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Supplementary material

The atmospheric chemical reaction of 4-*tert*-butylphenol initiated by OH radicals

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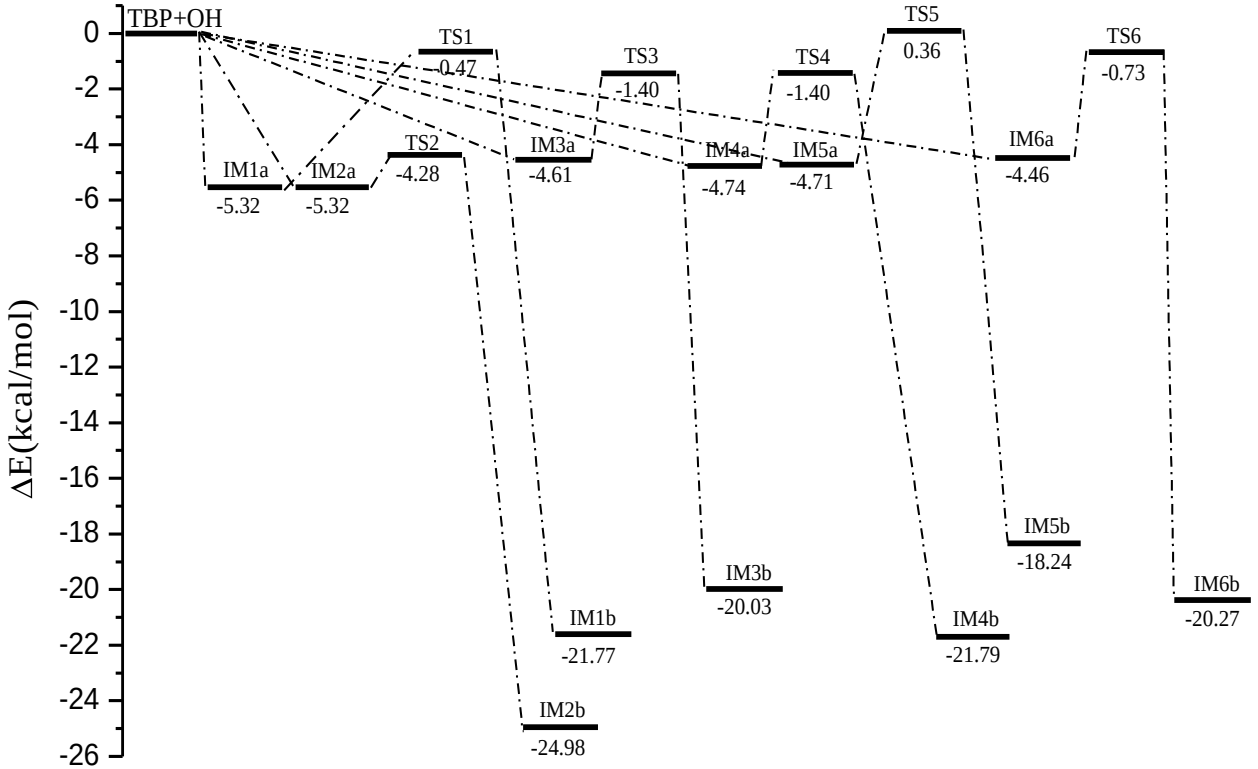

Fig. S1. The profile of the potential energy surface for the addition reactions of 4-*tert*-butylphenol (TBP) with OH radicals.

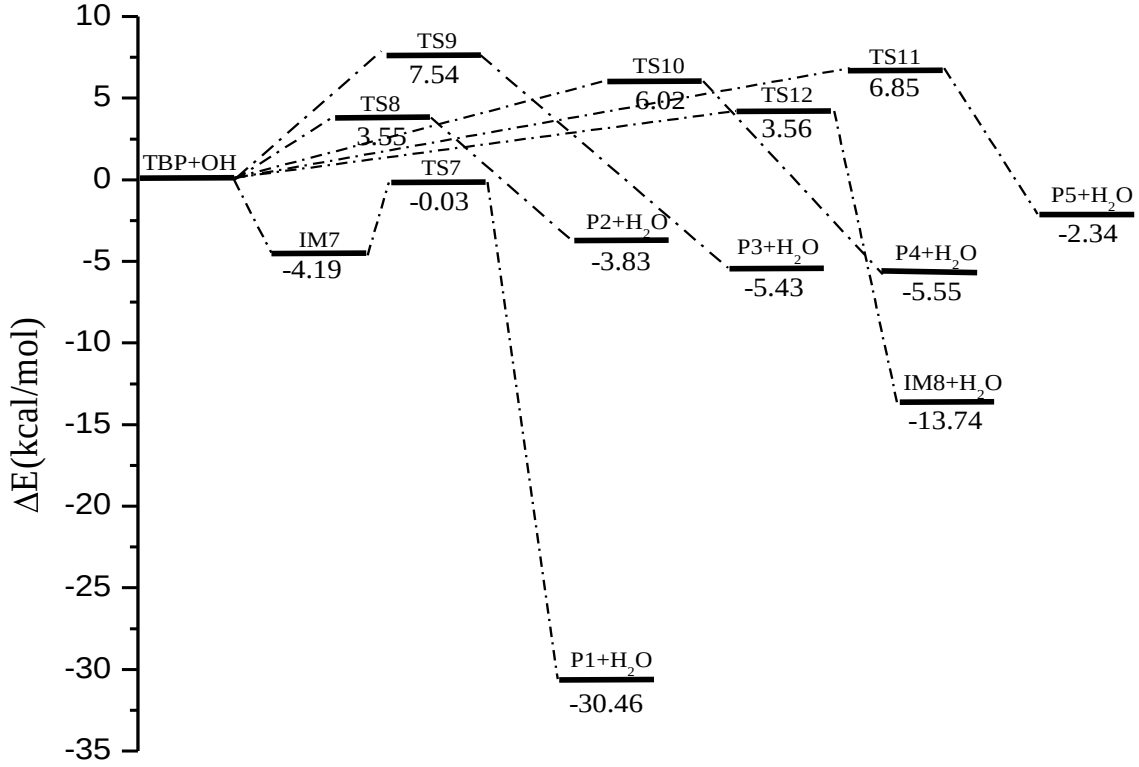

Fig. S2. The profile of the potential energy surface for the abstraction reactions of 4-*tert*-butylphenol (TBP) with OH radicals.

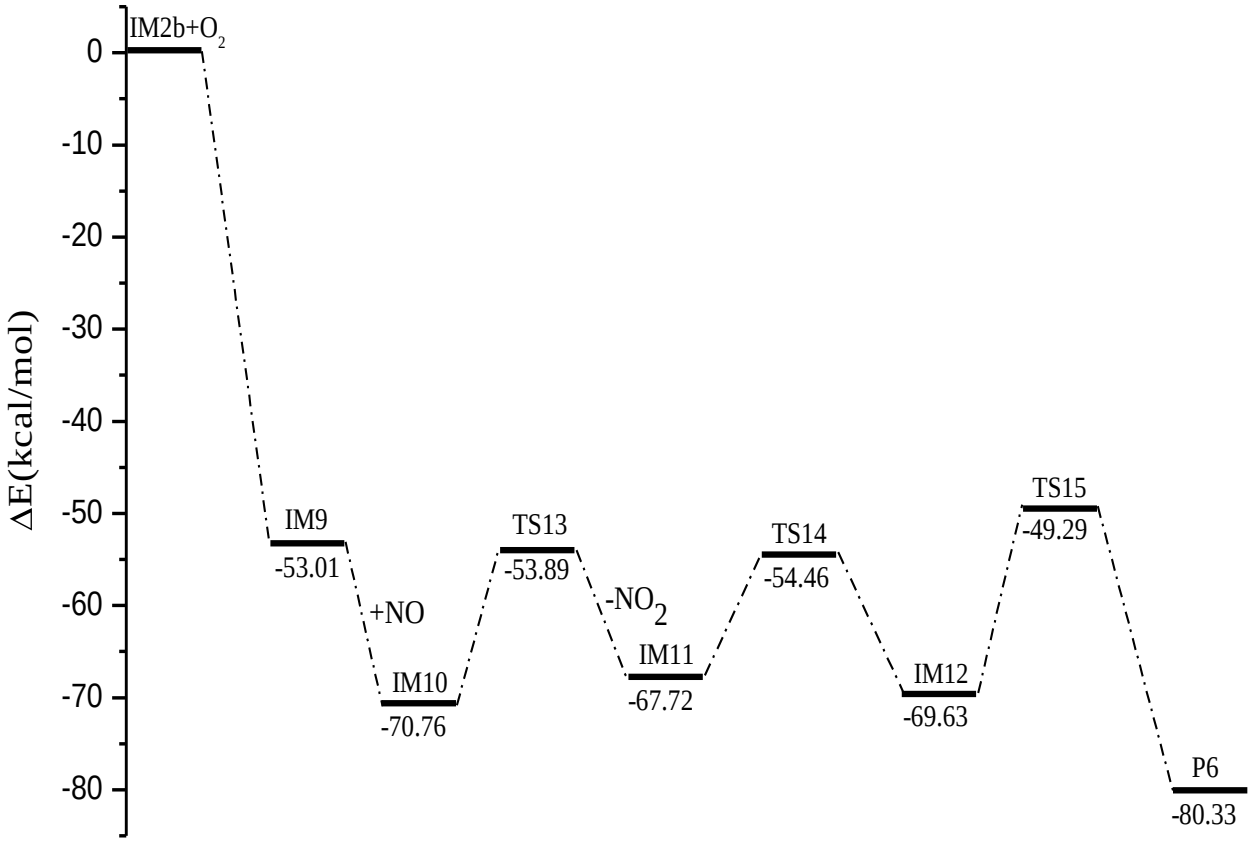

Fig. S3. The profile of the potential energy surface for IM2b reactions.

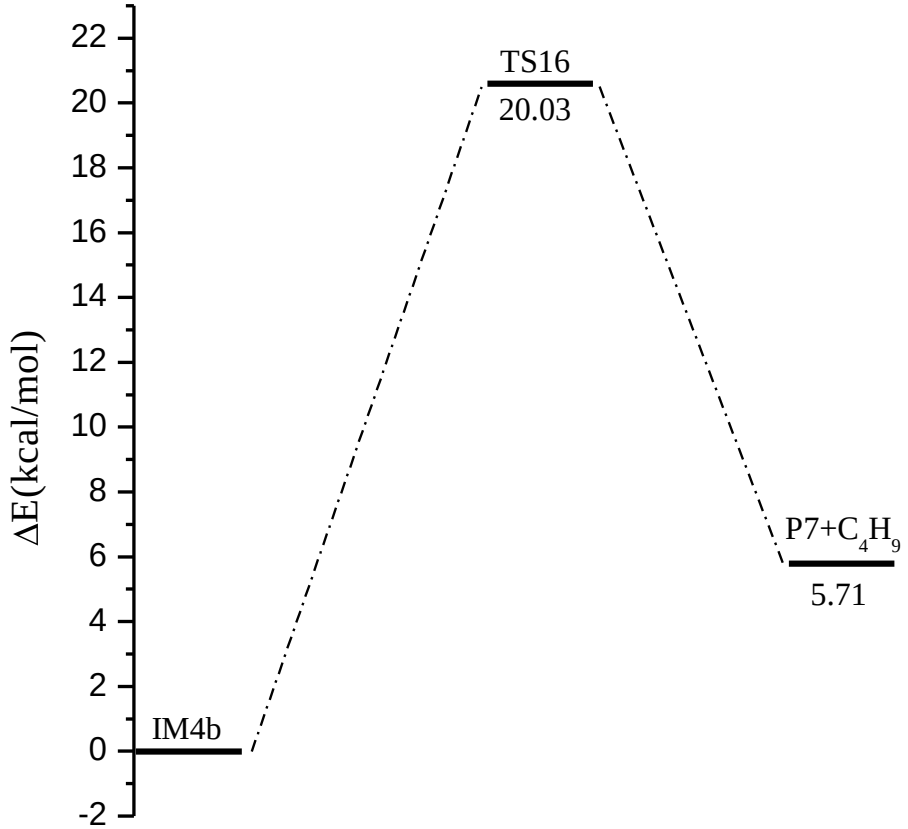

Fig. S4. The profile of the potential energy surface for IM4b reactions.

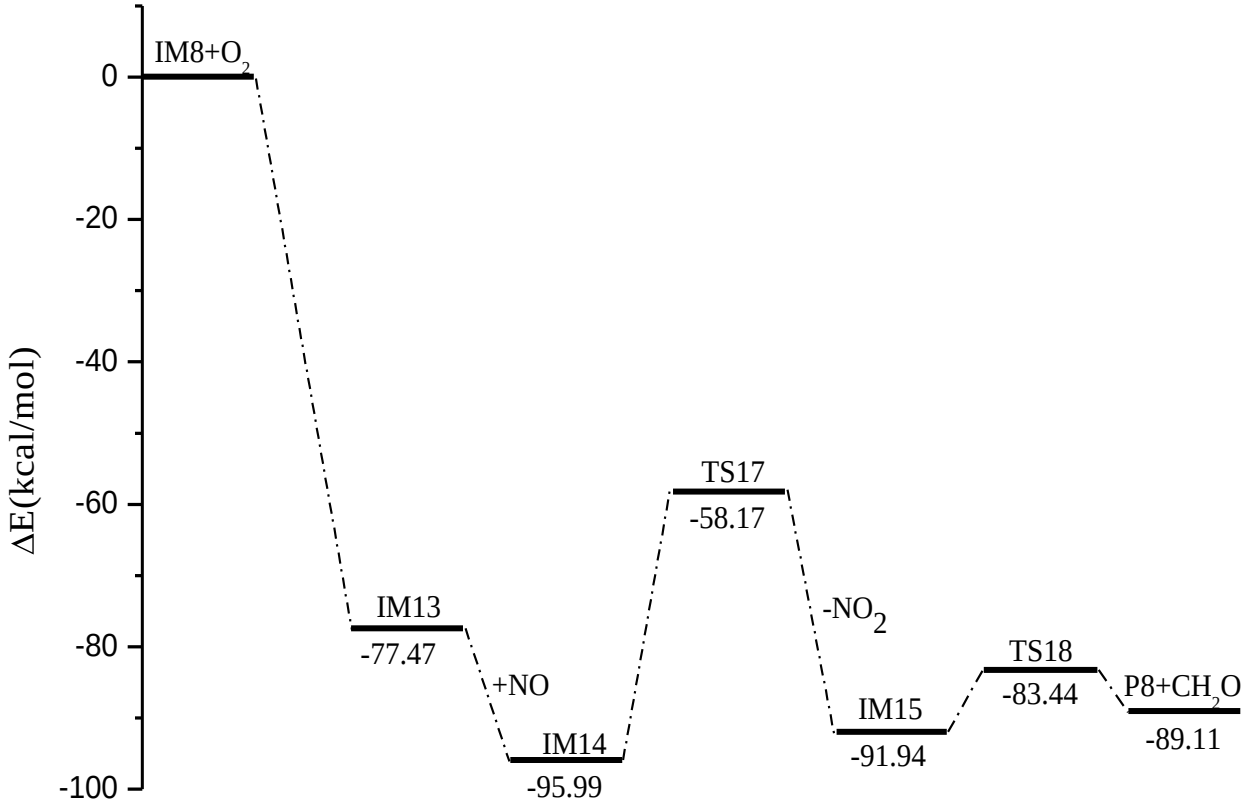

Fig. S5. The profile of the potential energy surface for IM8 reactions.

Table S1. The rate constants of addition reactions with the canonical variational transition with small-curvature tunnelling method at 200–500 K

The bold entries are the rate constants at room temperature, which are discussed in the manuscript

T (K)	Rate constants (cm^3 $molecule^{-1}$ s^{-1})					
	I	II	III	IV	V	VI
200	7.22×10^{-16}	1.01×10^{-14}	3.98×10^{-15}	6.50×10^{-15}	9.92×10^{-18}	9.94×10^{-16}
220	9.26×10^{-16}	1.01×10^{-14}	4.28×10^{-15}	7.04×10^{-15}	1.75×10^{-17}	1.33×10^{-15}
240	1.15×10^{-15}	1.03×10^{-14}	4.60×10^{-15}	7.62×10^{-15}	2.82×10^{-17}	1.71×10^{-15}
260	1.40×10^{-15}	1.06×10^{-14}	4.94×10^{-15}	8.24×10^{-15}	4.28×10^{-17}	2.14×10^{-15}
280	1.66×10^{-15}	1.09×10^{-14}	5.30×10^{-15}	8.88×10^{-15}	6.18×10^{-17}	2.60×10^{-15}
298.15	$\mathbf{1.93 \times 10^{-15}}$	$\mathbf{1.12 \times 10^{-14}}$	$\mathbf{5.64 \times 10^{-15}}$	$\mathbf{9.50 \times 10^{-15}}$	$\mathbf{8.28 \times 10^{-17}}$	$\mathbf{3.04 \times 10^{-15}}$
320	2.26×10^{-15}	1.17×10^{-14}	6.08×10^{-15}	1.03×10^{-14}	1.14×10^{-16}	3.64×10^{-15}
340	2.60×10^{-15}	1.22×10^{-14}	6.50×10^{-15}	1.10×10^{-14}	1.48×10^{-16}	4.20×10^{-15}
360	2.96×10^{-15}	1.30×10^{-14}	6.96×10^{-15}	1.18×10^{-14}	1.87×10^{-16}	4.78×10^{-15}
380	6.92×10^{-15}	1.36×10^{-14}	7.42×10^{-15}	1.27×10^{-14}	2.32×10^{-16}	5.40×10^{-15}
400	7.80×10^{-15}	1.43×10^{-14}	7.90×10^{-15}	1.36×10^{-14}	2.84×10^{-16}	6.02×10^{-15}
450	1.02×10^{-14}	1.61×10^{-14}	9.16×10^{-15}	1.59×10^{-14}	4.42×10^{-16}	7.58×10^{-15}
500	1.31×10^{-14}	1.82×10^{-14}	1.04×10^{-14}	1.86×10^{-14}	6.42×10^{-16}	9.06×10^{-15}

Table S2. The rate constants of the abstraction reactions with the canonical variational transition with small-curvature tunnelling method at 200–500 K

The bold entries are the rate constants at room temperature, which are discussed in the manuscript

T (K)	Rate constants (cm^3 $molecule^{-1}$ s^{-1})					
	VII	VIII	IX	X	XI	XII
200	1.78×10^{-16}	3.89×10^{-18}	4.75×10^{-21}	1.36×10^{-19}	2.32×10^{-20}	8.23×10^{-17}
220	3.44×10^{-16}	7.57×10^{-18}	1.91×10^{-20}	4.34×10^{-19}	6.91×10^{-20}	1.95×10^{-16}
240	6.01×10^{-16}	1.34×10^{-17}	6.17×10^{-20}	1.15×10^{-18}	1.74×10^{-19}	4.06×10^{-16}
260	9.71×10^{-16}	2.19×10^{-17}	1.69×10^{-19}	2.68×10^{-18}	3.85×10^{-19}	7.64×10^{-16}
280	1.48×10^{-15}	3.38×10^{-17}	4.07×10^{-19}	5.56×10^{-18}	7.68×10^{-19}	1.32×10^{-15}
298.15	$\mathbf{2.07 \times 10^{-15}}$	$\mathbf{4.80 \times 10^{-17}}$	$\mathbf{8.24 \times 10^{-19}}$	$\mathbf{1.00 \times 10^{-17}}$	$\mathbf{1.34 \times 10^{-18}}$	$\mathbf{2.07 \times 10^{-15}}$
320	2.98×10^{-15}	7.00×10^{-17}	1.75×10^{-18}	1.88×10^{-17}	2.44×10^{-18}	3.33×10^{-15}
340	4.01×10^{-15}	9.57×10^{-17}	3.25×10^{-18}	2.12×10^{-17}	3.97×10^{-18}	4.91×10^{-15}
360	5.25×10^{-15}	1.27×10^{-16}	5.66×10^{-18}	3.37×10^{-17}	6.19×10^{-18}	6.99×10^{-15}
380	6.71×10^{-15}	1.65×10^{-16}	9.40×10^{-18}	5.13×10^{-17}	9.27×10^{-18}	9.63×10^{-15}
400	8.41×10^{-15}	2.09×10^{-16}	1.49×10^{-17}	7.54×10^{-17}	1.34×10^{-17}	1.30×10^{-14}
450	1.38×10^{-14}	3.55×10^{-16}	4.08×10^{-17}	1.74×10^{-16}	3.01×10^{-17}	2.46×10^{-14}
500	2.09×10^{-14}	5.55×10^{-16}	9.42×10^{-17}	3.52×10^{-16}	5.94×10^{-17}	4.19×10^{-14}