08-Inorganic and Mineralogical Crystallography

PS-08.03.07
THE SYSTEM OF CLASSIFICATION AND THE BANK OF DATA FOR MINERALS.
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The problem of systematisation is urgent for the modern mineralogy.
We suggest the system of classification where the lower
taxon is a mineral species. We name by a mineral species a simple
substance of a chemical compound crystallized in the result of the
geo- or cosmo-chemical system. The basis of this classification
is the Periodic Table of the chemical elements. The suggested
classification is combined with the chemical classification. On
the first levels the classification is done by anions. The system of
the designations of minerals in decimal, connected with the position
of the chemical elements in the Periodic Table. An automatic
data bank of minerals realized on the basis of personal computer
will make it possible to enrich it with different information about
minerals.

08.04 - Inorganic Crystal Chemistry - II

PS-08.04.01
IS THE Au(I)...Au(I) 'AUROPHILIC' ATTRACTION DUE TO CORRELATION OR HYBRIDIZATION? By P. Pyrykk\\'\, J. Li, Department of Chemistry, University of Helsinki, E. Heuslerianina 4, SF-00100 Helsinki, Finland.

Ample crystallographic and some NMR evidence exists for an attraction between the sd^10 closed-shell cations Au(I)...Au(I) in pairs, oligomers, chains and sheets. Hoffmann et al. have attributed this attraction to sdsp3 hybridisation. In that case it should already appear at HF level in pseudopotential ab initio work.

We find however for (CuAuPb)_2 dimers, or the A-Enme Se(Au Pb) _2 no attraction at HF level. At MP2 or MP3 level the experimental secondary bond length (300–350 pm) and strength (7–8 kcal mol^{-1}) appear. This correlation-induced attraction is strongly enhanced by sublimation. Note that its strength equals that of the strongest hydrogen bonds. A particularly striking example is the observed geometry of Au(AuPb)_4 \(^{2-}\), which is C_4h and not T_d.


PS-08.04.02 NEUTRON DIFFRACTION INVESTIGATION OF Fe-N ALLOYS IN THE MARTENSITE STATE By T. A. Jno\\'c, E. A. El-zawi, S. Hamouda, F. Khalil and S. G. Toplouchev, Tajura Research Center, Tripoli-LIBYA.

In this investigation we use the \( \theta/2 \theta \), \( \omega \) and \( \varphi \) scanning to determine all remained austenite crystallites which have kept their orientations

after the martensitic transformation of the Fe-29.5
Ni alloys in the single crystal form. Pattems of
martenite crystallites which belong to the basis plane
of austenite (100) cannot be observed, but their
projections have been observed on this plane.

A total arrangement of the martensite crystallite
twins about the initial austenite can be described
by the \( \Omega \) point group. Neither symmetry nor arrange-
ment of martenite scattering vectors about
the austenite lattice in the present experimental
data are corresponding to the Mishiyama relations.

In this investigation where the horizontal and vertical
resolutions are adjusted to reach the best
experimental condition to reveal the orientation
matrices of martenite twins about the initial
austenite and moreover the symmetry relations of the
martenite transformation products.

Our work is a step in the procedure to create a rep-
resentative group communicating the initial and the
final products of the reconstructive martensitic
transformation through a common super group in ac-
cordance with crystallography.

PS-08.04.03 THE CRYSTAL STRUCTURE OF Cu(NH\(_2\)\(_2\))\(_4\) (ReO\(_2\))\(_2\), By O. Wittke, Universidad de Chile, Casilla 5487, Santiago, Chile and J. Costamagna and J. Garin, Universidad de Santiago, Casilla 10233, Santiago, Chile.

Blue crystals of the title compound were grown by slow precipitation from nearly saturated aqueous solutions of ammonium perchlorate and copper sulfate pentahydrate.

The molecular structure of the crystal was determined from data given by chemical analysis; IR spectrum and thermogravimetric behaviour.

The compound crystallizes with space group P1, Z = 1 and the following cell dimensions:

\[ a = 6.541(1) \text{ Å}, \quad b = 6.842(2) \text{ Å}, \quad c = 7.512(1) \text{ Å} \]
\[ a = 67.59(13), \quad \beta = 79.86(13), \quad \gamma = 70.93(12) \text{ °} \]

The structure was solved by Patterson for Ke and Cu, and by difference Fourier synthesis for N and O, using 2716 unique reflections with \( I > 2\sigma \) (Four-circle diffractometer, MoK\(_\alpha\) radiation, 8-28 scan), and refined by the full-matrix least-squares procedure. The refinement, assuming anisotropic temperature factors for all non-hydrogen atoms led to R = 3.9%. The molecular arrangement displays an essentially square planar configuration of the Cu(NH\(_2\)\(_2\))\(_2\) ion, where the copper atom is linked to two ReO\(_2\) tetrahedra. The ReO\(_2\) anions which are not centrosymmetrically related, are located above and below the plane of the complex, being distorted from a \( \Omega \) symmetry. Cu-N bond distances range from 2.012 to 2.129 Å, while the Cu-O (perchlorate) lengths are 2.416 and 2.577 Å. Distances in the ReO\(_2\) tetrahedra vary from 1.699 to 1.775 Å, the tetrahedral angles being in the range of 96.1 to 120.1°.