3)	5(3)	4(3)
C(3)	41(4)	66(4)	61(4)	-8(3)	-1(4)	-21(4)
C(4)	36(6)	38(4)	27(4)	0	-6(4)	0
C(5)	49(7)	40(5)	50(5)	0	1(5)	0
C(6)	80(6)	47(4)	85(5)	8(3)	-29(4)	7(4)
C(7)	32(7)	128(9)	72(7)	0	-13(6)	0
C(8)	70(8)	48(5)	30(5)	0	12(5)	0
C(11)	22(3)	47(3)	28(3)	-1(2)	-2(3)	-2(3)
C(12)	40(5)	50(3)	37(3)	-2(3)	10(3)	-2(3)
C(13)	43(5)	52(4)	41(4)	-16(3)	1(3)	10(3)
C(14)	40(4)	33(3)	54(4)	-6(3)	-10(4)	7(3)
C(15)	34(4)	36(3)	37(3)	3(3)	-5(3)	2(3)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (≈^{2}x 10 ^{3}) for **2**.

	x	y	z	U(eq)
H(3A)	13753	9253	5855	84
H(3B)	12327	9909	5501	84
H(3C)	13600	9354	4963	84
H(6A)	6717	8315	3045	106
H(6B)	6273	8837	3801	106
H(6C)	4747	8300	3380	106
H(7A)	4076	7500	4525	117
H(7B)	5569	6988	4951	117
H(8A)	10889	7500	3635	74
H(8B)	9452	6988	3175	74
H(12A)	6177	8234	8207	51
H(13A)	6206	9761	8075	54
H(14A)	7081	10367	6932	51
H(15A)	7803	9449	5944	43