Table 1. Crystal data and structure refinement for psty1m.

Identification code	psty1m	
Empirical formula	C16 H24 N2 Ni O5	
Formula weight	383.08	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.4282(16) Å	α= 101.786(4)°.
	b = 9.916(2) Å	β= 99.434(4)°.
	c = 12.270(3) Å	γ = 95.531(4)°.
Volume	864.9(3) $Å^3$	
Z	2	
Density (calculated)	1.471 Mg/m^3	
Absorption coefficient	1.149 mm^{-1}	
F(000)	404	
Crystal size	32.00 x 0.45 x 0.32 mm^3	
Theta range for data collection	1.73 to 23.36°.	
Index ranges	-8<=h<=8, -11<=k<=8, -12<=l<=13	
Reflections collected	3847	
Independent reflections	2484 [R(int) = 0.0341]	
Completeness to theta = 23.36°	98.6 %	
Absorption correction	Empirical	
Max. and min. transmission	0.7099 and 0.0123	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2484 / 0 / 221	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0607, wR2 = 0.1678	
R indices (all data)	R1 = 0.0650, wR2 = 0.1729	
Largest diff. peak and hole	1.126 and -0.885 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for psty1m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	1301(1)	4172(1)	3281(1)	24(1)
N(1)	2233(5)	5326(4)	4696(3)	25(1)
N(2)	600(6)	5736(4)	2836(3)	27(1)
O(1)	1894(5)	2556(3)	3684(3)	29(1)
O(2)	395(5)	3010(3)	1869(3)	28(1)
O(3)	-3489(5)	1374(3)	-1742(3)	36(1)
C(1)	1888(7)	6775(5)	4792(4)	30(1)
C(2)	1502(7)	7040(5)	3614(4)	33(1)
C(3)	-524(7)	5784(5)	1926(4)	28(1)
C(4)	-1319(6)	4606(5)	1029(4)	26(1)
C(5)	-2588(7)	4775(5)	101(4)	32(1)
C(6)	-3301(7)	3711(5)	-805(4)	32(1)
C(7)	-2747(6)	2398(5)	-820(4)	27(1)
C(8)	-1466(7)	2190(5)	77(4)	28(1)
C(9)	-764(6)	3268(5)	1025(4)	26(1)
C(10)	2723(7)	2439(5)	4674(4)	29(1)
C(11)	3269(7)	3521(5)	5590(4)	30(1)
C(12)	3024(6)	4930(5)	5602(4)	29(1)
C(13)	3671(7)	5973(5)	6712(4)	34(1)
C(14)	3003(8)	974(5)	4751(5)	41(1)
O(1S)	-2800(6)	-1087(4)	-1462(3)	46(1)
O(2S)	-7446(7)	1324(5)	-2322(5)	68(1)
C(1S)	-3644(9)	-1654(6)	-690(5)	46(1)
C(2S)	-8229(13)	-30(6)	-2456(6)	77(2)

Table 3. Bond lengths [Å] and angles [°] for psty1m.

Ni(1)-N(2)	1.839(4)
Ni(1)-O(1)	1.843(3)
Ni(1)-O(2)	1.853(3)
Ni(1)-N(1)	1.856(4)
N(1)-C(12)	1.320(7)
N(1)-C(1)	1.468(6)
N(2)-C(3)	1.292(7)
N(2)-C(2)	1.467(6)
O(1)-C(10)	1.302(6)
O(2)-C(9)	1.319(6)
O(3)-C(7)	1.355(6)
C(1)-C(2)	1.509(7)
C(3)-C(4)	1.433(7)
C(4)-C(5)	1.403(7)
C(4)-C(9)	1.427(7)
C(5)-C(6)	1.360(7)
C(6)-C(7)	1.400(7)
C(7)-C(8)	1.395(7)
C(8)-C(9)	1.397(7)
C(10)-C(11)	1.361(7)
C(10)-C(14)	1.506(7)
C(11)-C(12)	1.424(7)
C(12)-C(13)	1.507(7)
O(1S)-C(1S)	1.396(7)
O(2S)-C(2S)	1.377(7)
N(2)-Ni(1)-O(1)	177.14(15)
N(2)-Ni(1)-O(2)	93.97(16)
O(1)-Ni(1)-O(2)	83.83(14)
N(2)-Ni(1)-N(1)	86.54(17)
O(1)-Ni(1)-N(1)	95.68(16)
O(2)-Ni(1)-N(1)	179.31(15)
C(12)-N(1)-C(1)	119.6(4)
C(12)-N(1)-Ni(1)	125.9(3)

C(1)-N(1)-Ni(1)	114.4(3)
C(3)-N(2)-C(2)	119.2(4)
C(3)-N(2)-Ni(1)	127.1(3)
C(2)-N(2)-Ni(1)	113.7(3)
C(10)-O(1)-Ni(1)	126.6(3)
C(9)-O(2)-Ni(1)	127.5(3)
N(1)-C(1)-C(2)	108.2(4)
N(2)-C(2)-C(1)	107.9(4)
N(2)-C(3)-C(4)	125.0(4)
C(5)-C(4)-C(9)	118.8(4)
C(5)-C(4)-C(3)	119.9(4)
C(9)-C(4)-C(3)	121.2(4)
C(6)-C(5)-C(4)	122.4(4)
C(5)-C(6)-C(7)	119.1(5)
O(3)-C(7)-C(8)	122.7(4)
O(3)-C(7)-C(6)	116.9(4)
C(8)-C(7)-C(6)	120.4(4)
C(7)-C(8)-C(9)	120.9(4)
O(2)-C(9)-C(8)	118.8(4)
O(2)-C(9)-C(4)	122.9(4)
C(8)-C(9)-C(4)	118.4(4)
O(1)-C(10)-C(11)	124.2(4)
O(1)-C(10)-C(14)	114.4(4)
C(11)-C(10)-C(14)	121.3(5)
C(10)-C(11)-C(12)	125.1(5)
N(1)-C(12)-C(11)	122.5(4)
N(1)-C(12)-C(13)	120.4(4)
C(11)-C(12)-C(13)	117.1(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for psty1m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	29(1)	13(1)	27(1)	3(1)	6(1)	4(1)
N(1)	29(2)	16(2)	30(2)	2(2)	10(2)	0(2)
N(2)	38(2)	14(2)	30(2)	5(2)	11(2)	5(2)
O(1)	38(2)	18(2)	31(2)	5(1)	4(2)	7(1)
O(2)	37(2)	17(2)	27(2)	3(1)	1(1)	9(1)
O(3)	48(2)	25(2)	31(2)	7(2)	0(2)	8(2)
C(1)	32(3)	17(2)	38(3)	0(2)	9(2)	0(2)
C(2)	44(3)	14(2)	38(3)	2(2)	8(2)	4(2)
C(3)	37(3)	17(2)	38(3)	13(2)	14(2)	9(2)
C(4)	30(2)	20(2)	32(3)	9(2)	10(2)	8(2)
C(5)	39(3)	23(2)	39(3)	14(2)	11(2)	12(2)
C(6)	34(3)	34(3)	34(3)	17(2)	4(2)	11(2)
C(7)	30(2)	23(2)	31(3)	9(2)	7(2)	2(2)
C(8)	35(3)	19(2)	31(3)	7(2)	7(2)	7(2)
C(9)	29(2)	24(2)	28(3)	9(2)	11(2)	5(2)
C(10)	32(3)	24(3)	34(3)	11(2)	6(2)	6(2)
C(11)	32(3)	29(3)	30(3)	10(2)	3(2)	4(2)
C(12)	25(2)	27(3)	34(3)	7(2)	8(2)	-1(2)
C(13)	38(3)	29(3)	31(3)	3(2)	4(2)	-2(2)
C(14)	56(3)	29(3)	39(3)	9(2)	0(3)	14(2)
O(1S)	67(3)	25(2)	55(2)	12(2)	31(2)	22(2)
O(2S)	65(3)	51(3)	84(4)	18(3)	5(3)	7(2)
C(1S)	63(4)	32(3)	45(3)	9(3)	13(3)	11(3)
C(2S)	133(7)	30(3)	54(4)	4(3)	5(4)	-26(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for psty1m.

	x	y	z	U(eq)
H(3A)	-3241	623	-1621	53
H(1A)	2955	7400	5244	36
H(1B)	841	6934	5158	36
H(2A)	707	7758	3590	39
H(2B)	2643	7347	3396	39
H(3B)	-842	6648	1848	34
H(5A)	-2955	5646	106	38
H(6A)	-4145	3853	-1406	39
H(8A)	-1073	1323	43	33
H(11A)	3847	3324	6261	36
H(13A)	3432	6880	6615	51
H(13B)	4969	5985	6957	51
H(13C)	3024	5719	7272	51
H(14A)	2534	356	4026	62
H(14B)	2360	705	5307	62
H(14C)	4293	928	4967	62
H(1S)	-2147	-1629	-1743	55
H(2S)	-6321	1367	-2189	81
H(1S1)	-2719	-1772	-85	69
H(1S2)	-4341	-2540	-1068	69
H(1S3)	-4452	-1039	-387	69
H(2S1)	-7853	-342	-1773	116
H(2S2)	-7833	-611	-3075	116
H(2S3)	-9546	-82	-2614	116

Table 1. Crystal data and structure refinement for psty3m.

Identification code	psty3m	
Empirical formula	C15 H20 N2 O4 Pd	
Formula weight	398.73	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.2935(10) Å	α= 90°.
	b = 10.4320(10) Å	β= 90.984(2)°.
	c = 14.1939(14) Å	γ = 90°.
Volume	1523.9(3) $Å^3$	
Z	4	
Density (calculated)	1.738 Mg/m^3	
Absorption coefficient	1.237 mm^{-1}	
F(000)	808	
Crystal size	0.47 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.98 to 27.56°.	
Index ranges	-13<=h<=13, -13<=k<=13, -18<=l<=18	
Reflections collected	16923	
Independent reflections	3513 [R(int) = 0.0392]	
Completeness to theta = 27.56°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8863 and 0.5939	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3513 / 0 / 201	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0293, wR2 = 0.0731	
R indices (all data)	R1 = 0.0388, wR2 = 0.0767	
Largest diff. peak and hole	1.196 and -0.605 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for psty3m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5076(1)	1138(1)	9046(1)	19(1)
O(1)	4755(2)	2634(2)	9878(1)	27(1)
O(2)	3260(2)	1414(2)	8536(1)	25(1)
O(3)	-657(2)	374(2)	6987(2)	34(1)
N(1)	6882(2)	873(2)	9469(2)	25(1)
N(2)	5376(2)	-381(2)	8283(2)	23(1)
C(1)	7424(3)	-353(3)	9152(2)	33(1)
C(2)	6749(3)	-750(3)	8252(2)	33(1)
C(3)	4501(3)	-972(3)	7794(2)	25(1)
C(4)	3173(3)	-586(3)	7658(2)	23(1)
C(5)	2372(3)	-1410(3)	7106(2)	29(1)
C(6)	1115(3)	-1125(3)	6881(2)	29(1)
C(7)	584(3)	26(3)	7193(2)	26(1)
C(8)	1337(3)	869(3)	7733(2)	25(1)
C(9)	2626(3)	581(3)	7991(2)	22(1)
C(10)	5674(3)	3112(3)	10411(2)	27(1)
C(11)	6943(3)	2729(3)	10468(2)	29(1)
C(12)	7509(3)	1642(3)	10053(2)	26(1)
C(13)	8913(3)	1374(3)	10316(2)	36(1)
C(14)	5236(3)	4170(3)	11050(2)	35(1)
O(1S)	8104(3)	8601(2)	5955(2)	42(1)
C(1S)	8245(3)	8832(3)	4973(2)	36(1)

Table 3. Bond lengths [Å] and angles [°] for psty3m.

Pd(1)-N(2)	1.948(2)
Pd(1)-N(1)	1.963(2)
Pd(1)-O(1)	1.9877(19)
Pd(1)-O(2)	2.014(2)
O(1)-C(10)	1.300(3)
O(2)-C(9)	1.328(3)
O(3)-C(7)	1.355(4)
N(1)-C(12)	1.315(4)
N(1)-C(1)	1.469(4)
N(2)-C(3)	1.285(4)
N(2)-C(2)	1.465(4)
C(1)-C(2)	1.503(4)
C(3)-C(4)	1.436(4)
C(4)-C(5)	1.418(4)
C(4)-C(9)	1.426(4)
C(5)-C(6)	1.360(5)
C(6)-C(7)	1.395(4)
C(7)-C(8)	1.393(4)
C(8)-C(9)	1.403(4)
C(10)-C(11)	1.366(4)
C(10)-C(14)	1.504(4)
C(11)-C(12)	1.409(4)
C(12)-C(13)	1.512(4)
O(1S)-C(1S)	1.424(4)
N(2)-Pd(1)-N(1)	84.11(10)
N(2)-Pd(1)-O(1)	177.28(9)
N(1)-Pd(1)-O(1)	95.44(9)
N(2)-Pd(1)-O(2)	94.10(9)
N(1)-Pd(1)-O(2)	176.72(9)
O(1)-Pd(1)-O(2)	86.48(8)
C(10)-O(1)-Pd(1)	121.33(19)
C(9)-O(2)-Pd(1)	124.05(17)
C(12)-N(1)-C(1)	122.6(3)

C(12)-N(1)-Pd(1)	124.0(2)
C(1)-N(1)-Pd(1)	113.05(19)
C(3)-N(2)-C(2)	121.7(2)
C(3)-N(2)-Pd(1)	125.1(2)
C(2)-N(2)-Pd(1)	113.11(19)
N(1)-C(1)-C(2)	109.1(2)
N(2)-C(2)-C(1)	109.5(3)
N(2)-C(3)-C(4)	126.5(3)
C(5)-C(4)-C(9)	118.1(3)
C(5)-C(4)-C(3)	116.6(3)
C(9)-C(4)-C(3)	125.2(3)
C(6)-C(5)-C(4)	122.6(3)
C(5)-C(6)-C(7)	119.4(3)
O(3)-C(7)-C(8)	117.6(3)
O(3)-C(7)-C(6)	122.4(3)
C(8)-C(7)-C(6)	120.1(3)
C(7)-C(8)-C(9)	121.5(3)
O(2)-C(9)-C(8)	117.7(3)
O(2)-C(9)-C(4)	124.0(3)
C(8)-C(9)-C(4)	118.3(3)
O(1)-C(10)-C(11)	127.4(3)
O(1)-C(10)-C(14)	114.2(3)
C(11)-C(10)-C(14)	118.3(3)
C(10)-C(11)-C(12)	127.8(3)
N(1)-C(12)-C(11)	123.5(3)
N(1)-C(12)-C(13)	120.0(3)
C(11)-C(12)-C(13)	116.5(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for psty3m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	17(1)	18(1)	22(1)	1(1)	-1(1)	2(1)
O(1)	26(1)	25(1)	29(1)	-8(1)	-5(1)	2(1)
O(2)	21(1)	23(1)	30(1)	-8(1)	-5(1)	3(1)
O(3)	21(1)	40(1)	41(1)	-10(1)	-9(1)	-2(1)
N(1)	20(1)	26(1)	27(1)	4(1)	1(1)	2(1)
N(2)	20(1)	20(1)	28(1)	1(1)	3(1)	2(1)
C(1)	23(2)	37(2)	37(2)	0(1)	0(1)	8(1)
C(2)	26(2)	35(2)	38(2)	-6(1)	2(1)	7(1)
C(3)	35(2)	17(1)	23(1)	1(1)	6(1)	6(1)
C(4)	28(2)	21(1)	20(1)	1(1)	2(1)	-1(1)
C(5)	36(2)	21(1)	30(2)	-4(1)	3(1)	-1(1)
C(6)	32(2)	26(2)	29(2)	-3(1)	-2(1)	-9(1)
C(7)	23(2)	31(2)	24(2)	2(1)	2(1)	-5(1)
C(8)	22(2)	23(1)	30(2)	-6(1)	0(1)	2(1)
C(9)	24(1)	22(1)	20(1)	1(1)	1(1)	-3(1)
C(10)	33(2)	23(2)	25(2)	3(1)	-4(1)	-2(1)
C(11)	28(2)	31(2)	27(2)	1(1)	-5(1)	-8(1)
C(12)	23(2)	32(2)	23(1)	9(1)	-3(1)	-3(1)
C(13)	24(2)	46(2)	39(2)	2(2)	-4(1)	-1(1)
C(14)	39(2)	33(2)	31(2)	-8(1)	-5(1)	0(1)
O(1S)	48(2)	42(1)	35(1)	8(1)	-12(1)	-25(1)
C(1S)	35(2)	35(2)	38(2)	3(1)	-2(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for psty3m.

	x	y	z	U(eq)
H(3B)	-1018	-203	6664	52
H(1A)	7300	-1017	9641	39
H(1B)	8368	-260	9047	39
H(2A)	7166	-330	7710	40
H(2B)	6821	-1690	8170	40
H(3A)	4760	-1742	7492	30
H(5A)	2727	-2192	6883	34
H(6A)	603	-1705	6516	35
H(8A)	968	1657	7931	30
H(11A)	7510	3260	10830	35
H(13A)	9204	601	9988	54
H(13B)	8993	1243	10998	54
H(13C)	9452	2104	10132	54
H(14A)	4311	4343	10934	52
H(14B)	5740	4947	10925	52
H(14C)	5372	3911	11708	52
H(1S)	7673	7927	6032	62
H(1S1)	7892	9679	4815	54
H(1S2)	7771	8174	4613	54
H(1S3)	9167	8801	4815	54