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in many cases, when a new crystal structure is being reported, only a few of the strongest lines are reported in the pdf, and other lines, especially those with lower intensity, are not reported. the icsd data is not intended for the complete structure determination of unknown materials. the database contains reliable data for structure determination only in cases where reliable x-ray diffraction data are available. this type of data is an essential tool in mineralogy and geochemistry. it is also an important source of validation for structure determination. most pdf files do not contain enough information for an unambiguous structure determination, the database is not an ideal source for determining crystal structures, but it can be an invaluable tool for comparing structure of new materials. the reported structure was determined by the author of the paper. the crystallographic structure and the experimental crystal data (dipole moments, site occupancies, etc.) are stored in the card, the crystallographic data used for structure determination (primarily the diffraction intensities and their uncertainties) are stored in the database, as of may 2013, the structure description database contained 1 million+ entries, the structures are provided with their chemical formula, crystal symmetry, space group, and stoichiometry, an individual structure can be examined by the chemical formulae window, which provides an automated search for similar structures.

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fiz karlsruhe provides the scientific and the industrial community with the world's largest database for completely identified inorganic crystal structures, icsd. the icsd data are of excellent quality and its first records date back to 1913. only data which have passed thorough quality checks are included. each of the 50 000+ icsd entries is of excellent quality, they are published in the journal of crystal structure research, a peer reviewed scientific journal published by the international union of crystallography. the journal of crystal structure research is the official scientific journal of the international union of crystallography. a peer-reviewed process ensures that the scientific content of the database is appropriate for publication in this journal. information on the published icsd-pdf cards and the journal of crystal structure research can be found in the icsd homepage. each jcpds card contains the following information: the file number, the three strongest lines, the lowest angle line, the chemical formula, the data on diffraction method used, the crystallography in the journal of crystal structure research can be found in the icsd homepage. each jcpds card contains the following information: the file number, the file number is not possible. The journal of the journal of crystal structure research can be found in the icsd homepage. each jcpds card contains the following information: the file number, the file number, the file number is possible in the possible in the journal of crystal structure research can be found in the icsd h

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