PS08.01.41 A NEW LOOK AT SIMPLE STRUCTURES: THE ALKALINE EARTHS CHALCOGENIDES. A. Vegas and D. Tranqui. Instituto Rocasolano, CSIC, Serrano 119, E-28006 Madrid, Spain and Laboratoire de Cristallographie, CNRS, F-38042 Grenoble, France

The structures of the NaCl-type alkaline earths chalco­genides are analyzed on the basis of their fcc cation array which are compared with the structure of their parent metals as it has been reported for other compounds (1). The results are that, in most cases, the M-M distances in the compounds, reproduce the values observed in the pure metals.

In some cases, as in the sulfides and selenides of Ca and Sr, the coincidence is also in topology in such a way that the metal net is almost unaltered by the inclusion of the S or Se atoms. Thus, CaS, CaSe, SrS and SrSe can be described as S- and Se-stuffed elements as it was reported for CaF2 (2).

In the case of MgTe (M=Ca, Sr, Ba), the cation fcc-array is formed by (001) planes of the respective bcc-metal, in such a way that second-nearest neighbors distances of the metal are reproduced in the compounds. The general trend is that small anions as O2- tend to reproduce distances of the high pressure metallic phases and that greater anions as Te2- tend to reproduce distances of the high temperature metallic phases.


PS08.01.42 SPECIFIC FEATURES OF RARE-EARTH POLYHEDRA IN ALKALI LANTHANE CHLORIDES. A.G.Vigdorchik, Institute of Crystallography, Russian Acad. of Sci., Leninsky pr. 59, Moscow, 117333, Russia

This research was performed in the framework of a systematic study undertaken to explain the structure and properties of compounds of alkali rare-earth nitrates with common formula of (n-3m)A[(m)Ln(n)(NO3)(k)(H2O)](l)(H2O), A=n,alkali cat­ions; n,m,k,l=stoichiometric coeff. The analysis of crystal-chem­ical characteristics of Ln coordination polyhedra was carried out on the basis of our own experimental data (about 30 crystal com­pounds) and the data reported in literature. Their shape, symmetry and other properties were analyzed. In all compounds reviewed, the coordination numbers (CN) of the Ln atoms are close to 12, CN=12 is characteristic only of the elements of the cerium subgroup. Three types of coordination of the Ln-atoms by nitrate group were found: monodentate, bidentate and bridging bidentate. While reviewing structural data on the compounds in question, we face an exceedingly limited assortment of coordination polyhedra for high coordi­nation numbers - there are only three types: icosa­hedron, tetracapped trigonal prism, and bicapped tetragonal antiprism. All 12-vertex polyhedra appear as slightly distorted icosa­hedra. An atom of Ln tends to form a symmetrical coordination arrangement even in the case when it occupies a position without any symme­try elements. It should also be noticed that complexes with the different composition and stoichiometries may correspond to identical coordination polyhedra.