Electronic Supplementary Material (ESI) for RSC Advances.
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Electronic Supplementary Information for

"*Global* ab initio *exploration of potential energy surfaces for radical generation in the initial stage of benzene oxidation*"

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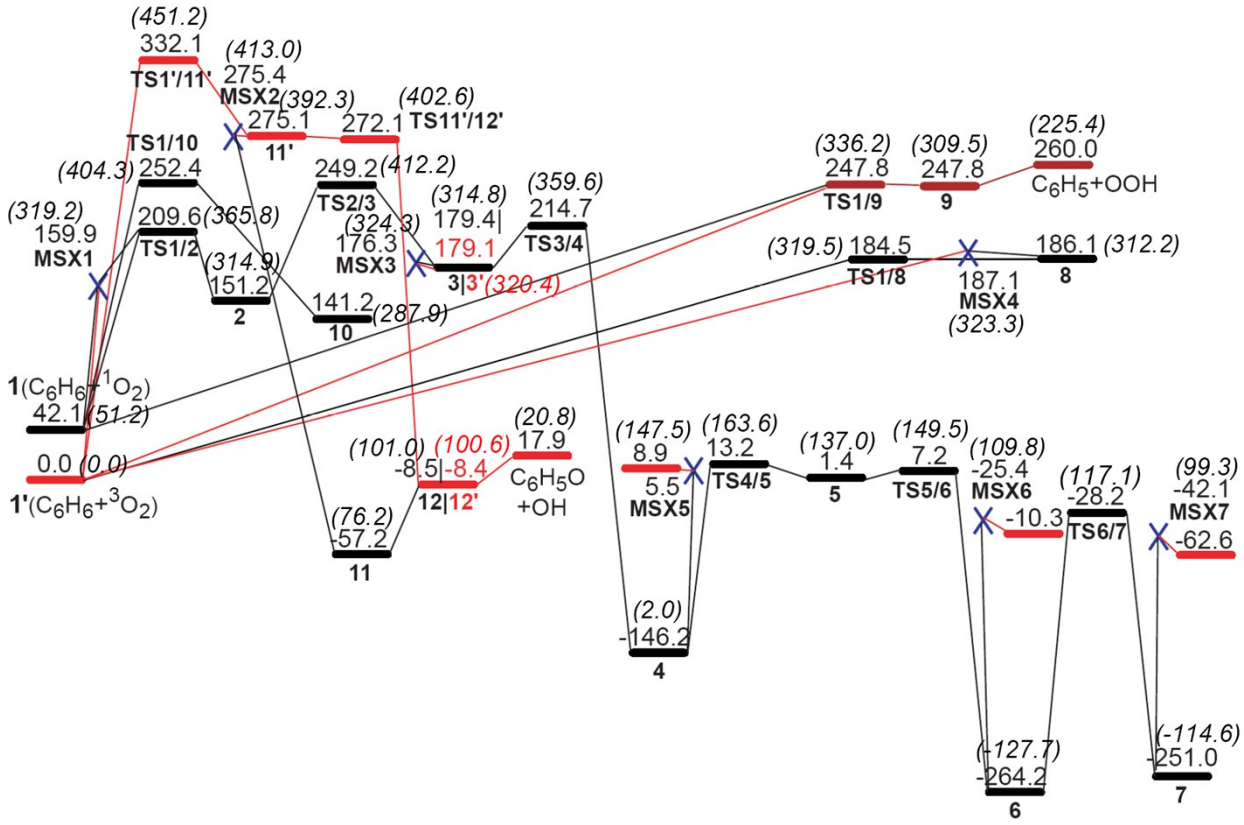
Figure S1. The potential energy surfaces (red for triplet and black for singlet) for benzene activation at UB3LYP/cc-pVTZ level. The data in parenthesis are Gibbs free energies calculated at 1000.0K. Energy values (in kJ/mol) are relative to triplet molecular oxygen plus benzene. The MESX points are shown with blue X. The corresponding structures are illustrated in Figure 1 of context.

Figure S2. The potential energy surfaces for the oxidation of intermediate **3** by triplet molecular oxygen at UB3LYP/cc-pVTZ level. The data in parenthesis are Gibbs free energies calculated at 1000.0K. Energy values (in kJ/mol) are relative to triplet molecular oxygen plus intermediate **3**.

Figure S3. The potential energy surfaces for the oxidation of intermediate **4** by triplet molecular oxygen at UB3LYP/cc-pVTZ level. The data in parenthesis are Gibbs free energies calculated at 1000.0K. Energy values (in kJ/mol) are relative to triplet molecular oxygen plus intermediate **4**.

Figure S4. The potential energy surfaces for the oxidation of intermediate **6** by triplet molecular oxygen at UB3LYP/cc-pVTZ level. The data in parenthesis are Gibbs free energies calculated at 1000.0K. Energy values (in kJ/mol) are relative to triplet molecular oxygen plus intermediate **6**.

Figure S5. The reaction path followed by the intrinsic reaction coordinate for **TS2/3** + O_2.



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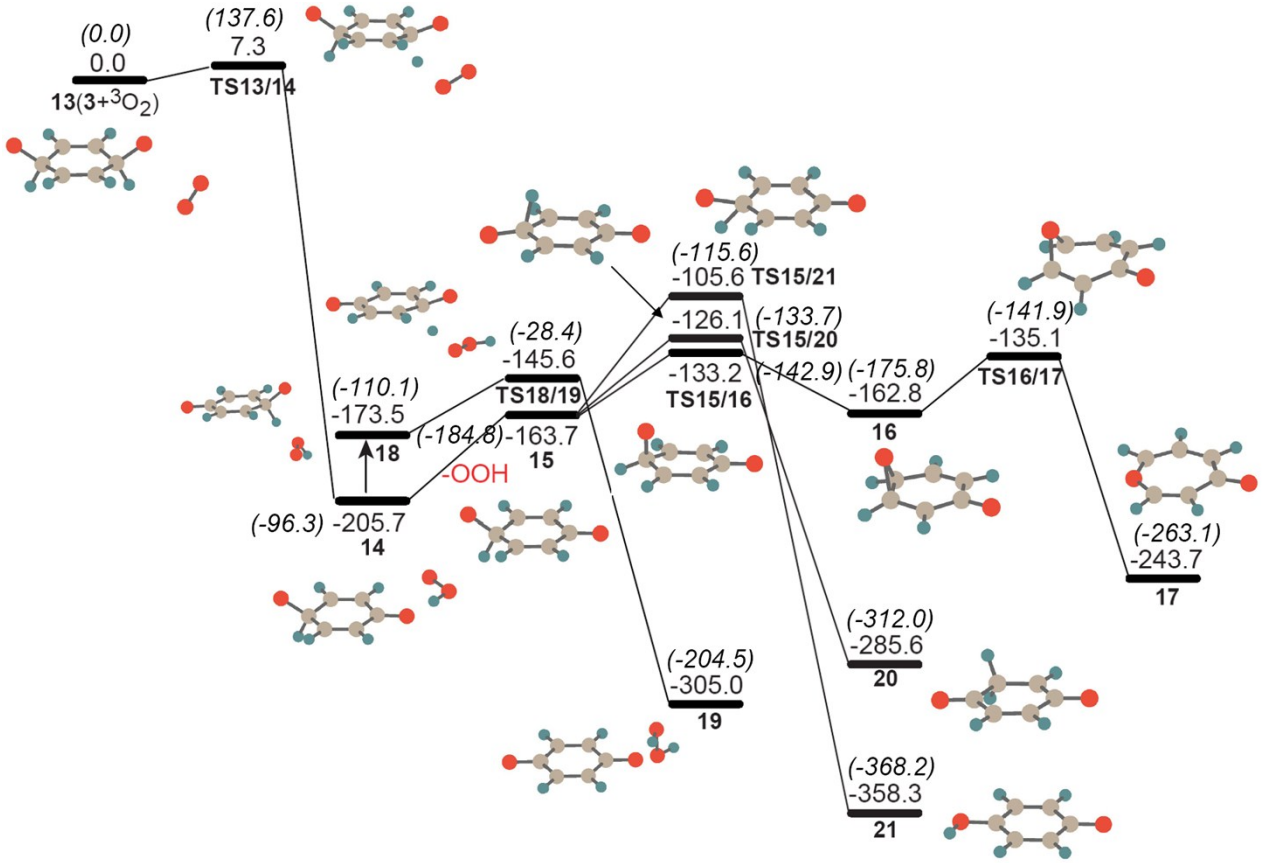

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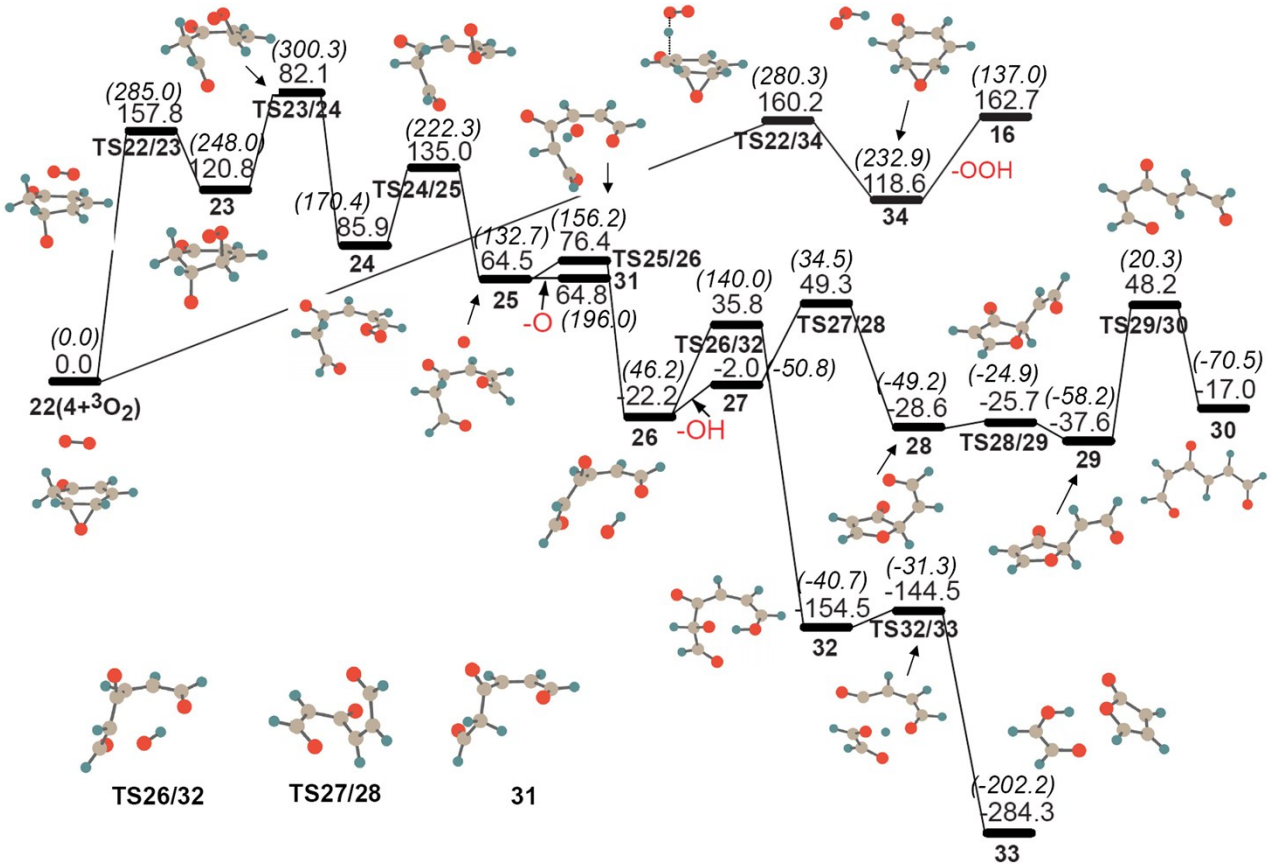

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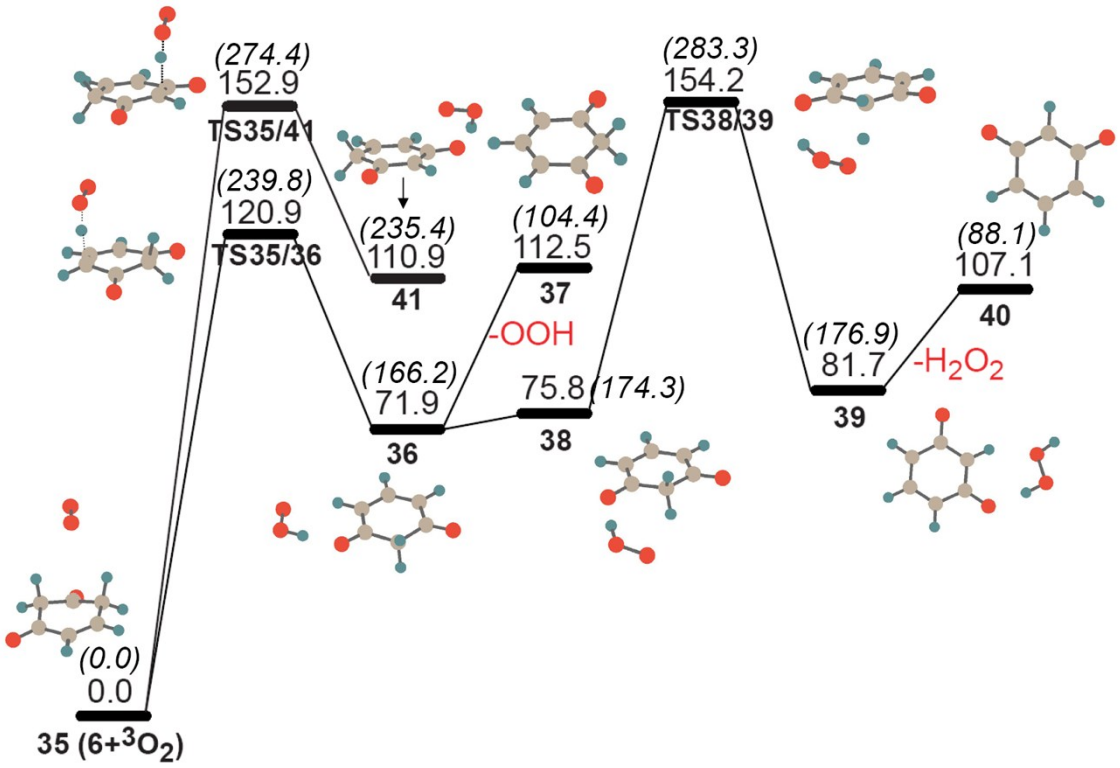

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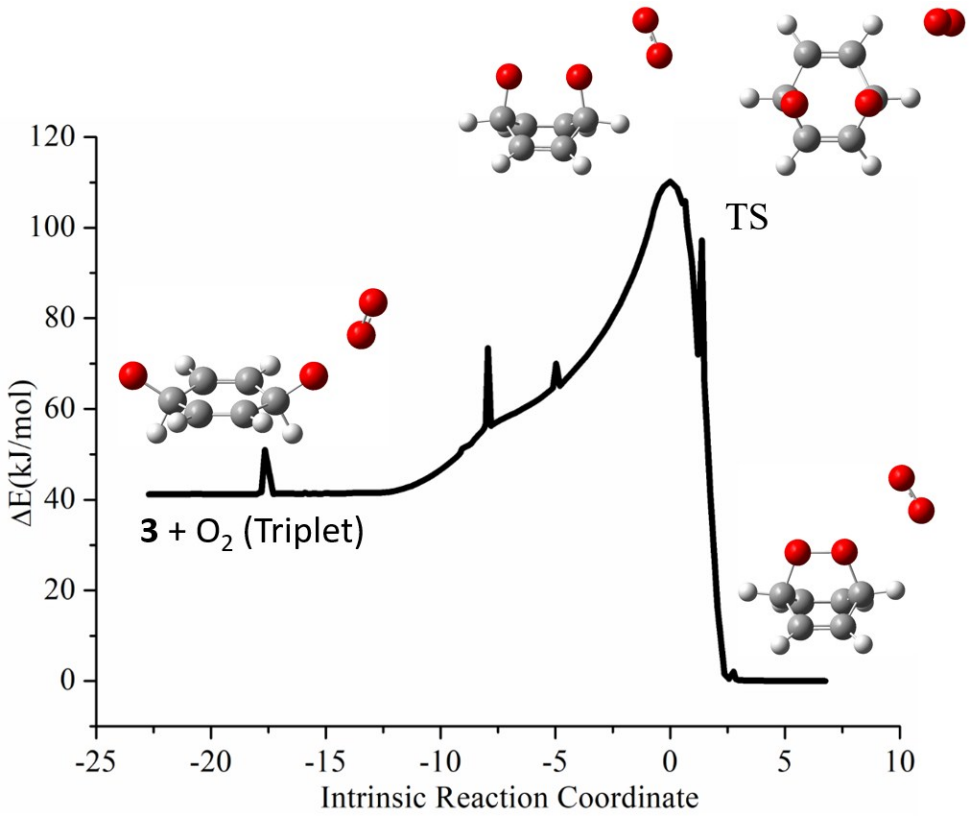

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