

LILLE SPECTROSCOPIC DATABASE FOR ASTROPHYSICALLY AND ATMOSPHERICALLY RELEVANT MOLECULES

R. A. MOTIYENKO, L. MARGULÈS, *UMR 8523 CNRS - Université de Lille, Laboratoire PhLAM, Villeneuve d'Ascq, France.*

The project of Lille Spectroscopic Database emerged from a large number of molecules of astrophysical and atmospheric interest exhibiting large amplitude motions studied in PhLAM laboratory in the last decade. To fit their spectra and to calculate spectral predictions, different codes were used: BELGI^a, RAM36^b, ERHAM^c or XIAM^d in the case of molecules with the internal rotation of a C_{3v} top, N. Ohashi code for the torsion-inversion problem of methylamine^e, ASFIT/ASROT^f programs for simple asymmetric tops, and SPFIT/SPCAT^g program suite for the treatments of other tunneling motions. While the latter is the main fitting/predicting tool for widely known CDMS and JPL databases^h, spectral predictions obtained with other codes are somehow scattered in the supplementary data of publications and are eventually available in the another well known Splatalogueⁱ database. For this reason, we decided to develop and maintain the Lille Spectroscopic Database which will contain the spectral predictions of the molecules studied in Lille. The new database will provide a typical functionality of other databases: predictions will be available in different formats including different intensity units, and at different temperatures; a search within the full database will be possible to limit the predictions for a particular range of frequencies, intensities or quantum numbers. We also plan to make publicly available the rotational spectra recorded in Lille, and a tool (software) for their analysis.

^aHougen, J. T. *et al*, 1994, *J. Mol. Spec.* **163**, 559

^bIlyushin, V.V. *et al*, 2010, *J. Mol. Spec.* **259**, 26.

^cP. Groner, *P. J. Chem. Phys.* **107**, 4483.

^dH.Hartwig H. *et al*, 1996, *Z. Naturforsch* **51a**, 923.

^eOhashi, N., *et al*. 1987, *J. Mol. Spec.*, **126**, 443

^fKisiel, Z. *et al*, 2019, *J. Mol. Spec.* **359**, 16.

^gPickett H. M., 1991, *J. Mol. Spec.* **148**, 371.

^hMüller, H. S. P., *et al.*, 2005, *J. Mol. Spec.* **327**, 95; Pickett, H. M., *et al.*, 1998, *JQSRT* **60**, 883

ⁱ<https://splatalogue.online>