Unprecedented insight into the carbonylation of dimethyl ether over Mordenite is provided through the identification of ketene (CH₂CO) as a reaction intermediate. The formation of ketene is predicted by detailed DFT calculations and verified experimentally by the observation of doubly deuterated acetic acid (CH₂DCOOD), when D₂O is introduced in the feed during the carbonylation reaction.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Center for Atomic-scale Materials Design, Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS, SUNCAT Center for Interface Science and Catalysis
Number of pages: 4
Pages: 7261-7264
Publication date: 2015
Peer-reviewed: Yes

Publication information
Volume: 54
Issue number: 25
ISSN (Print): 1433-7851
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 11.31 SJR 6.155 SNIP 2.165
Web of Science (2017): Impact factor 12.102
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.146
Web of Science (2016): Impact factor 11.994
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.13 SJR 5.888 SNIP 2.225
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 10.84 SJR 5.811 SNIP 2.307
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.7 SJR 5.702 SNIP 2.198
Web of Science (2013): Impact factor 11.336
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.55 SJR 6.407 SNIP 2.329
Web of Science (2012): Impact factor 13.734
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 10.75 SJR 6.063 SNIP 2.361
Web of Science (2011): Impact factor 13.455
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.921 SNIP 2.303
Web of Science (2010): Impact factor 12.73
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 5.571 SNIP 2.246
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 5.589 SNIP 2.153
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 4.528 SNIP 1.888
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 4.868 SNIP 2.165
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 4.797 SNIP 2.279
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 4.247 SNIP 2.198
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.559 SNIP 2.117
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 4.012 SNIP 2.142
Scopus rating (2001): SJR 3.788 SNIP 2.069
Scopus rating (2000): SJR 3.447 SNIP 2.1
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 3.529 SNIP 2.046
Original language: English
Keywords: Carbonylation, Density functional calculations, Heterogeneous catalysis, Reaction mechanisms, Zeolites
DOIs: 10.1002/anie.201410974
Source: FindIt
Source-ID: 275245236
Research output: Research - peer-review ; Journal article – Annual report year: 2015