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 fist levels the classification is done by anions. 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 computor 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 ?

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Ample crystallographic and some NMR evidence exists for an attraction between the $5d^{10}$ closed-shell cations Au(I)...Au(I) in pairs, oligomers, chains and sheets. Hoffmann et al. have attributed this attraction to 6s6p5d hybridization. In that case it should already appear at HF level in pseudopotential ab initio work.

We find however for $(ClAuPH_3)_2$ dimers, or the A-frame $Se(AuPH_3)_2$ 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 relativity. Note that its strength equals that of the strongest hydrogen bonds. A particularly striking example is the observed geometry of $As(AuPPh_3)_4^+$, which is C_{4v} and not T_d.

P. Pyykkö and Y.-F. Zhao, *Angew. Chem.* **103** (1991) 622.
J. Li and P. Pyykkö, *Chem. Phys. Lett.* **197** (1992) 586; *Inorg. Chem.* (subm.).

PS-08.04.02 NEUTRON DIFFRACTION INVESTIGATION OF Fe-Ni ALLOYS IN THE MARTENSITE STATE.

By T.T. Ajaal*, R.A. El-zawi, S. Hamouda, F. Khalf and S.G. Teplouchov. Tajura Research Center, Tripoli-LIBYA.

In this investigation we use the $\theta/2\theta$, ω and ψ-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 . Pattrens of martensite crystals which belong to the basis plane of austenite $(002)_\gamma$ cannot be observed , but their projections have been observed in this plane.

A total arrangement of the martensite crystallite twins about the initial austenite can be described by the O_h 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 $Cu(NH_3)_4(ReO_4)_2$.

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Blue crystals of the title compound were grown by slow precipitation from nearly saturated aqueous solutions of ammonium perrhenate 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:

$$a = 6.541(1), \quad b = 6.842(1), \quad c = 7.512(1) \quad Å$$

$$\alpha = 67.29(13), \quad \beta = 79.86(13), \quad \gamma = 70.93(12) \quad (°)$$

The structure was solved by Patterson for Re and Cu, and by difference Fourier synthesis for N and O, using 2736 unique reflections with $I > 3\sigma$ (Four-circle diffractometer, MoKα radiation, θ-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 $Cu(NH_3)_4$ ion, where the copper atom is linked to two ReO_4 tetrahedra. The ReO_4 anions which are not centrosymmetrically related, are located above and below the plane of the complex, being distorted from a T_d symmetry. Cu-N bond distances range from 2.012 to 2.128 Å, while the Cu-O (perrhenate) lengths are 2.416 and 2.577 Å. Distances in the ReO_4 tetrahedra vary from 1.690 to 1.775 Å, the tetrahedral angles being in the range of 96.1 to 120.1°.