

## METHOD LIMITATIONS IN THE TREATMENT OF NUCLEAR QUADRUPOLE COUPLING WITH INTERNAL ROTATION IN METHOXYFLURANE (C<sub>3</sub>H<sub>4</sub>Cl<sub>2</sub>F<sub>2</sub>O)

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The rotational spectrum of methoxyflurane was recorded using molecular jet FTMW spectroscopy. Methyl internal rotation and nuclear quadrupole coupling (NQC) of two chlorine nuclei (Cl) complicated the analysis. Codes that treat internal rotation often allow for simultaneous but approximate treatment of NQC, with significant errors for the NQC of Cl. In contrast, the well-known *SPFIT* code provides an exact treatment of NQC, which can be combined with separate fits for each internal rotation species. However, *SPFIT* local fits also have limitations; they only allow fitting of NQC off-diagonal elements and internal rotation parameters when the internal rotation axis and the coupling nucleus are coplanar, which is not the case in methoxyflurane. Still, with a "not-too-small" internal rotation barrier of 350 cm<sup>-1</sup>, a work-around is possible. The abstract-figure shows the  $J_{K_a, K_c} : 3_{2,1} - 2_{2,0}$  transition - experiment (black), simulations of species A (blue), E (red) and both combined (green). (A and E each scaled to match peak marked with an asterisk).

