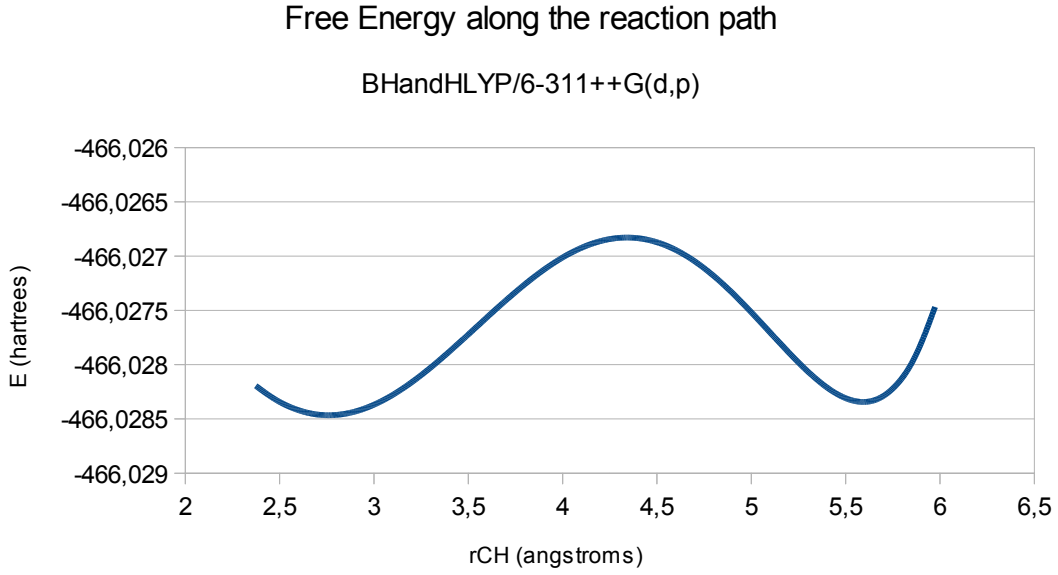
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

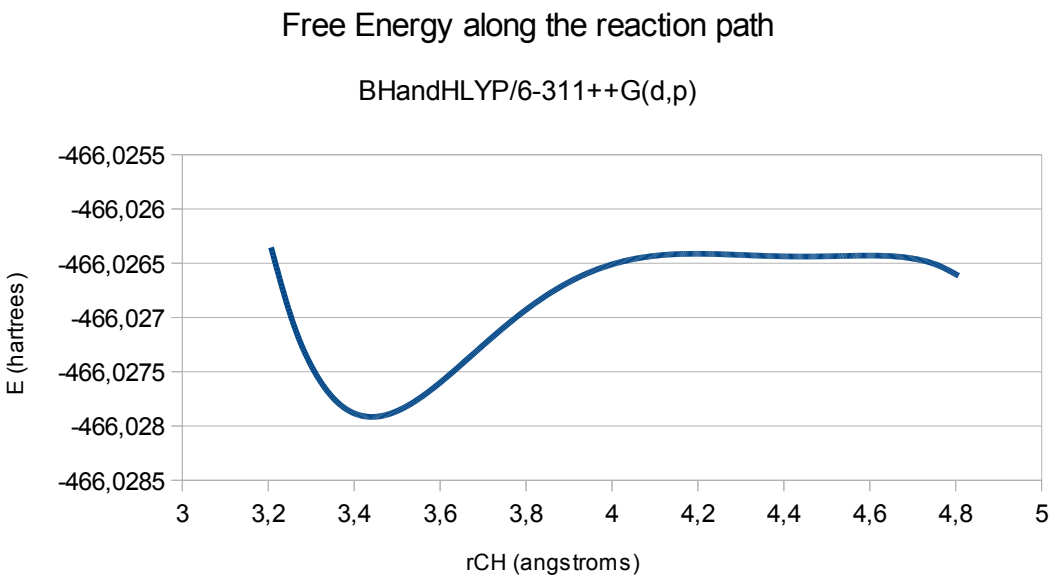
Supplementary Information:

Table 1: Thermochemical parameters for OH radical addition to carene's double bond. All values are in kcal mol^{-1}.

	$\Delta G^{\#}$	ΔG
	BHandHLYP/6-311G(d,p)	
Inter 1	9.37	-13.29
Inter 2	8.76	-11.52
Inter 3	10.06	-10.68
Inter 4	9.10	-11.86
$Complex_{bottom}$		3.75
$Complex_{top}$		4.68
	PBE1PBE/6-311G(d,p)	
Inter 1	2.55	-20.61
Inter 2	2.50	-19.02
Inter 3	3.74	-17.91
Inter 4		-19.32



(a)



(b)

Figure 1: Free energy profile for both pre-reactive complexes in the separated reactants at 298.15 K. A) $Complex_{bottom}$; b) $Complex_{top}$.

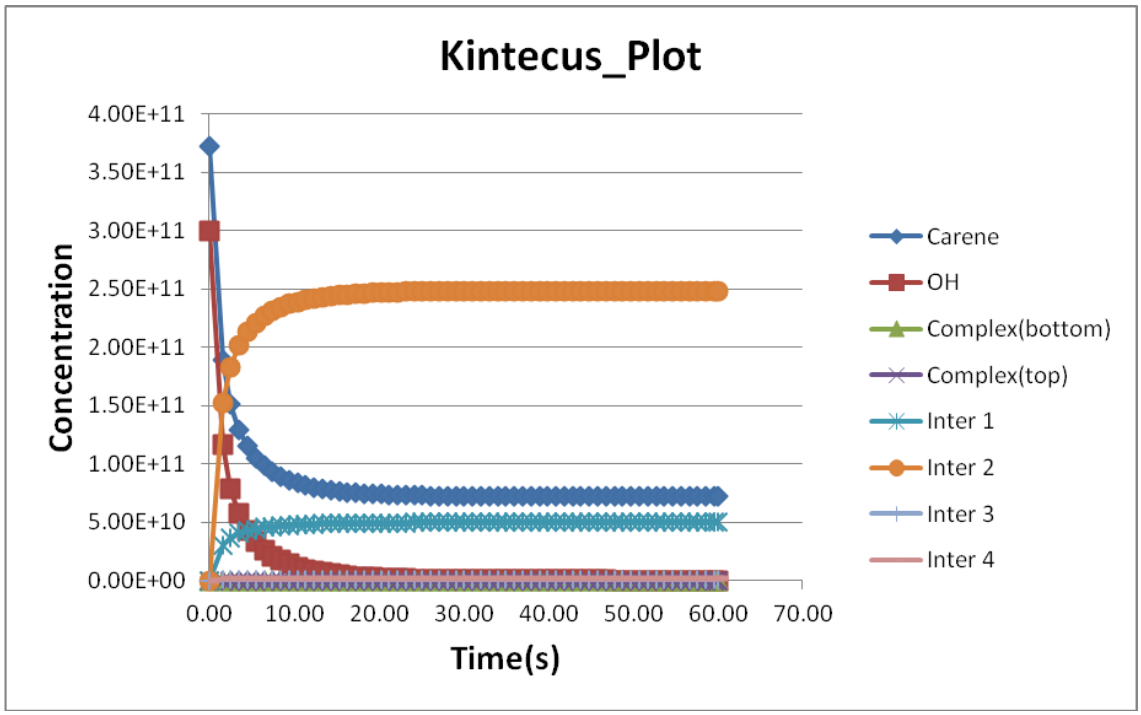


Figure 2: Numerical integration of rate equations for the addition of OH radical to carene's double bond. The initial concentration of carene and OH are $3.72\times10^{+11}$ molecule cm^{-3} and $3.00\times10^{+11}$ molecule cm^{-3}, respectively. The results shows that the concentration of both pre-reactive complexes remains nearly 0 along all simulation. This result indicates that the complexes obey the stead state approach.