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A permutation approach to crystal structures

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Hornfeck, W. (2012) Quantitative crystal structure descriptors from multiplicative congruential generators, *Acta Crystallographica Section A*, 68, 167–180.
Hornfeck, W. (2013) Quasirandom quasicrystals, *Acta Crystallographica Section A*, 69, accepted.
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Abstract: *A century after the first X-ray diffraction experiments of Friedrich, Knipping and von Laue a vast amount of crystal structures have been determined yielding detailed insight into the spatial organization of condensed matter. Symmetry, in particular space group theory, is invoked in order to describe and classify the wealth of crystal structure information in a likewise concise and comprehensive manner. Despite its successes symmetry gives only a partial picture conveying the qualitative features of crystal structures. It is well-known however that subtle interrelations may exist beyond the mere listing of atomic coordinates. This already founds it expression in the scientific work of Arthur L. Loeb (1923–2002) who devised what he called a 'modular algebra' for the description of crystal structures. Although his achievements appeared singular for several decades and somewhat less-well appreciated by contemporary crystallographers our recent work shows that many of Loeb's ideas regarding the description of the spatial patterns found in crystal structures transcend into a conceptual framework of a more general nature in which the combinatorial aspects of crystallography are highlighted – in an approach that could be called* crystallographic information theory. *In this framework the coordinate description of crystal structures is related to permutations in which symmetry is encoded in their cycle structures. Intriguingly, close relationships*

exist to the algorithmic generation of random numbers, thereby challenging and extending our understanding of condensed matter and its spatial organization into distinct ordered states.

Keywords: Multiplicative congruential generators, Bit-reversal sequences, Permutation structures, Combinatorial crystallography.
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