

Layered Structures and Disordered Polyanionic Nets in the Cation-Poor Polar Intermetallics $\text{CsAu}_{1.4}\text{Ga}_{2.8}$ and $\text{CsAu}_2\text{Ga}_{2.6}$

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Supporting information

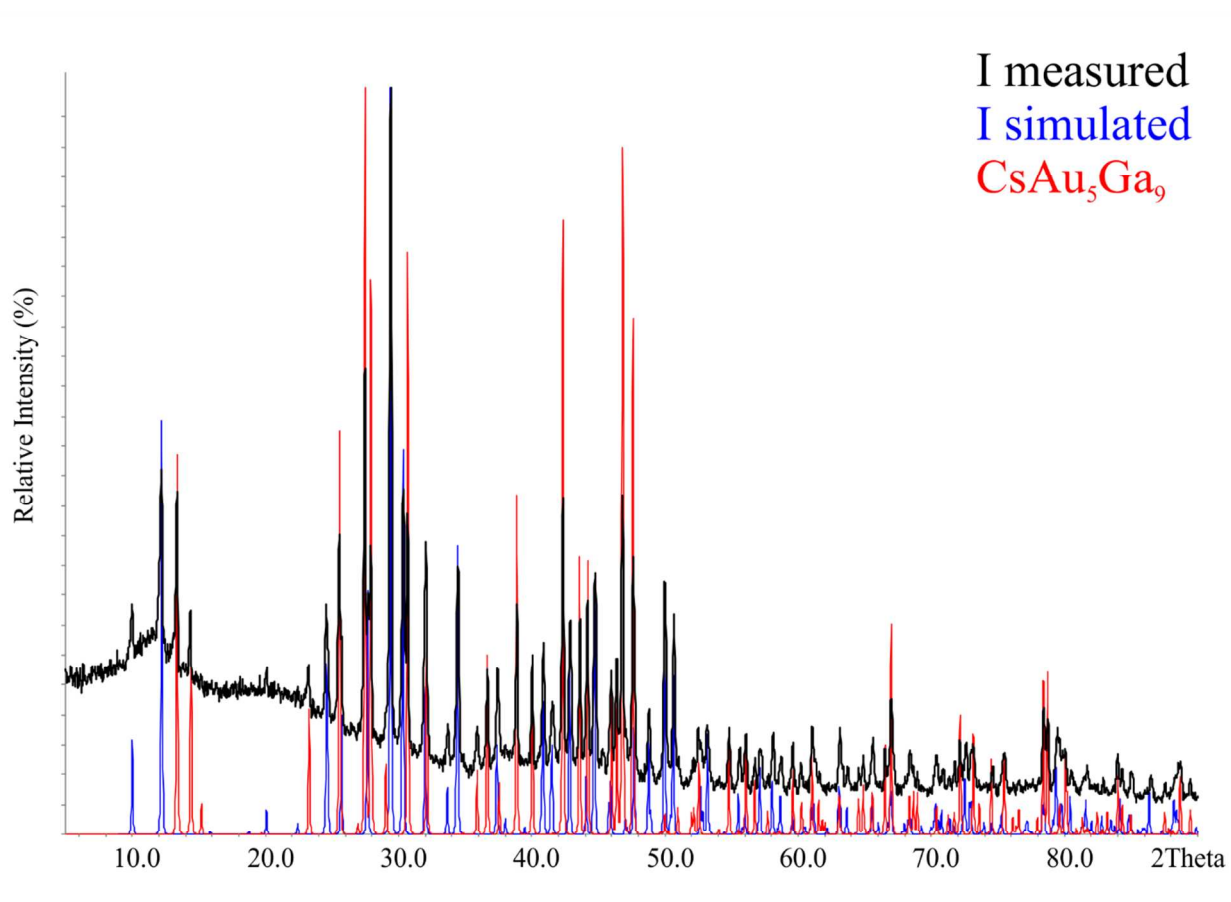


Figure S1. Measured and simulated powder pattern of $\text{CsAu}_{1.41}\text{Ga}_{2.76}$ (**I**) containing CsAu_5Ga_9 as an impurity.

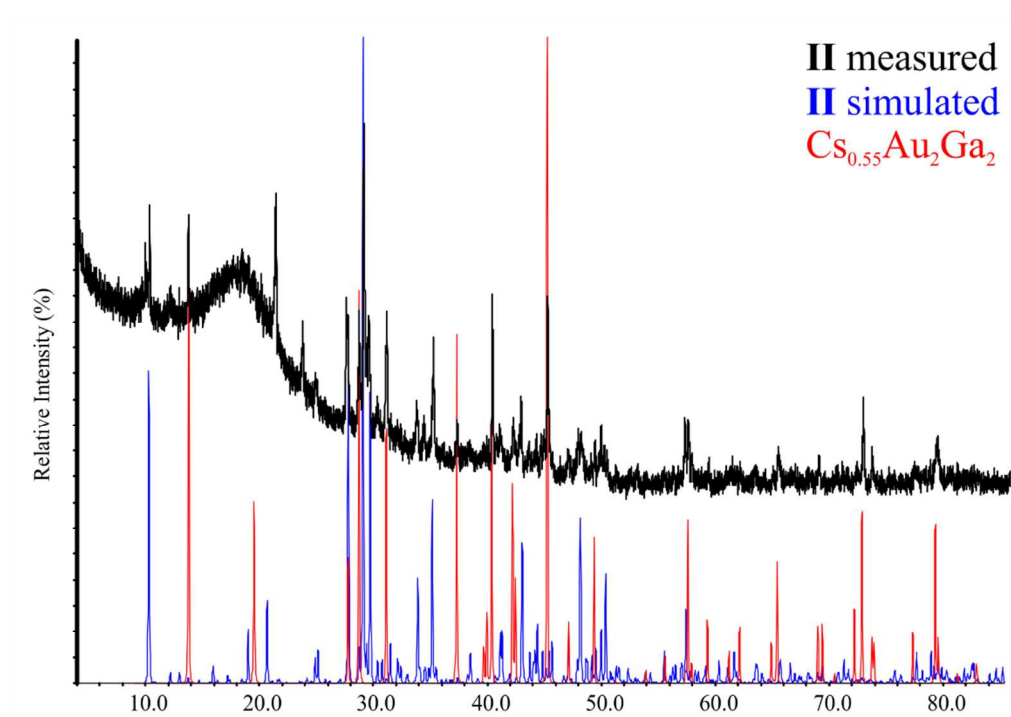


Figure S2. Measured and simulated powder pattern of $\text{CsAu}_{1.99}\text{Ga}_{2.58}$ (II) containing $\text{Cs}_{0.55}\text{Au}_2\text{Ga}_2$ as a main impurity.

Table S1. Anisotropic displacement parameters for CsAu_{1.41}Ga_{2.76} (**I**) and CsAu_{1.99}Ga_{2.58} (**II**).

Position	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I						
Cs1	0.0224(4)	0.0186(4)	0.0207(4)	-0.0012(3)	-0.0054(3)	0.0103(3)
Au1	0.0217(4)	0.0217(4)	0.0125(6)	0	0	0.0109(2)
Au2	0.0194(3)	0.0141(2)	0.0190(3)	-0.0010(2)	-0.0034(2)	0.0034(2)
Au3/Ga3	0.0159(6)	0.0146(6)	0.0333(8)	0.0046(4)	0.0028(4)	0.0058(4)
Ga4	0.0137(7)	0.0137(7)	0.0166(13)	0	0	0.0069(3)
Ga5	0.0139(6)	0.0169(7)	0.0167(7)	0.0000(6)	0.0013(6)	0.0075(6)
Ga6	0.0140(7)	0.0140(7)	0.0135(12)	0	0	0.0070(3)
Ga7	0.0153(7)	0.0153(7)	0.0165(13)	0	0	0.0077(4)
II						
Cs1	0.0249(8)	0.0241(8)	0.0423(11)	-0.0004(8)	0.0020(8)	0.0130(6)
Cs2	0.0275(8)	0.0262(8)	0.0203(8)	0.0026(7)	-0.0031(7)	0.0083(7)
Cs3	0.0209(7)	0.0222(8)	0.0429(11)	-0.0015(7)	-0.0057(8)	0.0128(6)
Au1	0.0202(6)	0.0202(6)	0.0158(9)	0	0	0.0101(3)
Au2	0.0174(9)	0.0174(9)	0.0223(14)	0	0	0.0087(5)
Ga2A	0.0174(9)	0.0174(9)	0.0223(14)	0	0	0.0087(5)
Au3	0.0197(5)	0.0197(5)	0.0164(9)	0	0	0.0099(3)
Au4	0.0196(5)	0.0161(5)	0.0161(6)	0.0007(4)	0.0001(4)	0.0117(4)
Au4A	0.0196(5)	0.0161(5)	0.0161(6)	0.0007(4)	0.0001(4)	0.0117(4)
Au5	0.0126(5)	0.0348(7)	0.0189(6)	-0.0022(5)	0.0007(5)	0.0030(5)
Ga5A	0.0126(5)	0.0348(7)	0.0189(6)	-0.0022(5)	0.0007(5)	0.0030(5)
Au6	0.0184(8)	0.0184(8)	0.0210(11)	0	0	0.0092(4)
Ga6A	0.0184(8)	0.0184(8)	0.0210(11)	0	0	0.0092(4)
Au6B	0.0184(8)	0.0184(8)	0.0210(11)	0	0	0.0092(4)
Ga6C	0.0184(8)	0.0184(8)	0.0210(11)	0	0	0.0092(4)
Au6D	0.0184(8)	0.0184(8)	0.0210(11)	0	0	0.0092(4)
Au7	0.0445(6)	0.0314(6)	0.0381(8)	-0.0046(5)	-0.0068(5)	0.0311(4)
Ga7A	0.0445(6)	0.0314(6)	0.0381(8)	-0.0046(5)	-0.0068(5)	0.0311(4)
Au8	0.022(1)	0.0223(14)	0.0135(19)	0	0	0.0111(7)
Ga8A	0.022(1)	0.0223(14)	0.0135(19)	0	0	0.0111(7)
Ga8B	0.022(1)	0.0223(14)	0.0135(19)	0	0	0.0111(7)
Au9	0.0276(9)	0.0248(9)	0.0146(9)	0.0010(7)	-0.0022(7)	0.0059(7)
Au9A	0.0276(9)	0.0248(9)	0.0146(9)	0.0010(7)	-0.0022(7)	0.0059(7)
Ga9A	0.0276(9)	0.0248(9)	0.0146(9)	0.0010(7)	-0.0022(7)	0.0059(7)
Ga9B	0.0276(9)	0.0248(9)	0.0146(9)	0.0010(7)	-0.0022(7)	0.0059(7)
Au10	0.0202(6)	0.0169(7)	0.026(1)	-0.0020(6)	-0.0005(7)	0.0089(5)
Ga10	0.0202(6)	0.0169(7)	0.026(1)	-0.0020(6)	-0.0005(7)	0.0089(5)
Au11	0.020(1)	0.020(1)	0.035(3)	0	0	0.0098(7)
Au12	0.018(2)	0.018(2)	0.021(3)	0	0	0.0090(8)
Ga12	0.018(2)	0.018(2)	0.021(3)	0	0	0.0090(8)
Au13	0.022(1)	0.020(1)	0.028(2)	0.004(1)	0.006(1)	0.011(1)
Ga13	0.022(1)	0.020(1)	0.028(2)	0.004(1)	0.006(1)	0.011(1)
Au14	0.039(1)	0.045(2)	0.065(2)	-0.032(1)	0.019(1)	-0.005(1)
Ga14	0.039(1)	0.045(2)	0.065(2)	-0.032(1)	0.019(1)	-0.005(1)
Ga1	0.023(2)	0.023(2)	0.014(2)	0	0	0.0116(9)
Ga2	0.010(2)	0.010(2)	0.020(3)	0	0	0.005(1)
Ga3	0.017(1)	0.031(1)	0.024(2)	-0.004(1)	0.0007(12)	0.012(1)

Ga4	0.026(1)	0.030(2)	0.019(2)	-0.001(1)	-0.003(1)	0.023(1)
Ga5	0.045(2)	0.037(2)	0.027(2)	-0.011(1)	-0.015(1)	0.028(1)
Ga6	0.015(1)	0.015(1)	0.021(3)	0	0	0.0076(8)
Ga7	0.019(2)	0.019(2)	0.017(3)	0	0	0.0092(8)
Ga8	0.015(3)	0.015(3)	0.017(4)	0	0	0.008(1)
Ga8C	0.015(3)	0.015(3)	0.017(4)	0	0	0.008(1)

bond	lengths (Å)	–ICOHP (eV/per bond)	bond	lengths (Å)	–ICOHP (eV/per bond)
Au–Ga	2.463	2.13	Ga–Ga	2.601	1.45
Au–Ga	2.633	1.55	Ga–Ga	2.651	1.34
Au–Ga	2.635	1.22	Ga–Ga	2.664	1.34
Au–Ga	2.645	1.33	Ga–Ga	2.611	1.05
Au–Ga	2.650	1.30	Ga–Ga	2.810	0.54
Au–Ga	2.667	1.21	Cs–Ga	3.838	0.004
Cs–Au	3.605	0.026	Cs–Ga	3.846	0.009
Cs–Au	3.636	0.014	Cs–Ga	3.621	0.023

Table S2. Bond length and corresponding –ICOHP values for the selected interatomic contacts in **I**