s1.m1.p3 **Quininium (R)-mandelate, an incommensu-rately modulated structure in superspace.** A. Schönleber, G. Chapuis, *Institut de Cristallographie, Université de Lausanne, BSP - Dorigny, CH-1015 Lausanne, Switzerland.*
Keywords: incommensurate, modulation, superspace.

Owing to very significant displacive modulations, quininium (R)-mandelate, $C_{20}H_{25}N_2O_2^+ \cdot C_8H_7O_3^-$, exhibits high order satellites in the diffraction patterns. On the basis of main reflections only, no average structure solution could be resolved. A commensurate approximation could only be obtained from the suitable selection of a supercell.

By iterating the use DIRDIF-96[1] (Patterson search methods) and SHELXL97[2], a model could be obtained and refined in two commensurate supercell approximations, a 3x5 supercell (in agreement with Gjerløv *et al.*[3]) and a 3x6 supercell. Both approximations have been performed in space group P2$_1$; the first supercell includes 15 formula units per asymmetric unit whereas the second includes 18 formula units per asymmetric unit.

The two approximations lead to a common starting model for the incommensurate refinement. The special reflection condition 0k00: k = 2n in a monoclinic basic cell (**b** unique) indicate the superspace-group P2$_1$(α0γ). The basic cell has one formula unit per asymmetric unit, the modulation vector is **q** = 0.333·**a*** - 0.276·**c***. The results of the incommensurate refinements with MSR[4] and JANA2000[5] in the superspace formalism will be presented. The different treatment of hydrogen atoms in these two programmes will be discussed

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s1.m1.p4 **The crystal structure of the tetragonal approximant Mn$_3$Ga$_5$.** M. Boström, *Structural Chemistry, Stockholm University, 10691 Stockholm, Sweden.*
Keywords: aperiodic, incommensurate.

The binary Mn-Ga alloy system is rich in phases, several with large unit cells and unknown structures. It has won renewed interest due to its close chemical relationship to the Mn-Al system where quasicrystals were first discovered[1]. A decagonal quasicrystal has also been identified in the Mn-Ga system[2]. The crystal structure of the tetragonal approximant Mn$_3$Ga$_5$ has been determined from single crystal X-ray diffraction data and is here described. The space group is P4$_2$/nmc with a = 12.659(2) Å and b = 24.616(6) Å. R$_w$=1.50 %. The structure is mainly made up of 38 atoms clusters isotypic to those found in γ-brass, Cu$_5$Zn$_8$.

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