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addenda and errata

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. Erratum

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Six printing errors are corrected in the Report by Tolédano *et al.* [*Acta Cryst.* (2001), A**57**, 614–626]. The first is in §2.1, the fourth last sentence of which should read ''Although such nicknames do not always describe the magnetic character of the substance explicitly, since 'AF' for example may be mistaken for antiferroelectric, this lack is compensated for by the fifth and sixth fields (see the examples in §§3.1–3.5).'' The second is in §3.4, second field of the AF phase, which should read '<260 K'. The third is in §4.5, the final sentence of which should be 'However, certain materials display ferroic properties in the incommensurate phase (*cf.* §5.3)'. The fourth is in §5.1, sixth field of phase II, which should read 'Incommensurate. Modulation: $\delta \sim 0.78$. Displacive modulation.'. The fifth is in §6, the third sentence of which should read ''While accepting this definition, it is necessary to point out, however, that the boundary between phases in the examples below need not be 'thermodynamically abrupt' (*i.e.* involve a latent heat and discontinuities in the physical quantities).''. The final error is in §6.1, sixth field of the FT phase, which should read 'FT | $0.45 < x < 1$ | *P*4*mm* (99) | $Z = 1$ | Ferroelectric and ferroelastic | All phases pseudo-cubic perovskites. No perovskite octahedral tilts; 6 variants.'.

References

Tolédano, J.-C., Berry, R. S., Brown, P. J., Glazer, A. M., Metselaar, R., Pandey, D., Perez-Mato, J. M., Roth, R. S. & Abrahams, S. C. (2001). *Acta Cryst.* A**57**, 614–626.

Diffraction physics. Erratum

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Owing to a copying error, the formula in §2.1(iv) of the paper by Authier & Malgrange [*Acta Cryst.* (1998), A**54**, 806–819] is erroneous and should be replaced by:

$$I_h = \frac{R^2\lambda^2(1+\cos^2 2\theta)}{2\sin^2\theta}\frac{t^2}{V^2}|F_{hkl}|^2\left[\frac{\sin(2\pi kt\cos\theta\Delta\theta)}{(2\pi kt\cos\theta\Delta\theta)}\right]^2.$$

References

Authier, A. & Malgrange, C. (1998). *Acta Cryst.* A**54**, 806–819.

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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[1]

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A general nomenclature applicable to the phases that form in any sequence of transitions in the solid state has been recommended by an IUCr Working Group [*Acta Cryst.* (1998). A**54**, 1028–1033]. The six-field notation of the first Report, hereafter I, was applied to the case of structural phase transitions, *i.e.* to transformations resulting from temperature and/or pressure changes between two crystalline (strictly periodic) phases involving modifications to the atomic arrangement. Extensive examples that illustrate the recommendations were provided. This second Report considers, within the framework of a similar six-field notation, the more complex nomenclature of transitions involving magnetic phases, incommensurate phases and transitions that occur as a function of composition change. Extension of the nomenclature to the case of phases with less clearly established relevance to standard schemes of transition in equilibrium systems, namely polytype phases, radiation-induced and other transient phases, quasicrystalline phases and their transitions is recommended more tentatively. A uniform notation for the translational periodicity, propagation vector or wavevector for magnetic and/or incommensurate substances is specified. The notation adopted for incommensurate phases, relying partly on the existence of an average structure, is also consistent with that for commensurate phases in a sequence. The sixth field of the nomenclature is used to emphasize the special features of polytypes and transient phases. As in I, illustrative examples are provided for each category of phase sequence.

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1. Introduction

A multiplicity of terminologies for distinguishing individual members of a sequence of crystalline phases that form as a function of temperature and/or pressure may be found in the crystallographic and other literature of the condensed state. Confusion caused by the lack of a unified nomenclature led the Commission on Crystallographic Nomenclature to establish a Working Group on Phase Transition Nomenclature.[2] The Working Group was charged with studying the multiple nomenclature in current use for naming such sequences of phases and with making such recommendations for its

[1] Established 15 February 1994 by the IUCr Commission on Crystallographic Nomenclature; following the resignation of two members upon acceptance of the first Report, three new members were appointed 18 July 1998. This second Report was received by the Commission 26 February 2001 and accepted 19 April 2001. The present Report, as all other Reports of the Commission, is available online at the Commission's webpage: http://www.iucr.org/iucr-top/comm/cnom.html.

[2] See footnote to paper title.

improvement as may be appropriate. The term 'phase-transition nomenclature', as used throughout this Report, applies to the nomenclature of phases that form as a consequence of one or more transitions; the nomenclature of materials that exist only in single phase form is adequately treated elsewhere, *e.g.* Leigh *et al.* (1998).

In I, the general purpose of the nomenclature was defined, the relevant information it should contain was specified, and a recommendation was made for the adoption of a six-field notation in the case of structural phase-transition nomenclature, *i.e.* of transitions between two crystalline (strictly periodic) phases that involve only a modification of the atomic arrangement. Extensive examples providing illustrative use of the nomenclature were presented for a variety of substances (metals, alloys, oxides and minerals) that undergo phase transitions as a function of temperature and/or pressure. The recommended notation is not only unambiguous; it also provides a full context for the transitions undergone by each phase.

The recommended nomenclature employs the following six-field notation for each phase with given chemical composition, each field being separated from the others by vertical bars:

Usual label in literature (α, I, ...)	Temp. (K) and pressure range (Pa)	Space-group symbol and number	Number of chemical formulas per unit cell	Ferroic properties	Comments

Full information concerning the content of each field is available in I, see also footnotes in §§6.1, 7.1.3, 7.2.2 and 7.3.3.

This second Report considers the more complex nomenclature required for transitions involving magnetic phases, incommensurate phases and transitions occurring as a function of composition change. The case of phases with a relevance to standard schemes of transition in equilibrium systems that is not yet clearly established is considered more tentatively; such phases include polytypes, see also Guinier *et al.* (1984), quasicrystalline, radiation-induced and other transient phases and their transitions.

The six-field nomenclature defined in I was found to be convenient and applicable to all the new systems above, provided a suitable adaptation of the content of each field is followed as recommended below. In addition, the present analysis led the Working Group to recommend, for every category of transition (including those considered in I), where known, that the order of the phase transition be noted as a comment in the sixth field.

2. Magnetic phases

Several major additional factors must be considered in the designation of a magnetic phase transition as compared with a structural phase transition. These include (*a*) the magnetic configuration, which must be specified as well as the atomic configuration, (*b*) the magnetic field, which is as relevant and controlling a parameter as the temperature and pressure, and (*c*) the magnetic periodicity of the system, which is not always unambiguously indicated by the number Z of structural units in the conventional cell.

Table 1
Recommended abbreviations for various magnetic categories.

Property	Abbreviation	Property	Abbreviation
Paramagnet	P	Exotic	EX
Ferromagnet	F	Amplitude modulated	IC
Antiferromagnet	AF	Helical	H
Spin flop	SF	Canted ferromagnet	CF
		Weak ferromagnet	WFM

A recommended adaptation of the six-field nomenclature to magnetic phase transitions is now presented.

2.1. First field

The usual name used in the literature for a magnetic phase tends to emphasize the magnetic behaviour of the phase. For instance, antiferromagnetic phases are often nicknamed AF1, AF2 *etc*; likewise, spin flop phases are nicknamed SF1, SF2 *etc*. In simple situations where either temperature or magnetic field is the dominant parameter controlling the phase diagram, the numeral in the nickname commonly increases with decreasing temperature (*e.g.* in antiferromagnetic phases), or commonly increases with increasing magnetic field (*e.g.* in spin flop phases). It is recommended that this practice of numeral increase be extended to newly discovered magnetic phases. In more complex situations involving an intricate phase diagram as a function of temperature and field, with the possibility of conflict between the assignment of increasing or decreasing numerals, it is recommended that the sequence due to an increasing magnetic field be given precedence. Although such nicknames do not always describe the magnetic character of the substance explicitly, since 'AF' for example may be mistaken for antiferroelectric, this lack is compensated for by the fifth and sixth fields (see the examples in §§31–3.5). A set of intuitively obvious notations for the different categories of magnetic behaviour is presented in Table 1. We recommend the assignment of nicknames as in this table. Two ferromagnetic phases in a sequence would hence be labelled F1 and F2.

2.2. Second field

The magnetic field range (H, in T) over which the phase is stable, if known, should be added to the temperature (T, in K) and pressure (P, in Pa) ranges used for structural phase transitions. Clearly, a summary of the detailed phase diagram of a given material as a function of three controlling parameters cannot be provided in a highly compact nomenclature. However, the present aim is to provide an immediate understanding of the experimental stability conditions for the material. If the phase is stable over a region bounded by all three variables T, P and H, then these ranges should be indicated by their end-values; in turn, the boundary conditions

Table 2
Definition of magnetic structure types.

Paramagnet	Normally the magnetically disordered phase stable at high temperatures
Ferromagnet	The magnetic phase with all spins parallel
Ferrimagnet	A spin array intermediate between that of a ferromagnet and an antiferromagnetic
Spin flop	A phase in which some fraction of the moment has been forced from antiferromagnetic to ferromagnetic order by the application of a field
Collinear	A unique magnetization direction exists
Non-collinear	Antiferromagnets with no unique magnetization direction
Canted ferromagnet	Small (<5°) non-collinearity producing weak ferromagnetism in a basically antiferromagnetic arrangement. Includes weak ferrromagnets of the Dzyaloshinski–Moriya type
Antiferromagnet	Commensurate in the strict sense that the propagation vector corresponds to a special point in the Brillouin zone. Could be modified by collinear or non-collinear spins
Amplitude modulated	Structures generated by a single modulation with wave vectors incommensurate in the sense given above
Helical	Structures generated by two orthogonal modulations in phase quadrature with the same incommensurate wave vector
Exotic	Cases not covered by the above descriptions
Weak ferromagnet	Commonly used name for a canted ferromagnet of the Dzyaloshinski–Moriya type

are separated by semicolons. §3.5 illustrates this notation for the intricate case of $EuAs_3$, the phase diagram of which is reproduced in Fig. 1. Since the magnetic field direction is of relevance, this information when available should be specified in the sixth field.

2.3. Third field

In the case of structural phase transitions, this field is devoted to the specification of the space-group symbol and number (to avoid ambiguities related to the setting); such information is insufficient for magnetic systems since it does not describe the nature of the magnetic ordering. An alternative might be to indicate the magnetic space group. However, the lack of a standard magnetic space-group notation leads us to recommend the use of the same crystallographic information (*i.e.* the crystallographic space-group symbol and number) in this field as for sequences of structural transitions. This does not detract from the total information provided since fields four and six contain additional information specifying the required magnetic structure (*i.e.* magnetic periodicity and spin configuration).

2.4. Fourth field

The recommendation in I for this field is to provide the number of chemical formulas per conventional unit cell, *i.e.* Z. The purpose is to specify the change of lattice periodicity occurring between phases or, in other terms, to indicate the onset of different superlattice reflections in the various phases of a sequence. Note that such information is analogous to (and less accurate than) the specification of the wavevector defining these superlattice reflections.

It is more convenient, for magnetic phases, to specify the magnetic propagation vector which fills the same function by providing information on the 'magnetic periodicity' of the phase. A similar option is adopted below for incommensurate systems (see §5). However, as in the latter systems, an ambiguity arises since the components of the propagation wavevector can be referred either to the reciprocal cell of the non-magnetic phase in the sequence or to that of the 'chemical structure' of the magnetic phase itself (which may differ from that of the non-magnetic phase). It is hence recommended, for the sake of clarity and consistency with the option chosen for incommensurate systems, see §4.4, that the reference phase be specified in the fourth field. Also, that the value of Z for the conventional chemical cell of the magnetic phase be indicated at the beginning of the fourth field.

2.5. Fifth field

The recommended information for this field, in the case of structural phase transitions, see I, is the name of the ferroic property. For magnetic phase transitions, specification of the magnetic type instead is recommended. The various magnetic types to be considered are listed in Table 2 together with their definitions.

2.6. Sixth field

This field may include complementary information such as the magnetic moment, its magnitude and direction for simple structures, the direction of the external magnetic field controlling the stability of the phases and any other information that contributes to the understanding of the magnetic configuration. Recommended descriptions for this field are given in Table 3.

The content of the various fields is summarized as follows

Usual magnetic label as used in literature (*e.g.* AF1, *cf.* Table 1)	Temp. (K), pressure (Pa) and magnetic field (T) range	Crystallographic space-group symbol and number	Reference phase, Z, and magnetic propagation vector	Magnetic type (*cf.* Table 2)	Magnetic configuration and comments (*cf.* Table 3).

3. Examples of magnetic phase-transition nomenclature

3.1. Fe (Geissler *et al.*, 1967)

P	>1040 K	*Im*3*m* (229)	P, $Z = 2$ 0, 0, 0	Paramagnet	–
F	<1040 K	*Im*3*m* (229)	P, $Z = 2$ 0, 0, 0	Ferromagnet	Easy magnetization direction ⟨110⟩.

Columns I, II, III and V above indicate that Fe undergoes a transition from paramagnetic to ferromagnetic at 1040 K

Table 3
Description of magnetic spin arrangements.

Screw spiral	Helical structure with spins in the plane perpendicular to the propagation vector
Cycloidal spiral	Helical structure with spins in the plane containing the propagation vector
Bunched spiral	Helical structure with spin directions bunched about particular directions in the plane in which they rotate
Sinusoidal modulation	The amplitudes of the spins in a collinear arrangement follow a sine curve
Square wave	The amplitudes of the spins in a collinear arrangement follow a square wave
Fan	A cycloidal structure with bunching
Antiphase domains	Regions of an antiferromagnetic structure related by inversion of all spins
k domains	Domains corresponding to different arms of the stars of the propagation vector
s domains	Domains with the same propagation vector, but different spin directions
Chirality domains	Domains corresponding to oppositely directed propagation vectors, when these are inequivalent, as for helical structures

without a change in crystallographic space group at T_c; column IV that both phases have two atoms in the conventional cubic unit cell and the reference of the *k* vector is the P phase.

3.2. NiO (Roth, 1958)

P	>523 K	*Fm*3*m* (225)	P, $Z = 4$ 0, 0, 0	Paramagnet	–
AF	<523 *K*	$R\bar{3}m$ (166)	P, $Z = 4$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	Antiferromagnet	Moments ferromagnetically coupled in (111) planes, adjacent layers antiferromagnetically coupled. Spins ∥ $[11\bar{2}]$. Four *k* domains each containing three *s* domains.

k domains differ in propagation vector direction, *s* domains in spin direction, *cf.* Table 3. The *Z* value refers to the conventional cell, hence the primitive cell in the AF phase (which is identical to the conventional cell) is quadruple that of the primitive cell in the P phase (one-fourth the cubic cell).

3.3. K_2IrCl_6 (Hutchings & Windsor, 1967)

P	>3.05 K	*Fm*3*m* (225)	P, $Z = 4$ 0, 0, 0	Paramagnet	–
AF	<3.05 K	*I*4/*m* (87)	P, $Z = 2$ 1, 0, $\frac{1}{2}$ in *Fm*3*m* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ in *I*4/*m*	Antiferromagnet	Spins ∥ [001], 6 *k* domains.

3.4. α-Fe_2O_3 (Shull *et al.*, 1951; Nathans *et al.*, 1964)

P	>945 K	$R\bar{3}c$ (167)	P, $Z = 4$ 0, 0, 0	Paramagnet	–
WFM	945–260 K	$R\bar{3}c$ (167)	P, $Z = 4$ 0, 0, 0	Canted ferromagnet	Moments in (111) ferromagnetically coupled. Nearly antiferromagnetic coupling between adjacent planes, moment directions in the planes. Three *s* domains.
AF	<206 K	$R\bar{3}c$ (167)	P, $Z = 4$ 0, 0, 0	Antiferromagnet	Moments in (111) ferromagnetically coupled. Exact antiferromagnetic coupling between planes. Moments parallel to [111].

3.5. $EuAs_3$ (Chattopadhyay & Brown (1987, 1988*a*,*b*,*c*)

P	>11.1 K, 0 T; 0 K, >6.5 T	*C*2/*m* (12)	P, $Z = 4$ 0, 0, 0	Paramagnet	–
IC	10.1–11.1 K, <0.83 T	*C*2/*m* (12)	P, $Z = 4$ 1, 1, $1/2 - \delta$	Amplitude modulated	$\delta = 0.15 - 0.075$, 11.12 – 10.17 K. Moments ∥ *b*, coupling as AF1.
AF1	0–10.1 K, 0 T; 0–9.8 K, 0.7 T. 0–10.1 K, <0.3 GPa; 5–9.8 K, <0.6 GPa	*C*2/*m* (12)	P, $Z = 4$ 1, 1, $\frac{1}{2}$	Antiferromagnet	Moments ∥ *b* and ferromagnetically coupled across the centre of symmetry at origin.
HP	0 K, >0.3 GPa; 5–9.8 K, >0.6 GPa	*C*2/*m* (12)	P, $Z = 4$ 0.11, 1, 0.22	Helical	Cycloid, moments in *ac* plane, coupling as AF1. Two chirality domains.
SF1	<9.5 K, 0.7 T; <7 K, 2.2 T	*C*2/*m* (12)	P, $Z = 4$ 0.1, 1, 0.25	Helical	Cycloid, moments in *ac* plane, coupling as AF1. Two chirality domains.
SF2	<5.8 K, 2.2 T; 0 K, 4.8 T	*C*2/*m* (12)	P, $Z = 4$ 0, 1, 0.25	Non-collinear ferromagnet	Antiferromagnetic components ∥ *c*, coupled as in AF1. Two chirality domains.
SF3	0 K, 4.8–5.5 T; 5.8 K, 2 T	*C*2/*m* (12)	P, $Z = 4$ 0.1, 1, 0.225	Exotic	Fan structure with antiferromagnetic components ∥ *c*, coupling as AF1.
SF4	9.6–10.8 K, 0.83T; 0 K, 5.5–6.5 T	*C*2/*m* (12)	P, $Z = 4$ 0.102, 1, 0.225	Exotic	As SF3 but with antiferromagnetic components at 8° to *c*.

The *P*–*T* and *H*–*T* phase diagrams of $EuAs_3$ are given in Fig. 1.

4. Incommensurate phases

A preliminary adaptation of the structural phase-transition nomenclature to the case of incommensurately modulated systems was proposed in I, §5, as illustrated by the example of K_2SeO_4. The requirement to keep the nomenclature as uniform as possible for the various types of phase system leads us to adopt the same convention in the fourth field as that used for magnetic systems, *i.e.* specifying the wavevector of the modulation rather than the approximate period of the modulation, see Chapuis *et al.* (1997).

Similarly, the possibility of substituting the multi-dimensional space group (Janssen *et al.*, 1992) for the usual (average) space group in the third field was considered but discarded for reasons similar to those for not using the magnetic space-group symbol (*viz*. the specialized nature of the topic and the possibility of ambiguity in the case of more than one direction of modulation). It is hence recommended that the space group of the average structure, *i.e.* the structure obtained by averaging the effects of the modulation, be inserted in this field.

We briefly summarize the content of each field.

4.1. First field

The common names used for incommensurate phases are identical to those for ordinary crystalline phases (*e.g.* I, II *etc*.). The incommensurate character appears in the fourth field (in which the wavevector of the modulation is specified) and, more explicitly, in the sixth field.

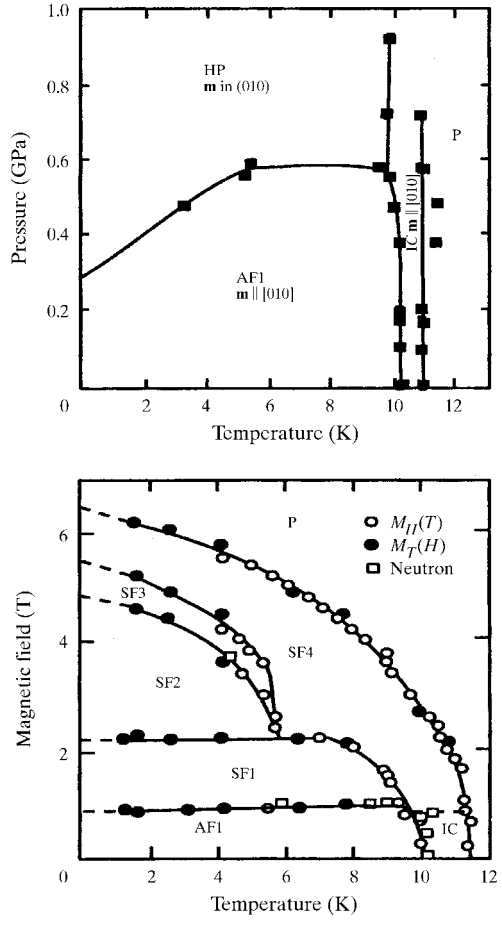

Figure 1
The *P*–*T* and *H*–*T* phase diagrams of $EuAs_3$

4.2. Second field

As in the case of magnetic materials, an additional controlling parameter, namely the electric field, E in V m^{-1}, is often relevant. Indeed, the stability range of modulated 'ferroelectric' phases is very sensitive to the application of an external electric field (which can play a rôle similar to that of the magnetic field in helical or sinusoidal magnets). Here, also, the option is taken of providing a simplified phase diagram; the approximate range of stability of the given phase, as a function of all three parameters T, P and E, is indicated by the appropriate stability intervals relative to each parameter, see also §2.2. Examples §§5.1–5.6 illustrate the application of this notation.

4.3. Third field

This field, for both the incommensurate and commensurate phases in a sequence, specifies the average space group of the structure, namely that obtained by averaging the modulated positions of the atoms. Each atom is located at the centre of the 'cloud' of positions determined by the modulation. In practice, this structure can be determined in many cases (if the modulation is not very large and not very anharmonic) by taking into account only the main reflections and ignoring the satellite reflections. If an incommensurate phase undergoes a transition to a commensurate phase on reducing the temperature, the exact space group of the latter, if known, should also be specified in the third field below the average space group in order to provide more accurate information.

4.4. Fourth field

This field contains the modulation propagation vector (the modulation wavevector), as referred to the reciprocal lattice of the phase specified therein (either the nonmodulated phase or the average structure of the modulated phase), following the nomenclature for magnetic phases. In the case of materials with a phase in which more than one modulation exists, *cf*. §5.5, the individual propagation vectors must be indicated with appropriate clarifying comments in the sixth field. On the other hand, it may be noted that, in a sequence involving one or several incommensurate phases, there may also exist phases that are strictly periodic, *i.e.* commensurate. These phases involve superlattice reflections, denoting a change in the unit cell. A comparable circumstance is taken into account for ordinary structural transitions in I by specifying, in the fourth field, the number of units in the unit cell of the average structure. We denote this number Z_A.

In the present case, however, the superlattice reflections in these commensurate phases are generally analogous to those observed in the incommensurate phase except for their commensurate location in reciprocal space. It is therefore recommended, for consistency in a sequence of phases, that, in addition to Z, the commensurate propagation vector be included in the fourth field. The Z_A value relative to the average structure of the incommensurate phase should also be included. The latter option has the advantage of lifting the ambiguity concerning the phase taken as reference for the

Table 4
Abbreviations used in the illustrative examples for composition-changed, transient-structural and quasicrystalline phases.

Property	Abbreviation
Ferroelectric orthorhombic	FO
Ferroelectric tetragonal	FT
Ferroelectric rhombohedral (high/low temperature)	FR (HT/LT)
Antiferroelectric	AF
Paraelectric	P
Quasicrystalline	Q
Approximant	A
Radical pair	RP
Metastable (higher temp.)	MS_1
Metastable (lower temp.)	MS_2
Rotator phase just below melting temperature	R_I
Non-rotator phase	T
Modulated quasicrystalline	MQ

modulation wavevector. It also provides a unified nomenclature scheme for the incommensurate and the magnetic systems, which may also be incommensurate.

4.5. Fifth field

It is recommended that, as with ordinary structural phase transitions, the 'average ferroic' properties be stated in the fifth field whenever they exist. In most examples, the point symmetry of the average structure is identical to that of the 'high-temperature' phase and no macroscopic ferroic properties exist. However, certain materials display ferroic properties in the incommensurate phase (*cf.* §5.2).

4.6. Sixth field

This field may include complementary information such as the incommensurate character and the nature of the structural modulation (*e.g.* onset of a modulated ferroelectric dipole of specified orientation or the modulated deformation of a specific group of atoms), as well as the possible occurrence of multiple k or several independent modulations.

The content of each nomenclature field is summarized as follows:

Usual label in literature (I, II, ...)	Relevant controlling parameters: temperature (K), pressure (Pa) and electric field (Vm^{-1})	Space-group symbol and number for the average structure	Z_A; modulation propagation vector (label of the reference phase). Z (for commensurate phases)	Ferroic type	Incommensurate character and nature of the modulation.

5. Examples of incommensurate phase-transition nomenclature

5.1. $SO_2(C_6H_4Cl)_2$ (Zúñiga *et al.*, 1993; Etrillard *et al.*, 1996)

A single phase transition at $T_i = 150$ K is reported; the incommensurate phase exists as low as 0.1 K.

I	>150 K	$I2/a$ (15)	$Z = 4$	Non-ferroic	–
II	$0.1 \leq T_i \leq 150$ K	$I2/a$ (15)	$Z_A = 4$ 0, δ, 0 referred to phase I	Non-ferroic	Icommensurate. Modulation: $\delta \sim 0.78$, displacive modulation.

5.2. K_2SeO_4 (Iizumi *et al.*, 1977)

The succession of four phases (three commensurate and one incommensurate) is denoted as follows:

I	>630 K	$P6_3/mmc$ (194)	$Z = 2$	Non-ferroic	–
II	630–130 K	$Pnam$ (62)	$Z = 4$	Ferroelastic	3 variants
III	130–93 K	$Pnam$ (62)	$Z_A = 4$ $(1/3 - \delta), 0, 0$ referred to phase II	Ferroelastic	Incommensurate. Modulation: $\delta \sim 0.05$, ferroelectric distortion of SeO_4 tetrahedra.
IV	<93 K	$Pnam$ (62) $Pna2_1$ (33)	$Z_A = 4$ 1/3, 0, 0 referred to phase II, $Z = 12$	Ferroelectric and ferroelastic	Commensurate; 6 variants.

5.3. $Ba_2NaNb_5O_{15}$ (Tolédano *et al.*, 1986)

I	>850 K	$P4/mbm$ (127)	$Z = 1$	Non-ferroic	–
II	850–570 K	$P4bm$ (100)	$Z = 1$	Ferroelectric	2 variants. Polarization along the 4 axis.
III	570–540 K	$Cmm2$ (35)	$Z_A = 2$ $(1 + \delta)/4$, $(1 + \delta)/4, \frac{1}{2}$ referred to phase I	Ferroelectric and ferroelastic	Incommensurate modulation ($\delta \sim 10^{-1}$): NbO_6 octahedral tilts. 4 ferroelectric–ferroelastic variants.
IV	540–110 K	$Cmm2$ (35) $Bbm2$ (40)	$Z_A = 2$ $(1 + \delta_0)/4$, $(1 + \delta_0)/4, \frac{1}{2}$ referred to phase I, $Z = 16$	Ferroelectric and ferroelastic	Commensurate $\delta_0 = 0$ in certain samples. Same variants as III.
V	<110 K	$P4bm$ (?) (100)	$Z_A = 1$ $(1 + \delta)/4$, $\pm(1 + \delta)/4, \frac{1}{2}$ referred to phase I, $Z = 32$	Ferroelectric	Re-entrant phase (sample dependent). Characteristics of k uncertain; 2 directions of modulation likely.

5.4. $(CH_3)_3NCH_2COO\cdot CaCl_2\cdot 2H_2O$ (Chaves & Almeida, 1990)

I	>164 K (4 GPa, >230 K)	*Pnma* (62)	$Z = 4$	Non-ferroic	–
II	164–129 K (4 GPa, 230–225 K)	*Pnma* (62)	$Z_A = 4$ 0, 0, δ referred to phase I	Non-ferroic	Incommensurate $\delta \sim 0.29$.
III	129–127 K (<2 GPa) (0.4 MV m^{-1} 143–122 K)	*Pnma* (62) *Pn*2$_1$*a* (33)	$Z_A = 4$ 0, 0, 2/7 referred to phase I, $Z = 28$	Ferroelectric	Commensurate ferroelectric polarization along *b*.
IV	127–117 K (4 GPa, 225–215 K) <0.2 MV m^{-1}	*Pnma* (62)	$Z_A = 4$ 0, 0, δ referred to phase I	Non-ferroic	Incommensurate $\delta \sim 0.27$.
V	117–116 K (0.4 MV m^{-1}, 120–110 K)	*Pnma* (62) *Pn*2$_1$*a* (33)	$Z_A = 4$ 0, 0, 4/15 referred to phase I, $Z = 60$	Ferroelectric	Commensurate ferroelectric polarization along *b*; electric field applied along *b*.
VI	116–80 K, $\leq$5GPa	*Pnma* (62) *P*2$_1$*ca* (29)	$Z_A = 4$ 0, 0, 1/4 referred to phase I $Z = 16$	Ferroelectric	Commensurate ferroelectric polarization along *a*.
VII–X111	4 GPa, $\sim$ 210–180 K	*Pnma* (62)	$Z_A = 4$ 0, 0, m/n referred to phase I, $Z = 4n$	Ferroelectric for m even, n odd or m odd, n even	Commensurate phases with $n = 7, 9, 11, 14, 17, 19$; the existence of some of these phases is uncertain.
XIV	78–57 K, $\leq$5 GPa, $\leq$ 0.2 MV m^{-1}	*Pnma* (62) *P*2$_1$2$_1$2$_1$ (19)	$Z_A = 4$ 0, 0, 1/5 referred to phase I, $Z = 20$	–	Commensurate. Electric field along *b*.
XV	57–50 K, <0.2 MV m^{-1}	*Pnma* (62) *P*2$_1$*ca* (29)	$Z_A = 4$ 0, 0, $\frac{1}{6}$ referred to phase I, $Z = 24$	Ferroelectric	Commensurate ferroelectric polarization along *a*. Electric field along *b*.
XVI	<50 K, 4 GPa, <180 K	*Pn*2$_1$*a* (33)	$Z = 4$	Ferroelectric	Nonmodulated ferroelectric polarization along *b*.

5.5. $TaSe_2$ (Fleming *et al.*, 1980; Bird *et al.*, 1985)

I	>123 K	*P*6$_3$/*mmc* (194)	$Z = 2$	Non-ferroic	–
II	123–112 K	*P*6$_3$/*mmc* (194)	$Z_A = 2$ $(1-\delta)/3, 0, 0$ $0, (1-\delta)/3, 0$ referred to phase I	Non-ferroic	Incommensurate. Triple-*k* modulation along three hexagonal directions: $\delta \sim 2\times10^{-2}$.
III	112–90 K	*Cmcm* (63)	$Z_A = 4$ $(1-\delta)/3, 0, 0$ $0, (1-\delta)/3, 0$ 1/3, 1/3, 0 referred to phase I	Ferroelastic	Double-*k* modulation. Commensurate along k_3.
IV	<90 K	*Cmcm* (63)	$Z_A = 4$ 1/3, 0, 0 0, 1/3, 0 referred to phase I, $Z = 36$	Ferroelastic	Commensurate. The amplitude of the modulation is equal along two directions and unequal in the third. There are three orientation domains each containing 9 translation domains.

5.6. $Bi_{2-x}Pb_xSr_2CaCu_2O_8$ (Tolédano *et al.*, 1990)

$Bi_{2-x}Pb_xSr_2CaCu_2O_8$ is an example of a material exhibiting incommensurate phases with two unusual characteristics: the first a compositional dependence of the wavevector, the second the presence of two modulations along the same direction.

I	$x = 0$	*Bbmb* (66)	$Z_A = 1$ 0, δ, 1/2	Twinned (ferroelastic?)	Incommensurate. Modulation: $\delta \sim 0.21$, 'buckling' of BiO planes.
II	$0.25 \geq x > 0.10$	*Bbmb* (66)	$Z_A = 1$ 0, δ, 1/2	Twinned (ferroelastic?)	Incommensurate. Modulation: $\delta \sim 0.21$, 'buckling' of BiO planes. $0.18 > \delta > 0.10$.
III	$0.10 > x \geq 0.05$ $x \sim 0.10$	*Bbmb* (66)	$Z_A = 1$ 0, δ, 1/2 0, δ, 0	Twinned (ferroelastic?)	Two modulations with characteristics close to that of phases I and II: $\delta_1 \sim 0.22$; $\delta_2 = (2/3)\delta_1$.

6. Composition-changed phases

A growing number of materials are being reported for which a change in composition results in a phase change; such materials are commonly referred to as morphotropic. IUPAC (Clark *et al.*, 1994) defines a morphotropic phase transition as 'an abrupt change in the structure of a solid solution with variation in composition'. If this definition is adopted, it is necessary to point out, however, that the boundary between phases in the examples below need not be 'thermodynamically abrupt' (*i.e.* involve a latent heat and discontinuities in the physical quantities). The abruptness, as in most phase transitions, concerns the structural changes (*e.g.* as specified by its space group) at a precisely defined composition. The nomenclature recommended in I and in §§2 and 4 of the

present Report is readily applicable to morphotropic phase transitions.

Composition limits for each phase should be given in the second field. The remaining fields follow the recommendations presented in I for structural phase transitions. Several examples illustrating the recommended nomenclature for composition-changed phases follow. In the illustrative examples chosen, the labelling of the phases is influenced by usage. Table 4 presents the meaning of these labels.

6.1. Examples of composition-changed phase nomenclature[3]

6.1.1. $PbZr_{1-x}Ti_xO_3$ phases at room temperature (Corker *et al.*, 1998).

FT	$0.45<x<1$	*P4mm* (99)	$Z=1$	Ferroelectric and ferroelastic	All phases pseudocubic perovskites. FT, no perovskite octahedral tilts; 6 variants.
FR(HT)	$0.35<x<0.45$	*R3m* (160)	$Z=3$	Ferroelectric and ferroelastic	No perovskite octahedral tilts; 8 variants.
FR(LT)	$0.06<x<0.35$	*R3c* (161)	$Z=6$	Ferroelectric and ferroelastic	$a^-a^-a^-$ perovskite octahedral tilt system. 8 variants.
AF	$0<x<0.06$	*Pbam* (55)	$Z=8$	Antiferroelectric and ferroelastic	$a^-a^-c^+$ perovskite octahedral tilt system.

The symbols $a^-a^-a^-$ and $a^-a^-c^+$ are from Glazer's (1972) system of specifying the anion octahedral tilts in perovskite structures. The perovskite structure consists of corner-linked octahedra that can tilt about any combination of pseudocubic axes, a_p, b_p and c_p. The three letters refer to each axis in turn and indicate equivalence or non-equivalence of the angle of tilt. Equivalence is indicated by repeating a letter. If successive tilts about an axis are in the same sense, then a superscript + is used; if in opposing senses, then a superscript − is used. Thus the symbol $a^-a^-a^-$ means that all octahedra tilted about the a_p axis are tilted in alternating senses. The same is true for the octahedra viewed down b_p and down c_p. All tilts are of equivalent magnitude; the net effect is to create a rhombohedral structure.

6.1.2. $KTa_{1-x}Nb_xO_3$ (Perry *et al.*, 1976). The end members of this solid solution undergo transitions as a function of temperature (for $KNbO_3$, $T_c \sim 698$ K; for $KTaO_3$, $T_c \sim 1$–3 K). All transitions described below are a function of composition at room temperature, except for the FR phase.

P	$0<x<0.37$	*Pm3m* (55)	$Z=1$	Paraelectric	–
FT	$0.37<x<0.54$	*P4mm* (99)	$Z=1$	Ferroelectric and ferroelastic	P_s along [001] of phase P, 6 variants.
FO	$0.54<x<1$	*Bmm2* (38)	$Z=2$	Ferroelectric and ferroelastic	P_s along [110] of phase P, 6 variants.
FR	$0.45<x<1$	*R3m* (160)	$Z=1$	Ferroelectric and ferroelastic	P_s along [111] of phase P at $T=200$ K; 6 variants.

6.1.3. $La_{2-x}Sr_xCuO_4$ (Torrance *et al.*, 1989; Burns, 1992). The $La_{2-x}Sr_xCuO_4$ solid solutions have been widely studied for their interest in the important field of high-temperature superconductivity. Elucidation of the phase diagram by the work of many authors has revealed a rich diversity of fields. The example given here illustrates the phases at $T=300$ K; superconducting and other phases form at lower temperatures.

I	$0.07<x$	*I4/mmm* (139)	$Z=2$	Prototype	At $T=300$ K, metallic conductor.
II	$0<x<0.07$	*Abma* (64)	$Z=4$	Ferroelastic	At $T=300$ K, metallic conductor.

7. Tentative nomenclature for other systems

Each of the systems considered in this section have aspects that can lead to an adequate description within the framework of a six-field nomenclature. Thus, polytypes form sequences of phases that can be crystallographically and physically defined in the same way as commensurate and incommensurate phases. Further, the existence of large sequences of phases in these systems is an essential feature and therefore particularly relevant to the objectives of the present nomenclature. However, they also raise a specific difficulty since the conditions of phase stability (defined by a controlling parameter such as temperature and pressure) are ill-defined and, so far, it has not been possible to determine an acceptable phase diagram giving stability fields for the known polytypes of materials such as SiC, ZnS or CdI_2. The relevant parameters in this case are hence concerned with the method and conditions of phase stabilization.

A similar situation is also applicable in the case of transient or metastable phases obtained through the irradiation of samples by light or particle beams. Moreover, the physical characterization of the phases observed often leads to a different categorization than for the phases dealt with in the preceding sections (*viz*. ferroic properties). Quasicrystals raise even greater difficulties since, in addition to the former features (metastability, specific characterization of the physical properties), the atomic structure can only be very roughly specified without making use of the specialized nomenclature of six-dimensional crystallography; unlike the situation in incommensurate systems, it is not possible with quasicrystals to 'bypass' this abstract description by use of a modulation wavevector and an 'average space group'.

In view of this situation, the following proposals for the nomenclature of these systems must be considered as tentative.

[3] See footnotes **4** for the third and fourth, **5** for the sixth and **6** for the fifth fields as defined in Report I. *Second field*, Report I: If the phase is stable over a thermal range, then the temperature limits should be given in kelvins; if over a pressure range, in pascals. SI prefixes should be used as required. If no pressure range is indicated, the observations correspond to atmospheric pressure; similarly, if no temperature range is indicated, the observations correspond to room temperature.

7.1. Polytypic phases

Polytypic transitions are defined by IUPAC (Clark *et al.*, 1994) as transitions from 'a crystalline structure into one or more forms which differ in the way identical layers of atoms are stacked'.

7.1.1. First field. The IUCr (Guinier *et al.*, 1984) has recommended two kinds of symbolism for use with either simple or complicated polytypic structures. The first consists of 'indicative symbols' in a modified Gard notation, the second of 'descriptive symbols' based on earlier proposals by Dornberger-Schiff, Ďurovič and Zvyagin. Use of the term '*nN*', commonly used to designate the stacking sequence of layers (*n*) and the crystal system (*N*), is recommended for the first field. Guinier *et al.* (1984) recommend the upper-case letters that follow for the crystal system. Note that the common meaning of *n*, *i.e.* the number of layers, may depend on the system. Thus, as in the examples below, *n* is either the smallest number of layers necessary to describe a sequence or is the entire number of layers required to define the unit cell. The intent of the convention used becomes apparent in the fifth field:

Cubic	*C*
Hexagonal	*H*
Trigonal (with hexagonal Bravais lattice)	*T*
Trigonal (with rhombohedral Bravais lattice)	*R*
Tetragonal (quadratic)	*Q*
Orthorhombic	*O*
Monoclinic	*M*
Triclinic (anorthic)	*A*

7.1.2. Second field. As stated in the introduction to §7, these systems do not have a generally established stability range. Hence, the second field can indicate either a temperature and/or a composition range that corresponds to the conditions for *practical* stabilization of the individual phase. Certain metastable phases in these systems transform on annealing above a threshold temperature that provides a sufficient activation energy. It is recommended that a comment be inserted in the sixth field in order to clarify the content of the second field.

7.1.3. Third and fourth fields. These two fields follow the recommendations presented in I for structural phase transitions by providing the crystallographic characteristics of the phases.[4]

7.1.4. Fifth and sixth fields. In principle, the fifth field of the nomenclature should specify the ferroic properties of the phase but this is likely to be blank for most polytypes; it is hence recommended that this field should instead provide the essential stacking sequence information. The detailed descriptive symbols recommended by Guinier *et al.* (1984) to specify stacking sequences have not been widely used in the literature. Instead, a simple notation in which 'c' is taken for cubic and 'h' for hexagonal packing appears to be in common use and is adopted here. The sixth field should contain the preparation conditions and structure type or related information. Six examples illustrating the recommended nomenclature for polytypic phases follow.

7.2. Examples of polytypic phase nomenclature

7.2.1. $Ca_2Ta_2O_7$ (Grey *et al.*, 1999; Grey & Roth, 2000).

7*M*	>1673 K	*C*2 (5)	*Z* = 28	hcccchcccccc	Stable high-temperature polytype.
3*T*	<1673 K	$P3_121$ (152)	*Z* = 6	Unknown	Metastable low-temperature form. Not reversible from higher temperature.
6*M*	Unknown	*Cc* (9)	*Z* = 24	hcccchcccch	Obtainable with either a $Ca_2V_2O_7$ or a $Ca_2B_2O_5$ flux.

7.2.2. $Ca_{2-x}Mg_xTa_{2-y}Nb_yO_7$ (Grey & Roth, 2000)[5].

7*M*	$0<x<0.002$ $0<y<\sim 0.15$	*C*2 (5)	*Z* = 28	hcccchcccccc	Heated to 1773 K.
5*M*	$x \sim 0.002$ $\sim 0.15<y<0.36$	*C*2 (5)	*Z* = 20	hccchccccc	Formed only with very minor Mg impurity, cation ordering in c blocks. Type = *pyrochlore*.

7.2.3. $Ca_{2-x}Sm_xTa_{2-y}Ti_yO_7$ (Grey & Roth, 2000).

6*T*	$\sim 0.1<x<\sim 0.2$ $\sim 0.1<y<\sim 0.2$	$P3_1$ (144)	*Z* = 12	All cubic packing	Related to 3*T* weberite structure.
5*M*	$\sim 0.2<x<\sim 0.25$ $\sim 0.2<y<\sim 0.25$	*C*2 (5)	*Z* = 20	hccchccccc	Cation ordering in c blocks. Type = *weberite*.

7.2.4. $Ca_{2-x}Nd_xTa_{2-y}Zr_yO_7$ (Grey & Roth, 2000).

3*T*	$x \sim 0.1, y \sim 0.1$	$P3_121$ (152)	*Z* = 6	All cubic stacking	Heated at 1500°C, from $Ca_2V_2O_7$ flux.
4*M*	$x \sim 0.1, y \sim 0.1$	*C*2 (5)	*Z* = 16	All cubic stacking	From $Ca_2V_2O_7$ flux.
5*M*	*x*, *y* unknown	Unknown	*Z* = 20	All cubic stacking	From $Ca_2V_2O_7$ flux.

7.2.5. ZnS (Pandey *et al.*, 1994).

2*H*	>1297 K	$P6_3mc$ (186)	*Z* = 2	All hexagonal packing	May exist metastably at room temperature and transform irreversibly to 3*C* above 673 K.
3*C*	<1297 K	$F\bar{4}3m$ (216)	*Z* = 4	All cubic packing	Transforms into 2*H* martensitically.

[4] See footnotes **3** for the second, **5** for the sixth and **6** for the fifth fields as defined in Report I. *Third field*, Report I: The space-group symbol and number of the phase, as used in *International Tables for Crystallography* (1996), should be given. When incomplete crystallographic information is available, these data may be replaced by specifying the point group (*e.g.* 4*mm*) or the crystal system (*e.g.* tetragonal). *Fourth field*, Report I: The number of chemical formula units per conventional cell should be entered; if undetermined, the field should contain only a dash. The (tripled) hexagonal unit-cell setting in rhombohedral systems should be used.

[5] See footnotes **3** for the second, **4** for the third and fourth, and **6** for the fifth fields as defined in Report I. *Sixth field*, Report I: If the phase crystallizes with a standard structure type, then the sixth field should begin with an entry in the format | Type = *XXXX*. Typical structure type names are, for instance, *XXXX* = *NaCl*, *pyrite*, *sphalerite*, *etc*., with the name in italics or, alternatively, structure-type formulas such as *XXXX* = *GXX* ′, *T*3(*T*′/*L*)*X*4 *etc*. with the formula in italics.

7.2.6. SiC (Ramsdell, 1947; Pandey & Krishna, 1982). The SiC family is probably the best known of all polytypes. No temperature, pressure or compositional differences have been proven for long-period modifications of SiC. Shaffer (1969) reports 74 different polytypes. Pandey & Krishna (1982) have listed 60 polytypes, with complete stacking sequences of layers, the more common of which are listed below.

2*H*	<1673 K	$P6_3mc$ (186)	$Z = 2$	11 h	Transforms irreversibly above 1673 K to 3*C* and above 2273 K to 6*H*.
3*C*	<2273 K	$F\bar{4}3m$ (216)	$Z = 4$	∞ c	Transforms irreversibly above 2273 K to 6*H*.
6*H*	>2273 K	$P6_3mc$ (186)	$Z = 6$	33 cchcch	2*H* and 3*C* transform irreversibly to 6*H* above 2273 K. Most common form in α-SiC.
15*R*	Unknown	$R3m$ (160)	$Z = 15$	$(32)_3$ cchch	Second most common form in α-SiC.
4*H*	Unknown	$P6_3mc$ (186)	$Z = 4$	22 chch	Third most common form in α-SiC. Can occur in melt-grown crystals below 2273 K.

7.3. Transient-structural phases

It has recently become possible to study a range of photo-induced and other transient phases with lifetimes of order ranging from picoseconds to hours. Studies of short-duration phases by use of synchrotron radiation, see *e.g.* Helliwell & Rentzepis (1997), are being reported with increasing frequency in the current literature. The lower limit is likely to be reduced further by the introduction of femtosecond synchrotron radiation (see *e.g.* Schoenlein *et al.*, 2000). On the other hand, phases can be stabilized outside their ordinary stability range by irradiation with various types of beams, *e.g.* high-energy ions (Dammak *et al.*, 1996). For these categories of transitions, not all variables have yet been fully explored, hence the recommended nomenclature that follows may later require revision. The usage recommended in I, as modified in §§2 and 4 of the present Report, is readily adapted to radiation-induced phases as follows.

7.3.1. First field. As in I (§3.1) and in §4.1 of the present Report. The significance of the labels used is indicated in Table 4.

7.3.2. Second field. In addition to the temperature/pressure stability range of each phase in the system, the wavelength (nm) and radiant flux (W m^{-2}) necessary to obtain the irradiated phase should be given. In the case of other types of irradiation, equivalent specifications for the radiation used should be given.

7.3.3. Third, fourth and fifth fields. As in I (§§3.3–3.5).[6] In most examples below, information pertaining to the fifth field (ferroic property) is unavailable.

7.3.4. Sixth field. A brief description of each transient phase in the system should be given. Comments should include an indication of the experimental conditions used for phase onset, phase lifetime and preparation.

7.4. Examples of transient-structural phase-transition nomenclature

7.4.1. $Na_2[Fe(CN)_5NO]\cdot 2H_2O$ (Carducci *et al.*, 1997).

GS	Zero irradiation at 50 K	$Pnnm$ (58)	$Z = 4$	–	Ground-state structure. Crystallized from aqueous solution.
MS_1	488 nm, 1 kW m^{-2} at 50 K	$Pnnm$ (58)	$Z = 4$	–	Metastable state I. Laser-excited. Heated to 165 K for 5 min, recooled to 50 K.
MS_2	1064 nm, 0.7 kW m^{-2} at 50 K	$Pnnm$ (58)	$Z = 4$	–	Metastable state II. Longer wavelength laser-excited.

7.4.2. *n*-Hexadecane, $C_{16}H_{34}$ (Sirota & Herhold, 1999).

R_I	289.66 K	$Fmmm$ (69)	$Z = 4$	–	Transient (<10 s) rotator phase. Forms on slow cooling from the melt.
T	<289.66 K	$P\bar{1}$ (2)	$Z = 1$	–	Non-rotator phase. Transforms from R_I phase, melts at 291.5 K.

7.4.3. 2,2′-Di(orthochlorophenyl)-4,4′,5,5′-tetraphenylbiimidazole (*o*-Cl-HABI) (Kawano *et al.*, 1999).

GS	>103 K	$Pbca$ (61)	$Z = 16$	–	Ground state, two independent molecules, *A* and *B*. Pale yellow. Irradiated as for RP, warmed to 300 K giving GS, then cooled to 103 K.
RP	High-pressure Hg lamp, 20 min irradiation at 103 K	$Pbca$ (61)	$Z = 16$	–	0% *A* molecules, 10% *B* molecules converted into radical pairs at 103 K. Reddish-brown. Cleavage of the C–N bond gives two planar radicals in an RP.

7.4.4. Titanium under high-energy ion irradiation (Dammak *et al.*, 1996).

α	T<1200 K, p<500 MPa	$P6_3/mmc$ (194)	$Z = 2$	Twinned	–
ω	>2 × 10^{13} ions cm^{-2}, ~ 1 GeV, 80 K; p>500 MPa	$P6/mmm$ (191)	$Z = 3$	Twinned	Phase stable at high pressure, stabilized at room pressure by irradiation with high-energy lead ions. 3 twin orientations (c_ω along a_α).
β	T>1200 K	$Im3m$ (229)	$Z = 2$	–	–

7.5. Quasicrystalline phases

Reversible phase transitions have been observed between ordered and disordered quasicrystals, also between quasicrystalline phases and either orientationally twinned crystalline approximant phases or modulated quasicrystals (Fettweis *et al.*, 1995; Steurer, 2000; Zurkirch *et al.*1998). A rigorous definition of any of these phase categories has not yet been

[6] See footnotes **3** for the second, **4** for the third and fourth, and **5** for the sixth fields as defined in Report I. *Fifth field*, Report I: Contains the name of the ferroic property exhibited by the phase, see Clark *et al.* (1994). If this property has not actually been observed experimentally but is nevertheless probable on crystallographic grounds, a comment indicating this situation should be added in the sixth field. An unknown property is denoted by a dash (see *e.g.* §7.4.1).

achieved (*cf.* Launois, 1999, and references therein). The present tentative adaptation of the nomenclature in I to these systems hence uses the simplest pragmatic definitions available even if these do not adequately explain all the complex situations observed. A quasicrystalline phase is thus considered to be characterized by the absence of an average Bravais lattice and/or the observation of 'forbidden' crystallographic symmetry (*e.g.* decagonal).

An *approximant phase* is a crystalline phase with large unit cell and diffraction pattern closely resembling that of a quasicrystalline phase in the sequence. In practice, approximant phases of different coherent or incoherent orientations coexist, forming twinned structures. Such twinning can produce a diffraction pattern that exhibits 'forbidden symmetry'. *Modulated quasicrystals* are systems with a diffraction pattern that displays two sets of reflections: the first is a set of strong 'main' reflections, characteristic of a quasicrystal. The second is a set of weaker 'satellite' reflections that symmetrically surround the main reflections. The two sets are interpreted as the presence of a periodic modulation of atomic positions in the quasicrystal. We consider hereunder the adaptation of each nomenclature field to the specific features of these systems.

7.5.1. First field. Unless a label has been applied previously to the phase, we suggest the abbreviations given in Table 4. Additional numbering is used, *e.g.* Q1, if phases of the same type in a sequence are to be distinguished. If more complex phases are involved in a given sequence, then an appropriate label may be similarly defined.

7.5.2. Second field. Temperature appears to be the relevant controlling parameter in all transitions observed hitherto between quasicrystalline and other phases. The standard conventions in I hence remain applicable. However, since phase-transition irreversibility may be of importance in considering these systems, it is recommended that this be specified, if present, in field six.

7.5.3. Third and fourth fields. It is recommended, for quasicrystalline phases, that these fields provide only an elementary description of the structural geometry. Both the dimensionality and type of the system point symmetry (crystallographic or noncrystallographic) should be specified in field three. This information immediately distinguishes (Steurer, 1990; Launois, 1999) one-dimensional quasicrystals, in which ordinary crystalline order is observed in two dimensions, from two-dimensional quasicrystals, in which only one dimension is periodic, and both from three-dimensional quasicrystals. In the two-dimensional case, the forbidden symmetries already observed are pentagonal, octagonal, decagonal or dodecagonal. Three-dimensional crystals generally have icosahedral symmetry; however, examples of lower symmetries have recently been found. Since an average/structural space group cannot be defined, unlike the case of incommensurate/magnetic systems, see §§4 and 2, higher-dimensional space groups may be indicated if available, see Janssen *et al.* (1999). The diffraction pattern of a quasicrystalline phase displays a multiplicity of characteristic spacings between spots. However, by combining integer coefficients, six basic spacings allow the reproduction of an entire set of reciprocal positions. These basic spacings are derived from a 'hypercell' in the n-dimensional (n = 4, 5 or 6) description of the structure. The fourth field should contain an indication of the hypercell parameters, if available. Such information is analogous to the specification of Z for a crystalline phase.

The third field, for modulated quasicrystalline phases as for incommensurate phases in §4.3, should specify the *average quasicrystal* (corresponding to the main reflections). Field four should provide the propagation wavevector of the modulation, either as a fraction of the 'hypercell' reciprocal-lattice vectors, or in absolute units (Å^{-1}). For approximant phases, the normal space group should be given in the third field, while the fourth field should contain the dimensions of the large cell or the number of formulas in the large cell.

7.5.4. Fifth field. The recommendations of I are applicable, if relevant, see footnote **5**; if not, as is generally the case for this class of phases, the field contains only a dash.

7.5.5. Sixth field. Phases in alloys that display quasicrystalline phases are often characterized by small changes in the *measured* composition, with respect to that of the average composition. Whenever available, this information should be stated. In addition, the type of twinning in approximant phases should be indicated, including the forbidden symmetry thus generated. If the phase transition is irreversible, this should be noted here, see §7.5.2.

7.6. Examples of quasicrystalline phase nomenclature

7.6.1. $Al_{63}Cu_{17.5}Co_{17.5}Si_2$ (Fettweis *et al.*, 1995).

Q1	>1070 K	Two-dimensional decagonal $P10_5/mmc$	–	–	Reversible transition with 100 K hysteresis.
A1	<1000 K	Orthorhombic base-centred	$a \sim b \sim 51.5$, $c \sim 4.1$ Å	–	5 variants rotated by 72°.

7.6.2. $Al_{69}Pd_{22}Mn_9$ (de Boissieu *et al.*, 1998; Boudard *et al.*, 1992).

Q1	>1013 K	3-dimensional icosahedral $Fm\bar{3}\bar{5}$ or $F235$	–	–	Composition $Al_{68.8}Pd_{22}Mn_{9.2}$.
$Q2/F2_M$	<1013 K	3-dimensional hypercubic F lattice	6d hypercubic cell $a = 12.90$ Å	Twinned	Composition $Al_{69.3}Pd_{22}Mn_{8.7}$. 5 variants related to the lowering of orientational symmetry with respect to Q1.
Q3/F2	<920 K	3-dimensional icosahedral	Icosahedral cell $a' = 2a$	–	Metastable between Q1 and Q2. Composition $Al_{69.8}Pd_{21.4}Mn_{8.8}$. Superlattice of phase Q2.

8. Discussion

Wide acceptance of new nomenclature in any branch of science is achievable only if the clarity of communication within that field is thereby evidently improved. The presen-

tation of this second and final Report offers an opportunity to re-emphasize the advantages of the recommended phase-transition nomenclature. This may be illustrated by comparing it with the typical use of earlier nomenclature found in two recent reports of new crystal structures and their phase transitions. The first, by Haile & Wuensch (2000*a*) on α-$K_3NdSi_6O_{15}\cdot xH_2O$, with $2 \geq x \geq 0$, appeared in the course of preparing the present recommendations and summarized the sequence of transitions in this rare-earth silicate as:

$$\alpha \text{ (or } \alpha') \overset{400\,(30)\,\mathrm{K}}{\longleftrightarrow} \alpha_{\mathrm{I}} \quad \text{and} \quad \alpha_{\mathrm{I}} \overset{415\,(25)\,\mathrm{K}}{\longleftrightarrow} \alpha_{\mathrm{II}},$$

where the designation α distinguishes the dihydrate from its polymorphic anhydride β-$K_3NdSi_6O_{15}$ (Haile & Wuensch, 2000*b*). The recommended six-field notation for the sequence in α-$K_3NdSi_6O_{15}\cdot 2H_2O$, retaining the original phase labels, is:

α_{II}	>1373−415 K	–	–	Non-ferroic $\sigma_{11}(873\,\mathrm{K}) = 34\,\mathrm{M\Omega\,m^{-1}}$ $\sigma_{33}(873\,\mathrm{K}) = 170\,\mathrm{M\Omega\,m^{-1}}$	Anhydrous.
α_{I}	415 (25)−400 (30) K	–	–	Non-ferroic insulator	May or may not contain H_2O.
α'	300 K>6 months	*Pnnm* (58)	$Z = 8$	Non-ferroic insulator	Room-temperature ordering of α.
α	<400 (30) K	*Pbam* (55)	$Z = 4$	Non-ferroic insulator	Hydrothermally grown.

The second, by Gaudin *et al.* (2000) on Cu_7PSe_6 in the same journal issue, summarized its sequence of phase transformations as $\alpha \rightarrow \beta$ at 250 (1) K and $\beta \rightarrow \gamma$ at 320 (1) K. The recommended six-field notation for the transitions in Cu_7PSe_6, retaining the original phase labels, is:

γ	≥ 320 (1) K	$F\bar{4}3m$ (216)	$Z = 4$	Non-ferroic ionic conductor	Type = *argyrodite*.
β	320−250 K	$P2_13$ (198)	$Z = 4$	Non-ferroic	Type = *argyrodite*.
α	≤ 250 (1) K	–	–	Non-ferroic	Type = *argyrodite*.

These reports were probably submitted without knowledge of the nomenclature recommendations in I. An obvious advantage of the Working Group's notation for the first case is that the properties of the phase sequence are immediately apparent, rather than dispersed over many pages (the β phase is reported to grow hydrothermally under conditions similar to the α phase but not to undergo a transition to the α phase). In both cases, and quite generally, the recommended notation instantly reveals the potential interest that any material exhibiting a phase transition might have for the reader, in a short and standard format, without a need to search the literature. It also reveals the conditions and order under which the sequence of phases form; in the event that a single parameter, such as temperature, is the only variable investigated, it enhances the possibility that other variables might be considered. Important missing information associated with the phase transition(s) is immediately revealed; in the case of α-$K_3NdSi_6O_{15}\cdot 2H_2O$, the space group and structure of both higher-temperature phases is unknown. In the case of α-Cu_7PSe_6, its structure has not yet been given but is to be published. The present primary interest in both materials is related to their conductance.

Further examples of the notation in other structural phase transitions may be found in the first Report (Tolédano *et al.*, 1998). As noted in I, §5, it is recommended that, following first use of the full six-field notation in a paper for identifying a given phase transition, the first two fields only need be used thereafter unless the phase is not associated with a label. In that case, the second two fields suffice for phase identification.

Finally, it is appropriate to address the question of the potential for computer use of the nomenclature. The exchange, storage and retrieval of structural data over the last decade has been greatly strengthened by the adoption of the Crystallographic Information File (CIF; Hall *et al.*, 1991) as the method for submitting manuscripts electronically to the IUCr for publication. The following discussion of a possible adaptation of this approach to the nomenclature recommended for structural phase transitions in our first Report (Tolédano *et al.*, 1998) and to that in the present Report is based upon an analysis by I. D. Brown, Chair of the Committee for the Maintenance of the Crystallographic Information File Standard (COMCIFS).

All symbols used in the recommended nomenclature are readily represented by ASCII characters using various text conventions. However, the intent of the CIF goes beyond simple text transcription by using a tag–value pair to identify particular items of information with a name that labels the item and a value for that item. A dictionary defining these tags enables the computer to relate given items to any other item in the CIF. The computer, for example, may thus locate other structures with the same item value.

The recommended nomenclature symbols are necessarily defined rather informally. For example, the label in the first field is defined as that in common use; another user, however, may assign a different label. This field is hence not, in general, unique. The alternative policy of recommending a uniform rational system for label assignment to each phase is regarded as unlikely to be successful, in view of the long-established tradition of nickname assignment and the diversity of disciplines in which phase transitions are studied. Similarly, the numerical range(s) of the variable(s) defining the stability field is experimental, hence open to change as techniques improve; thus, the second of the six nomenclature fields is in general also bound to lack uniqueness, as are the two final fields.

A consequence of the necessarily imprecise phase identifiers is that, while the recommended nomenclature *per se* is computer readable, its need to provide a compact identification for each phase that is both intuitive and informative conflicts with the computer requirements for labels that are unique and precise. This conflict represents a major problem that besets the present development of computer-based chemical and physical crystallographic information systems.

It is a pleasure to thank Dr David D. Cox for discerning comments on an early draft of the nomenclature proposed for magnetic phases, Dr Eric B. Sirota for a discussion of *n*-hexadecane, Professor Y. Ohashi for discussions of photo-induced structural changes, Professor I. D. Brown for

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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 τ in two orthogonal directions in the quasiperiodic plane of the two-dimensional decagonal quasicrystal.

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