Structural Investigation of ScAuSi and ScAuGe using ^{45}Sc Solid State NMR

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The hexagonal scandium compounds ScAuSi ($P\bar{6}m2$, a = 421.7(1), c = 680.7(1) pm) and ScAuGe ($P6_3mc$, a = 431.03(9), c = 685.5(1) pm) were synthesized in X-ray pure form *via* arc-melting of the elements. The structures are derived from the AlB_2-type. The gold and silicon (germanium) atoms build up strongly puckered layers of Au_3Si_3 and Au_3Ge_3 hexagons. Due to a different puckering pattern and stacking sequence of the hexagons, the ScAuGe structure has one and the ScAuSi structure two crystallographically independent scandium sites, which can be unambiguously distinguished on the basis of ^{45}Sc–^{29}Si magnetic dipole-dipole interactions measured in a site selective fashion on an isotopically enriched material by solid state NMR.

Key words: Scandium, Intermetallics, Crystal Chemistry, Solid State NMR