A GLOBAL RAM METHOD FOR FITTING ASYMMETRIC TOPS WITH ONE METHYL INTERNAL ROTOR AND TWO ^{14}N NUCLEI: APPLICATION OF THE BELGI-2N CODE TO THE MICROWAVE SPECTRA OF THE METHYLIMIDAZOLE ISOMERS.

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A number of internal rotation codes can deal with the combination of one or two internal rotor(s) with one ^{14}N quadrupole nucleus, but not many treats the internal rotations with two ^{14}N nuclei. Here we present the extended version of our internal rotor program (BELGI-C_s), called BELGI-2N using the Rho-Axis Method (RAM)[a] global approach to deal with the compounds containing one methyl top and two weakly coupling ^{14}N nuclei. For molecules containing a ^{14}N nucleus with a nuclear spin I equal to 1, all rotational transitions of the rigid rotor split into several hyperfine components. The quadrupole moment is relatively small and can be treated using a first order perturbation approximation. To test our new code, we applied it to the microwave data previously recorded for N-, 2-, 4- and 5-methylimidazole, using a chirped-pulse Fourier transform microwave spectroscopy in the 7.0–18.5 GHz frequency range[b]. Compared to this study, we were able to perform global fits with root-mean-square deviations within the experimental accuracy and to increase the number of assigned lines with the high predictive power of the fits.

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[a] J. T. Hougen, I. Kleiner, and M. Godefroid, J. Mol. Spectrosc. 163, 559 (1994)

[b] E. Gougoula, C. Medcraft, J. Heitkämper, and N. R. Walker, J. Chem. Phys. 151, 144301 (2019)