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This Week's Citation Classic

Roth R S. Classification of perovskite and other ABO_3-type compounds.
J. Res. Nat. Bur. Stand. **58**:75-88, 1957.
[National Bureau of Standards, Washington, DC]

It was shown in this paper that the structure, and therefore the electronic properties, of solid solutions between various perovskite type compounds can be predicted by a three-dimensional classification based on the radii of the constituent ions as well as the polarizability of the larger cation. [The *SCI*® indicates that this paper has been cited over 120 times since 1961.]

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"In 1951, I was hired as a new PhD by the National Bureau of Standards (NBS) to utilize a new high angle x-ray powder diffractometer as part *of* a team studying phase equilibria in the uranium-beryllium-carbon system.[1] The x-ray patterns of this system were so boring that I had to solicit specimens to examine from all my colleagues engaged in more interesting ceramic research. Other research on crystalline materials in the division was devoted principally to refractories and dielectric ceramics. Many interesting crystal chemistry problems were thus uncovered by my curiosity, as it quickly became obvious to me that ox-ides offered better research opportunities than carbides. This utilization of the x-ray equipment resulted in further collaboration with the other teams in the division.

"One of the most interesting and important of these collaborations was the study of piezoelectric ceramics in the solid solution series $PbZrO_3$-$PbTiO_3$[2] and the effect of the addition of other oxides on their crystal chemistry and piezoelectric properties.[2] These studies aroused my curiosity concerning the crystallographic symmetry exhibited by the perovskite compounds encountered. These slight symmetry changes were obviously connected with very important changes in the electronic properties –ferroelectricity, piezoelectricity, dielectric constant, etc. Any systematic classification of such phases based on bibliographic information was hopeless, as the literature was riddled with false and misleading information. The incorrect early results were apparently due mostly to the poor resolution of early x-ray diffraction equipment.

"With my new instrument and the collaboration of my expert ceramist colleagues, I was in a position to correct the earlier data and arrive at a classification which might be useful for predicting future results. I thus gathered up all the old specimens I could find lying around the division which might contribute to my knowledge of ABO_3-type chemical compositions and even prepared a few specimens myself. The end result of this study was a list of all possible chemical reactions in $A^{+2}B^{+4}O_3$ and $A^{+3}B^{+3}O_3$ compounds and a classification which enabled future researchers to predict the crystallographic symmetry, and therefore the electronic properties, of any desired solid solution combination.

"This paper has thus been used as a reference so often because it is unnecessary to refer to earlier literature (it all was reviewed here) and all new work in the field is (relatively) accurately predicted by this reference (see reference 3). More than 200 reprints of this article were distributed. This paper was reproduced by the Physical Society of Japan[4] in an effort to increase its international availability. Although many of my colleagues and coauthors between 1951 and 1957 helped greatly in this work, I probably owe most to the then president of the US, Harry S. Truman, who in 1951 granted me a presidential deferment from induction into the Army so I could help the war effort at NBS rather than in Korea."

1. **Burdick M D, Parker H S, Roth R S & McGandy E L.** An x-ray study of the system uranium raonocarbide-uranium dicarbide-berylliura carbide. *J. Res. Nat. Bur. Stand.* **54**:217-29, 1955.
2. **Jaffe B, Roth R S & Marzullo S.** Properties of piezoelectric ceramics in the solid solution series lead titanate-lead zirconate-lead oxide: tin oxide and lead titanate-lead hafnate. *J. Res. Nat. Bur. Stand.* **55**:239-54, 1955.
3. **Goodenoagh J B & Longo J M.** Crystallographic and magnetic properties of perovskite and perovskite related compounds. (Landolt-Boernstein Numerical Data and Functional Relations in Science and Technology Group 3, ed.) *Crystal and solid state physics*. Berlin: Springer-Verlag, 1970. Vol. 4. Pt. A. p. 126-275.
4. **Roth R S.** Classification of perovskite and other ABC_3-type compounds. (Physical Society of Japan, ed.) *Series of selected papers in physics—ferroelectrics*. Tokyo: Physical Society of Japan, 1961. p. 11-24.