# NOTATION CONFUSION OF SYMMETRY SPECIES FOR MOLECULES WITH SEVERAL LARGE-AMPLITUDE INTERNAL MOTIONS

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The Mulliken convention [a] has become the standard notation for symmetry species (irreducible representations) of point groups for quasi-rigid molecules. No such convention exists for symmetry species of symmetry groups for semi-rigid or non-rigid molecules with large amplitude internal motions (LAMs). As a result, we have a situation where we create notations in a do-it-yourself fashion or adopt them from the literature, sometimes even without proper reference to its derivation or to the character table on which it is based. This may be just a nuisance for those who are comfortable enough with group theory and molecular symmetry groups to figure "it" out, but it represents a real problem for everybody else.

The notation confusion is illustrated with examples from the literature (both old and new) on molecules with two or more LAMs. Most authors use the notation introduced by Myers and Wilson [b] for molecules such as acetone or propane. No universal notation is in use for molecules with two methyl groups but lower overall symmetry. For example, the notation $G_{18}$ is used for one of these groups. As it turns out, different people use the same notation for different groups. This presentation is an attempt to bring some light into the dark and to combat confusion with a call for an anti-confusion convention.

[a] R. S. Mulliken, Phys. Rev. 43, 279 (1933).

[b] R. J. Myers, E. B. Wilson, J. Chem. Phys. 33, 186 (1960).