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FIZnews

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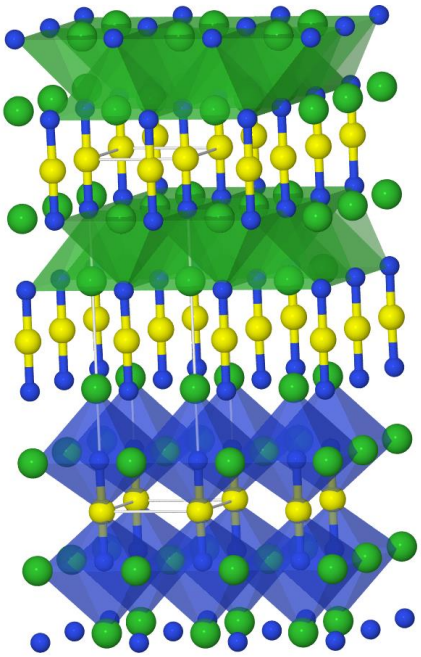
ICSD on a steep growth track – 300,000 structures mark cracked

the 300,000 structure is a nitridometallate structure

Karlsruhe, 23 May 2024— The 300,000 structure in ICSD is Ca2NiN2 and was described by Simon D. Kloß and J. Paul Attfield in the article "Low-dimensional magnetism in calcium nitridonickelate(II) Ca2 NiN2" (DOI: 10.1039/d1cc04001d). In nitridometalates, Ni with oxidation state +II is very unusual. The compound could only be synthesized at high temperature and pressure.

The crystalline Ca_2NiN_2 can be assigned to the Na_2HgO_2 structure type. The coordination spheres of the different elements are interesting here. For example, the Ni^{2+} features a linear complex anion, the stability of which is probably significantly influenced by the covalent Ni-N multiple bonding and the associated short Ni-N bond distances. The calcium and nitrogen ions form layers of edge-sharing square pyramids (CaN5; shown in green in the image) and octahedra (NCa5Ni; shown in blue in the image), respectively. The successful synthesis of Ca_2NiN_2 paves the way for a new class of late transition metal nitrides that may exhibit interesting electronic properties. This makes the compound a typical representative of inorganic compounds in ICSD that can potentially be used in research into new materials. This compound will be included in the next ICSD release 2024.2 under the collection code 149497.



ICSD is the world's largest database for fully determined inorganic crystal structures. These high-quality data date back to the first records from 1913. Only data that have passed thorough quality checks are documented. All important crystal structure data are available, including experimental inorganic and organometallic as well as theoretical structures. This thorough data curation was one of the reasons why the service was recently awarded the Core Trust Seal.

The ICSD was founded in 1977 at the University of Bonn, FIZ Karlsruhe has been significantly involved in the production and provision of the database since 1985. The 100,000 structure mark was reached only 30 years after the foundation of ICSD in 2007. Just 11 years later, the 200,000th structure was included in ICSD in 2018. The fact that the ICSD has grown to 300,000 structures just 6 years later is largely due to the expansion of the content to include experimental organometallic structures and theoretical inorganic structures.

For more information, visit https://icsd.products.fiz-karlsruhe.de/

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