metals

MDPI

Article

Synthesis of complex concentrated nanoparticles by Ultrasonic Spray Pyrolysis and Lyophilisation – Supplementary materials

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Structure data for detected phases, output generated by CrystalDiffract 6 for macOS

Name and formula

1. Reference code: 00-007-0218

Compound name:	Ammonium Platinum Chloride
PDF index name:	Ammonium Platinum Chloride
Empirical formula:	$Cl_6H_8N_2Pt$
Chemical formula:	$(NH_4)_2PtCl_6$

Crystallographic parameters

Crystal system:	Cubic
Space group:	Fm3m
Space group number:	225
a (A):	9.8580
b (A):	9.8580
c (A):	9.8580
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	90.0000

Calculated density (g/cm^3):	3.08
Volume of cell (10^6 pm^3):	958.00
Z:	4.00
RIR:	-

Subfiles and quality

Subfiles:	Common Phase
	Forensic
	Inorganic
	NBS pattern
Quality:	Star (S)

Comments

Color:	Yellow
Creation Date:	1/1/1970
Modification Date:	1/1/1970
Optical Data:	A=1.835
Color:	Yellow
Sample Preparation:	Sample prepared at NBS from NH_4Cl and H_2PtCl_6
Analysis:	Spectroscopic analysis shows <0.1% Na; <0.01% Si; <0.001% Ca, Fe, Mg
Temperature of Data Collection:	Pattern made at 25 C. Merck Index, 8th Ed., p. 71.

References

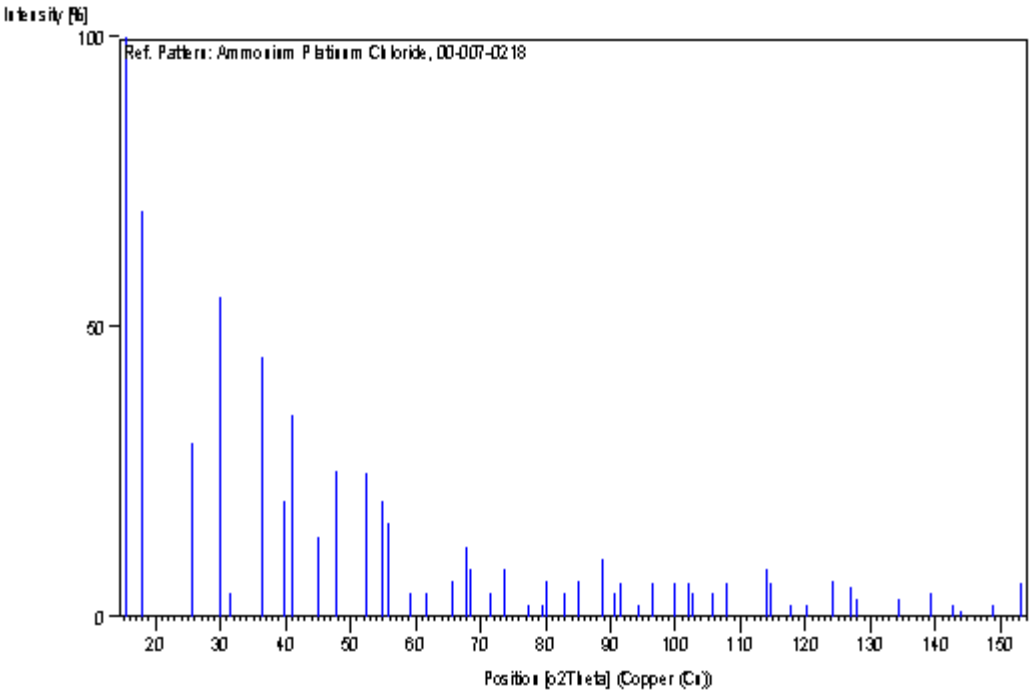
Primary reference:	*Natl. Bur. Stand. (U.S.), Circ. 539*, **5**, 3, (1955)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	1	1	1	5.69700	15.542	100.0
2	2	0	0	4.92900	17.982	70.0
3	2	2	0	3.48500	25.539	30.0
4	3	1	1	2.97310	30.032	55.0
5	2	2	2	2.84640	31.403	4.0
6	4	0	0	2.46550	36.412	45.0
7	3	3	1	2.26180	39.823	20.0
8	4	2	0	2.20460	40.902	35.0
9	4	2	2	2.01240	45.012	14.0

10	5	1	1	1.89710	47.913	25.0
11	4	4	0	1.74270	52.465	25.0
12	5	3	1	1.66620	55.072	20.0
13	6	0	0	1.64310	55.914	16.0
14	6	2	0	1.55890	59.225	4.0
15	5	3	3	1.50340	61.644	4.0
16	4	4	4	1.42300	65.547	6.0
17	7	1	1	1.38050	67.833	12.0
18	6	4	0	1.36720	68.584	8.0
19	6	4	2	1.31730	71.572	4.0
20	7	3	1	1.28330	73.776	8.0
21	8	0	0	1.23250	77.363	2.0
22	7	3	3	1.20420	79.536	2.0
23	8	2	0	1.19560	80.223	6.0
24	6	6	0	1.16170	83.070	4.0
25	7	5	1	1.13820	85.184	6.0
26	8	4	0	1.10210	88.684	10.0
27	9	1	1	1.08200	90.783	4.0
28	8	4	2	1.07550	91.487	6.0
29	6	6	4	1.05070	94.299	2.0
30	9	3	1	1.03330	96.400	6.0
31	8	4	4	1.00600	99.940	6.0
32	7	7	1	0.99070	102.070	6.0
33	8	6	0	0.98580	102.777	4.0
34	10	2	0	0.96660	105.673	4.0
35	9	5	1	0.95290	107.875	6.0
36	9	5	3	0.91920	113.861	8.0
37	10	4	0	0.91530	114.615	6.0
38	10	4	2	0.89990	117.737	2.0
39	11	1	1	0.88880	120.149	2.0
40	8	8	0	0.87130	124.277	6.0
41	11	3	1	0.86140	126.822	5.0
42	10	4	4	0.85800	127.737	3.0
43	11	3	3	0.83610	134.234	3.0
44	12	0	0	0.82150	139.329	4.0
45	11	5	1	0.81310	142.654	2.0
46	12	2	0	0.81030	143.844	1.0
47	12	2	2	0.79960	148.883	2.0
48	11	5	3	0.79180	153.235	6.0

Stick Pattern



2. Reference code: 00-052-0746

Compound name:	Ammonium Nickel Platinum Chloride Hydrate
PDF index name:	Ammonium Nickel Platinum Chloride Hydrate
Empirical formula:	$Cl_6H_{19}N_6NiO_{0.5}Pt$
Chemical formula:	$(NH_3)_6NiPtCl_6 \times 0.5H_2O$

Crystallographic parameters

Crystal system:	Cubic
Space group:	Pa-3
Space group number:	205
a (A):	11.6320
b (A):	11.6320
c (A):	11.6320
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	90.0000

Volume of cell (10^6 pm^3):	1573.85
Z:	4.00
RIR:	-

Subfiles and quality

Subfiles:	Inorganic
Quality:	Indexed (I)

Comments

Color:	Yellow
Creation Date:	1/1/1970
Modification Date:	1/1/1970
Color:	Yellow
Sample Preparation:	Ni (NH_3)$_6Cl_2$ was dissolved in aqueous ammonia, then added to a solution of $Na_2PtCl_6 \cdot 6H_2O$. Both solutions were cooled to 0 C before mixing
Analysis:	Chemical analysis (wt.%): Pt 33.5, Ni 10.1, Cl 37.2, N 14.7, H 3.3.

References

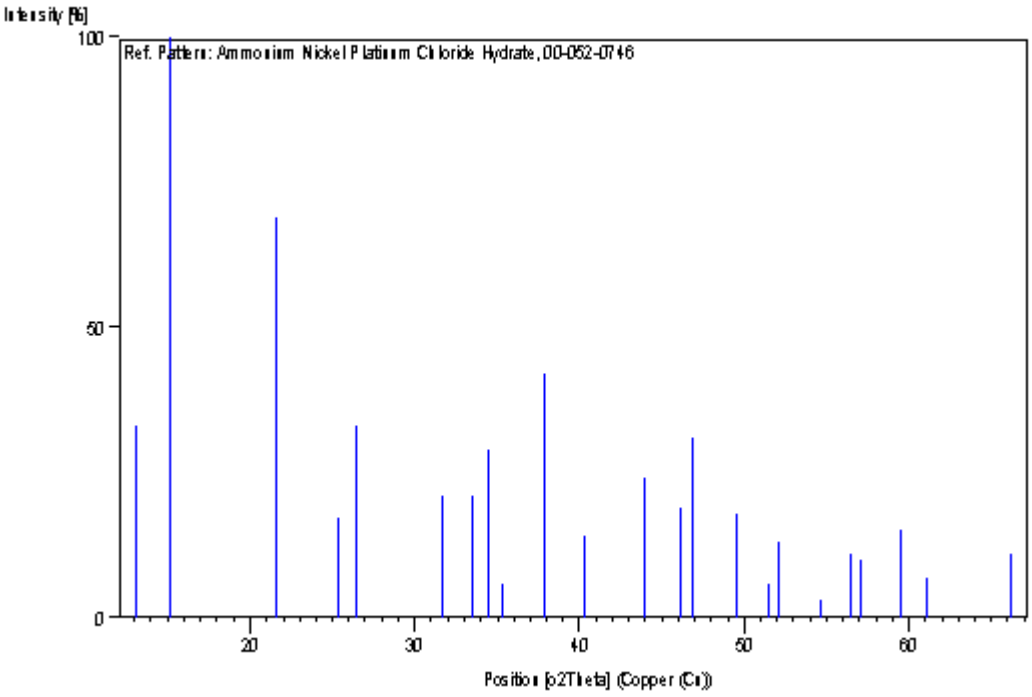
Primary reference: Val'kovskii, M., Bol'shakova, L., Lapkin, V., *Russ. J. Inorg. Chem. (Engl. Transl.)*, **41**, 213, (1996)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	1	1	1	6.74786	13.110	33.0
2	2	0	0	5.84795	15.138	100.0
3	2	2	0	4.12350	21.533	69.0
4	3	1	1	3.52017	25.280	17.0
5	2	2	2	3.36343	26.479	33.0
6	3	2	2	2.82257	31.675	21.0
7	3	3	1	2.67104	33.523	21.0
8	4	2	0	2.60183	34.442	29.0
9	4	2	1	2.54044	35.302	6.0
10	4	2	2	2.37569	37.839	42.0
11	3	3	3	2.23947	40.237	14.0

12	4	4	0	2.05700	43.984	24.0
13	5	3	1	1.96610	46.132	19.0
14	4	4	2	1.93718	46.861	31.0
15	6	2	0	1.83787	49.559	18.0
16	5	3	3	1.77284	51.507	6.0
17	6	2	2	1.75385	52.106	13.0
18	4	4	4	1.67938	54.604	3.0
19	5	5	1	1.62818	56.472	11.0
20	6	4	0	1.61250	57.071	10.0
21	6	4	2	1.55356	59.449	15.0
22	5	5	3	1.51553	61.097	7.0
23	6	4	4	1.41032	66.212	11.0

Stick Pattern



Reference code: **01-074-0925**

Compound name:	Platinum Ammine Chloride
Common name:	Magnus green salt
ICSD name:	Platinum Ammine Chloride
Empirical formula:	$Cl_4H_{12}N_4Pt_2$
Chemical formula:	$Pt_2(NH_3)_4Cl_4$

Crystallographic parameters

Crystal system:	Tetragonal
Space group:	P4/mnc
Space group number:	128
a (A):	9.0300
b (A):	9.0300
c (A):	6.4900
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	90.0000
Calculated density (g/cm^3):	3.77
Volume of cell (10^6 pm^3):	529.20
Z:	2.00
RIR:	13.31

Subfiles and quality

Subfiles:	Corrosion
	Inorganic
	Modelled additional pattern
Quality:	Calculated (C)

Comments

ICSD collection code:	026615
Creation Date:	1/1/1970
Modification Date:	1/1/1970
ICSD Collection Code:	026615
Calculated Pattern Original Remarks:	ATOM H 1 +1 24.00 Atoms not located in unit cell
Test from ICSD:	At least one TF missing
Test from ICSD:	Calc. density unusual but tolerable
Additional Patterns:	See PDF 34-193.

References

Primary reference: *Calculated from ICSD using POWD-12++*, (1997)

Structure: Atoji, M., Richardson, J.W., Rundle, R.E., *J. Am. Chem. Soc.*, **79**, 3017, (1957)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	1	1	0	6.38517	13.858	100.0
2	1	0	1	5.27007	16.809	1.4
3	2	0	0	4.51500	19.646	34.0
4	2	1	0	4.03834	21.993	0.6
5	2	1	1	3.42875	25.966	1.6
6	0	0	2	3.24500	27.464	20.0
7	2	2	0	3.19259	27.924	5.1
8	1	1	2	2.89286	30.886	23.7
9	3	1	0	2.85554	31.300	20.9
10	3	0	1	2.73061	32.771	0.3
11	2	0	2	2.63503	33.995	14.9
12	3	1	1	2.61372	34.281	4.3
13	2	1	2	2.52954	35.459	0.3
14	3	2	0	2.50447	35.826	0.1
15	3	2	1	2.33653	38.498	0.1
16	2	2	2	2.27580	39.568	4.1
17	4	0	0	2.25750	39.902	8.5
18	4	1	0	2.19010	41.185	0.1
19	3	1	2	2.14371	42.118	16.8
20	3	3	0	2.12839	42.436	4.5
21	1	0	3	2.10380	42.956	0.2
22	4	1	1	2.07513	43.580	0.3
23	4	2	0	2.01917	44.852	9.3
24	3	2	2	1.98265	45.725	0.1
25	4	2	1	1.92801	47.098	0.1
26	2	1	3	1.90695	47.650	0.2
27	4	0	2	1.85316	49.123	8.2
28	4	1	2	1.81533	50.217	0.1
29	4	3	0	1.80600	50.494	0.2
30	3	3	2	1.77972	51.293	4.4
31	5	1	0	1.77093	51.567	4.8
32	3	0	3	1.75669	52.016	0.1
33	5	0	1	1.73989	52.556	0.1
34	3	1	3	1.72436	53.066	0.9
35	4	2	2	1.71438	53.400	10.1
36	5	1	1	1.70847	53.599	5.5

37	5	2	0	1.67683	54.694	0.1
38	3	2	3	1.63714	56.136	0.1
39	5	2	1	1.62250	56.688	1.7
40	4	4	0	1.59629	57.705	1.6
41	4	3	2	1.57806	58.436	0.3
42	1	1	4	1.57253	58.661	2.9
43	5	1	2	1.55450	59.409	5.6
44	5	3	0	1.54863	59.657	3.3
45	4	1	3	1.53908	60.065	0.2
46	2	0	4	1.52690	60.595	2.2
47	5	3	1	1.50634	61.511	1.0
48	5	2	2	1.48969	62.274	0.1
49	6	1	0	1.48452	62.515	0.1
50	4	2	3	1.47610	62.913	0.1
51	6	1	1	1.44643	64.356	0.9
52	4	4	2	1.43237	65.065	2.1
53	6	2	0	1.42777	65.301	2.3
54	3	1	4	1.41069	66.192	3.4
55	5	3	2	1.39763	66.892	3.5
56	6	2	1	1.39442	67.066	1.8
57	4	3	3	1.38639	67.506	0.1
58	5	4	1	1.37809	67.968	0.1
59	5	1	3	1.37033	68.406	0.1
60	6	0	2	1.36531	68.693	0.7
61	3	2	4	1.36172	68.899	0.4
62	6	1	2	1.34996	69.585	0.1
63	6	3	0	1.34611	69.813	0.1
64	6	3	1	1.31752	71.558	2.0
65	6	2	2	1.30686	72.233	2.4
66	4	1	4	1.30371	72.435	1.3
67	3	3	4	1.29033	73.308	1.2
68	7	1	0	1.27703	74.198	1.6
69	7	0	1	1.26477	75.041	2.8
70	5	3	3	1.25924	75.428	0.5
71	7	1	1	1.25224	75.924	0.8
72	6	3	2	1.24338	76.562	0.1
73	7	2	0	1.24037	76.782	0.1
74	2	1	5	1.23574	77.123	0.1
75	6	4	1	1.22956	77.582	0.1
76	6	1	3	1.22404	77.998	0.1
77	7	2	1	1.21831	78.435	0.1
78	4	3	4	1.20696	79.318	0.1

79	5	1	4	1.19632	80.165	1.8
80	7	1	2	1.18833	80.815	2.4
81	7	3	0	1.18570	81.032	2.0
82	6	4	2	1.16827	82.501	1.1
83	5	2	4	1.16601	82.696	0.6
84	7	2	2	1.15861	83.341	0.1
85	6	5	0	1.15617	83.557	0.1
86	6	3	3	1.14292	84.749	0.1
87	6	5	1	1.13790	85.211	0.8
88	8	0	0	1.12875	86.069	0.3
89	5	3	4	1.12025	86.883	1.4
90	7	3	2	1.11368	87.525	1.3
91	8	1	1	1.10340	88.552	0.3
92	6	1	4	1.09505	89.407	1.1
93	4	2	5	1.09186	89.739	0.6

Stick Pattern