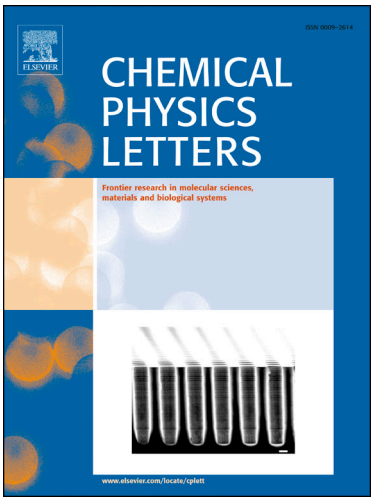

Research paper

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PII: S0009-2614(17)30764-9
DOI: http://dx.doi.org/10.1016/j.cplett.2017.08.003
Reference: CPLETT 35013

To appear in: *Chemical Physics Letters*

Received Date: 22 May 2017
Revised Date: 1 August 2017
Accepted Date: 3 August 2017

Please cite this article as: C. Plascencia, J. Wang, A.K. Wilson, Importance of the ligand basis set in *ab initio* thermochemical calculations of transition metal species, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.08.003

Importance of the ligand basis set in *ab initio* thermochemical calculations of transition metal species

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Abstract: The impact of basis set choice has been considered for a series of transition metal (TM) species. The need for higher level correlation consistent basis sets on both the metal and ligand has been investigated, and permutations in the pairings of basis set used for TM's and basis set used for ligands can lead to effective routes to complete basis set (CBS) limit extrapolations of thermochemical energetics with little change in thermochemical predictions as compared to those resulting from the use of traditional basis set pairings, while enabling computational cost savings. Basis set superposition errors (BSSE) that can arise have also been considered.

Keywords: correlation consistent basis set, transition metal, extrapolation, basis set superposition error, counterpoise correction, complete basis set limit.

1.1 Introduction

The reliable prediction of thermochemical properties of transition metal (TM) species is important in areas from catalyst design[1,2] to biomedical applications.[3,4] A route towards reliable prediction is via *ab initio* electron correlation methods, however, the modeling of TM atoms and complexes brings many theoretical challenges. These challenges include the need to account for

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