

Symmetry-Adapted Tensorial Formalism to Model Rovibrational and Rovibronic Molecular Spectra

V. Boudon

Laboratoire de Physique de l'Université de Bourgogne – CNRS UMR 5027, 9 Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France

This talk aims present a short review on the tensorial formalism developed by the Dijon group to solve molecular spectroscopy problems. This approach, originally devoted to the rovibrational spectroscopy of highly symmetrical species (spherical tops) has been recently extended in several directions: quasi-spherical tops, some symmetric and asymmetric tops and rovibronic spectroscopy of spherical tops in a degenerate electronic state.

Despite their apparent complexity (heavy notations, quite complex mathematical tools), these group theoretical tensorial methods have a great advantage of flexibility: a systematic expansion of effective terms for any rovibrational/rovibronic problem up to a given order is automatically generated. Inclusion of all possible interaction terms for any polyad scheme is therefore easy. This makes such an approach suitable for many types of molecular problems, not only the most symmetric ones.

I will first detail the questions of the symmetrization of molecular states. Then, I will detail the tensorial construction of the Hamiltonian and transition moment operators (dipole moment and polarizability) for different types of molecular symmetry (including the case of approximate symmetries). Then, I will address the problem of rovibronic spectroscopy in a degenerate electronic state. Finally, I will finish with some recent examples of results obtained using such models.

Some relevant references :

- J.-P. Champion, M. Loëte and G. Pierre, “*Spherical Top Spectra*” in “*Spectroscopy of the Earth's Atmosphere and Interstellar Medium*” K. Narahari Rao and A. Weber editors, Academic Press, San Diego, 1992, pp. 339–422.
- M. Rey, V. Boudon, M. Loëte, *J. Mol. Struct.*, **599**, 125–137 (2001).
- M. Rey, V. Boudon, Ch. Wenger, G. Pierre, B. Sartakov, *J. Mol. Spectrosc.*, **219**, 313–325 (2003).
- V. Boudon, M. Rey, M. Rotger and M. Loëte, “*Open-shell octahedral molecules: A first insight into the full rovibronic problem*”, Proceedings of SPIE, “*XIVth Symposium on High Resolution Molecular Spectroscopy, HighRus 2003, (July 6–11 2003, Krasnoyarsk – Yenisseisk – Krasnoyarsk, Russia)*”, **5311**, 1–13 (2003).
- V. Boudon, J.-P. Champion, T. Gabard, M. Loëte, F. Michelot, G. Pierre, M. Rotger, Ch. Wenger and M. Rey, *J. Mol. Spectrosc.*, **228**, 620–634 (2004).
- A. El Hilali, V. Boudon and M. Loëte, *J. Mol. Spectrosc.*, **239**, 41–50 (2006).