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A note on crystallographic notation.

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THERE exists a bewildering variety of notations for the thirty-two classes of crystal-symmetry and for the 230 groups of symmetry-movements which control the arrangements of atoms building up a crystalline medium. The notation which has found most favour has been that of Schoenflies's 'Krystallsysteme und Krystallstructur' (1891).[1] This was followed in Hilton's 'Mathematical Crystallography' (1903) (see the second column of the table given below), and more recently in

[1] A comparison of this with other notations was given by the present author in Philosophical Magazine, 1902, ser. 6, vol. 3, p. 203, and Centralblatt Min., 1901, p. 746.

Niggli's 'Geometrische Kristallographie des Diskontinuums' (1919). The object of these two authors was doubtless to avoid a still further increase in the number of notations already in existence. But the 230 groups of movements have attained to a vastly increased importance owing to recent X-ray experiments, and it has become necessary to ensure that a notation likely to come into general and permanent use is really the best possible.

Now Schoenflies's notation suffers from two very serious drawbacks. The first is that it is based on a wrong principle. He takes the rotation and rotatory-reflection as fundamental operations, whereas it is absolutely essential for crystal-structure purposes to take the rotation and rotatory-inversion. This is obvious on a comparison of 'Krystallsysteme und Krystallstructur', §§ 23 and 24 (pp. 146–149), or 'Mathematical Crystallography', ch. vii, §§ 1 and 2 (p. 73). A second drawback is that Schoenflies's notation is troublesome and expensive to print; a very serious practical handicap, if it is to become the standard notation adopted by other authors.

The question arises as to whether it is possible to devise a notation which shall be based on correct principles, easy to write and print, and acceptable to the crystallographic world in general. An attempt was made in Hilton's 'Finite Groups' (1908), pp. 113–115. Its nature will be clear from the third column of the table given below. For instance, C_m is the class with a single m-al rotation axis, c_m that with a single m-al rotatory-inversion axis, Γ_m that with a single m-al rotation-axis combined with a centre of symmetry, and so on. This notation was based on correct principles and is easier to print than that of Schoenflies. But the suffixes and the changes from English to Greek type are not satisfactory from the printer's point of view. I suggest, therefore, the notation given in the fourth column of the table. In this A, B, D, E, F suggest respectively the existence of a predominant 1-al, 2-al, 4-al, 3-al, 6-al rotation-axis (the first being trivial). They are put in this order, for it is convenient in structure-theory to take the trigonal and hexagonal systems together, and also the orthorhombic and tetragonal systems together. Moreover, a, b, d, e, f suggest respectively the existence of a 1-al, 2-al, 4-al, 3-al, 6-al rotatory-inversion-axis, the first implying merely the existence of a centre of symmetry, and the second being the normal to a symmetry-plane. Again C or c imply that the class is derived from B or b respectively by adding on a perpendicular 2-al rotation-axis. Also T and O imply respectively the existence of the rotation-axes of the regular tetrahedron or octahedron. These symbols once fixed in the memory, the rest of the notation is easy. For instance, *Eb* is the class generated by a 3-al rotation-axis and a perpendicular 2-al rotatory-inversion-axis (i.e. a 3-al rotation-axis and a plane of symmetry through it); *fB* is the class generated by a 6-al rotatory-inversion-axis and a perpendicular 2-al rotation-axis; *Oa* is the class generated by adding on a centre of symmetry to *O*; *dc* is the class generated by a 4-al rotatory-inversion-axis and the movements of *c* (the rotatory-inversion-axis of *d* coinciding with one rotatory-inversion-axis of *c*); and so on.

The suggestion is that a class should be known by its symbol. Thus we should talk of the '*T, a*' class, not of the 'regular-parallel-faced-hemihedral' class, nor even of the 'pyritohedral' class, which would lead to confusion, if, for example, future research should show that pyrites did not belong to this class after all.

The notation for the groups of movements will be obvious. Thus, for example, Schoenflies's C_{4v}^{12} (figured in 'Mathematical Crystallography', fig. 147) would be called '*Db*12'. It is true that Schoenflies's numbering of the groups attached to any particular crystal-class might perhaps be revised with advantage. But it is beyond the scope of this brief note to enter into details on this matter.

	Schoenflies (1891).[1]	Hilton I (1908).	Hilton II (1922).	
1.	C_1	C_1	A	Triclinic
2.	C_i	c_1	a	
3.	C_2	C_2	B	Monoclinic
4.	C_s	c_2	b	
5.	C_{2h}	Γ_2	Ba	
6.	$\mathfrak{Q}$	D	C	Orthorhombic
7.	C_{2v}	δ_2	c	
8.	Q_h	Δ	Ca	
9.	C_4	C_4	D	Tetragonal
10.	C'_4	c_4	d	
11.	D_4	D_4	DB	
12.	D_{2d}	d_4	dB	
13.	C_{4h}	Γ_4	Da	
14.	C_{4v}	δ_4	Db	
15.	D_{4h}	Δ_4	dc	

[1] As adapted in Hilton's 'Mathematical Crystallography,' 1903.

16.	C_3	C_3	E	
17.	C_{3i}	Γ_3	e	
18.	D_3	D_3	EB	Trigonal
19.	C_{3v}	δ_3	Eb	
20.	D_{3d}	Δ_3	eB	
21.	C_6	C_6	F	
22.	C_{3h}	c_6	f	
23.	D_6	D_6	FB	
24.	D_{3h}	d_6	fB	Hexagonal
25.	C_{6h}	Γ_6	Fa	
26.	C_{6v}	δ_6	Fb	
27.	D_{6h}	Δ_6	fC	
28.	T	T	T	
29.	T_h	Θ	Ta	
30.	T_d	θ	Tb	Regular
31.	O	O	O	
32.	O_h	Ω	Oa	