boundary in the region below room temperature. The theory suggests that morphotropy is preserved, i.e., that the phase boundary occurs at nearly the same composition right down to 0 K. The rhombohedral ($R3m$)-rhombohedral ($R3c$) phase transition was investigated for a composition $PbZr_{0.6}Ti_{0.4}O_3$ using neutron diffraction. Structures in both phases were refined by the Rietveld profile fitting technique. The transition behavior in this composition was indicative of a diffuse-type phase transition, with a transition temperature somewhere between 250 and 300 K. The diffuse nature of this transition is perhaps due to short-range ordering of Zr and Ti. However, neutron powder diffraction is not ideal for determining critical behavior; therefore, it is difficult to make a quantitative conclusion in this respect. Values of the spontaneous polarization were obtained from the (Zr/Ti) shifts, and compared to those deduced from phenomenological theory.

Synthesis and Structure of an Infinite Chain Form of ZrI_2 (α). J. D. Corbett* and D. H. Guthrie, Department of Chemistry, Iowa State University, Ames, Iowa 50011. The synthesis of a second polymorph of ZrI_2 has been achieved by a transport reaction between ZrI_4 and zirconium metal under a 750/850°C gradient in a sealed tantalum tube. The black lath-like crystals produced in the 775°C region occur in space group $P2_1/m$ with $a = 6.821(2)$ Å, $b = 3.741(1)$ Å, $\beta = 95.66(3)°$, $Z = 4$. A total of 669 independent reflections with $2\theta \leq 50°$ and $I > 3\sigma(I)$ were measured at room temperature on a four-circle automated diffractometer with monochromatized MoK_α radiation and were corrected for absorption ($\mu = 190$ cm^{-1}). The structure was solved by direct methods and full-matrix least-squares refinement of all atoms with anisotropic thermal parameters to give final residuals $R = 0.064$ and $R_w = 0.079$. This phase is isoelectronic and isostructural with β-$MoTe_2$, a distorted CdI_2-type structure in which the zirconium atoms are displaced 0.440 Å from the octahedral centers along a to form infinite zig-zag metal chains ($d_{Zr-Zr} = 3.182(3)$ Å) parallel to b. The phase is a diamagnetic semiconductor at room temperature ($E_g \sim 0.1$ eV).

Correlation of Metal–Metal Bonding in Halides and Chalcides of the Early Transition Elements with That in the Metals. J. D. Corbett,* Department of Chemistry, Iowa State University, Ames, Iowa 50011. Values of the average Pauling metal–metal bond order n per metal valence electron (PBO/e) are reported for about 110 metal-rich compounds of transition groups III–VI (including the lanthanides) which are structurally well characterized. The calculations include bond orders over all metal–metal separations with $n > \sim 0.07$ and assume only the presence of closed-shell anions, the Pauling equation $D_n = D_1 - 0.60 \log n$, and D_1 values likewise calculated from the respective metals. Matrix effects—usually anion–anion repulsions that restrict metal–metal bonding—are shown to yield plausible and predictable reductions in PBO/e values, these effects being greater with high nonmetal:metal ratios, large anion or small metallic radii, in M_6X_{12}-type clusters, and in layered and rock-salt-type structures. On the other hand, 32 metal-rich halides and chalcides are found to be relatively free of matrix effects and to be strongly metal–metal bonded relative to their respective metals by the criterion $0.80 \leq$ PBO/$e < 1.05$, these being principally M_6X_8-type clusters and extended (condensed) metal networks. Three special circumstances are considered: reduced metal–metal bonding in the molybdenum chalcides (but not halides) which arises from strong heteroatom bonding and nonmetal repulsions between clusters; a few errant examples with low concentrations of metallic electrons in which core sizes dictate separations (e.g., Ca_2N, PBO/e = 22.4); and some clusters of Nb, Mo, and Mo containing only oxide and fluoride in which nonmetal π contributions evidently give effective bond orders >1.0.

Phase Diagram and Infrared Spectral Investigation of the $2TeO_2 \cdot V_2O_5$–$Na_2O \cdot V_2O_5 \cdot 2TeO_2$ System. Y. Dimitriev,* M. Arnaudov, and V. Dimitrov. Higher Institute of Chemical Technology, Sofia - 1156, Bulgaria. The phase diagram of the $2TeO_2 \cdot V_2O_5$–$Na_2O \cdot V_2O_5 \cdot 2TeO_2$ system is studied by X-ray diffraction, ir spectroscopy, and DTA. A new compound with a compositin of $Na_2O \cdot 3V_2O_5 \cdot 6TeO_2$ is established. The ir spectra of the alkaline trivanadates are interpreted. They are considered as structural analogs of the new phase. As a result of this comparison, the postulate is made that the main structural units in the $Na_2O \cdot 3V_2O_5 \cdot 6TeO_2$ compound are V_2O_8 groups, while tellurium is present both in TeO_3 and TeO_4 groups. Conversely to the crystal phases, in glasses the transition from VO_5 toward VO_4 does not proceed through the formation of new structural units of vanadium, but rather a gradual transition of the structure is observed with a change in the composition from $2TeO \cdot V_2O_5$ to $Na_2O \cdot V_2O_5 \cdot 2TeO_2$.