s11.m2.p1 **Computer modeling of the mixing properties of MO-M'O solid solutions.** V.S. Urusov, T.G. Petrova, N.N. Eremin, *Department of Crystallography and Crystal Chemistry, Moscow State University, 119899, Moscow, Russia.*
Keywords: solid solutions, computer modeling, ionic and partially covalent potentials.

Atomistic semi-empirical potentials were applied to calculate the mixing energy, mixing volume and elastic properties of CaO-MgO, CaO-SrO, BaO-SrO solid solutions by the using of the GULP code [1]. The calculations were performed both with purely ionic and partially covalent approximations for 7:1, 3:1, 1:1, 1:3, 1:7 mixed cation compositions.

For all compositions we used 64-ion primitive supercell with doubled parameters of the unit cell. The calculations were made for a number of different degrees s of short-range ordering in the mixed cation sublattice. It was found that for all systems there are evident tendentions of solid solutions to be ordered: the minimum of the mixing energy for a given composition as a function of s appears to be in the range of $s = 0.5$-0.6. By extrapolation of the obtained values of the mixing properties to $s=0$ the corresponding properties of a random solid solution were theoretically estimated and compared with available structural and thermochemical data. The dependences of mixing volume, bulk modulus and oxygen position shift from composition were plotted.

It was shown that using such kind of extrapolation within partially covalent model of atomic interactions allows one to improve sufficiently the agreement between the calculated mixing properties and those obtained by means of semi-empirical model [2] and *ab initio* approach [3].

s11.m2.p2 **Computer modeling of structure and properties of Mn-oxides using atomization energy minimization.** V.S. Urusov, O.V. Obolenskiy, N.N. Eremin. *Departament of Crystallography and Crystal Chemistry, Moscow State University, Moscow, Russia.*
Keywords: computer modeling, partially covalent potentials, charge-transfer energy.

Previously developed by the authors [1] VALUES program code was modified to describe ionization process of transition metal atoms with s- p- and d- valence electron levels. For example, the ionization of Mn in different valence states was reproduced using the orbital electronegativities equilization principle. The modified code was used to calculate the value of minimum atomization energy consisting of effective electrostatic, repulsion and charge-transfer energy terms. This technique was testified on the following manganese oxides: pyrolusite (MnO_2), manganosite (MnO) and curnakite (Mn_2O_3).

The modeling of the structures and elastic properties was performed with the help of GULP code [2]. The optimal value of MnO_2 atomization energy was found at the Mn-O bond ionicity degree (f) equal to $f=0.54$, while for Mn_2O_3 $f = 0.68$ and for MnO $f=0.83$.

As a result of this modeling it was found that at the atomization energy minimum the structural, energetic and elastic properties of minerals under investigation are in better agreement with available experimental data when compared with purely ionic procedure. This demonstrates that the modified charge-transfer energy correction allows one to predict the effective ionicity degree rather correctly and the optimal values of Mn-O pair potential parameters may be used for modeling of more complex manganese oxide compounds.

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