

## **Supplementary Material:**

### **Experimental and Modeling Study of Benzaldehyde Oxidation**

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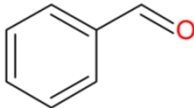
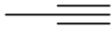
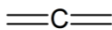
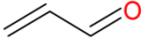

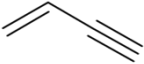
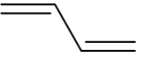

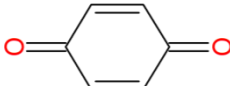
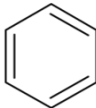
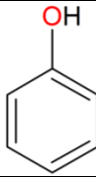
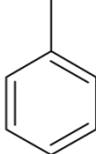
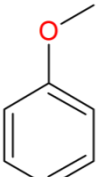
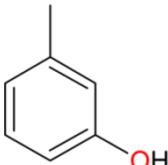
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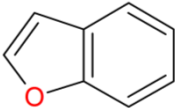
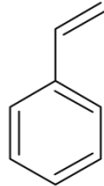
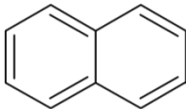
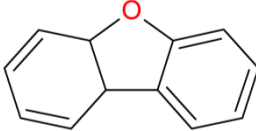
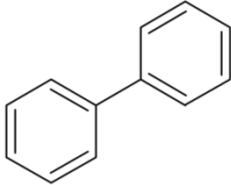
### **Summary**

1. **Molecule nomenclature**
2. **Benzaldehyde and some radicals enthalpy of formations**
3. **Carbon balances and conversion charts**
4. **Additional sensitivity analyses**

## 1. Molecule nomenclature

Table 1. Information about the molecules named in the main manuscript

Name	Formula	Model Name	Structure
Benzaldehyde	$C_7H_6O$	C6H5CHO	
Propyne	$C_3H_4$	C3H4-P	
Allene	$C_3H_4$	C3H4-A	
Acrolein	$C_3H_4O$	C2H3CHO	
Propene	$C_3H_6$	C3H6	
Butenyne	$C_4H_4$	C4H4	
1-3 Butadiene	$C_4H_6$	C4H6	
Cyclopentadiene	$C_5H_6$	C5H6	
Benzoquinone	$C_6H_4O_2$	C6H4O2	
Benzene	$C_6H_6$	C6H6	
Phenol	$C_6H_6O$	C6H5OH	
Toluene	$C_7H_8$	C7H8	
Anisole	$C_7H_8O$	C6H5OCH3	
Cresol	$C_7H_8O$	CRESOL	

Name	Formula	Model Name	Structure
Benzofuran	C <sub>8</sub> H <sub>6</sub> O	BZFUR	
Styrene	C <sub>8</sub> H <sub>8</sub>	C6H5C2H3	
Naphtalene	C <sub>10</sub> H <sub>8</sub>	C10H8	
Dibenzofuran	C <sub>12</sub> H <sub>8</sub> O	DIBZFUR	
Biphenyl	C <sub>12</sub> H <sub>10</sub>	BIPHENYL	

## 2. Benzaldehyde and some radicals enthalpy of formations

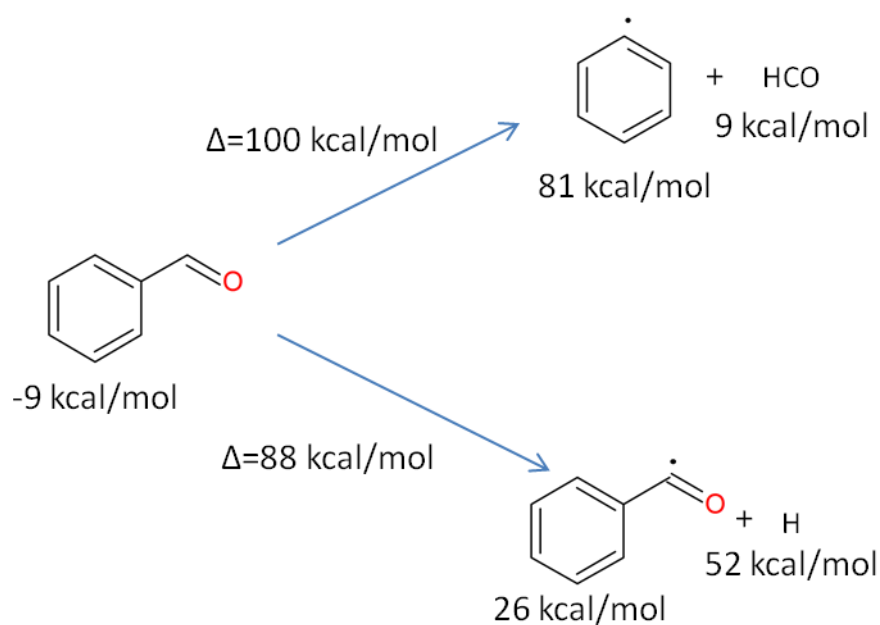


Figure 1. Unimolecular decomposition pathways of benzaldehyde, considered in the model. The values correspond to the enthalpies of formation (uncertainties  $\pm 1$  kcal/mol)

### 3. Carbon balances and conversion charts

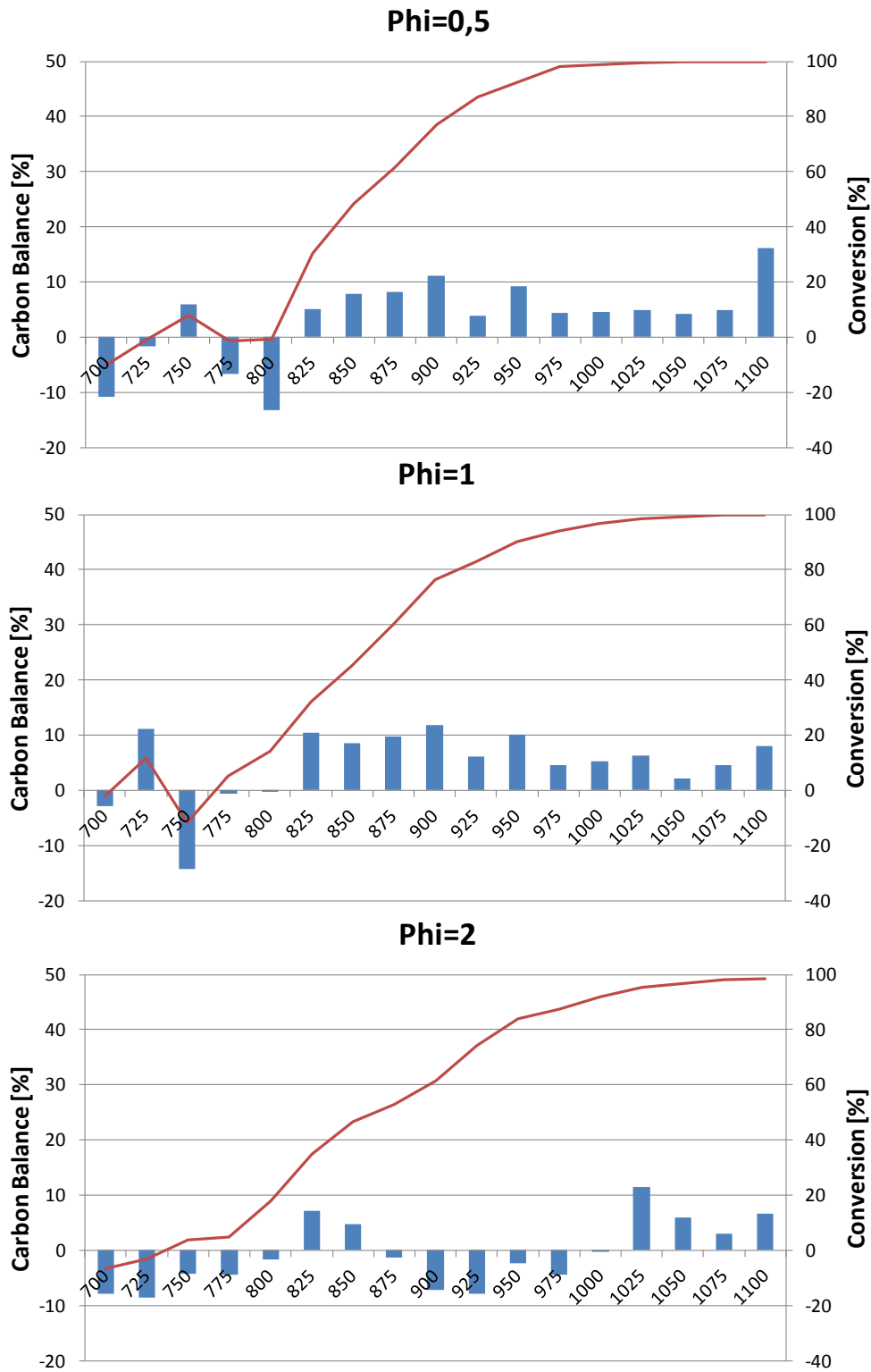


Figure 2. Carbon balances (blue bars) and fuel conversions (red line) as a function of the temperature [K] for benzaldehyde at the three studied equivalence ratios.

#### 4. Additional sensitivity analyses

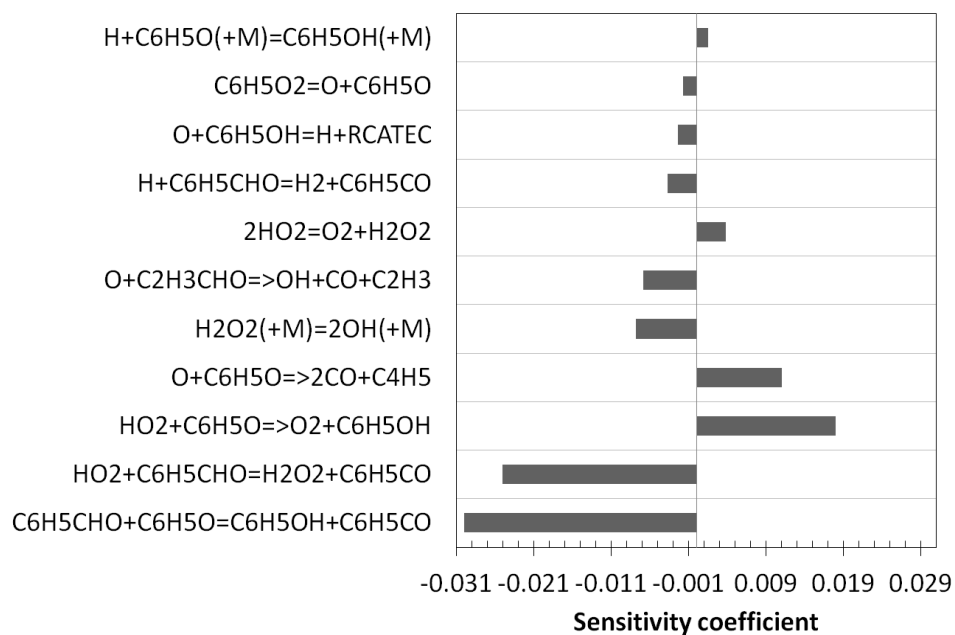
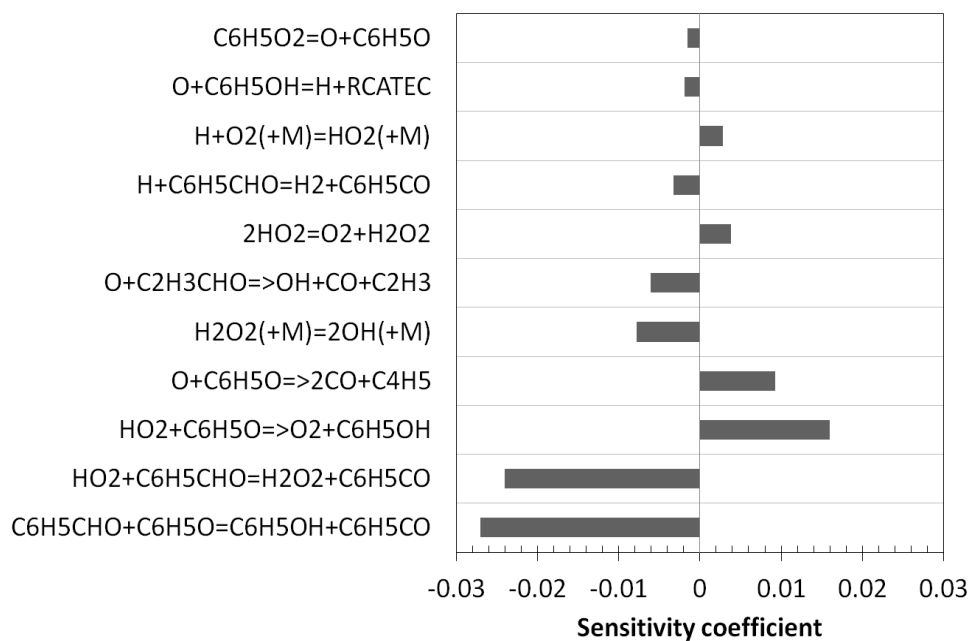


Figure 3. Sensitivity analyses of benzaldehyde oxidation to rate constants at T=770K and for  $\phi=0.5$  (top) and  $\phi=2$  (bottom)