

# The Chemistry of Scopus & Web of Science

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Science Librarian  
York University


# Scopus & Web of Science

- Coverage: [JCR](#) and [SCImago](#)
- Affiliation search versus departmental search
- Subject and author keywords
- Open access content and patents
- Caveats in both databases


# Scopus & Web of Science Chemistry Journals Coverage

- Scopus (using ScImago): **487**

SJR is developed by:



Data source:



### Journal Indicators

Ranking Parameters

Subject Area: Chemistry

Subject Category: All categories of selected Area

Country:

Order By:

Display journals with at least:

Year: 2007

Refresh

Subject Area: Chemistry.  
Year: 2007.

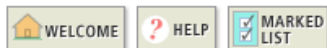
Download data in MS Excel format (107 Kb)

1 - 50 of 487 << First | < Previous | Next > | Last >>

## Web of Science (from JCR): **448**

ISI Web of Knowledge<sup>SM</sup>

Journal Citation Reports<sup>®</sup>



2007 JCR Science Edition

Journal Summary List

[Journal Title Changes](#)

Journals from: subject categories CHEMISTRY, ANALYTICAL; CHEMISTRY, APPLIED; CHEMISTRY, INORGANIC & NUCLEAR; CHEMISTRY, MEDICINAL; CHEMISTRY, MULTIDISCIPLINARY; CHEMISTRY, ORGANIC; CHEMISTRY, PHYSICAL

[VIEW CATEGORY SUMMARY LIST](#)

Sorted by: Journal Title


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# WoS: Coverage

## Subject Category Summary List

[Journal Title Changes](#)

Category data from: subject categories BIOCHEMICAL RESEARCH METHODS; BIOCHEMISTRY & MOLECULAR BIOLOGY; CHEMISTRY, ANALYTICAL; CHEMISTRY, APPLIED; CHEMISTRY, INORGANIC & NUCLEAR; CHEMISTRY, MEDICINAL; CHEMISTRY, MULTIDISCIPLINARY; CHEMISTRY, ORGANIC; CHEMISTRY, PHYSICAL  [VIEW JOURNAL SUMMARY LIST](#)

Sorted by:  

Categories 1 - 9 (of 9)

|<<< [ 1 ] >>>|

Page 1 of 1

*Ranking is based on your category and sort selections.*

Rank	Category (linked to category information)	Total Cites	Median Impact Factor	Aggregate Impact Factor	Aggregate Immediacy Index	Aggregate Cited Half-Life	# Journals	Articles
1	<a href="#">BIOCHEMISTRY &amp; MOLECULAR BIOLOGY</a>	2383087	2.550	4.225	0.812	6.7	263	48051
2	<a href="#">CHEMISTRY, MULTIDISCIPLINARY</a>	973867	1.032	3.463	0.649	6.3	127	29835
3	<a href="#">CHEMISTRY, PHYSICAL</a>	839377	1.739	2.676	0.437	5.8	110	32287
4	<a href="#">CHEMISTRY, ANALYTICAL</a>	435144	1.601	2.555	0.421	6.5	70	17428
5	<a href="#">CHEMISTRY, APPLIED</a>	189615	0.862	1.768	0.321	6.4	62	10635
6	<a href="#">BIOCHEMICAL RESEARCH METHODS</a>	339628	2.135	3.270	0.513	5.8	60	12571
7	<a href="#">CHEMISTRY, ORGANIC</a>	489970	1.808	2.666	0.567	6.3	56	19182
8	<a href="#">CHEMISTRY, INORGANIC &amp; NUCLEAR</a>	286910	1.260	2.192	0.434	7.1	43	11616
9	<a href="#">CHEMISTRY, MEDICINAL</a>	187782	1.817	2.516	0.428	5.8	41	8860

# WoS: Coverage - Organic Chemistry

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2007 JCR Science Edition

## Journal Summary List

[Journal Title Changes](#)

Journals from: subject categories CHEMISTRY, ORGANIC

Sorted by:

Journals 1 - 20 (of 56)

◀◀◀ [ 1 | 2 | 3 ] ▶▶▶

Page 1 of 3

*Ranking is based on your journal and sort selections.*

Mark	Rank	Abbreviated Journal Title (linked to journal information)	ISSN	JCR Data						Eigenfactor <sup>TM</sup> Metrics	
				Total Cites	Impact Factor	5-Year Impact Factor	Immediacy Index	Articles	Cited Half-life	Eigenfactor <sup>TM</sup> Score	Article Influence <sup>TM</sup> Score
<input type="checkbox"/>	1	<a href="#">ADV CARBOHYD CHEM BI</a>	<a href="#">0065-2318</a>	744	1.200	1.800		0	>10.0	0.00023	0.661
<input type="checkbox"/>	2	<a href="#">ADV HETEROCYCL CHEM</a>	<a href="#">0065-2725</a>	865	2.150	2.022	0.750	8	>10.0	0.00058	0.555
<input type="checkbox"/>	3	<a href="#">ADV ORGANOMET CHEM</a>	<a href="#">0065-3055</a>	994	4.176			0	>10.0	0.00146	
<input type="checkbox"/>	4	<a href="#">ADV PHYS ORG CHEM</a>	<a href="#">0065-3160</a>	450	2.667	2.519		0	>10.0	0.00068	1.089
<input type="checkbox"/>	5	<a href="#">ADV SYNTH CATAL</a>	<a href="#">1615-4150</a>	6277	4.977	5.193	0.852	317	3.1	0.04328	1.714

# Scopus Coverage – Organic Chemistry



SCImago  
Journal & Country  
Rank

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## Journal Indicators

### Ranking Parameters

Subject Area:  Chemistry  
 Subject Category:  Organic Chemistry  
 Country: All Year: 2007  
 Order By: SJR  
 Display journals with at least: 0 Citable Docs. (3 years) Refresh

Subject Area: **Chemistry**.  
 Subject Category: **Organic Chemistry**.  
 Year: **2007**.

 Download data in MS Excel format (18 Kb)

 1 - 50 of 85 << First | < Previous | Next > | Last >>

	Title	SJR	H index	Total Docs. (2007)	Total Docs. (3years)	Total Refs.	Total Cites (3years)	Citable Docs. (3years)	Cites / Doc. (2years)	Ref. / Doc.	Country
1	Chemistry and Biology	1,198	92	163	575	5.775	2.494	435	5,30	35,43	UNITED KINGDOM
2	Aldrichimica Acta	1,032	32	9	21	944	224	20	11,54	104,89	UNITED STATES
3	Medicinal Research	0,880	56	30	81	5.067	600	79	6,96	168,90	UNITED STATES

SJR is developed by:



Data source:

SCOPUS


# Scopus: Affiliation Search

## Make Affiliation Selection

### Affiliation

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E.g., university of toronto

 Search

Clear



The Scopus Affiliation Identifier is the world's first tool to help you identify and group an organization's complete body of work. It turns a time-consuming process into a simple task.

[More information...](#)

Refined with: ( LIMIT-TO(AFFILCOUNTRY, "Canada") AND (LIMIT-TO(AFFILCITY, "Toronto") AND (LIMIT-TO(AFFILCITY, "Toronto"))

### Refine Results

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Country

☐ Canada (2)

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Select one or more affiliations and click **show documents**.

### Affiliation Results: 2

Page 1 of 1

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Affiliations		Documents	City	Country
1.	<input type="checkbox"/> <b>York Universite</b> York University <a href="#">Find unmatched affiliations</a>	<a href="#">Details</a> <a href="#">16205</a>	Toronto	Canada
2.	<input type="checkbox"/> <b>Norman Bethune College</b> York University Bethune College <a href="#">Find unmatched affiliations</a>	<a href="#">Details</a> <a href="#">20</a>	Toronto	Canada

# Scopus: Research Outputs

Name variants **York University**

## Research

Documents [16,205](#) [Add to list](#) [E-mail alert](#) | [RSS](#)

Authors [4,652](#)

Web Results [232](#)

Patent Results [9,727](#)

Sources [194](#) Vision Research  
[184](#) Dissertation Abstracts International A the Humanities and Social Sciences  
[136](#) Journal of Chemical Physics  
[122](#) Inorganic Chemistry  
[110](#) Astronomical Journal  
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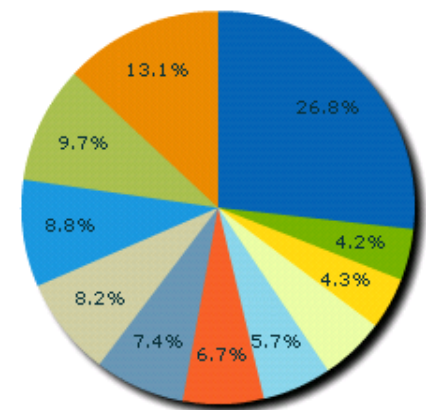
[Find unmatched affiliations](#)

## Collaborating Affiliations

Affiliation Name	Documents
University of Toronto	<a href="#">1,110</a>
McGill University	<a href="#">242</a>
The University of British Columbia	<a href="#">208</a>
McMaster University	<a href="#">202</a>
University of Alberta	<a href="#">176</a>
<a href="#">More...</a>	

## Subject Areas

[Chart](#) | [Data](#)



- Social Sciences
- Medicine
- Psychology
- Physics and Astronomy
- Biochemistry, Genetics and ...
- Earth and Planetary Sciences
- Mathematics
- Chemistry
- Environmental Science



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Source Title	Author Name	Year	Document Type	Subject Area
<input type="checkbox"/> Vision Research (194)	<input type="checkbox"/> Bohme, D.K. (228)	<input type="checkbox"/> 2009 (358)	<input type="checkbox"/> Article (12,611)	<input type="checkbox"/> Social Sciences (3,124)
<input type="checkbox"/> Dissertation Abstracts International A the Humanities and Social Sciences (184)	<input type="checkbox"/> Lever, A.B.P. (201)	<input type="checkbox"/> 2008 (1,176)	<input type="checkbox"/> Conference Paper (1,098)	<input type="checkbox"/> Medicine (2,321)
<input type="checkbox"/> Journal of Chemical Physics (136)	<input type="checkbox"/> Burke, R.J. (181)	<input type="checkbox"/> 2007 (1,129)	<input type="checkbox"/> Review (1,014)	<input type="checkbox"/> Psychology (2,114)
<a href="#">More...</a>	<a href="#">More...</a>	<a href="#">More...</a>	<a href="#">More...</a>	<a href="#">More...</a>
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Source Title	Author Name	Year	Document Type	Subject Area
<input type="checkbox"/> Vision Research (194)	<input type="checkbox"/> Bohme, D.K. (228)	<input type="checkbox"/> 2009 (358)	<input type="checkbox"/> Article (12,611)	<input type="checkbox"/> Social Sciences (3,124)
<input type="checkbox"/> Dissertation Abstracts International A the Humanities and Social Sciences (184)	<input type="checkbox"/> Lever, A.B.P. (201)	<input type="checkbox"/> 2008 (1,176)	<input type="checkbox"/> Conference Paper (1,098)	<input type="checkbox"/> Medicine (2,321)
<input type="checkbox"/> Journal of Chemical Physics (136)	<input type="checkbox"/> Burke, R.J. (181)	<input type="checkbox"/> 2007 (1,129)	<input type="checkbox"/> Review (1,014)	<input type="checkbox"/> Psychology (2,114)
<input type="checkbox"/> Inorganic Chemistry (122)	<input type="checkbox"/> Hopkinson, A.C. (162)	<input type="checkbox"/> 2006 (985)	<input type="checkbox"/> Dissertation (193)	<input type="checkbox"/> Physics and Astronomy (1,967)
<input type="checkbox"/> Astronomical Journal (110)	<input type="checkbox"/> Mahaney, W.C. (137)	<input type="checkbox"/> 2005 (934)	<input type="checkbox"/> Letter (129)	<input type="checkbox"/> Biochemistry, Genetics and Molecular Biology (1,782)
<input type="checkbox"/> Journal of Geophysical Research D Atmospheres (103)	<input type="checkbox"/> Stauffer, A.D. (121)	<input type="checkbox"/> 2004 (823)	<input type="checkbox"/> Note (128)	<input type="checkbox"/> Earth and Planetary Sciences (1,603)
<input type="checkbox"/> Journal of the American Chemical Society (98)	<input type="checkbox"/> Shepherd, G.G. (104)	<input type="checkbox"/> 2003 (709)	<input type="checkbox"/> Article in Press (100)	<input type="checkbox"/> Mathematics (1,372)
<input type="checkbox"/> Astrophysical Journal (87)	<input type="checkbox"/> Wu, J. (102)	<input type="checkbox"/> 2002 (642)	<input type="checkbox"/> Book (91)	<input checked="" type="checkbox"/> Chemistry (1,277)
<input type="checkbox"/> Geophysical Research Letters (85)	<input type="checkbox"/> McEachran, R.P. (93)	<input type="checkbox"/> 2001 (583)	<input type="checkbox"/> Editorial (83)	<input type="checkbox"/> Environmental Sciences (1,023)
<input type="checkbox"/> Personality and Individual Differences (84)	<input type="checkbox"/> Regan, D. (92)	<input type="checkbox"/> 2000 (579)	<input type="checkbox"/> Short Survey (57)	<input type="checkbox"/> Agricultural and Biological Sciences (1,012)
<input type="checkbox"/> Lecture Notes in Computer Science Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics (74)	<input type="checkbox"/> Heddle, J.A. (91)	<input type="checkbox"/> 1999 (502)	<input type="checkbox"/> Erratum (23)	<input type="checkbox"/> Engineering (972)
<input type="checkbox"/> Topology and Its Applications (73)	<input type="checkbox"/> Pritchard, H.O. (89)	<input type="checkbox"/> 1998 (638)	<input type="checkbox"/> Conference Review (1)	<input type="checkbox"/> Computer Science (871)
<input type="checkbox"/> Chemical Physics Letters (72)	<input type="checkbox"/> Flett, G.L. (88)	<input type="checkbox"/> 1997 (641)	<input type="checkbox"/> Undefined (600)	<input type="checkbox"/> Neuroscience (817)
<input type="checkbox"/> Physics Letters Section B Nuclear Elementary Particle and High Energy Physics (71)	<input type="checkbox"/> Howard, I.P. (85)	<input type="checkbox"/> 1996 (683)	<a href="#">Less...</a>	<input type="checkbox"/> Arts and Humanities (776)

# WoS: Departmental Search

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	 <i>Example: National Center</i>		
AND	<input type="text" value=""/>	in	<input type="text" value="Publication Name"/>
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Timespan:

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- ☐ From  to  (default is all years)

## Tandem mass spectrometry and multiple reaction monitoring using an atmospheric pressure quadrupole mass spectrometer for product identification in atmospherically important reactions

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Author(s): Auld J (Auld, Janeen), Hastie DR (Hastie, Donald R.)<sup>1</sup>

Source: INTERNATIONAL JOURNAL OF MASS SPECTROMETRY Volume: 282 Issue: 3 Pages: 91-98 Published: MAY 1 2005

Times Cited: 0 References: 22  Citation Map

**Abstract:** An atmospheric pressure chemical ionization triple quadrupole mass spectrometer has been coupled to a smog chamber for the study of hydrocarbon oxidation reactions. Traditional MS and MS/MS scan modes were used to identify ion signals arising from possible reactions. This method was used to follow a number of these as target  $\rightarrow$  fragment ion pairs over the course of the reaction. Mechanistic information has been obtained from these signals. MRM profiling has allowed the identification of interferences that occur due to isobaric ions resulting from the formation of isobaric ions undetectable using the MS and MS/MS modes. Differences in product formation rate results in variations of their MRM ion pair onset times being observed. This method was tested during a study of the products of the HO radical oxidation of  $\beta$ -pinene. The oxidation product pinic acid was identified at its (M+H)<sup>+</sup>, m/z 139, being more accurately monitored using its (M+H+H<sub>2</sub>O)<sup>+</sup> cluster ion pairs, 157  $\rightarrow$  139 and 157  $\rightarrow$  111 has led to the identification of a more highly oxidized acid-aldehyde product. It has been determined that an organic dependence relative to pinic acid cannot be the expected simple C<sub>10</sub> hydroxynitrone product but rather a more highly oxidized C<sub>9</sub> nitrone. This reaction time has proven to be a valuable addition to existing mass spectrometric acquisition modes for reaction product determination.

Document Type: Article


Language: English

**Author Keywords:** Mass spectrometry; Atmospheric pressure chemical ionization;  $\beta$ -Pinene; Oxidation

**KeyWords Plus:** PARTICULATE PRODUCTS; BETA-PINENE; OXIDATION; OZONE; OH; MONOTERPENES; MECHANISM; H&(H<sub>2</sub>O)N

**Reprint Address:** Hastie, DR (reprint author), York Univ, Dept Chem, 4700 Keele St, Toronto, ON M3J 1P3 Canada

### Addresses:

1. York Univ, Dept Chem, Toronto, ON M3J 1P3 Canada 
2. York Univ, Ctr Atmospher Chem, Toronto, ON M3J 1P3 Canada

**E-mail Addresses:** [Hastie@Yorku.ca](mailto:Hastie@Yorku.ca)

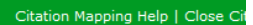
### Funding Acknowledgement:

Funding Agency	Grant Number
Natural Sciences and Engineering Research Council of Canada (NSERC)	

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WoS

## Heterogeneous reactions of glyoxal on particulate matter: Identification of acetals and sulfate esters

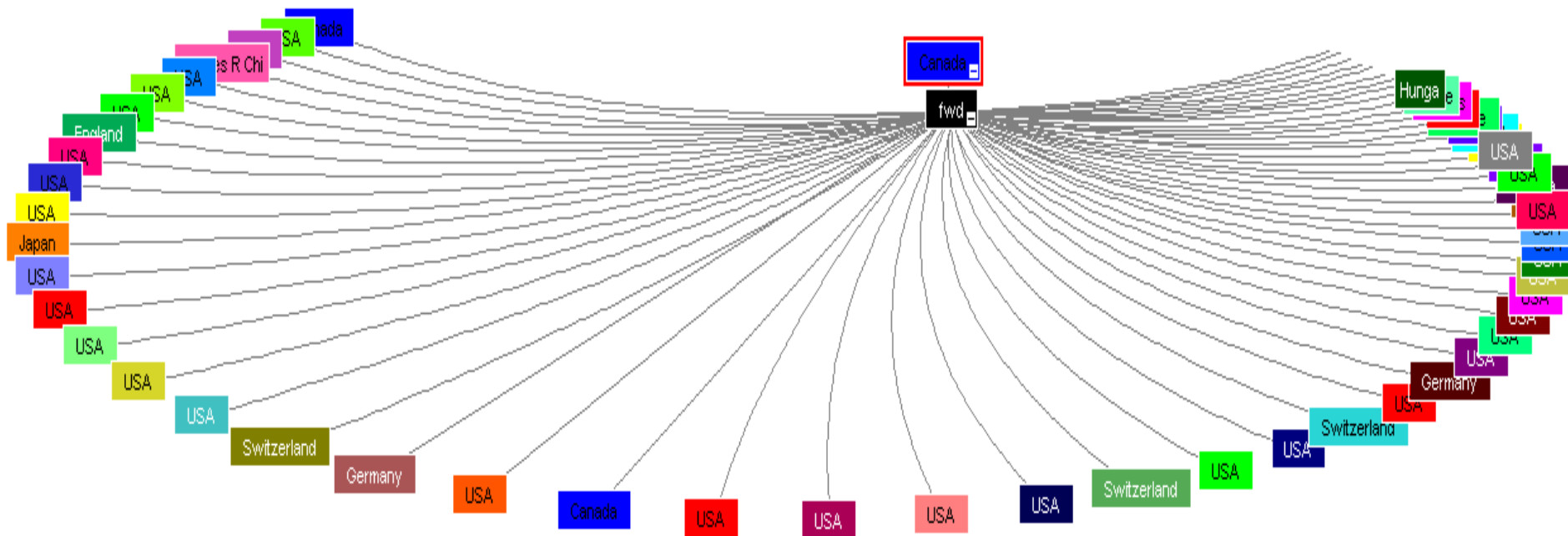


Choose Forward to see records that cite the target record, choose Backward to see records the target record cites — to see both types, choose Forward and Backward

	Primary Author	Journal Name	Article title
⇒	Reemtsma, T	2006-ANALYTICAL CHEMISTRY	Identification of fulvic acids and sulfated and nitrated analogues in atmospheric aerosol by electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry
⇒	Surratt, JD	2008-JOURNAL OF PHYSICAL CHEMISTRY A	Organosulfate formation in biogenic secondary organic aerosol
⇒	Ieda, T	2006-TELLUS SERIES B-CHEMICAL AND PHYSICAL METEOROLOGY	Diurnal variations and vertical gradients of biogenic volatile and semi-volatile organic compounds at the Tomakomai larch forest station in Japan
⇒	Myriokefalitakis,	2008-ATMOSPHERIC	The influence of natural and anthropogenic secondary sources on the

Displaying 1 - 10 of 62
 « 1 2 3 4 5 »
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 Records per page

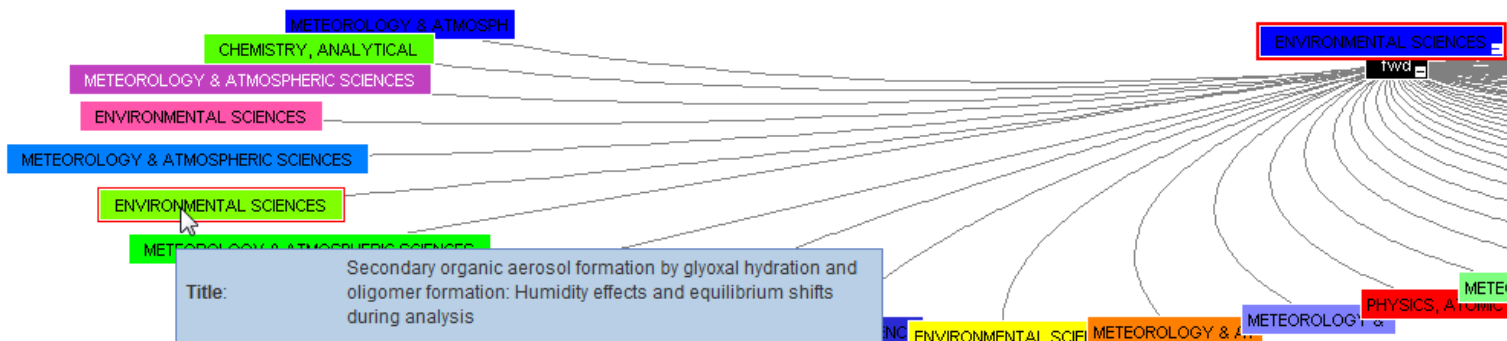
Heterogeneous reactions of glyoxal on particulate matter: Identification of acetals and sulfate esters	
Number / Title	<a href="#">143355829 / Heterogeneous reactions of glyoxal on particulate matter: Identification of acetals and sulfate esters</a>
Journal Title	ENVIRONMENTAL SCIENCE & TECHNOLOGY
Publication Year	2005
Author	Liggio, J
Group Author	
Source	ENVIRON SCI TECHNOL



# Citation Mapper: Sort by Country

# WoS: Mapper: By subject

Heterogeneous reactions of glyoxal on particulate matter: Identification of acetals and sulfate esters



Source: ISI Web of Knowledge™, www.thomsonscientific.com

Record details for the nodes are displayed below (double-click)

Primary Author	Journal Name	
⇒ Reemtsma, T	2006-ANALYTICAL CHEMISTRY	Identification of atmospheric cyclotrisulfonates
⇒ Surratt, JD	2008-JOURNAL OF PHYSICAL CHEMISTRY A	Organic aerosol formation by glyoxal hydration and oligomer formation: Humidity effects and equilibrium shifts during analysis
⇒ Ieda, T	2006-TELLUS SERIES B-CHEMICAL AND PHYSICAL	Diurnal variations and vertical gradients of biogenic volatile and semi-volatile organic compounds at the Tomakomai larch forest station

**Title:** Secondary organic aerosol formation by glyoxal hydration and oligomer formation: Humidity effects and equilibrium shifts during analysis  
**Authors:** Hastings, WP; Koehler, CA; Bailey, EL ...  
**Journal title:** ENVIRONMENTAL SCIENCE & TECHNOLOGY  
**Volume:** 39  
**Page:** 8728-8735  
**Publish year:** 2005  
**DOI:** DOI 10.1021/es0504461  
**Document type:** Article  
**Subject category:** ENVIRONMENTAL SCIENCES  
**Language:** English  
**Country:** USA  
**Institution:** Univ San Diego

Heterogeneous reactions of glyoxal on particulate matter: Identification of acetals and sulfate esters

Number / Title	143355829 / Heterogeneous reactions of glyoxal on particulate matter: Identification of acetals and sulfate esters
Journal Title	ENVIRONMENTAL SCIENCE & TECHNOLOGY
Publication Year	2005
Author	Liggio, J

# WoS: Research Outputs

555 records. Address=(Dept Chem SAME York Univ SAME Canada)

Rank the records by this field:	Analyze:	Set display
<div> <div>Language</div> <div>Publication Year</div> <div>Source Title</div> <div>Subject Area</div> </div>	Up to <input type="text" value="500"/> records.	Show the top <input type="text" value="25"/> results. Minimum record count (threshold): <input type="text" value="2"/>

Analyze

Use the checkboxes below to view the records. You can choose to view those selected records, or you can exclude them ( and view the others).

**Note:** The number of records displayed may be greater than the listed Record Count

if the original set contained more records than the number of records analyzed.

<input type="checkbox"/> View Records <input checked="" type="checkbox"/> Exclude Records		Field: Subject Area	Record Count	% of 500	Bar Chart	Save Analysis Data to File
<input type="checkbox"/>		CHEMISTRY, PHYSICAL	117	23.4000 %	<div></div>	
<input type="checkbox"/>		PHYSICS, ATOMIC, MOLECULAR & CHEMICAL	114	22.8000 %	<div></div>	
<input type="checkbox"/>		CHEMISTRY, MULTIDISCIPLINARY	91	18.2000 %	<div></div>	
<input type="checkbox"/>		CHEMISTRY, ANALYTICAL	68	13.6000 %	<div></div>	
<input type="checkbox"/>		CHEMISTRY, INORGANIC & NUCLEAR	61	12.2000 %	<div></div>	
<input type="checkbox"/>		SPECTROSCOPY	60	12.0000 %	<div></div>	
<input type="checkbox"/>		CHEMISTRY, ORGANIC	46	9.2000 %	<div></div>	
<input type="checkbox"/>		METEOROLOGY & ATMOSPHERIC SCIENCES	27	5.4000 %	<div></div>	
<input type="checkbox"/>		BIOCHEMICAL RESEARCH METHODS	24	4.8000 %	<div></div>	
<input type="checkbox"/>		BIOCHEMISTRY & MOLECULAR BIOLOGY	19	3.8000 %	<div></div>	
<input type="checkbox"/>		ENVIRONMENTAL SCIENCES	12	2.4000 %	<div></div>	
<input type="checkbox"/>		CRYSTALLOGRAPHY	11	2.2000 %	<div></div>	
<input type="checkbox"/>		CHEMISTRY, APPLIED	10	2.0000 %	<div></div>	
<input type="checkbox"/>		GEOSCIENCES, MULTIDISCIPLINARY	8	1.6000 %	<div></div>	
<input type="checkbox"/>		CHEMISTRY, PHYSICAL	7	1.4000 %	<div></div>	



# Scopus: Extra Coverage

Scopus (16,205)

More... (0)

Web: 232

Patents (9,727)

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- ☐ Radboud University Nijmegen (41)
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| <input type="checkbox"/> issue date   | <input type="checkbox"/> scope of activity               | <input type="checkbox"/> southern queensland           |
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## Synthesis, spectroscopic and a ZINDO study of cis- and trans-(X-2)bis(4,4'-dicarboxylic acid-2,2'-bipyridine)ruthenium(II) complexes (X = Cl<sup>-</sup>, H<sub>2</sub>O, NCS<sup>-</sup>)

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Author(s): Nazeeruddin MK, Zakeeruddin SM, Humphry-Baker R, Gorelsky SI, Lever ABP, Gratzel M

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Source: COORDINATION CHEMISTRY REVIEWS Volume: 208 Pages: 213-225 Published: OCT 2000

Times Cited: 70 References: 45 [Citation Map](#)

**Abstract:** Ruthenium complexes of the type trans-[Ru(dcbpyH(2))(2)(Cl)(2)], trans-[Ru(dcbpyH(2))(2)(H<sub>2</sub>O)(2)] and trans-[Ru(dcbpyH(2))(2)(NCS)(2)] (dcbpyH(2) = 4,4'-dicarboxylic acid-2,2'-bipyridine) were synthesized and characterized by NMR, UV-vis absorption and emission spectroscopy. The proton NMR spectra of the trans isomers, in the aromatic region, show only three peaks corresponding to the two dcbpy ligands in which all the pyridine rings are trans to each other and magnetically equivalent. The C-13-NMR spectrum of the trans isomer is characterized by a relatively simple pattern of resonances from the four equivalent pyridine rings. The lowest energy metal-to-ligand charge-transfer transition maximum of the trans-[Ru(dcbpyH(2))(2)(Cl)(2)] complex is at 14500 cm<sup>-1</sup> in DMF solution and shows onset of weak and broad emission signals above 11100 cm<sup>-1</sup>. This is a significantly larger red shift compared with any of the trans ruthenium(II) polypyridyl complexes reported to date. The absorption and emission maxima of the trans complexes are red shifted compared with the cis analogues, which is due to the CO<sub>2</sub>H contribution in the trans isomer that stabilizes the LUMO relative to the LUMO of the cis isomer. The enhanced red response of the trans complexes renders them as suitable dyes for dye-sensitized titanium dioxide mesoporous electrodes. The electronic spectra of cis- and trans-[Ru(dcbpyH(2))(2)(Cl)(2)] complexes were calculated by ZINDO/S and compared with the experimental data. (C) 2000 Elsevier Science S.A. All rights reserved.

**Document Type:** Proceedings Paper

**Language:** English


**Author Keywords:** spectroscopic; ZINDO study; ruthenium complexes; cis-trans isomers; sensitizers

**Keywords Plus:** EFFECTIVE CORE POTENTIALS; NANOCRYSTALLINE TiO<sub>2</sub>; CRYSTAL-STRUCTURE; MOLECULAR CALCULATIONS; ELECTRON-TRANSFER; SOLAR-CELLS; DYE; RUTHENIUM; ABINITIO; FILMS

**Reprint Address:** Nazeeruddin, MK (reprint author), Swiss Fed Inst Technol, Inst Phys Chem, Lab Photon & Interfaces, CH-1015 Lausanne, Switzerland

### Addresses:

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**Publisher:** ELSEVIER SCIENCE SA, PO BOX 564, 1001 LAUSANNE, SWITZERLAND

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## Tau protein binds single-stranded DNA sequence specifically - The proof obtained in vitro with non-equilibrium capillary electrophoresis of equilibrium mixtures

Krylova, S.M.<sup>a</sup> , Musheev, M.<sup>a</sup> , Nutiu, R.<sup>b</sup> , Li, Y.<sup>b</sup> , Lee, G.<sup>c</sup> , Krylov, S.N.<sup>a</sup>   

<sup>a</sup> Department of Chemistry, York University, Toronto, Ont. M3J 1P3, Canada

<sup>b</sup> Depts. of Biochemistry and Chemistry, McMaster University, Hamilton, Ont. L8N 3Z5, Canada

<sup>c</sup> Departments of Internal Medicine, University of Iowa, 200 Hawkins Drive, Iowa City, IA 52242, United States

### Abstract

**Tau** is a microtubule-associated **protein**, which plays an important role in physiology and pathology of neurons. **Tau** has been recently reported to **bind** double-stranded **DNA** (dsDNA) but not to **bind single-stranded DNA** (ssDNA) [Cell. Mol. Life Sci. 2003, 60, 413-421]. Here, we prove that **tau binds** not only dsDNA but also ssDNA. This finding was facilitated by using two kinetic capillary electrophoresis methods: (i) non-equilibrium capillary electrophoresis of equilibrium mixtures (NECEEM); (ii) affinity-mediated NECEEM. Using the new approach, we observed, for the first time, that **tau** could induce dissociation of strands in dsDNA by binding one of them in a sequence-specific fashion. Moreover, we determined the equilibrium dissociation constants for all **tau-DNA** complexes studied. © 2005 Federation of European Biochemical Societies. Published by Elsevier B.V. All rights reserved.

### Language of Original Document

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### Author Keywords

Alzheimer disease; Non-equilibrium capillary electrophoresis of equilibrium mixture; **Protein-DNA** interaction; ssDNA-binding **protein**; **Tau protein**

### Index Keywords

→ **EMTREE drug terms:** double **stranded DNA**; **single stranded DNA**; **tau protein**

→ **EMTREE medical terms:** article; capillary electrophoresis; dissociation; **DNA** sequence; nonhuman; priority journal; **protein DNA** binding

→ **MeSH:** Animals; Base Sequence; **DNA**, **Single-Stranded**; Electrophoresis, Capillary; Escherichia coli; **Protein** Binding; Substrate Specificity; **tau Proteins**; Thermodynamics  
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## Keywords

## Tau protein binds single-stranded DNA sequence specifically - the proof obtained in vitro with non-equilibrium capillary electrophoresis of equilibrium mixtures

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**Author(s):** Krylova SM, Musheev M, Nutiu R, Li YF, Lee G, Krylov SN

**Source:** FEBS LETTERS **Volume:** 579 **Issue:** 6 **Pages:** 1371-1375 **Published:** FEB 28 2005

**Times Cited:** 17 **References:** 24  **Citation Map**

**Abstract:** Tau is a microtubule-associated protein, which plays an important role in physiology and pathology of neurons. Tau has been recently reported to bind double-stranded DNA (dsDNA) but not to bind single-stranded DNA (ssDNA) [Cell. Mol. Life Sci. 2003, 60, 413-421]. Here, we prove that tau binds not only dsDNA but also ssDNA. This finding was facilitated by using two kinetic capillary electrophoresis methods: (i) non-equilibrium capillary electrophoresis of equilibrium mixtures (NECEEM); (ii) affinity-mediated NECEEM. Using the new approach, we observed, for the first time, that tau could induce dissociation of strands in dsDNA by binding one of them in a sequence-specific fashion. Moreover, we determined the equilibrium dissociation constants for all tau-DNA complexes studied. (C) 2005 Federation of European Biochemical Societies. Published by Elsevier B.V. All rights reserved.

**Document Type:** Article


**Language:** English

**Author Keywords:** tau protein; protein-DNA interaction; Alzheimer disease; non-equilibrium capillary electrophoresis of equilibrium mixture; ssDNA-binding protein


**KeyWords Plus:** HUMAN NEUROBLASTOMA-CELLS; NUCLEAR-TAU; IDENTIFICATION; INHIBITION; RNA

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




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
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
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## Where does the electron go? Electron distribution and reactivity of peptide cation transfer in the gas phase

[Tureček, F.](#)<sup>a</sup>  , [Chen, X.](#)<sup>a b</sup> , [Hao, C.](#)<sup>a c</sup>  

<sup>a</sup> Department of Chemistry, Bagley Hall, University of Washington, Seattle, WA 98195-1700, United States

<sup>b</sup> National Institutes of Health (NIH), 9000 Rockville Pike, Bethesda, MD 20892, United States


<sup>c</sup> [Department of Chemistry, York University, Toronto, ON, Canada](#)

### Abstract

We report the first detailed analysis at correlated levels of ab initio theory of experimentally studied peptide cations undergoing electron transfer and competitive dissociations by loss of H atoms, ammonia, and N-C<sub>α</sub> bond cleavage in the gas phase. Doubly protonated (KK + 2H)<sup>2+</sup>, are each calculated to exist as two major conformers in the gas phase. Electron transfer to conformers via exothermic dissociation by loss of ammonia from the Gly residue, which occurs from the ground (X) electronic state of atoms is predicted to occur from the first excited (A) state of the charge-reduced ions. The X and A states are nearly degenerate in energy. This calculation indicates that the electron transfer process is highly sensitive to the conformation of the peptide cation. This calculation indicates that the electron transfer process is highly sensitive to the conformation of the peptide cation.

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

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Author(s): Turecek F (Turecek, Frantisek)<sup>1</sup>, Chen XH (Chen, Xiaohong)<sup>1</sup>, Hao CT (Hao, Changtong)<sup>1</sup>

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY Volume: 130 Issue: 27 Pages: 8818-8833 Published: JUL 9 2008

Times Cited: 4 References: 95 [Citation Map](#)

**Abstract:** We report the first detailed analysis at correlated levels of ab initio theory of experimentally studied peptide cations undergoing charge reduction by collisional electron transfer and competitive dissociations by loss of H atoms, ammonia, and N-C-alpha bond cleavage in the gas phase. Doubly protonated Gly-Lys, (GK + 2H)(2+), and Lys-Lys, (KK + 2H)(2+), are each calculated to exist as two major conformers in the gas phase. Electron transfer to conformers with an extended lysine chain triggers highly exothermic dissociation by loss of ammonia from the Gly residue, which occurs from the ground (X) electronic state of the cation radical. Loss of Lys ammonium H atoms is predicted to occur from the first excited (A) state of the charge-reduced ions. The X and A states are nearly degenerate and show extensive delocalization of unpaired electron density over spatially remote groups. This delocalization indicates that the captured electron cannot be assigned to reduce a particular charged group in the peptide cation and that superposition of remote local Rydberg-like orbitals plays a critical role in affecting the cation-radical reactivity. Electron attachment to ion conformers with carboxyl-solvated Lys ammonium groups results in spontaneous isomerization by proton-coupled electron transfer to the carboxyl group forming dihydroxymethyl radical intermediates. This directs the peptide dissociation toward N-C-alpha bond cleavage that can proceed by multiple mechanisms involving reversible proton migrations in the reactants or ion-molecule complexes. The experimentally observed formations of Lys z(+center dot) fragments from (GK + 2H)(2+) and Lys c(+) fragments from (KK + 2H)(2+) correlate with the product thermochemistry but are independent of charge distribution in the transition states for N-C-alpha bond cleavage. This emphasizes the role of ion-molecule complexes in affecting the charge distribution between backbone fragments produced upon electron transfer or capture.

Document Type: Article

Language: English

**KeyWords Plus:** N-C-ALPHA; CAPTURE-INDUCED DISSOCIATION; HYDROGEN-ATOM ADDUCTS; REIONIZATION MASS-SPECTROMETRY; DENSITY-FUNCTIONAL THEORY; CHARGED PROTEIN CATIONS; ION-BEAM SPECTROSCOPY; AB-INITIO; NEUTRALIZATION-REIONIZATION; PROTON AFFINITY

**Reprint Address:** Turecek, F (reprint author), Univ Washington, Dept Chem, Bagley Hall, Box 351700, Seattle, WA 98195 USA

**Addresses:**

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**E-mail Addresses:** [turecek@chem.washington.edu](mailto:turecek@chem.washington.edu)

**Publisher:** AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA

**Subject Categories:** Chemistry, Multidisciplinary





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











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**Abstract:** The reactions of water cluster anions (H<sub>2</sub>O)(n)<sup>-</sup>, n = 30-70, with hydrogen chloride have been studied by Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry. The first HCl taken up by the clusters is presumably ionically dissolved. The solvated electron recombines with the proton, which is thereby reduced to atomic hydrogen and evaporates from the cluster. This process is accompanied by blackbody radiation and collision induced loss of water molecules. Subsequent collisions lead to uptake of HCl and loss of H<sub>2</sub>O, yielding mixed clusters Cl-(HCl)(m)(H<sub>2</sub>O)(n) until they are saturated with HCl. Those saturated clusters lose H<sub>2</sub>O and HCl in a characteristic sequence. The final stage of the reaction, involving clusters with m = 0-4 and n = 0-6, is studied in detail with density functional theory calculations. The Cl-(HCl)(4)(H<sub>2</sub>O)(6) cluster represents an example for supramolecular self-organization in the gas phase: it consists of a tetrahedral Cl-(HCl)(4), connected on one side of the tetrahedron to a compact water hexamer.

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## Reactions of large water cluster anions with hydrogen chloride: Formation of atomic hydrogen and p in the gas phase

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### Abstract

The reactions of water cluster anions  $(\text{H}_2\text{O})_n^-$ ,  $n = 30-70$ , with hydrogen chloride have been studied by Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry. The first HCl taken up by the clusters is presumably ionically dissolved. The solvated electron recombines with the proton, which is then atomic hydrogen and evaporates from the cluster. This process is accompanied by blackbody radiation and collision induced loss of water molecules: collisions lead to uptake of HCl and loss of  $\text{H}_2\text{O}$ , yielding mixed clusters  $\text{Cl}^-(\text{HCl})_m(\text{H}_2\text{O})_n$  until they are saturated with HCl. Those saturated clusters show a characteristic sequence. The final stage of the reaction, involving clusters with  $m = 0-4$  and  $n = 0-6$ , is studied in detail with density functional theory (DFT). The  $\text{Cl}^-(\text{HCl})_4(\text{H}_2\text{O})_6$  cluster represents an example for supramolecular self-organization in the gas phase: it consists of a tetrahedral  $\text{Cl}^-(\text{HCl})_4$  core, converted from the tetrahedron to a compact water hexamer. © 2007 American Chemical Society.