THE SYMMETRIZATION OF ANGULAR MOMENTUM WAVEFUNCTIONS AND ITS APPLICATIONS TO MOLECULAR SPECTROSCOPY

V. BOUDON, M. REY, CH. WENGER, G. PIERRE, *Laboratoire de Physique de l'Université de Bourgogne, CNRS UMR 5027, 9, Avenue Alain Savary, BP 47870, F-21078 Dijon Cedex, France*; B. SARTAKOV, *General Physics Institute RAS, Vavilov str. 38, 119991 Moscow, Russia*.

In molecular spectroscopy problems, the use of symmetrized wavefunctions, *i.e.* basis vectors transforming according to irreducible representations of the molecular point group, helps to classify the quantum states according to their symmetries. This is very useful when considering the selection rules for transitions and it also facilitates the calculations of eigenvalues. Thus, the symmetrization can be used as a powerful tool in the analysis of high-resolution molecular spectra. While this process is easy to perform in the case of symmetric- and asymmetric-top molecules thanks to projection methods, it is much harder in the case of spherical-tops (tetrahedral or octahedral molecules).

After briefly reviewing the general principles of this topic, we propose a detailed method for the symmetrization of the standard basis $|j, m\rangle$ into the O_h or T_d point group[a]. This is realized by means of an orientation matrix called G determined following the ideas developed formerly by Moret-Bailly[b]. It allows matrix element calculations for rovibronic spectroscopic problems concerning octahedral or tetrahedral molecules. A numerical calculation of all the G matrix elements for both integer and half-integer j values up to $399/2$ has been performed. Such high angular momentum values are necessary for the case of heavy molecules with high rotational excitation. The complete list of these coefficients can be obtained freely at the URL: `http://www.u-bourgogne.fr/LPUB/group.html`. As an illustration, we also present briefly an application to a case where both high and half angular momentum values are to be considered: the ν_3 band of ReF_6 (an open-shell molecule with an odd number of electrons and a fourfold degenerate electronic ground state)[c].

[a] M. Rey, V. Boudon, Ch. Wenger, G. Pierre and B. Sartakov, *J. Mol. Spectrosc.*, in press (2003).

[b] J. Moret-Bailly, *Cah. Phys.*, **15**, 237–316 (1961); J.-P. Champion, G. Pierre, F. Michelot and J. Moret-Bailly, *Can. J. Phys.*, **55**, 515–520 (1977).

[c] V. Boudon, M. Rotger, Y. He, H. Hollenstein, M. Quack and U. Schmitt, *J. Chem. Phys.*, **117**(7), 3196–3207 (2002).