Electronic Supplementary Information for: 'Pressure Suppression of Charge Order without Metallisation in $Cs_2Au_2I_6$' by Kesmartseva et al

Crystal structure parameters (cell parameters, atomic positions and isotropic U–factors) and the derived Au-I bond distances for $Cs_2Au_2I_6$ from Rietveld fits to the high pressure synchrotron X-ray diffraction data shown in Fig. 1 .

Pressure	0 kbar			47 kbar			89 kbar			89 kbar			120 kbar		
S.G.	*I4/mmm*			*I4/mmm*			*I4/mmm*			*P4/mmm*			*P4/mmm*		
a (Å)	8.2831(6)			7.973(3)			8.003(2)			5.483(1)			5.339(15)		
c (Å)	12.0929(9)			11.577(5)			10.840(3)			5.670(2)			5.517(4)		
Vol./f.u. (Å^3)	207.42(2)			184.0(1)			173.6(1)			170.5(1)			157.3(5)		
	x	y	z	x	Y	z	x	y	z	x	y	z	x	y	Z
Au 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
U_{iso} (Å^2)		0.002(3)			0.003(4)			0.005(4)			0.005(4)			0.01(1)	
Au 2	½	½	0	½	½	0	½	½	0						
U_{iso} (Å^2)		0.002			0.003			0.005							
I 1	0.2276(9)	0.2276(9)	0	0.228(3)	0.228(3)	0	0.230(2)	0.230(2)	0	½	0	0	½	0	0
U_{iso} (Å^2)		0.014(5)			0.004(5)			0.053(10)			0.016(7)			0.00(1)	
I 2	½	½	0.219(2)	½	½	0.218(3)	½	½	0.221(3)	0	0	½	0	0	½
U_{iso} (Å^2)		0.088(9)			0.004			0.053			0.016			0.00	
Cs	0	½	¼	0	½	¼	0	½	¼	½	½	½	½	½	½
U_{iso} (Å^2)		0.043(5)			0.044(10)			0.075(5)			0.075			0.11(1)	

Bond distances (Å)	0 kbar	47 kbar	89 kbar	89 kbar	120 kbar
Au1-I1 x4	2.666(7)	2.57(2)	2.70(6)	2.741(1)	2.670(8)
Au1-I2 x2	3.39(2)	3.25(3)	2.99(9)	2.794(1)	2.759(2)
<Au^{I}-I>	2.907(15)	2.797(36)	2.80(10)		
<Au^{II}-I>				2.758(2)	2.70(1)
Au2-I1 x4	3.191(7)	3.07(2)	2.97(6)		
Au2-I2 x2	2.62(2)	2.54(3)	2.45(9)		
<Au^{III}-I>	3.011(17)	2.893(35)	2.80(10)		