Electronic Supplementary Information

Density Functional Theory Study on the Reaction of Triazol-3-one with Nitronium: Direct Nitration versus Acidic Group-Induced Nitration

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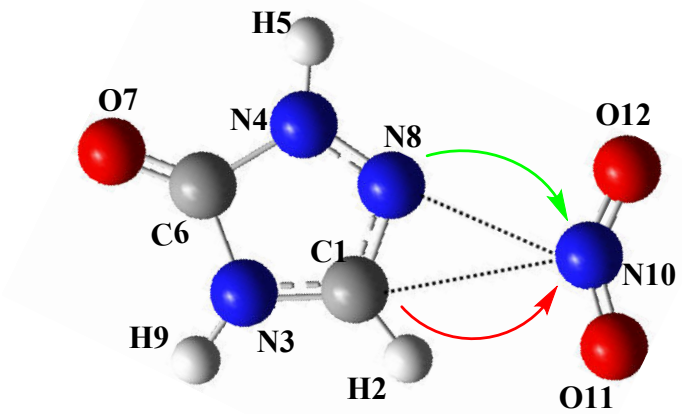

Fig. S1 Schematic diagram for the attraction of NO_2^+ by TO molecule during the nitration process.

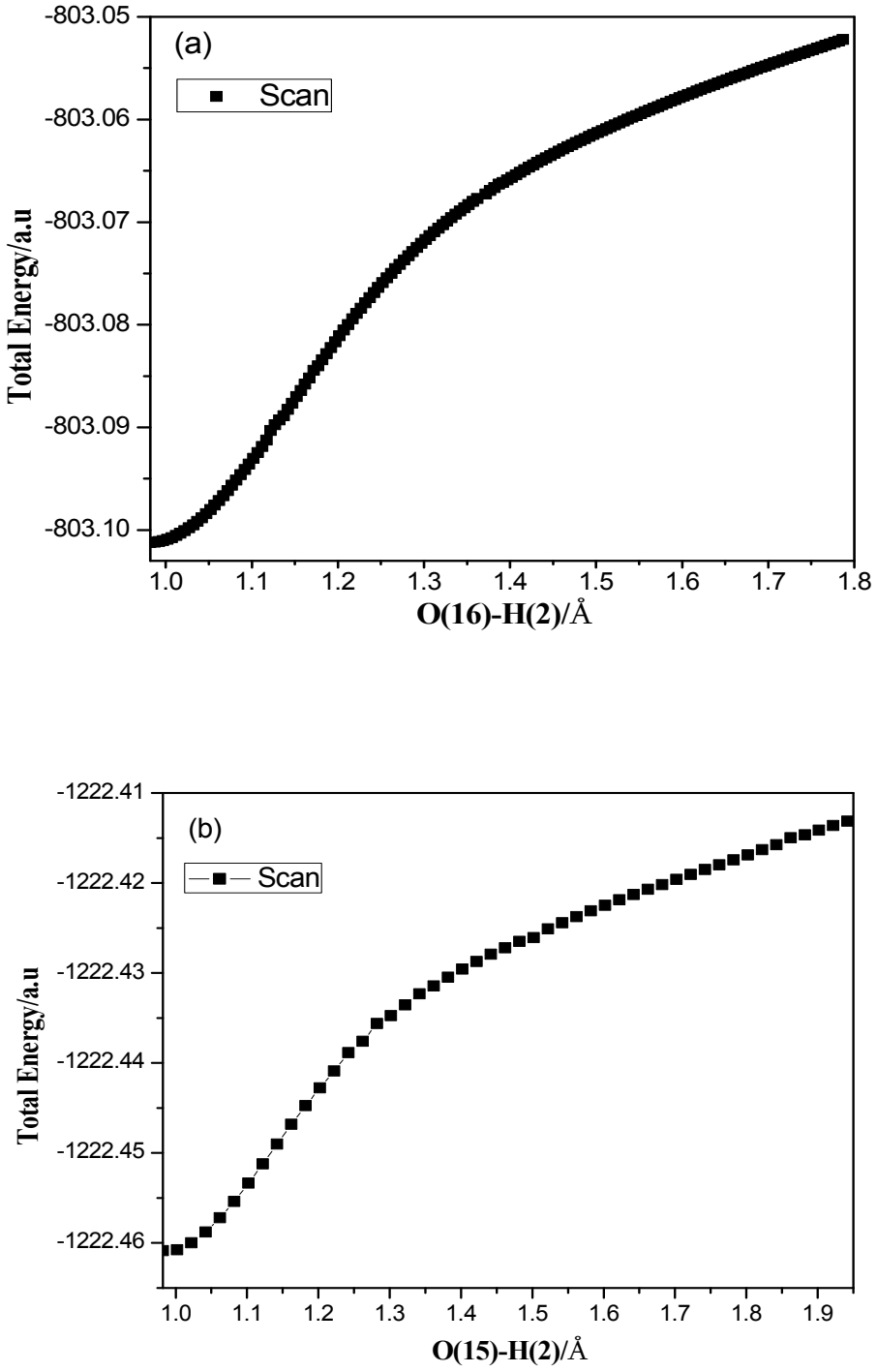

Fig. S2 (a) The potential energy surface scan of O(16)-H(2) in An-IM4 calculated at the B3LYP/6-311G(d,p) level. (b) The potential energy surface scan of O(15)-H(2) in As-IM4 calculated at the B3LYP/6-311G(d,p) level.

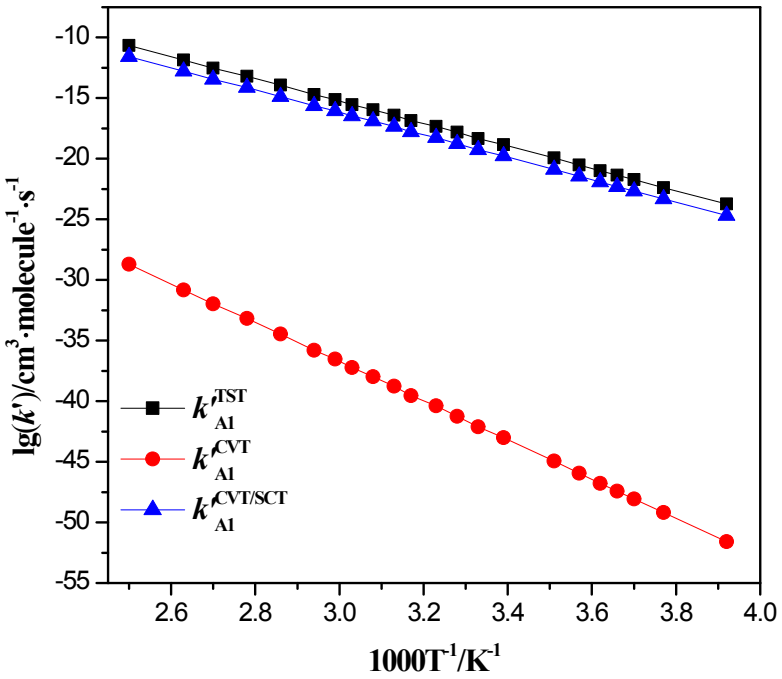

Fig. S3 The calculated rate constants of the rate-determining step of path A1 via TST, CVT and CVT/SCT within temperature ranges of 225-400 K.