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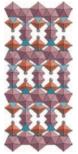
CONTENTS

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Regular Articles

New open-framework in the uranyl vanadates $A_3(UO_2)_7(VO_4)_5O$ (A = Li, Ag) with intergrowth structure between $A(UO_2)_4(VO_4)_3$ and $A_2(UO_2)_3(VO_4)_2O$ S. Obbade, C. Renard and F. Abraham *Page 413*

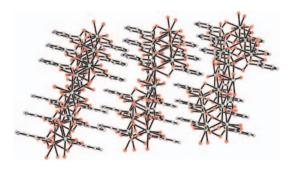


A view of the three-dimensional structure of Li₃(UO₂)₇(VO₄)₅O.

Syntheses, structures and photoluminescence of a series of lanthanide-organic frameworks involving in situ ligand formation

Xiandong Zhu, Shuiying Gao, Yafeng Li, Hongxun Yang, Guoliang Li, Bo Xu and Rong Cao

Page 421

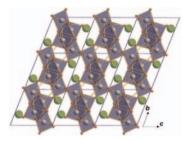


A series of lanthanide-organic frameworks with aromatic pyridinecarboxylate ligands have been successfully synthesized and characterized. Complexes 3 and 5 exhibit strong fluorescent emissions in the visible region at room temperature.

Regular Articles—Continued

A new triclinic modification of the pyrochlore-type KOs_2O_6 superconductor

S. Katrych, Q.F. Gu, Z. Bukowski, N.D. Zhigadlo, G. Krauss and J. Karpinski *Page 428*

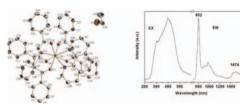


A new modification of KOs₂O₆, the representative of a new structural type (Pearson symbol aP18, a=5.5668(1)Å, b=6.4519(2)Å, c=7.2356(2)Å, α =65.377(3)°, β =70.572(3)°, γ =75.613(2)° space group P-1, no. 2 was synthesized employing high pressure technique. The structure can be described as two OsO₆ octahedral chains relating to each other through inversion and forming big voids with K atoms inside.

Synthesis, characterization, and near-infrared luminescent properties of the ternary thulium complex covalently bonded to mesoporous MCM-41

Jing Feng, Shu-Yan Song, Yan Xing, Hong-Jie Zhang, Zhe-Feng Li, Li-Ning Sun, Xian-Min Guo and Wei-Qiang Fan

Page 435

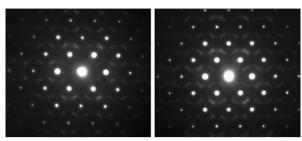


The crystal structure of Tm(DBM)₃phen complex (DBM = dibenzoylmethane; phen = 1, 10-phenanthroline). The complex is successfully covalently bonded to MCM-41 (Tm(DBM)₃phenMCM-41). After ligand-mediated excitation, the emission spectrum of Tm(DBM)₃phen-MCM-41 shows the bands 802 and 1474 nm. The FWHM of the 1474-nm band for Tm(DBM)₃phen-MCM-41 is 110 nm, such a broad spectrum enables a wide gain bandwidth for optical amplification.

Lanthanum pyrochlores and the effect of yttrium addition in the systems $La_{2-x}Y_xZr_2O_7$ and $La_{2-x}Y_xHf_2O_7$

Karl R. Whittle, Lachlan M.D. Cranswick, Simon A.T. Redfern, Ian P. Swainson and Gregory R. Lumpkin

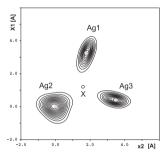
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Short-range ordering has been seen in the defect fluorites $Y_2Zr_2O_7$ and $Y_2Hf_2O_7$, where they previously were thought to be entirely disordered. Evidence suggests the correlation length changes with composition, but is not commensurate with unit cell sizes.

Silver transfer in proustite Ag₃AsS₃ at high temperatures: Conductivity and single-crystal X-ray studies

Anna Gągor, Antoni Pawłowski and Adam Pietraszko *Page 451*



Anomalous lattice parameter increase in alkali earth aluminium substituted tungsten defect pyrochlores

Gordon J. Thorogood, Brendan J. Kennedy, Vanessa K. Peterson, Margaret M. Elcombe, Gordon J. Kearley, John V. Hanna and Vittorio Luca *Page 457*

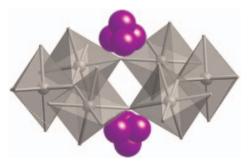
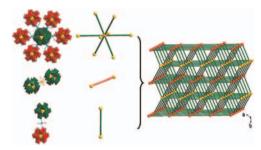


Diagram showing general disorder of K cations in $KAl_{0.33}W_{1.67}O_6$.

A series of pure inorganic eight-connected self-catenated network based on Silverton-type polyoxometalate

Huaqiao Tan, Weilin Chen, Yang-Guang Li, Ding Liu, Limin Chen and Enbo Wang

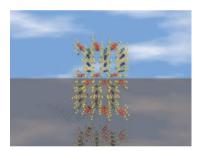
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Three extended frameworks based on Silverton-type polyoxometalate have been successfully synthesized. In these compounds, $[Ce^{IV}Mo_{12}O_{42}]^{8-}$ clusters are connected by lanthanide, transition metal and Li⁺ to form a $4^{24}56^3$ network.

Syntheses, crystal structures and spectroscopic properties of $Ag_2Nb[P_2S_6][S_2]$ and $KAg_2[PS_4]$

Yuandong Wu and Wolfgang Bensch *Page 471*

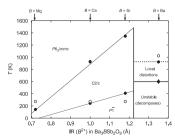


The thiophosphates $Ag_2Nb[P_2S_6][S_2]$ and $KAg_2[PS_4]$ crystallize as three-dimensional networks. A remarkable structural feature of the former compound is a $[Ag_2S_4]$ chain composed of $[AgS_4]$ tetrahedra and $[AgS_3]$ triangles.

Structures, phase transitions and microwave dielectric properties of the 6H perovskites $Ba_3BSb_2O_9$, B=Mg, Ca, Sr, Ba

Chris D. Ling, Budwy Rowda, Maxim Avdeev and Robert Pullar

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Thermodynamic phase diagram for $Ba_3BSb_2O_9$, B=Mg, Ca, and Sr, as a function of temperature T and effective ionic radius (IR) of the B^{2+} cation.

High-pressure synthesis and crystal structure of the mixed-valent titanium borate $Ti_5B_{12}O_{26}$

Almut Haberer and Hubert Huppertz *Page 484*

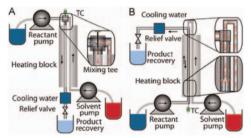


High-pressure/high-temperature synthesis (multianvil technique) led to the first mixed-valent titanium borate Ti₅B₁₂O₂₆, which is exclusively built up from corner-sharing BO₄-tetrahedra, showing structural relations to the Zintl phase NaTl.

Comparison of T-piece and concentric mixing systems for continuous flow synthesis of anatase nanoparticles in supercritical isopropanol/water

Lars L. Toft, David F. Aarup, Martin Bremholm, Peter Hald and Bo B. Iversen

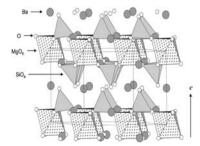
Page 491



Direct experimental comparison of T-piece and concentric mixing geometries in supercritical continuous flow synthesis of anatase nanoparticles.

Superstructure of a phosphor material Ba₃MgSi₂O₈ determined by neutron diffraction data

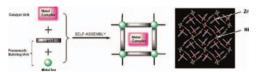
Cheol-Hee Park, Seung-Tae Hong and Douglas A. Keszler *Page 496*



Crystal structure of $Ba_3MgSi_2O_8$ viewed along the c direction. Superstructure reflections, observed only in the neutron diffraction data, provided the means to establish the true unit cell and a chemically reasonable structure.

Synthesis, structural characterization and selectively catalytic properties of metal-organic frameworks with nanosized channels: A modular design strategy

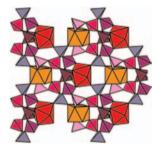
Ling-Guang Qiu, Li-Na Gu, Gang Hu and Li-De Zhang *Page 502*



A modular design strategy has been developed to synthesize microporous metal-organic frameworks with potential catalytic activity by self-assembly of the framework-building blocks and the catalyst unit.

Synthesis and crystal structure determination of yttrium ultraphosphate YP_5O_{14}

A. Mbarek, M. Graia, G. Chadeyron, D. Zambon, J. Bouaziz and M. Fourati *Page 509*

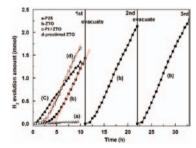


The crystal structure of the monoclinic C2/c polymorph of YP_5O_{14} has been refined from single-crystal X-ray diffraction data. The luminescence properties of the Eu^{3+} ion incorporated in this matrix as local structural probe show that the Eu^{3+} ions are distributed over the two Y^{3+} crystallographic sites of C_2 symmetry of this structure.

Hydrothermal synthesis, characterization, and photocatalytic properties of Zn_2SnO_4

Xianliang Fu, Xuxu Wang, Jinlin Long, Zhengxin Ding, Tingjiang Yan, Guoying Zhang, Zizhong Zhang, Huaxiang Lin and Xianzhi Fu

Page 517

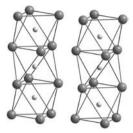


Nanosized Zn_2SnO_4 (ZTO) was successfully synthesized by hydrothermal process. Photocatalytic test showed that the samples exhibited high activity and durability for photodegradation of methyl orange (MO) and photocatalytic production H_2 from ethanol aqueous solution.

Low- and high-temperature crystal structures of TiI₃

Joachim Angelkort, Andreas Schönleber and Sander van Smaalen

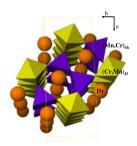
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 TiI_3 undergoes a first-order phase transition at $T_c=323\,\mathrm{K}$. The dimerization of chains of metal atoms at low temperatures is larger in TiI_3 than in corresponding chlorides and bromides, and thus provides an explanation for the larger inclination of TiI_3 towards dimerization, despite metal–metal bonds being weaker than in chlorides and bromides.

Preparation, structural and magnetic characterization of $DyCrMnO_{5}$

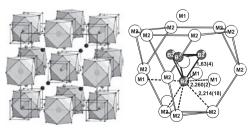
M.J. Martínez-Lope, M. Retuerto, M. García-Hernández and J.A. Alonso *Page 532*



DyCrMnO₅ is isostructural with DyMn₂O₅, belonging to the *Pbam* space group. The crystal structure contains infinite chains of edge-sharing $Mn^{4+}O_6$ octahedra, interconnected by dimer units of $Cr^{3+}O_5$ square pyramids. The low-temperature neutron powder diffraction (NPD) patterns do not show any magnetic contribution, indicating that a full long-range magnetic ordering is not established down to low temperature, although the Dy^{3+} magnetic moments are susceptible to be polarized by an external magnetic field at the lowest temperature of 5 K.

Single crystal studies on Co-containing τ -borides $Co_{23-x}M_xB_6$ (M = Al, Ga, Sn, Ti, V, Ir) and the boron-rich τ -boride $Co_{12.3}Ir_{8.9}B_{10.5}$

Dominik Kotzott, Martin Ade and Harald Hillebrecht *Page 538*

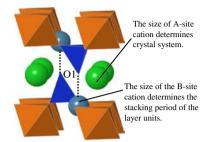


Single crystal investigations on τ -borides Co/M/B with M=Al, Ga, In, Sn, V, Ti, Ir explained the substitution processes. Furthermore the yielded the first binary boride, Co₂₃B₆, and a boron-rich Co_{12.3}Ir_{8.9}B_{10.5} containing B₄-tetrahedra.

Crystal structure of Eu²⁺-doped M₃MgSi₂O₈ (M: Ba, Sr, Ca) compounds and their emission properties

Yoshinori Yonesaki, Takahiro Takei, Nobuhiro Kumada and Nobukazu Kinomura

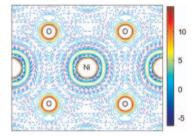
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Structure of glaserite-type $M_3MgSi_2O_8$ illustrated with MgO_6 octahedra and SiO_4 tetrahedra.

Charge density measurement and bonding character in LiNiO₂

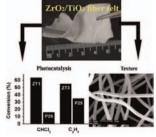
Jiefeng Cao, Chao Guo and Huamin Zou *Page 555*



Combining electron and X-ray diffraction data of $LiNiO_2$ in multipole refinement, charge density distribution, topological properties at bond critical points and 3d orbital populations of Ni atoms were obtained.

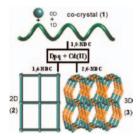
Structural characterization and photocatalytic activity of hollow binary ZrO₂/TiO₂ oxide fibers

Baochao Wu, Rusheng Yuan and Xianzhi Fu *Page 560*



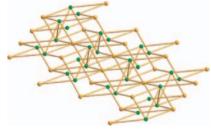
The final $\rm ZrO_2/TiO_2$ products composed of hollow fibers are in the form of felt on the centimeter scale and possess certain strength and flexibleness. Moreover, they exhibit excellent efficiency and durable activity stability for photodegradation of gaseous ethylene and trichloromethane, reaching about 136% and 387% of the $\it P25$ activity after 10 h, respectively.

Ligand-controlled assembly of Cd(II) coordination polymers based on mixed ligands of naphthalene-dicarboxylate and dipyrido[3,2-d:2',3'-f]quinoxaline: From 0D+1D cocrystal, 2D rectangular network (4,4), to 3D PtS-type architecture Guocheng Liu, Yongqiang Chen, Xiuli Wang, Baokuan Chen and Hongyan Lin *Page 566*



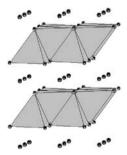
Three novel Cd(II) compounds have been synthesized under hydrothermal conditions exhibiting a systematic variation of architecture by the employment of three structurally related naphthalene-dicarboxylate ligands.

A 3D porous zinc MOF constructed from a flexible tripodal ligand: Synthesis, structure, and photoluminescence property Lili Wen, Dong'e Wang, Chenggang Wang, Feng Wang, Dongfeng Li and Kejian Deng *Page 574*



Synthesis of $\text{Li}_{(x)}\text{Na}_{(2-x)}\text{Mn}_2\text{S}_3$ and LiNaMnS_2 through redox-induced ion exchange reactions

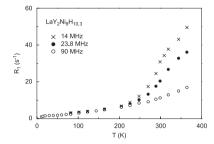
Joshua A. Luthy, Phillip L. Goodman and Benjamin R. Martin *Page 580*



Structure of LiNaMnS₂. Li and Mn are statistically distributed in edge-shared tetrahedral environments linked into infinite planes. Sodium ions occupy interlayer sites.

Nuclear magnetic resonance study of hydrogen mobility in $LaY_2Ni_9H_x$ and $CeY_2Ni_9H_x$

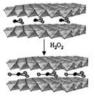
A.V. Soloninin, A.L. Buzlukov, A.V. Skripov,M. Latroche and V. Paul-BoncourPage 586



The temperature dependences of the proton spin–lattice relaxation rates R_1 measured at 14, 23.8 and 90 MHz for LaY₂Ni₉H_{10.3}. The frequency-dependent increase in R_1 at T > 250 K indicates the onset of the motional contribution to the relaxation rates.

Synthesis and intracrystalline oxidation of nitriteintercalated layered double hydroxides

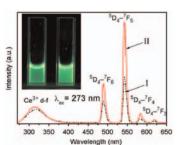
Nygil Thomas, G. Pradeep Kumar and Michael Rajamathi *Page* 592



Nitrite intercalated LDHs were prepared by a two -stage process. The interlayer nitrite ions could be quantitatively oxidized to nitrate ions using H₂O₂

Nitrite-intercalated LDHs could be prepared by a two-stage process that involves coprecipitation in the presence of nitrite ions followed by stirring the product with excess of nitrite ions. The interlayer nitrite ions in these LDHs could be quantitatively oxidized to nitrate ions.

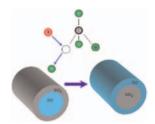
Synthesis of highly fluorescent LaF₃:Ln³⁺/LaF₃ core/shell nanocrystals by a surfactant-free aqueous solution route Meng-Yin Xie, Liao Yu, Hui He and Xue-Feng Yu *Page 597*



The LaF_3 : Ce^{3+} , Tb^{3+} nanocrystals with LaF_3 shells exhibited much stronger emission than the original cores.

Hydrogen activated axial inter-conversion in SiC nanowires Mark H. Rümmeli, David B. Adebimpe, Ewa Borowiak-Palen, Thomas Gemming, Paola Ayala,

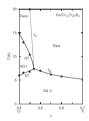
Nicholas Ioannides, Thomas Pichler, Andrzej Huczko, Stanisław Cudziło, Martin Knupfer and Bernd Büchner *Page 602*



SiC and SiO₂/SiCNWs are shown to be structurally modified through a hydrogen activated replacement route which can even lead to the axial inter-conversion of species. The process could be exploited as a viable route to manipulate a variety of nanostructures and films for doping and etching and structural manipulation.

Evolution from a ferromagnetic to a spin-glass regime in the spinel-type $Cu(Cr_{1-x}Ti_x)_2S_4$

Fumihiro Kariya, Shuji Ebisu and Shoichi Nagata *Page 608*

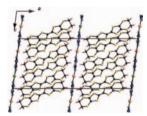


An enlargement of the magnetic phase diagram for $\operatorname{Cu}(\operatorname{Cr}_{1-x}\operatorname{Ti}_x)_2\operatorname{S}_4$ at a constant field of 100 Oe over the range of $0.40 \leqslant x \leqslant 0.70$. The curves give a guide to the eye: para, paramagnetic; ferro, ferromagnetic; SGI, spin-glass I (GT-phase), and SGII: spin-glass II (AT-phase). Three characteristic temperatures of T_c , T_{GT} , and T_{AT} merge into 7.40 K at x=0.47 in H=100 Oe. This is a multicritical point.

The first polymorph, κ'' -(ET)₂Cu[N(CN)₂]Cl, in the family of κ -(ET)₂Cu[N(CN)₂]X (X= Cl, Br, I) radical cation salts N.D. Kushch, A.V. Kazakova, L.I. Buravov, A.N. Chekhlov, A.D. Dubrovskii, E.B. Yagubskii

A.N. Chekhlov, A.D. Dubrovskii, E.B. Yagubskii and E. Canadell

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The first polymorph, κ'' -(ET)₂Cu[N(CN)₂]Cl, of the well known family of isostructural κ -salts (ET)₂Cu[N(CN)₂]X (X=Cl, Br, I) has been prepared and its crystal and electronic structures have been examined. The main structural differences between the monoclinic and orthorhombic polymorphic κ -salts are that in the first the anion sheets are disordered and the ET molecules are less planar. The new polymorph shows metallic type resistivity down to 4.2 K.

IM-16: A new microporous germanosilicate with a novel framework topology containing *d4r* and *mtw* composite building units

Yannick Lorgouilloux, Mathias Dodin, Jean-Louis Paillaud, Philippe Caullet, Laure Michelin, Ludovic Josien, Ovidiu Ersen and Nicolas Bats

Page 622

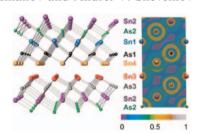


The synthesis and the structure of IM-16 a new germanosilicate with a novel zeolitic topology prepared hydrothermally with the ionic liquid 3-ethyl-1-methyl-3*H*-imidazol-1-ium as the organic structure-directing agent are reported. This new zeolite framework type contains 10-MRs channels and may be described from the *d4r* and *mtw* composite building units.

Sn₄As₃ revisited: Solvothermal synthesis and crystal and electronic structure

Kirill Kovnir, Yury V. Kolen'ko, Alexey I. Baranov, Inés S. Neira, Alexey V. Sobolev, Masahiro Yoshimura, Igor A. Presniakov and Andrei V. Shevelkov

Page 630



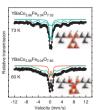
Solvothermally synthesized tin arsenide reveals non-centrosymmetric crystal structure and a complicated chemical bonding pattern including multi-center bonds and lone pairs.

Rapid Communication

Mössbauer spectroscopy analysis of 57 Fe-doped YBaCo₄O_{7+ δ}: Effects of oxygen intercalation

E.V. Tsipis, J.C. Waerenborgh, M. Avdeev and V.V. Kharton

Page 640



Mössbauer spectroscopy of layered YBaCo $_{3.96}$ Fe $_{0.04}$ O $_{7+\delta}$ ($\delta=0.02$ and 0.80), with 1% 57 Fe isotope substituted for cobalt, revealed no evidence of charge ordering at 4–293 K. The predominant state of iron cations was found trivalent, irrespective of their coordination and oxygen stoichiometry variations determined by thermogravimetric analysis. Decreasing temperature below 75–80 K leads to gradual freezing of the iron magnetic moments in inverse correlation with the content of extra oxygen extending the temperature range where the paramagnetic and frozen states coexist down to $45–50\,\mathrm{K}$.

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