

AUTOMATED, CONTEXT-FREE ASSIGNMENT OF ASYMMETRIC ROTOR MICROWAVE SPECTRA

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We present a new algorithm, Robust Automated Assignment of Rigid Rotors (RAARR), for assigning rotational spectra of asymmetric tops. The RAARR algorithm can automatically assign experimental spectra under a broad range of conditions, including spectra comprised of multiple mixture components, in about 100 seconds or less. The RAARR algorithm exploits constraints placed by the conservation of energy to find sets of connected lines in an unassigned spectrum. The highly constrained structure of these sets eliminates all but a handful of plausible assignments for a given set, greatly reducing the number of potential assignments that must be evaluated. We successfully apply our algorithm to automatically assign 15 experimental spectra, including 5 previously unassigned species, without prior estimation of molecular rotational constants. In 9 of the 15 cases, the RAARR algorithm successfully assigns two or more mixture components.