

Nano-ball allophane is a naturally occurring aluminum silicate mineral with hollow spherical morphology. Diameter of the mineral is observed as 3.5 to 5.0 nm with TEM, and cation exchange experiments have proven the existence of some pores along the spherule wall. Chemical structure of the wall is similar to that of imogolite with nano-tube structure, where orthosilicates are bonded inside of gibbsite vacant site (imogolite sheet). However, whole chemical structure of the nano-ball has not been clarified. We succeeded to tentatively construct the whole chemical structure of the ball by assuming an expanded truncated octahedron composed of hexagonal imogolite sheets. By changing size of the imogolite sheets, diameters of the ball become 1.5 nm, 3.0 nm, 4.5 nm, and so on. Here we present full-structural optimization results for the nano-ball with diameter of 1.5 nm. Gaussian 03 for UNIX revision C.01 with HF/6-31G(d) method was used for calculations. The 6-coordinated Al and the 4-coordinated Si atom in the optimized structure were stable and no change in its ball shape structure. The calculated O · · · O atom distance in the vacant octahedral site that is substituted with orthosilicate has average 2.62 Å. Meanwhile, in the outer vacant octahedral sheet, the distance has average value of 4.25 Å for. It can be said that these contractions from substituted Si atom cause transformation of a planar gibbsite sheet to a material with spherical shape. Until now, there are no reports on the evidence of smallest nano-ball allophane except with diameter of 3.5 to 5.0 nm. However, our calculation result confirmed that the smallest of nano-ball allophane is stable and possible exists in the soil natural environmental.

Keywords: nano-ball allophane, *ab initio*, perfect mineral

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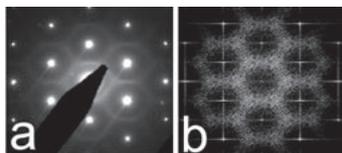
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Crystal structures and diffuse scattering of compounds with graphite-like (B,C)-nets

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The crystal structures of the new compounds Ca(B,C)₆ (hexagonal, $a = 4.563(1)\text{Å}$, $c = 4.396(1)\text{Å}$) and Ca(B,C)₈ (hexagonal, $a = 2.588(1)\text{Å}$, $c = 4.434(1)\text{Å}$) were determined from powder diffraction data. The compounds consist of planar graphite-like (B,C)-nets, intercalated by calcium atoms. In Ca(B,C)₆ one third of the hexagonal prismatic voids formed by the (B,C)-layers is occupied by Ca. In Ca(B,C)₈ the Ca-atoms are disordered, which gives rise to honeycomb-like diffuse scattering visible in the electron diffraction pattern (Fig. 1a). A model for the calcium distribution was developed and the diffuse scattering could be simulated successfully with the program DISCUS [1] (Fig. 1b).

[1] Proffen T., T., J. Appl. Cryst., 1997, 30, 171



Keywords: diffuse diffraction, powder diffraction, intercalation chemistry

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Synthesis and crystal structure of some indole derivatives complexes

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Schiff bases of hydrazone derivatives were synthesized from a condensation reaction involving hydrazones or amines and carbonyl containing compounds via reflux in ethanol for several hours. The crystal structure of the some complexes has different topology such as C18H20N8S2Ni which has a layer structure.

Keywords: indole, complexes, layer structure

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Preparation of ferrites MFe₂O₄ (M=Co,Ni) nanoporous ribbons structure and their magnetic properties

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Spinel ferrites, MFe₂O₄ (M=Co, Ni), ribbons with nanoporous structure were prepared by electrospinning combined with sol-gel technology. The ribbons were formed through the agglomeration of magnetic nanoparticles with PVP as structure directing template. The length of the polycrystalline ribbons can reach several hundred micrometers and the width of the ribbons can be tuned from several micrometers to several hundred nanometers by changing the concentration of precursor. Nanoporous structure was formed during the decomposition of PVP and inorganic salts. The ribbons exhibited weak saturation magnetizations and low coercivities at room temperature, but at low temperature, saturation magnetizations and coercivities increased a lot, especially for CoFe₂O₄ ribbons, reaching to 72 emu/g and 1.45 T at 2 K respectively. These novel magnetic ribbons can potentially be used in micro/nano electronic devices, magnetic sensors and flexible magnets.

Keywords: synthesis inorganic, magnetic oxides, ferrites

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Controllable synthesis and properties of ferric oxide nanostructural materials

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The design and synthesis of nanostructural materials have been among the important research topics of nanoscience due to their