Supporting Information

Defining the qualities of high-quality palladium on carbon catalysts for hydrogenolysis

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TEM and XRD of 5% Pd/C (pre-treated) recycled catalyst

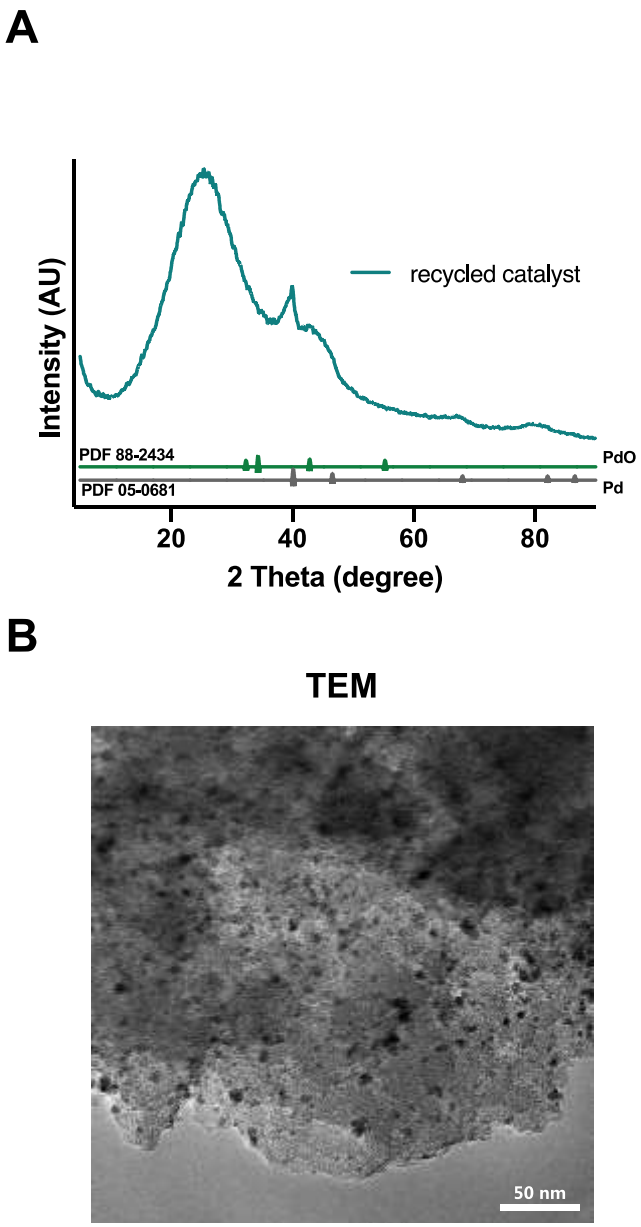
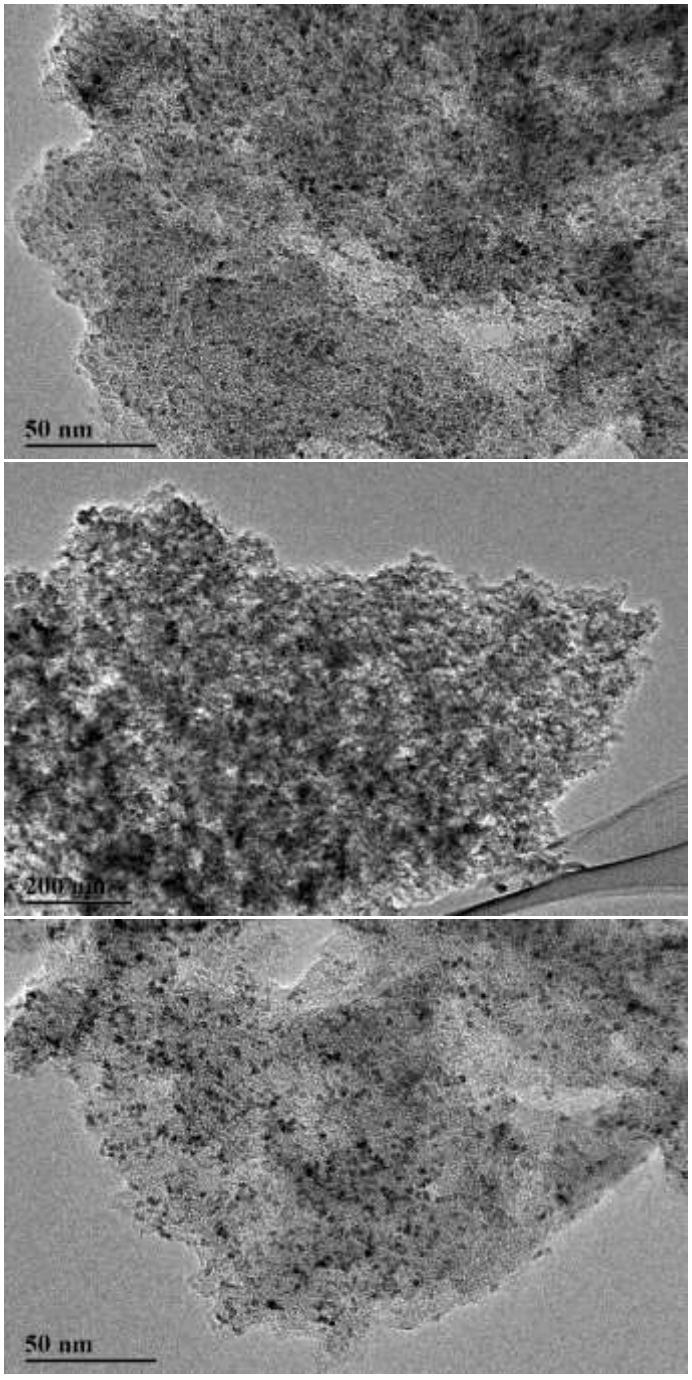
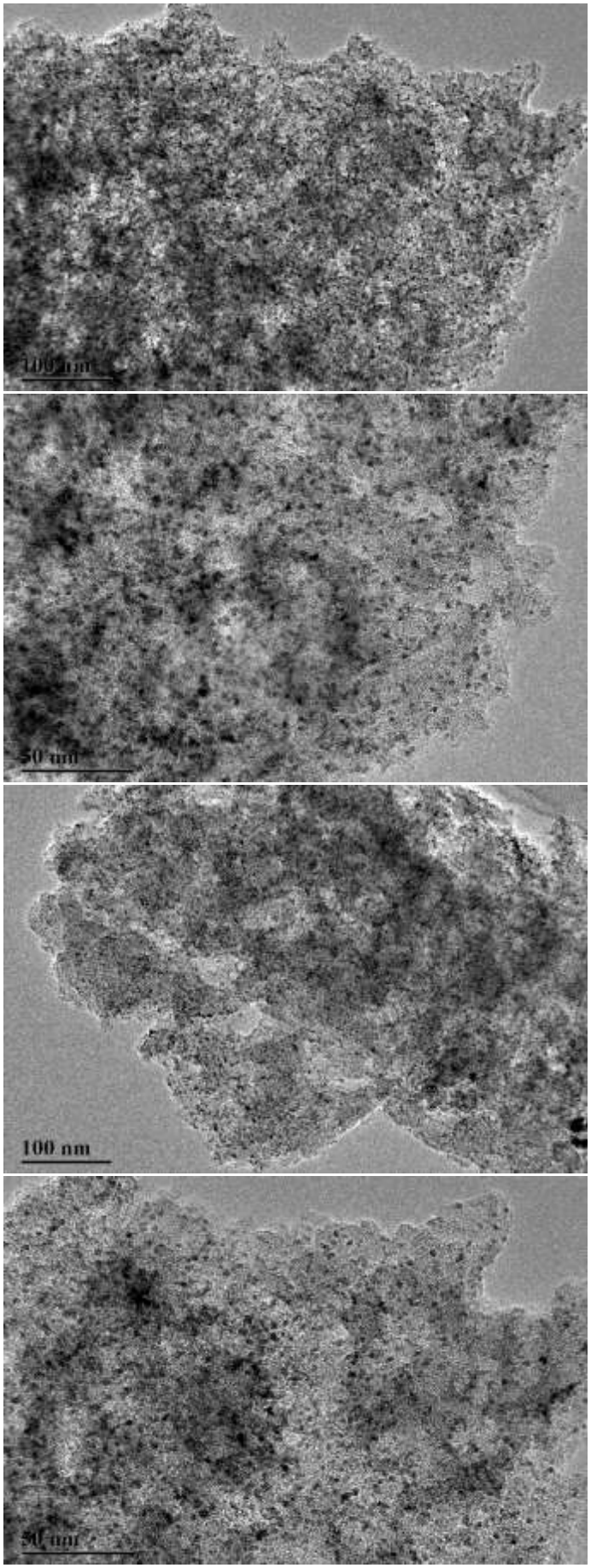
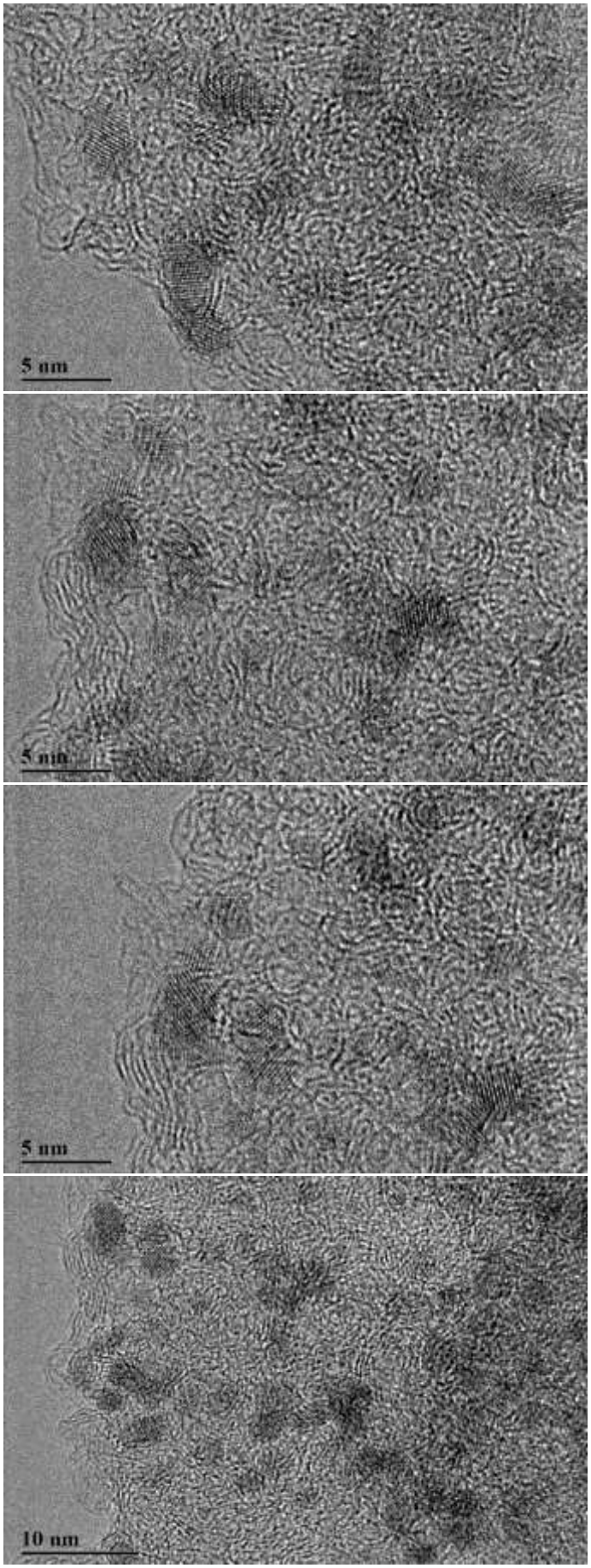


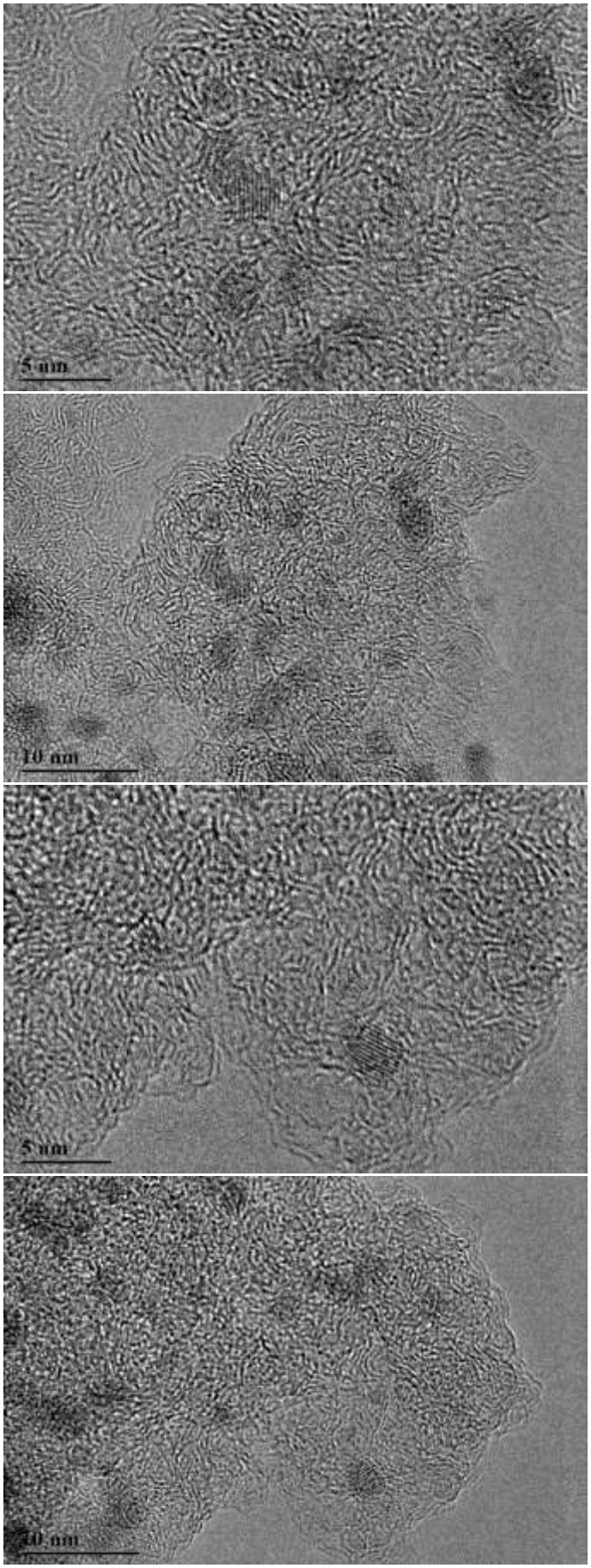
Figure S1. TEM and XRD of 5% Pd/C (pre-treated) recycled catalyst

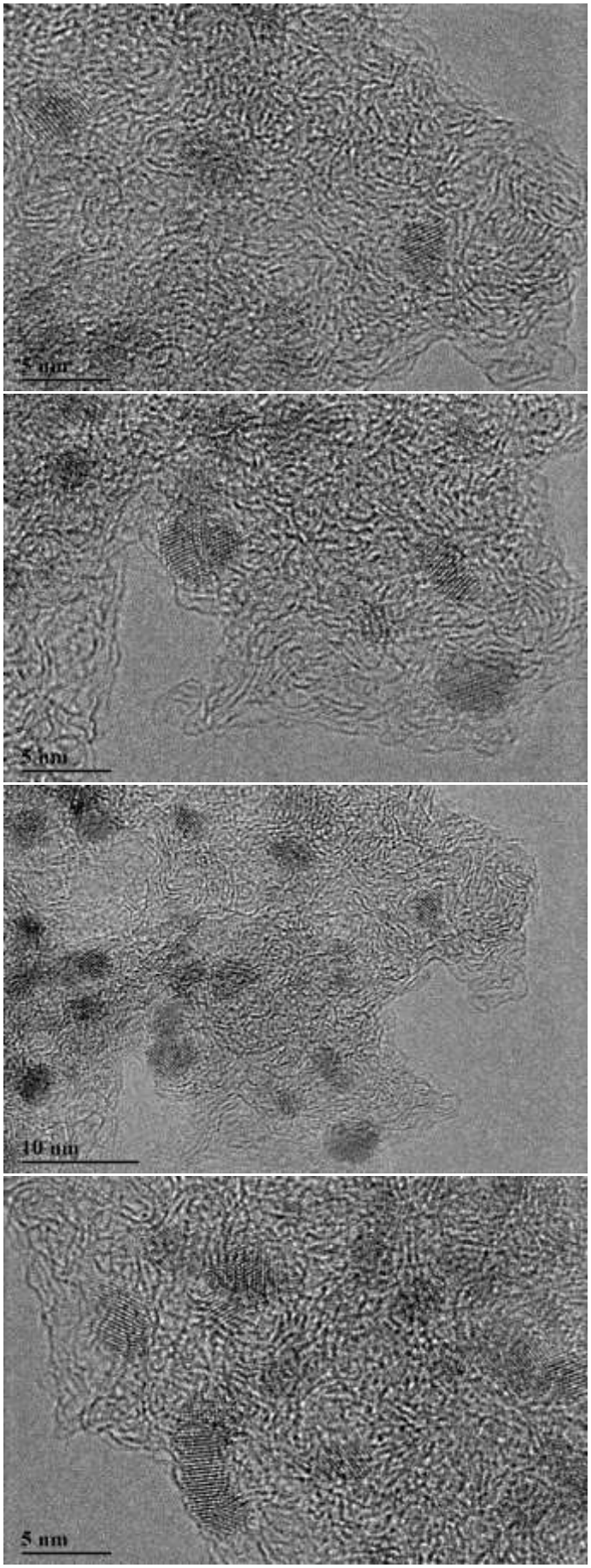
TEM of 5% Pd/C STREM Chemicals (1#)



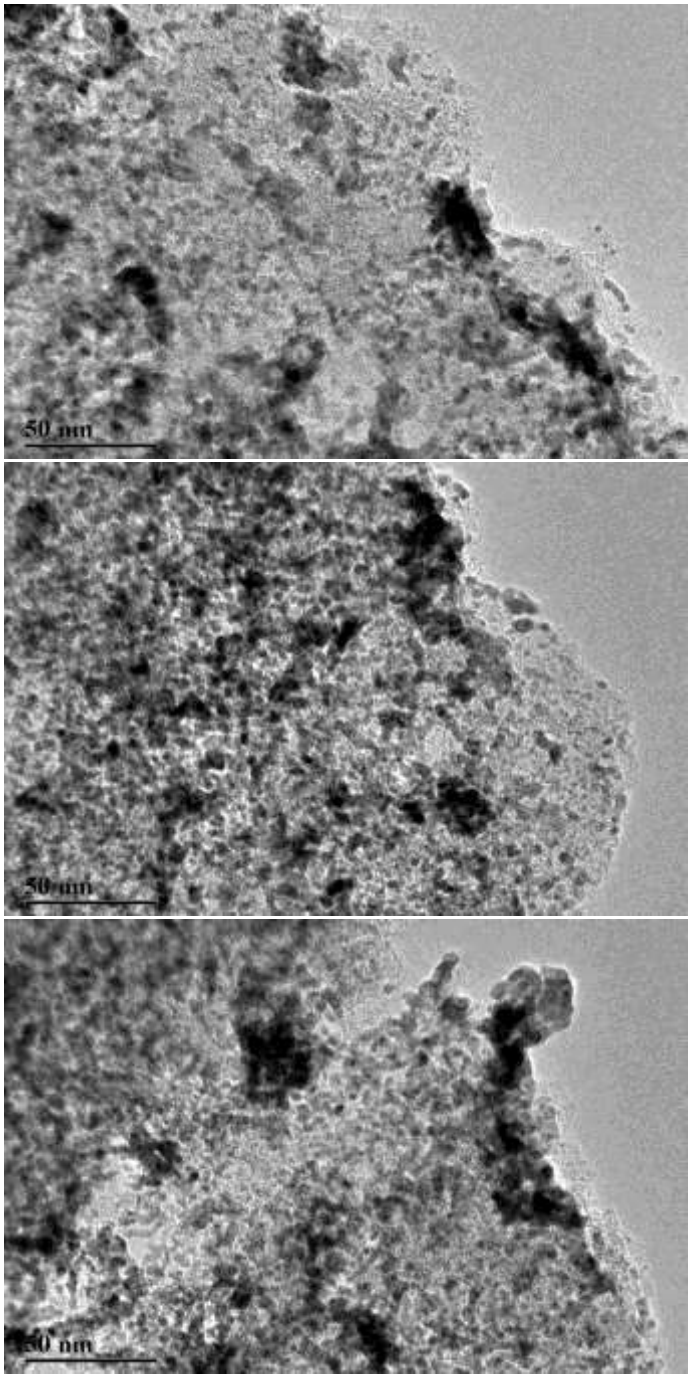

100 nm
50 nm
100 nm

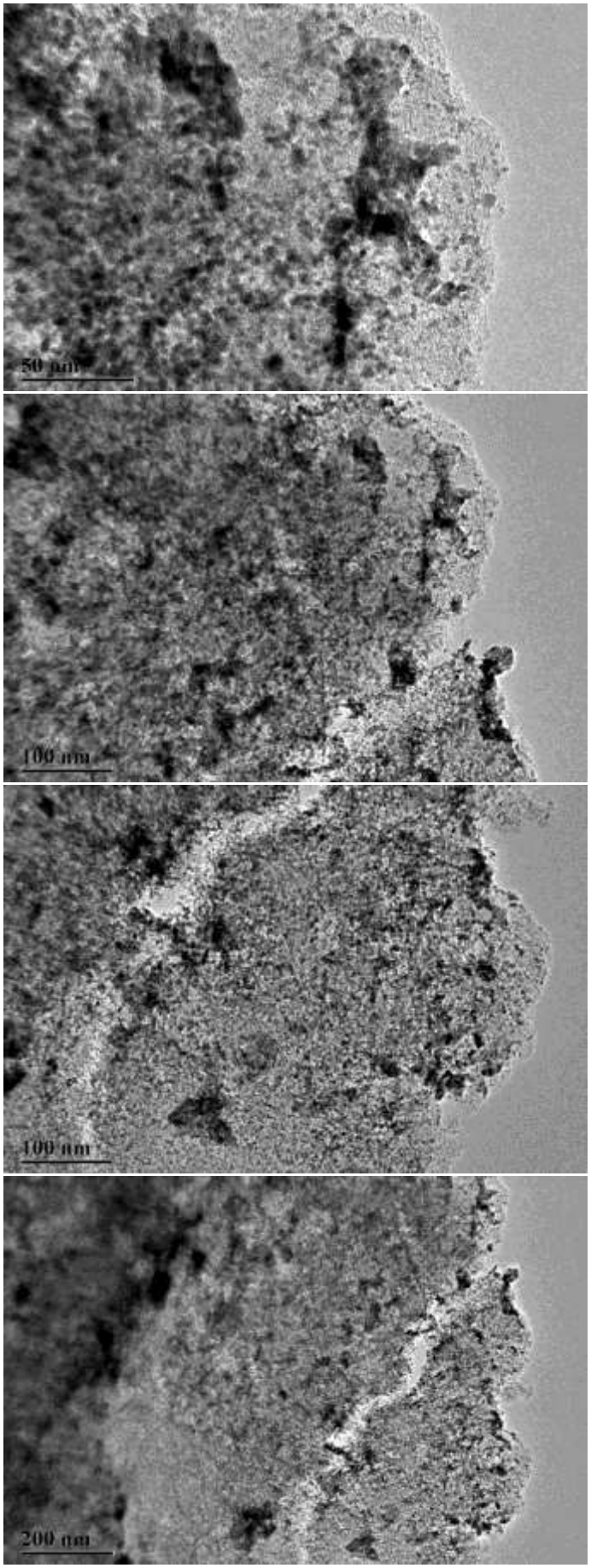

5 nm
5 nm
5 nm
10 nm

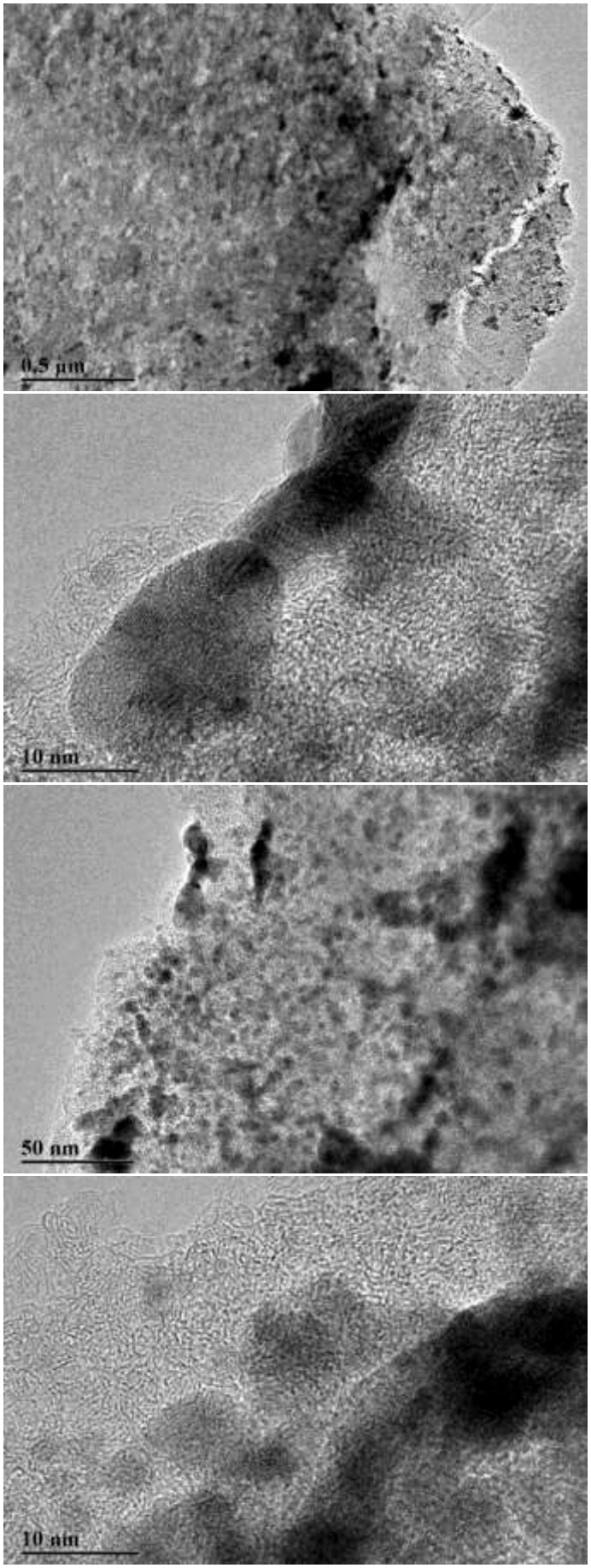

5 nm
10 nm
5 nm
20 nm

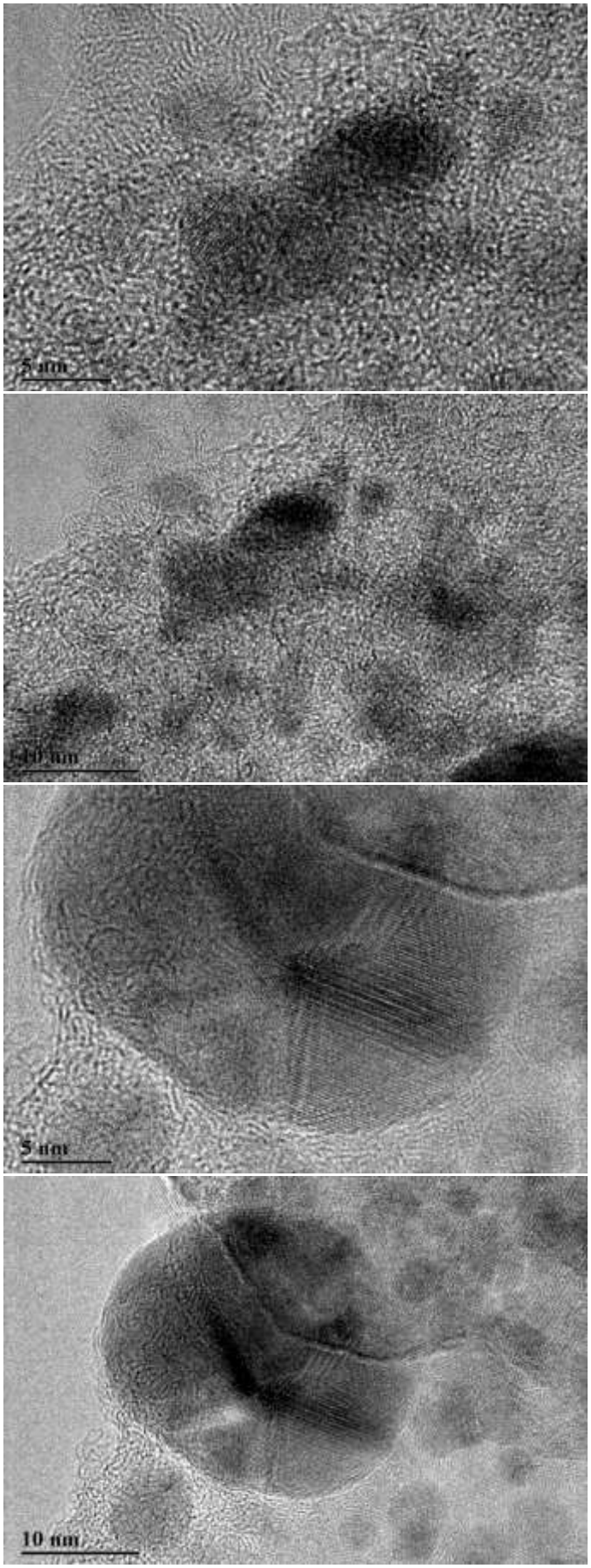

5 nm
5 nm
10 nm
5 nm

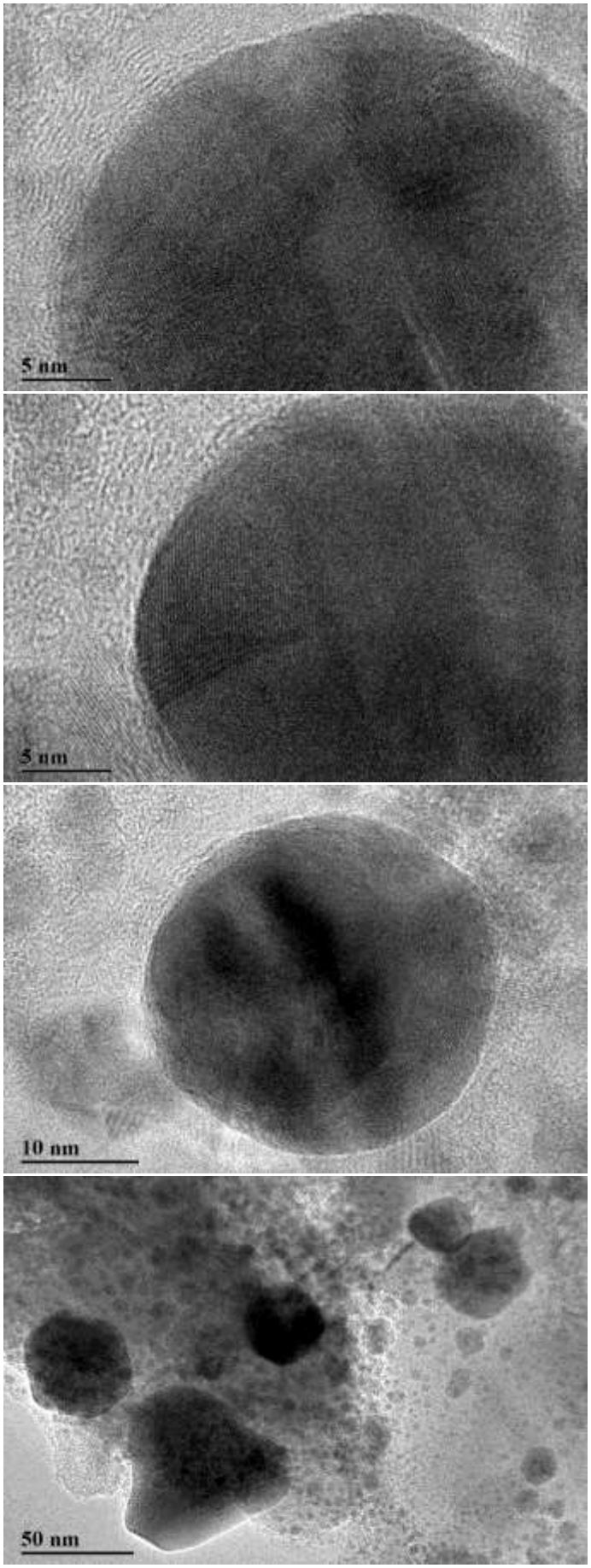
TEM 10% Pd/C Sigma-Aldrich (2#)

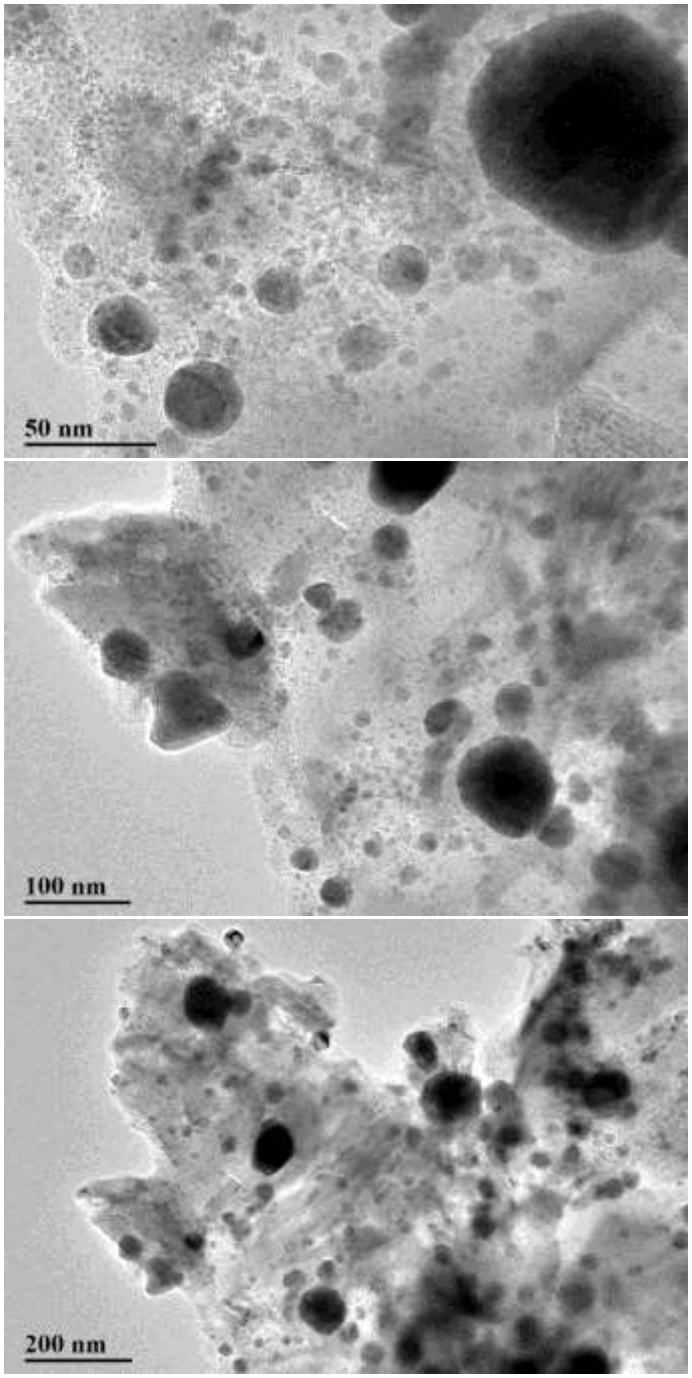



50 nm
100 nm
100 nm
200 nm

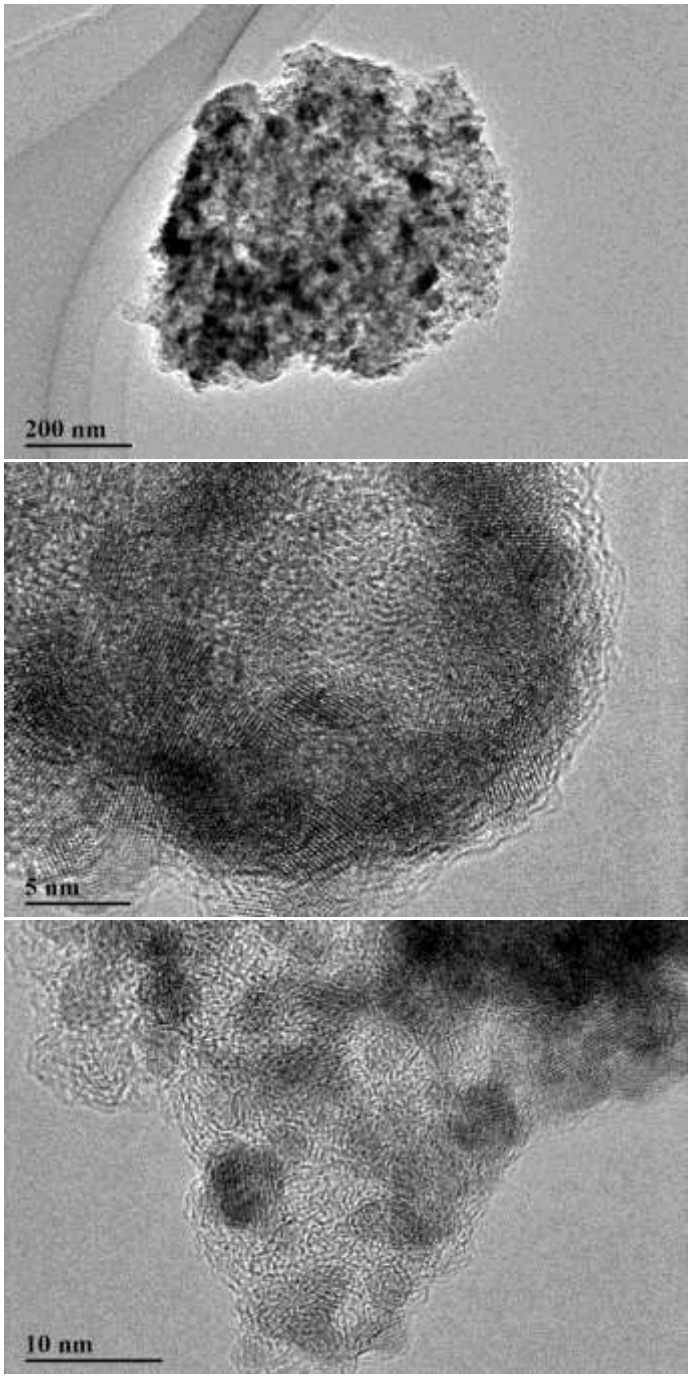

0,5 µm
10 nm
50 nm
10 nm

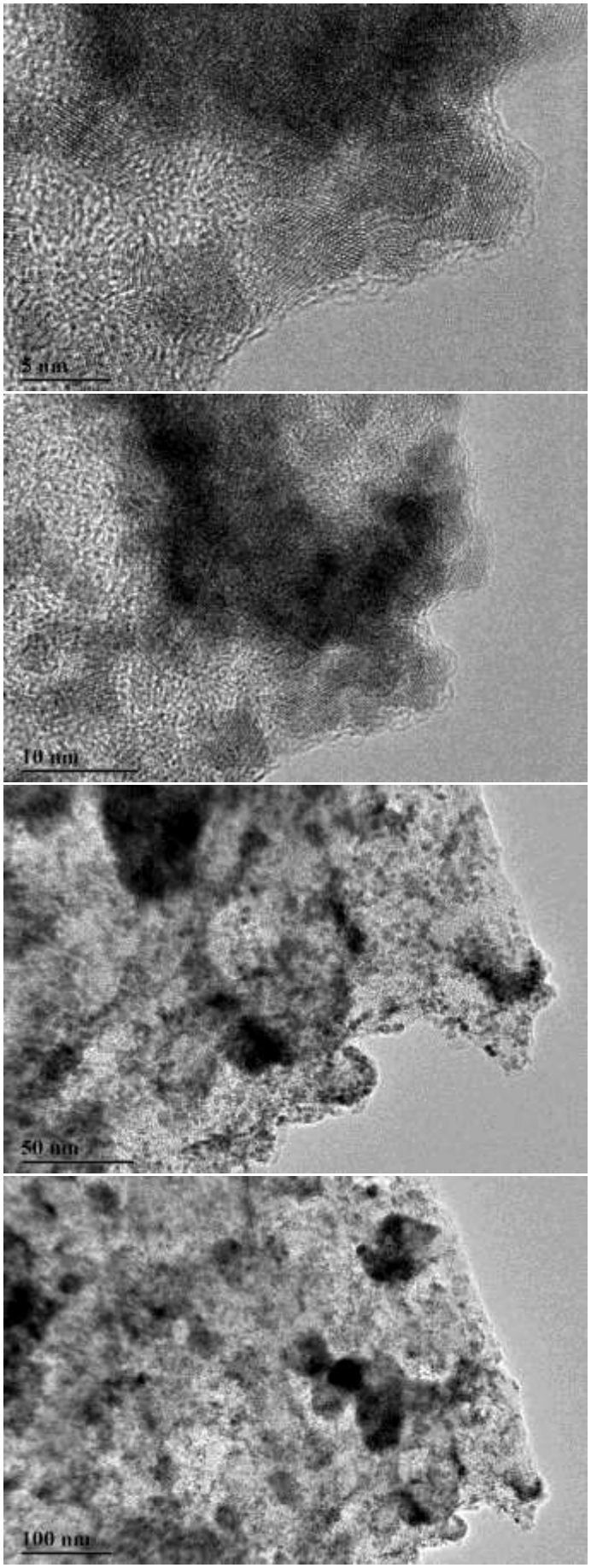

5 nm
5 nm
10 nm

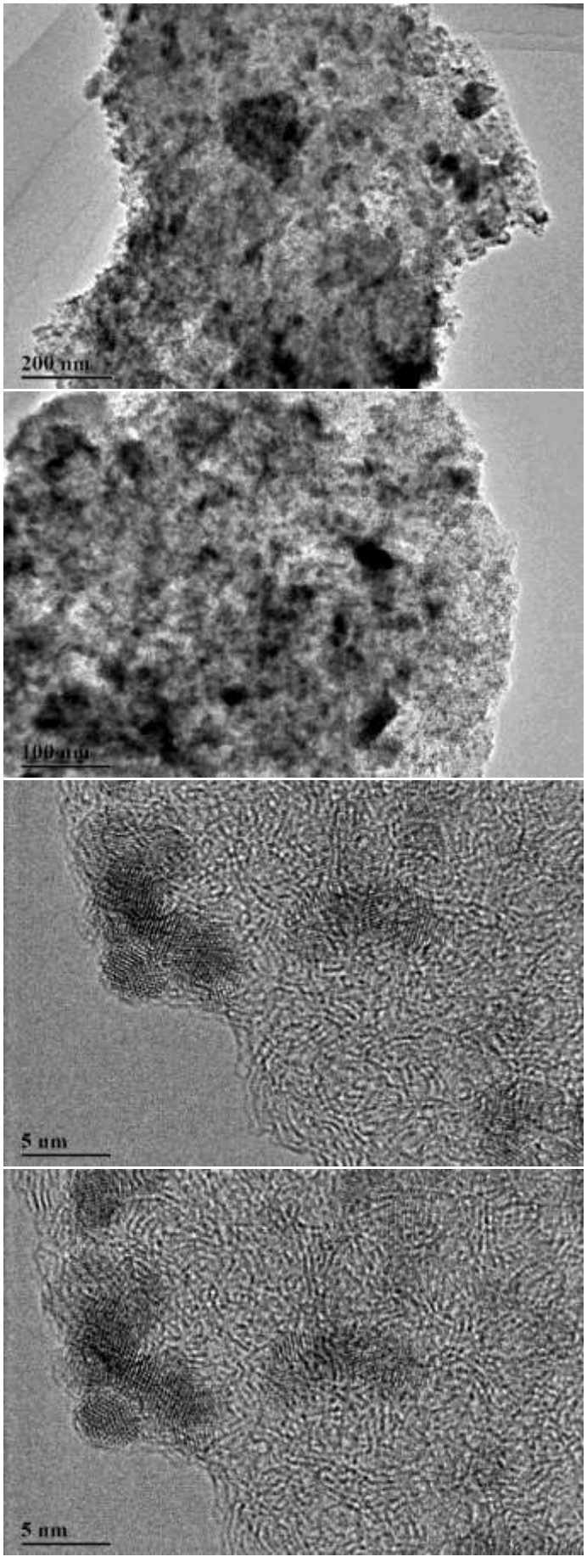

5 nm
5 nm
10 nm
50 nm

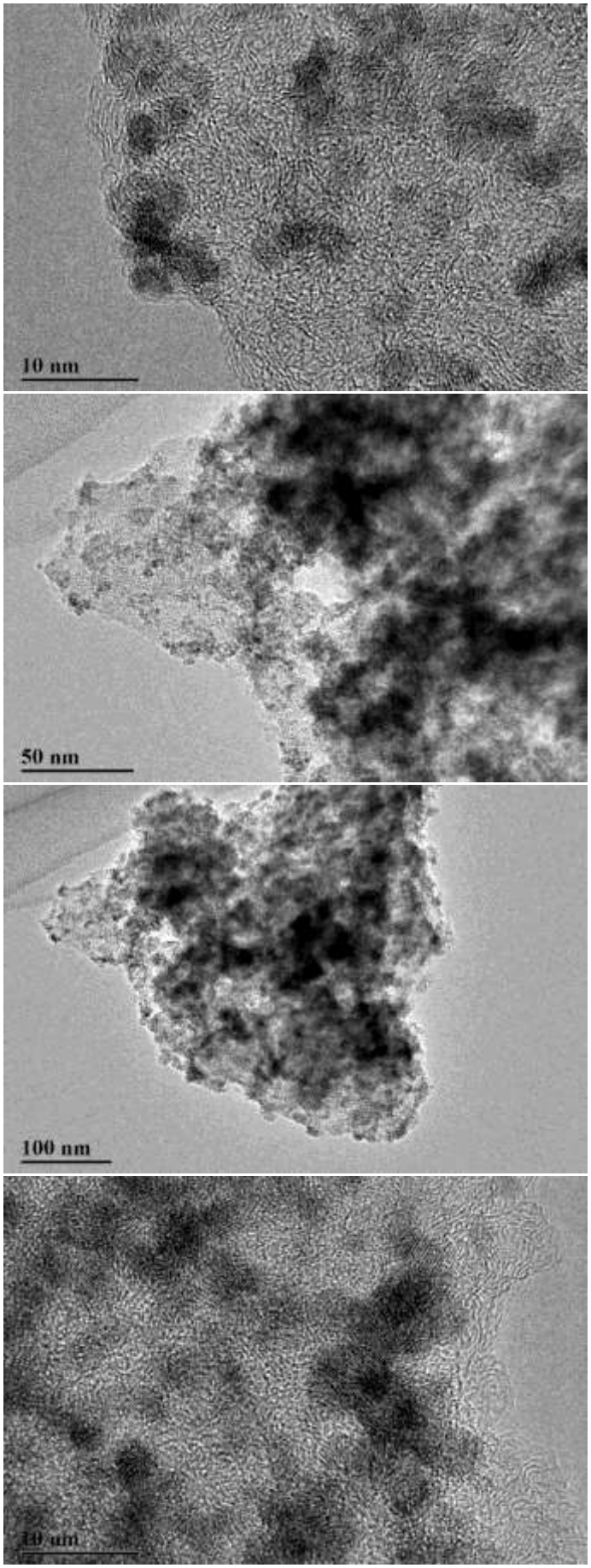

50 nm
100 nm
200 nm

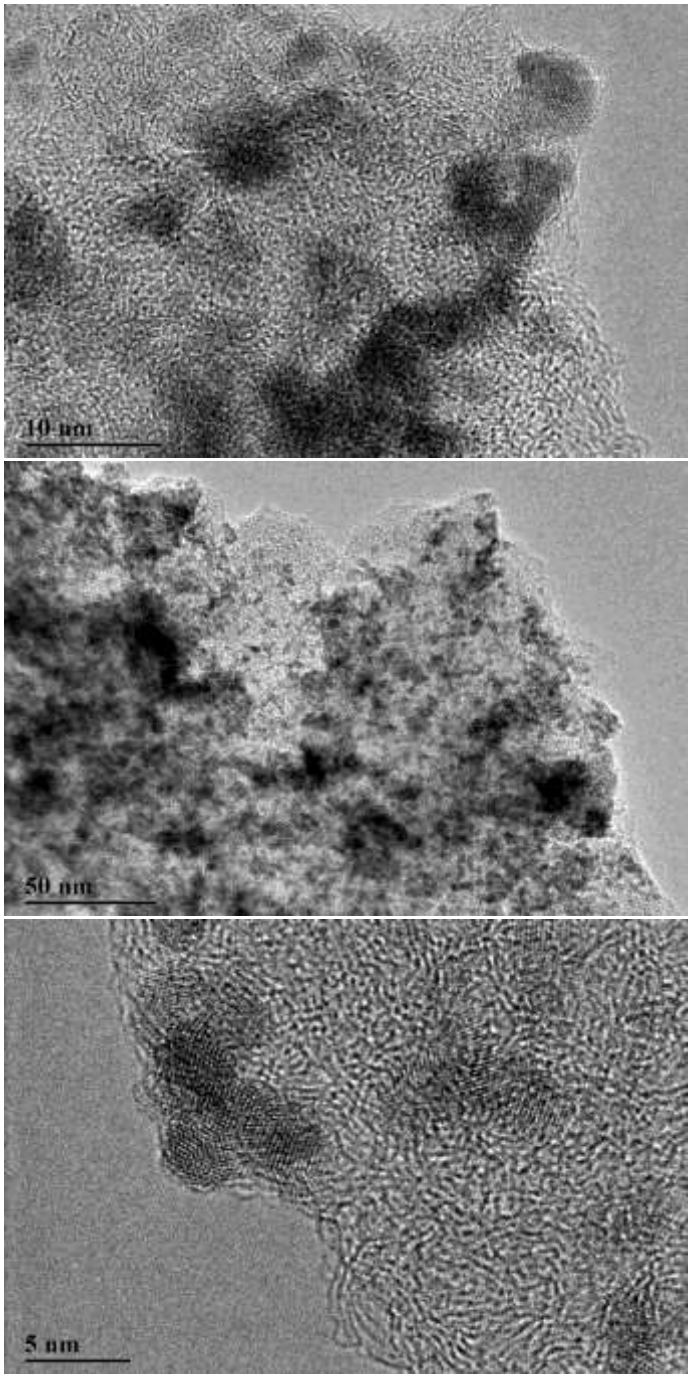
TEM of 20% $Pd[OH]_2/C$ Sigma-Aldrich (3#).



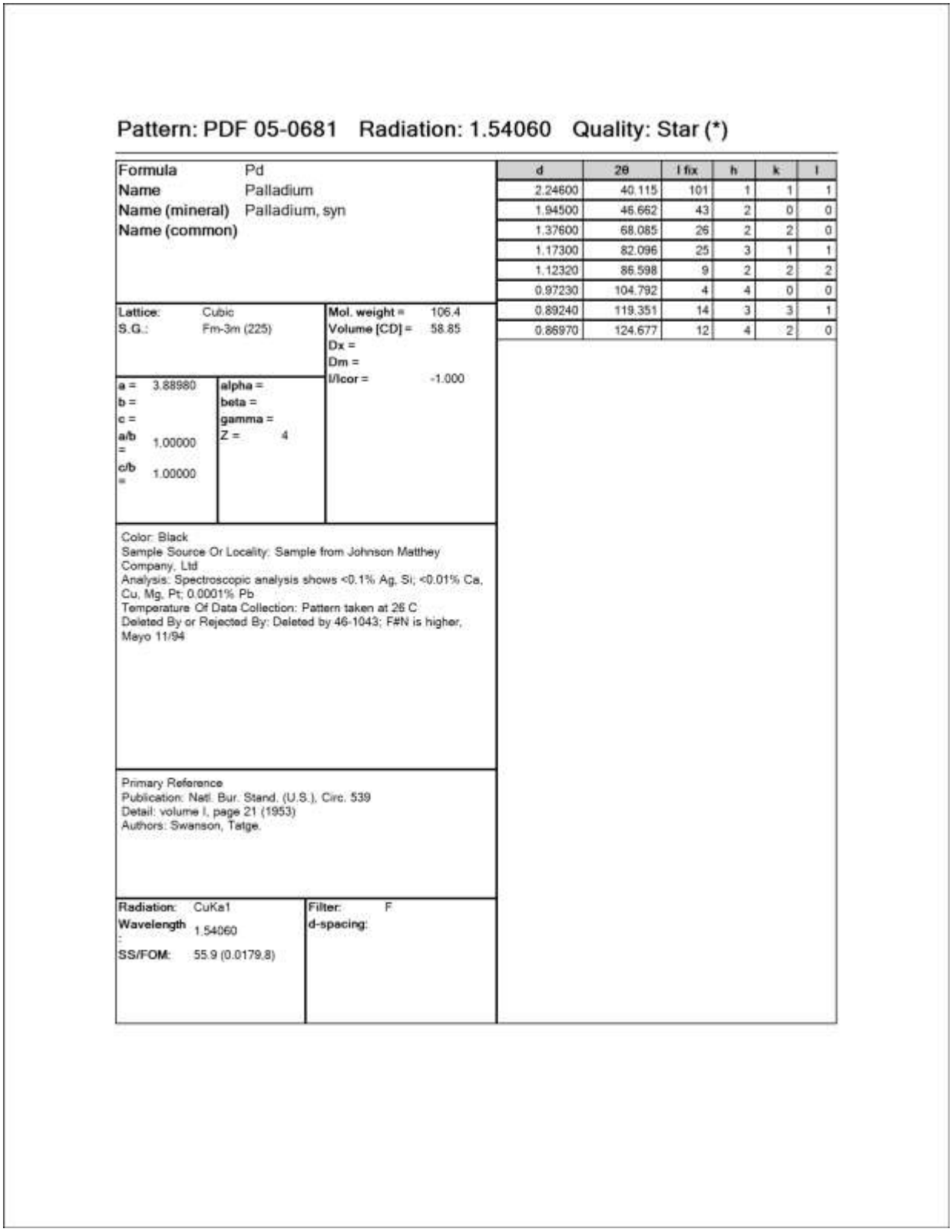

5 nm
10 nm
50 nm
100 nm


200 nm
100 nm
5 nm
5 nm


10 nm
50 nm
100 nm
10 nm


10 nm
50 nm
5 nm

Palladium: PDF 05-0681



Pattern: PDF 05-0681 Radiation: 1.54060 Quality: Star (*)

Formula	Pd
Name	Palladium
Name (mineral)	Palladium, syn
Name (common)	

Lattice:	Cubic
S.G.:	Fm-3m (225)

Mol. weight =	106.4
Volume [CD] =	58.85
Dx =	
Dm =	
I/Icor =	-1.000

a =	3.88980	alpha =	
b =		beta =	
c =		gamma =	
a/b =	1.00000	Z =	4
c/b =	1.00000		

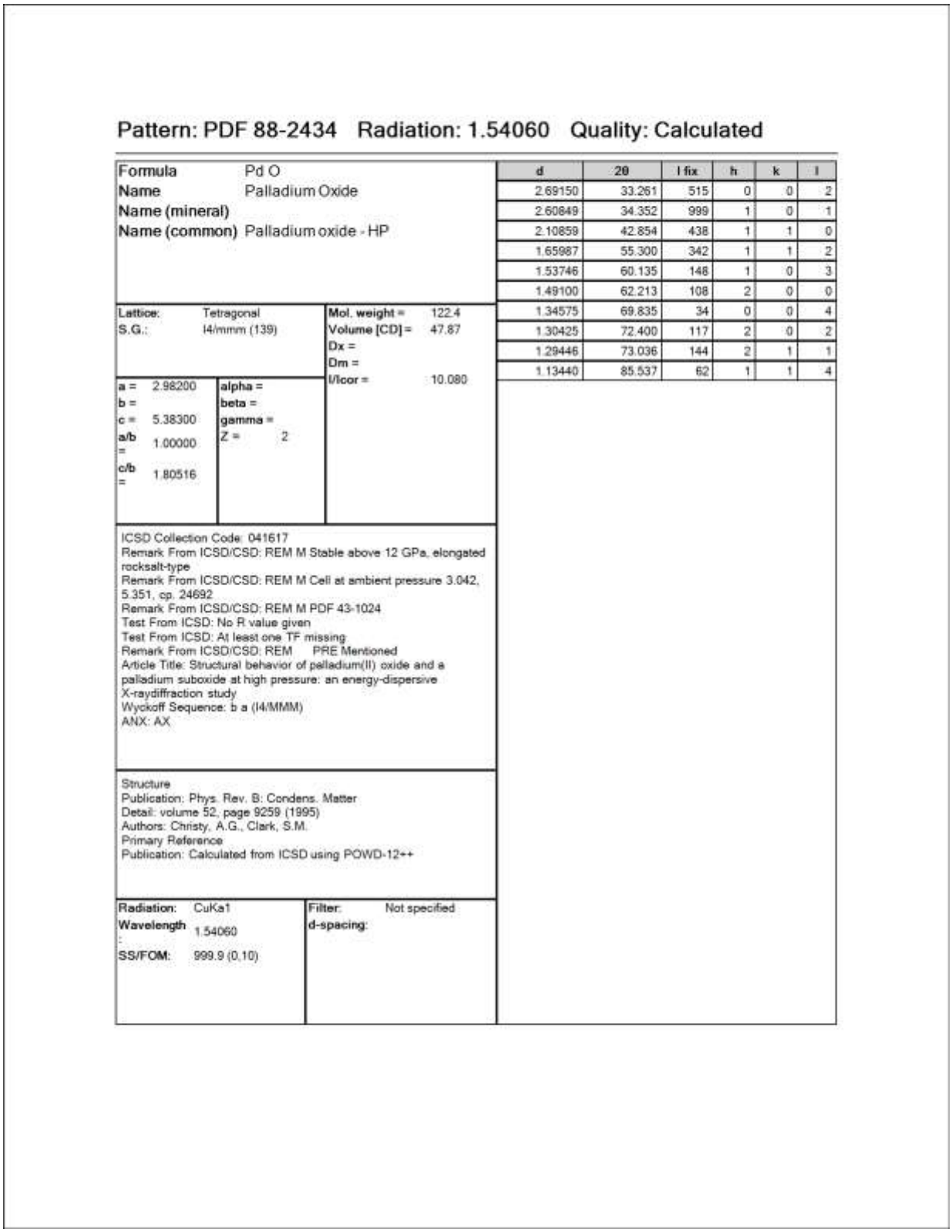
Color: Black
Sample Source Or Locality: Sample from Johnson Matthey Company, Ltd
Analysis: Spectroscopic analysis shows <0.1% Ag, Si; <0.01% Ca, Cu, Mg, Pt; 0.0001% Pb
Temperature Of Data Collection: Pattern taken at 26 C
Deleted By or Rejected By: Deleted by 46-1043; F#N is higher, Mayo 11/94

Primary Reference
Publication: Natl. Bur. Stand. (U.S.), Circ. 539
Detail: volume I, page 21 (1953)
Authors: Swanson, Tatge.

Radiation:	CuKa1	Filter:	F
Wavelength:	1.54060	d-spacing:	
SS/FOM:	55.9 (0.0179,8)		

d	2θ	I fix	h	k	l
2.24600	40.115	101	1	1	1
1.94500	46.662	43	2	0	0
1.37600	68.085	26	2	2	0
1.17300	82.096	25	3	1	1
1.12320	86.598	9	2	2	2
0.97230	104.792	4	4	0	0
0.89240	119.351	14	3	3	1
0.86970	124.677	12	4	2	0

Palladium oxide: PDF 88-2434



Pattern: PDF 88-2434 Radiation: 1.54060 Quality: Calculated

Formula	Pd O
Name	Palladium Oxide
Name (mineral)	
Name (common)	Palladium oxide - HP

Lattice:	Tetragonal
S.G.:	I4/mmm (139)

Mol. weight =	122.4
Volume [CD] =	47.87
Dx =	
Dm =	
I/Icor =	10.080

a =	2.98200
b =	
c =	5.38300
a/b =	1.00000
c/b =	1.80516

alpha =	
beta =	
gamma =	
Z =	2

ICSD Collection Code: 041617
Remark From ICSD/CSD: REM M Stable above 12 GPa, elongated rocksalt-type
Remark From ICSD/CSD: REM M Cell at ambient pressure 3.042, 5.351, cp. 24692
Remark From ICSD/CSD: REM M PDF 43-1024
Test From ICSD: No R value given
Test From ICSD: At least one TF missing
Remark From ICSD/CSD: REM PRE Mentioned
Article Title: Structural behavior of palladium(II) oxide and a palladium suboxide at high pressure: an energy-dispersive X-raydiffraction study
Wyckoff Sequence: b a (I4/MMM)
ANX: AX

Structure
Publication: Phys. Rev. B: Condens. Matter
Detail: volume 52, page 9259 (1995)
Authors: Christy, A.G., Clark, S.M.
Primary Reference
Publication: Calculated from ICSD using POWD-12++

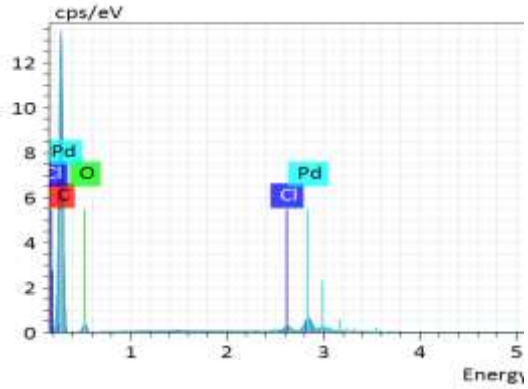
Radiation:	CuKa1
Wavelength:	1.54060
SS/FOM:	999.9 (0.10)

Filter:	Not specified
d-spacing:	

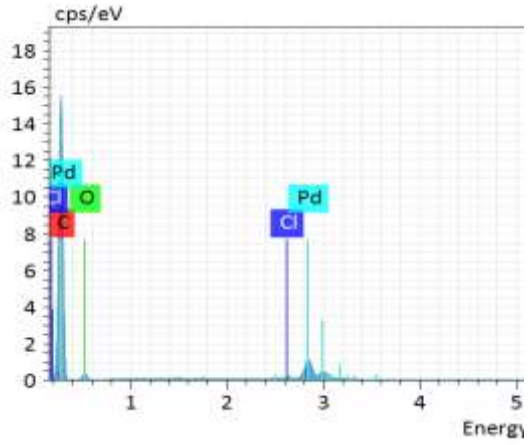
d	2θ	I fix	h	k	l
2.69150	33.261	515	0	0	2
2.60849	34.352	999	1	0	1
2.10859	42.854	438	1	1	0
1.65987	55.300	342	1	1	2
1.53746	60.135	148	1	0	3
1.49100	62.213	108	2	0	0
1.34575	69.835	34	0	0	4
1.30425	72.400	117	2	0	2
1.29446	73.036	144	2	1	1
1.13440	85.537	62	1	1	4

SEM-EDS

1# Sample, Pd/C STREM Chemicals: Cl=1.7%$_{wt}$



2# Sample, Pd/C Sigma-Aldrich: Cl=0.8%$_{wt}$



3# Sample, Pd[OH]$_2$ /C Sigma-Aldrich: negligible