

New Ag₈PtO₆: synthesis, crystal structure, physical properties and theoretical analyses

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Table S1. Bond lengths [Å] and angles [°] for Ag₈PtO₆.

Ag(1)-O(1)	2.053(3)
Ag(1)-O(1)#1	2.053(3)
Ag(2)-O(4)#2	2.114(3)
Ag(2)-O(1)	2.153(3)
Ag(3)-O(3)	2.120(3)
Ag(3)-O(5)#3	2.189(3)
Ag(4)-O(3)	2.225(3)
Ag(4)-O(1)#4	2.252(3)
Ag(5)-O(2)#2	2.159(3)
Ag(5)-O(3)	2.191(3)
Ag(6)-O(4)#2	2.171(3)
Ag(6)-O(6)#5	2.198(3)
Ag(7)-O(2)#3	2.137(3)
Ag(7)-O(5)#5	2.161(3)
Ag(8)-O(6)#4	2.155(3)
Ag(8)-O(6)#5	2.155(3)
Ag(9)-O(5)#6	2.170(3)
Ag(9)-O(6)#5	2.176(3)
Pt(1)-O(2)	2.006(3)
Pt(1)-O(4)	2.011(3)
Pt(1)-O(1)	2.021(3)
Pt(1)-O(3)	2.026(3)
Pt(1)-O(6)	2.027(3)
Pt(1)-O(5)	2.033(3)
O(1)-Ag(4)#4	2.252(3)
O(2)-Ag(7)#3	2.137(3)
O(2)-Ag(5)#7	2.159(3)
O(4)-Ag(2)#7	2.114(3)
O(4)-Ag(6)#7	2.171(3)
O(5)-Ag(7)#8	2.161(3)
O(5)-Ag(9)#9	2.170(3)
O(5)-Ag(3)#3	2.189(3)
O(6)-Ag(8)#8	2.155(3)
O(6)-Ag(9)#8	2.176(3)
O(6)-Ag(6)#8	2.198(3)
O(1)-Ag(1)-O(1)#1	180.0
O(4)#2-Ag(2)-O(1)	167.74(11)

O(3)-Ag(3)-O(5)#3	166.42(11)
O(3)-Ag(4)-O(1)#4	154.60(10)
O(2)#2-Ag(5)-O(3)	169.28(11)
O(4)#2-Ag(6)-O(6)#5	163.63(10)
O(2)#3-Ag(7)-O(5)#5	176.93(11)
O(6)#4-Ag(8)-O(6)#5	180.0
O(5)#6-Ag(9)-O(6)#5	165.70(11)
O(2)-Pt(1)-O(4)	94.13(12)
O(2)-Pt(1)-O(1)	174.53(11)
O(4)-Pt(1)-O(1)	82.57(11)
O(2)-Pt(1)-O(3)	90.10(11)
O(4)-Pt(1)-O(3)	86.22(11)
O(1)-Pt(1)-O(3)	85.34(11)
O(2)-Pt(1)-O(6)	94.01(11)
O(4)-Pt(1)-O(6)	94.93(11)
O(1)-Pt(1)-O(6)	90.62(11)
O(3)-Pt(1)-O(6)	175.63(11)
O(2)-Pt(1)-O(5)	89.32(11)
O(4)-Pt(1)-O(5)	176.53(11)
O(1)-Pt(1)-O(5)	93.97(11)
O(3)-Pt(1)-O(5)	93.44(11)
O(6)-Pt(1)-O(5)	85.16(11)
Pt(1)-O(1)-Ag(1)	127.81(14)
Pt(1)-O(1)-Ag(2)	119.46(13)
Ag(1)-O(1)-Ag(2)	89.12(11)
Pt(1)-O(1)-Ag(4)#4	118.41(13)
Ag(1)-O(1)-Ag(4)#4	84.48(10)
Ag(2)-O(1)-Ag(4)#4	110.17(12)
Pt(1)-O(2)-Ag(7)#3	126.06(14)
Pt(1)-O(2)-Ag(5)#7	111.73(13)
Ag(7)#3-O(2)-Ag(5)#7	89.74(10)
Pt(1)-O(3)-Ag(3)	122.14(14)
Pt(1)-O(3)-Ag(5)	114.21(13)
Ag(3)-O(3)-Ag(5)	89.53(11)
Pt(1)-O(3)-Ag(4)	97.15(11)
Ag(3)-O(3)-Ag(4)	120.73(13)
Ag(5)-O(3)-Ag(4)	114.38(12)
Pt(1)-O(4)-Ag(2)#7	114.46(13)
Pt(1)-O(4)-Ag(6)#7	127.45(14)
Ag(2)#7-O(4)-Ag(6)#7	89.95(10)
Pt(1)-O(5)-Ag(7)#8	116.79(13)
Pt(1)-O(5)-Ag(9)#9	115.17(13)
Ag(7)#8-O(5)-Ag(9)#9	118.95(13)
Pt(1)-O(5)-Ag(3)#3	100.14(12)
Ag(7)#8-O(5)-Ag(3)#3	86.96(10)
Ag(9)#9-O(5)-Ag(3)#3	113.01(12)
Pt(1)-O(6)-Ag(8)#8	113.70(13)
Pt(1)-O(6)-Ag(9)#8	114.40(13)
Ag(8)#8-O(6)-Ag(9)#8	99.46(11)
Pt(1)-O(6)-Ag(6)#8	113.19(13)

Ag(8)#8-O(6)-Ag(6)#8 88.53(10)
 Ag(9)#8-O(6)-Ag(6)#8 122.97(13)

Symmetry transformations used to generate equivalent atoms:

1. -x+1,-y,-z+1
2. x-1,y,z
3. -x+1,-y+1,-z
4. x-1,y+1,z
5. -x+1,-y+1,-z+1
6. x,y+1,z
7. x+1,y,z
8. x+1,y-1,z
9. x,y-1,z

Table S2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Ag_8PtO_6 . The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ag(1)	5(1)	4(1)	4(1)	1(1)	0(1)	-2(1)
Ag(2)	5(1)	6(1)	5(1)	0(1)	-1(1)	-1(1)
Ag(3)	8(1)	5(1)	4(1)	0(1)	0(1)	-2(1)
Ag(4)	8(1)	5(1)	5(1)	-1(1)	-1(1)	-1(1)
Ag(5)	5(1)	6(1)	5(1)	0(1)	0(1)	-2(1)
Ag(6)	10(1)	4(1)	5(1)	0(1)	1(1)	-3(1)
Ag(7)	6(1)	6(1)	4(1)	0(1)	0(1)	-2(1)
Ag(8)	6(1)	6(1)	4(1)	1(1)	-1(1)	-1(1)
Ag(9)	5(1)	6(1)	5(1)	0(1)	0(1)	-2(1)
Pt(1)	3(1)	3(1)	2(1)	0(1)	0(1)	-1(1)
O(1)	6(1)	6(1)	3(1)	1(1)	2(1)	-2(1)
O(2)	5(1)	7(1)	6(1)	0(1)	3(1)	-2(1)
O(3)	5(1)	5(1)	6(1)	1(1)	-1(1)	1(1)
O(4)	5(1)	5(1)	6(1)	0(1)	-3(1)	-2(1)
O(5)	7(1)	8(1)	4(1)	-1(1)	1(1)	-4(1)
O(6)	5(1)	4(1)	6(1)	0(1)	0(1)	0(1)

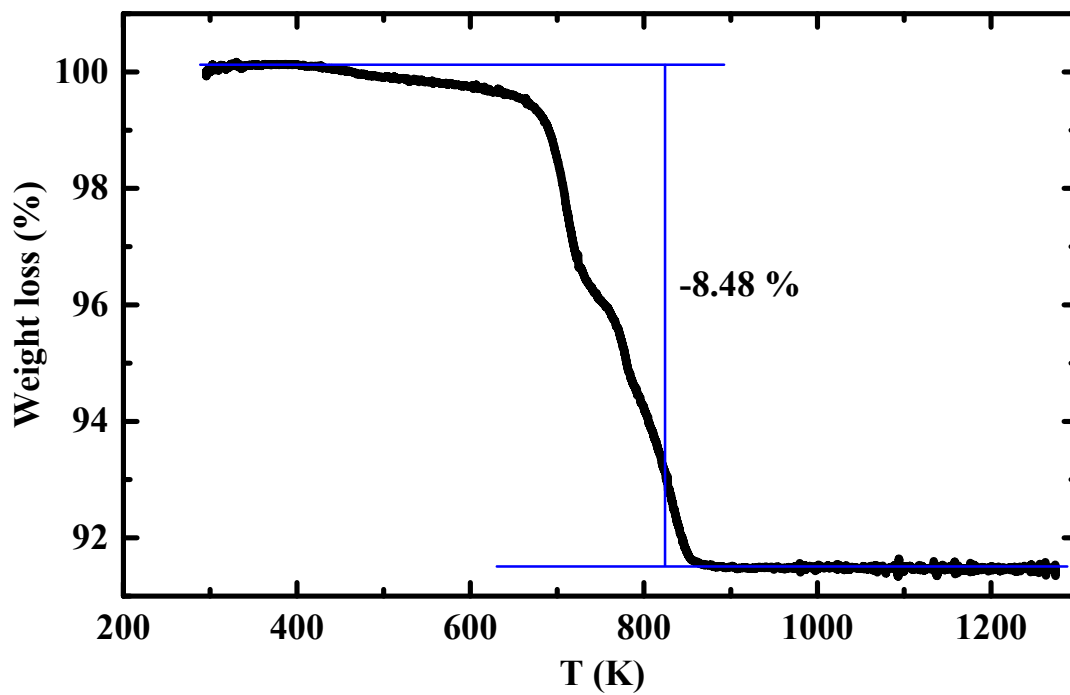


Figure S1. Thermal decomposition profile of Ag_8PtO_6 .