

## Supplementary Material

### Characterization of organic isomers: CID fragmentation technique on protonated hydroxybenzophenone isomers

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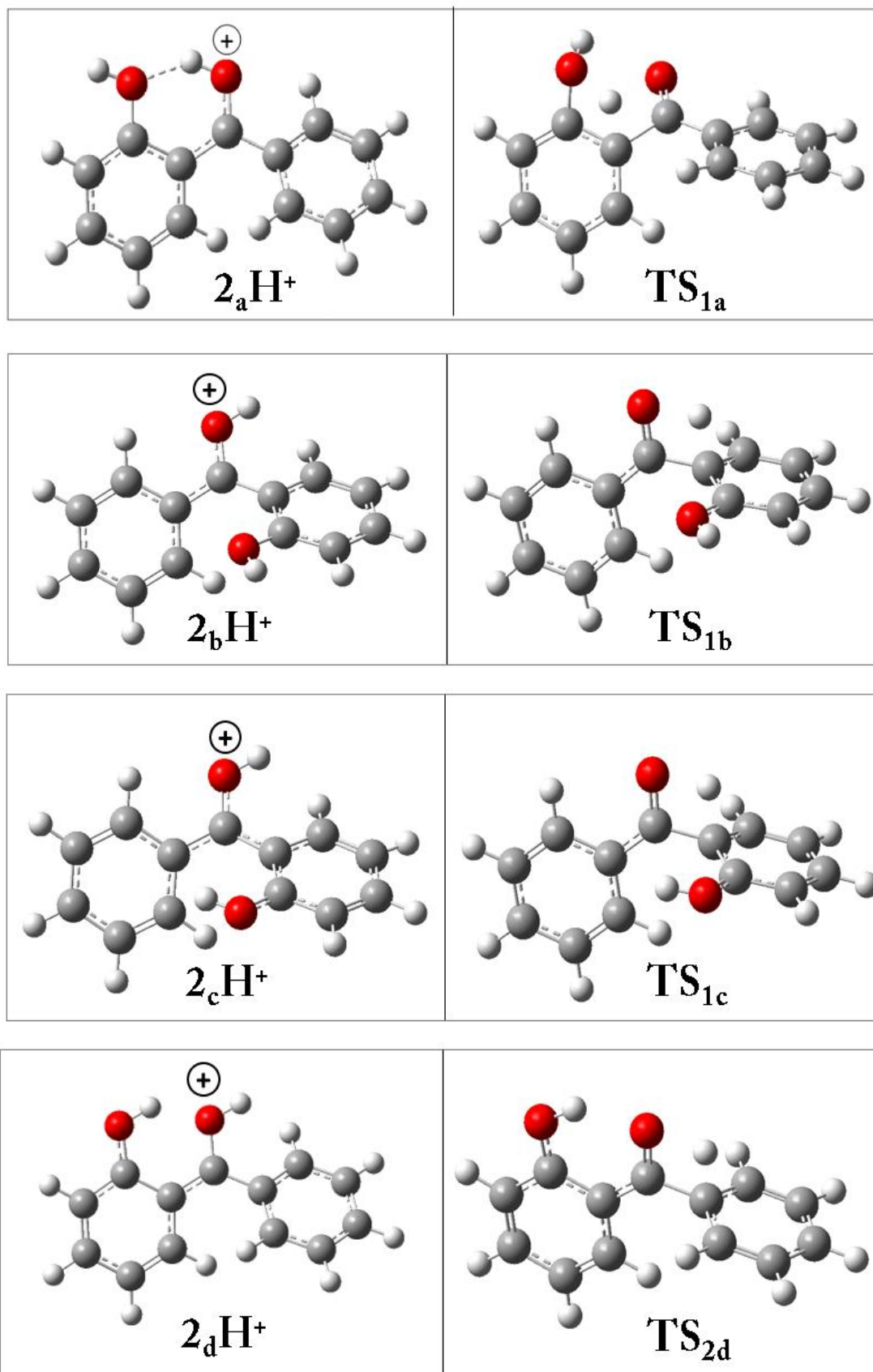
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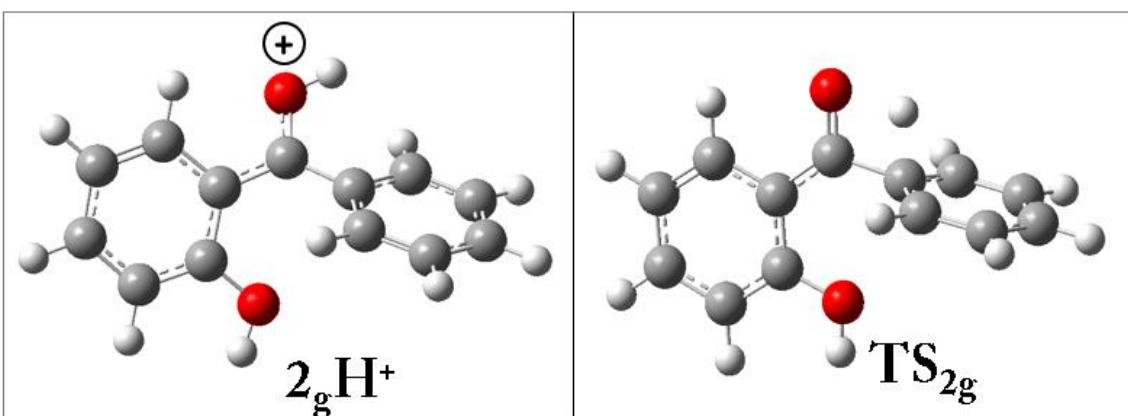
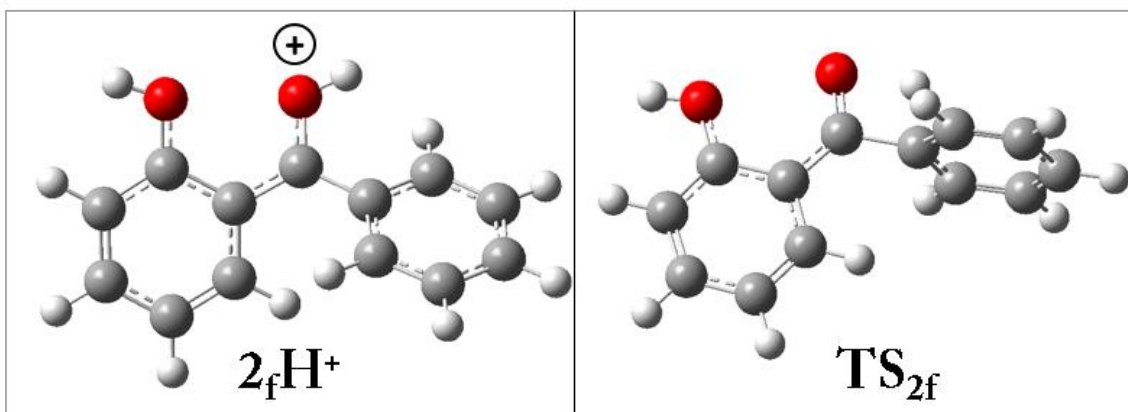
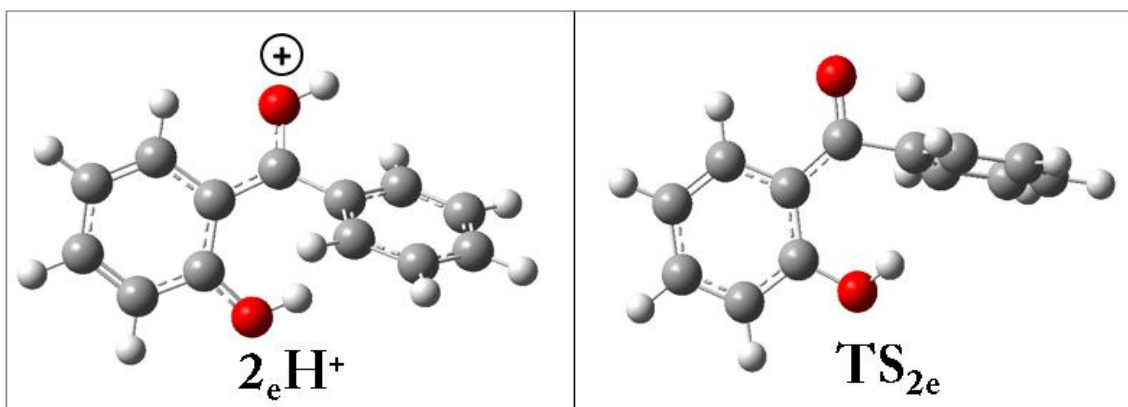
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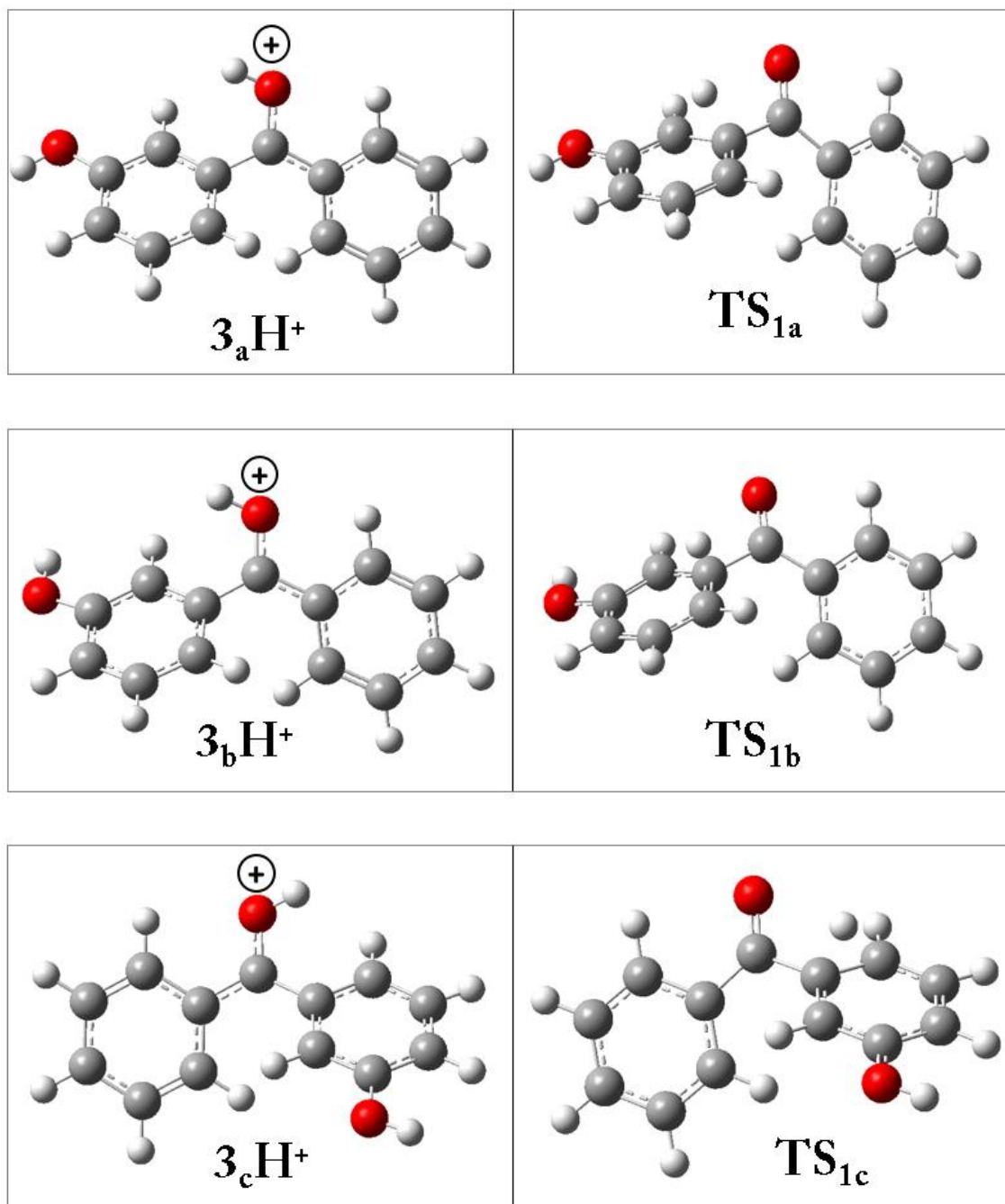
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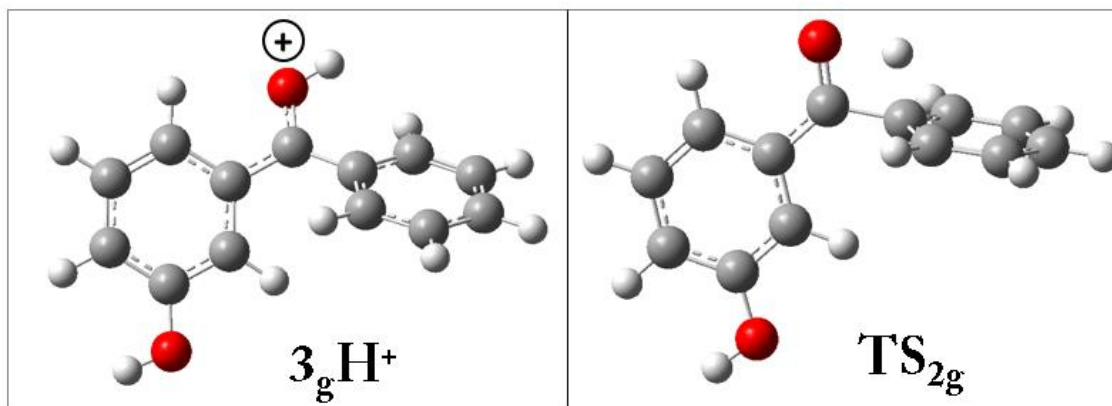
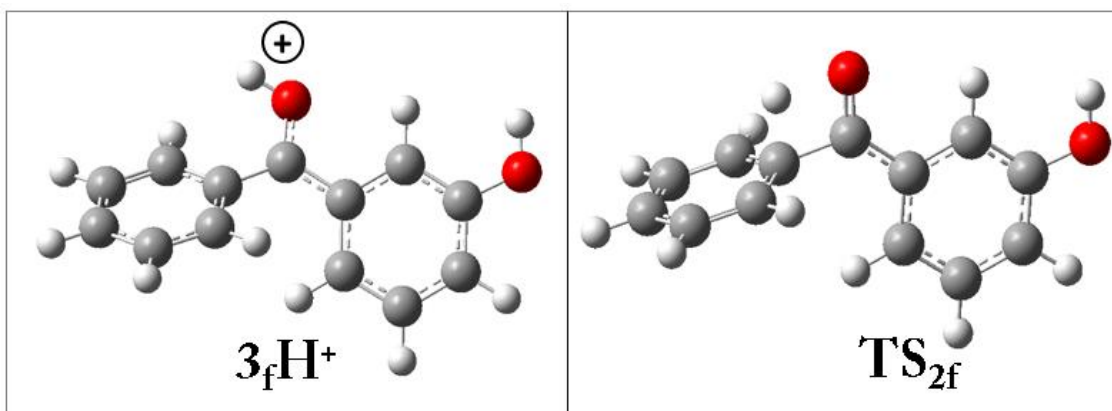
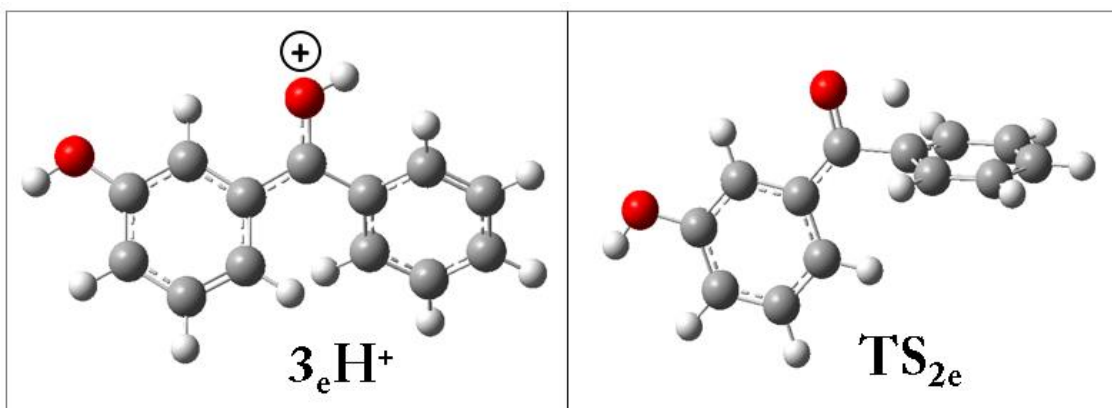
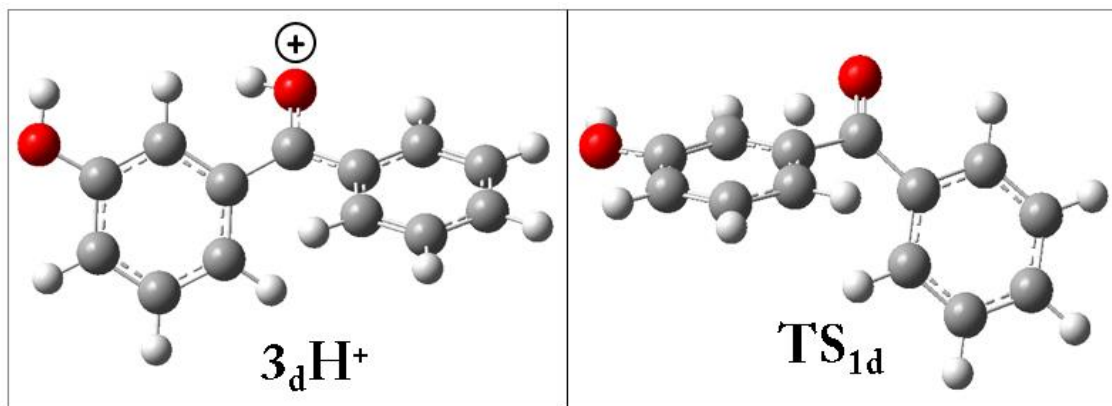
**Figure S1.** Optimized geometries, at the B3LYP/6-311++G(d,p) level of theory, of the of  $2\text{H}^+$  rotamers and the transition states of their corresponding fragmentation routes.

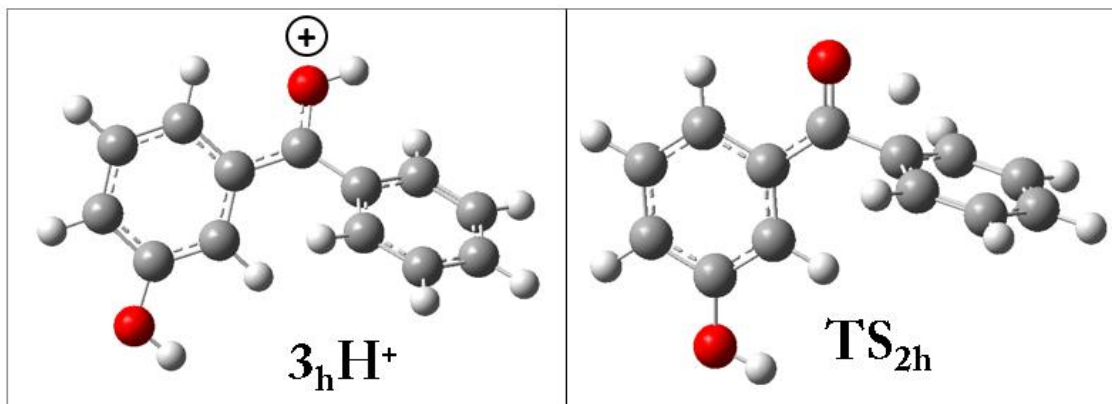




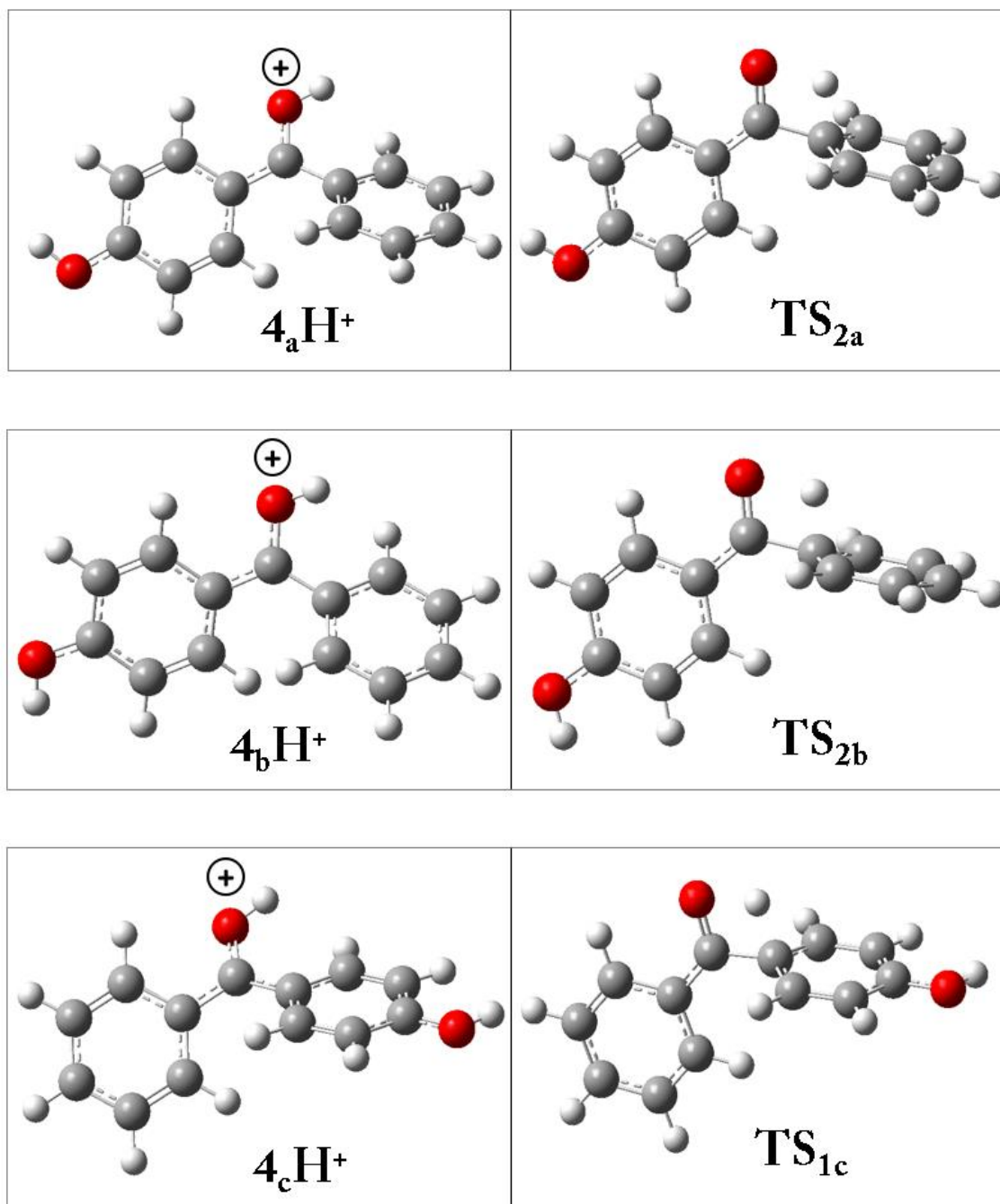
**Figure S2.** Optimized geometries, at the B3LYP/6-311++G(d,p) level of theory, of the of  $3\text{H}^+$  rotamers and the transition states of their corresponding fragmentation.

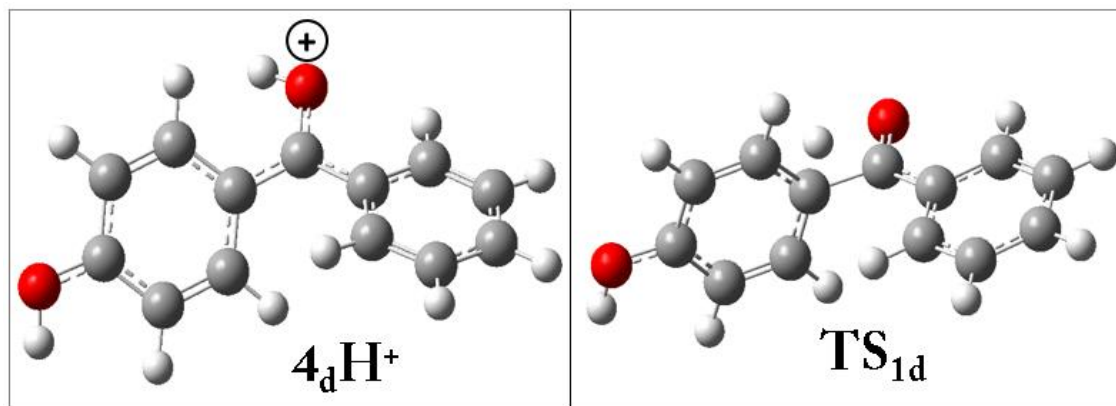






**Figure S3.** Optimized geometries, at the B3LYP/6-311++G(d,p) level of theory, of the of  $4\text{H}^+$  rotamers and the transition states of their corresponding fragmentation routes.







**Figure S4.** Optimized geometries, at B3LYP/6-311++G(d,p) level of theory, of fragments 105  $m/z$  and 121  $m/z$ .

