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# letters to the editor

## Comments on quasicrystalline phases and examples of quasicrystalline phase nomenclature in *Nomenclature of magnetic, incommensurate, composition-changed morphotropic, polytype, transient-structural and quasicrystalline phases undergoing phase transitions. II. Report of an IUCr Working Group on Phase Transition Nomenclature* by J.-C. Tolédano *et al.* (2001). *Acta Cryst.* A57, 614–626

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In this Report, some suggestions for the nomenclature of quasicrystalline phases and their crystalline approximants have been put forward and examples have been given, about which I should like to make the following comments:

**1.** In §7.5 of this Report, there is a statement "quasicrystalline phase is thus considered to be characterized by the absence of an averaged Bravais lattice and/or the observation of 'forbidden' crystallographic symmetry (*e.g.* decagonal)." The use of 'and/or' in this sentence means two alternatives. In the 'or' case, 'the absence of an averaged Bravais lattice' is no longer a necessary condition for quasicrystals. It is well known that a quasicrystalline phase is characterized by its quasiperiodicity and a consequence of this is the absence of a Bravais lattice. The majority of quasicrystals do have forbidden rotational symmetry, but some quasicrystals with conventional rotational symmetry, such as cubic and hexagonal, also exist. However, in the 'and' case, "the observation of 'forbidden' crystallographic symmetry" is emphasized without mentioning the possibility of conventional rotational symmetry. In order to remove any ambiguity, it is perhaps better to use 'with/without' rather than 'and/or' or not to mention the rotational symmetry at all. In fact, the definition for aperiodic crystals including quasicrystals suggested by the *Ad Interim* Commission on Aperiodic Crystals of the IUCr (International Union of Crystallography, 1992) only laid stress on the absence of the Bravais lattice. It reads "By 'crystal' we mean any solid having an essentially discrete diffraction diagram, and by 'aperiodic crystal' we mean any crystal in which three-dimensional lattice periodicity can be considered to be absent."

**2.** The definition for a crystalline approximant given in §7.5 is: 'An approximant phase is a crystalline phase with large unit cell and diffraction pattern closely resembling that of a quasicrystalline phase in the sequence.' It is well known that the structure of both icosahedral and decagonal quasicrystals is characterized by the irrational golden number $\tau = (1 + 5^{1/2})/2$ [$\cos 36^\circ = \tau/2$, $\cos 72^\circ = (\tau - 1)/2$] and this irrational number can be successively approximated by a rational ratio of two consecutive Fibonacci numbers, such as 1/0, 1/1, 2/1, 3/2, ..., $F_n/F_{n-1}$, ... , and as $n \rightarrow \infty$, $F_n/F_{n-1} \rightarrow \tau$. As $n$ increases, 'one obtains a sequence of (periodic) cubic structures with corresponding lattice constants $a$, $a\tau$, $a\tau^2$' (Elser & Henley, 1985) and these periodic phases are called 'approximants'. For the Al–Mn–Si icosahedral quasicrystal and its 1/1 cubic approximant ($a$ = 12.68 Å), Elser & Henley (1985) found that the strong diffraction peaks in the [100] electron diffraction pattern of the latter agree extremely well with the positions of peaks of the twofold pattern of the former. It is understood that this icosahedral quasicrystal and its approximant have not only similar composition but also similar local structure or subunits. Thus, it is the strong diffraction peaks but not the whole diffraction pattern of the approximant closely resembling the diffraction pattern of the quasicrystal.

**3.** In §7.6.1, the lattice parameters given for the base-centred orthorhombic approximant of the $Al_{63}Cu_{17.5}Co_{17.5}Si_2$ decagonal quasicrystal are: $a \sim b \sim 51.5$, $c \sim 4.1$ Å. The original data for this approximant (Fettweis *et al.*, 1995) in fact are 'base-centred orthorhombic (rhombic unit-cell parameters at $T = 300^\circ$C; $a = b \approx 51.5$, $c \approx 4.13$ Å and $\gamma = 108^\circ$)'. Since the rhombic unit cell is not a three-dimensional Bravais lattice, its use should perhaps be avoided. Moreover, it might be misleading too, as the omission of rhombic unit cell and $\gamma = 108^\circ$ in the above case. The lattice parameters for the base-centred orthorhombic approximant of the $Al_{63}Cu_{17.5}Co1_{7.5}Si_2$ decagonal quasicrystal are: $a \approx 2 \times 51.5 \sin 36^\circ = 60.5$ Å, $b \approx 2 \times 51.5 \cos 36^\circ = 83.3$ Å and $c \approx 4.13$ Å. Similar $a$ and $b$ parameters have been obtained earlier by Zhang & Kuo (1990) when two suitable rational ratios of Fibonacci numbers are used to substitute for the irrational $\tau$ in two orthogonal directions in the quasiperiodic plane of the two-dimensional decagonal quasicrystal.

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