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Solid-State Chemistry of Inorganic Materials III

EDITORS

Margret J. Geselbracht

John E. Greedan

David C. Johnson

M.A. Subramanian

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Symposium held November 27–30, 2000, Boston, Massachusetts, U.S.A.

EDITORS:

Margret J. Geselbracht
Reed College
Portland, Oregon, U.S.A.

John E. Greedan
BIMR, McMaster University
Hamilton, Ontario, Canada

David C. Johnson
University of Oregon
Eugene, Oregon, U.S.A.

M.A. Subramanian
Dupont Central Research & Development
Experimental Station
Wilmington, Delaware, U.S.A.

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PREFACE

Solid-state chemistry is an interdisciplinary field, attracting investigators from a diverse set of backgrounds including materials science and engineering, ceramics, chemistry, chemical engineering, mineralogy/geology, and condensed-matter physics. Researchers share the common challenge of understanding, controlling, and predicting the structures and properties of solids at the atomic level. Symposium GG, "Solid-State Chemistry of Inorganic Materials," held November 27–30 at the 2000 MRS Fall Meeting in Boston, Massachusetts, was the third in a biennial series, all held at the MRS Fall Meetings. This symposium continues to provide an international, interdisciplinary forum for the presentation and discussion of recent fundamental advances in the solid-state chemistry of inorganic materials and the impact of these advances on the development of practical applications.

Symposium GG was the third largest symposium at the 2000 MRS Fall Meeting with a total of 175 contributed papers, including 73 oral presentations and 102 poster presentations. The symposium attracted a large gathering of scientists, including a significant number of international speakers, working in this core discipline of inorganic materials research. The program lasted four days and included the presentations of 14 invited speakers and three evening poster sessions. The topics covered included novel synthetic methods leading to new materials, solving complex crystal structures using four dimensional crystallography, magnetic interactions in superconductors and colossal magnetoresistive solids, solid-state ionics, microwave dielectrics, microporous and hybrid inorganic/organic materials, negative thermal expansion and thermoelectric materials. A highlight of the symposium was an afternoon session dedicated to Professor J.M. Honig in recognition of his many contributions to the discipline of solid-state chemistry and his stewardship of the Journal of Solid State Chemistry.

The organizers would like to thank all of the people who attended and participated in this symposium and those of you who chose to contribute to these proceedings. This first experience with exclusively electronic handling of manuscripts presented a number of challenges to both authors and reviewers, and we appreciate your patience and cooperation as we navigated these challenges. Your enthusiastic participation in this symposium made it a resounding success and underscored the pivotal role that this forum plays in the solid-state chemistry community. The success of this symposium would not have been possible without the financial support received from Academic Press, DuPont Central Research & Development, Elsevier Science, and the National Science Foundation. We would like to express our sincere gratitude to David Nelson, program director of Solid-State Chemistry in NSF's Division of Materials Research, for his enthusiastic and generous financial support of this symposium.

Margret J. Geselbracht
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Structure Determination of $Ba_8CoRh_6O_{21}$, a New Member of the 2H-Perovskite Related Oxides

H.-C. zur Loye*, M. D. Smith, K. E. Stitzer
Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, 29208, USA, email: zurloye@sc.edu

A. El Abed† and J. Darriet
Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB-CNRS), Avenue du Dr. Schweitzer, 33608 Pessac Cedex, France
† Permanent Address: Mohamed I Univ., Facultédes Sciences, Oujda, Morocco.

ABSTRACT

Single crystals of $Ba_8CoRh_6O_{21}$ were grown out of a potassium carbonate flux. The structure was solved by a general method using the superspace group approach. The superspace group employed was $R\bar{3}m(00\gamma)0s$ with a = 10.0431(1) Å, c_1 = 2.5946(1) Å and c_2 = 4.5405(1) Å, V = 226.60(1) Å^3. $Ba_8CoRh_6O_{21}$ represents the first example of an m = 5, n = 3 member of the $A_{3n+3m}A'_nB_{3m+n}O_{9m+6n}$ family of 2H hexagonal perovskite related oxides and contains chains consisting of six consecutive RhO_6 octahedra followed by one distorted CoO_6 trigonal prism. These chains in turn are separated from each other by $[Ba]_\infty$ chains.

INTRODUCTION

Low-dimensional magnetic systems have attracted much interest historically due to the presence of magnetic behavior unique to structurally highly anisotropic systems. [1-3] Insights into such behavior can be gained from structural families where it is possible to systematically vary either the structure or the composition independently. For this reason, perovskite and perovskite-related oxides in particular have long provided excellent candidates for structural and physical property studies, due to the compositional and structural flexibility of this huge extended oxide family. Recently, much interest has been focussed on a large and varied group of oxides closely akin to the pseudo-one-dimensional 2H hexagonal perovskites, with the general formula $A_{3n+3m}A'_nB_{3m+n}O_{9m+6n}$ (n, m = integers, A = alkaline earth; A', B = large assortment of metals including alkali, alkaline earth, transition, main group and rare earth metals). [4-25] An early general structural classification of these materials based on the filling of interstitial sites generated by the stacking of $[A_3O_9]$ and $[A_3A'O_6]$ layers was developed by Darriet and Subramanian. [26-27] This approach easily describes the structural composition of all the commensurate members of this family of structures and can be extended to encompass members that form incommensurately modulated (aperiodic) structures.

An alternate, complementary description that highlights the low-dimensional nature of these compounds is the composite structure approach. In this structural description, these oxides consist of two crystallographically independent sub-structures, $[A]_\infty$ chains and $[(A',B)O_3]_\infty$ columns made up of distinct ratios of face-sharing octahedra and trigonal prisms. In many cases, the ratio of the repeat distances of the two chains is not a rational number and, consequently, the structure is incommensurately modulated along the chain direction. As shown previously, a better structural formulation of such composites is $A_{1+x}(A'_xB_{1-x})O_3$, where $x = n/(3m+2n)$ and