THE SYSTEM OF CLASSIFICATION AND THE BANK OF DATA FOR MINERALS.

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The problem of systematization 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 such 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 analogs. The system of the designations of minerals is 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.

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PS-08.04.01 IS THE Au(I)...Au(I) 'AUOPHILIC' ATTRACTION DUE TO CORRELATION OR HYBRIDIZATION? By P. Pyrykö and J. Li, Department of Chemistry, University of Helsinki, E. Hesperiankatu 4, SF-00160 Helsinki, Finland.

Ample crystallographic and some NMR evidence exists for an attraction between the 5d10 closed-shell cations Au(I)...Au(I) in pairs, oligomers, chains and sheets. Hoffmann et al. have attributed this attraction to 6sp6d hybridization. In that case it should already appear at HF level in pseudopotential ab initio work.

We find however for (ClAuPPh3)2 dimers, or the A-emme Se(AuPPh3)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 relaxation. Note that its strength equals that of the strongest hydrogen bonds. A particularly striking example is the observed geometry of Au2(AuPPh3)4, which is C2h and not T₄.


PS-08.04.02 NEUTRON DIFRACTION INVESTIGATION OF Fe-N ALLOYS IN THE MARTENSITE STATE By T. A. Abolatova, E. A. El-Zawi, S. Ramoda, F. Khall and S. G. Topouchov, Tajura Research Center, Tripoli-LIBYA.

In this investigation we used the 3/2⁰, 2θ and ω-scanning to determine all remained austenite crystallites which have kept their orientations after the martensitic transformation of the Fe-29.5 Ni alloys is the single crystal form. Pattersons of martensite crystals which belong to the basis plane of austenite 1002 cannot be observed, but their projections have been observed in this plane.

A total arrangement of the martensite crystallites twins about the initial austenite can be described by the 0₀₁₀ point group. Neither symmetry nor arrangement of the martensite scattering vectors about the austenite lattice in the present experimental data are corresponding to the Nishiyama relations.

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

Our work is a step in the procedure to create a representative group communicating the initial and the final products of the reconstructive martensitic transformation through a common super group in accordance with crystallography.

PS-08.04.03 THE CRYSTAL STRUCTURE OF Cu(NH3)4(ReO4)2 By O. Wittke, Universidad de Chile, Casilla 5487, Santiago, Chile and J. Costamagna and J. Garín, 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 permanganate 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:

\[ a = 6.54(1), \quad b = 6.842(2), \quad c = 7.512(1) \, \text{Å} \]

\[ a = 67.39(13), \quad \beta = 79.86(13), \quad \gamma = 70.93(12) \, ^{\circ} \]

The structure was solved by Patterson for Ke and Cu, and by difference Fourier synthesis for N and O, using 2716 unique reflections with \( I > 3 \sigma \) (four-circle diffractometer, MoKα radiation, 8-2θ 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 discloses an essentially square planar configuration of the Cu(NH3)4 ion, where the copper atom is linked to two ReO4 tetrahedra. The ReO4 anions which are not centrosymmetrically related, are located above and below the plane of the complex, being distorted from a Tet symmetry. Cu-N bond distances range from 2.012 to 2.129 Å, while the Cu-O (peroxide) lengths are 2.416 and 2.577 Å. Distances in the ReO4 tetrahedra vary from 1.690 to 1.775 Å, the tetrahedral angles being in the range of 95.1 to 120.1°.