A Theoretical Study on the Formation and Photolysis of Nitrosamines (CH_3CH_2NHNO and $(CH_3CH_2)_2NNO$) under Atmospheric Conditions

Sopporting Information

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Figure S1. The optimized geometries of reactants and products at the B3LYP/6-311++G(d,p), B3LYP/aug-cc-pVDZ, MP2/6-311++G(d,p), and MP2/aug-cc-pVDZ levels for the CH_3CH_2NH +NO and $(CH_3CH_2)_2N$ +NO reactions. Bond distances are in angstrom and bond angles are in degrees. From top to bottom, the values are obtain at the B3LYP/6-311++G(d,p), B3LYP/aug-cc-pVDZ, MP2/6-311++G(d,p), and MP2/aug-cc-pVDZ levels.

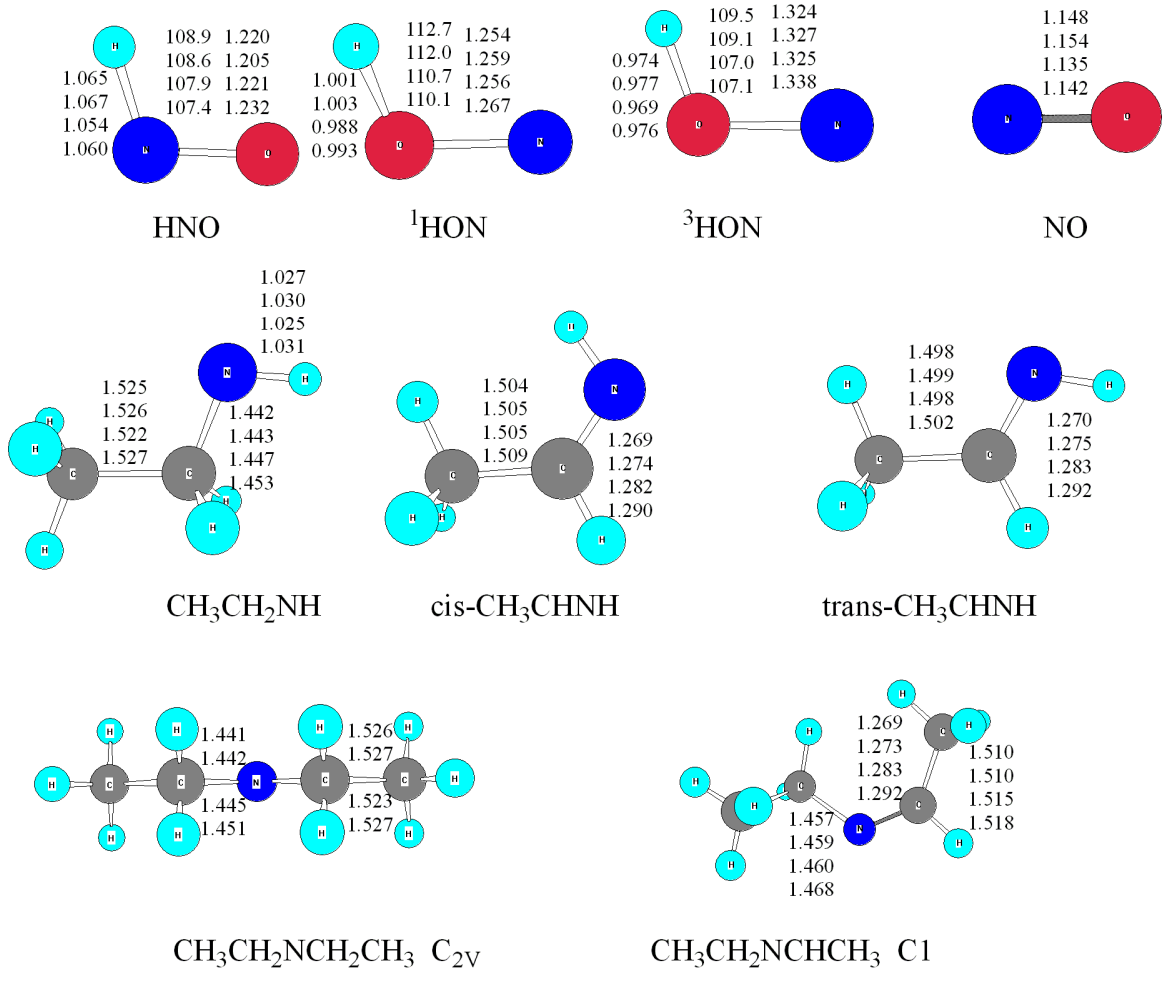
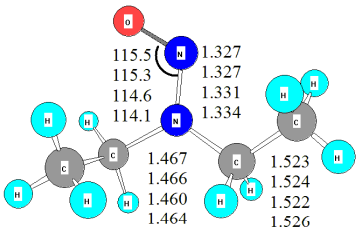
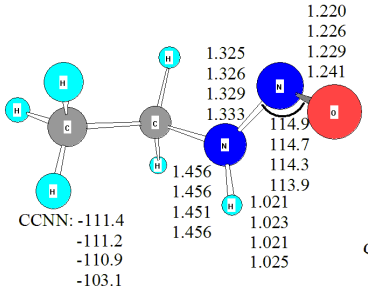


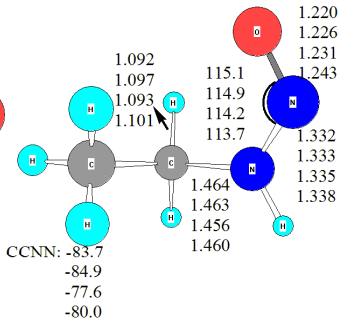
Figure S2. The optimized geometries of intermediates (IM) and transition states (TS) at the B3LYP/6-311++G(d,p), B3LYP/aug-cc-pVDZ, MP2/6-311++G(d,p), and MP2/aug-cc-pVDZ levels for the CH_3CH_2NH + NO and $(CH_3CH_2)_2N$ + NO reactions. Bond distances are in angstrom and bond angles are in degrees. From top to bottom, the values are obtain at the B3LYP/6-311++G(d,p), B3LYP/aug-cc-pVDZ, MP2/6-311++G(d,p), and MP2/aug-cc-pVDZ levels. For TS11, the values are from the B3LYP/6-311++G(d,p) and B3LYP/aug-cc-pVDZ levels.



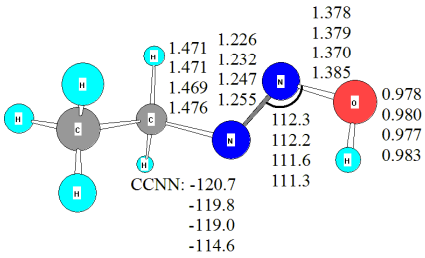
$(CH_3CH_2)_2NNO$ (IM1)



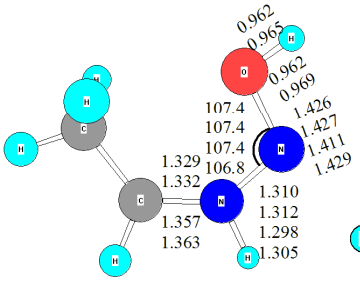
syn-CH_3CH_2NHNO (IM2)



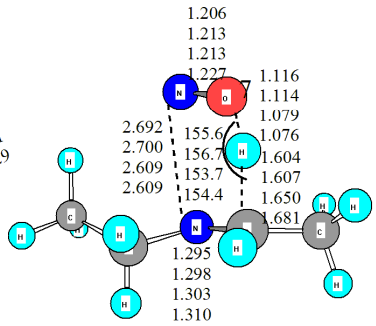
anti-CH_3CH_2NHNO (IM3)



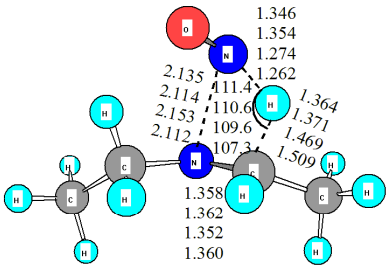
IM4



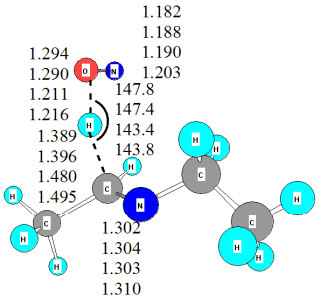
IM5



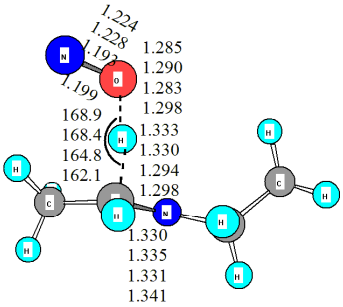
TS1



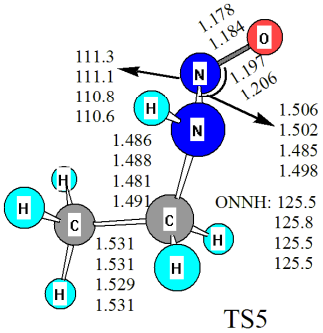
TS2



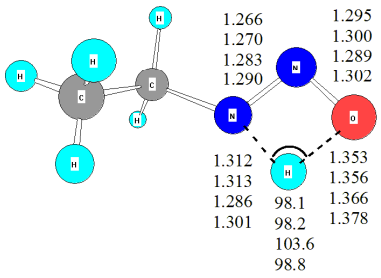
TS3



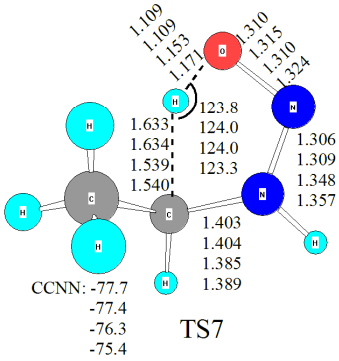
TS4



TS5



TS6



TS7

Figure S2 continued.

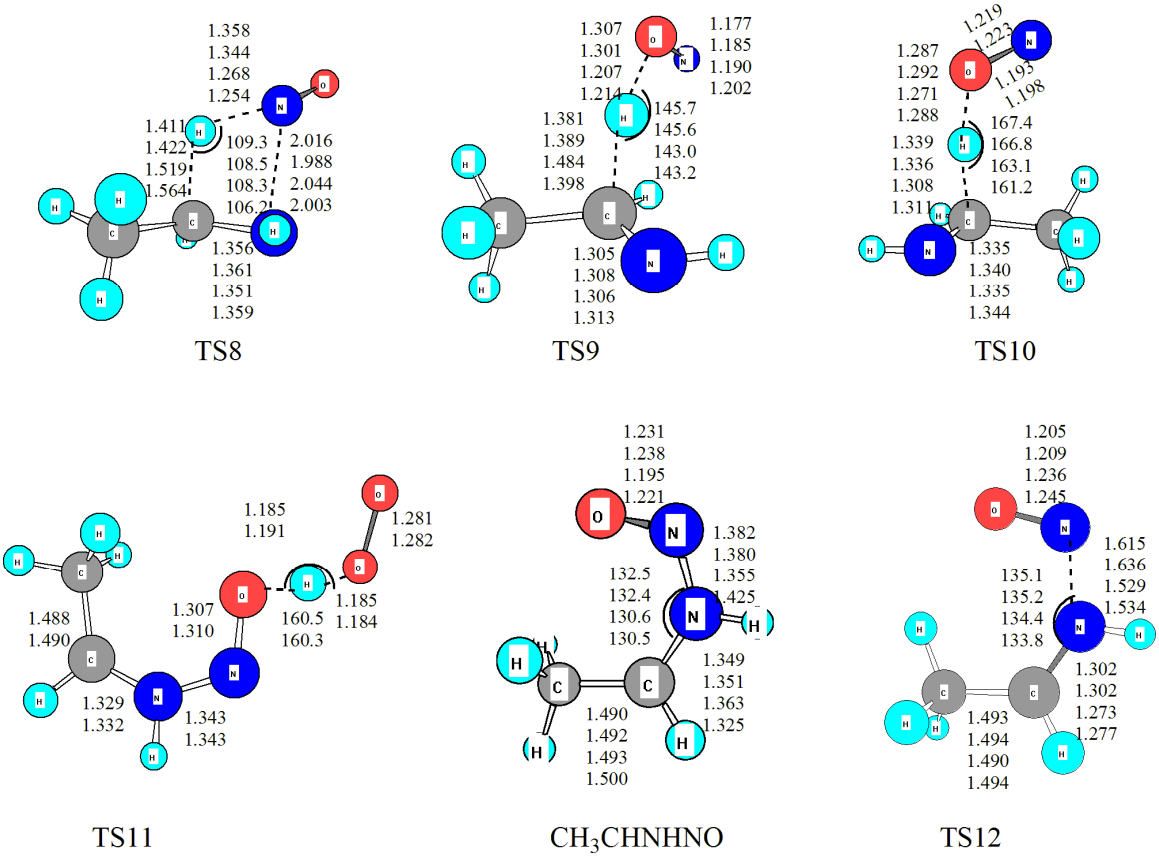


Table S1. The excitation energy (in eV) and oscillator strength (in atomic units) of the first excited state (1A") of the CH_3CH_2NHNO, $(CH_3CH_2)_2NNO$, $CH_3CHNHNOH$ and CH_3CH_2NNOH at B3LYP/basis set//B3LYP/6-311++G(d,p) level.

Species	6-311++G(d,p)	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-aug-pVDZ	cc-aug-pVTZ
CH_3CH_2NHNO	3.36 0.0012	3.37 0.0013	3.37 0.0010	3.37 0.0010	3.37 0.0009	3.37 0.0009
$CH_3CHNHNOH$	3.45 0.0016	4.30 0.0004	4.12 0.0007	3.95 0.0010	3.42 0.0018	3.43 0.0017
CH_3CH_2NNOH	4.65 0.0001	4.70 0.0000	4.68 0.0000	4.67 0.0000	4.66 0.0001	4.65 0.0001
$(CH_3CH_2)_2NNO$	3.38 0.0008	3.38 0.0008	3.39 0.0007	3.39 0.0006	3.39 0.0006	3.39 0.0006

Table S2. The excitation energy (in eV) and oscillator strength (in atomic units) of the first excited state (1A") of the CH_3CH_2NHNO, $(CH_3CH_2)_2NNO$, $CH_3CHNHNOH$ and CH_3CH_2NNOH at B3LYP/basis set//B3LYP/basis set.

Species	6-311++G(d,p)	cc-pVDZ	cc-pVTZ	cc-aug-pVDZ	cc-aug-pVTZ
CH_3CH_2NHNO	3.36 0.0012	3.36 0.0013	3.39 0.0011	3.35 0.0009	3.38 0.0009
$CH_3CHNHNOH$	3.45 0.0016	4.28 0.0004	4.13 0.0007	3.42 0.0018	3.44 0.0017
CH_3CH_2NNOH	4.65 0.0001	4.71 0.0000	4.71 0.0000	4.65 0.0001	4.67 0.0001
$(CH_3CH_2)_2NNO$	3.38 0.0008	3.37 0.0008	3.40 0.0007	3.37 0.0006	3.40 0.0006