Supporting Information

Electrophilic Aromatic Substitution: New Insights into an Old Class of Reactions

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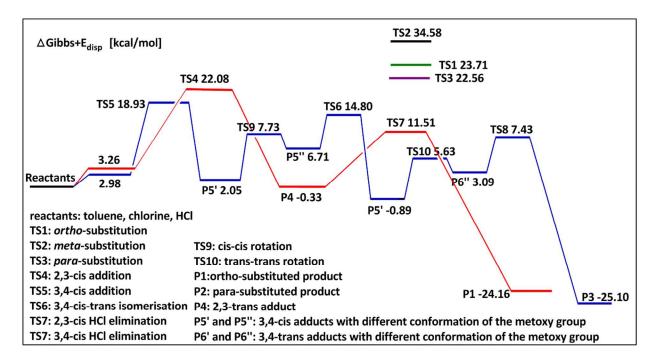


Figure S1. Computed potential free energy surface (PES) for anisole- Cl_2 reactions, catalyzed by HCl, in simulated CCl_4 solution at B2-PLYP+D3/6-311+G(2d,2p)//B3LYP/6-311+G(2d,2p). Cis-trans isomerization and elimination transition states, leading to formation of *m*-substituted product are not included.

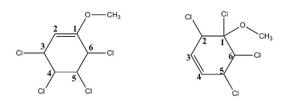


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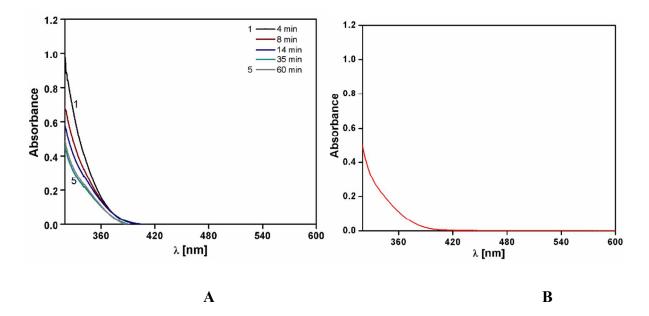


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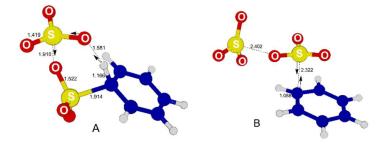


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Cartesian coordinates

The Cartesian coordinates of the optimized structures discussed in the text can be found in the Supporting Information files of the following publications:

Anisole chlorination: SI to Ref. 15.

Toluene chlorination: SI to Ref. 16.

Benzene bromination: SI to Ref. 17.

Benzene nitration: SI to Ref. 18.

Benzene sulfonation: SI to Ref. 19.