Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Selective Formation of Silver(I) Bis-phospholane Macrocycles and Further Evidence that Gold(I) is Smaller than Silver(I)

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Table S1. Summary of data collection, structure solution and refinement details for **4**, **5**, **6**, **7**.

Compound	**4**	**5**	**6**	**7**
Formula	$C_{26}H_{52}Ag_2P_4$,2(BF_4), C_7H_8, 2(CH_2Cl_2)	$C_{30}H_{60}Ag_2P_4$, 2(BF_4)	$C_{34}H_{68}Ag_2P_4$, 2(BF_4), 0.5 C_7H_8	$C_{38}H_{76}Ag_2P_4$, 2(BF_4)
Formula weight	1139.90	934.02	1036.19	1046.23
Temperature [K]	130(2)	130(2)	130(2)	130(2)
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P2_1/n$	$P\bar{1}$	$P\bar{1}$
Crystal description	colorless prism	colorless prism	colorless prism	colorless needle
Unit cell				
a [pm]	1022.9(5)	901.7(5)	1034.8(5)	1295.70(5)
b [pm]	1033.2(5)	1756.2(5)	1143.1(5)	1832.00(8)
c [pm]	1251.6(5)	1239.9(5)	2051.2(5)	2288.40(7)
α [deg]	72.496(5)	90	81.509(5)	103.656(3)
β [deg]	71.499(5)	97.526(5)	80.136(5)	94.894(3)
γ [deg]	87.663(5)	90	87.890(5)	92.006(3)
V [nm^3]	1.1941(9)	1.947(1)	2.364(2)	4.7918(3)
Z	1	2	2	4
$\rho_{calcd.}$ [g/cm^3]	1.585	1.594	1.456	1.450
μ [mm^{-1}]	1.234	1.230	1.020	1.008
F(000)	578	952	1066	2160
Crystal size [mm]	0.4×0.4×0.2	0.3×0.15×0.15	0.25×0.12×0.03	0.25×0.03×0.03
Θ_{Min} - Θ_{Max} [deg]	3.13 - 36.32	2.85 - 36.32	2.86 - 25.35	2.86 - 25.35
Collected reflections	23349	65409	17344	30683
Indep. reflections (R_{int})	11560 (0.0175)	9412 (0.0316)	8649 (0.0258)	17372 (0.0531)
Completeness to Θ_{Max}	99.9 %	100.0 %	99.8 %	99.0 %
restraints/parameters	102 / 318	82 / 264	177 / 552	69 / 980
GooF (F^2)	1.019	1.068	1.054	1.007
R1, wR2 (I>2σ(I))	0.0308, 0.0685	0.0282, 0.0609	0.0559, 0.1360	0.0643, 0.1093
R1, wR2 (all data)	0.0400, 0.0735	0.0358, 0.0640	0.0774, 0.1493	0.1311, 0.1325
Residual electron density [$e \cdot Å^{-3}$]	0.922 / –1.019	0.876 / –0.441	1.952 / –2.678	0.869 / –0.761

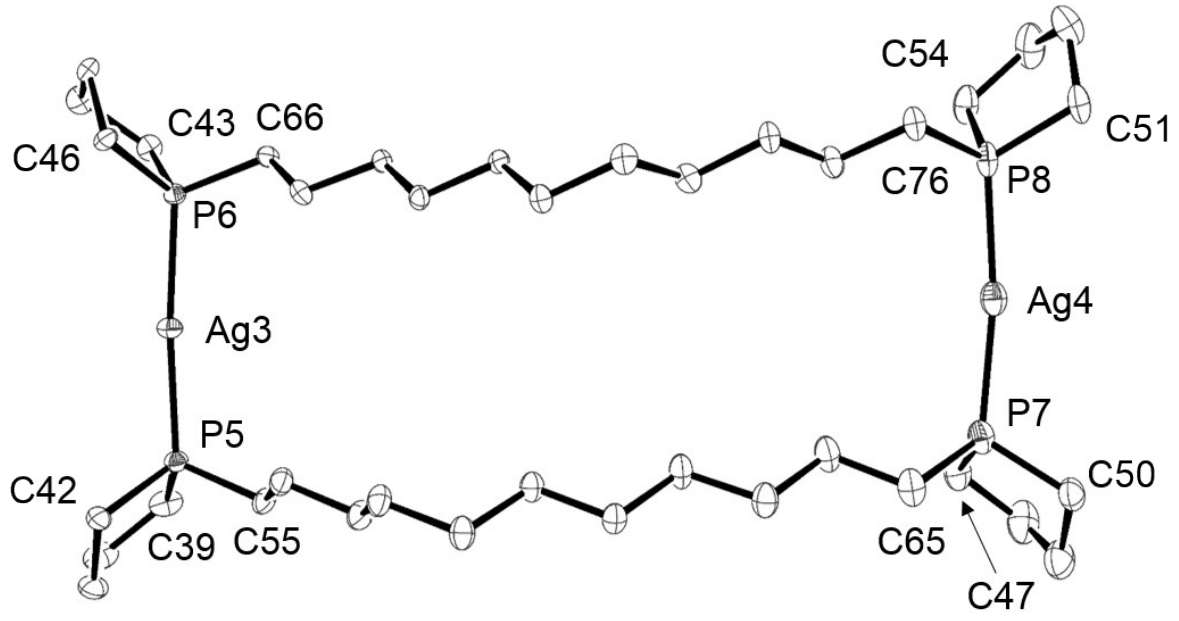

Figure S1. Second independent molecule of **7**. Ellipsoids are drawn at the 30% probability level. H atoms and counter ions are omitted for clarity.