

## AUTOMATED SPECTROSCOPIC ANALYSIS USING THE PARTICLE SWARM OPTIMIZATION ALGORITHM: IMPLEMENTING A GUIDED SEARCH ALGORITHM TO AUTOFIT

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While rotational spectra can be rapidly collected, their analysis (especially for complex systems) is seldom straightforward, leading to a bottleneck. The AUTOFIT program<sup>a</sup> was designed to serve that need by quickly matching rotational constants to spectra with little user input and supervision. This program can potentially be improved by incorporating an optimization algorithm in the search for a solution. The Particle Swarm Optimization Algorithm (PSO) was chosen for implementation. PSO is part of a family of optimization algorithms called heuristic algorithms, which seek approximate best answers. This is ideal for rotational spectra, where an exact match will not be found without incorporating distortion constants, etc., which would otherwise greatly increase the size of the search space. PSO was tested for robustness against five standard fitness functions and then applied to a custom fitness function created for rotational spectra. This talk will explain the Particle Swarm Optimization algorithm and how it works, describe how Autofit was modified to use PSO, discuss the fitness function developed to work with spectroscopic data, and show our current results.

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<sup>a</sup>Seifert, N.A., Finneran, I.A., Perez, C., Zaleski, D.P., Neill, J.L., Steber, A.L., Suenram, R.D., Lesarri, A., Shipman, S.T., Pate, B.H., J. Mol. Spec. 312, 13-21 (2015)