

Co-ligands Triphenylphosphine/Alkynyl-Stabilized Undecagold

Nanocluster with a Capped Crown StructureExperimental

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Supplementary Information

Table S1. Crystallographic data of the gold cluster **1**.

Identification code	[Au ₁₁ (PPh ₃) ₈ (C≡CPhCF ₃) ₂](SbF ₆)
Formula	C ₁₆₂ H ₁₂₈ Au ₁₁ F ₁₂ P ₈ Sb
Formula weight	4838.78
Crystal size/mm ³	0.2×0.06×0.03
Temperature/K	150.2(1)
Crystal system	Triclinic
Space group	P -1
a (Å)	16.0672(3)
b (Å)	17.0707(3)
c (Å)	32.9542(3)
α (°)	80.8164(10)
β (°)	82.7276(10)
γ (°)	63.1499(17)
V (Å ³)	7945.5(2)
Z	2
D _c /(g·cm ⁻³)	2.023
F(000)	4496
Radiation	Cu Kα (λ= 1.54184 Å)
Theta (°) range	2.722 to 65.693
Index ranges	-18 ≤ h ≤ 18, -20 ≤ k ≤ 20, -38 ≤ l ≤ 29
Refls. Total	26720
Unique	23105
Parameters	1773
R _{int}	0.0628
R ₁ /wR ₂ [I>2σ(I)]	0.0650/0.1760
R ₁ /wR ₂ (all data)	0.0748/0.01851
Completeness	0.973
GoF	1.030

Table S2 Selected bond lengths (Å) for compound **1**.

Parameter	value	Parameter	value
Au(1)-Au(2)	2.6721(7)	Au(4)-Au(9)	2.9812(8)
Au(1)-Au(3)	2.7192(5)	Au(4)-Au(10)	2.9749(7)
Au(1)-Au(4)	2.7279(7)	Au(4)-C(1)	1.982(15)
Au(1)-Au(5)	2.6734(7)	Au(5)-Au(6)	3.2442(8)
Au(1)-Au(6)	2.6890(7)	Au(5)-Au(10)	2.9357(7)
Au(1)-Au(7)	2.7174(7)	Au(5)-Au(11)	3.2182(7)
Au(1)-Au(8)	2.6273(8)	Au(5)-P(3)	2.295(3)
Au(1)-Au(9)	2.6938(7)	Au(6)-Au(7)	2.8722(9)
Au(1)-Au(10)	2.6880(7)	Au(6)-Au(11)	2.9580(7)
Au(1)-Au(11)	2.6559(7)	Au(6)-P(4)	2.305(3)
Au(2)-Au(3)	2.8791(8)	Au(7)-Au(8)	2.9000(9)
Au(2)-Au(4)	3.0583(7)	Au(7)-C(2)	2.026(18)
Au(2)-Au(5)	2.9461(7)	Au(8)-Au(9)	2.9362(8)
Au(2)-Au(6)	2.9376(8)	Au(8)-Au(11)	3.0521(8)
Au(2)-Au(7)	3.3125(9)	Au(8)-P(6)	2.277(4)
Au(2)-P(1)	2.283(4)	Au(9)-Au(10)	2.9215(7)
Au(3)-Au(4)	2.9247(8)	Au(9)-P(7)	2.279(3)
Au(3)-Au(7)	2.8062(8)	Au(10)-Au(11)	2.8943(7)
Au(3)-Au(9)	2.8549(7)	Au(10)-P(8)	2.288(3)
Au(3)-P(2)	2.271(3)	Au(11)-P(5)	2.298(3)
Au(4)-Au(5)	2.9781(7)		

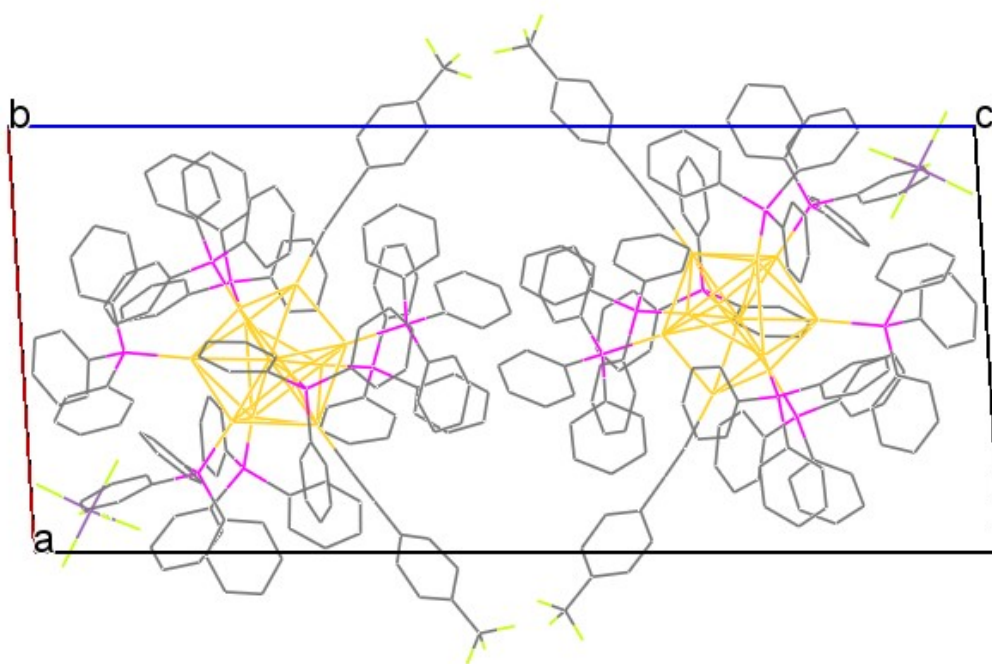


Figure S1 Packing structure of $[\text{Au}_{11}(\text{PPh}_3)_8(\text{C}\equiv\text{CPhCF}_3)_2](\text{SbF}_6)$ clusters in a unit cell along b-axis. Color legend: yellow spheres, Au; pink spheres, P; green spheres, F; grey spheres, C. All hydrogen atoms are omitted for clarity.

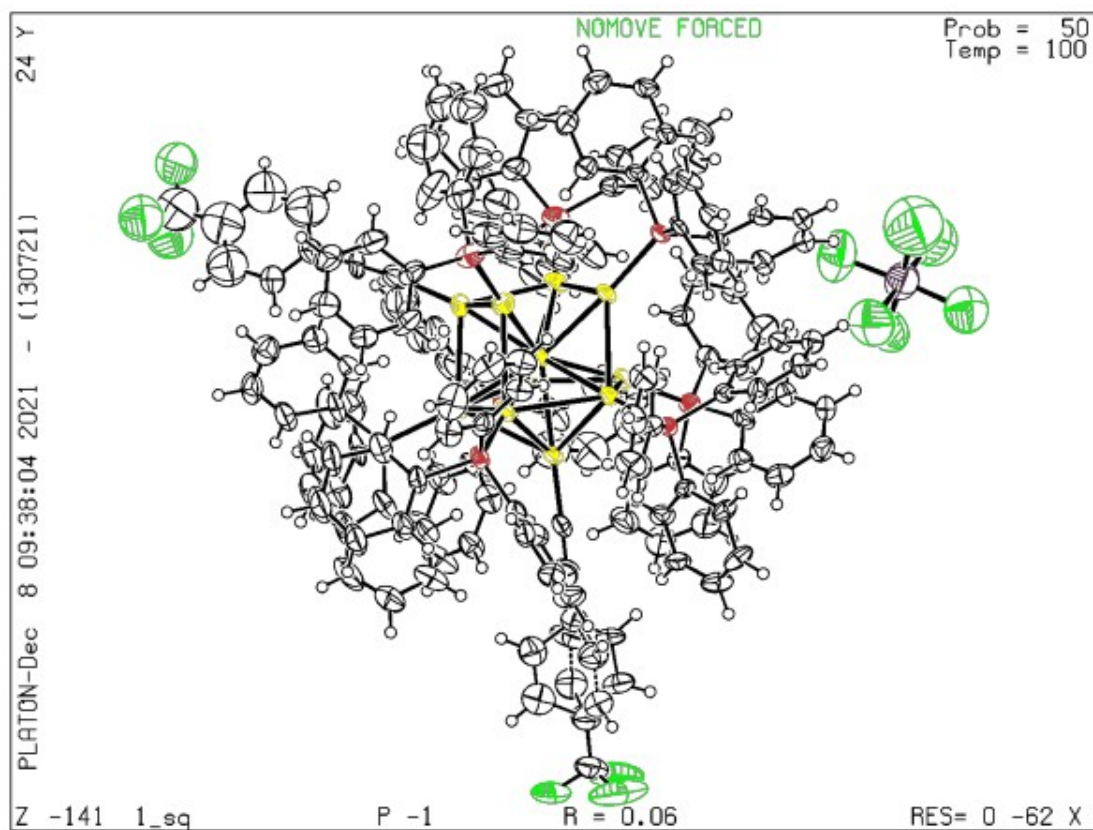


Figure S2 ORTEP diagram of $[\text{Au}_{11}(\text{PPh}_3)_8(\text{C}\equiv\text{CPhCF}_3)_2](\text{SbF}_6)$ (**1**) with the thermal ellipsoids at 50% probability.

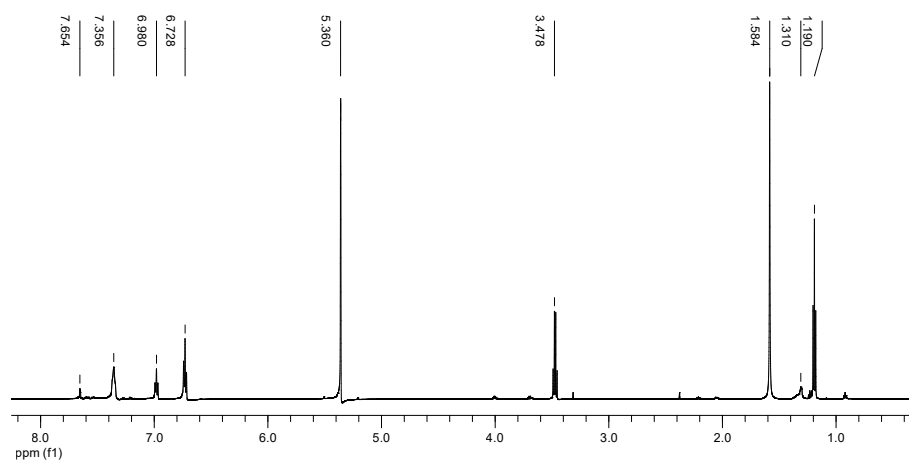


Figure S3 ^1H NMR for the pure triphenylphosphine/alkynyl-stabilized undecagold clusters recorded in CDCl_3 .