

## 3.6. CLASSIFICATION AND USE OF MACROMOLECULAR DATA

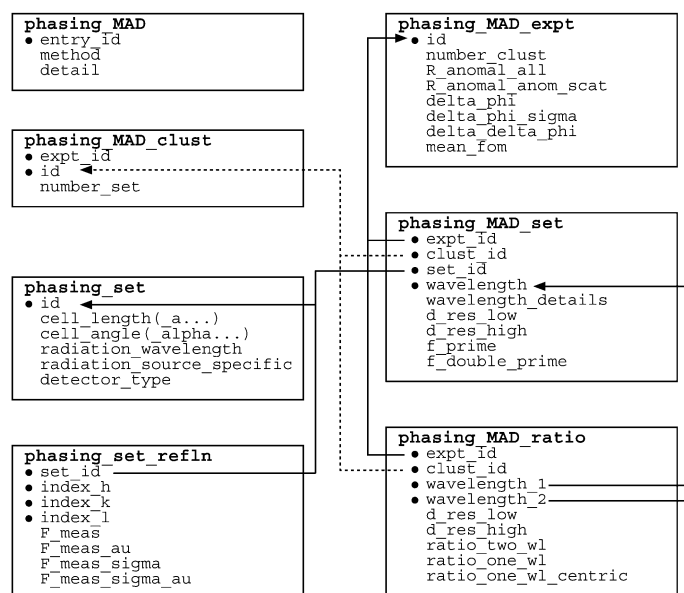


Fig. 3.6.6.1. The family of categories used to describe MAD phasing. Boxes surround categories of related data items. Data items that serve as category keys are preceded by a bullet (•). Lines show relationships between linked data items in different categories with arrows pointing at the parent data items.

The relationships between categories describing MAD phasing are shown in Fig. 3.6.6.1.

Data items in the PHASING\_MAD category allow a brief overview of the method that was used to be given and allow special aspects of the phasing strategy to be noted; data items in this category are analogous to the data items in the other overview categories describing phasing techniques.

In the data model for MAD phasing used in the present version of the mmCIF dictionary, a collection of data sets measured at different wavelengths can be used to construct more than one set of phases. These phase sets will produce electron-density maps with different local properties. The model of the structure is often constructed using information from a collection of these maps. The collections of multiple phase sets are referred to as ‘experiments’ and the groups of data sets that contribute to each experiment are referred to as ‘clusters’. Data items in PHASING\_MAD\_EXPT identify each experiment and give the number of contributing clusters. Additional data items record the phase difference between the structure factors due to normal scattering from all atoms and from only the anomalous scatterers, the standard uncertainty of this quantity, the mean figure of merit, and a number of other indicators of the quality of the phasing.

Data items in the PHASING\_MAD\_CLUST category can be used to label the clusters of data sets and give the number of data sets allocated to each cluster. In Example 3.6.6.4 two experiments are described. The first experiment contains two clusters, one of which contains four data sets and the second of which contains five data sets. The second experiment contains a single cluster of five data sets. Note that the author has chosen informative labels to identify the clusters (‘four wavelength’, ‘five wavelength’). Carefully chosen labels can help someone reading the mmCIF to trace the complex relationships between the categories.

Data items in the PHASING\_MAD\_RATIO category can be used to record the ratios of phasing statistics (Bijvoet differences) between pairs of data sets in a MAD phasing experiment, within shells of resolution characterized by `_phasing_MAD_ratio.d_res_high` and `*.d_res_low`.

The data sets used in the MAD phasing experiments are described using data items in the PHASING\_MAD\_SET category.

Each data set is characterized by resolution shell and wavelength, and by the  $f'$  and  $f''$  components of the anomalous scattering factor at that wavelength. The actual observations in each data set and the experimental conditions under which they were made are recorded using data items in the PHASING\_SET and PHASING\_SET\_REFLN categories.

## 3.6.6.1.5. Phasing via multiple isomorphous replacement

The data items in these categories are as follows:

## (a) PHASING\_MIR

- `_phasing_MIR.entry_id`  
→ `_entry.id`
- `_phasing_MIR.details`
- `_phasing_MIR.d_res_high`
- `_phasing_MIR.d_res_low`
- `_phasing_MIR.FOM`
- `_phasing_MIR.FOM_acentric`
- `_phasing_MIR.FOM_centric`
- `_phasing_MIR.method`
- `_phasing_MIR.reflns`
- `_phasing_MIR.reflns_acentric`
- `_phasing_MIR.reflns_centric`
- `_phasing_MIR.reflns_criterion`

## (b) PHASING\_MIR\_SHELL

- `_phasing_MIR_shell.d_res_high`
- `_phasing_MIR_shell.d_res_low`
- `_phasing_MIR_shell.FOM`
- `_phasing_MIR_shell.FOM_acentric`
- `_phasing_MIR_shell.FOM_centric`
- `_phasing_MIR_shell.loc`
- `_phasing_MIR_shell.mean_phase`
- `_phasing_MIR_shell.power`
- `_phasing_MIR_shell.R_cullis`
- `_phasing_MIR_shell.R_kraut`
- `_phasing_MIR_shell.reflns`
- `_phasing_MIR_shell.reflns_acentric`
- `_phasing_MIR_shell.reflns_anomalous`
- `_phasing_MIR_shell.reflns_centric`

## (c) PHASING\_MIR\_DER

- `_phasing_MIR_der.id`  
`_phasing_MIR_der.d_res_high`  
`_phasing_MIR_der.d_res_low`  
`_phasing_MIR_der.der_set_id`  
→ `_phasing_set.id`
- `_phasing_MIR_der.details`
- `_phasing_MIR_der.native_set_id`  
→ `_phasing_set.id`
- `_phasing_MIR_der.number_of_sites`
- `_phasing_MIR_der.power_acentric`
- `_phasing_MIR_der.power_centric`
- `_phasing_MIR_der.R_cullis_acentric`
- `_phasing_MIR_der.R_cullis_anomalous`
- `_phasing_MIR_der.R_cullis_centric`
- `_phasing_MIR_der.reflns_acentric`
- `_phasing_MIR_der.reflns_anomalous`
- `_phasing_MIR_der.reflns_centric`
- `_phasing_MIR_der.reflns_criteria`

## (d) PHASING\_MIR\_DER\_REFLN

- `_phasing_MIR_der_refl.der_id`  
→ `_phasing_MIR_der.id`
- `_phasing_MIR_der_refl.index_h`
- `_phasing_MIR_der_refl.index_k`
- `_phasing_MIR_der_refl.index_l`
- `_phasing_MIR_der_refl.set_id`  
→ `_phasing_set.id`
- `_phasing_MIR_der_refl.F_calc`
- `_phasing_MIR_der_refl.F_calc_au`
- `_phasing_MIR_der_refl.F_meas`
- `_phasing_MIR_der_refl.F_meas_au`
- `_phasing_MIR_der_refl.F_meas_sigma`
- `_phasing_MIR_der_refl.F_meas_sigma_au`
- `_phasing_MIR_der_refl.HL_A_iso`
- `_phasing_MIR_der_refl.HL_B_iso`
- `_phasing_MIR_der_refl.HL_C_iso`