JET-COOLED SPECTROSCOPY OF THE *M*-XYLYL RADICAL IN A CORONA-EXCITED SUPERSONIC EXPANSION: HYPER-CONJUGATION AND CONFORMATIONAL DEPENDENCE IN VIBRONIC TRANSITIONS

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ABSTRACT

The electronically hot but jet-cooled *m*-xylyl radical was produced from the precursor *m*-xylene in a corona-excited supersonic expansion (CESE), and its vibronic emission spectrum was recorded. Theoretical studies of the ground and excited state structures, as well as the hyper-conjugative interaction of the *m*-xylyl radical, were carried out. The preferred geometry of the methyl rotor in the ground state is switched in the excited state. The vibronic emission spectrum of the *m*-xylyl radicals corresponded to the $D_1 \rightarrow D_0$ electronic transition and determined the electronic transition energy depending on the initial change in the methyl conformations.

Keywords: Spectroscopy, *m*-xylyl radical, corona discharge, hyper-conjugation, natural bond orbital.