The PCOD and P2D2 databases (P for Predicted)

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The Predicted Crystallography Open Database (PCOD) [1] is an online searchable tool (http://www.crystallography.net/pcod/) offered to the scientific community. Five years after its foundation, the PCOD passed a major milestone in 2008, by archiving the 100000th entry in an attempt to gather all these theoretical crystal structures which will very probably soon exceed in number the really observed ones. Up to now, the PCOD contains essentially inorganic compounds, N- and N-N'-connected 3D nets (N = 3, 4, 5, 6) predicted with the help of the GRINSP software [2].

Research about structure prediction appears closely related to powder diffraction. The fact is that structure determination from single crystal data is currently almost totally efficient at solving any problem, provided one suitable single crystal is available. The consequence is that most efforts are now concentrated on cases still unsolved, due to the absence of this essential, large and well organized-enough single crystal. Too much complexity can preclude the structure determination by powder diffractometry (SDPD) in spite of a successful indexing. Moreover, there are cases where indexing is not realized at all. However even if showing strong iso or anisotropic line broadening, precluding indexing, the powder diffraction pattern remains a fingerprint which can be used for the selection of the best model, if any, among the generally too numerous predictions. In February 2007, from the PCOD data, was created the P2D2 (Predicted Powder Diffraction Database) [3] allowing for identification by search-match procedures in a way similar as done from the PDF (Powder Diffraction File) [4], using powder patterns calculated from the predicted crystal structures. Immediate structure solution (before indexing) is shown to be possible if the discrepancies between the predicted crystal structure cell parameters and the actual ones are < 1%.

It remains to convince more scientists to deposit their high quality virtual crystal structures into the PCOD/P2D2 as soon as they are simulated, published or not. The uses of PCOD/P2D2 already realized in external database interfaces include the integration of the data inside of the EVA search-match software [5] for identification through calculated powder patterns, the development of an user interface [6] to the PCOD (and the COD containing ~70000 actual crystal structures) allowing for visualization, importing, exporting data to other applications like GULP to calculate energies, phonon properties, molecular dynamics, free energies and so on. These realizations are the clear consequence of the open character of the PCOD data. The COD Advisory Board (see ref. [1] authors, adding S. Gražulis, Y. Matsushita, P. Moeck, M. Quirós Olozábal) encourages the scientific community to extend their uses of these open tools in an unlimited way.

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[3] Le Bail A., Powder Diffraction, in the press (2008).
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