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AN AUTOMATIC MOLECULAR LINE IDENTIFICATION USING MILLIMETER OBSERVATIONS

A. Farafontova and M. Kirsanova

Institute of Astronomy of the RAS,
119017, Moscow, Pyatnitskaya St. 48, Russia

E-mail: farafontova@inasan.ru
kirsanova@inasan.ru

Observations conducted with modern telescopes in the sub- and millimeter range have provided key insights about processes within star-forming regions. These instruments deliver high-resolution ($\lambda/\Delta\lambda = 10^7$) spectra across broad bandwidths, revealing a dense forest of molecular emission lines which can serve as tracers of kinematic, physical, and chemical conditions in sources. Line profiles can provide information about gas dynamics and excitation mechanisms.

The identification of emission lines requires rigorous cross-matching of observed frequencies with laboratory spectroscopic catalogs, while accounting for source-specific excitation conditions. To address this, we developed an automated line identification pipeline. In this pipeline we applied a consecutive Gaussian fitting algorithm to determine the observed central frequencies of emission lines and a procedure to automatically cross-match these values with entries in molecular spectroscopic databases (CDMS and JPL). In six observational spectra toward the young stellar object we resolved >400 emission lines, attributing 99% to rotational transitions of SO, OCS, SiO, HCO, H_2CO, SO_2, H_2CS, complex organic molecules CH_3OH, CH_3CCH and CH_3CN ladder transitions, CH_3OCH_3, CH_3OCHO, CH_3CHO, C_2H_3CN etc. We found up to 9-atom molecules like C_2H_5CN, isotopologues $^{13}CH_3OH$, $S^{33}O$, $S^{33}O_2$, $S^{34}O$, $OC^{34}S$, $H_2C^{33}S$, $H_2C^{34}S$ and deuterated species like HDO. Application of this pipeline reduced spectral line analysis time from ∼40 hours per spectrum (manual processing) to <10 minutes, achieving a limit of $\geq 5\sigma$ for line detections. This work was supported by RSF grant 24-22-00097.