

FTMW SPECTROSCOPY OF THE METHYL-VINYL CRIEGEE INTERMEDIATE

YASUKI ENDO, CHEN-AN CHUNG, YUAN-PERN LEE, *Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan.*

Pure rotational transitions of the methyl-vinyl Criegée intermediate have been observed by FTMW spectroscopy. The species was produced by discharging a mixture, 1,3-diiodo-but-2-en and O₂ diluted in Ar. Among four possible isomers for this species with energy less than 3 kcal/mol, only the lowest energy isomer, the *syn-trans* isomer was detected. Thirty rotational transitions with internal rotation splitting for the methyl top were observed. The observed frequencies were analyzed by the XIAM program,¹ yielding the rotational constants, which agree very well for the lowest energy isomer, giving definite assignment of the isomer observed. Furthermore, the internal rotation barrier was determined to be 702.8(28) cm⁻¹, which also reasonably agrees with that of an *ab initio* calculation 680 cm⁻¹ at CCSD(T)/cc-pVTZ.

1. H. Hartwig and H. Dreizler, Z. Naturforsch. A 51, 923 (1996).