

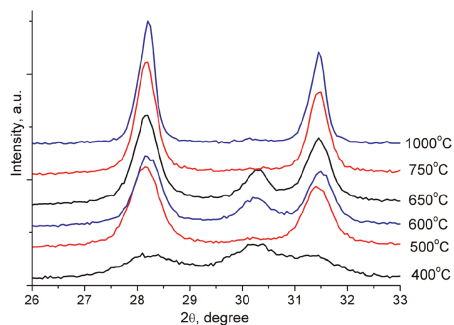
CONTENTS

Regular Articles

X-ray, Raman and FTIRS studies of the microstructural evolution of zirconia particles caused by the thermal treatment

Dmitry A. Zyuzin, Svetlana V. Cherepanova, Ella M. Moroz, Elena B. Burgina, Vladislav A. Sadykov, Victor G. Kostrovskii and Valerii A. Matyshak

Page 2965

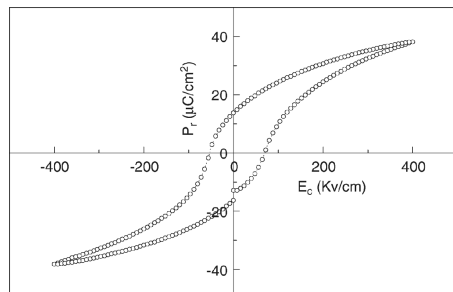


Appearance of the (111) peak of cubic phase at $2\theta \sim 30.5^\circ$ in the diffraction patterns of zirconia samples calcined at 600 and 650 °C could be explained by polysynthetic twinning in zirconia crystallites along the (001) direction.

Ferroelectric and dielectric properties of $\text{Ba}_{0.5}\text{Sr}_{0.5}(\text{Ti}_{0.80}\text{Sn}_{0.20})\text{O}_3$ thin films grown by the soft chemical method

I.A. Souza, A.Z. Simões, S. Cava, L.S. Cavalcante, M. Cilense, E. Longo and J.A. Varela

Page 2972



P-E hysteresis loops for BST:Sn film annealed at 700 °C for 2 hours in oxygen atmosphere.

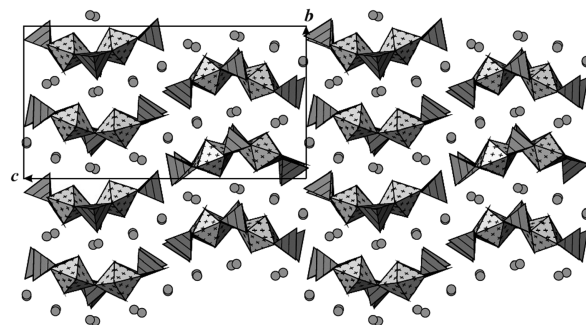
Regular Articles—Continued

One-dimensional chains in uranyl tungstates:

Syntheses and structures of $A_8[(\text{UO}_2)_4(\text{WO}_4)_4(\text{WO}_5)_2]$ ($A = \text{Rb}, \text{Cs}$) and $\text{Rb}_6[(\text{UO}_2)_2\text{O}(\text{WO}_4)_4]$

Evgeny V. Alekseev, Sergey V. Krivovichev, W. Depmeier, T. Armbruster, H. Katzke, Evgeny V. Suleimanov and Evgeny V. Chuprunov

Page 2977

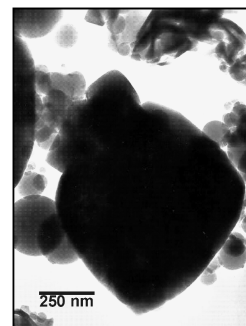


One-dimensional chains in the structure of $\text{Cs}_8[(\text{UO}_2)_4(\text{WO}_4)_4(\text{WO}_5)_2]$.

Calcium aluminates hydration in presence of amorphous SiO_2 at temperatures below 90 °C

J.M. Rivas Mercury, X. Turrillas, A.H. de Aza and P. Pena

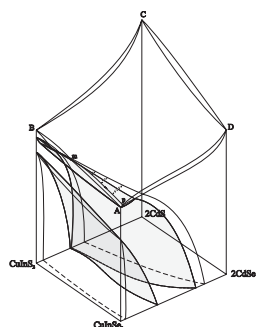
Page 2988



Katoite, $\text{Ca}_3\text{Al}_2(\text{SiO}_4)_{3-x}(\text{OH})_{4x}$ ($0 \leq 3-x \leq 0.334$), was identified besides gibbsite, $\text{Al}(\text{OH})_3$, as a crystalline stable hydration product in $\text{Ca}_3\text{Al}_2\text{O}_6$, $\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$ and CaAl_2O_4 hydrated with added amorphous silica between 40 and 90 °C.

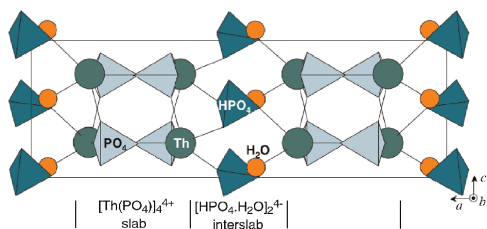
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The reciprocal $\text{CuInS}_2 + 2\text{CdSe} \rightleftharpoons \text{CuInSe}_2 + 2\text{CdS}$ system—Part II: Liquid–solid equilibria in the system
 O.V. Parasyuk, I.D. Oleksyuk, V.I. Zaremba,
 O.A. Dzham, Z.V. Lavrynyuk, L.V. Piskach,
 O.G. Yanko, S.V. Volkov and V.I. Pekhnyo
 Page 2998



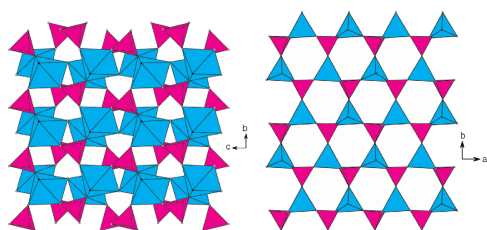
Perspective view of the reciprocal system $\text{CuInS}_2 + 2\text{CdSe} \rightleftharpoons \text{CuInSe}_2 + 2\text{CdS}$.

From thorium phosphate hydrogenphosphate hydrate to β -thorium phosphate diphosphate: Structural evolution to a radwaste storage ceramic
 Gilles Wallez, Nicolas Clavier, Nicolas Dacheux,
 Michel Querton and Wouter van Beek
 Page 3007



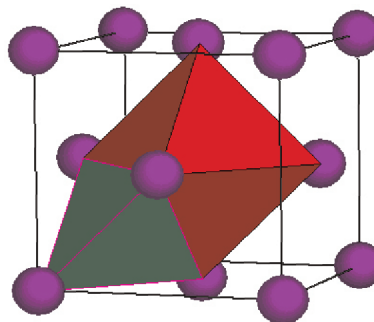
The 2D structure of the TPHPH precursor that sustains first the HPO_4 condensation and dehydration in the interslabs then a shearing of the slabs leading to stable β -TPD, a 3D framework suitable for long-term storage of actinide elements.

Layered metal phosphonates containing pyridyl groups: Syntheses and characterization of $\text{Mn}_2(2\text{-C}_5\text{H}_4\text{NPO}_3)_2(\text{H}_2\text{O})$ and $\text{Zn}(6\text{-Me-2-C}_5\text{H}_4\text{NPO}_3)$
 Yun-Sheng Ma, Yi-Fan Yang, Song Gao, Yi-Zhi Li and Li-Min Zheng
 Page 3017



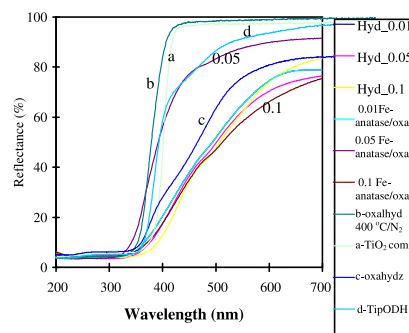
A layered manganese compound $\text{Mn}_2(2\text{-C}_5\text{H}_4\text{NPO}_3)_2(\text{H}_2\text{O})$ (1) in which chains of aqua-bridged $\{\text{Mn}_2\text{O}_2\}$ dimers are connected by $\{\text{CPO}_3\}$ tetrahedra through corner-sharing and a zinc compound $\text{Zn}(6\text{-Me-2-C}_5\text{H}_4\text{NPO}_3)$ (2) with a honeycomb layer structure are reported in this paper. Weak antiferromagnetic interactions are propagated between the Mn(II) centers in 1.

Crystal structure of $\text{Mg}_{0.65}\text{Sc}_{0.35}\text{D}_x$ deuterides studied by X-ray and neutron powder diffraction
 M. Latroche, P. Kalisvaart and P.H.L. Notten
 Page 3024



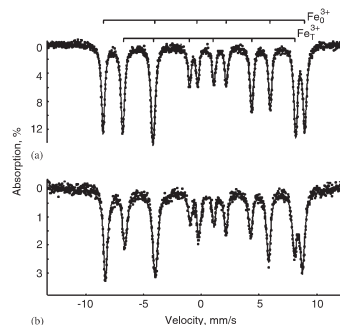
3D view of the crystal structure of $\text{Mg}_{0.65}\text{Sc}_{0.35}\text{D}_{2.2}$.

Visible light-sensitive yellow $\text{TiO}_{2-x}\text{N}_x$ and Fe–N co-doped $\text{Ti}_{1-y}\text{Fe}_y\text{O}_{2-x}\text{N}_x$ anatase photocatalysts
 K.S. Rane, R. Mhalsiker, S. Yin, T. Sato, Kuk Cho,
 E. Dunbar and Pratim Biswas
 Page 3033



DRS of TiO_2 , N/Fe–N doped TiO_2 .

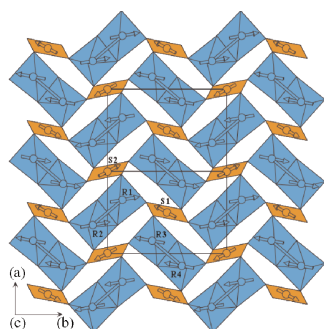
Oxygen-ion and electron conductivity in $\text{Sr}_2(\text{Fe}_{1-x}\text{Ga}_x)_2\text{O}_5$
 I.A. Leonidov, M.V. Patrakeev, J.A. Bahteeva,
 K.V. Pohlolok, D.S. Filimonov, K.R. Poeppelmeier and V.L. Kozhevnikov
 Page 3045



The ^{57}Fe Mössbauer spectra for $\text{Sr}_2(\text{Fe}_{1-x}\text{Ga}_x)_2\text{O}_5$ at 80 K: $I = 0$ (a) and $x = 0.2$ (b).

Magnetic susceptibility, specific heat and magnetic structure of $\text{CuNi}_2(\text{PO}_4)_2$

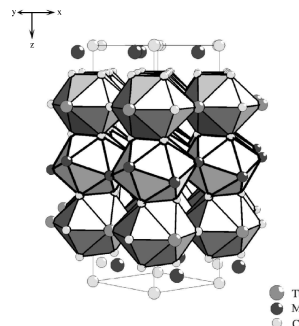
Jaione Escobal, José L. Pizarro, José L. Mesa, Aitor Larrañaga, Jesús Rodríguez Fernández, María I. Arriortua and Teófilo Rojo
Page 3052



Magnetic structure of $\text{CuNi}_2(\text{PO}_4)_2$.

Rare earth–copper–magnesium compounds RECu_9Mg_2 ($\text{RE} = \text{Y, La–Nd, Sm–Ho, Yb}$) with ordered CeNi_3 -type structure

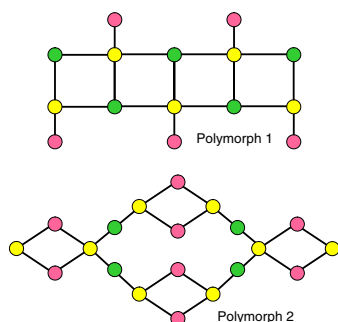
P. Solokha, V. Pavlyuk, A. Saccone, S. De Negri, W. Prochwicz, B. Marciniak and E. Różycka-Sokołowska
Page 3073



The perspective view of the arrangement of the icosahedrons and anti-cubooctahedrons in the structure of TbCu_9Mg_2 .

Synthesis and structural characterization of two polymorphs of $\text{Fe}(\text{2,2'–bpy})(\text{HPO}_4)(\text{H}_2\text{PO}_4)$

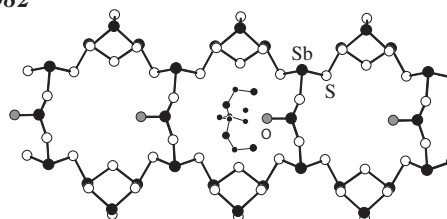
Wen-Jung Chang, Yau-Chen Jiang, Sue-Lein Wang and Kwang-Hwa Lii
Page 3059



Schematic representation of a section of a chain in polymorph 1 and a layer in polymorph 2.

$[\text{C}_6\text{H}_{21}\text{N}_4][\text{Sb}_9\text{S}_{14}\text{O}]$: Solvothermal synthesis, crystal structure and characterization of the first non-centrosymmetric open Sb–S–O framework containing the new $[\text{SbS}_2\text{O}]$ building unit

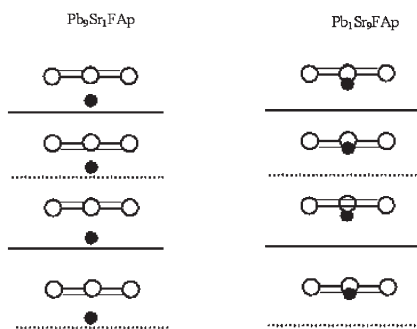
Ragnar Kiebach, Christian Näther, C. Peter Sebastian, Bernd D. Mosel, Rainer Pöttgen and Wolfgang Bensch
Page 3082



The $[\text{Sb}_9\text{S}_{14}\text{O}]^{3-}$ chain in $[\text{C}_6\text{H}_{21}\text{N}_4][\text{Sb}_9\text{S}_{14}\text{O}]$ directed along the b -axis with the organic template molecule acting like a tetradentate ligand around the O atom of the $[\text{SbS}_2\text{O}]$ group.

Structural investigations of lead–strontium fluoroapatites

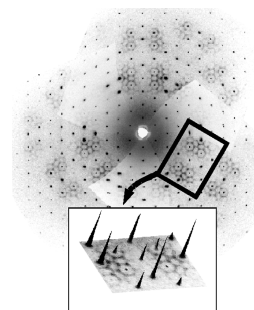
Béchir Badraoui, Abdallah Aissa, Adriana Bigi, Mongi Debbabi and Massimo Gazzano
Page 3065



The structural refinements carried out on five $\text{Pb}_{(10-x)}\text{Sr}_x(\text{PO}_4)_6\text{F}_2$ samples evidence preferential distribution of cations in metal sites and a progressive shift of the F^- ion.

Polycationic disorder in $[\text{Bi}_6\text{O}_4(\text{OH})_4](\text{NO}_3)_6$: Structure determination using synchrotron radiation and microcrystal X-ray diffraction

N. Henry, O. Mentré, F. Abraham, E.J. MacLean and P. Roussel
Page 3087

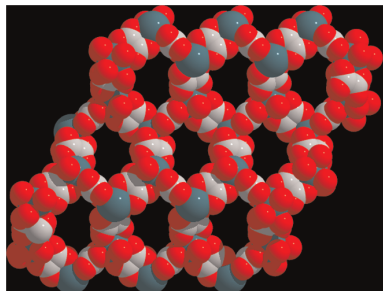


Reconstructed $hk0$ precession layer showing intense Bragg peaks and large amount of diffuse scattering.

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Two novel 3-D bismuth oxalates with organic amines protruding in channels

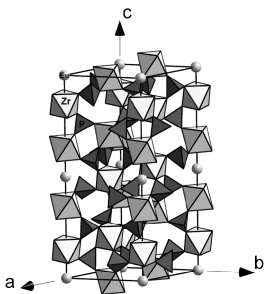
Xiaohong Yu, Hanhui Zhang, Yanning Cao, Zhongjian Hu, Yiping Chen and Zhen Wang
Page 3095



In this work, two novel 3-D oxalate-containing bismuth compounds with channels were obtained by hydrothermal method. In compound **1**, the connectivity between Bi and three oxalates gives rise to a honeycomb-like layer, with a 12-membered aperture in the *ac* plane. Then the layers are also connected through oxalate ligands, creating the 3-D structure with a channel about $5.0 \text{ \AA} \times 5.0 \text{ \AA}$ along the *c*-axis. The uncoordinated water molecules and protonated imidazole molecules were located in the channels.

Crystal structures of lanthanide and zirconium phosphates with general formula $Ln_{0.33}Zr_2(PO_4)_3$, where $Ln = Ce, Eu, Yb$

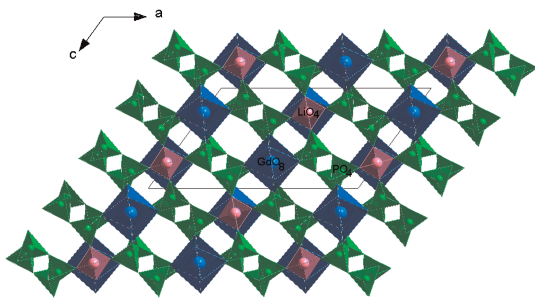
D.M. Bykov, E.R. Gobechiya, YuK Kabalov, A.I. Orlova and S.V. Tomilin
Page 3101



Fragment of structure of synthetic phosphate $Eu_{0.33}Zr_2(PO_4)_3$.

The crystal structure, thermal behaviour and ionic conductivity of a novel lithium gadolinium polyphosphate $LiGd(PO_3)_4$

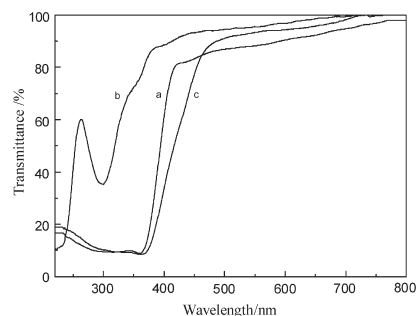
Hasna Ettis, Houcine Naïli and Tahar Mhiri
Page 3107



The structural arrangement of $LiGd(PO_3)_4$ viewed in the (010) plane.

Preparation of 5-benzotriazolyl-4-hydroxy-3-sec-butylbenzenesulfonate anion-intercalated layered double hydroxide and its photostabilizing effect on polypropylene

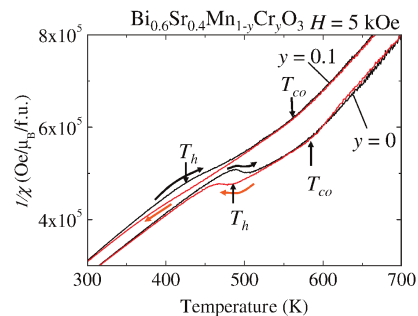
Dianqing Li, Zhenjun Tuo, David G. Evans and Xue Duan
Page 3114



Intercalation of an organic UV absorber in a layered double hydroxide host leads to an enhancement of its photo- and thermal stability.

Effect of Cr-doping on charge ordering stability in $Bi_{1-x}Sr_xMn_{1-y}Cr_yO_3$

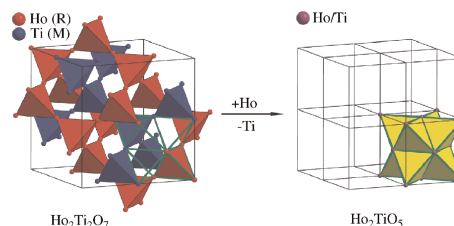
Shigeki Yamada, Eri Sugano and Taka-hisa Arima
Page 3121



Temperature dependence of $Bi_{0.6}Sr_{0.4}Mn_{1-y}Cr_yO_3$ ($y = 0, 0.1$). The abbreviation 'f.u.' denotes the formula unit. T_{co} and T_h are represented kinks or anomalies that involve hysteresis, respectively.

Stuffed rare earth pyrochlore solid solutions

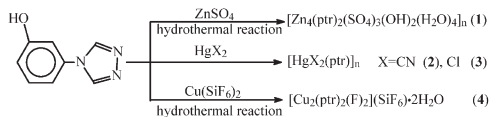
G.C. Lau, B.D. Muegge, T.M. McQueen, E.L. Duncan and R.J. Cava
Page 3126



A simplified model of the transition from pyrochlore to fluorite in the series $Ln_2(Ti_{2-x}Ln_x)O_{7-x/2}$ ($Ln = Tb-Lu, 0 \leq x \leq 0.67$), with Ho as an example. The separate corner sharing tetrahedral lattices of cations in the pyrochlore structure develop into edge sharing tetrahedra as extra *Ln* is stuffed in place of Ti. The increased spin connectivity in these new materials represents a new avenue of study in the well-known rare earth titanate pyrochlores in view of geometrical magnetic frustration.

Four triazole-bridging coordination polymers containing (*m*-phenol)-1,2,4-triazole: Syntheses, structures and properties of fluorescence and magnetism

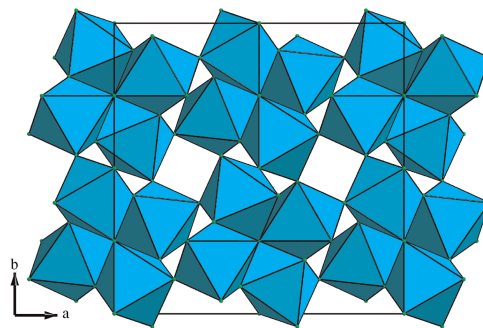
Bing Liu, Guo-Cong Guo and Jin-Shun Huang
Page 3136



Four triazole-bridging coordination complexes, $[Zn_4(ptr)_2(SO_4)_3(\mu_3-OH)_2(H_2O)_4]_n$ (1), $[Hg(CN)_2(ptr)]_n$ (2), $[Hg(Cl)_2(ptr)]_n$ (3) and $[Cu_2(\mu_2-ptr)_2(\mu_2-F)_2]_n(SiF_6)_n \cdot 2nH_2O$ (4), were synthesized with (*m*-phenol)-1,2,4-triazole (*ptr*). Compounds 1–4 with extended structures of 4-substituted 1,2,4-triazole are rarely reported.

Hypothetical AlF_3 crystal structures

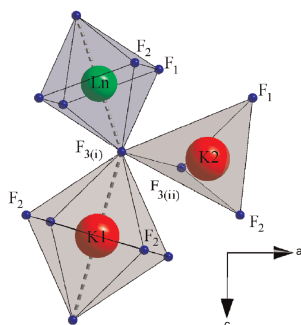
Armel Le Bail and Florent Calvayrac
Page 3159



Hypothetical AlF_3 structure with a dense packing of corner-sharing AlF_6 octahedra packed in tetrahedral blocks.

Crystal structure and vibrational properties of new luminescent hosts K_3YF_6 and K_3GdF_6

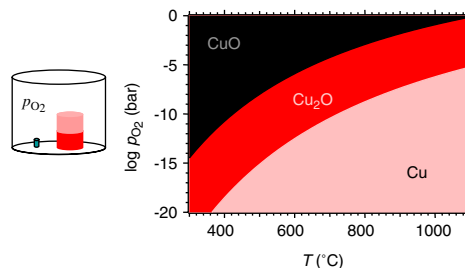
Marek Adam Gusowski, Anna Gągor, Monika Trzebiatowska-Gusowska and Witold Ryba-Romanowski
Page 3145



The coordination polyhedra of *Ln*, K(1) and K(2) atoms along *b* direction in K_3LnF_6 .

Nonstoichiometry in oxides and its control

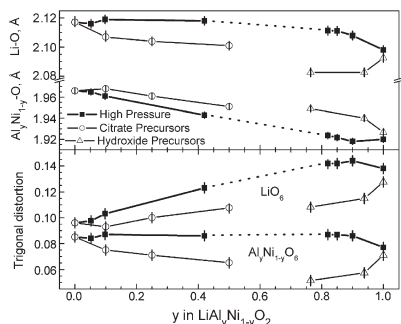
Pavel Karen
Page 3167



Oxygen nonstoichiometry control by p_{O_2} buffer.

Formation of $LiAl_yNi_{1-y}O_2$ solid solutions under high and atmospheric pressure

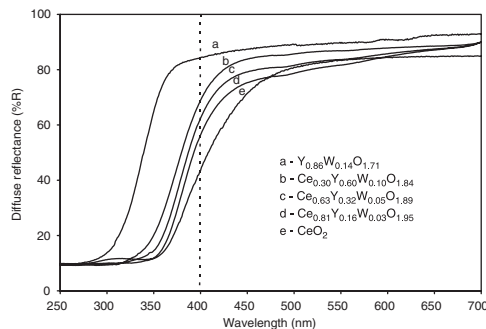
E. Shinova, E. Zhecheva and R. Stoyanova
Page 3151



The incorporation of Al into the layered structure of $LiNiO_2$ is limited.

UV absorption properties of ceria-modified compositions within the fluorite-type solid solution $CeO_2-Y_6WO_{12}$

François Cheviré, Francisco Muñoz, Charles F. Baker, Franck Tessier, Olivier Larcher, Souhir Boujday, Christophe Colbeau-Justin and Roger Marchand
Page 3184

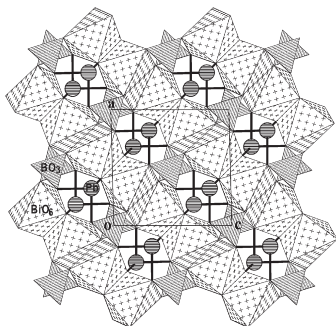


Diffuse reflectance spectra of the Ce-Y-W-O samples calcined at 1000 °C.

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Synthesis and crystal structure of a novel ternary oxoborate, PbBiBO_4

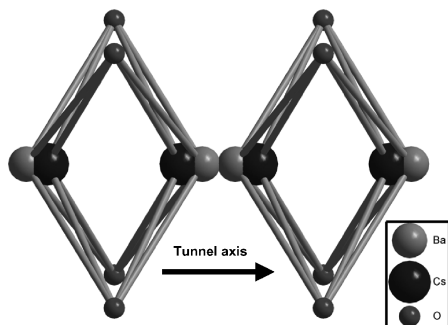
Xuean Chen, Jianlong Zuo, Xinan Chang, Yinghua Zhao, Hegui Zang and Weiqiang Xiao
Page 3191



PbBiBO_4 represents a new structure type in which $2_{\infty}[\text{BiO}_4]^{5-}$ layers are bridged by B atoms of BO_3 triangles to give rise to a three-dimensional framework. Channels parallel to the [010] direction accommodate Pb^{2+} cations.

Synthesis and characterization of hollandite-type material intended for the specific containment of radioactive cesium

A.Y. Leinekugel-le-Cocq, P. Deniard, S. Jobic, R. Cerny, F. Bart and H. Emerich
Page 3196



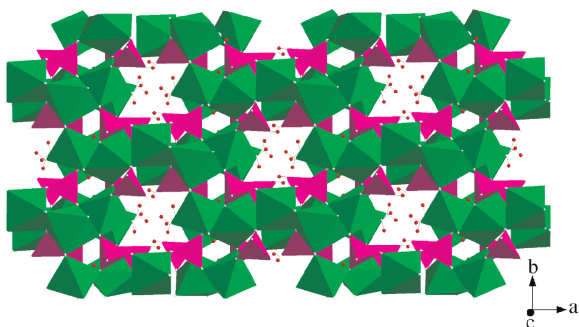
Ba and Cs location along the tunnel axis in $\text{BaCs}_{0.28}\text{Fe}_{0.82}\text{Al}_{1.46}\text{Ti}_{5.72}\text{O}_{16}$.

A new three-dimensional cobalt phosphate:



Zhangang Han, Aixiang Tian, Jun Peng and Xueliang Zhai

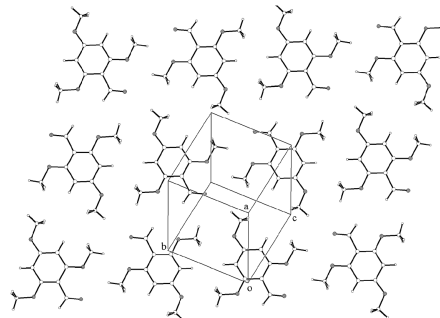
Page 3209



A 3D cobalt phosphate with a neutral framework, $\text{Co}_5(\text{OH}_2)_4(\text{HPO}_4)_2(\text{PO}_4)_2$ (**1**), has been synthesized and characterized. Compound **1** exhibits a complex net architecture based on edge- and corner-sharing of CoO_6 and PO_4 polyhedra. Its magnetic property was researched.

Solid-state structural properties of 2,4,6-trimethoxybenzene derivatives, determined directly from powder X-ray diffraction data in conjunction with other techniques

Zhigang Pan, Mingcan Xu, Eugene Y. Cheung, James A. Platts, Kenneth D.M. Harris, Edwin C. Constable and Catherine E. Housecroft
Page 3214

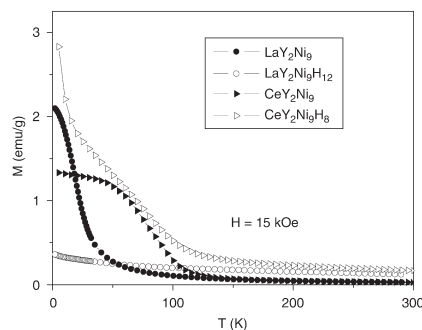


Final Rietveld refinement for 2,4,6-trimethoxyacetophenone.

Magnetic properties of RY_2Ni_9 compounds and their hydrides ($R = \text{La}, \text{Ce}$)

V. Paul-Boncour, M. Latroche and A. Percheron-Guégan

Page 3224

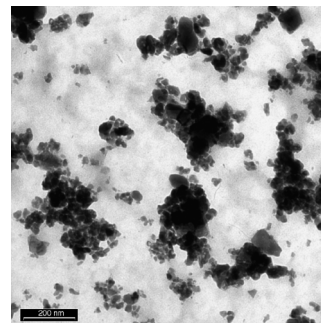


This figure shows the isofield magnetization measured at 15 KOe of the RY_2Ni_9 compounds and their hydrides ($R = \text{La}, \text{Ce}$).

Solvothermal synthesis and characterisation of $\text{La}_{1-x}\text{A}_x\text{MnO}_3$ nanoparticles

Carlos Vázquez-Vázquez and M. Arturo López-Quintela

Page 3229

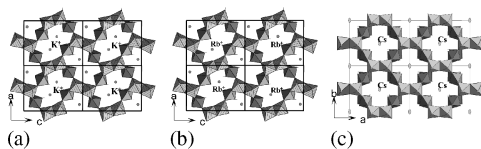


TEM of $\text{LaMnO}_3 + \delta$ calcined at 600 °C.

The $A_{1-x}\text{UNbO}_{6-x/2}$ compounds ($x=0$, $A=\text{Li, Na, K, Cs}$ and $x=0.5$, $A=\text{Rb, Cs}$): from layered to tunneled structure

S. Surblé, S. Obbade, S. Saad, S. Yagoubi, C. Dion and F. Abraham

Page 3238

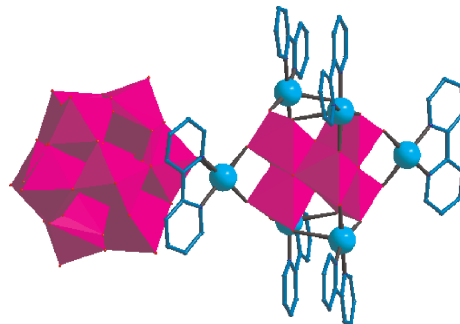


Occupation of the tunnels of the uranium niobium polyhedra framework by the alkaline metal in (a) KUNbO_6 , (b) $\text{Rb}_{0.5}\text{UNbO}_{5.75}$ and (c) $\text{Cs}_{0.5}\text{UNbO}_{5.75}$.

A novel 1D organic–inorganic hybrid based on alternating heteropolyanions $[\text{GeMo}_{12}\text{O}_{40}]^{4-}$ and isopolyanions $[\text{Mo}_6\text{O}_{22}]^{8-}$

Jing-Ping Wang, Xiao-Di Du and Jing-Yang Niu

Page 3260



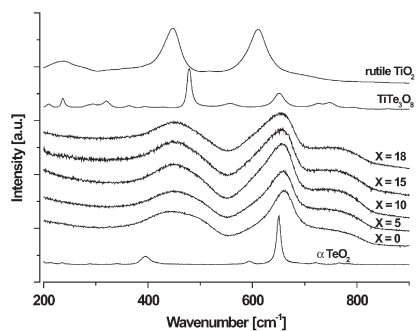
A novel polyoxometalate $[\{\text{Cu}(2,2'\text{-bpy})\}_6(\text{Mo}_6\text{O}_{22})][\text{GeMo}_{12}\text{O}_{40}] \cdot \text{H}_2\text{O}$, which represents the first example of 1D organic–inorganic hybrid based on a Keggin-type heteropolyanion $[\text{GeMo}_{12}\text{O}_{40}]^{4-}$ and an unprecedented isopolyanion $[\text{Mo}_6\text{O}_{22}]^{8-}$.

Rapid Communications

Thermal characteristics, Raman spectra and structural properties of new tellurite glasses within the $\text{Bi}_2\text{O}_3\text{--TiO}_2\text{--TeO}_2$ system

M. Udovic, P. Thomas, A. Mirgorodsky, O. Durand, M. Soulis, O. Masson, T. Merle-Méjean and J.C. Champarnaud-Mesjard

Page 3252



Raman spectra of the titanium tellurite glasses and of the relevant crystalline compounds.

NOTICE

The Keyword Index for Volume 179 will appear in the December 2006 issue as part of a cumulative index for the year 2006.