OCCASIONALLY IRRATIONAL SYMMETRIES PROVIDE THE OPTIMUM OF CLOSE PACKING IN CRYSTALS

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Under non ideal conditions Nature seems to be able to crystallize molecules with unusual symmetries which are irrational in the realm of the 230 space groups known commonly since the nineties of the 19th century. Whenever the ideal formations of crystals are hindered Nature, instead of letting molecular packing remain in chaos, attempts to form pseudosymmetries especially in unusual position like (2n- 1) 1/8 which are then accompanied by *asymmetric* translation ($q = 1/4 \rightarrow 3/4$) generated by their complementary operators. The latter is induced by the presence of a crystallographic inversion center. These irregular symmetries have been discovered in the course of a symmetry analysis of triclinic crystals published with space group P 1 and four molecules in the asymmetric unit. So far more than half dozen triclinic crystals have been found among the structures retrieved from the Cambridge Structural Database to exhibit pseudo symmetries of $*2_1$ and *c type accompanied by screw axes and glide planes in unusual position of (2n-1)1/8 , respectively. In particular three structures, which could be transformed into centered monoclinic unit cells exhibit two forms (1,3) of the irregular topologies: (1) $2_1/c_q$, *(2)* $2_q/c$ and (3) $2q/n_q$, inferred from the most popular space group $P2_1/c$ (No. 14) by a linear combination of the parameters ($\alpha,\beta,\gamma = 0$, 1/8, 1/4) in the symmetry triplet

$$2\tau(\alpha,Y,\beta) <\!-\!> c\tau(X,y,Z) = \bar{1}\ (0,0,0)$$

where τ is either regular 1/2, or irregular $q = 1/4(3/4)$ translation, while X,Y,Z indicate the infinite extension(s) of the commutative (<->) operators and 1 (0,0,0) is a crystallographic inversion center located in the origin. These three irrational topologies ought to be regarded as the 231st 232nd and 233th space groups if their perfect (100%) formation were permitted. Of course, this would violate the absolute priority of standard space group(s) using only regular (I/2) translations.