

Dear David:

Many thanks for your Discussion Paper #7 on phase ID and all the thought, with which I am in general agreement, that has clearly gone into it. Specific suggestions for possible incorporation into the draft Report to be considered by the Working Group follow:

1. The IUCr phase nomenclature divides fields by a vertical bar ($\bar{}$), not a solidus ($/$). Since the former symbol is found on all keyboards, I propose retaining it in the IChI symbol.
2. In §2.1, having provided an IChI example you note “The following is an explanation of the above IChI as far as I can figure it out.” Since our Report should certainly incorporate an authoritative explanation of all IChI abbreviations to be used, why not run that explanation by the IChI group so that possible misunderstandings, including case sensitivity, may be eliminated.
3. In §3.2 under COMPOSITION, an example of a formula unit in which ‘one or more of the multipliers is non-integral, so that the size of the formula unit is indeterminate and only the relative multipliers are meaningful’ should be given for clarity. Similarly for cases in which ‘non-integral multipliers are encountered’, the ‘tolerance factor to allow for experimental uncertainties’ should be defined and a clarifying example given.

Under PH, I suggest we add each of the crystalline states for which a specific nomenclature is given in the second IUCr phase nomenclature Report, namely magnetic, incommensurate, composition-changed morphotropic, polytype and transient-structural in addition to quasicrystalline phases. Incidentally, the abbreviation ‘amp’ for amorphous is not very intuitive; perhaps a five-letter symbol would be clearer, *e.g.*

liquid	liquid
amphs	amorphous
solid	solid of unknown form
cryst	crystal
liqcr	liquid crystal
magcr	magnetic crystal
incr	incommensurate crystal
comcr	composition-changed morphotropic crystal
polcr	polytype crystal
trncr	transient-structural crystal
quasi	quasicrystal

4. Responding to your invitation that we suggest ‘the best’ way in which the IChI phase identifier could be incorporated into the IUCr phase transition nomenclature, I would argue that a union of the two symbolic systems has greater value than the sum of the two used separately, at least when first introduced. As suggested by the examples below, the united symbol indicates to the potential user a means of searching the literature for a given inorganic or organic crystalline phase for all cases in which that phase can be appropriately identified.

You also ask for some additional examples under §3.3. Combining the two requests, an example taken from each of the two IUCr Phase Nomenclature Reports is presented. A pair of vertical bars (all bars are in bold type below, for emphasis) is used to separate the IChI from the IUCr symbol, as follows:

K_2TeBr_6 |PH:xtl|SG:14:*ae4*||III|<400K| $P2_1/n(14)$ |Z=2|Ferroelastic|12 variants

$(CH_3)_3NCH_2COO \cdot CaCl_2 \cdot 2H_2O$ |PH:xtl(incr)|SG:33:*a28*||XVI|<50K, 4GPa,<180K|
 $Pn2_1a(33)$ |Z=4|Ferroelectric|Nonmodulated ferroelectric polarization along *b*

[I had hoped that Jean-Claude Tolédano might endorse or improve Suggestion 4 but suspect he may be out of town.]

Best wishes

