COD (Crystallography Open Database) and PCOD (Predicted)

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The COD was created in March 2003 and was built on the PDB model of open access on the Internet. It is intended that this database [1] consist of any small or medium crystal structure (inorganic, organic, organometallic). Currently the total entry number is close to 15.000, including 6.600 entries from the American Mineralogist Crystal Structure Database (AMCSD) [2], and CIF files donations from a few laboratories in Europe or from individuals. The distribution is made through an Apache/MYSQL/PHP system that takes queries on chemistry, ranges of cell parameters, volumes, etc, as well as combination of fields, and can download or upload CIF files. A large donation of CIFs is anticipated from the IUCr.

The PCOD, created in December 2003, is a COD subset of crystal structures predicted by the GRINSP computer program [3]. It is growing fast and already contains > 1000 CIF files corresponding to M_2X_3, MX_2, MX_3 or $M_aM'_bX_c$ formulations (X = O, F; M/M' = B, Na, Si, Al, P, Ca, V, Fe, Ga, Re, Zr, etc), including hypothetical zeolites and other binary compounds with N-connected 3D frameworks of M atoms (N = 3, 4, 5, 6) as well as ternary compounds with mixed M/M' frameworks. The PCOD is open for search, download and upload of predicted crystal structures (coming from any prediction computer program, inorganic or small and medium organic molecules).

Crystallographers are invited to deposit their data as CIF files.

[1] http://www.crystallography.net/ [2] http://www.geo.arizona.edu/AMS/amcsd.php [3] http://www.cristal.org/grinsp/

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