Investigation of the Alkaline Earth Phosphates: Crystal Structure of a New Strontium Hydrogen Phosphate Form. L.B. Taher and L. Smiri\textsuperscript{11}, Y. Laligant and V. Maisonneuve\textsuperscript{12}, \textsuperscript{11}Laboratoire de Chimie Inorganique et Structurale, Faculté des Sciences de Bizerte, 7021 Jarzouma, Tunisie; \textsuperscript{12}Laboratoire des Fluorures, UPRES-A CNRS 6510, Faculté des Sciences, Université du Maine, Avenue O. Messiaen, 72085 Le Mans Cedex 9, France.

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The X-ray single-crystal structure is reported for a new form of strontium hydrogen phosphate ($\gamma$-SrHPO$_4$) ($\gamma$-Sr). The cell is orthorhombic (Pbcn) with $a_o=8.131(3)\,\text{Å}$, $b_o=9.258(5)\,\text{Å}$, $c_o=18.084(7)\,\text{Å}$, $V=1361.31(2)\,\text{Å}^3$, $Z=16$, and $R=0.039$. The atomic arrangement consists of a succession along [001] of two kinds of HPO$_4^{2-}$ alternating planes denoted as P(1) and P(2). These sheets are held together by Sr$^{2+}$ cations. Here we find the same arrangement as observed in the monoclinic CaBa(HPO$_4$)$_2$ (CaBa). Further interaction linkages are provided by strong hydrogen bonds established within the phosphate sheets. The features of the hydrogen bonding system (dimers in P(1) and infinite chains in P(2)) are defined by the HPO$_4^{2-}$ ratio as has been found in CaBa and some sulfate structures e.g. KHSO$_4$, where H/SO$_4$ ratio is also 1. The unit cell deformation of CaBa ($b_o$=$a_o$, $a_o$=$b_o$, $c_o$=1/2$c_o$) can be directly related to the nature of the cations coordination: one kind of ninefold ions (2Sr$^{2+}$) with average distances 2.703 Å for Sr(1)O$_6$ and 2.660 Å for Sr(2)O$_6$, is replaced by (Ba$^{2+}$, Ca$^{2+}$) ions with <Ba-O>=2.846 Å and <Ca-O>=2.462 Å in BaO$_6$ and CaO$_7$ polyhedra, respectively. The lattice distortion is coupled with small rotation of the HPO$_4$ tetrahedra along the $a_o$ axis. Moreover, the slight increase of $a_o$ (8.131Å) compared to $b_o$ (7.930Å) is caused by: (i) a radius change of the ions, where two Sr$^{2+}$ cations (r$_{\text{Sr}}$(Sr$^{2+}$)=1.31Å) are replaced by a relatively small Ca$^{2+}$ (r$_{\text{Ca}}$(Ca$^{2+}$)=1.07Å) and large Ba$^{2+}$ (r$_{\text{Ba}}$(Ba$^{2+}$)=1.47 Å) cations, (ii) a reduction in the distance between Ba$^{2+}$ atoms along the infinite phosphate chains in CaBa (4.280Å as compared to 4.369Å for $\gamma$-Sr). This decrease in the P-P distance is accompanied by a decrease in the P(2)-P(2) angle (137.06° to 135.77°). The approximately doubling of $c_o$ ($c_o$=9.865 Å) is due to the orientation of the tetrahedra in two successive layers either of P(1) type or of P(2) type.

