

**MS23-1-2 1/1 and 2/1 QC approximant in the Ce-Au-Al System
#MS23-1-2**

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Abstract

Since the discovery of the stable binary Cd_{5.7}Yb [1] and Cd_{5.7}Ca [2] icosahedral quasicrystals (QCs), there has been an increasing interest in these quasicrystalline structures and their approximants. These quasicrystalline phases, known as Tsai-type QCs, and their related approximants (1/1: YbCd₆ Type, SG: *Im-3*, and 2/1: Yb₁₃Cd₇₆ SG : *Pa-3*) are built from similar clusters consisting of concentric shells of disordered tetrahedra, dodecahedra, icosahedra, icosidodecahedra and defected triacontahedra from the inside out.

Similar approximant structures, called 1/1 QC approximant, crystallizing with the body centred space group *Im-3*, have been reported in ternary systems like RE-Au-X [3-5], RE-Ag-X [6] with RE = Rare earth, Ca [7] or Na [8] and X a metalloid element or in Sc-Mg-Zn system [9]. All these systems have similar clusters but differ significantly by their respective composition. For example, gold systems usually crystallize with composition around RE₁₅Au₆₅X₂₀, for silver it is approximately around RE₂₀Ag₄₀In₄₀ and for the Sc-Mg-Zn the 1/1 composition is Sc₁₄Mg_{0.8}Zn₈₄ [10]. The same behaviour can be observed for the 2/1 approximant.

In this frame, we will concentrate here on the Ce-Au-Al systems, where Kondo effect behaviour have been reported recently [10], but without complete structural determination. Indeed to date both quasicrystal approximants have been only reported in the Sc-Mg-Zn [9] and in the Ca-Au-Sn[7] systems. Therefore, this paper will report the structural characterization of both 1/1 and 2/1 approximants in a ternary system where magnetic element like cerium is involved. In both cases, the two approximants' structures have been characterized by powder and single crystal X-ray diffraction.

The single crystal XRD analysis performed on the as-cast sample reveals the existence of two types of structure. First, a body centred cubic structure (*Im-3*) isotypic to those previously reported for the Ge or Sn-containing systems [3,4] was observed with $a_{1/1} = 14.927 \text{ \AA}$ for the 1/1 approximant. In agreement with the X-ray powder diagram a second crystal analysis reveals the existence of a primitive cubic unit cell with $a_{2/1} = 24.12 \text{ \AA}$, crystallizing with the *Pa-3* space group and in agreement with the 2/1 approximant reported for the Sc-Mg-Zn and Ca-Au-Sn systems. This paper will precisely describe these two related structures explaining their structural relationship and differences with those already reported in similar systems.

References

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