HIGH LEVEL AB INITIO STUDY OF THE ROVIBRONIC SPECTRUM OF SULFUR MONOXIDE (SO): DIABATIC REPRESENTATION

RYAN BRADY, *Department of Physics and Astronomy, University College London, London, UK*; GAP-SUE KIM, *Dharma college of Dongguk, University in Seoul, Seoul, Korea*; WILFRID SOMOGYI, SERGEI N. YURCHENKO, JONATHAN TENNYSON, *Department of Physics and Astronomy, University College London, London, UK*.

We present a high level ab initio study of the rovibronic spectra of Sulfur Monoxide (SO) using internally contracted multireference configuration interaction (IC-MRCI) method using aug-cc-pv5z basis sets and a fully diabatised model for the molecule. The diabatic model covers the lowest 13 singlet and triplet electronic states of SO $X^3\Sigma^-$, $a^1\Delta$, $b^1\Sigma^+$, $c^1\Sigma^-$, $A^{3\prime}\Delta$, $A^{3\prime\prime}\Sigma^+$, $A^3\Pi$, $B^3\Sigma^-$, $C^3\Pi$, $C^{3\prime}\Pi$, $d^1\Pi$, $e^1\Pi$, and $(3)^1\Pi$ ranging up to 66,800 cm^{-1}. The ab initio spectroscopic model includes potential energy curves, dipole and transition dipole moment curves, spin-orbit curves and electronic angular momentum curves. A diabatic representation is built by removing avoiding crossings between the $C^3\Pi$–$C^{3\prime}\Pi$ and $e^1\Pi$–$(3)^1\Pi$ states through a unitary transformation who's rotation angle is determined on the fly by enforcing smoothness properties of the diabatic potential energy curves. A rovibronic line list of SO is computed covering the wavelength range up to 167 nm.