
We find a justification for this phenomenology in terms of a very simple molecular orbital model for the interactions between atoms A and B. By using a slightly more rigorous molecular orbital treatment, we produce superior structural sorting diagrams for all AB compounds, and hence shed light on the reasons underpinning structural preference, and the tendency to undergo polymorphic phase transitions, in terms of the number of valence electrons, and the relative positions of the energy levels of the constituent atoms.

08.1-11 CATION DISTRIBUTION AND CATION SOLUBILITY STUDIES BASED ON SOLID SOLUTIONS OF THE $\gamma$-Zn$_m$(PO$_4$)$_2$ STRUCTURE TYPE. By A.G. Nord and T. Stefanidis. Section of Mineralogy, Swedish Museum of Natural History, S-104 05 Stockholm, and Dept. of Inorganic and Structural Chemistry, Archenius Laboratory, S-106 91 Stockholm, Sweden.

The aim of this study is to correlate solubility, cation radius, unit cell dimensions and cation distribution for (Me,Mg)$_m$(PO$_4$)$_2$ orthophosphate solid solutions of the isotypic compounds $\gamma$-Zn$_m$(PO$_4$)$_2$, Mg$_m$(PO$_4$)$_2$, the mineral farringtonite, and Ca$_m$(PO$_4$)$_2$ (space group $P_2_1_3$). This structure type is interesting because two thirds of the cations, M(1), are five-coordinated (distorted trigonal bipyramids) and one third, M(2), are six-coordinated (almost regular octahedra). All solid solutions are equilibrated at $\approx$1070 K. Divalent cations of Mg, Mn, Fe, Co, Ni, Cu, Mn, and Cd were included in the study. The orthophosphates of zinc (γ phase), magnesium and cobalt are almost completely soluble in each other at 1070 K. Fe and Mn show intermediate solubility, while the solubility of Ni$^{2+}$, Cd$^{2+}$ and Cd$^{2+}$ in the three base structures is comparatively slight. The observed change of unit cell dimensions is clearly correlated to the incorporated cation's radius. The cation distributions in some (Mg,Mn)$_m$(PO$_4$)$_2$ solutions have been determined with the described profile-refinement technique based on X-ray powder data. The M(1) site preference order is $\gamma$-Mn$^{2+}$$\rightarrow$Cd$^{2+}$$\rightarrow$P$^{6+}$$\rightarrow$Mg$^{2+}$$\rightarrow$Mn$^{2+}$. Mössbauer studies at Uppsala University have confirmed part of these results (H. Annersten, T. Ericsson and A.G. Nord; J. Phys. Chem. Solids (1980) 41 1235-1240). The cation distribution studies are not yet complete but additional neutron diffraction studies are in progress.