



FIZnews

New ICSD Scientific Manual 2025 – an insight into the world’s largest database for inorganic crystal structures

Karlsruhe, 10.02.2025 — [ICSD \(Inorganic Crystal Structure Database\)](#) is the world's largest database for fully determined inorganic crystal structures. It contains crystallographic data of published inorganic and organometallic structures as well as theoretically calculated structure models - a total of over 16,000 new entries per year. This well indexed content makes ICSD an indispensable tool for materials science and crystallography.

With the new Scientific Manual 2025, FIZ Karlsruhe offers a comprehensive overview of the content in ICSD and its curation as well as the latest content enhancements.

Important new features:

A significant novelty is the expanded representation and analysis of coordination polyhedra. In addition, uniform naming and classification of minerals have been introduced as part of mineral standardization. A further improvement is the integration of external links that allow users to access additional data sources for further information.

ICSD enables a precise search for structure types, contains physico-chemical keywords and allows the simulation of powder diffraction data. Data quality is ensured through continuous selection, verification and enrichment. ICSD has also been certified with the Core Trust Seal since 2023.

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Page 1 of 2



[The manual is available online](#) and is presented by us at specialist conferences. Our team will be happy to answer any questions about the content.

Page 2 of 2

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