

Dynamics of Nitro-Nitrite Rearrangement in Nitromethane Radical Cation

MI'KAYLA D WORD, HUGO A. LOPEZ PENA, DERRICK AMPADU BOATENG, KATHARINE MOORE TIBBETTS, *Department of Chemistry, Virginia Commonwealth University, Richmond, Virginia, USA.*

- NM^+ dissociates into CH_3^+ , NO^+ , and NO_2^+
- NO_2^+ is assigned to the $D_0 \rightarrow D_2$ transition
- NO^+ is assigned to the population of D_2 and relaxation to D_0 to undergo the NNR in ~ 435 fs.
- CH_3^+ is assigned to the $D_0 \rightarrow D_2$ transition within geometry with C-N bond distance of 1.88 \AA

$$S(\tau) = ae^{-\tau/T_1} + be^{-\tau/T_2} + ce^{-\tau/T_3} + d$$

