materials (conventional superconductors, superconductor reaction products, superconductor-related and high-T_c superconductors), terpenes and thermoelectric materials. There is an educational package for classroom use, and the complete PDF is available for educational use on a time-limited basis. A primary purpose of the subfile system is to limit the size of the search universe by applying prior knowledge of the system being studied. This greatly reduces the number of false positives in a database that contains hundreds of thousands of materials. Field experts are consulted to guide the criteria for subfile selection, allowing novices to use the subfiles without being a subject expert.

3.7.2.1. *Sources and formats of the PDF*

The data incorporated into the Powder Diffraction File are acquired through contributions from individual scientists, corporate laboratories, literature surveys and a Grant-in-Aid programme. Approximately 200 leading scientific journals are searched manually for powder-diffraction data. Additional literature surveys covering patents, dissertations and the remaining open literature are performed using various online resources and search techniques.

Release 2019 (the current release as of this writing) contains more than 893 400 unique material data sets. The large size and comprehensive coverage of the PDF is achieved through the ICDD's historical sources of powder data (searches of the original literature, contributions and the Grant-in-Aid programme) as well as current and historic collaborations with crystallographic database organizations. Each PDF entry is assigned a unique identifying number of the format *ss-mmm-nnnn*. The integer *ss* indicates the source of the data: 00, ICDD location/generation of powder data; 01, Inorganic Crystal Structure Database; 02, Cambridge Structural Database; 03, NIST (a short-term collaboration focused on metals and alloys); 04, Pearson's Crystal Data; 05, ICDD extraction of atomic coordinates from published sources (including incommensurate/modulated structures). Powder-diffraction data for sources 01 through 05 are computed from the crystal structures provided by these sources.

The Powder Diffraction File is designed and produced in several different formats in order to serve different groups of users. The PDF-2 database is designed for phase identification of inorganic materials; many common organic materials have also been added to this database. The PDF-4+ database is the most advanced database and is designed for both phase identification and quantitative analysis. This database has comprehensive coverage of inorganic materials and contains numerous additional features such as digitized (raw) patterns, molecular graphics and atomic coordinates to facilitate Rietveld refinements. The PDF-4+ database is also available as a portable full-function WEBPDF-4+ version. The PDF-4/Minerals database is a subset of the PDF-4+ database, and is the most comprehensive collection of mineral diffraction data. The PDF-4/Organics database is designed for phase identification of organic and coordination compounds. It contains data from ICDD sources (both experimental powder patterns and extraction of coordinates) as well as patterns calculated from CSD entries.

Advances in hardware, software and computing power have led to the collection of higher-quality powder data, and thus have necessitated higher-quality reference data to perform more complex multiphase analyses and total-pattern analyses. The PDF now includes tools that permit users to evaluate different types of data collected using different types of detectors and different sources, including X-rays, neutrons and electrons. The goal is to include ideal specimen patterns in the PDF, patterns that can be modified by the user to correspond to the current experiment. The user can select the wavelength type and various instrumental parameters to simulate the whole diffraction pattern. A crystallite size calculation was added in 2007 and an orientation function in 2011.

Since 2006, the ICDD has begun to include several types of less-crystalline materials in the database, materials for which too much information is lost when reducing the raw data to a list of *d*-spacings and intensities. These materials include clays and other layered materials, mixed-crystallinity polymers, amorphous materials and nanomaterials.

Nanomaterials often contain crystalline and amorphous fractions, and their powder patterns are difficult to generate from an ideal crystal structure. The ICDD has developed quality-evaluation methods for noncrystalline materials, and has established two additional quality marks: 'good' (G) and 'minimal acceptable' (M). These marks reflect the quality of the supporting data used to characterize the material. An amorphous material with a G quality mark has been characterized by independent analyses verifying the stated composition or thermogravimetric/differential scanning calorimetry analyses confirming the physical stability or the presence of a glass transition. A G quality mark indicates that the editors are satisfied that the pattern is representative of both the diffraction conditions and the stated chemistry and have confidence that the user can reproduce the pattern using similar conditions. The quality mark M indicates that the ICDD received some supporting documentation but it was insufficient for structural interpretation and classification of the material.

Great care needs to be taken in interpreting the patterns of mixtures of crystalline and amorphous phases, particularly in the definition and subtraction of the background. Significant work is under way to develop and adapt numerical techniques for processing full patterns of low-crystallinity materials.

3.7.2.2. *Quality marks in the PDF*

All data are critically reviewed and evaluated by the PDF editorial staff. Each pattern must pass through a four-tiered editorial review process before it can be included in the PDF. As technology evolves, the quality requirements for reference data also evolve. As a result, the information in the PDF is continuously reviewed and upgraded for accuracy and quality.

For many years, a quality mark has been assigned to each experimental PDF entry. A Star (*/S) pattern represents high-quality diffractometer or Guinier data. Several criteria must be satisfied for a pattern to be assigned a Star quality mark:

(i) The chemical composition must be well characterized.
(ii) The intensities must have been measured objectively; no visual estimation is allowed.
(iii) The pattern has a good range and an even spread of intensities.
(iv) The completeness of the pattern is sensible.
(v) The *d*-spacing of each reflection with $d \leq 2.500$ Å is given to at least three decimal places. The *d*-spacings of reflections with $d \leq 1.2000$ Å are given to at least four decimal places.
(vi) No serious systematic errors exist.
(vii) The $|\Delta 2\theta|$ value (*i.e.* the difference between the observed peak position and the position calculated from the unit