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be generated by applying the symmetry operations of the space group to the representative special position whose coordinates are included. Although the multiplicity and site symmetry of a given special position can be calculated if the symmetry operations are known, the Wyckoff letter cannot be calculated since it is assigned arbitrarily and is setting-independent.

As with the symmetry operations, it is possible to include the special positions of more than one space group, each space group being identified by `_space_group_Wyckoff.sg_id`.

3.8.4. Future developments

Version 1.0 of the symmetry CIF dictionary contains only the basic items needed to define the properties of the three-dimensional space groups. It is only the first step in the definition of a more comprehensive symmetry dictionary. Future versions will define items needed to describe the higher-dimensional symmetries that have recently proved popular for describing modulated structures and quasicrystals, and items to make it easier for computers to explore the relationships between a space group and its super- and subgroups.

The addition of methods in future versions of the DDL will permit the dictionary to include the expressions for calculating each item from other items in the CIF. Methods will be particularly useful in the symmetry CIF dictionary, since almost all its items can be calculated from a single item: a symmetry generator name. The symmetry CIF dictionary is an essential component in the plan to make the suite of CIF dictionaries a self-contained online compendium of crystallographic knowledge.

References

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