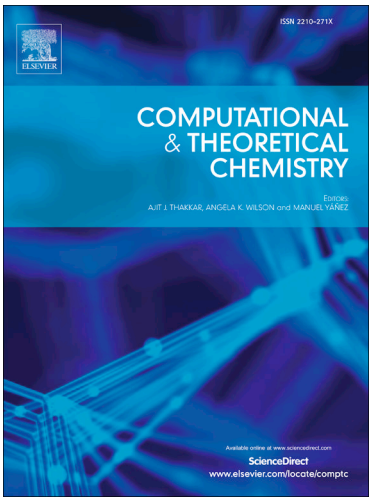

Theoretical Study on Abnormal Trans-Effect of Chloride, Bromide and Iodide ligands in Iridium Complexes

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PII: S2210-271X(18)30182-8
DOI: https://doi.org/10.1016/j.comptc.2018.05.015
Reference: COMPTC 2801

To appear in: *Computational & Theoretical Chemistry*

Received Date: 13 January 2018
Revised Date: 1 May 2018
Accepted Date: 23 May 2018

Please cite this article as: C. Wang, Y-Y. Jiang, Theoretical Study on Abnormal Trans-Effect of Chloride, Bromide and Iodide ligands in Iridium Complexes, *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.05.015

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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