and space-group setting. For data sets with unknown space group, the cell parameters have been standardized assuming the space group of lowest symmetry in agreement with the Pearson symbol, *e.g. P*222 for *oP** or *o***.

Standardized data are described with respect to the standard settings described in *International Tables for Crystallography* Volume A, with the following additional restraints: inversion centre at the origin, unique *b* axis and 'best' cell for monoclinic structures (Parthé & Gelato, 1985), triple-hexagonal cell for rhombohedral structures or Niggli reduced cell for triclinic structures. As a consequence, they can easily be incorporated into any program handling crystallographic data. The systematic standardization of the crystallographic data also greatly simplifies the classification of crystal structures into different prototypes.

A conversion tool to standardize cell parameters and/or compute the Niggli reduced cell is included in the software of Pearson's Crystal Data.

3.7.5.4. *Consequent prototype assignment*

The prototype is a well known concept in inorganic chemistry, where a large number of compounds often crystallize with very similar atom arrangements. The compilation *Strukturbericht* started to catalogue crystal structures into types named by codes such as A1, B1 or A15. These notations are still in use; however, today prototypes are generally referred to by the name of the compound for which this particular kind of atom arrangement was first identified, *i.e.* Cu, NaCl and Cr_3Si for the types enumerated above. Pearson's Crystal Data uses a longer notation which also includes the Pearson symbol and the space-group number: Cu,cF4,225, NaCl,cF8,225 and Cr_3Si,cP8,223. In a few cases several prototypes correspond to the same code, for example several polytypes of CdI_2 have the same notation. A similar situation occurs for the wrong and the correct structure proposals for FeB, which have the same Pearson code and space group. In these cases a letter is added after the type-defining compound, for example the correct FeB type will be referred to as FeB-b,oP8,62.

Each prototype is defined on a particular PCD database entry. In principle, this data set represents a recent refinement of the structure of the type-defining compound, but no effort has been made to find or use the most recent determination.

All of the data sets with published coordinates in Pearson's Crystal Data have been classified into prototypes following the criteria defined in *TYPIX* (Parthé *et al.*, 1993, 1994). According to this definition, isotypic compounds must crystallize in the same space group and have similar cell-parameter ratios; the atoms should occupy the same Wyckoff positions in the standardized description and have similar positional coordinates. If all of these criteria are fulfilled, the atomic environments should be similar. Note that H^+ (protonic hydrogen) is ignored in the assignment of the prototype as well as in the Wyckoff sequence, Pearson symbol/code and atomic environments. Isopointal substitution variants are usually distinguished; however, no distinction is made between structures with fully and partly occupied atom sites. At present, 29 470 prototypes are represented.

When possible, a prototype has also been assigned to data sets without published atom coordinates. The prototype is often stated in the publication; in other cases the editors have assigned it. The editor will have added the exact space-group setting to which the cell parameters refer when this was not published. It is important to note that a prototype has been assigned at two different levels. The first is intimately related to the published data (entry level), whereas the second is assigned at the phase level and may, in some cases, be inconsistent with the crystallographic data listed below.

For partly investigated structures, the available structural information is given using a similar way, for example the complete Pearson symbol may be replaced by *t*** (tetragonal) or *cI** (cubic body-centred) and the place of the type-defining compound is occupied by an asterisk.

3.7.5.5. *Assigned atom coordinates*

In order to give an approximate idea of the actual structure, a complete set of positional coordinates and site occupancies is proposed for data sets where a prototype could be assigned but the atom coordinates were not determined. The coordinates of the type-defining entry are proposed as a first approximation. The atom distribution is inserted by an *ESDD* module that compares the chemical formula of the type-defining entry with the chemical formula of the isotypic compound where the chemical elements have been reordered by the editor so that the first element is expected to occupy the same atom sites as the first element in the type-defining formula, and so on. Depending on the character of the prototype, substitutions and/or vacancies are either distributed over all atom sites occupied by the corresponding element or are expected to occur selectively on particular atom sites.

For this category of database entries, structure drawings, diffraction patterns and interatomic distances have also been computed. The structural portion of the database is thus more extensive than the primary literature.

3.7.5.6. *External links*

When relevant, the database entries contain links to external data sources, including ASM International Alloys Phase Diagrams Centre Online, SpringerMaterials (The Landolt–Börnstein Database incorporating Inorganic Solid Phases PAULING FILE Multinaries Edition – 2010 in SpringerMaterials) and the original publication (through https://www.crossref.org/). A (static) reference to the Powder Diffraction File entry number is provided for database entries that are included in the PDF4+ product.

3.7.5.7. *Retrievable database fields*

In addition to bibliographic (*e.g.* a particular institute) and chemical (*e.g.* sulfates) searches, many characteristics of the experiment and data processing (*e.g.* single crystal, neutron diffraction, range of temperature or reliability factors) or additional studies (*e.g.* pressure-dependence studies, magnetic structure) can be used as search criteria. Published crystal data, standardized crystal data and the Niggli reduced cells can be searched, as well as crystallographic classifications such as crystal class, Pearson symbol, Pearson code, Wyckoff sequence, structure prototype or structure class. Such searches can be very valuable in identifying a structural model for a new composition and saving the work of an *ab initio* structure determination.

The Quick Search pane includes commonly used searches on chemical elements (including cations in a particular oxidation state for oxides and halides), the number of elements and functional groups. The chemical selection (and/or/not) can be combined with selection on structure prototypes, space-group numbers and symbols or the crystal system. Retrieval on cell parameters (with ranges) and bibliographic information is also