Supporting Information for

Theoretical and Experimental Study on the Degradation Mechanism of Atrazine in Fenton Oxidation Treatment

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**Figure Captions**

**Figure S1** The dealkylation and alkyl oxidation process of IM11 in aqueous medium by Fenton oxidation technology

**Figure S2** Optimized geometries for the transition states involved in the dealkylation and alkyl oxidation process. Distances are in angstroms
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Figure S2 Optimized geometries for the transition states involved in the dealkylation and alkyl oxidation process. Distances are in angstroms.