Electronic Supplementary Information for PCCP

SUPPORTING INFORMATION

Isolation, structure, and stability of a dodecanethiolate-protected Pd_1Au_{24} cluster

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Part I. Characterization of 3

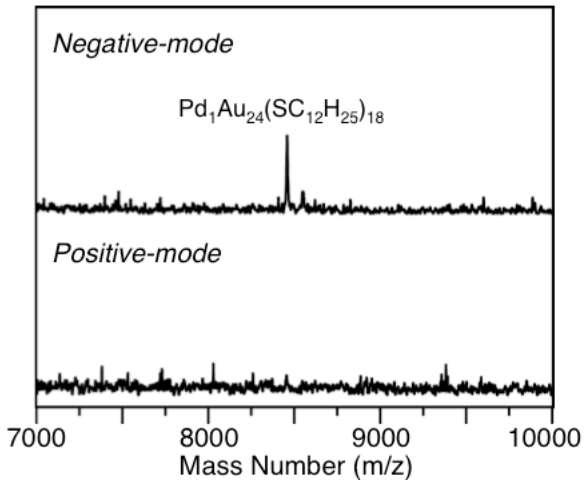

Fig. S1 MALDI mass spectra of the residual fraction that remained after extraction by acetone. No significant ion peaks were observed for $Pd_nAu_{25-n}(SC_{12}H_{25})_{18}$ ($n \cong 2$) in either the negative- or positive-ion mass spectrum.

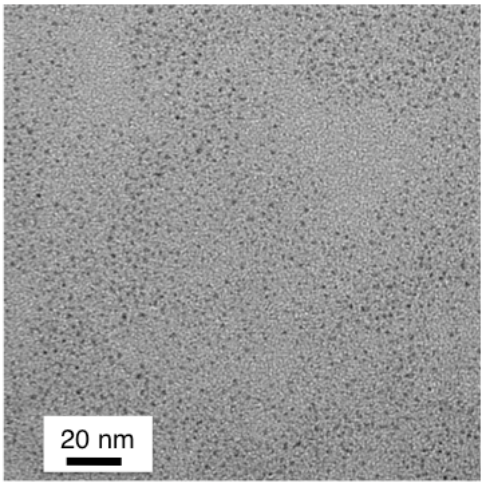

Fig. S2 TEM image of fraction **3**. Particles with a size of ~1 nm are barely discernible.

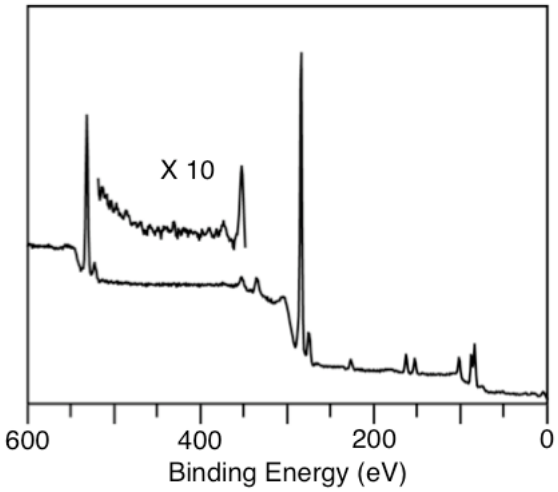

Fig. S3 XPS spectrum of fraction **3**. No significant peaks were observed for N (N 1s:401.1 eV).

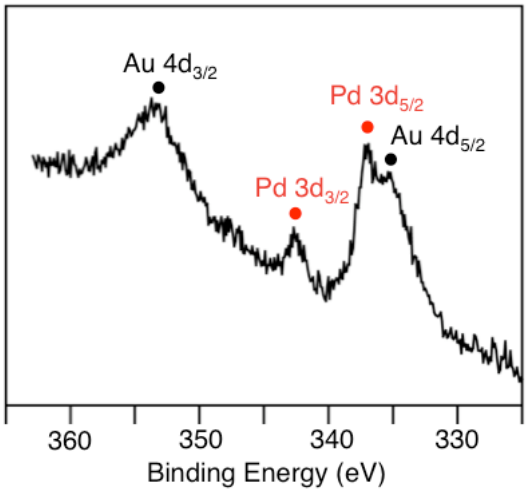

Fig. S4 Pd 3d spectrum of fraction **3**. Weak peaks assigned to Pd 3d (337.2 and 342.7 eV) were observed, together with strong peaks assigned to Au 4d (335.4 and 353.4 eV)

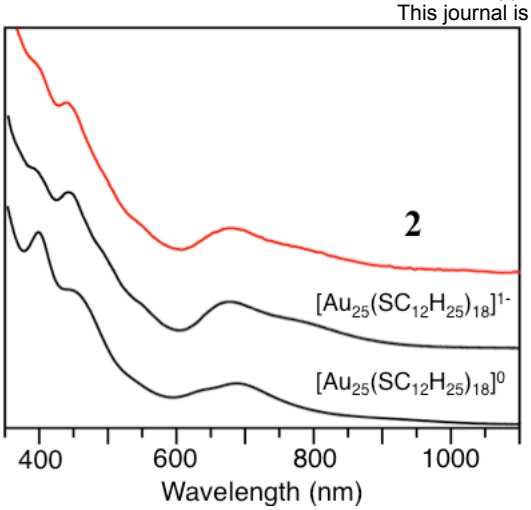

Fig. S5 Absorbance spectra of fraction **2**, $[Au_{25}(SC_{12}H_{25})_{18}]^{1-}$, and $[Au_{25}(SC_{12}H_{25})_{18}]^{0}$. The absorbance spectrum of fraction **2** is quite similar to that of $[Au_{25}(SC_{12}H_{25})_{18}]^{1-}$, indicating that **2** is the anionic species $[Au_{25}(SC_{12}H_{25})_{18}]^{1-}$.

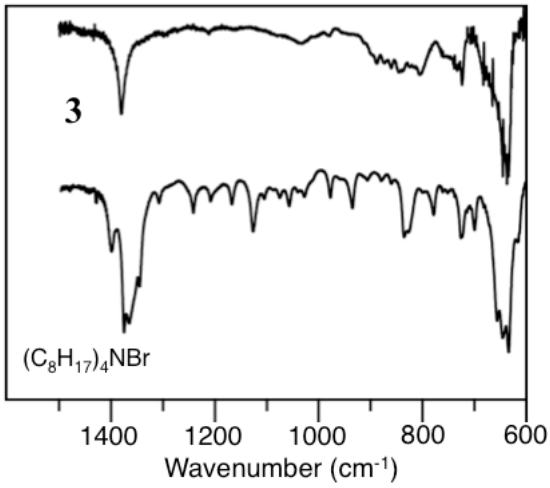

Fig. S6 FT-IR spectrum of fraction **3** and $(C_8H_{17})_4NBr$. In the spectrum of fraction **3**, no significant peaks were observed for C-N stretching vibration mode (1030 - 1230 cm^{-1}).

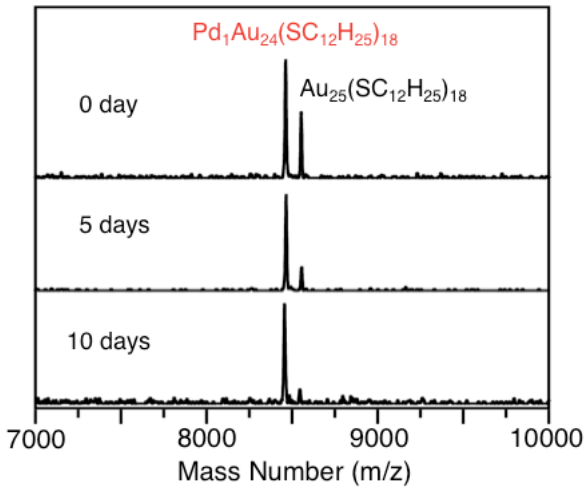

Fig. S7 Chemical composition of a toluene solution containing **2** and **3** ([**2**]:[**3**] = 0.6:1) at 60 ℃ as followed by MALDI mass spectrometry.

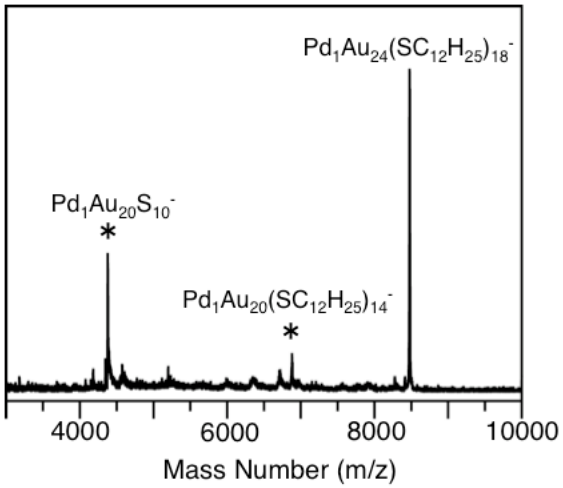

Fig. S8 Negative-ion MALDI mass spectrum of fraction **3** observed with a fluence slightly higher than that used for the observation of nondestructive mass spectrum (fig. 1(b)). The asterisks indicate the main fragment ions.

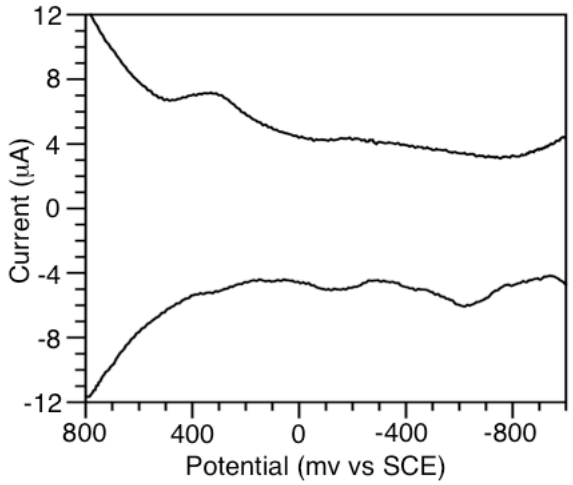

Fig. S9 Square wave voltammograms (pulse height, 25 mV; pulse cycling time, 100 ms) recorded at a scan rate of 30 mV/s of **3** (5.9 mg) in a dichloromethane solution of tetrabutylammonium perchlorate (0.1 M, 3 ml) under Ar atmosphere at 300 K.

Part II. Optimized Coordinate for 3'

Pd	0.0000000	0.0000000	0.0000000
Au	0.5345863	-1.1404296	-2.6216302
Au	-0.6094433	-2.8430759	-0.3528277
Au	-2.1608341	-0.6445066	-1.7959108
Au	2.0962795	-1.9565868	-0.2772498
Au	2.1697840	1.1615938	-1.4892539
Au	4.0284291	-1.5341801	-3.0051129
Au	-1.7154879	0.0387790	-5.1014728
Au	1.7088503	-4.3827572	-2.5982807
Au	-3.8751795	2.0480966	-2.8632164
Au	-0.5011217	1.7247008	-2.2918990
Au	-1.7281975	-4.4726790	2.4776502
Au	-3.8597204	-3.4869270	-0.3795343
S	-3.7183084	1.3529954	-5.1532033
S	3.8239703	-3.8466826	-3.5961280
S	-0.1115012	3.7224742	-3.8113166
S	4.4050767	0.7527340	-2.4160545
S	-3.4522590	-5.3584408	1.0624120
S	4.2666479	-2.7040043	0.6002140
S	0.2207290	-1.3678888	-5.1271644
S	-0.3837336	-5.0180976	-1.6369820
S	-4.3915383	-1.6718587	-1.8367333
C	0.6757188	3.0551093	-5.3363304
C	-0.4786081	-3.0439079	-5.4361624
C	0.0205037	-6.3860780	-0.4735510
C	3.5243996	-3.8239256	-5.4135740
C	4.3898932	1.6174628	-4.0417676
C	-4.9602058	-5.5008226	2.1093656
C	-4.5301235	-2.4370071	-3.5057856
C	-3.2992590	2.8935798	-6.0711847
C	4.1287976	-4.5405497	0.6304782
H	1.4984932	2.3659444	-5.0984086
H	-0.0948452	2.5072441	-5.9034898
H	1.0536547	3.8964166	-5.9397452
H	-0.8453129	-3.0895011	-6.4743166

H	0.3286231	-3.7806262	-5.2933111
H	-1.2968587	-3.2763149	-4.7387803
H	0.7558467	-6.0727370	0.2825719
H	-0.9163009	-6.6828583	0.0245689
H	0.4164737	-7.2363125	-1.0519154
H	3.2424566	-4.8413878	-5.7288313
H	2.7328664	-3.1086133	-5.6830484
H	4.4675529	-3.5357180	-5.9052299
H	5.3503587	1.4159473	-4.5439320
H	3.5615610	1.2735883	-4.6775236
H	4.2870917	2.6986410	-3.8548677
H	-5.7888092	-5.8319784	1.4631560
H	-4.7704314	-6.2614722	2.8836347
H	-5.2228209	-4.5424845	2.5807165
H	-5.4426314	-3.0547803	-3.5217057
H	-4.6213223	-1.6252087	-4.2451367
H	-3.6552885	-3.0606533	-3.7408612
H	-4.1980553	3.5309688	-6.0819153
H	-2.4684650	3.4339451	-5.5924404
H	-3.0327272	2.6177617	-7.1040867
H	5.0053146	-4.9398767	1.1661277
H	3.2051355	-4.8703944	1.1281091
H	4.1382197	-4.8977759	-0.4118682
Au	-0.5345863	1.1404296	2.6216302
Au	0.6094433	2.8430759	0.3528277
Au	2.1608341	0.6445066	1.7959108
Au	-2.0962795	1.9565868	0.2772498
Au	-2.1697840	-1.1615938	1.4892539
Au	-4.0284291	1.5341801	3.0051129
Au	1.7154879	-0.0387790	5.1014728
Au	-1.7088503	4.3827572	2.5982807
Au	3.8751795	-2.0480966	2.8632164
Au	0.5011217	-1.7247008	2.2918990
Au	1.7281975	4.4726790	-2.4776502
Au	3.8597204	3.4869270	0.3795343
S	3.7183084	-1.3529954	5.1532033
S	-3.8239703	3.8466826	3.5961280

S	0.1115012	-3.7224742	3.8113166
S	-4.4050767	-0.7527340	2.4160545
S	3.4522590	5.3584408	-1.0624120
S	-4.2666479	2.7040043	-0.6002140
S	-0.2207290	1.3678888	5.1271644
S	0.3837336	5.0180976	1.6369820
S	4.3915383	1.6718587	1.8367333
C	-0.6757188	-3.0551093	5.3363304
C	0.4786081	3.0439079	5.4361624
C	-0.0205037	6.3860780	0.4735510
C	-3.5243996	3.8239256	5.4135740
C	-4.3898932	-1.6174628	4.0417676
C	4.9602058	5.5008226	-2.1093656
C	4.5301235	2.4370071	3.5057856
C	3.2992590	-2.8935798	6.0711847
C	-4.1287976	4.5405497	-0.6304782
H	-1.4984932	-2.3659444	5.0984086
H	0.0948452	-2.5072441	5.9034898
H	-1.0536547	-3.8964166	5.9397452
H	0.8453129	3.0895011	6.4743166
H	-0.3286231	3.7806262	5.2933111
H	1.2968587	3.2763149	4.7387803
H	-0.7558467	6.0727370	-0.2825719
H	0.9163009	6.6828583	-0.0245689
H	-0.4164737	7.2363125	1.0519154
H	-3.2424566	4.8413878	5.7288313
H	-2.7328664	3.1086133	5.6830484
H	-4.4675529	3.5357180	5.9052299
H	-5.3503587	-1.4159473	4.5439320
H	-3.5615610	-1.2735883	4.6775236
H	-4.2870917	-2.6986410	3.8548677
H	5.7888092	5.8319784	-1.4631560
H	4.7704314	6.2614722	-2.8836347
H	5.2228209	4.5424845	-2.5807165
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H	4.1980553	-3.5309688	6.0819153
H	2.4684650	-3.4339451	5.5924404
H	3.0327272	-2.6177617	7.1040867
H	-5.0053146	4.9398767	-1.1661277
H	-3.2051355	4.8703944	-1.1281091
H	-4.1382197	4.8977759	0.4118682