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Crystal structure and electrical properties of the $Bi_{2-y}Sr_yIr_2O_7$ α-pyrochlore solid solution CARLOS COSIO-CASTANEDA, GUSTAVO TAVIZON, Facultad de Quimica, PABLO DE LA MORA, Facultad de Ciencias, UNAM, FRANCISCO MORALES, Instituto de Materiales — In this work we report the synthesis and crystal structure of the $Bi_{2-y}Sr_yIr_2O_7$. From structural Rietveld refinements we show that in this system the local geometry of the IrO_6 passes from a trigonal antiprism (y<0.4); a regular octahedron (y=0.5), reaching a new trigonal antiprism at the end compositions (y>0.5). Experimentally, this is a metallic system with a conductivity that decreases as a function of the Sr content in the (10-300 K) low temperature range. By means of electronic structure calculations, using WIEN2k to study $Bi_2Ir_2O_7$ and two hypothetical compounds, $BiSrIr_2O_7$ and h-$BiSrIr_2O_7$, we show that a) the main contribution to conductivity come from the shift of the oxygen towards the Ir atoms; b) the lattice imperfections (random occupation of Sr) and lattice vibrations are responsible for the drop of the electrical conductivity, and c) the IrO_6 local geometry (and crystal field configuration, $t_{2g}^5\ e_g^0/e_g^4 a_{1g}^1 b_{2g} b_{1g}$ change), this last one does not seem to affect the electrical conductivity.

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