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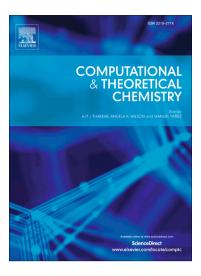
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Theoretical Study on Abnormal Trans-Effect of Chloride, Bromide and Iodide ligands in

Iridium Complexes

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Abstract: Iridium complexes have been widely applied to energy and chemical industry,

pharmaceutical industry, and organic synthesis. As a parameter reflecting the interaction

between ligands and metal centers, trans-effect plays an important role in the

kinetics/thermodynamic stability, the reactivity and the catalytic performance of transition

metal complexes. A systematic study was conducted herein to address the abnormal

trans-effect of iridium halide complexes reported by Werneke et al. It is found that the

observed unconventional trans-effect mainly results from the different cis-to-trans

isomerization energies of different tetra-coordinated iridium complexes. The relevant results

provide deeper insights into understanding the trans-effect based on the experimentally

measured bond dissociation energies, and thus benefit the design and development of new,

highly effective hydrogen fuel carrier metal complexes.

Keywords: Iridium Complexes; Trans-Effect; Theoretical Calculations; Bond Dissociation

Energy

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