Studies on the Compounds in Ba–Fe–S System. I. Linear Chain Antiferromagnetism of Ba_2FeS_3 and Related Compounds Ba_2CoS_3 and Ba_2MnS_3. N. NAKAYAMA, K. KOSUGE, S. KACHI, T. SHINJO, AND T. TAKADA, Department of Chemistry, Faculty of Science, Kyoto University, Kyoto 606, Japan. Magnetic susceptibilities of Ba_2FeS_3, Ba_2CoS_3, and Ba_2MnS_3 show rounded maxima at 130, 125, and 100°K, respectively, which are due to quasi-one-dimensional antiferromagnetic short-range ordering. Intrachain interactions, J/k, are estimated to be −20, −15, and −12°K, respectively. ^{57}Fe Mössbauer spectra of Ba_2FeS_3 and ^{57}Fe-doped Ba_2CoS_3 and Ba_2MnS_3 at 4.2 K show long-range antiferromagnetic ordering, due to the interchain interaction. The profile of Mössbauer spectra at 4.2°K is analyzed based on the coexistence of magnetic hyperfine and quadrupole interactions, and magnetic hyperfine fields at 4.2°K are estimated to be 36, 29, and 59 kOe, respectively.

Synthesis of $Ba(V_{1-x}Ti_x)S_3$ $(0 \leq x \leq 1.0)$ Compounds and Their Structural Transitions. T. WADA, M. SHIMADA, AND M. KOIZUMI, The Institute of Scientific and Industrial Research, Osaka University, Suita, Osaka 565, Japan. The two-layer hexagonal perovskites $Ba(V_{1-x}Ti_x)S_3$ $(0 \leq x \leq 1.0)$ are prepared in a H_2S stream. A structural phase transition from a hexagonal to an orthorhombic form takes place for the powder samples with $0 \leq x \leq 0.4$ and their transition temperatures are determined to be 250°K for $x = 0$, 240°K for $x = 0.1$, 222°K for $x = 0.2$, 195°K for $x = 0.3$, and 160°K for $x = 0.4$, respectively. The phase transformation does not occur down to 90°K for the materials above $x = 0.5$.

Lattice Dynamics and Hyperfine Interactions of the Intercalation Compounds Fe_xTiS_2 $(x = \frac{1}{4}, \frac{1}{3}, \frac{1}{2})$ and $Fe_{1/3}NbS_2$ from ^{57}Fe Mössbauer Spectroscopy. MOTOMI KATADA AND R. H. HERBER, Department of Chemistry, Rutgers, The State University, New Brunswick, New Jersey 08903. The intercalates Fe_xTiS_2 $(x = \frac{1}{4}, \frac{1}{3}, \frac{1}{2})$ and $Fe_{1/3}NbS_2$ have been prepared and characterized by ^{57}Fe Mössbauer effect spectroscopy. From isomer shift systematics it is inferred that the electron configuration of the iron atom in these compounds is formally +2, high spin. $Fe_{1/2}TiS_2$ shows magnetic ordering at temperatures below about 140°K, and the internal field at 4.2°K is approximately 30 kOe. Temperature-dependent Mössbauer measurements permit a calculation of the effective vibrating mass of the resonant moiety and a lattice temperature as probed by the Mössbauer atom. The former is nearly constant and that expected for a "bare" iron atom, while the latter varies over a significant range for the four title compounds, despite the similarity in the nearest-neighbor environment around the metal atom in all cases. This variation can be accounted for by the differences in the sulfur bonding modes in these compounds.

Synthesis and Structural Study of the New Rare Earth Magnesium Borates $LnMgB_5O_{10}$ (Ln = La . . . Er). BERNADETTE SAUBAT, MARCUS VLASSE, AND CLAUDE FOUASSIER, Laboratoire de Chimie du Solide CNRS, Université de Bordeaux I, 351 cours de la Libération, 33405 Talence, Cedex, France. To obtain rare earth luminescent materials with weak concentration quenching, the B_2O_3-rich portion of the ternary diagram $Ln_2O_3-MgO-B_2O_3$ (Ln = rare earth) has been investigated. A ternary phase of composition $LnMgB_5O_{10}$ has been found for Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, and Er. These compounds crystallize all in the monoclinic space group $P2_1/c$. The structure has been determined on a $LaMgB_5O_{10}$ crystal. A full-matrix least-squares refinement leads to $R = 0.039$. The structure can be described as being made of $(B_5O_{10}{}^{5-})_n$ two-dimensional layers linked together by the lanthanum and magnesium ions. The rare earth atom coordination polyhedra form isolated chains. These borates are isostructural with some rare earth cobalt borates.

The Ionic Model Applied to Vacancy Ordering in NaCl-Type Materials. HUGO F. FRANZEN AND JEAN A. MERRICK, Ames Laboratory–DOE and Department of Chemistry, Iowa State University, Ames, Iowa 50011. An order–disorder transition in $Sc_{0.8}S$ (NaCl structure type) was studied by high-temperature X-ray diffraction and 700 ± 20°C was found to be the ordering temperature. A group of ordered sublattices on the rock salt lattice was generated and a Madelung energy and a configurational entropy were calculated for each assuming the lattice was made up of point charges. Mean field and pair interaction approximations were used to model long-range and short-range orderings, respectively. Results indicate that the ionic model is seriously in error in predicting short-range orderings of the type observed.

Comparaison Des Champs De Force Des Niobates, Tantalates, Et Antimoniates De Structure Columbite Et Trirutile. E. HUSSON, Y. REPELIN, AND H. BRUSSET, Laboratoire de Chimie et Physico-Chimie Minerales, Institut de Chimie, Ecole Centrale des Arts et Manufactures, 92290 Chatenay-Malabry, France. A comparison is made between the force fields calculated for the $M^{II}Nb_2^{V}O_6$ and $M^{II}Ta_2^{V}O_6$