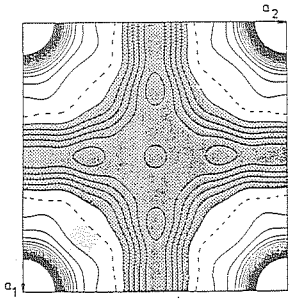
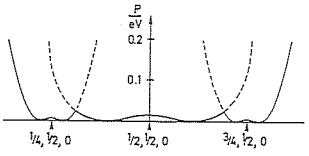
We have determined such atomic potentials for several fast ionic conductors (e.g. Ag_3SI, Ag_2S, AgI, Li_3N , $LiAlSiO_4$). These potentials can then be used to measure the activation energy. Furthermore they give hints on phase transitions. For example the Ag-potential in α-Ag_3SI allows already to predict the phase transition to the low temperature γ-phase and to estimate the temperature of the phase transition.



α-Ag_3SI (space group Im3m). Electron density at z=0. I atoms at the corners. Ag density is grey shadowed. Ag positions at (1/2,1/2,0) and (1/2,1/4,0)



Ag potential in α-Ag_3SI. Black line: Potential for an Ag ion diffusing (1/4⇔3/4,1/2,0). Black and dotted line: Potential including Repulsion terms.

07.4-01 THE CRYSTAL STRUCTURE OF $Ru_6Cu_2C(CO)_{16}(MeCN)_2$. Gerald B. Ansell, M. E. Leonowicz and Michelle A. Modrick, Analytical and Information Department and J. S. Bradley, Corporate Research Laboratories, Exxon Research and Engineering Company, P. O. Box 45, Linden, NJ 07036.

The title compound is one of several ruthenium/copper carbonyl clusters which have been synthesized as models of potential catalysts for reactions between carbon monoxide and hydrogen. The cluster was synthesized by reacting $Ru_6C(CO)_{16}^{2-}$ with $Cu(CH_3CN)_4^+$ in acetone. Single crystals were grown from methylene chloride/hexane solution and for diffraction purposes were sealed in a capillary tube with mother liquor. The crystals are triclinic with cell-dimensions a = 10.122(2), b = 16.364(2), c = 9.874(2) Å, α = 97.35(1), β = 96.58(2), γ = 77.89(1)° and have a space-group PT. The structure was solved by direct methods and 6215 independent reflections have been refined to an R value of 0.059. The structure has a unique eight metal-atom cluster containing an almost regular octahedron of six ruthenium atoms. One copper atom is situated almost at the center of one of the triangular faces of the octahedron and the second almost over the center of one of the sides of the same triangle, 2.68Å from the first copper atom. A carbido carbon is found at the center of the Ru_6 cluster. Metal-metal bond distances are 2.80-3.07 Å for Ru-Ru, 2.55-2.81 for Ru-Cu. There are 13 terminal and 3 bridged carbonyls linked to Ru_6 octahedra. Each copper atom retains one acetonitrile ligand.

07.5-01 STRUCTURAL ORDERING IN $TbFe_2$ AND YFe_2. By P. D'Antonio and J. H. Konnert, Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, D. C. 20375, and J. J. Rhyne and C. Hubbard, National Bureau of Standards, Washington, D. C. 20234.

Experimental radial distribution functions (RDF) for sputtered amorphous rare earth-transition metal compounds of YFe_2 and $TbFe_2$ have been determined. Errors due to an incorrect background, scaling of the data and termination effects have been minimized. Total neutron diffraction data were analyzed for YFe_2, whereas both total neutron and x-ray diffraction data were used for $TbFe_2$ in order to verify peak assignments in the RDF curves. The coordination numbers, internuclear distances and disorder parameters for the first six coordination spheres have been determined using the RADILS program (P. D'Antonio and J. H. Konnert, J. Appl. Cryst. (1979), 12, 634-635). The bonding topology in these materials is different than that found in their crystalline Laves phase structures. The radial distribution function, rG(r), corresponding to the topology in crystalline YFe_2-C is shown at the top of the figure. The transition metal substructure consisting of corner sharing tetrahedra is preserved in the metallic glass but the tetrahedral coordination of the rare earth atoms is not. The experimental rG(r) functions corresponding to the raw unsmoothed neutron data for YFe_2-R, the smoothed neutron data for YFe_2-N and $TbFe_2$-N and the smoothed x-ray data for $TbFe_2$-X are illustrated in the figure. The data were smoothed with a new variable filter digital FFT smoothing routine. The bulk density, ρ_o, and error estimates based on random errors in the unsmoothed, σ, and smoothed, σ_s, intensities are also shown.