**Exploration in the Sc-Al-Cu system: evidence for *i*-ScAl2.4Cu3.2 quasicrystal and new data for five crystal phases.**

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Supplemental material



Figure S1. Experimental XRD powder patterns (2 theta, Cu-Kα)   
recorded for the quasicrystalline ScAl2.4Cu3.2 phase (red) (Cu/Al ratio 1.33)  
calculated (black) for the crystalline phases: from top to bottom hexagonal (Cu/Al ratio 0.40 and 1.20), tetragonal (1.25), orthorhombic (1.60) and cubic (2.0).

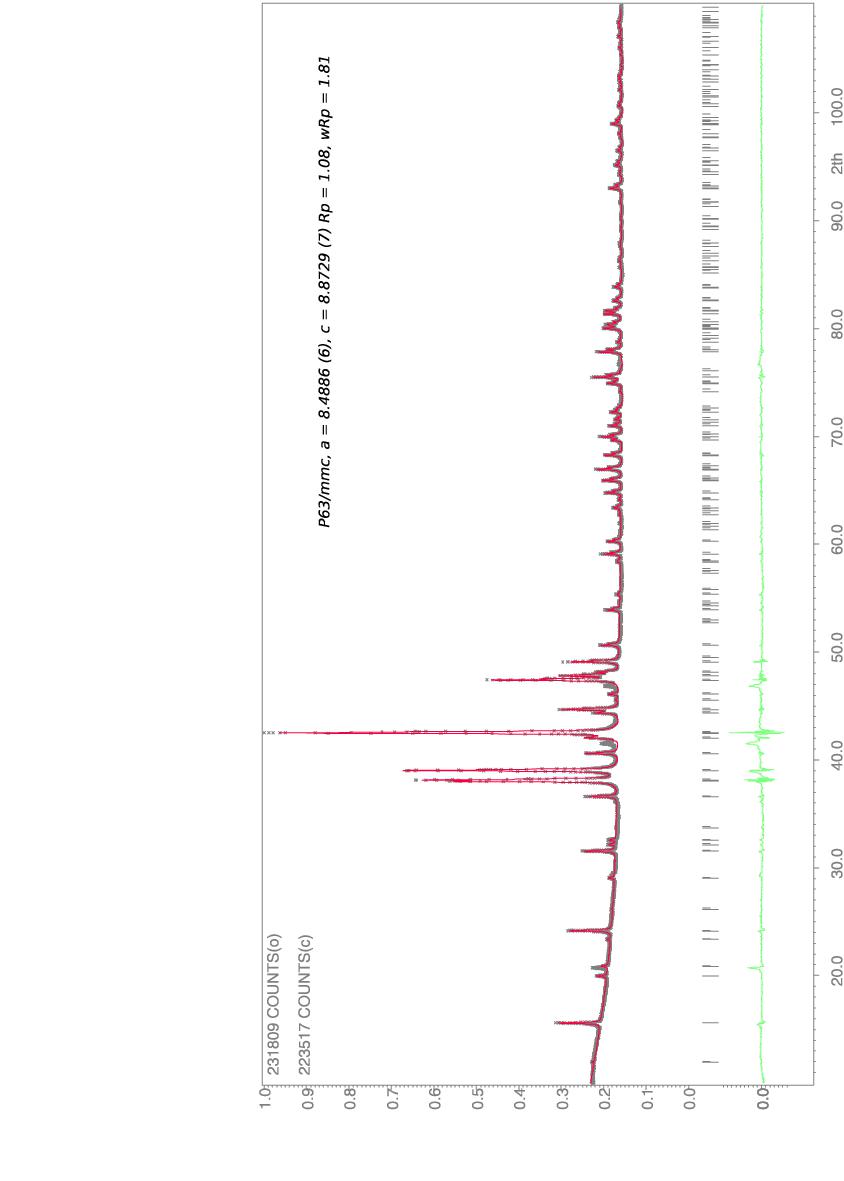


Figure S2. Profile refinement for the experimental XRD powder pattern (Cu-Kα) recorded for the hexagonal phase ScAl2.4Cu2.9

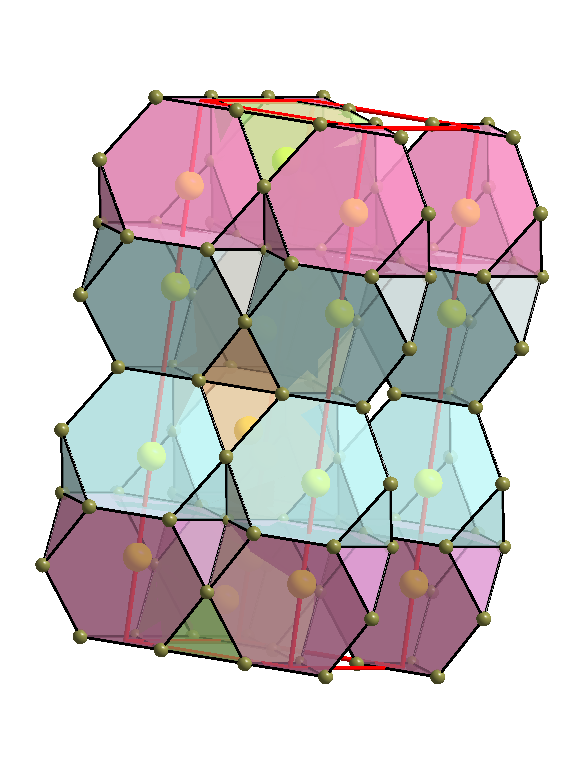
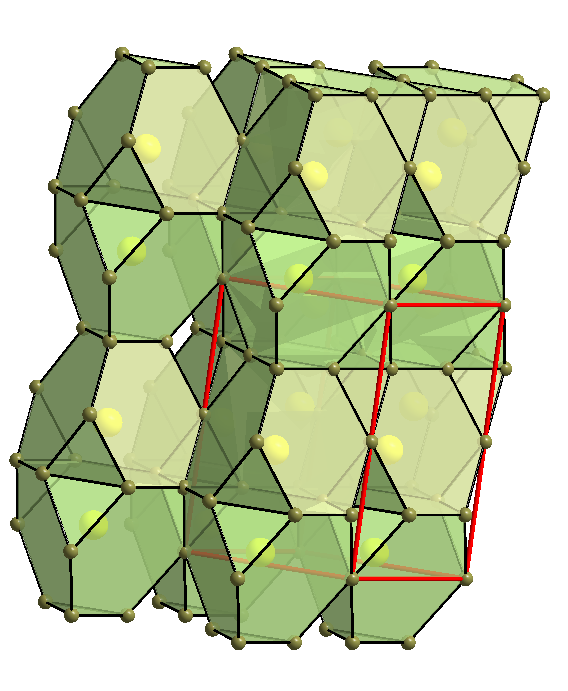
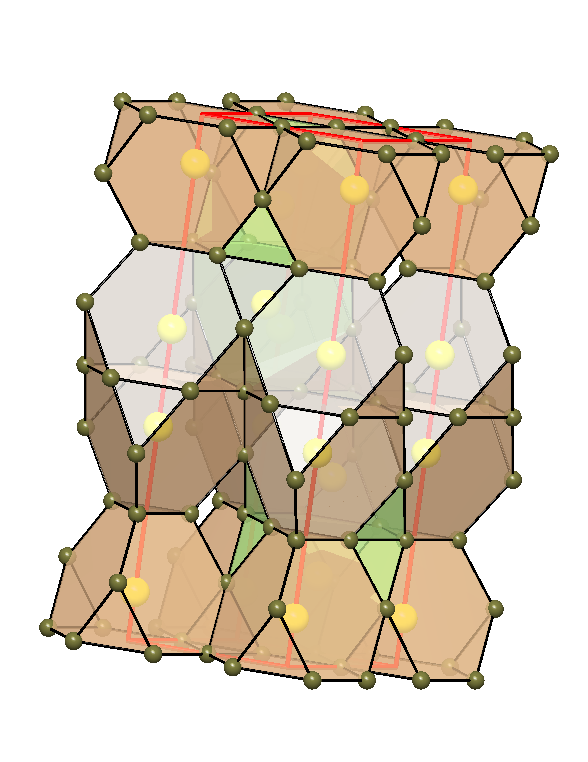


Figure S3. Structural representation of 12-vertex (Franck-Kasper) polyhedral packing approximately viewed along [-1 -1 0] direction.   
From left to right: ScAl1.4Cu0.6 (P63/*mmm*, 2 Sc independent sites), ScAlCu (P63/*mmm*, one Sc site) and ScAl1.1Cu0.9 (P*m2*, 4 Sc independent sites).

Tables S1–S7. Atom coordinates and equivalent isotropic displacement parameters (Å2×103). Ueq is defined as one third of the trace of the orthogonalized Uij tensor.

**Table S1. ScAl2.43Cu2.91,** crystal S34, a = 8.4928(2), c = 8.8743(2), P63/*mmc*

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site Cu/Al content x y z Ueq

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Sc(1) ***6h***  0.1984(1) 0.3968(2) 0.25 9(1)

M(1) ***12k*** 0.47/0.53(1) 0.1574(1) 0.3148(1) 0.5913(1) 14(1)

M(2) ***6h*** 0.37/0.63(1) 0.5660(1) 0.1321(2) 0.25 9(1)

M(3) ***6g*** 0.86/0.14(1) 0.5 0 0 9(1)

M(4) ***4f*** 0.09/0.91(1) 0.3333 0.6667 0.0081(3) 9(1)

M(5) ***2a*** 0.45/0.55(1) 0 0 0.25 30(1)

M(6) ***2b*** 0.12/0.88(2) 0 0 0 35(2)

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**Table S2. ScAl2.44Cu2.88,** crystal S35, a = 8.4920(5), c = 8.8714(6), P63/*mmc*

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site Cu/Al content x y z Ueq

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Sc(1) ***6h***  0.1984(1) 0.3967(2) 0.25 8(1)

M(1) ***12k*** 0.47/0.53(1) 0.1573(1) 0.3146(1) 0.5912(1) 14(1)

M(2) ***6h*** 0.38/0.62(1) 0.5660(1) 0.1321(2) 0.25 9(1)

M(3) ***6g*** 0.87/0.13(1) 0.5 0 0 10(1)

M(4) ***4f*** 0.09/0.91(1) 0.3333 0.6667 0.0085(2) 9(1)

M(5) ***2a*** 0.45/0.55(1) 0 0 0.25 32(1)

M(6) ***2b*** 0.10/0.90(1) 0 0 0 32(2)

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**Table S3. ScAl2.19Cu3.42**, crystal S37, a = 21.8869(7), b = 8.3311(2), c = 8.3238(2), C*mmm*

\* M2 position is split into Cu2 and Al2. \*\*Al content is the complement to unity

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site x y z Ueq Cu content\*\*

this work [1]

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Sc1 ***8o*** 0.81290(7) 0 0.7051(2) 0.0289(3)

Sc2 ***4g*** 0.38542(9) 0 0 0.0291(4)

Sc3 ***4j*** 0 0.3044(2) 0.5 0.0283(4)

Al2\* ***8p*** 0.2521(3) 0.168(1) 0 0.062(3) 0.12(1) 0.48

Cu2\* ***4g*** 0.2575(2) 0 0 0.053(2) 0.245(9) 0.02

M1 ***4k***  0 0 0.2631(2) 0.0297(5) 0.95(1) 0.95

M3 ***4i*** 0 0.2590(2) 0 0.0296(5) 0.82(1) 0.89

M4 ***8o***  0.40573(5) 0 0.3480(1) 0.0272(3) 0.745(9) 0.88

M5 ***4h***  0.0699(1) 0 0.5 0.0288(8) 0.13(1) 0.12

M6 ***4g*** 0.06009(7) 0 0 0.0300(5) 0.76(1) 0.78

M7 ***4f*** 0.25 0.25 0.5 0.0257(7) 0.25(1) 0.32

M8 ***16r***  0.30741(4) 0.16054(9) 0.23744(9) 0.0303(3) 0.800(8) 0.72

M9 ***8p*** 0.65294(6) 0.3382(1) 0 0.0355(4) 0.900(11) 0.85

M10 ***8q*** 0.63246(4) 0.2548(1) 0.5 0.0264(3) 1 1

M11 ***4l*** 0 0.5 0.1857(3) 0.0264(6) 0.37(1) 0.22

M12 ***4h*** 0.30329(8) 0 0.5 0.0249(5) 0.56(1) 0.31

M13 ***16r*** 0.57975(6) 0.2767(2) 0.7749(2) 0.0288(4) 0.212(7) 0.07

[1] T. Ishimasa, A. Hirao, T. Honma and M. Mihalkovic, Philos. Mag. 91 (2011) p. 2594.

**Table S4. ScAl5.34Cu6.66**, crystal S36, a = 8.5605(3), c = 5.0061(3), I4/*mmm*

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site Cu/Al content x y z Ueq

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Sc ***2a*** 0 0 0 14(1)

M(2) ***8j*** 0.581/0.419(7) 0.2813(2) 0.5 0 21(1)

Cu(3) ***8f*** 1.0/0.0 0.25 0.25 0.25 15(1)

M(4) ***8i*** 0.085/0.915(6) 0.3461(2) 0 0 17(1)

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**Table S5. ScAl1.03Cu2.00**, crystal S42, a = 6.1958(6), F*m**m*

**ScAl0.97Cu2.00**, crystal S45, a = 6.1976(2), F*m**m* *(\* italic)*

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site x y z Ueq *(\*)Ueq*

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Cu ***8c***  0.25 0.25 0.25 13(1) *9(1)*

Sc ***4b*** 0.5 0 0 9(1) *5(1)*

Al ***4a*** 0 0 0 8(1) *5(1)*

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**Table S6. ScAl1.12Cu0.88**, crystal S6, a = 5.2237(5), c = 16.8872(3), P2*m*

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site Cu/Al content x y z Ueq

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Sc(1) ***2g*** 0 0 0.8443(1) 8(1)

Sc(2) ***2h*** 0.3333 0.6667 0.9063(1) 9(1)

Sc(3) ***2g*** 0 0 0.3429(1) 8(1)

Sc(4) ***2h*** 0.3333 -0.3333 0.4066(1) 8(1)

M(1) ***6n*** 0.456/0.544(5) 0.4959(1) 0.5041(1) 0.7505(1) 9(1)

M(2) ***3k***  0.516/0.484(6) 0.3284(3) 0.1642(2) 0.5 9(1)

M(3) ***3j*** 0.430/0.570(6) 0.8360(2) 0.1640(2) 0 8(1)

M(4) ***2i***  0.296/0.704(7) 0.6667 0.3333 0.8757(2) 8(1)

M(5) ***2i*** 0.419/0.581(7) 0.6667 0.3333 0.6254(1) 10(1)

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**Table S7. ScAl1.13Cu0.87**, crystal S7, a = 5.2215(1), c = 16.8861(4), P2*m*

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site Cu/Al content x y z Ueq

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Sc(1) ***2g*** 0 0 0.8448(1) 9(1)

Sc(2) ***2h*** 0.3333 0.6667 0.9059(1) 10(1)

Sc(3) ***2g*** 0 0 0.3424(1) 9(1)

Sc(4) ***2h*** 0.3333 -0.3333 0.4069(1) 7(1)

M(1) ***6n*** 0.468/0.532(7) 0.4979(2) 0.5021(2) 0.7507(1) 9(1)

M(2) ***3k*** 0.524/0.476(9) 0.3247(4) 0.1624(2) 0.5 9(1)

M(3) ***3j*** 0.384/0.616(9) 0.8384(2) 0.1616(2) 0 10(1)

M(4) ***2i*** 0.263/0.737(9) 0.6667 0.3333 0.8750(2) 10(1)

M(5) ***2i*** 0.441/0.559(9) 0.6667 0.3333 0.6266(2) 9(1)

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