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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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