

Table S1

**New ternary phases from the *R*–Au–Ga systems:
atom coordinates, isotropic displacement parameters and occupancies**

1) RAu₃Ga₇**GdAu₃Ga₇**

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Gd	6 <i>b</i>	0	0	0	0.94(7)	1Gd
Au	18 <i>e</i>	0.31803(14)	0	1/4	0.95(3)	1Au
Ga1	6 <i>a</i>	0	0	1/4	1.27(14)	1Ga
Ga2	36 <i>f</i>	0.0120(4)	0.2089(3)	0.13533(12)	1.11(5)	1Ga

Refinement composition: GdAu₃Ga₇. Reliability factors: *R*_B = 5.12 %, *R*_F = 3.83 %.

TbAu₃Ga₇

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Tb	6 <i>b</i>	0	0	0	1.08(8)	1Tb
Au	18 <i>e</i>	0.31779(17)	0	1/4	1.07(3)	1Au
Ga1	6 <i>a</i>	0	0	1/4	1.32(16)	1Ga
Ga2	36 <i>f</i>	0.0143(5)	0.2107(4)	0.13521(14)	1.00(6)	1Ga

Refinement composition: TbAu₃Ga₇. Reliability factors: *R*_B = 6.84 %, *R*_F = 4.70 %.

DyAu₃Ga₇

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Dy	6 <i>b</i>	0	0	0	1.01(8)	1Dy
Au	18 <i>e</i>	0.31834(17)	0	1/4	0.99(3)	1Au
Ga1	6 <i>a</i>	0	0	1/4	1.22(16)	1Ga
Ga2	36 <i>f</i>	0.0122(5)	0.2090(4)	0.13489(13)	0.97(6)	1Ga

Refinement composition: DyAu₃Ga₇. Reliability factors: *R*_B = 6.30 %, *R*_F = 3.45 %.

HoAu₃Ga₇

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Ho	6 <i>b</i>	0	0	0	1.21(9)	1Ho
Au	18 <i>e</i>	0.31883(16)	0	1/4	0.95(3)	1Au
Ga1	6 <i>a</i>	0	0	1/4	1.29(15)	1Ga
Ga2	36 <i>f</i>	0.0127(4)	0.2093(4)	0.13474(13)	0.95(6)	1Ga

Refinement composition: HoAu₃Ga₇. Reliability factors: *R*_B = 6.13 %, *R*_F = 3.45 %.

ErAu₃Ga₇

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Er	6 <i>b</i>	0	0	0	1.13(7)	1Er
Au	18 <i>e</i>	0.31960(16)	0	1/4	0.99(3)	1Au
Ga1	6 <i>a</i>	0	0	1/4	1.12(14)	1Ga
Ga2	36 <i>f</i>	0.0117(4)	0.2087(3)	0.13499(12)	0.97(6)	1Ga

Refinement composition: ErAu₃Ga₇. Reliability factors: *R*_B = 4.89 %, *R*_F = 3.54 %.

2) RAu_{3±x}Ga_{3±x}

GdAu_{3±x}Ga_{3±x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Gd	24 <i>g</i>	0	0.1845(3)	0.3008(3)	1.00(10)	1Gd
M1	12 <i>d</i>	0.4131(16)	0	0	1.28(6)	1Ga
M2	12 <i>e</i>	0.2040(10)	0	1/2	1.28(6)	0.055(13)Au+0.945(13)Ga
M3	16 <i>f</i>	0.1555(3)	0.1555(3)	0.1555(3)	1.28(6)	0.38(2)Au+0.62(2)Ga
M4	24 <i>g</i>	0	0.4011(4)	0.3531(3)	1.28(6)	1Au
M5	24 <i>g</i>	0	0.2474(6)	0.0947(6)	1.28(6)	0.524(16)Au+0.476(16)Ga
M6	24 <i>g</i>	0	0.0614(11)	0.1058(10)	1.28(6)	0.274(16)Au+0.059(16)Ga
M7	48 <i>h</i>	0.1184(3)	0.3392(3)	0.2007(4)	1.28(6)	0.456(9)Au+0.544(9)Ga

Refinement composition: GdAu_{2.99}Ga_{3.01}. Reliability factors: *R*_B = 8.29 %, *R*_F = 7.36 %.

TbAu_{3±x}Ga_{3±x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Tb	24 <i>g</i>	0	0.1832(4)	0.3014(4)	1.00(13)	1Tb
M1	12 <i>d</i>	0.4191(13)	0	0	1.21(5)	1Ga
M2	12 <i>e</i>	0.2040(8)	0	1/2	1.21(5)	0.093(12)Au+0.907(12)Ga
M3	16 <i>f</i>	0.1567(3)	0.1567(3)	0.1567(3)	1.21(5)	0.394(17)Au+0.606(17)Ga
M4	24 <i>g</i>	0	0.3997(3)	0.3522(3)	1.21(5)	1Au
M5	24 <i>g</i>	0	0.2477(6)	0.0948(5)	1.21(5)	0.573(13)Au+0.427(13)Ga
M6	24 <i>g</i>	0	0.0641(11)	0.1052(9)	1.21(5)	0.243(13)Au+0.090(13)Ga
M7	48 <i>h</i>	0.1203(3)	0.3388(3)	0.2013(4)	1.21(5)	0.430(8)Au+0.570(8)Ga

Refinement composition: TbAu_{2.98}Ga_{3.02}. Reliability factors: *R*_B = 7.36 %, *R*_F = 6.61 %.

DyAu_{3±x}Ga_{3±x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Dy	24 <i>g</i>	0	0.1839(4)	0.3032(4)	1.00(10)	1Dy
M1	12 <i>d</i>	0.4207(11)	0	0	1.18(5)	0.065(15)Au+0.935(15)Ga
M2	12 <i>e</i>	0.2033(8)	0	1/2	1.18(5)	0.094(12)Au+0.906(12)Ga
M3	16 <i>f</i>	0.1566(3)	0.1566(3)	0.1566(3)	1.18(5)	0.450(17)Au+0.550(17)Ga
M4	24 <i>g</i>	0	0.3988(3)	0.3512(3)	1.18(5)	1Au
M5	24 <i>g</i>	0	0.2473(5)	0.0942(4)	1.18(5)	0.569(12)Au+0.431(12)Ga
M6	24 <i>g</i>	0	0.0647(10)	0.1035(9)	1.18(5)	0.243(12)Au+0.090(12)Ga
M7	48 <i>h</i>	0.1187(3)	0.3380(3)	0.2020(4)	1.18(5)	0.446(8)Au+0.554(8)Ga

Refinement composition: DyAu_{3.08}Ga_{2.92}. Reliability factors: *R*_B = 8.58 %, *R*_F = 7.73 %.

HoAu_{3±x}Ga_{3±x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Ho	24 <i>g</i>	0	0.1845(3)	0.3022(3)	0.93(8)	1Ho
M1	12 <i>d</i>	0.4148(9)	0	0	1.02(3)	0.066(12)Au+0.934(12)Ga
M2	12 <i>e</i>	0.2003(6)	0	1/2	1.02(3)	0.119(9)Au+0.881(9)Ga
M3	16 <i>f</i>	0.1578(2)	0.1578(2)	0.1578(2)	1.02(3)	0.410(13)Au+0.590(12)Ga
M4	24 <i>g</i>	0	0.4008(2)	0.3502(2)	1.02(3)	1Au
M5	24 <i>g</i>	0	0.2488(4)	0.0945(4)	1.02(3)	0.516(10)Au+0.484(10)Ga
M6	24 <i>g</i>	0	0.0666(10)	0.0957(9)	1.02(3)	0.162(9)Au+0.171(9)Ga
M7	48 <i>h</i>	0.1184(2)	0.3394(2)	0.2032(3)	1.02(3)	0.506(7)Au+0.494(7)Ga

Refinement composition: HoAu_{3.06}Ga_{2.94}. Reliability factors: *R*_B = 6.07 %, *R*_F = 7.83 %.

ErAu_{3±x}Ga_{3±x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Er	24 <i>g</i>	0	0.1850(4)	0.3050(4)	0.51(11)	1Er
M1	12 <i>d</i>	0.4049(10)	0	0	1.06(5)	0.35(2)Au+0.65(2)Ga
M2	12 <i>e</i>	0.2023(8)	0	1/2	1.06(5)	0.148(13)Au+0.852(13)Ga
M3	16 <i>f</i>	0.1602(3)	0.1602(3)	0.1602(3)	1.06(5)	0.484(18)Au+0.516(18)Ga
M4	24 <i>g</i>	0	0.3981(3)	0.3500(3)	1.06(5)	1Au
M5	24 <i>g</i>	0	0.2406(6)	0.0913(5)	1.06(5)	0.605(17)Au+0.395(17)Ga
M6	24 <i>g</i>	0	0.0870(14)	0.0774(13)	1.06(5)	0.215(13)Au+0.118(13)Ga
M7	48 <i>h</i>	0.1184(3)	0.3383(3)	0.2024(4)	1.06(5)	0.511(11)Au+0.489(11)Ga

Refinement composition: ErAu_{3.41}Ga_{2.59}. Reliability factors: *R*_B = 8.73 %, *R*_F = 10.9 %.

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

$Er_{14}Au_{34+x}Ga_{17-x}$						
Atom	Site	x	y	z	$B_{iso} (\text{\AA}^2)$	Occupation G
Er1	2e	0	0	0.3044(11)	0.74(8)	1Er
Er2	6j	0.1187(5)	0.3934(5)	0	0.74(8)	1Er
Er3	6k	0.4653(5)	0.1326(6)	1/2	0.74(8)	1Er
M1	2c	1/3	2/3	0	1.06(4)	0.91(2)Au+0.09(2)Ga
M2	4h	1/3	2/3	0.2951(11)	1.06(4)	0.250(17)Au+0.750(17)Ga
M3	6j	0.0365(13)	0.1399(10)	0	1.06(4)	0.228(13)Au+0.272(13)Ga
M4	6k	0.0601(5)	0.2334(5)	1/2	1.06(4)	0.501(16)Au+0.499(16)Ga
M5	12l	0.4894(3)	0.1085(3)	0.1494(5)	1.06(4)	0.524(11)Au+0.476(11)Ga
M6	12l	0.2704(3)	0.0708(3)	0.2298(4)	1.06(4)	0.746(12)Au+0.254(12)Ga
M7	12l	0.1156(2)	0.4466(2)	0.3388(4)	1.06(4)	0.969(13)Au+0.031(13)Ga

Refinement composition: $Er_{14}Au_{34.1}Ga_{16.9}$. Reliability factors: $R_B = 6.80\%$, $R_F = 5.02\%$.

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

$GdAu_{1+x}Ga_{2-x}$						
Atom	Site	x	y	z	$B_{iso} (\text{\AA}^2)$	Occupation G
Gd	4c	0	0.4096(2)	1/4	1.30(9)	1Gd
M1	4c	0	0.70278(19)	1/4	0.77(8)	0.816(12)Au+0.184(12)Ga
M2	8f	0	0.1189(2)	0.0525(4)	1.03(11)	0.180(8)Au+0.820(8)Ga

Refinement composition: $GdAu_{1.18}Ga_{1.82}$. Reliability factors: $R_B = 5.76\%$, $R_F = 3.22\%$.

$TbAu_{1+x}Ga_{2-x}$						
Atom	Site	x	y	z	$B_{iso} (\text{\AA}^2)$	Occupation G
Tb	4c	0	0.4101(2)	1/4	1.20(8)	1Tb
M1	4c	0	0.70255(16)	1/4	0.84(7)	0.840(11)Au+0.160(11)Ga
M2	8f	0	0.11923(19)	0.0524(3)	1.02(9)	0.216(8)Au+0.784(8)Ga

Refinement composition: $TbAu_{1.27}Ga_{1.73}$. Reliability factors: $R_B = 7.77\%$, $R_F = 3.74\%$.

DyAu_{1+x}Ga_{2-x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Dy	4 <i>c</i>	0	0.4107(2)	1/4	1.29(9)	1Dy
M1	4 <i>c</i>	0	0.70280(19)	1/4	0.94(7)	0.819(13)Au+0.181(13)Ga
M2	8 <i>f</i>	0	0.1195(2)	0.0516(4)	0.75(11)	0.173(9)Au+0.827(9)Ga

Refinement composition: DyAu_{1.17}Ga_{1.83}. Reliability factors: *R*_B = 7.90 %, *R*_F = 3.84 %.

HoAu_{1+x}Ga_{2-x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Ho	4 <i>c</i>	0	0.4120(2)	1/4	1.30(10)	1Ho
M1	4 <i>c</i>	0	0.70258(16)	1/4	0.76(7)	0.875(10)Au+0.125(10)Ga
M2	8 <i>f</i>	0	0.11931(19)	0.0511(3)	0.78(10)	0.254(8)Au+0.746(8)Ga

Refinement composition: HoAu_{1.38}Ga_{1.62}. Reliability factors: *R*_B = 6.25 %, *R*_F = 3.55 %.

ErAu_{1+x}Ga_{2-x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Er	4 <i>c</i>	0	0.4110(3)	1/4	1.02(13)	1Er
M1	4 <i>c</i>	0	0.7033(2)	1/4	0.96(10)	0.870(17)Au+0.130(17)Ga
M2	8 <i>f</i>	0	0.1179(3)	0.0497(5)	1.01(16)	0.158(12)Au+0.842(12)Ga

Refinement composition: ErAu_{1.18}Ga_{1.82}. Reliability factors: *R*_B = 8.67 %, *R*_F = 4.95 %.

5) RAu_{1+x}Ga_{3-x} and R₃Au_{3+x}Ga_{8-x}**GdAu_{1+x}Ga_{3-x}**

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Gd	2 <i>a</i>	0	0	0	1.07(7)	1Gd
M1	4 <i>d</i>	0	1/2	1/4	1.21(7)	0.105(4)Au+0.895(4)Ga
M2	4 <i>e</i>	0	0	0.38854(16)	0.89(5)	0.466(6)Au+0.534(6)Ga

Refinement composition: GaAu_{1.14}Ga_{2.86}. Reliability factors: *R*_B = 6.42 %, *R*_F = 4.08 %.

Tb₃Au_{3+x}Ga_{8-x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Tb1	2 <i>a</i>	0	0	0	0.89(13)	1Tb
Tb2	4 <i>i</i>	0	0	0.3178(2)	0.53(9)	1Tb
M1	2 <i>d</i>	1/2	0	1/2	1.41(23)	1Ga
M2	4 <i>h</i>	0	0.2142(4)	1/2	0.93(14)	0.391(10)Au+0.609(10)Ga
M3	8 <i>l</i>	0	0.2745(4)	0.1444(3)	0.75(10)	1Ga
M4	8 <i>l</i>	0	0.3686(2)	0.3383(2)	1.49(8)	0.484(14)Au+0.516(14)Ga

Refinement composition: Tb₃Au_{2.72}Ga_{8.28}. Reliability factors: *R*_B = 6.49 %, *R*_F = 5.38 %.

Dy₃Au_{3+x}Ga_{8-x}

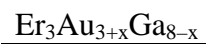
Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Dy1	2 <i>a</i>	0	0	0	1.25(15)	1Dy
Dy2	4 <i>i</i>	0	0	0.3167(2)	0.43(10)	1Dy
M1	2 <i>d</i>	1/2	0	1/2	1.19(23)	1Ga
M2	4 <i>h</i>	0	0.2147(4)	1/2	0.99(10)	0.449(7)Au+0.551(7)Ga
M3	8 <i>l</i>	0	0.2736(5)	0.1418(4)	1.09(12)	1Ga
M4	8 <i>l</i>	0	0.3680(2)	0.3375(2)	1.25(8)	0.451(6)Au+0.549(6)Ga

Refinement composition: Dy₃Au_{2.70}Ga_{8.30}. Reliability factors: *R*_B = 6.57 %, *R*_F = 5.59 %.

Ho₃Au_{3+x}Ga_{8-x}

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso} (Å ²)	Occupation G
Ho1	2 <i>a</i>	0	0	0	1.38(17)	1Ho
Ho2	4 <i>i</i>	0	0	0.3154(3)	0.52(11)	1Ho
M1	2 <i>d</i>	1/2	0	1/2	0.44(20)	0.058(11)Au+0.942(11)Ga
M2	4 <i>h</i>	0	0.2152(4)	1/2	0.76(9)	0.600(8)Au+0.400(8)Ga
M3	8 <i>l</i>	0	0.2766(4)	0.1414(3)	0.72(11)	0.069(5)Au+0.931(5)Ga
M4	8 <i>l</i>	0	0.3671(2)	0.3380(2)	1.23(8)	0.627(9)Au+0.373(9)Ga

Refinement composition: Ho₃Au_{4.05}Ga_{6.95}. Reliability factors: *R*_B = 7.82 %, *R*_F = 5.52 %.



Atom	Site	x	y	z	$B_{\text{iso}} (\text{\AA}^2)$	Occupation G
Er1	$2a$	0	0	0	1.61(16)	1Er
Er2	$4i$	0	0	0.3159(3)	0.63(10)	1Er
M1	$2d$	1/2	0	1/2	0.66(22)	0.024(10)Au+0.976(10)Ga
M2	$4h$	0	0.2119(4)	1/2	1.28(11)	0.423(7)Au+0.577(7)Ga
M3	$8l$	0	0.2764(5)	0.1427(4)	0.87(13)	1Ga
M4	$8l$	0	0.3665(2)	0.3383(3)	0.98(9)	0.436(7)Au+0.564(7)Ga

Refinement composition: $\text{Er}_3\text{Au}_{2.61}\text{Ga}_{8.39}$. Reliability factors: $R_B = 8.09\%$, $R_F = 7.47\%$.