A Study of the Phase $\text{Mg}_2\text{Cu}_6\text{Ga}_5$, Isotypic with $\text{Mg}_2\text{Zn}_{11}$. A Route to an Icosahedral Quasicrystal Approximant

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Table S1. Crystal data and structure refinement for $\text{Mg}_2\text{Cu}_6\text{Ga}_5$

formula weight	778.46
Temperature	293(2) K
wavelength, Å	0.71073
crystal system, space group, Z	cubic, $Pm\bar{3}$ (No. 200), 3
unit cell dimension, Å	8.278(1)
volume, Å ³	567.3(1)
density (calc)	6.836 Mg/m ³
absorp. coeff. (Mo K α), mm ⁻¹	34.06 mm ⁻¹
F(000)	1059
crystal size, mm	0.2 × 0.18 × 0.2
θ range for data collection, deg.	3.48 to 28.18
Index ranges	$-10 \leq h \leq 10, -10 \leq k \leq 8, -10 \leq l \leq 9$
reflections collected	2630 [$R_{\text{int}} = 0.0470$]
independent obs. reflections ($2\sigma_I$)	280
completeness of $\theta = 28.18^\circ$	97.9%
absorption correction	SADABS
refinement method	full-matrix least-squares on F^2
data / restraints / parameters	280 / 0 / 24
goodness-of-fit on F^2	1.145
final R indices [$I > 2\sigma_I$]	$R1 = 0.0477, wR2 = 0.1282$
[all data]	$R1 = 0.0480, wR2 = 0.1288$
extinction coefficient	0.011(3)
largest diff. peak and hole	1.481 and -2.233 Å^3

Table S2. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Mg}_2\text{Cu}_6\text{Ga}_5$. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atoms	Wyck.	symm.	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
Ga1	1 <i>a</i>	<i>m</i> 3.	0	0	0	18(1)
Ga2	6 <i>g</i>	<i>mm</i> 2..	0.3364(2)	½	0	21(1)
Ga3	8 <i>i</i>	.3.	0.2824(1)	<i>x</i>	<i>x</i>	22(1)
Cu1	6 <i>h</i>	<i>mm</i> 2..	0.2750(2)	½	½	20(1)
Cu2	12 <i>j</i>	<i>m</i> ..	0	0.1637(1)	0.2573(1)	19(1)
Mg	6 <i>f</i>	<i>mm</i> 2..	0.1812(6)	0	½	25(1)

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Mg}_2\text{Cu}_6\text{Ga}_5$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + \dots + 2hka^*b^* U_{12}]$

atoms	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ga1	18(1)	18(1)	18(1)	0	0	0
Ga2	25(1)	20(1)	19(1)	0	0	0
Ga3	22(1)	22(1)	22(1)	-2(1)	-2(1)	-2(1)
Cu1	22(1)	18(1)	21(1)	0	0	0
Cu2	18(1)	21(1)	19(1)	0	0	0
Mg	28(2)	23(2)	24(2)	0	0	0

Figure S1. Environment of Mg in Mg₂Cu₆Ga₅