Classification of Rotational Energy Levels within the Complete Nuclear Permutation Inversion Group

Mira Diekmann[a] and Robert Berger[a]

[a] *Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg, Germany*
Diekmann@students.uni-marburg.de

For the classification of molecular energy levels and spectroscopic transitions group theory is an important tool. Whereas for rigid systems conventional point group concepts are usually sufficient, for non-rigid systems, in which for example tunneling has to be considered, the more general concept of permutation-inversion groups is needed.[1] The complete nuclear permutation and inversion (CNPI) group, which includes all permutations of identical nuclei, however has the disadvantage, that it is very large even for small molecules. Therefore subgroups, which only include feasible permutations, are usually used.

We use a system of 4 atoms as a minimal example for symmetry classification of rotational energy levels of a chiral system within the CNPI group. Within this group restrictions due to nuclear spin can be included as well as splitting of energy levels due to tunneling between enantiomers or between different versions of the enantiomer.

References

1. J. T. Hougen, *J. Phys.Chem.* **90** (1986), 562.