Table S2

New ternary phases from the *R*–Au–Ga systems: interatomic distances and coordination numbers

1) RAu_3Ga_7

R	Gd	Tb	Dy	Ho	Er	Tm	CN
R –							18
– 6Ga2	3.265(2)	3.262(3)	3.250(2)	3.246(2)	3.247(2)	3.241(3)	
– 6Au	3.274(1)	3.271(1)	3.267(1)	3.263(1)	3.258(1)	3.255(1)	
– 6Ga2	3.377(2)	3.359(3)	3.372(3)	3.368(2)	3.370(2)	3.373(2)	
Au –							9
– 2Ga2	2.564(2)	2.562(3)	2.568(3)	2.571(3)	2.566(2)	2.568(3)	
– 1Ga1	2.589(1)	2.584(1)	2.586(1)	2.589(1)	2.594(1)	2.593(1)	
– 2Ga2	2.632(2)	2.616(3)	2.620(3)	2.611(3)	2.612(2)	2.609(3)	
– 2Ga2	2.669(3)	2.680(3)	2.662(3)	2.663(3)	2.657(3)	2.654(3)	
– 2R	3.274(1)	3.271(1)	3.267(1)	3.263(1)	3.258(1)	3.255(1)	
Ga1 –							9
– 3Au	2.589(1)	2.584(1)	2.586(1)	2.589(1)	2.594(1)	2.593(1)	
– 6Ga2	2.903(2)	2.905(3)	2.904(2)	2.905(2)	2.898(2)	2.893(3)	
Ga2 –							10
– 1Au	2.564(3)	2.562(3)	2.568(3)	2.571(3)	2.566(2)	2.568(3)	
– 1Au	2.632(3)	2.616(3)	2.620(3)	2.611(3)	2.612(2)	2.609(3)	

– 1Au	2.669(3)	2.680(3)	2.662(3)	2.663(3)	2.657(3)	2.654(3)
– 1Ga2	2.785(3)	2.762(4)	2.765(4)	2.755(4)	2.766(3)	2.770(4)
– 2Ga2	2.864(2)	2.872(3)	2.859(3)	2.859(3)	2.855(2)	2.842(2)
– 1Ga1	2.903(3)	2.905(3)	2.904(2)	2.905(2)	2.898(2)	2.893(3)
– 1Ga2	2.938(4)	2.962(5)	2.943(5)	2.950(5)	2.932(4)	2.932(5)
– 1R	3.265(3)	3.262(3)	3.250(2)	3.246(2)	3.247(2)	3.241(3)
– 1R	3.377(2)	3.359(3)	3.372(3)	3.368(2)	3.370(2)	3.373(2)

2) $RAu_{3\pm x}Ga_{3\pm x}$

R	Gd	Tb	Dy	Ho	Er	Tm	CN
R –							17
– 2M7	3.102(6)	3.086(6)	3.080(6)	3.054(4)	3.052(6)	3.039(5)	
– 2M5	3.112(6)	3.085(6)	3.095(6)	3.092(5)	3.120(7)	3.069(5)	
– 2M7	3.121(6)	3.100(6)	3.110(6)	3.133(4)	3.113(6)	3.116(6)	
– 2M3	3.122(5)	3.111(6)	3.127(6)	3.113(4)	3.138(6)	3.096(5)	
– 1M5	3.132(10)	3.133(9)	3.158(8)	3.140(7)	3.188(9)	3.139(7)	
– 1M1	3.139(13)	3.152(12)	3.156(10)	3.122(8)	3.035(9)	3.097(13)	
– 2M7	3.183(6)	3.194(7)	3.171(7)	3.158(5)	3.164(7)	3.120(6)	
– 1M4	3.238(7)	3.219(7)	3.184(7)	3.200(5)	3.144(7)	3.159(6)	
– 2M4	3.278(5)	3.261(6)	3.240(6)	3.235(4)	3.216(6)	3.234(4)	
– 1M2	3.318(8)	3.306(8)	3.280(8)	3.306(6)	3.251(8)	3.280(8)	
– 1M6	3.351(16)	3.322(15)	3.363(15)	3.434(14)	3.577(20)	3.498(22)	
M1 –							9

– 1M1	2.526(33)	2.342(27)	2.293(22)	2.461(18)	2.746(20)	2.519(32)	
– 2M5	2.774(22)	2.835(18)	2.853(16)	2.759(13)	2.713(15)	2.690(21)	
– 4M4	2.867(11)	2.838(9)	2.844(8)	2.872(6)	2.956(8)	2.870(11)	
– 2R	3.139(13)	3.152(12)	3.156(10)	3.122(8)	3.035(9)	3.097(13)	
M2 –							10
– 2M4	2.600(13)	2.590(11)	2.591(10)	2.596(8)	2.590(10)	2.581(8)	
– 2M4	2.625(10)	2.613(8)	2.609(8)	2.610(6)	2.606(8)	2.592(12)	
– 4M7	2.903(4)	2.912(4)	2.904(4)	2.882(3)	2.893(4)	2.910(4)	
– 2R	3.318(8)	3.306(8)	3.280(8)	3.306(6)	3.251(8)	3.280(8)	
M3 –							10
– 1M6	2.739(10)	2.738(10)	2.735(9)	2.781(9)	2.810(12)	2.776(14)	
– 3M5	2.770(7)	2.772(6)	2.768(6)	2.785(4)	2.772(6)	2.758(6)	
– 3M7	2.802(6)	2.764(6)	2.759(6)	2.763(4)	2.710(6)	2.752(6)	
– 3R	3.122(5)	3.111(6)	3.127(6)	3.113(4)	3.138(6)	3.096(5)	
M4 –							12
– 1M2	2.600(13)	2.590(11)	2.591(10)	2.596(8)	2.590(10)	2.581(8)	
– 1M2	2.625(10)	2.613(8)	2.609(8)	2.610(6)	2.606(8)	2.592(12)	
– 2M7	2.797(6)	2.782(5)	2.793(5)	2.800(4)	2.786(5)	2.801(5)	
– 2M1	2.867(11)	2.838(9)	2.844(8)	2.872(6)	2.956(8)	2.870(11)	
– 1M4	2.875(8)	2.904(6)	2.927(6)	2.865(4)	2.942(6)	2.887(6)	
– 2M7	2.946(6)	2.929(6)	2.894(6)	2.867(4)	2.865(6)	2.875(6)	
– 1R	3.238(7)	3.219(7)	3.184(7)	3.200(5)	3.144(7)	3.159(6)	
– 2R	3.278(5)	3.261(6)	3.240(6)	3.235(4)	3.216(6)	3.234(4)	
M5 –							10

– 1M6	2.632(15)/ 2.708(18)	2.645(14)/ 2.662(18)	2.644(16)/ 2.656(13)	2.632(16)/ 2.771(13)	2.226(22)/ 2.977(19)	2.726(20)/ 2.763(24)	
– 2M7	2.667(8)	2.673(8)	2.664(7)	2.665(6)	2.736(8)	2.669(7)	
– 1M5	2.753(12)	2.744(10)	2.724(8)	2.730(8)	2.636(10)	2.671(8)	
– 2M3	2.770(7)	2.772(6)	2.768(6)	2.785(4)	2.772(6)	2.758(6)	
– 1M1	2.774(22)	2.835(18)	2.853(16)	2.759(13)	2.713(15)	2.690(21)	
– 2R	3.112(6)	3.085(6)	3.095(6)	3.092(5)	3.120(7)	3.069(5)	
– 1R	3.132(10)	3.133(9)	3.158(8)	3.140(7)	3.188(9)	3.139(7)	
M6 –							6
– 2M5	2.632(15)	2.645(14)	2.656(13)	2.771(13)	2.977(19)	2.726(20)	
– 1M5	2.708(18)	2.662(18)	2.644(16)	2.632(16)	2.226(22)	2.763(24)	
– 2M3	2.739(10)	2.738(10)	2.735(9)	2.781(9)	2.810(12)	2.776(14)	
– 1R	3.351(16)	3.322(15)	3.363(15)	3.434(14)	3.577(20)	3.498(22)	
M7 –							10
– 1M5	2.667(8)	2.673(8)	2.664(7)	2.665(6)	2.736(8)	2.669(7)	
– 2M7	2.762(7)	2.712(7)	2.729(7)	2.718(5)	2.726(7)	2.657(7)	
– 1M4	2.797(6)	2.782(5)	2.894(6)	2.800(4)	2.786(5)	2.801(5)	
– 1M3	2.802(6)	2.764(6)	2.759(6)	2.763(4)	2.710(6)	2.752(6)	
– 1M2	2.903(4)	2.912(4)	2.904(4)	2.882(3)	2.893(4)	2.910(4)	
– 1M4	2.946(6)	2.782(5)	2.894(6)	2.867(4)	2.865(6)	2.875(6)	
– 1R	3.102(6)	3.086(6)	3.080(6)	3.054(4)	3.052(6)	3.039(5)	
– 1R	3.121(6)	3.100(6)	3.110(6)	3.133(4)	3.113(6)	3.116(6)	
– 1R	3.183(6)	3.194(7)	3.171(7)	3.158(5)	3.164(7)	3.120(6)	

3) $R_{14}Au_{34+x}Ga_{17-x}$

R		Er	Tm	CN
R1 –				16
	– 6M6	3.079(3)	3.071(5)	
	– 6M4	3.141(7)	3.156(9)	
	– 3M3	3.160(10)	3.126(14)	
	– 1R1	3.536(14)	3.592(19)	
R2 –				14
	– 1M3	2.771(14)	2.755(20)	
	– 2M6	3.025(7)	3.000(10)	
	– 2M5	3.051(7)	3.035(11)	
	– 1M1	3.082(5)	3.094(6)	
	– 2M7	3.137(4)	3.121(5)	
	– 2M5	3.146(6)	3.129(8)	
	– 2M6	3.152(4)	3.122(7)	
	– 2M5	3.160(7)	3.168(10)	
R3 –				15
	– 2M7	2.961(7)	2.962(10)	
	– 2M7	3.007(7)	2.991(10)	
	– 2M7	3.034(6)	3.035(8)	
	– 2M2	3.101(7)	3.131(10)	
	– 1M4	3.150(10)	3.177(8)	
	– 1M4	3.180(5)	3.195(14)	
	– 2M5	3.211(5)	3.220(7)	

– 2M6	3.243(5)	3.268(9)	
– 1R3	3.783(12)	3.651(16)	
M1 –			11
– 2M2	2.668(10)	2.605(14)	
– 6M5	2.875(3)	2.853(7)	
– 3R2	3.082(5)	3.094(8)	
M2 –			10
– 1M1	2.668(10)	2.605(14)	
– 3M7	2.736(2)	2.713(4)	
– 3M5	2.860(6)	2.822(8)	
– 3R3	3.101(7)	3.131(10)	
M3 –			9
– 2M3	2.693(11)	2.638(16)	
– 2M6	2.757(12)	2.765(12)	
– 1R2	2.771(14)	2.755(20)	
– 2M6	2.781(8)	2.783(19)	
– 2R1	3.160(11)	3.126(15)	
M4 –			12
– 2M4	2.596(5)	2.596(8)	
– 2M7	2.782(6)	2.779(9)	
– 2M6	2.843(5)	2.849(8)	
– 2M6	2.892(5)	2.904(8)	
– 2R1	3.141(8)	3.156(11)	
– 1R3	3.150(5)	3.177(15)	

	– 1R3	3.180(10)	3.195(8)
M5 –			11
	– 1M6	2.611(6)	2.589(10)
	– 1M5	2.701(6)	2.672(10)
	– 1M7	2.771(5)	2.769(8)
	– 1M5	2.824(6)	2.834(11)
	– 1M2	2.860(6)	2.822(8)
	– 1M1	2.875(3)	2.853(5)
	– 1M7	3.004(4)	3.017(7)
	– 1R2	3.051(4)	3.035(7)
	– 1R2	3.146(6)	3.129(10)
	– 1R2	3.160(5)	3.168(9)
	– 1R3	3.211(5)	3.220(7)
M6 –			12
	– 1M5	2.611(6)	2.589(10)
	– 1M3	2.757(4)/ 2.781(9)	2.765(14)/ 2.783(7)
	– 1M4	2.843(4)	2.849(7)
	– 1M4	2.892(5)	2.904(7)
	– 1M7	2.928(5)	2.923(9)
	– 2M6	3.004(3)	3.000(5)
	– 1M7	3.011(3)	2.978(5)
	– 1R2	3.025(3)	3.000(6)
	– 1R1	3.079(4)	3.071(7)
	– 1R2	3.152(6)	3.122(9)
	– 1R3	3.243(5)	3.268(9)

M7 –			11
	– 1M2	2.736(2)	2.713(4)
	– 1M5	2.771(4)	2.769(7)
	– 1M4	2.782(6)	2.779(9)
	– 1M7	2.914(5)	2.965(6)
	– 1M6	2.928(3)	2.923(5)
	– 1R3	2.961(4)	2.962(6)
	– 1M5	3.004(5)	3.016(8)
	– 1R3	3.007(4)	2.991(6)
	– 1M6	3.011(5)	2.978(8)
	– 1R3	3.034(6)	3.035(9)
	– 1R2	3.137(4)	3.121(5)

4) $RAu_{1+x}Ga_{2-x}$

R	Gd	Tb	Dy	Ho	Er	Tm	CN
R –							17
– 1M1	3.025(3)	3.006(3)	2.994(3)	2.971(3)	2.980(4)	2.970(3)	
– 4M2	3.033(2)	3.024(1)	3.013(2)	3.008(1)	2.989(2)	3.006(2)	
– 2M1	3.100(2)	3.090(2)	3.082(2)	3.083(2)	3.062(3)	3.054(2)	
– 2M2	3.276(3)	3.267(3)	3.263(3)	3.273(3)	3.271(4)	3.261(3)	
– 4M2	3.384(2)	3.369(2)	3.358(2)	3.342(2)	3.333(3)	3.312(2)	
– 2M1	3.527(1)	3.524(1)	3.524(1)	3.532(1)	3.518(1)	3.541(1)	
– 2R	3.818(1)	3.807(1)	3.797(1)	3.787(1)	3.783(2)	3.769(1)	
M1 –							9
– 2M2	2.729(3)	2.722(2)	2.710(3)	2.710(2)	2.698(3)	2.693(3)	
– 4M2	2.745(2)	2.732(1)	2.726(2)	2.721(1)	2.723(2)	2.706(2)	
– 1R	3.025(3)	3.006(3)	2.994(3)	2.971(3)	2.980(4)	2.970(3)	
– 2R	3.100(2)	3.090(2)	3.082(2)	3.083(2)	3.062(3)	3.054(2)	
M2 –							10
– 1M2	2.552(3)	2.549(3)	2.544(3)	2.533(3)	2.493(4)	2.534(3)	
– 1M2	2.631(4)	2.631(3)	2.640(4)	2.651(3)	2.659(5)	2.621(4)	
– 1M1	2.729(3)	2.722(2)	2.710(3)	2.710(2)	2.698(3)	2.693(3)	
– 2M1	2.745(2)	2.732(1)	2.726(2)	2.721(1)	2.723(2)	2.706(2)	
– 2R	3.033(2)	3.024(1)	3.013(2)	3.008(1)	2.989(2)	3.006(2)	
– 1R	3.276(3)	3.267(3)	3.263(3)	3.273(3)	3.271(4)	3.261(3)	
– 2R	3.384(2)	3.369(2)	3.358(2)	3.342(2)	3.333(3)	3.312(2)	

5) $RAu_{1+x}Ga_{3-x}$ and $R_3Au_{3+x}Ga_{8-x}$

$GdAuGa_3$

R		Gd	CN
R –			16
	– 8M2	3.200(1)	
	– 8M1	3.465(1)	
M1 –			12
	– 4M2	2.590(1)	
	– 4M1	2.953(1)	
	– 4R	3.465(1)	
M2 –			9
	– 1M2	2.465(3)	
	– 4M1	2.590(1)	
	– 4R	3.200(1)	

$R_3Au_{3+x}Ga_{8-x}$

R	Tb	Dy	Ho	Er	Tm	CN
R1 –						20
– 8M4	3.210(2)	3.210(2)	3.203(2)	3.194(2)	3.171(2)	
– 4M3	3.283(4)	3.252(5)	3.269(4)	3.270(5)	3.306(5)	
– 4M2	3.559(3)	3.548(3)	3.539(3)	3.559(3)	3.556(3)	
– 2R2	3.967(2)	3.939(2)	3.915(4)	3.908(4)	3.873(4)	
– 2R1	4.244(1)	4.232(1)	4.223(1)	4.210(1)	4.202(1)	
R2 –						19
– 2M1	3.110(2)	3.111(2)	3.116(3)	3.101(3)	3.121(3)	
– 2M2	3.124(3)	3.129(3)	3.139(4)	3.105(4)	3.121(4)	
– 4M3	3.132(3)	3.139(4)	3.116(3)	3.107(4)	3.078(4)	
– 4M4	3.166(2)	3.146(2)	3.137(3)	3.137(3)	3.107(3)	
– 2M3	3.495(4)	3.492(5)	3.503(5)	3.488(5)	3.476(5)	
– 2M4	3.694(2)	3.683(2)	3.671(2)	3.660(2)	3.685(2)	
– 1R1	3.967(2)	3.939(2)	3.915(4)	3.908(4)	3.873(4)	
– 2R2	4.244(1)	4.232(0)	4.223(1)	4.210(1)	4.202(1)	
M1 –						12
– 4M3	2.886(4)	2.867(5)	2.836(4)	2.842(5)	2.826(5)	
– 4M2	3.015(3)	3.012(3)	3.010(3)	2.981(3)	2.972(3)	
– 4R2	3.110(2)	3.111(2)	3.116(3)	3.101(3)	3.121(3)	
M2 –						12
– 2M4	2.541(3)	2.535(3)	2.517(3)	2.524(4)	2.534(4)	
– 4M3	2.787(2)	2.757(3)	2.747(2)	2.750(3)	2.760(3)	

– 2M1	3.015(3)	3.012(3)	3.010(3)	2.981(3)	2.972(3)	
– 2R2	3.124(3)	3.129(3)	3.139(4)	3.105(4)	3.121(4)	
– 2R1	3.559(3)	3.548(3)	3.539(3)	3.559(3)	3.556(3)	
M3 –						13
– 2M4	2.568(3)	2.558(3)	2.564(3)	2.552(3)	2.579(3)	
– 1M4	2.597(4)	2.610(6)	2.602(4)	2.581(6)	2.563(6)	
– 2M2	2.787(2)	2.757(3)	2.747(2)	2.750(3)	2.760(3)	
– 1M1	2.886(4)	2.867(5)	2.836(4)	2.842(5)	2.826(5)	
– 2R2	3.132(3)	3.139(4)	3.116(3)	3.107(4)	3.078(4)	
– 1R1	3.283(4)	3.252(5)	3.269(4)	3.270(5)	3.306(5)	
– 2M3	3.419(4)	3.456(6)	3.465(4)	3.429(6)	3.399(5)	
– 1R2	3.495(4)	3.492(5)	3.503(5)	3.488(5)	3.476(5)	
– 1M3	3.605(5)	3.528(7)	3.510(5)	3.531(7)	3.575(7)	
M4 –						9
– 1M2	2.541(3)	2.535(3)	2.517(3)	2.524(4)	2.534(4)	
– 2M3	2.568(3)	2.558(3)	2.564(3)	2.552(3)	2.579(3)	
– 1M3	2.597(4)	2.610(6)	2.602(4)	2.581(6)	2.563(6)	
– 1M4	2.627(3)	2.636(2)	2.650(3)	2.659(3)	2.598(3)	
– 2R2	3.166(2)	3.146(2)	3.137(3)	3.137(3)	3.107(3)	
– 2R1	3.210(2)	3.210(2)	3.203(2)	3.194(2)	3.171(2)	