Schoenflies and Mulliken Notations

At the end of the 19th century Arthur Schoenflies developed the point group system shown in the table below to describe the external morphology of crystals. Crystallographers long ago abandoned this system in favour of the international (herman-maguin) approach but molecular scientists continue to use it. To find the equivalent point group in generator notation just compare the Schoneflies symbol with the generator symbol in the same position of the table.

Point groups in three dimensions - Schoenflies

Partition	System	G		$\bar{G}$	Gi
[1,1,1]	Triclinic	C_1			C_i
	Monoclinic	C_2		C_s	C_{2h}
	Orthogonal	D_2	C_{2v}		D_{2h}
[2,1]	Trigonal	C_3			S_6
		D_3	C_{3v}		D_{3d}
	Tetragonal	C_4		S_4	C_{4h}
		D_4	C_{4v}	D_{2d}	D_{4h}
	Pentagonal	C_5			S_{10}
		D_5	C_{5v}		D_{5d}
	Hexagonal	C_6		C_{3h}	C_{6h}
		D_6	C_{6v}	D_{3h}	D_{6h}
	Heptagonal	C_7			S_{14}
		D_7	C_{7v}		D_{7d}
	Octagonal	C_8		S_8	C_{8h}
		D_8	C_{8v}	D_{4d}	D_{8h}
		…………………			
	Infinity	C_∞			$C_{\infty h}$
		D_∞	$C_{\infty v}$		$D_{\infty h}$
[3]	Tetrahedral	T			T_h
	Octahedral	O		T_d	O_h
	Icosahedral	I			I_h

Irreducible representations in Mulliken notation

Mulliken notation for irreducible representations is closely associated with the Schoenflies notation for groups. For example, $\bar{n}$ and $\bar{n}2$ when $n/2$ is an odd number have a peculiar standard Mulliken notation that includes primes ($'$ and $''$). These groups are labeled C_{nh} and D_{nh} except for the special monoclinic case

Monoclinic $\bar{2}$	Schoneflies (C_s)
A	A'
B	A''

Hexagonal $\bar{6}2$	Schoneflies (C_{3h}/D_{3h})
A_1	$A_1{}'$
A_2	$A_2{}'$
B_1	$A_1{}''$
B_2	$A_2{}''$
E_1	E''
E_2	E'

Dodecagonal $\overline{10}2$	Schoneflies (C_{5h}/D_{5h})
A_1	$A_1{}'$
A_2	$A_2{}'$
B_1	$A_1{}''$
B_2	$A_2{}''$
E_1	$E_1{}''$
E_2	$E_2{}'$
E_3	$E_2{}''$
E_4	$E_1{}'$

In groups $\bar{n}$ and $\bar{n}2$ when $n/2$ is an even number all of the 2D irrep subscripts are reversed relative to the rotational group. Cyclic groups $\bar{n}$ are Schoneflies S_n while $\bar{n}2$ are $D_{(n/2)d}$. $\bar{4}$ is no problem because there is only one 2D irrep.

Octagonal $\bar{8}2$	Schoneflies S_8
A_1	A_1
A_2	A_2
B_1	B_1
B_2	B_2
E_1	E_3
E_2	E_2
E_3	E_1

Higher order groups follow the same complicated pattern