THEORETICAL PREDICTION OF THE ROTATIONAL CONSTANTS FOR PROTONATED METHANOL ($CH_3OH_2^+$): A MISSING PLAYER IN HOT CORE CHEMISTRY

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Protonated molecules play important roles in the ion-molecule chemistry of hot cores. Protonated methanol, $CH_3OH_2^+$, is thought to contribute significantly to the gas phase formation of other known organic species such as methyl formate and dimethyl ether. While the protonated forms of many of the most common astromolecules have previously been detected, $CH_3OH_2^+$ remains unidentified to date due to the absence of an experimental rotational spectrum. In order to provide theoretical predictions to assist anticipated new laboratory work, various levels of quantum chemical methodology were employed to predict the structure of $CH_3OH_2^+$ and to convert its equilibrium rotational constants to A_0, B_0, and C_0. Potentials for the inversion and rotation of OH_2^+ with respect to the CH_3 group were also determined. This work built upon a benchmark study of methylamine discussed elsewhere (INSERT CODE).