Abstract Submitted for the NWS08 Meeting of The American Physical Society

Purpose and Features of Web-Based Open-Access Crystallographic Databases PETER SONDERGELD, PETER MOECK, Portland State University, BORIS DUSEK, HYNEK HANKE, Charles University, Prague, Czech Republic — Roughly 5,000 new crystal structures are added to the (approximately 104,000 entry) Inorganic Crystal Structure Database each year (see http://icsdweb.fiz-karlsruhe.de/index.php for an approximately 4,000 entry demonstration version). Other commercial crystallographic databases specialize in organics, metals and alloys, and "non-organics" including minerals. This presentation gives an overview over these databases and evaluates the potential of open-access databases such as the (approximately 68,000 entry) Crystallography Open Database (http://crystallography.net/) and Portland State University's (PSU's) Wiki Crystallography Database, Crystal Morphology Database, and Nano-Crystallography Database (http://nanocrystallography.research.pdx.edu/CIF-searchable). Key features of open-access crystallographic databases are: a universal data exchange format, unrestricted internet access to the actual data (including downloads), search capabilities, and crystal structure identification functionalities. Interactive threedimensional structure or morphology visualizations are also available at PSU's site. Most recently, we implemented at PSU community-based, Wikipedia-inspired data upload and database content management provisions. A selection of all of these features will be demonstrated (online) during the presentation.

> Peter Moeck Portland State University

Date submitted: 18 Apr 2008

Electronic form version 1.4