Supplementary Material

Triphenylphosphine-(N,N-dimethyldithiocarbamato)-gold(I) methanol solvate

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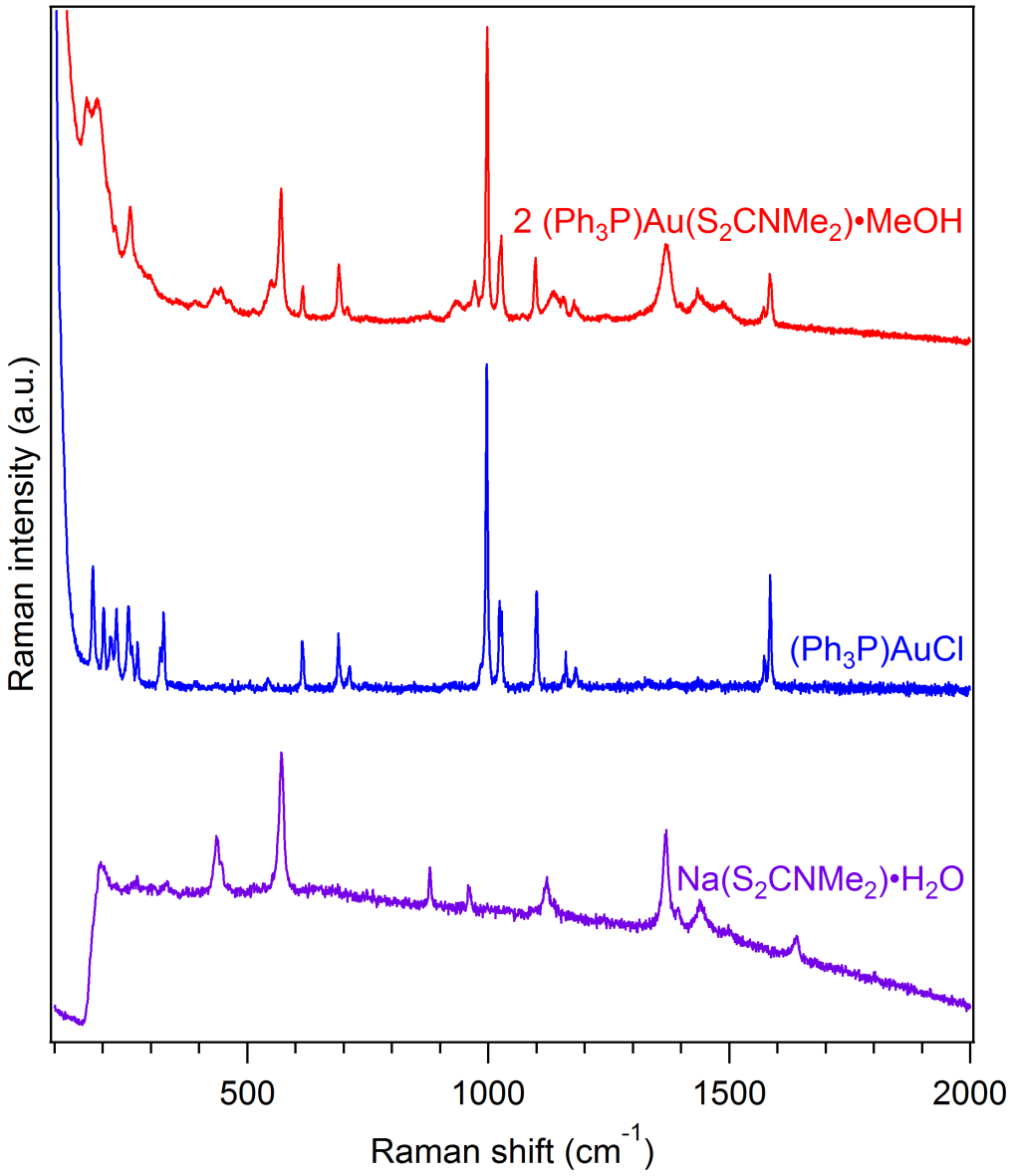

Figure S1. Raman spectra of the synthesized compound 2 $(Ph_3P)Au(S_2CNMe_2)•CH_3OH$ and of its precursors. Raman spectra were measured at room temperature with an excitation wavelength of 785 nm are offset along the vertical axis for clarity.

Table S1. Atoms' coordinates of the DFT-optimized ground-state structure of $(Ph_3P)Au(S_2CNMe_2)$ in the gas-phase (Gaussian 09, PBE1PBE/Lanl2dz).

Atoms	X	Y	Z
Au	-0.87588900	-0.67903400	-0.02762700
S	-3.14402200	-1.54232200	-0.07028100
P	1.38395700	0.01536700	-0.00368800
C	-3.98645200	0.05624200	0.01374900
C	1.66124600	1.54880100	-1.02340400
C	2.00846000	0.42348900	1.70419000
C	2.58865400	-1.24185600	-0.66830100
S	-3.09692500	1.55272300	0.08945700
N	-5.34339800	0.05503000	0.02182600
C	2.89287400	1.80537000	-1.65007100
C	0.59871200	2.46089300	-1.15176300
C	1.65851300	-0.43803300	2.75947200
C	2.80318200	1.55306000	1.95618100
C	2.18471300	-2.04556400	-1.74869600
C	3.87529300	-1.39165700	-0.12506300
C	-6.17364600	-1.15230500	-0.03093500
C	-6.07426300	1.32699600	0.09047900
H	3.70596700	1.08809400	-1.57661000
C	3.06510700	2.98179000	-2.39350000
C	0.77962600	3.63817400	-1.89182400
H	-0.36625700	2.24666200	-0.69598200
H	1.01959100	-1.29737900	2.57027000
C	2.11744300	-0.17862000	4.05724200
C	3.25450100	1.81359700	3.25915900
H	3.05697600	2.23563200	1.15013500
H	1.17931700	-1.94683200	-2.15101900
C	3.07182800	-2.98342600	-2.29349200
C	4.75787500	-2.33741300	-0.66824600
H	4.18451300	-0.78844800	0.72425400
H	-6.80235800	-1.21397800	0.86602800
H	-5.54818500	-2.04308900	-0.08253700
H	-6.82041400	-1.12353700	-0.91659100
H	-5.82029100	1.96361700	-0.76375800
H	-5.80716300	1.87622800	0.99962100
H	-7.14660000	1.11409500	0.08782000
H	4.01550600	3.17589700	-2.88237200
C	2.01095600	3.90101200	-2.51081700
H	-0.04451000	4.33797900	-1.99187300
H	1.84140900	-0.84483900	4.86914700

C	2.91688700	0.94754800	4.30904700
H	3.86221500	2.69306100	3.45141500
H	2.75516600	-3.60310900	-3.12716700
C	4.35958300	-3.13040400	-1.75442100
H	5.74986700	-2.45503200	-0.24169100
H	2.14555000	4.81038400	-3.08979500
H	3.26433300	1.15346300	5.31743000
H	5.04362300	-3.86349500	-2.17240700

Table S2. Comparison between experimental and DFT-calculated (Gaussian 09, PBE1PBE/Lanl2dz) Raman shifts for the main Raman peaks.

Raman shift (cm^{-1})		Assignment*
Exp.	Calc.	
168	218 and 214	C-P-C angle deformation
189	252	C-P-C angle deformation
257	293	N-C-S (uncoord.) angle deformation
433	423	Me-N-Me angle deformation + symm. C-S stretching
445	453, 450 and 448	453: P-C stretching + out-of-plane C-C-C (Ph) deformation + out-of-plane C-H deformation (Ph) 450: C(Me)-N-C(dtc) angle deformation + N-C-S (dtc) angle deformation 448: C-P-C out-of-plane deformation + out-of-plane C-C-C (Ph) deformation + out-of-plane C-H deformation (Ph)
463	460	Au-P stretching + out-of-plane C-C-C (Ph) deformation + out-of-plane C-H deformation (Ph)
550	556	Symm. C-S stretching + CH_3 rocking
570		
615	636, 635 and 634	In-plane C-C-C (Ph) angle deformation
690	703	P-C stretching + in-plane C-C-C (Ph) angle deformation
707	719 and 718	P-C stretching + in-plane C-C-C (Ph) angle deformation
972	989, 986, 980 and 978	989 and 986: Out-of-plane C-H (Ph) deformation + antisymm. C-S stretching + CH_3 rocking 980 and 978: Out-of-plane C-H (Ph) deformation
998	1024 and 1023	In-plane C-C-C (Ph) angle deformation
1023	1059 and 1058	In-plane C-C-H (Ph) angle deformation + in-plane C-C-C (Ph) angle deformation
1027		
1098	1138, 1135, 1134, 1128, 1124 and 1121	1138, 1135 and 1134: in-plane C-C-H (Ph) angle deformation + P-C stretching 1128: CH_3 rocking 1124 and 1121: in-plane C-C-H (Ph) angle deformation

1136	1183 and 1177	1183: CH_3 rocking + out-of-plane deformation centered on the Me_2N-C fragment (dtc) 1177: H-C-H angle deformation (dtc) + C-N (dtc) stretching
1156	1215	In-plane C-C-H (Ph) angle deformation
1179	1242, 1237 and 1236	In-plane C-C-H (Ph) angle deformation
1370	1405 and 1404	C-C (Ph) stretching + in-plane C-C-H (Ph) angle deformation
1399	1440	C-N (dtc) stretching + H-C-H (dtc) angle deformation
1435	1514, 1504, 1482, 1481 and 1479	1514, 1504, 1482 and 1481: H-C-H (dtc) angle deformation 1479: CH_3 umbrella mode
1488	1559, 1531 and 1530	1559: C-N (dtc) stretching + H-C-H (dtc) angle deformation 1531 and 1530: H-C-H (dtc) angle deformation
1571	1655 and 1654	C-C (Ph) stretching + in-plane C-C-H (Ph) angle deformation
1585	1668, 1667 and 1666	C-C (Ph) stretching + in-plane C-C-H (Ph) angle deformation

*dtc : dithiocarbamate moiety