ISOMERS OF SO_2: INFRARED ABSORPTION OF SOO IN SOLID AR

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Sulfur dioxide (SO_2) isolated in solid argon at 12K was irradiated with light at 193 nm from an ArF excimer laser. Preliminary results show that new absorption lines observed at 1006.1 and 739.9 cm^{-1} are assigned to sulfur superoxide (SOO). Theoretical calculations using the B3-LYP/cc-pVTZ density functional method were carried out for SOO and cyclic SO_2; predicted vibrational wavenumbers are (1079,763, and 472) and (1009, 739, and 682) cm^{-1}, respectively. Although observed wavenumbers fit better with those predicted for cyclic SO_2, the observed relative IR intensities and O-18 isotopic shifts are in excellent agreement with those predicted for SOO.