Appendix

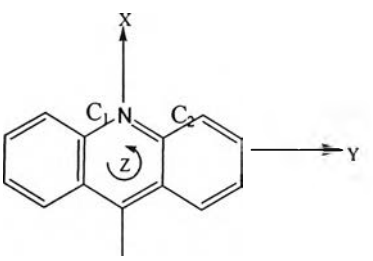
In chemistry, the "elements" of a mathematical group are actually symmetry operations that involve rotation, reflection etc. which maintain the original structure.

The symmetry that a molecule possesses is important to its chemical properties:

1) Chemical Reactivity

2) Electronic Structure

For symmetrical molecules the application of group theory has proven to be very helpful. Examples where group theory can be applied successfully are molecular orbital theory, molecular spectroscopy. For instance, the model for π- π * transitions in acridine have been classified using the group theory. The acridine molecule belongs to C_{2v} symmetry and lie in the xy plane with x axis. The electronic properties have been investigated using NDDO-G with SIBIQ program.



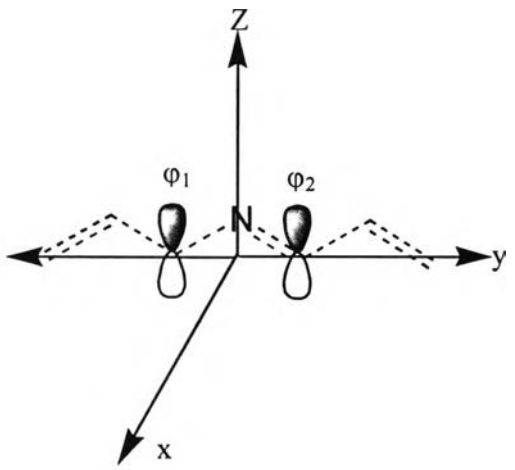
The important electronic transitions in acridine can be understood by considering only C1 and C2. Let's consider a part of calculation out put.

Eigenvalues (eV) and eigenvectors

MO#	31	32	33	34	35
	-9.9972	-9.3336	-8.5740	-1.0429	-0.2872
OCC#	2.00	2.00	**2.00**	**0.00**	0.00
Atom C1 AO: s, px, py, pz					
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.1474	-0.4062	**0.0442**	**0.1404**	0.4254
Atom C2 AO: s, px, py, pz					
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	-0.1473	0.4059	**0.0450**	**0.1407**	-0.4254

The highest occupied molecular orbital and lowest unoccupied molecular orbital are presented at the thirty-third and thirty-fourth molecular orbital, respectively. They have been from a basis for b1 representation.

In this point group we have the following operations:



E = identity φ no change

$C_2(x)$ = 180 rotation about z $\varphi_1 \rightarrow -\varphi_1$ and $\varphi_2 \rightarrow -\varphi_2$

$\sigma(xy)$ = reflection through xy plane $\varphi_1 \rightarrow -\varphi_1$ and $\varphi_2 \rightarrow -\varphi_2$

$\sigma(xz)$ = reflection through xy plane $\varphi_1 \rightarrow \varphi_1$ and $\varphi_2 \rightarrow \varphi_2$

The electronic configuration of the excited state is $(b_1)(b_1)$. The direct product of these two single electron orbitals is 1 1 1 1 which corresponds to a A_1 configuration.

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PUBLICATIONS

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