Supporting Information for

Insights into the Mechanism and Kinetics for Gas-phase atmospheric Reaction of 9-Chloroanthracene with NO_3 Radical in the Presence of NO_X

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Six pages

Contains four figures

Figure S1. The H abstraction reaction scheme of 9-ClAnt embedded with the potential barrier Δ*E* (in kJ/mol) and reaction heat Δ*H* (in kJ/mol). Δ*H* is calculated at 0 K.

Figure S2. The isomerization reaction schemes of IM1, IM2, IM3 and IM4 embedded with the potential barrier Δ*E* (in kJ/mol) and reaction heat Δ*H* (in kJ/mol).

Figure S3. The unimolecular decomposition reaction scheme of the NO_3-9-ClAnt adducts embedded with the potential barrier Δ*E* (in kJ/mol) and reaction heat Δ*H* (in kJ/mol).

Figure S4. Configuration for the transition states of H abstractions from 9-ClAnt optimized at the BB1K/6-31+G(d,p) level of theory. Distances are in angstrom.

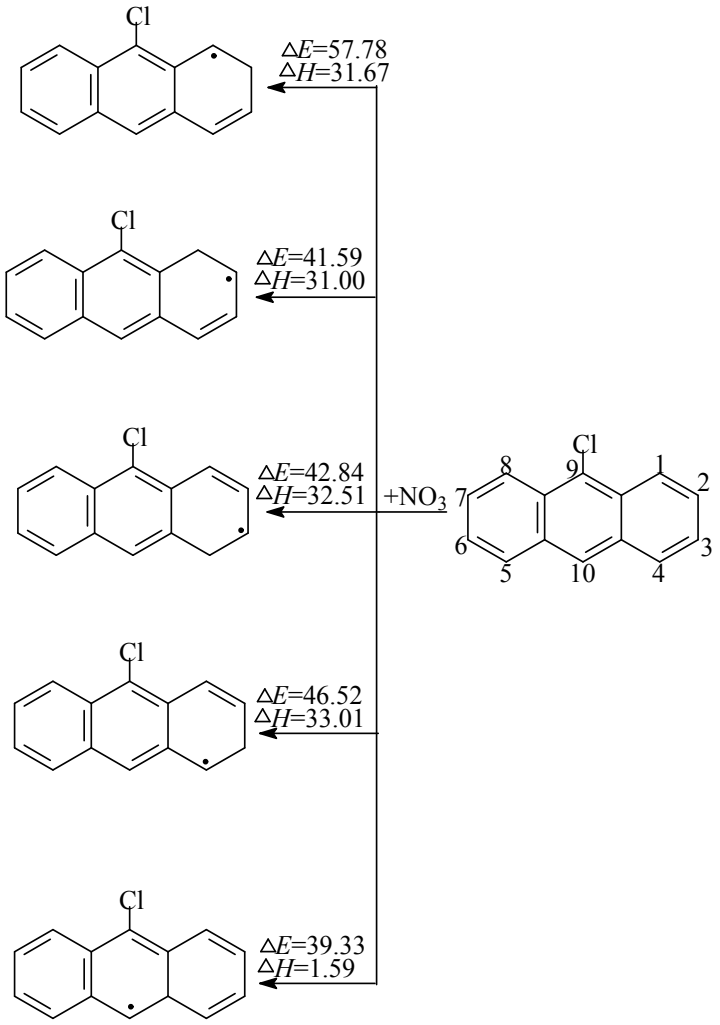
Cl
ΔE=57.78
ΔH=31.67
Cl
ΔE=41.59
ΔH=31.00
Cl
ΔE=42.84
ΔH=32.51
+NO3
Cl
1
2
3
4
5
6
7
8
9
10
Cl
ΔE=46.52
ΔH=33.01
Cl
ΔE=39.33
ΔH=1.59

Figure S1

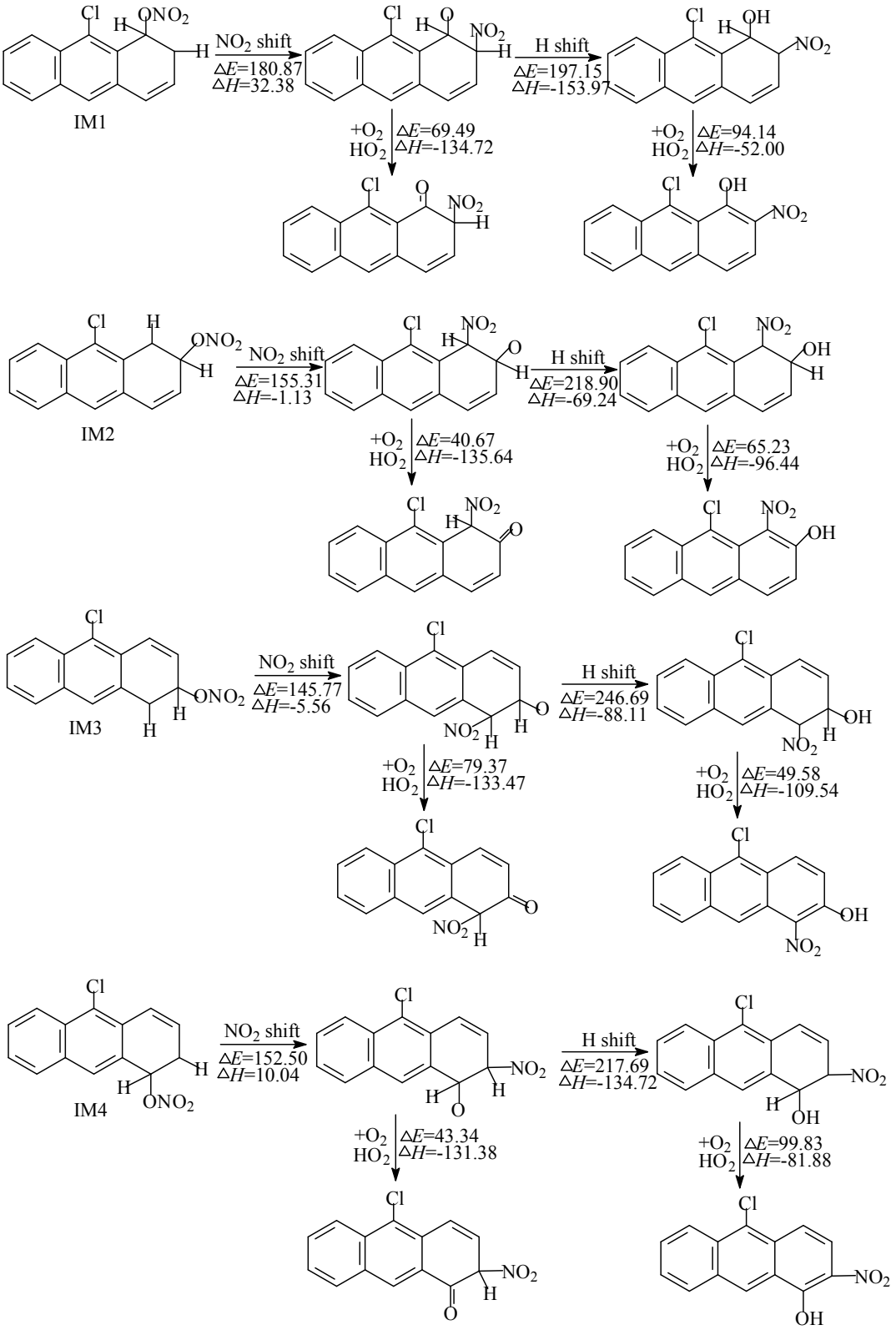
IM1
NO2 shift
ΔE=180.87
ΔH=32.38
H shift
ΔE=197.15
ΔH=-153.97
+O2
HO2
ΔE=69.49
ΔH=-134.72
ΔE=94.14
ΔH=-52.00
IM2
NO2 shift
ΔE=155.31
ΔH=-1.13
H shift
ΔE=218.90
ΔH=-69.24
ΔE=40.67
ΔH=-135.64
ΔE=65.23
ΔH=-96.44
IM3
NO2 shift
ΔE=145.77
ΔH=-5.56
H shift
ΔE=246.69
ΔH=-88.11
ΔE=79.37
ΔH=-133.47
ΔE=49.58
ΔH=-109.54
IM4
NO2 shift
ΔE=152.50
ΔH=10.04
H shift
ΔE=217.69
ΔH=-134.72
ΔE=43.34
ΔH=-131.38
ΔE=99.83
ΔH=-81.88

Figure S2

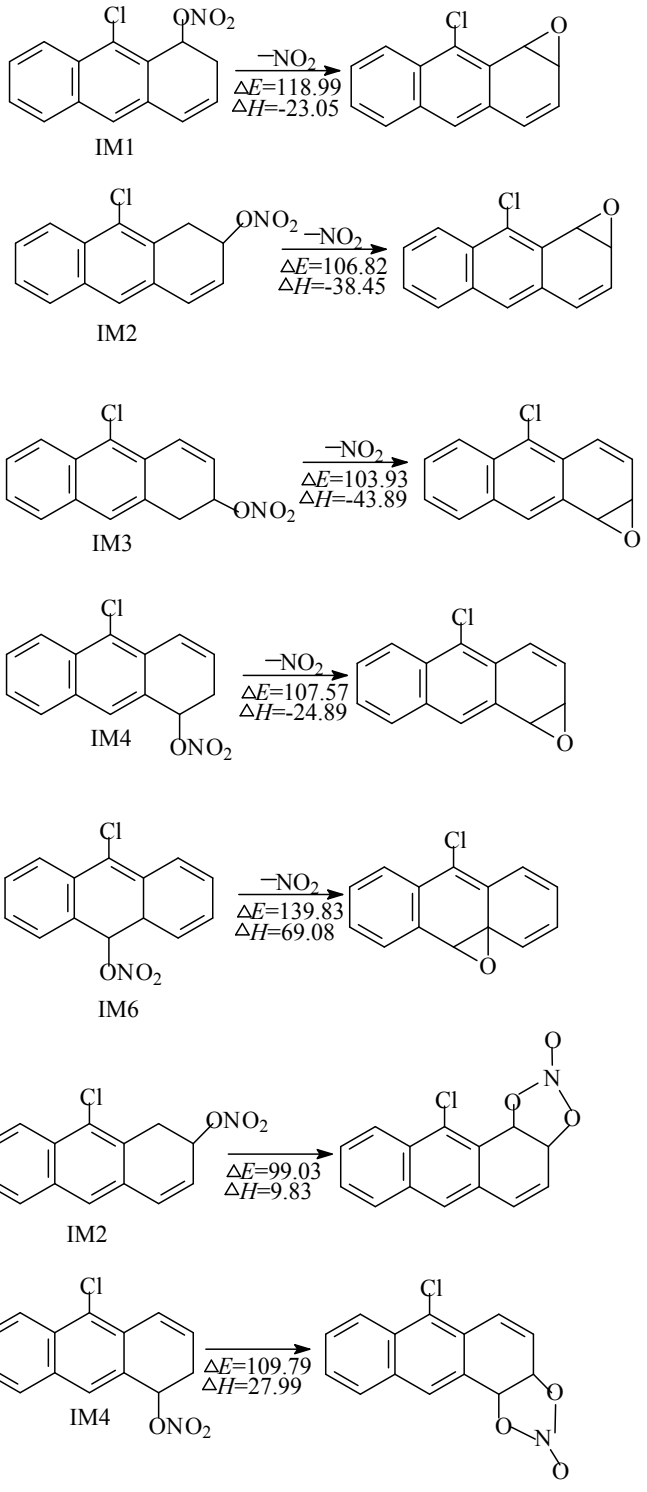
Cl
ONO2
−NO2
ΔE=118.99
ΔH=-23.05
IM1
Cl
O
Cl
ONO2
−NO2
ΔE=106.82
ΔH=-38.45
IM2
Cl
O
Cl
ONO2
−NO2
ΔE=103.93
ΔH=-43.89
IM3
Cl
O
Cl
ONO2
−NO2
ΔE=107.57
ΔH=-24.89
IM4
Cl
O
Cl
ONO2
−NO2
ΔE=139.83
ΔH=69.08
IM6
Cl
O
Cl
ONO2
ΔE=99.03
ΔH=9.83
IM2
Cl
O
N
O
O
Cl
ONO2
ΔE=109.79
ΔH=27.99
IM4
Cl
O
N
O
O

Figure S3

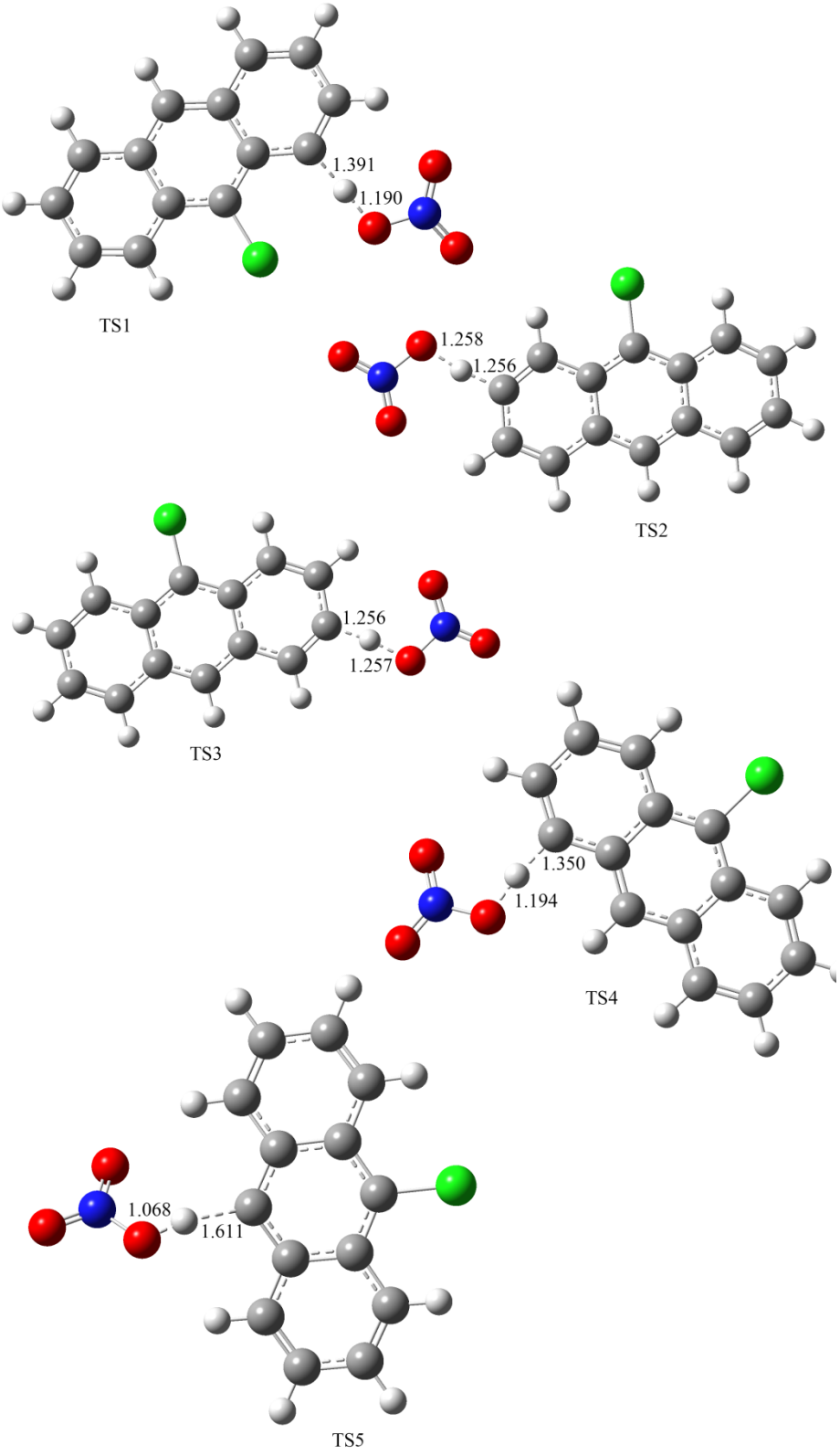
1.391
1.190
TS1
1.258
1.256
TS2
1.256
1.257
TS3
1.350
1.194
TS4
1.068
1.611
TS5

Figure S4