

## LABORATORY DETECTION OF THE *TRANS-GAUCHE* CONFORMER OF ETHYL FORMATE.

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Ethyl formate has two coordinates of conformational flexibility, in the ester (O=C-O-C) and ethyl (C-O-C-C) dihedral angles. Two conformers, one with a *cis* ester and *trans* ethyl orientation, the other with a *cis* ester and *gauche* ethyl orientation, have been previously detected by rotational spectroscopy.<sup>a</sup> In addition, the *cis-trans* isomer, the lowest-energy conformer, has recently been detected in the SgrB2(N) hot core.<sup>b</sup> The third conformer of ethyl formate, with a *trans* ester orientation and *gauche* ethyl orientation, is significantly higher in energy than the *cis-trans* conformer according to electronic structure calculations (1900 cm<sup>-1</sup>, or 1330 K), but there is a barrier of 2870 cm<sup>-1</sup> (2000 K) for this conformer to relax into the more stable *cis* ester potential well, and so local thermodynamic equilibrium between these conformers is not expected in the interstellar medium. Similar behavior is found for the *trans* ester conformer of methyl formate, for which a tentative detection in SgrB2(N) was presented at this meeting last year, with a column density roughly 1% of that of the more stable *cis* isomer.<sup>c</sup> Here we report the laboratory detection of *trans-gauche* ethyl formate using Fourier transform microwave spectroscopy; its low population at room temperature equilibrium has been enhanced by the use of a pulsed discharge nozzle. The spectrum is complicated by a low barrier (140 cm<sup>-1</sup>) to tunneling between equivalent structures.

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<sup>a</sup>J.M. Riveros and E.B. Wilson, *J. Chem. Phys.* **46**, 4605 (1967).

<sup>b</sup>A. Belloche. *et al.*, *A&A* **499**, 215 (2009).

<sup>c</sup>M.T. Muckle *et al.*, RH15, 64th International Symposium on Molecular Spectroscopy (2009).