modulation of the atom-site properties. They fall naturally into families describing the modulation of atomic displacement, of site occupation or of thermal parameters.

New data items are added to several categories in the core CIF dictionary that describe molecular or packing geometry. There are also new data items to describe superspace-group symmetry.

3.4.3.3.1. *Atom sites*

Data items in these categories are as follows:

(*a*) ATOM_SITE

```
_atom_site_displace_modulation_flag
_atom_site_occ_modulation_flag
_atom_site_subsystem_code
      → _cell_subsystem_code
_atom_site_U_modulation_flag
```

(*b*) ATOM_SITE_PHASON

```
• _atom_site_phason_atom_site_label
      → _atom_site_label
  _atom_site_phason_coeff
  _atom_site_phason_formula
```

The bullet (•) *indicates a category key. The arrow* (→) *is a reference to a parent data item.*

The ATOM_SITE category is extended in the msCIF dictionary by the addition of a small number of items that may appear in the main looped list of atom-site information (see Section 3.2.4.1.1). The `*_flag` items indicate whether each individual atom site has been modelled through modulation of atomic displacement, site occupation or thermal parameters. In each case, the default value of the item is `no`, so that any or all of the flags may be omitted when that particular type of modulation has not been applied to the structural model.

`_atom_site_subsystem_code` identifies the cell subsystem to which the atom site must be assigned in the description of composite structures. Each value of `_atom_site_subsystem_code` must match one of the values of `_cell_subsystem_code` in the overall description of the subsystems defined for a composite.

The ATOM_SITE_PHASON category allow details of an atom-dependent phason correction, as implemented in *JANA2000*, to be given. The use of these phason corrections is discouraged.

3.4.3.3.2. *Modulation functions as Fourier series*

Data items in these categories are as follows:

(*a*) ATOM_SITE_DISPLACE_FOURIER

```
• _atom_site_displace_Fourier_id
  _atom_site_displace_Fourier_atom_site_label
      → _atom_site_label
  _atom_site_displace_Fourier_axis
  _atom_site_displace_Fourier_wave_vector_seq_id
      → _atom_site_Fourier_wave_vector_seq_id
```

(*b*) ATOM_SITE_DISPLACE_FOURIER_PARAM

```
• _atom_site_displace_Fourier_param_id
      → _atom_site_displace_Fourier_id
  _atom_site_displace_Fourier_param_cos
  _atom_site_displace_Fourier_param_modulus
  _atom_site_displace_Fourier_param_phase
  _atom_site_displace_Fourier_param_sin
```

(*c*) ATOM_SITE_FOURIER_WAVE_VECTOR

```
  _atom_site_Fourier_wave_vector_description
  _atom_site_Fourier_wave_vector_seq_id
  _atom_site_Fourier_wave_vector_x
  _atom_site_Fourier_wave_vector_y
  _atom_site_Fourier_wave_vector_z
```

(*d*) ATOM_SITE_OCC_FOURIER

```
• _atom_site_occ_Fourier_id
  _atom_site_occ_Fourier_atom_site_label
      → _atom_site_label
  _atom_site_occ_Fourier_wave_vector_seq_id
      → _atom_site_Fourier_wave_vector_seq_id
```

(*e*) ATOM_SITE_OCC_FOURIER_PARAM

```
• _atom_site_occ_Fourier_param_id
      → _atom_site_occ_Fourier_id
  _atom_site_occ_Fourier_param_cos
  _atom_site_occ_Fourier_param_modulus
  _atom_site_occ_Fourier_param_phase
  _atom_site_occ_Fourier_param_sin
```

(*f*) ATOM_SITE_ROT_FOURIER

```
• _atom_site_rot_Fourier_id
  _atom_site_rot_Fourier_atom_site_label
      → _atom_site_label
  _atom_site_rot_Fourier_axis
  _atom_site_rot_Fourier_wave_vector_seq_id
      → _atom_site_Fourier_wave_vector_seq_id
```

(*g*) ATOM_SITE_ROT_FOURIER_PARAM

```
• _atom_site_rot_Fourier_param_id
      → _atom_site_rot_Fourier_id
  _atom_site_rot_Fourier_param_cos
  _atom_site_rot_Fourier_param_modulus
  _atom_site_rot_Fourier_param_phase
  _atom_site_rot_Fourier_param_sin
```

(*h*) ATOM_SITE_U_FOURIER

```
• _atom_site_U_Fourier_id
  _atom_site_U_Fourier_atom_site_label
      → _atom_site_label
  _atom_site_U_Fourier_tens_elem
  _atom_site_U_Fourier_wave_vector_seq_id
      → _atom_site_Fourier_wave_vector_seq_id
```

(*i*) ATOM_SITE_U_FOURIER_PARAM

```
• _atom_site_U_Fourier_param_id
      → _atom_site_U_Fourier_id
  _atom_site_U_Fourier_param_cos
  _atom_site_U_Fourier_param_modulus
  _atom_site_U_Fourier_param_phase
  _atom_site_U_Fourier_param_sin
```

(*j*) ATOM_SITES_DISPLACE_FOURIER

```
  _atom_sites_displace_Fourier_axes_description
```

(*k*) ATOM_SITES_MODULATION

```
  _atom_sites_modulation_global_phase_t_1
  _atom_sites_modulation_global_phase_t_2
  _atom_sites_modulation_global_phase_t_3
  _atom_sites_modulation_global_phase_t_4
  _atom_sites_modulation_global_phase_t_5
  _atom_sites_modulation_global_phase_t_6
  _atom_sites_modulation_global_phase_t_7
  _atom_sites_modulation_global_phase_t_8
```

(*l*) ATOM_SITES_ROT_FOURIER

```
  _atom_sites_rot_Fourier_axes_description
```

The bullet (•) *indicates a category key. The arrow* (→) *is a reference to a parent data item.*

It is common to represent a modulated structure using a reference periodic structure on which are superimposed atomic modulation functions expanded as Fourier series. (A full discussion of this is given in Section 3.4.4.3.) The msCIF dictionary provides separate categories for listing the modulated parameters that apply to atom positions, site occupancies and thermal parameters. The structuring of the data items within each of these categories follows a similar pattern.

For example, consider the modulation of the atomic displacements. The ATOM_SITE_DISPLACE_FOURIER category allows a listing of the axis along which the displacement occurs (`*_axis`) and the wave vectors contributing to that displacement component (`*_wave_vector_seq_id`) for each relevant atom site (labelled by `_atom_site_displace_Fourier_atom_site_label`).