it is evidenced that the second layer molecules are found to adsorb
directly on top of the underlying layer.


**Keywords:** quasicrystal, pentacene, adsorption

**MS63.P24**


Structure solution of decagonal ZnMgDy quasicrystal
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Here we report the first structure solution of decagonal ZnMgDy
quasicrystal (d-ZnMgDy) based on single crystal X-ray diffraction
data. Samples with the composition (Zn$_x$Mg$_{1-x}$Dy$_{0.6}$) were prepared by
induction melting followed by annealing at 375°C for 10 months. The
alloys were then quenched to room temperature. The resulting samples
consist mainly of a hexagonal phase with the d-ZnMgDy existing as the
secondary phase. The morphology of the decagonal phase is typically
needle-like. These grains are of 50 µm in length and approximately 15
µm in other dimensions. X-ray diffraction experiments were carried out
both in-house (Oxford Xcalibur PX diffractometer, CCD detector,
Mo Kα radiation) and at the Synchrotron facility in Swiss-Norwegian
beam line, ESRF, Grenoble (λ=0.6980 Å).

The Laue group was specified to be $10/mmm$ with a periodicity
of 5.22 Å along the periodic direction. No systematic extinctions
were observed. SUPERFLIP program package [1] (based on charge
flipping and low density elimination algorithms) was used for structure
solution.

786-790.

**Keywords:** quasicrystal, decagonal

**MS63.P25**


Analysis of structure and chemical order in a ternary Yb$_3$Mg$_{15}$Cd$_{68}$
quasicrystal
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The atomic structure of the ternary Yb$_3$Mg$_{15}$Cd$_{68}$ quasicrystal has
been refined from single crystal X-ray data. The ternary quasicrystal
is related to the binary i-Yb$_3$Cd$_{68}$ parent phase,[1] 2 and suffers from
chemical disorder mainly due to mixing between Mg and Cd. Studies
on related ternary approximants however indicate that this chemical
disorder is only partial, and that there are strong selection rules in
several ternary systems that govern the choice of a particular atom at a
specific site. The purpose of this work is thus to elucidate the chemical
order between the constituent elements in the ternary Yb$_3$Mg$_{15}$Cd$_{68}$
quasicrystal and its relation to ternary approximants in other RE-Mg-
Cd (RE=Rare Earth) systems. The structure refinements performed
on the Yb$_3$Mg$_{15}$Cd$_{68}$ quasicrystal clearly indicate that it is composed of
similar atomic clusters as the binary i-Yb$_3$Cd$_{68}$ phase and that there is
a strong selection rule that mainly determines the chemical order at the
cluster level. Similar observations have also been made in other related
ternary approximant phases. The structure refinement is the first of its
kind performed on a ternary Yb-Cd-related quasicrystal, and the results
indicate that the structures and chemical order of ternary quasicrystals
can be understood by extracting and combining information from
structure refinements on both quasicrystals and related approximants.

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**Keywords:** quasicrystal, approximant, chemical order

**MS63.P26**


Ab-initio calculations on the stability of heptagonal ordering in
Gallium
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Sevenfold symmetry is the lowest rotational symmetry not yet
observed in quasicrystals. However, there are several strong hints
that indicate the existence of heptagonal quasicrystals (QCs) [1]. In
a previous ab-initio study [2] it was shown that theoretical sevenfold
approximants, designed from promising known boride and borocarbide
structure types by using a supertile approach, were acceptably stable
within the range of error. Due to the fact that these structures and their
associated tilings are ternary, the weak matching rules automatically
imposed on the edges of the tiles only allow for a limited number of
possible structural arrangements.

The configurational degrees of freedom can be increased by
investigating the structure of monatomic γ-Ga, a metastable low
temperature phase that forms when undercooling liquid Ga to below
-35.6°C. Its structure consists of regular sevenfold antiprisms centered
by a single Ga atom. Additionally it can be described as a periodic
arrangement of one of the three heptagonal rhombic unit tiles, namely
the “fat” tile with an ideal acute angle of 3π/7 (= 77.12°, in the structure
76.15°).

For the missing two unit tiles (with acute angles π/7 and 2π/7),
decorations were be designed by using similar atomic arrangements
as for the fat tile (i.e. γ-Ga). As only periodic structures can be
accessed by means of ab-initio total energy calculations, the unit
tiles were subsequently used to decorate approximants. Therefore
various theoretical structure types were generated, either by periodic
arrangement of single tiles or hexagon supertiles of the rhomb-tiles, or
by creating rational heptagonal approximants using the cut-and-project
method.

The first-principles DFT calculations were performed with the VASP
code [3], using a plane-wave basis set, the GGA algorithm and PAW-
PBE pseudopotentials. Total energies were calculated for all theoretical
Ga structure types, as well as the electron localization function (ELF),
and the atom relaxation movements were investigated.

The possibility of stabilizing the designed structures by dopant
atoms was also explored: the rational approximant structures mentioned
above exhibit a small number of voids or holes too large for Ga-atoms,