SCREW AXES OF SYMMETRY AND THEIR SYMBOLS*

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Abstract

The usefulness of Mauguin symbolism is demonstrated by its adaptation in slightly modified form for the characterization of screw axes. The symbols of all screws isomorphous with any given rotary axis and the geometrical properties essential for their visualization can be found by simple arithmetical means. The otherwise difficult subject of non-crystallographic chain symmetry groups is thus greatly simplified.

Screw axes are elements of symmetry of chain groups and space groups (the digonal screw also occurs in net groups). They are the controlling elements of operations of translatory rotation. In space groups we only have the fifteen crystallographic screw axes with Mauguin symbols 2, 2_1, 3, 3_1, 3_2, 4, 4_1, 4_2, 4_3, 6, 6_1, 6_2, 6_3, 6_4, 6_5. In chain groups, however, where translation is admitted in only one dimension, we have an infinite number of non-crystallographic screws, some of which may conceivably be found in chain molecules, which do not crystallize to nets or lattices. The principle of Mauguin symbolism can be adapted to characterize screws in general and combinations of screw axes with rotary axes in the same line.

A *pure* screw axis is one which is not combined with a rotary axis in the same line. The symbol of a pure screw is given in the Mauguin form p_q. We interpret the symbol as follows: p operations (the single operation is rotation around the axis through the angle α and translation through the distance τ/p parallel to the axis) result in q complete revolutions around the axis and a total translation τ, which is the period of identity. Therefore $\alpha = q\cdot 360°/p$ is the rotational component of the screw and τ/p is the translational component. In consequence it must be stipulated that p and q be integers without common divisor. Also $p > q$, as otherwise $\alpha > 360°$. When $p = q$, $\alpha = 360°$, so that 1_1 can be used as a symbol for periodicity along the screw axis.

Every screw can be interpreted as a *right* or a *left* screw. If the right screw has the rotational component α, the corresponding left screw has the rotational component $(360° - \alpha)$. If we imagine a screw motion towards us along an axis, we call the axis a right screw when the rotation is counter clockwise through the smallest angle $\alpha < 180°$ which will produce coverage of equivalent points. When $\alpha = 180°$, the screw is both right and left and can be called *neutral.*

p_q is a right screw when $p > 2q$
p_q is a left screw when $p < 2q$
2_1 is the only neutral pure screw.

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Two screws p_q and $p_{(p-q)}$ can be enantiomorphous, one being the mirror picture of the other. One is right and the other left, for if p_q has the rotational component α, then $p_{(p-q)}$ has the component $360° - \alpha = -\alpha$, so $p_q = -p_{(p-q)} = p_{(q-p)}$. The use of negative symbols is usually unnecessary, the above relation being given mainly to show that when calculation yields values with $q > p$, we can subtract p from q repeatedly until $q < p$.

Combination of Axes of Rotation and Screw Axes

We combine n (rotary axis) and p_q in one line and write n, p_q. This combination produces further elements $p'_{q'}$ in the same line. If $\sigma = 360°/n$ is the smallest angle of rotation of n, and $\alpha = q \cdot 360°/p$ is the smallest rotational component of p_q, then the rotational component of the implied axes $p'_{q'}$ is $(\alpha + a\sigma)$, where a is any integer.

$$p'/q' = 360°/(\alpha + a\sigma) = np/(nq + ap)$$

$$n,\ p_q = n,\ np_{(nq+ap)} \tag{1}$$

The translational component is n/p, where p has its maximum value. In computing the different symbols for the same axis by means of the above equation, the procedure is to make $np > (nq + ap)$ by subtraction of np from the latter term when necessary, and then to treat $np_{(nq+ap)}$ as a fraction and reduce it to its lowest form.

The calculated different expressions for a given combination of rotary and screw axes yield significant information on the geometrical properties of screws. For instance, the Mauguin screw 6_3 is written more significantly as 3, 6_1, which shows that it is a combination of a trigonal rotary axis and a right hexagonal screw. Use of equation (1) reveals that 3, 6_5 and 3, 2_1 are synonymous expressions and we see that the screw is neutral.

Isomorphous Axes

All axes which reduce to p on suppression of translation are said to be *isomorphous* with the class (point group) p. Isomorphous axes have the following properties in common: equivalent points lie on equally spaced parallel lines on a cylinder surface. There are p such lines, all of which must carry equivalent points. All multiples of $\sigma = 360°/p$ must therefore result from the symmetry operation.

This is realized for all axes p_q (p and q have no common divisor and $p > q$). Thus we have, for instance, four pure screw axes isomorphous with the point group 5. They are 5_1, 5_2, 5_3, 5_4, with the angular components 72°, 144°, 216°(−144°), and 288°(−72°), respectively, as computed from $\alpha = q \cdot 360°/p$. The first two are right screws and the others left. The fifth axis isomorphous with 5 is 5, 1_1 which is the periodic repetition of 5. Thus when p is prime we can immediately write the symbols of all the isomorphous axes p, 1_1, p_1, p_2, $- p_{(p-2)}$, $p_{(p-1)}$.

When p is not prime, the procedure is to write down the symbols p_q where q is all integers from 1 to p. The pure screws are obtained by picking out the symbols with numbers without common divisor. When p_q has a common divisor n, an axis n, 1_1 is indicated and we write n, np_q. This symbol stands for a combination of n, 1_1 with np_q (which is treated as a fraction and reduced to its lowest form). When $p=q$ we get p, p_1 which is equal to p, 1_1.

We thus have p axes isomorphous with p, as q assumes all integral values from 1 to p. When p is even, we have a neutral screw $p/2$, p_1. For instance, $p_q=4_2$, then the axis is 2, 4_1, a right screw. The symbol of the substitutable left screw 2, 4_3 is obtained from equation (1).

We now have a simple method for determining and symbolizing all screws isomorphous with any given rotary axis, and of ascertaining their geometrical properties. The table shows the symbols of the screws isomorphous with the axes 2 to 12.

Special Cases

In screw axes, the rotational component can be an irrational fraction of 360°. The period of identity then becomes infinitely large, although the translational component of the screw is finite. Translation is not a subgroup of irrational screws. The symbol of this class of screws is r_1, where r is an irrational number. There is an infinite number of screws r_1 and n, r_1, which are isomorphous with rotary axes (as yet unsymbolized), which themselves are perhaps only sub-groups of the axis ∞. Here the symbol ∞ designates a rotary axis, the angle of rotation being a free variable, i.e. assuming all angular values. Thus the axis ∞ establishes equivalence of *all* the points of a circle. It would seem that although the equivalent points due to an irrational screw r_1 form a dense circle on supression of the translational component, this circle does not have the symmetry ∞, because an infinite number of points, corresponding to rational angles, are missing. This problem awaits investigation.

Finally there are the helices, continuous screws, all the points of which are equivalent. The symbols are ∞_1 and n, ∞_1. We can distinguish between right and left helices by use of a negative symbol for the left one.

The group ∞, ∞_1 is equal to the group $\infty/m\ m$ (with free variable translation), representing the symmetry of a cylinder surface, all the points of which are equivalent.

Combination of Screw Axes with Other Elements of Symmetry in Chain Groups

All screw axes n, p_q (also n, r_1 and n, ∞_1) can be combined with digonal axes normal to them, to form chain groups n, p_q2 (n, r_12 and n, ∞_1 2),

Symbols of Screw Axes Isomorphous with Rotary Axes 2 to 12
Computed from: n, $p_q=n$, $np_{nq}+ap$

Rotary Axis	Pure Right Screws	Pure Left Screws	Combination of Axes of Rotation and Right Screws	Combination of Axes of Rotation and Left Screws	Neutral Screws	
2					$2,1_1$	2_1
3	3_1	3_2			$3,1_1$	
4	4_1	4_3			$4,1_1$	$2,4_1=2,4_3$
5	5_1 5_2	5_3 5_4			$5,1_1$	
6	6_1	6_5	$2,6_1=2,3_2$	$2,3_1=2,6_5$	$6,1_1$	$3,6_1=3,2_1=3,6_5$
7	7_1 7_2 7_3	7_4 7_5 7_6			$7,1_1$	
8	8_1 8_3	8_5 8_7	$2,8_1=2,8_5$	$2,8_3=2,8_7$	$8,1_1$	$4,8_1=4,8_3=4,8_5=4,8_7$
9	9_1 9_2 9_4	9_5 9_7 9_8	$3,9_1=3,9_4=3,9_7$	$3,9_2=3,9_5=3,9_8$	$9,1_1$	
10	10_1 10_3	10_7 10_9	$2,10_1=2,5_3$ $2,10_3=2,5_4$	$2,5_1=2,10_7$ $2,5_2=2,10_9$	$10,1_1$	$5,10_1=5,10_3=5,2_1=5,10_7=5,10_9$
11	11_1 11_2 11_3 11_4 11_5	11_6 11_7 11_8 11_9 11_{10}			$11,1_1$	
			$2,12_1=2,12_7$	$2,12_5=2,12_{11}$	$12,1_1$	
12	12_1 12_5	12_7 12_{11}	$3,12_1=3,12_5=3,4_3$	$3,4_1=3,12_7=3,12_{11}$	$6,12_1=6,4_1=6,12_5=6,12_7=6,4_3=6,12_{11}$	
			$4,12_1=4,3_1=4,12_7=4,6_5$	$4,6_1=4,12_5=4,3_2=4,12_{11}$		

but combination with planes normal to or containing the screw axis, or with centers of symmetry, is only possible for neutral screws, i.e. n, 1_1 or n, $p_q = n$, $p_{(p-q)}$.

Sub-Groups

Sub-groups are groups of operations which cover only a fraction of the equivalent points of the whole group. Thus translation 1_1 is a sub-group of all screws excepting irrational ones.

A pure screw p_q has sub-groups $p_{q(1+a)}$ where a assumes all integral values from 1 to $p-2$, translational component $(1+a)/p$. The addition of translation will yield the equivalent points of the operation p_q which have been skipped by the operation $p_{q(1+a)}$, but only when p and $q\ (1+a)$ have no common divisor. The pure left screw 6_5, for instance, has the sub-groups 1_1, 6_1, 2_1, 3_1, and 3_2. In addition to the sub-groups of its screw n, p_q of course has sub-groups n, 1_1 and d, 1_1 where d is a divisor of n. Further sub-groups are n, $p_{q(1+a)}$, d, $p_{(1+a)}$, and d, p_q.

Finally, all pure screws, rational and irrational, are sub-groups of the helix.