

ASSIGNMENT OF THE PERFLUOROPROPIONIC ACID-FORMIC ACID COMPLEX AND THE DIFFICULTIES OF INCLUDING HIGH K_a TRANSITIONS.

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We recently began an investigation into the perfluoropropionic acid···formic acid complex using broadband microwave spectroscopy. This study aims to examine the possible double proton transfer between the two interacting carboxylic acid groups. The spectrum presented as a doubled set of lines, with spacing between transitions of < 1 MHz. Transitions appeared to be a -type, R branch transitions for an asymmetric top. Assignment of all $K_a = 1, 0$ transitions yields decent fits to a standard rotational Hamiltonian. Treatment of the doubling as either a two state system (presumably with a double proton transfer) or as two distinct, but nearly identical conformations of the complex produce fits of similar quality. Including higher K_a transitions for the a -type, R-branch lines greatly increases the error of these fits. A previous study involving the trifluoroacetic acid···formic acid complex published observed similar high K_a transitions, but did not include them in the published fit.^a We hope to shed more light on this conundrum. Similarities to other double-well potential minimum systems will be discussed.

^aMartinache, L.; Kresa, W.; Wegener, M.; Vonmont, U.; and Bauder, A. *Chem. Phys.* **148** (1990) 129-140.