"Facile One-Pot Preparation and Catalytic Application of Tunable Silica-Coated Aqueous Gold Nanoparticles"

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Supporting Information

TMSP-PEI Au NP Characterization:

Nanoparticle size analysis was conducted using TEM images with the NIH program ImageJ. The resulting data is shown below.

Table S1. Nanoparticle size analysis of TMSP-PEI nanoparticles in ratios 1-1.6, 1-3.5, and 1-14.

1-1.6 Ratio		1-3.5 Ratio		1-14 Ratio	
#	Length (nm)	#	Length (nm)	#	Length (nm)
1	11.267	1	3.91	1	5.591
2	10.267	2	3.963	2	7.103
3	11.846	3	3.754	3	9.066
4	12.593	4	4.848	4	8.611
5	10.95	5	5.288	5	10.817
6	9.587	6	6.62	6	7.443
7	10.961	7	4.639	7	7.762
8	16.624	8	4.667	8	6.957
9	12.935	9	5.67	9	5.592
10	6.425	10	5.575	10	9.729
11	10.438	11	6.665	11	9.136
12	10.553	12	4.745	12	7.739
13	12.596	13	5.71	13	8.451
14	8.139	14	5.256	14	6.986
15	10.746	15	7.941	15	9.313
16	9.539	16	7.54	16	7.994
17	11.477	17	7.705	17	10.439
18	11.425	18	5.269	18	9.809
19	11.275	19	4.291	19	8.298
20	4.756	20	5.885	20	9.161
21	9.323	21	5.604	21	8.101
22	9.049	22	6.021	22	7.634
23	11.437	23	7.236	23	8.364
24	8.445	24	4.689	24	6.838
25	12.638	25	3.91	25	7.793
26	11.28	26	5.944	26	8.576

27	11.662	27	5.505	27	8.236
28	9.797	28	7.121	28	10.025
29	11.597	29	5.545	29	8.282
30	15.531	30	4.518	30	6.073
31	10.688	31	4.973	31	7.56
32	10.325	32	6.662	32	10.035
33	11.848	33	7.654	33	10.219
34	11.912	34	5.532	34	7.576
35	12.138	35	5.441	35	6.756
36	9.186	36	4.905	36	6.341
37	12.862	37	4.873	37	7.883
38	11.004	38	6.877	38	8.359
39	8.614	39	6.877	39	7.06
40	4.809	40	6.451	40	9.725
41	10.226	41	5.831	41	7.385
42	12.72	42	6.562	42	6.438
43	8.885	43	5.315	43	5.239
44	9.776	44	5.206	44	10.744
45	10.212	45	6.434	45	10.035
46	9.785	46	6.727	46	9.48
47	12.932	47	7.295	47	10.859
48	13.337	48	6.622	48	5.61
49	8.617	49	6.383	49	9.638
50	5.237	50	5.43	50	11.801
51	7.326	51	4.605	51	13.822
52	7.376	52	6.889	52	12.071
53	12.485	53	8.175	53	8.781
54	10.401	54	8.404	54	9.038
55	7.384	55	5.866	55	9.378
56	9.326	56	5.562	56	7.646
57	12.128	57	5.572	57	8.849
58	3.329	58	7.808	58	9.179
59	7.558	59	6.341	59	5.061
60	10.913	60	9.232	60	9.943
61	8.089	61	5.914	61	4.231
62	9.934	62	7.083	62	11.705
63	13.918	63	6.717	63	10.4
64	14.708	64	7.816	64	11.674
65	9.102	65	5.396	65	8.418
66	12.258	66	6.252	66	11.9
67	15.561	67	6.239	67	7.711
68	10.867	68	7.956	68	8.657
69	12.286	69	8.818	69	10.963

70	9.149	70	7.721	70	9.765
71	12.126	71	7.265	71	8.813
72	12.943	72	7.758	72	9.313
73	8.952	73	6.382	73	4.117
74	16.638	74	9.216	74	13.052
75	11.298	75	8.131	75	6.574
76	13.463	76	8.596	76	11.453
77	6.439	77	7.455	77	9.231
78	6.864	78	9.677	78	3.813
79	9.854	79	6.914	79	8.915
80	9.805	80	6.586	80	5.263
81	12.369	81	6.93	81	10.337
82	9.369	82	9.296	82	3.536
83	12.995	83	6.788	83	3.779
84	10.783	84	10.341	84	9.536
85	10.846	85	9.197	85	7.81
86	13.305	86	5.285	86	4.882
87	11.278	87	7.026	87	7.854
88	13.389	88	7.113	88	6.209
89	10.563	89	7.375	89	9.669
90	8.731	90	5.229	90	4.53
91	12.586	91	8.394	91	8.127
92	13.723	92	8.322	92	6.429
93	11.259	93	6.093	93	3.689
94	8.508	94	6.433	94	10.788
95	8.141	95	6.411	95	9.762
96	16.708	96	6.932	96	5.129
97	10.491	97	5.649	97	3.419
98	10.809	98	7.067	98	11.862
99	12.258	99	7.975	99	8.81
100	12.451	100	5.595	100	6.667
Average (nm):	10.73313	Average (nm):	6.47881	Average (nm):	8.27222

The average diameter of the nanoparticles calculated with the program, ImageJ, and the initial mass of Gold (III) Chloride Trihydrate was used to determine the concentrations of the nanoparticle solutions. The calculations are provided below.

Mass of pure Au in reaction = (Mass of $HAuCl_4 \cdot 3H_2O$) · Mass fraction Au
$= 0.0393\ g \cdot 0.5 = 1.97 \times 10^{-2}\ g$

Volume of Au added = Mass of Au added ÷ Density of Au
$= 1.97 \times 10^{-2}\ g \div 19.32\ g \cdot cm^3 = 1.02 \times 10^{-3}\ cm^3$

Volume of 1 Au NP $= \frac{4}{3} \cdot \pi \cdot r_{AuNP}{}^3 = \frac{4}{3} \cdot \pi \cdot (10.7\ nm)^3 = 5{,}130\ nm^3$ (1-1.6 ratio)
$= \frac{4}{3} \cdot \pi \cdot (6.47\ nm)^3 = 1{,}050\ nm^3$ (1-3.5 ratio)

$= \frac{4}{3} \cdot \pi \cdot (8.27\ \text{nm})^3 = 2{,}230\ \text{nm}^3$ (1-14 ratio)

Number of NPs in solution = Volume of Au added ÷ Volume of 1 Au NP in cm^3

= $1.02 \times 10^{-3}\ cm^3 \div 5.13 \times 10^{-18}\ cm^3 = 1.98 \times 10^{14}$ (1-1.6 ratio)

= $1.02 \times 10^{-3}\ cm^3 \div 1.05 \times 10^{-18}\ cm^3 = 9.68 \times 10^{14}$ (1-3.5 ratio)

= $1.02 \times 10^{-3}\ cm^3 \div 2.23 \times 10^{-18}\ cm^3 = 4.56 \times 10^{14}$ (1-14 ratio)

Concentration of stock Au NP solution = (Number of NPs in solution ÷ 6.022×10^{23} 1/mol) 0.1 L

= $(1.98 \times 10^{14} \div 6.022 \times 10^{23}\ 1/\text{mol}) \div 0.05\ \text{L} = 6.58 \times 10^{-9}$ M (1-1.6 ratio)

= $(9.68 \times 10^{14} \div 6.022 \times 10^{23}\ 1/\text{mol}) \div 0.05\ \text{L} = 3.22 \times 10^{-8}$ M (1-3.5 ratio)

= $(4.56 \times 10^{14} \div 6.022 \times 10^{23}\ 1/\text{mol}) \div 0.05\ \text{L} = 1.51 \times 10^{-8}$ M (1-14 ratio)