Supplementary Material

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

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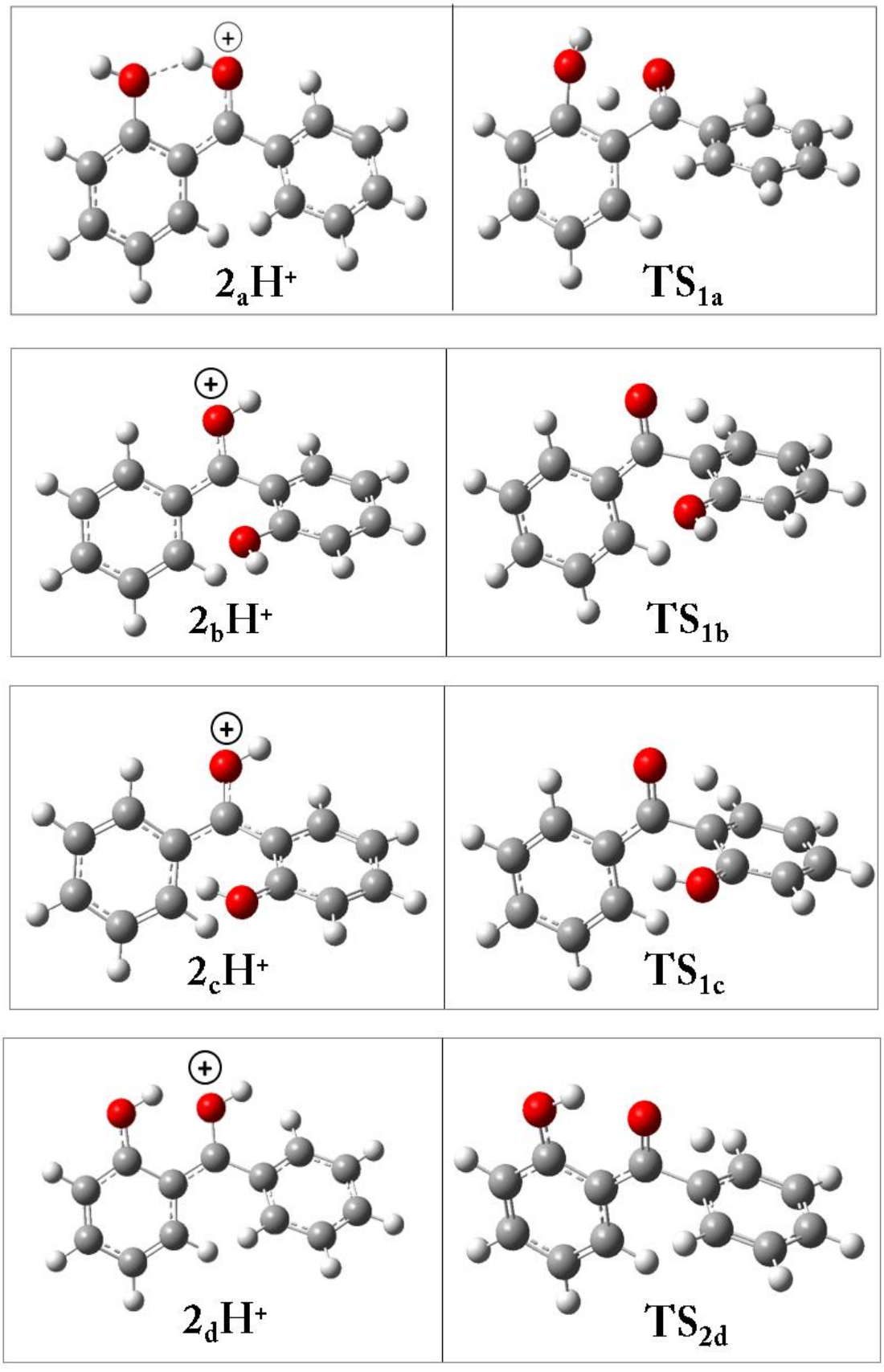


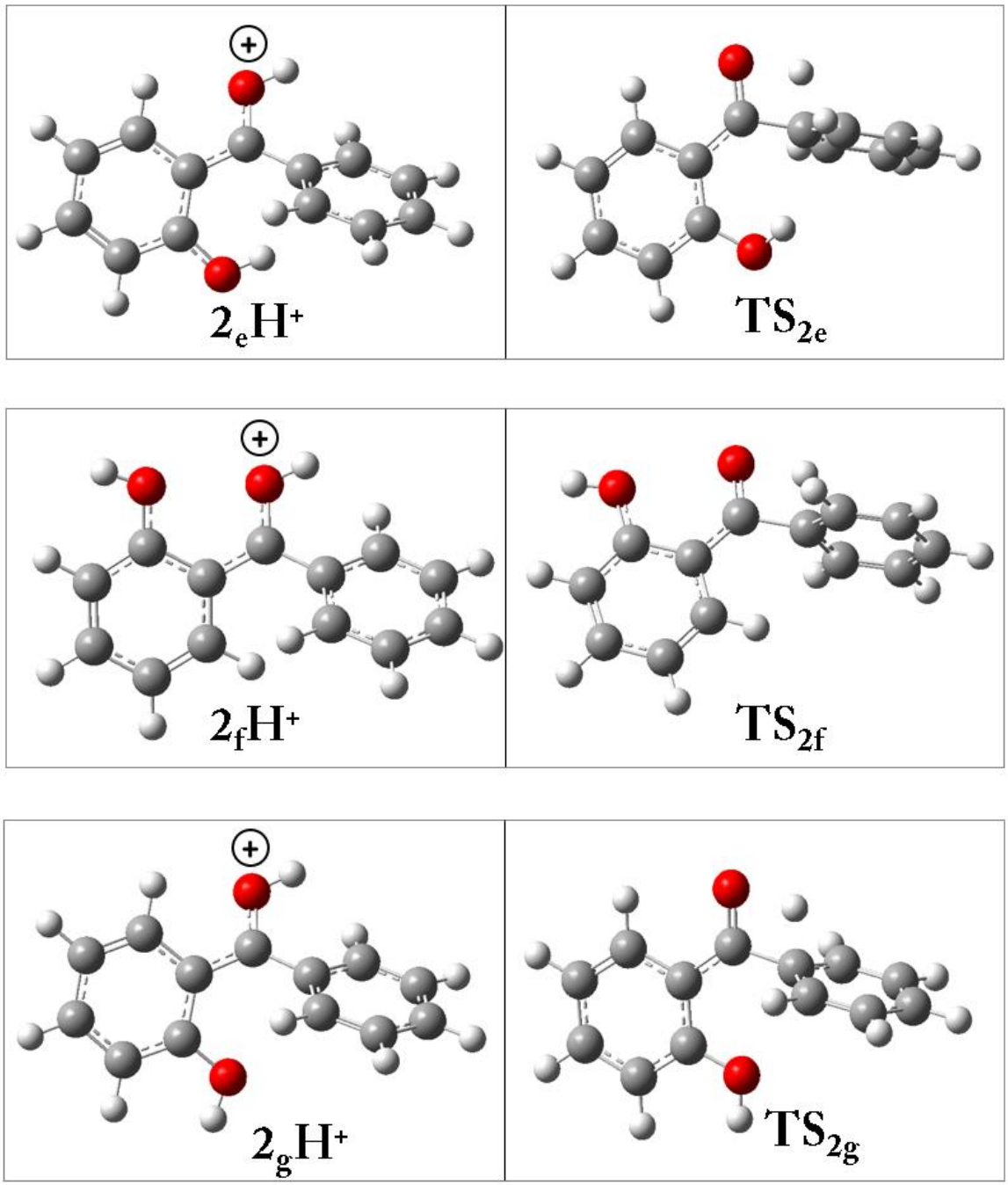
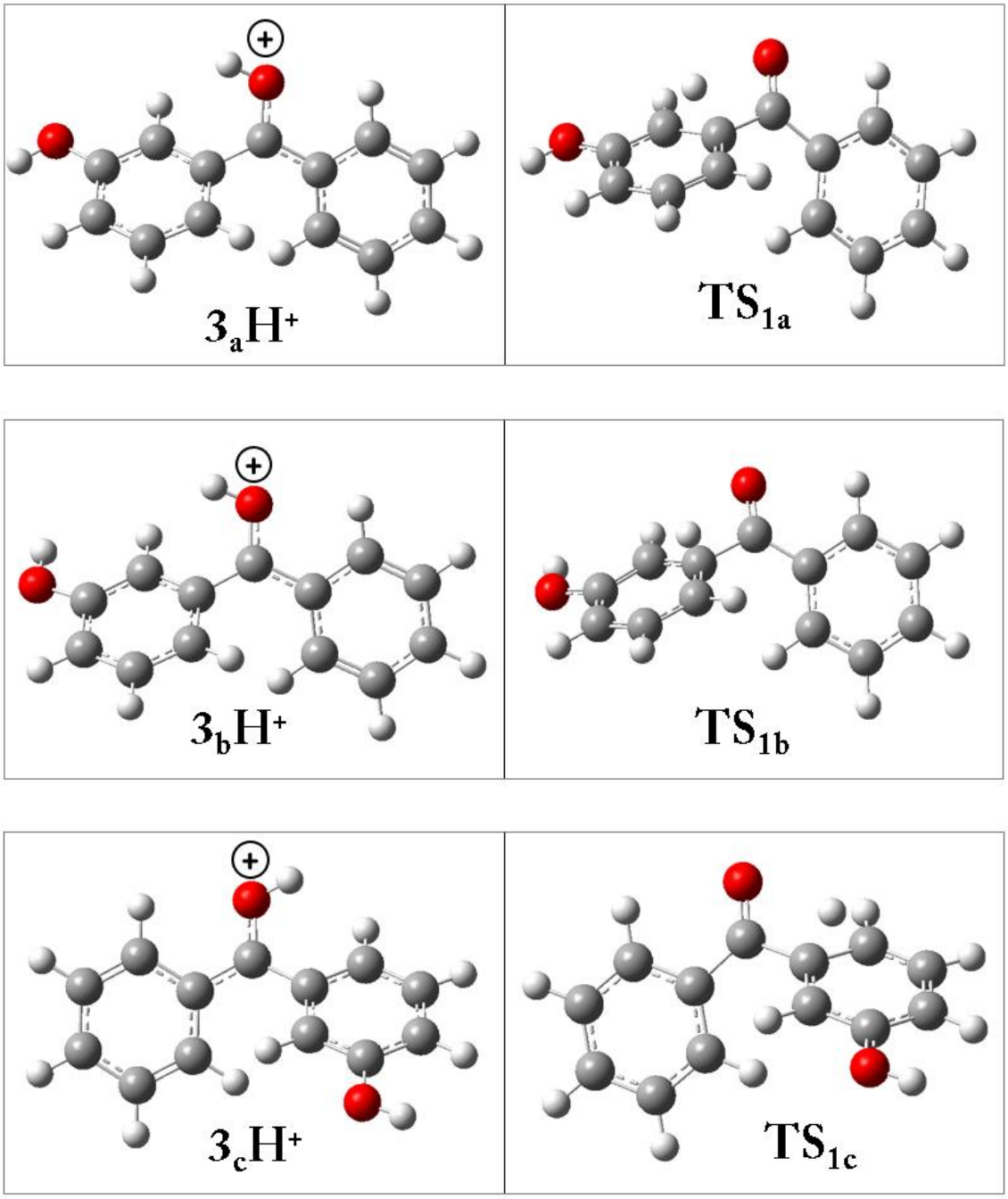
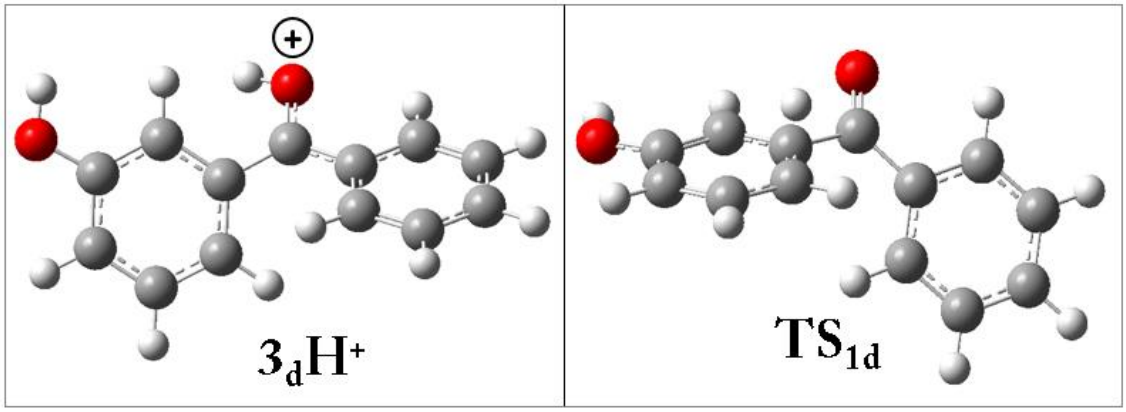
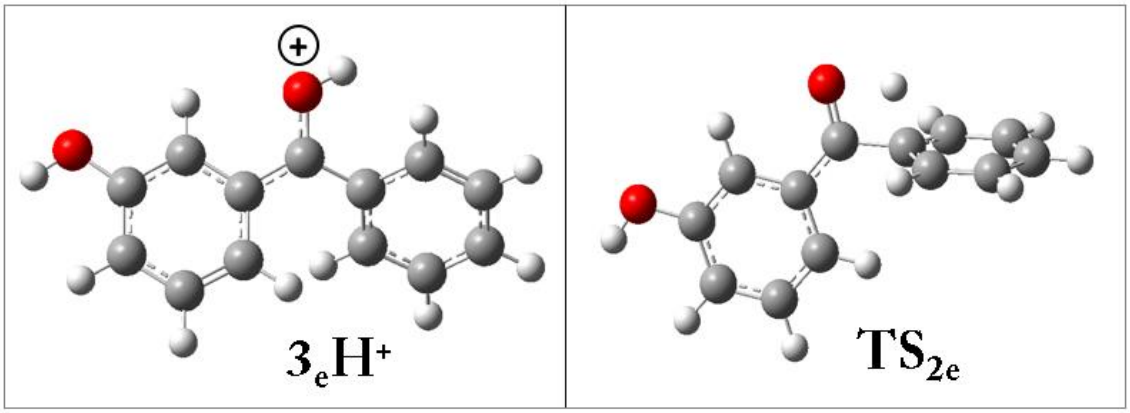
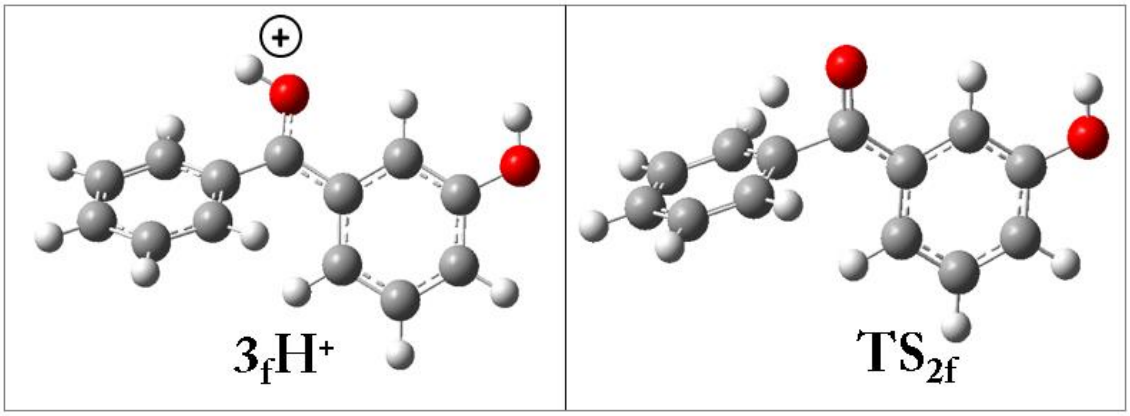


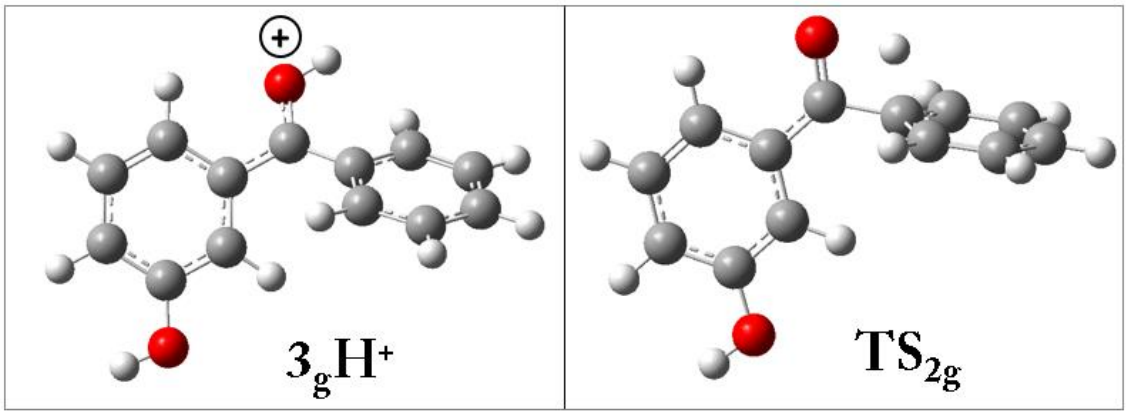
Figure S2. Optimized geometries, at the B3LYP/6-311++G(d,p) level of theory, of the of **3**H^+ rotamers and the transition states of their corresponding fragmentation.











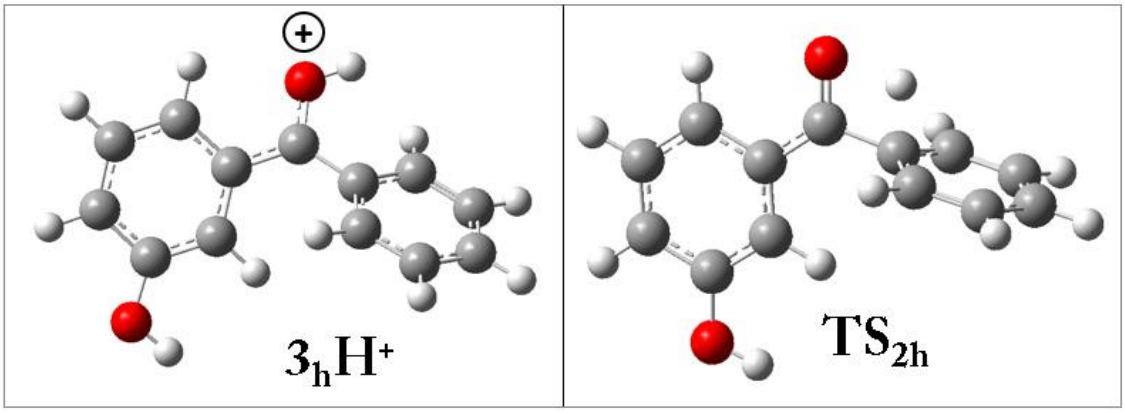
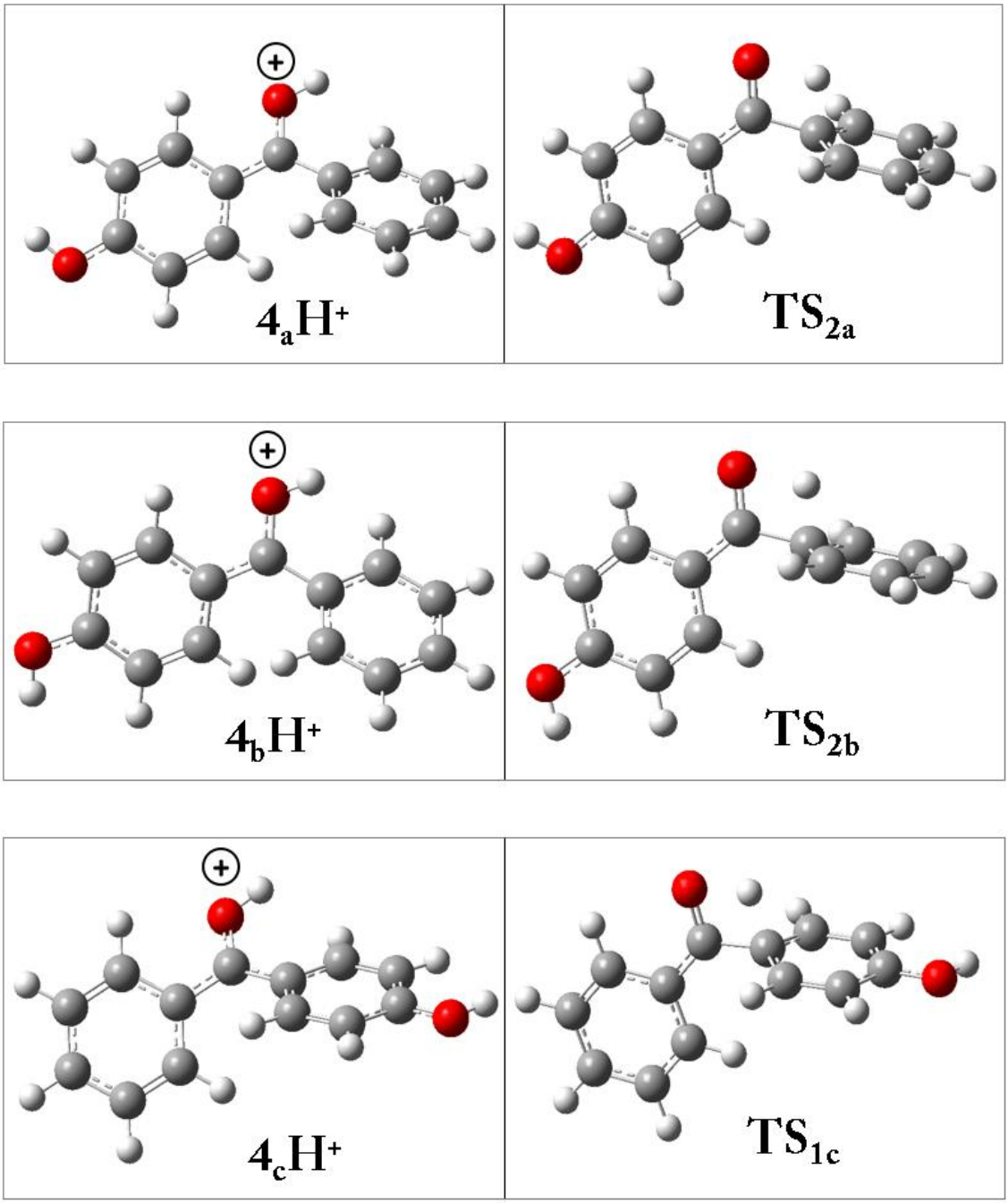


Figure S3. Optimized geometries, at the B3LYP/6-311++G(d,p) level of theory, of the of **4**H^+ rotamers and the transition states of their corresponding fragmentation routes.



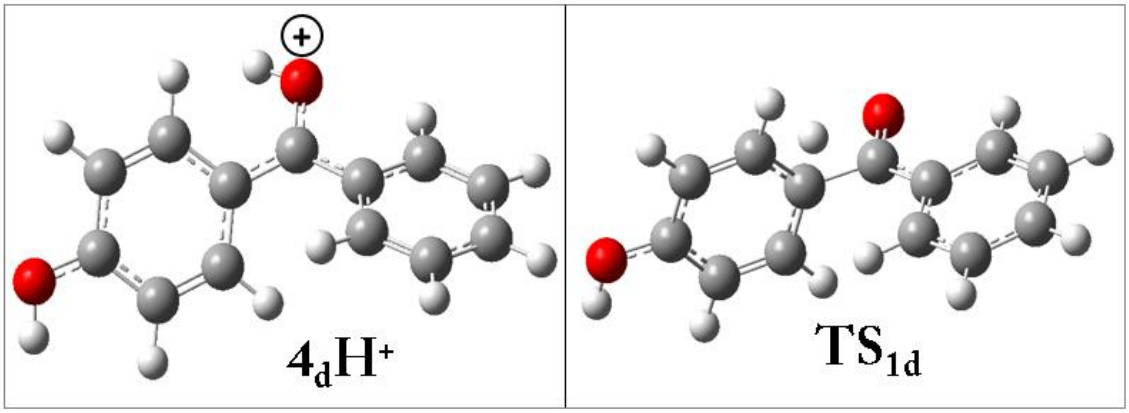


Figure S4. Optimized geometries, at B3LYP/6-311++G(d,p) level of theory, of fragments 105 *m/z* and 121 *m/z*.