3. CIF DATA DEFINITION AND CLASSIFICATION

```
_phasing_MIR_der_refln.HL_D_iso
_phasing_MIR_der_refln.phase_calc
```

(*e*) PHASING_MIR_DER_SHELL
- `_phasing_MIR_der_shell.d_res_high`
- `_phasing_MIR_der_shell.d_res_low`
- `_phasing_MIR_der_shell.der_id`
      → `_phasing_MIR_der.id`
  `_phasing_MIR_der_shell.fom`
  `_phasing_MIR_der_shell.ha_ampl`
  `_phasing_MIR_der_shell.loc`
  `_phasing_MIR_der_shell.phase`
  `_phasing_MIR_der_shell.power`
  `_phasing_MIR_der_shell.R_cullis`
  `_phasing_MIR_der_shell.R_kraut`
  `_phasing_MIR_der_shell.reflns`

(*f*) PHASING_MIR_DER_SITE
- `_phasing_MIR_der_site.der_id`
      → `_phasing_MIR_der.id`
- `_phasing_MIR_der_site.id`
  `_phasing_MIR_der_site.atom_type_symbol`
      → `_atom_type.symbol`
+ `_phasing_MIR_der_site.B_iso`
+ `_phasing_MIR_der_site.Cartn_x`
+ `_phasing_MIR_der_site.Cartn_y`
+ `_phasing_MIR_der_site.Cartn_z`
  `_phasing_MIR_der_site.details`
+ `_phasing_MIR_der_site.fract_x`
+ `_phasing_MIR_der_site.fract_y`
+ `_phasing_MIR_der_site.fract_z`
  `_phasing_MIR_der_site.occupancy`
  `_phasing_MIR_der_site.occupancy_anom`
  `_phasing_MIR_der_site.occupancy_anom_su`
  `_phasing_MIR_der_site.occupancy_iso`
  `_phasing_MIR_der_site.occupancy_iso_su`

The bullet (●) indicates a category key. Where multiple items within a category are marked with a bullet, they must be taken together to form a compound key. The arrow (→) is a reference to a parent data item. Data items marked with a plus (+) have companion data names for the standard uncertainty in the reported value, formed by appending the string `_esd` *to the data name listed.*
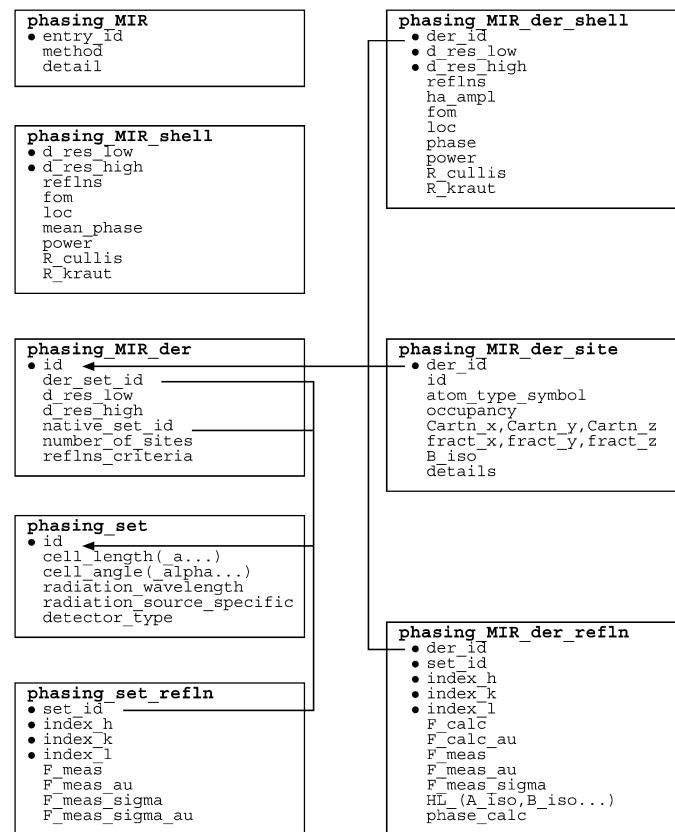

Fig. 3.6.6.2. The family of categories used to describe MIR phasing. Boxes surround categories of related data items. Data items that serve as category keys are preceded by a bullet (●). Lines show relationships between linked data items in different categories with arrows pointing at the parent data items.

PHASING_MIR and related categories provide information about phasing by methods involving multiple isomorphous replacement (MIR). These same categories may also be used to describe phasing by related techniques, such as single isomorphous replacement (SIR) and single or multiple isomorphous replacement plus anomalous scattering (SIRAS, MIRAS). The relationships between the categories describing MIR phasing are shown in Fig. 3.6.6.2.

As with the other overview categories described in this section, the PHASING_MIR category contains data items that can be used for text-based descriptions of the method used and any special aspects of its application. There are also items for describing the resolution limit of the reflections that were phased, the figures of merit for all reflections and for the acentric reflections phased in the native data set, and the total numbers of reflections and their inclusion threshold in the native data set. Statistics for the phasing can be given by shells of resolution using data items in the PHASING_MIR_SHELL category.

An MIR phasing experiment involves one or more derivatives. The remaining categories in this group are used to describe aspects of each derivative (Example 3.6.6.5). A derivative in this context does not necessarily correspond to a data set; for instance, the same data set could be used to one resolution limit as an isomorphous scatterer and to a different resolution (and with a different sigma cutoff) as an anomalous scatterer. These would be treated as two distinct derivatives, although both derivatives would point to the same data sets *via* `_phasing_MIR_der.der_set_id` and `_phasing_MIR_der.native_set_id` (see Fig. 3.6.6.2).

Data items in the PHASING_MIR_DER category can be used to identify and describe each derivative. The resolution limits for the individual derivatives need not match those of the overall phasing experiment, as the phasing power of each derivative as a function of resolution will vary. Many of the statistical descriptors of phasing given in the PHASING_MIR category are repeated in this category, as derivatives vary in quality and their contribution to the phasing must be assessed individually. These same statistical measures can be given for shells of resolution in the PHASING_MIR_DER_SHELL category.

Data items in the PHASING_MIR_DER_REFLN category can be used to provide details of each reflection used in an MIR phasing experiment. The pointer `_phasing_MIR_der_refln.set_id` links the reflection to a particular set of experimental data and `_phasing_MIR_der_refln.der_id` points to a particular derivative used in the phasing (as mentioned above, derivatives in this context do not equate to data sets). The phase assigned to each reflection and the measured and calculated values of its structure factor can be given. (It is not necessary to include the measured values of the structure factors in this list, since they are accessible in the PHASING_SET_REFLN category, but it may be convenient to present them here). Data items are also provided for the *A*, *B*, *C* and *D* phasing coefficients of Hendrickson & Lattman (1970).

The heavy atoms identified in each derivative can be listed using data items in the PHASING_MIR_DER_SITE category. Most of the data names are clear analogues of similar items in the ATOM_SITE category; an exception is `_phasing_MIR_der_site.occupancy_anom`, which specifies the relative anomalous occupancy of the atom type present at a heavy-atom site in a particular derivative.

references