Kinetic Isotope Effects (KIE) and Density Functional Theory (DFT): A Match Made in Heaven? - DTU Orbit (03/01/2019)

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Determination of experimental kinetic isotope effects (KIE) is one of the most useful tools for the exploration of reaction mechanisms in organometallic chemistry. The approach has been further strengthened during the last decade with advances in modern computational chemistry. This allows for the calculation of a theoretical KIE that can often be compared directly to the experimental value. This combined experimental/theoretical approach can be particularly useful in cases where the value of the experimental KIE is not directly associated with one particular reaction step (e.g., in a catalytic reaction). The approach is highlighted by using recent examples from both stoichiometric and catalytic reactions, homogeneous and heterogeneous catalysis, and enzyme catalysis to illustrate the expected accuracy and utility of this approach.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Contributors: Christensen, N. J., Fristrup, P.
Number of pages: 6
Pages: 508-513
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: SYNLETT: Accounts and Rapid Communications in Chemical Synthesis
Volume: 26
Issue number: 4
Article number: st-2014-d1004-l
ISSN (Print): 0936-5214
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.87 SJR 0.83 SNIP 0.446
Web of Science (2017): Impact factor 2.369
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.84 SJR 0.857 SNIP 0.458
Web of Science (2016): Impact factor 2.151
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2 SJR 0.865 SNIP 0.489
Web of Science (2015): Impact factor 2.323
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.09 SJR 0.978 SNIP 0.584
Web of Science (2014): Impact factor 2.419
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.08 SJR 1.041 SNIP 0.572
Web of Science (2013): Impact factor 2.463
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.1 SJR 1.17 SNIP 0.631
Web of Science (2012): Impact factor 2.655
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.43 SJR 1.308 SNIP 0.666
Web of Science (2011): Impact factor 2.71
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.241 SNIP 0.641
Web of Science (2010): Impact factor 2.447
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.291 SNIP 0.702
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.507 SNIP 0.748
Scopus rating (2007): SJR 1.557 SNIP 0.818
Scopus rating (2006): SJR 1.535 SNIP 0.842
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.327 SNIP 0.8
Scopus rating (2004): SJR 1.42 SNIP 0.846
Scopus rating (2003): SJR 1.391 SNIP 0.924
Scopus rating (2002): SJR 1.742 SNIP 0.947
Scopus rating (2001): SJR 1.505 SNIP 0.906
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.306 SNIP 0.87
Scopus rating (1999): SJR 1.426 SNIP 0.876
Original language: English
Keywords: Kinetic isotope effect, Competition experiments, Density functional calculations, Catalysis
DOIs:
Source: PublicationPreSubmission
Source-ID: 105452601
Research output: Research - peer-review › Journal article – Annual report year: 2015