LLWP – UPDATES ON A NEW LOOMIS-WOOD SOFTWARE AT THE EXAMPLE OF ACETONE- $^{13}C_1$

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Acetone- ${}^{13}C_1$ is a complex organic molecule with two internal methyl (-CH₃) rotors having relatively low barriers to internal rotation of 251 cm⁻¹ [1]. This leads to two low-lying torsional modes and five internal rotation components resulting in a dense and complex spectrum. Similar conditions can be found in many complex molecules, with isotopologues, hyperfine structure, and interactions being additional factors for the presence of even more crowded spectra than that of acetone.

Measurements of acetone- ${}^{13}C_1$ were performed with an isotopically enriched sample in the frequency range from 37-1102 GHz. Loomis-Wood plots (LWPs) are one approach to improve and fasten the analysis of such crowded spectra. Here, an updated version of the LLWP software was used which relies on LWPs for fast and confident assignments. Additionally, LLWP focuses on being user-friendly, intuitive, and applicable to a broad range of assignment tasks. The software will be presented here and is available together with its full documentation at llwp.astro.uni-koeln.de. Predictions of acetone- ${}^{13}C_1$ created with ERHAM [2] allow for future radio astronomical searches.

[1] P. Groner, J. Mol. Struct. 550-551 (2000) 473-479.

- [2] P. Groner, J. Chem. Phys. 107 (1997) 4483-4498.
- [3] P. Groner, J. Mol. Spectrosc. 278 (2012) 52-67.