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Halogen atom transfer mechanism of iron-catalyzed direct arylation to form biaryl using Density Functional Theory calculations

Qinghua Ren, Shanshan An, Zhilei Huang, Ningning Wu, Xiaoyan Shen

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$$\begin{array}{c|c} & Fe(OAc)_2 \\ \hline & + & \\ \hline & \frac{bathophenanthroline}{t\text{-BuOK}, 80^{\circ}C} \end{array}$$

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