LLWP - A NEW LOOMIS-WOOD SOFTWARE AT THE EXAMPLE OF PROPANONE-$^{13}C_1$

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Spectra of complex molecules are dense and complicated, especially if isotopologues, low-lying vibrationally excited states, hyperfine structure or other interactions are present. Analysis of these spectra can be difficult due to line confusion. One approach to accommodate this challenge are Loomis-Wood plots (LWPs), which are a visual aid for displaying series of transitions in a spectrum in order to ease assignments. Programs utilizing LWPs exist already in the literature, e.g. AABS [1], Pgopher [2] and LWW [3]. Here, we present a newly developed software which focuses on being intuitive and user friendly while simultaneously allowing for fast and confident assignments of molecular spectra. The software is called LLWP and is written in Python. The core functionality and selected features are presented on the example of first results of the analysis of isotopically enriched propanone-$^{13}C_1$ ($^{13}CH_3COCH_3$), which was synthesized as its signal at natural abundance only allowed for a very limited analysis [4, 5]. The software and its full documentation are available at ltotheois.github.io/LLWP.

[1] Z. Kisiel et al., J. Mol. Spectrosc. **233** (2005) 231 – 243.
[2] C. M. Western, J. Quant. Spectrosc. Radiat. Transf. **186** (2017) 221 – 242.
[3] W. Lodyga et al., J. Mol. Spectrosc. **243** (2007) 182 – 188.
[4] F. J. Lovas and P. Groner, J. Mol. Spectrosc. **236** (2006) 173.
[5] M. H. Ordu et al., Astron. Astrophys. **629** (2019) A72.