The Chemistry of Scopus & Web of Science

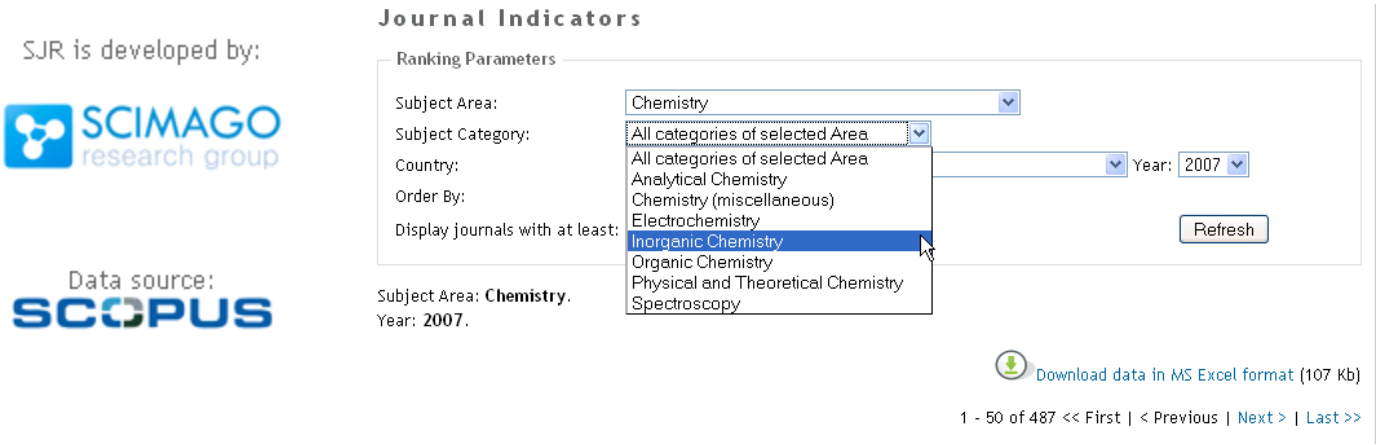
Rajiv Nariani
Science Librarian
York University

Scopus & Web of Science

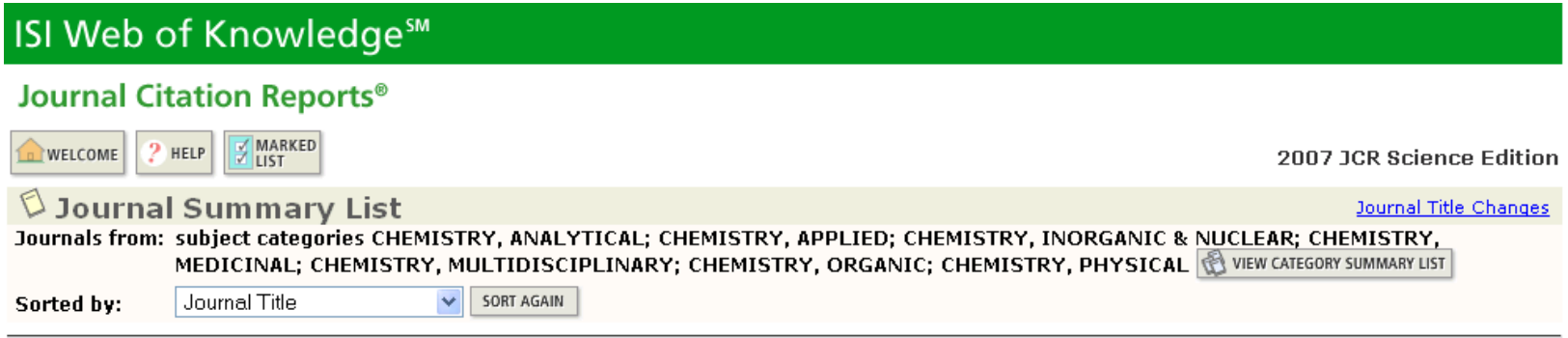
- Coverage: JCR and SCImago
- Affiliation search versus departmental search
- Subject and author keywords
- Open access content and patents
- Caveats in both databases

Scopus & Web of Science Chemistry Journals Coverage

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



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



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: # Journals SORT AGAIN

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	BIOCHEMISTRY & MOLECULAR BIOLOGY	2383087	2.550	4.225	0.812	6.7	263	48051
2	CHEMISTRY, MULTIDISCIPLINARY	973867	1.032	3.463	0.649	6.3	127	29835
3	CHEMISTRY, PHYSICAL	839377	1.739	2.676	0.437	5.8	110	32287
4	CHEMISTRY, ANALYTICAL	435144	1.601	2.555	0.421	6.5	70	17428
5	CHEMISTRY, APPLIED	189615	0.862	1.768	0.321	6.4	62	10635
6	BIOCHEMICAL RESEARCH METHODS	339628	2.135	3.270	0.513	5.8	60	12571
7	CHEMISTRY, ORGANIC	489970	1.808	2.666	0.567	6.3	56	19182
8	CHEMISTRY, INORGANIC & NUCLEAR	286910	1.260	2.192	0.434	7.1	43	11616
9	CHEMISTRY, MEDICINAL	187782	1.817	2.516	0.428	5.8	41	8860

WoS: Coverage - Organic Chemistry

ISI Web of Knowledge℠

Journal Citation Reports®

WELCOME | HELP

2007 JCR Science Edition

Journal Summary List

Journal Title Changes

Journals from: subject categories CHEMISTRY, ORGANIC | VIEW CATEGORY SUMMARY LIST

Sorted by: Journal Title | SORT AGAIN

Journals 1 - 20 (of 56)

[1 | 2 | 3]

Page 1 of 3

MARK ALL | UPDATE MARKED LIST

Ranking is based on your journal and sort selections.

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

Scopus Coverage – Organic Chemistry

SJR SCImago Journal & Country Rank

"EST MODUS IN REBUS" Horatio (Satire 1,1,106)

Home
> Journal Indicators
Journal Search
Country Indicators
Country Search
Compare
Map Generator
Help
About Us

How to cite this website?

SJR is developed by: SCIMAGO research group

Data source: SCOPUS

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

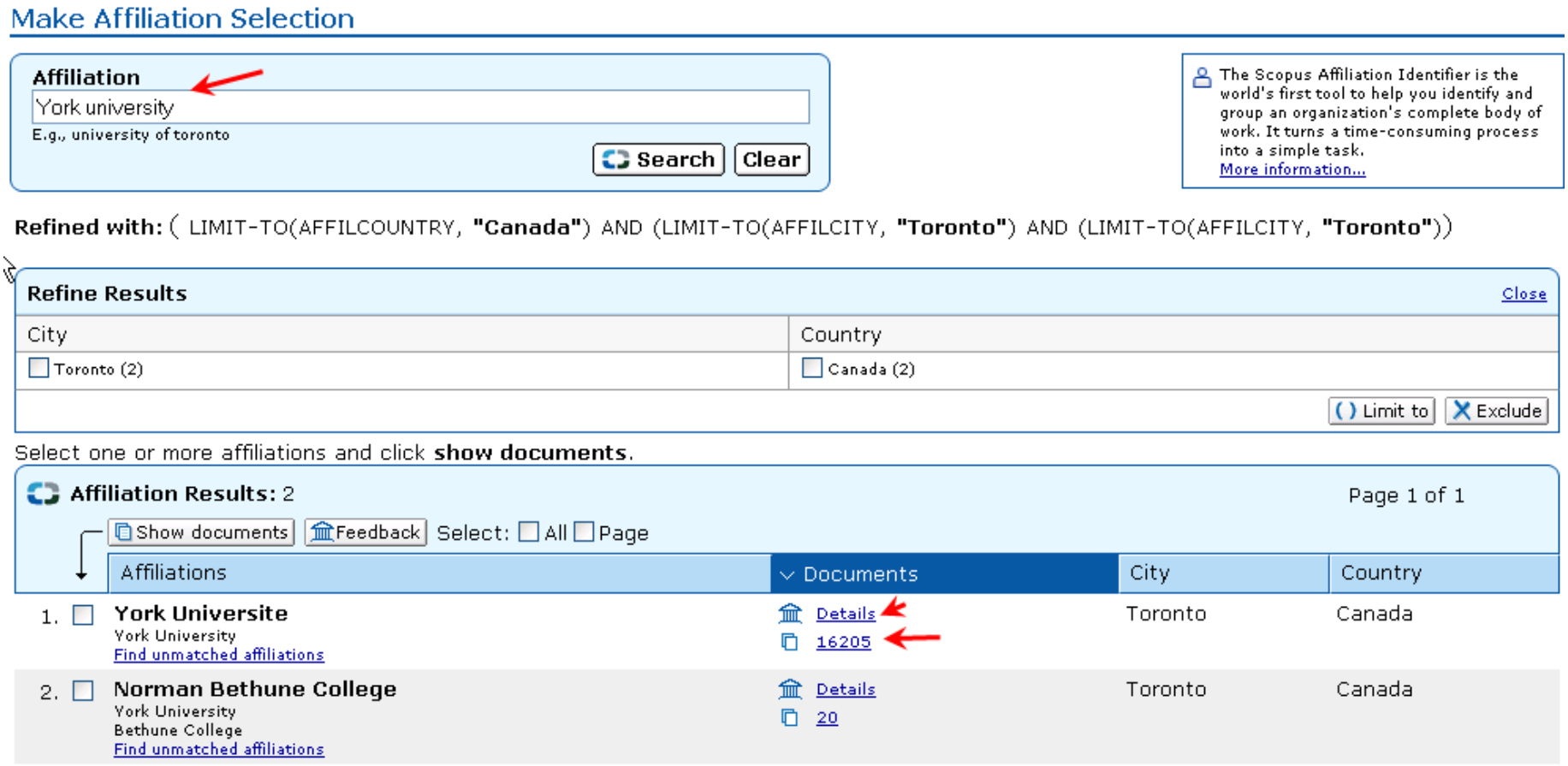
Subject Area: **Chemistry**.
Subject Category: **Organic Chemistry**.
Year: **2007**.

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

Scopus: Affiliation Search



Scopus: Research Outputs

Name variants	**York University**

Research

Documents	16,205 Add to list E-mail alert |
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
	More...

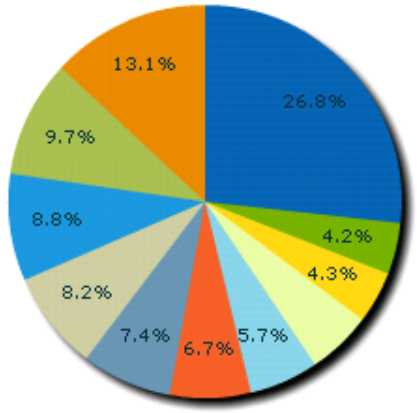
⊞ Find unmatched affiliations

Collaborating Affiliations

Affiliation Name	Documents
University of Toronto	1,110
McGill University	242
The University of British Columbia	208
McMaster University	202
University of Alberta	176

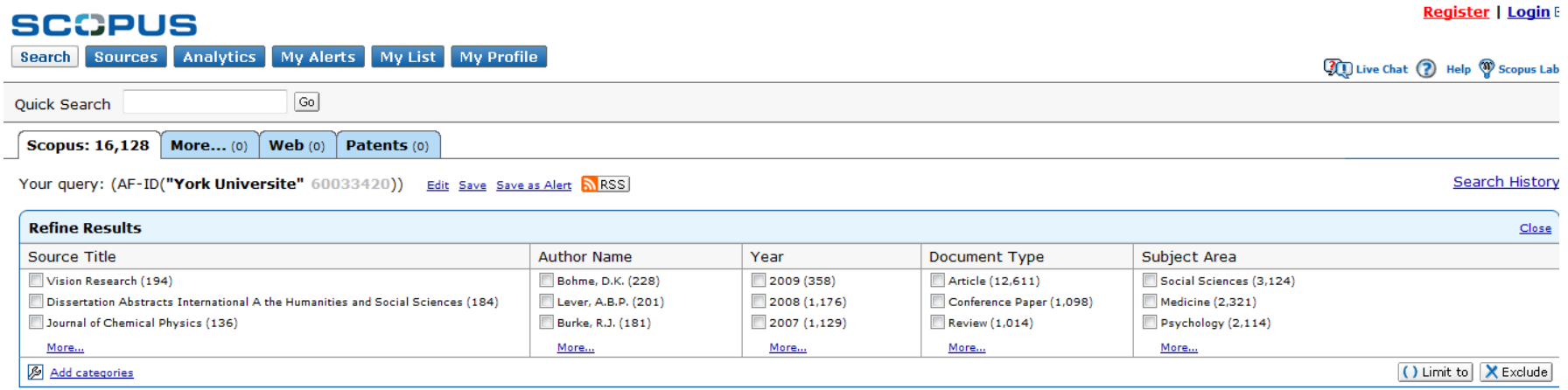
More...

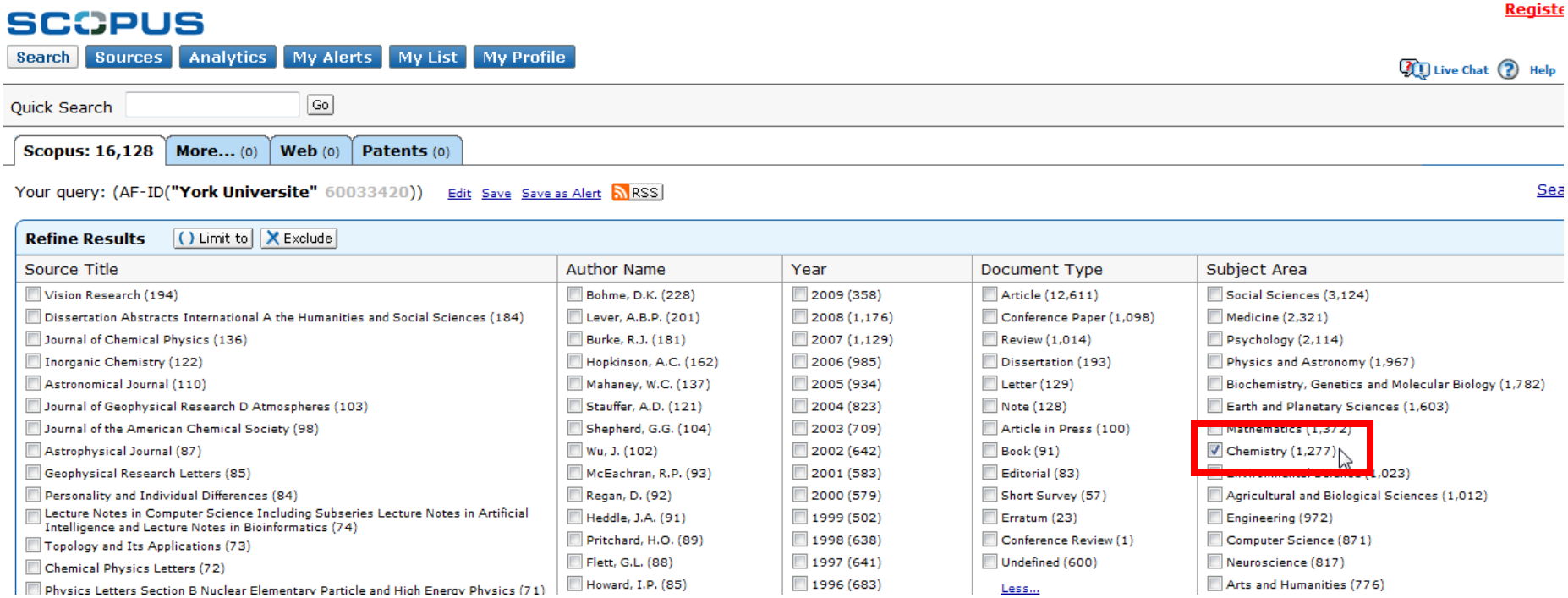
Subject Areas Chart | Data



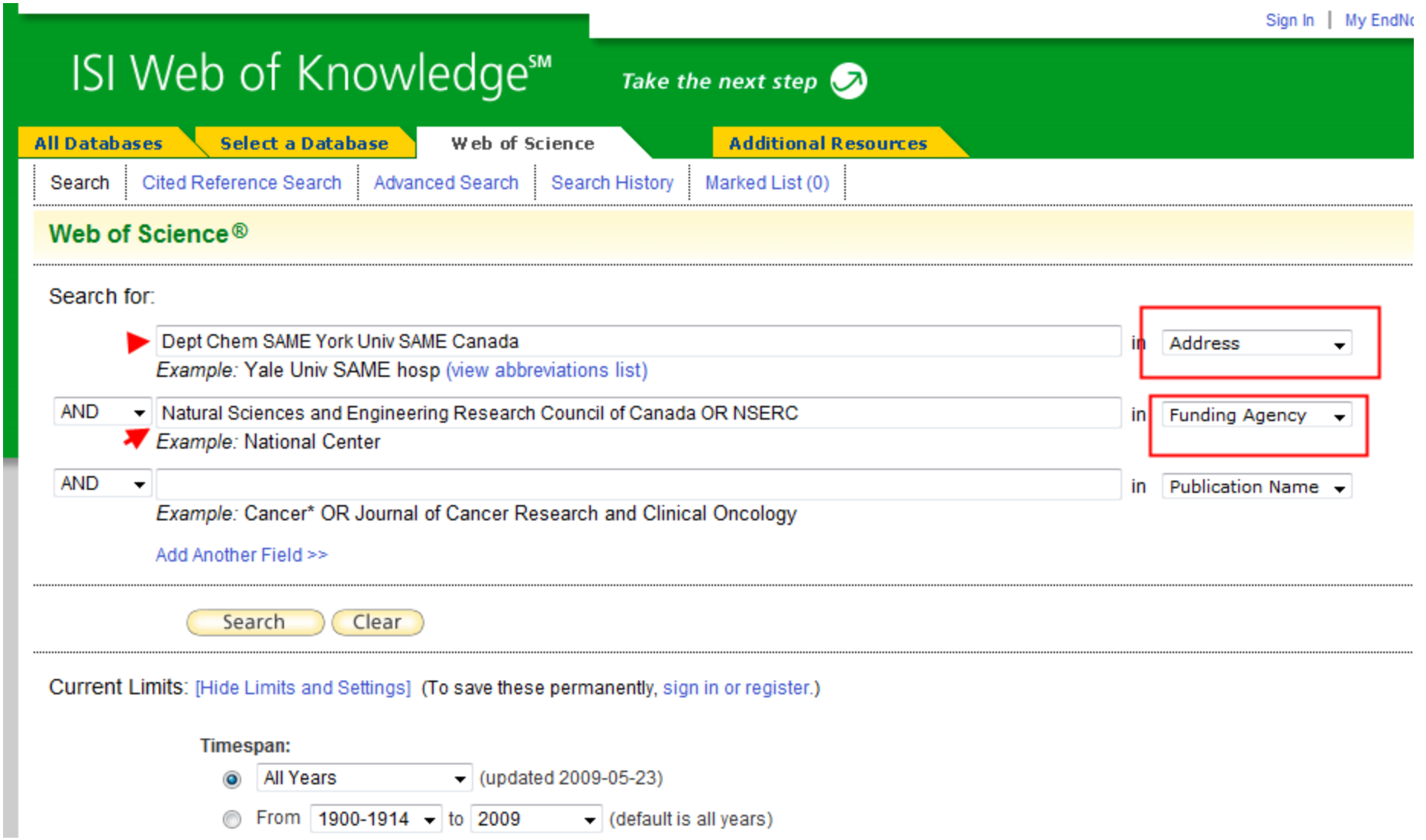
- Social Sciences
- Medicine
- Psychology
- Physics and Astronomy
- Biochemistry, Genetics and ...
- Earth and Planetary Sciences
- Mathematics
- Chemistry
- Environmental Science

Scopus : Subject search





WoS: Departmental Search



Tandem mass spectrometry and multiple reaction monitoring using an atmospheric pressur quadrupole mass spectrometer for product identification in atmospherically important reacti

Find it York | Print | E-mail | Add to Marked List | Save to EndNote

Author(s): Auld J (Auld, Janeen), Hastie DR (Hastie, Donald R.)[1]

Source: INTERNATIONAL JOURNAL OF MASS SPECTROMETRY **Volume:** 282 **Issue:** 3 **Pages:** 91-98 **Published:** MAY 1 20

Times Cited: 0 **References:** 22 Citation Map

Abstract: An atmospheric pressure chemical ionization triple quadrupole mass spectrometer has been Coupled to a smog chambe hydrocarbon oxidation reactions. Traditional MS and MS/MS scan modes were used to identify ion signals arising from possible reac was used to follow a number of these as target -> fragment ion pairs over the course of the reaction. Mechanistic information has bee signals. MRM profiling has allowed the identification of interferences that occur due to isobaric ions resulting from the formation of isc undetectable using the MS and MS/MS modes. Differences in product formation rate results in variations of their MRM ion pair onset a observed. This method was tested during a Study of the products of the HO radical oxidation of P-pinene. The oxidation product pinak interferences at its (M+H)(+), m/z 139. being more accurately monitored using its (M+H+H2O)(+) cluster ion pairs, 157 -> 139 and 157 ion pair 157 -> 111 has lead to the identification of a More highly oxidized acid-aldehyde product. It has been determined that an orga dependence relative to pinaketone cannot be the expected simple C10 hydroxynitrate product but rather a more highly oxidized C9 nitr reaction time has proven to be a valuable addition to existing mass spectrometric acquisition modes for reaction product determinati

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&(H2O)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

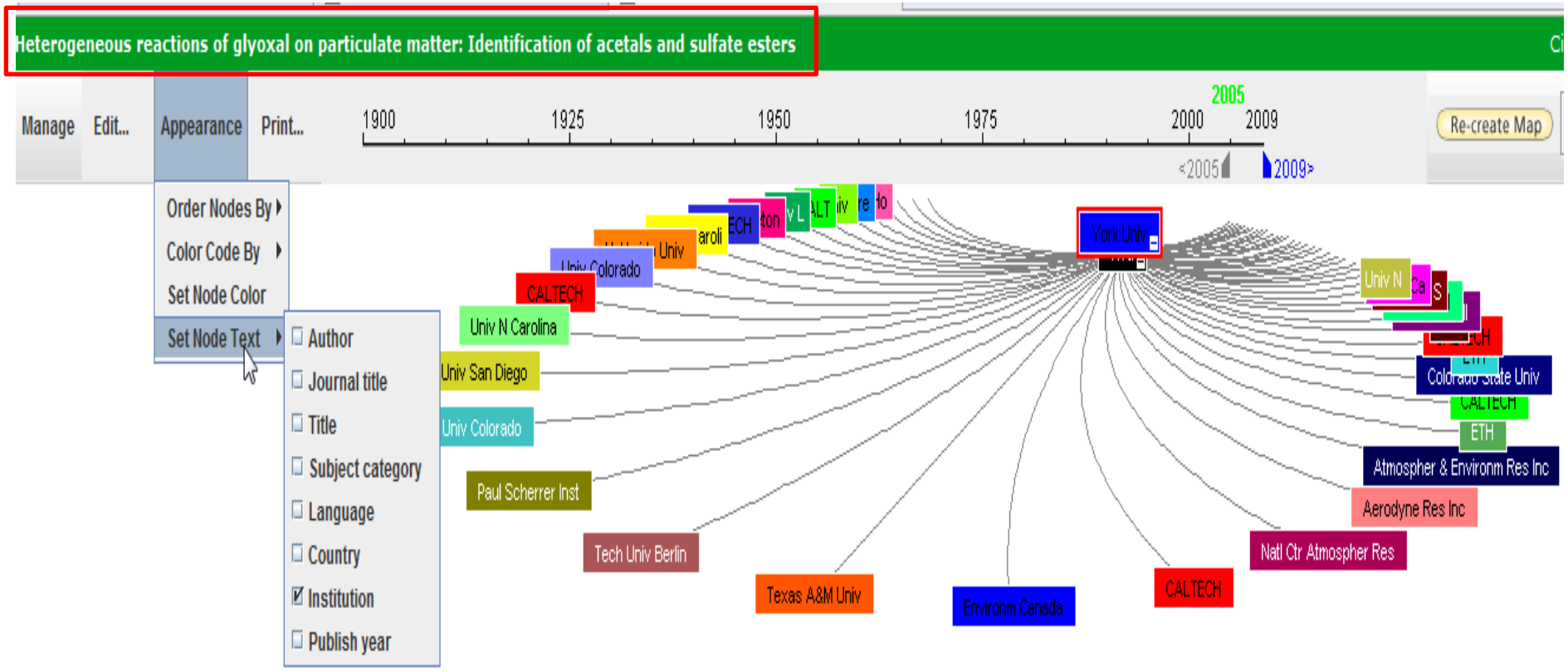
E-mail Addresses: Hastie@Yorku.ca

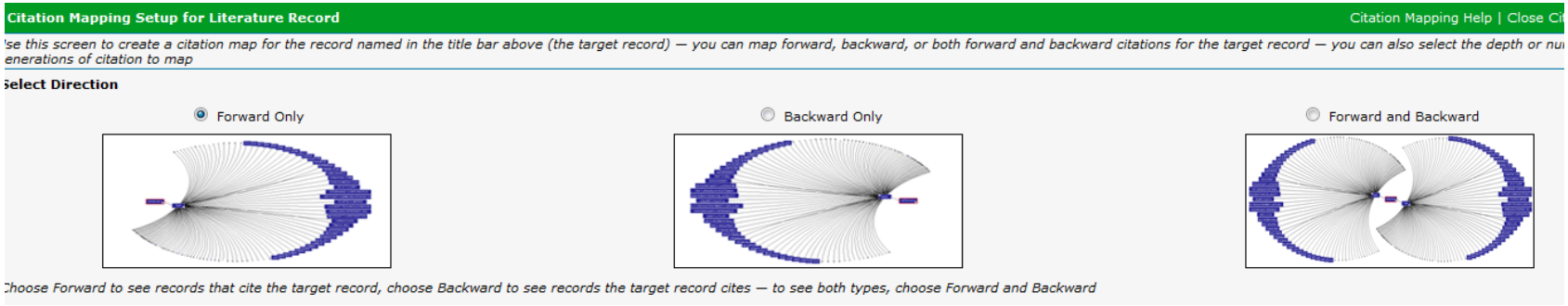
Funding Acknowledgement:

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

FUNDING AGENCIES WoS

Citation Mapper: Sort by University





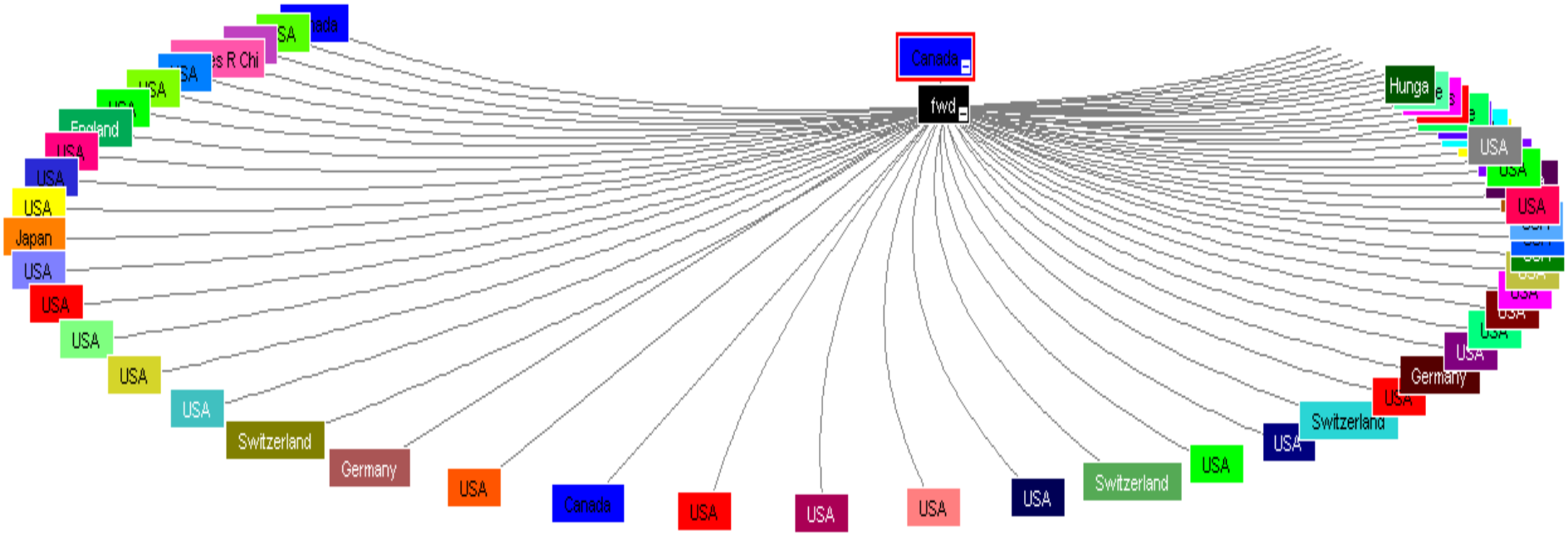
Record details for the nodes are displayed below (double-click a node to show its details). Click a checkbox below to locate that node above.

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 › » Display 10 Records per page

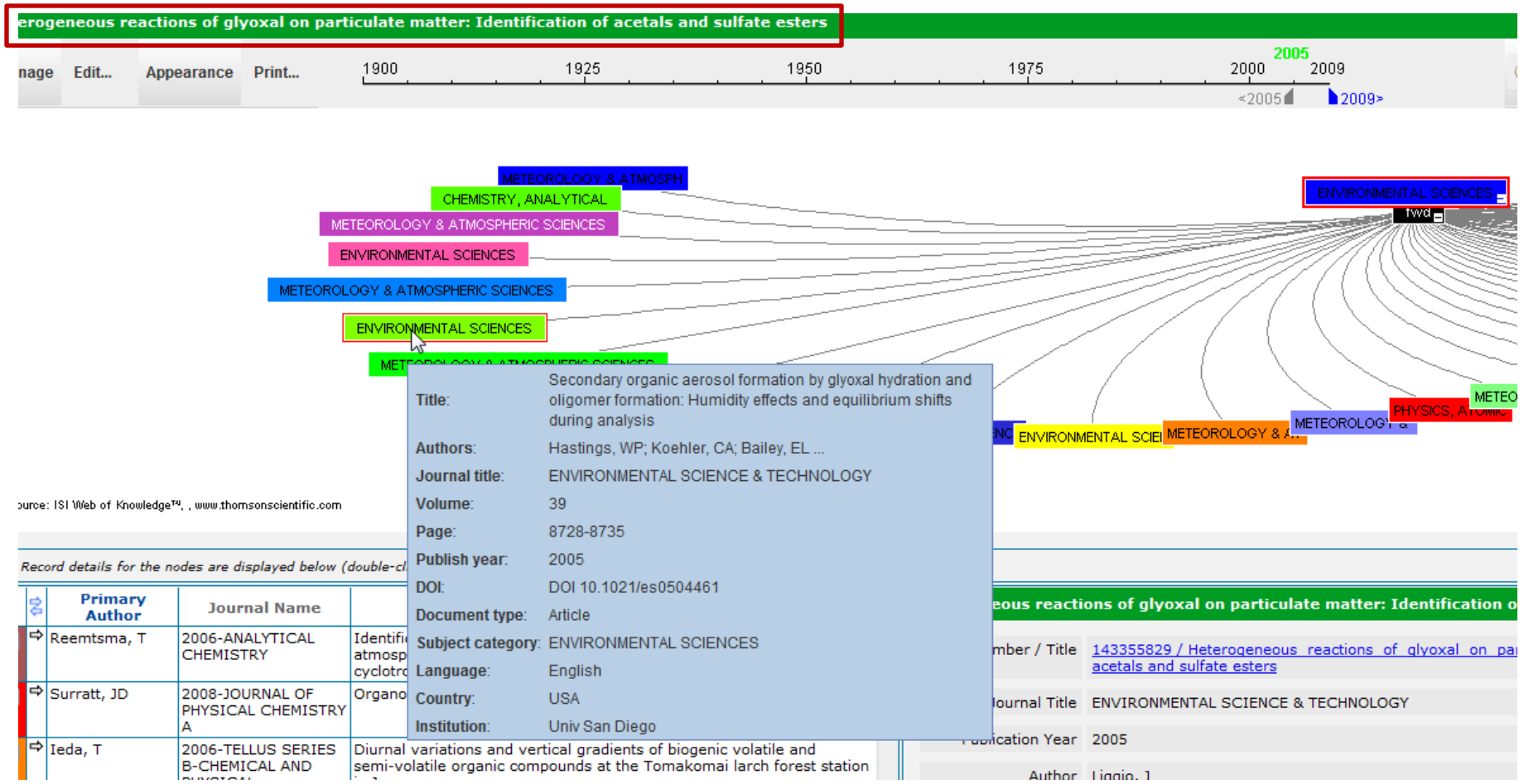
Heterogeneous reactions of glyoxal on particulate matter: Identification of acetals and sulfate esters

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
Group Author	
Source	ENVIRON SCI TECHNOL



Citation Mapper: Sort by Country

WoS: Mapper: By subject



WoS: Research Outputs

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

Rank the records by this field:	Analyze:	Set displa
Language Publication Year Source Title Subject Area	Up to 500 records.	Show the top 25 results. Minimum record count (threshold): 2

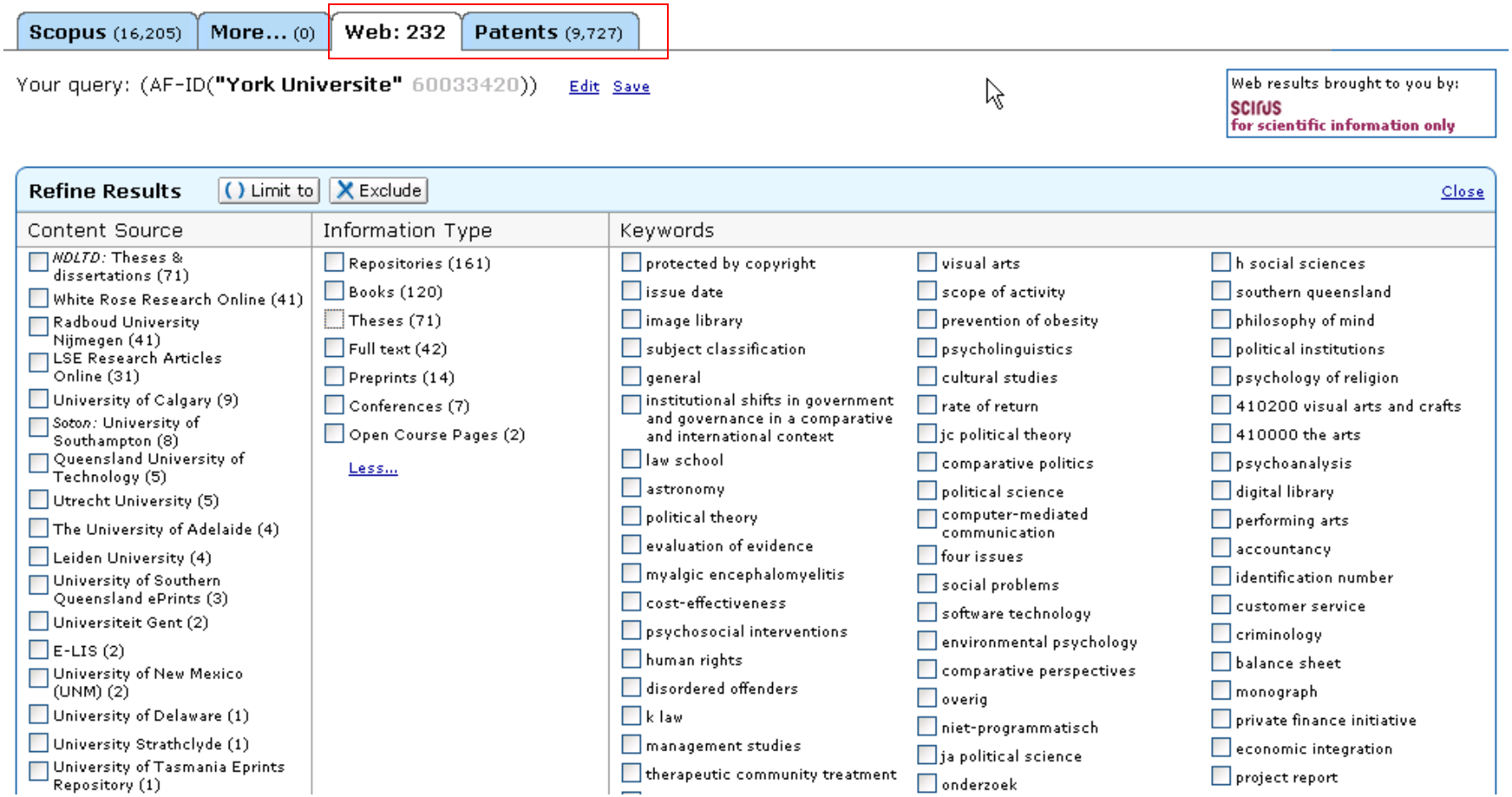
Analyze

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.

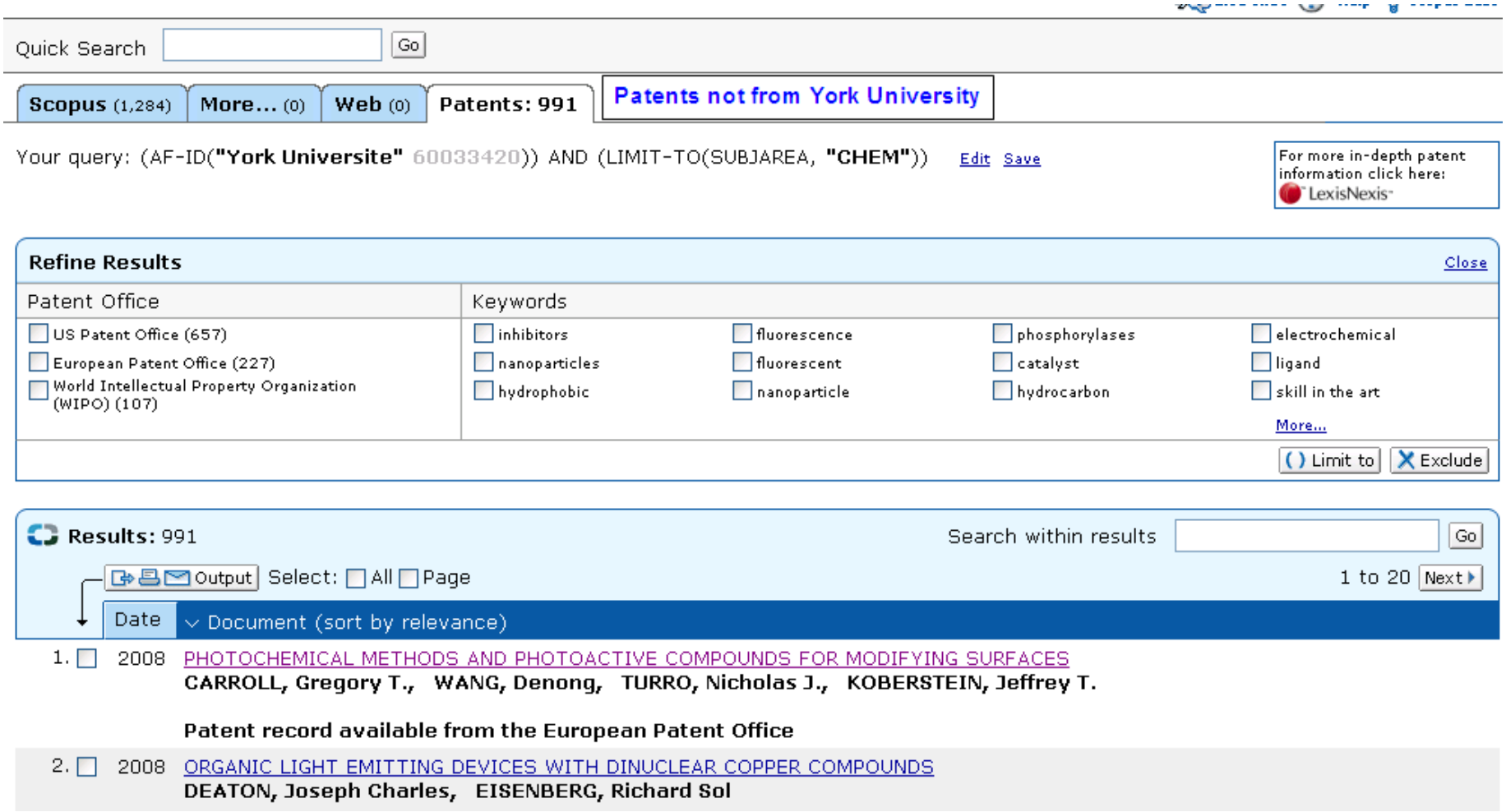
View Records | Exclude Records | Save Analysis Data to File

Field: Subject Area	Record Count	% of 500	Bar Chart
CHEMISTRY, PHYSICAL	117	23.4000 %	
PHYSICS, ATOMIC, MOLECULAR & CHEMICAL	114	22.8000 %	
CHEMISTRY, MULTIDISCIPLINARY	91	18.2000 %	
CHEMISTRY, ANALYTICAL	68	13.6000 %	
CHEMISTRY, INORGANIC & NUCLEAR	61	12.2000 %	
SPECTROSCOPY	60	12.0000 %	
CHEMISTRY, ORGANIC	46	9.2000 %	
METEOROLOGY & ATMOSPHERIC SCIENCES	27	5.4000 %	
BIOCHEMICAL RESEARCH METHODS	24	4.8000 %	
BIOCHEMISTRY & MOLECULAR BIOLOGY	19	3.8000 %	
ENVIRONMENTAL SCIENCES	12	2.4000 %	
CRYSTALLOGRAPHY	11	2.2000 %	
CHEMISTRY, APPLIED	10	2.0000 %	
GEOSCIENCES, MULTIDISCIPLINARY	8	1.6000 %	
CELL BIOLOGY	7	1.4000 %	

Scopus: Extra Coverage



Scopus Patent Coverage



WoS: Clarity required

<< Back to results list ◄ Record 9 of 555 ►

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-, H2O, NCS-)

Find it York | Print | E-mail | Add to Marked List | Save to EndNote Web | Save to EndNote, RefMan, ProCite | more options

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

Who is from York?

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)(H2O)(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(-1) in DMF solution and shows onset of weak and broad emission signals above 11100 cm(-1), 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 CO2H 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 TIO2; 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:
1. Swiss Fed Inst Technol, Inst Phys Chem, Lab Photon & Interfaces, CH-1015 Lausanne, Switzerland
2. York Univ, Dept Chem, Toronto, ON M3J 1P3 Canada ◄

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

Subject Category: Chemistry, Inorganic & Nuclear

IDS Number: 365AL

ISSN: 0010-8545

View at Publisher | Find it York

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

Krylova, S.M.[a], Musheev, M.[a], Nutiu, R.[b], Li, Y.[b], Lee, G.[c], Krylov, S.N.[a]

[a] Department of Chemistry, York University, Toronto, Ont. M3J 1P3, Canada
[b] Depts. of Biochemistry and Chemistry, McMaster University, Hamilton, Ont. L8N 3Z5, Canada
[c] 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

English

SCOPUS

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

Medline is the source for the MeSH terms of this document.

Keywords

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

Find it York | Print | E-mail | Add to Marked List | Save to EndNote Web | Save to EndNote, RefMan, ProC

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 dou 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. Th facilitated by using two kinetic capillary electrophoresis methods: (i) non-equilibrium capillary electrophoresis of equilibrium mixtures (NECEEM); (ii) affinity-mediate 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 fashio determined the equilibrium dissociation constants for all tau-DNA complexes studied. (C) 2005 Federation of European Biochemical Societies. Published by Elsevie reserved.

Document Type: Article

Language: English

ISI Web of Knowledge℠

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

Web of Science: Abbreviated Author names

Subject: Re: [PAMNET] web of science
From: "Davidoff, Gary N." <gdavidoff@anl.gov>
Sender: PAMnet
Reply-To: "Davidoff, Gary N." <gdavidoff@anl.gov>
Date: 28/04/2009 1:31 PM
To: PAMNET@LISTSERV.ND.EDU

Subject: web of science

Recently one of my faculty members asked for help locating some of his "lost" articles. We discovered that his name was spelled incorrectly in 19 articles.

Some database vendors are happy to receive notification of an error and fix the problem in a timely matter.

The response that I got from Web of Science: "Due to our editorial policy we are not currently able to make any updates based on the data change that you requested."

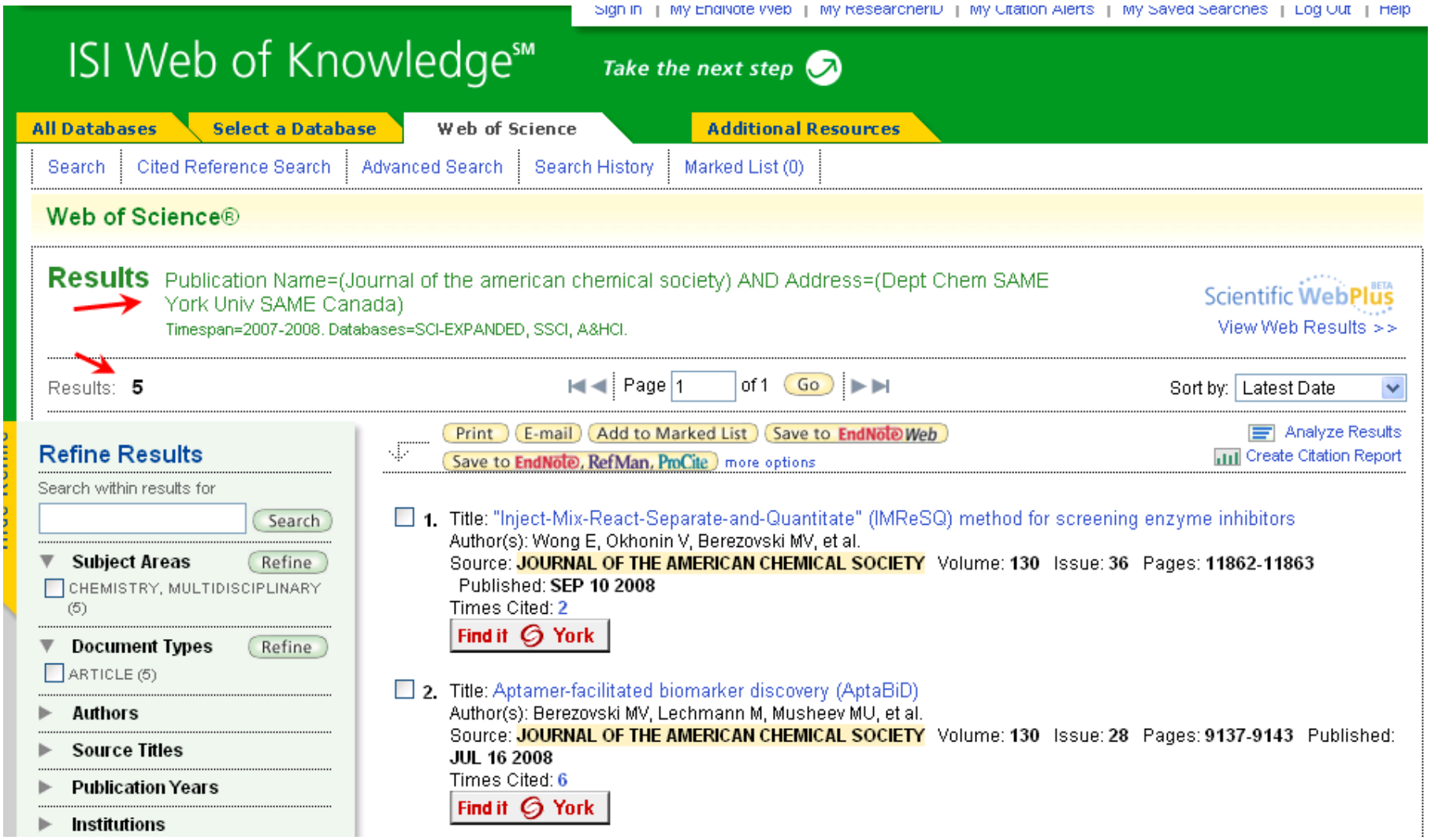
The question becomes do we want to support a system that has that attitude?!

Cheers,

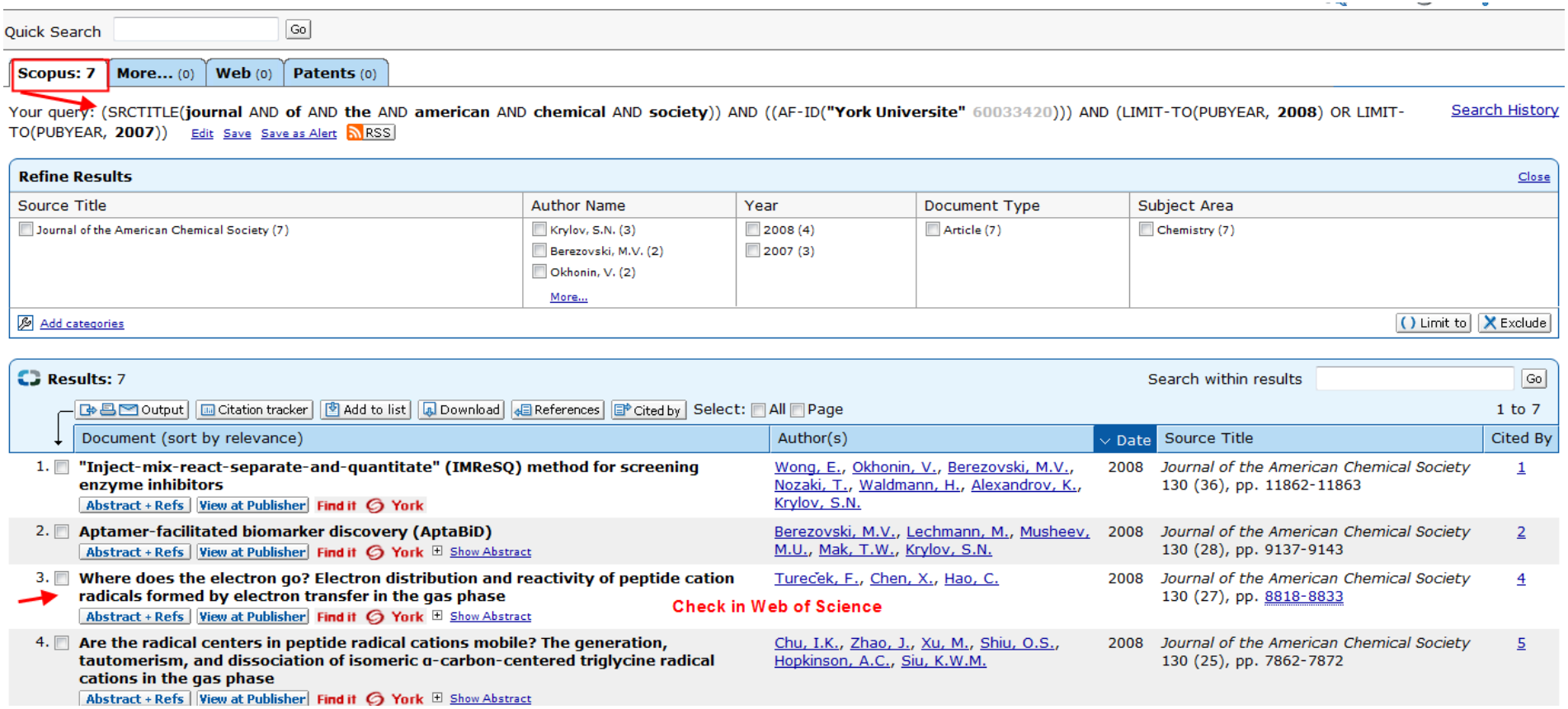
--

Physics & Astronomy Librarian Edna McConnell Clark
Physical Sciences Library Clark Hall Cornell University Ithaca, NY
14853-2501
Voice: 607-255-0067

JACS 2007 & 2008 in WoS



JACS 2007 & 2008 in Scopus



Quick Search Go

Scopus: 7 | More... (0) | Web (0) | Patents (0)

Your query: (SRCTITLE(**journal** AND **of** AND **the** AND **american** AND **chemical** AND **society**)) AND ((AF-ID("**York Universite**" 60033420))) AND (LIMIT-TO(PUBYEAR, **2008**) OR LIMIT-TO(PUBYEAR, **2007**)) Edit Save Save as Alert RSS Search History

Refine Results Close

Source Title	Author Name	Year	Document Type	Subject Area
Journal of the American Chemical Society (7)	Krylov, S.N. (3) Berezovski, M.V. (2) Okhonin, V. (2) More...	2008 (4) 2007 (3)	Article (7)	Chemistry (7)

Add categories Limit to Exclude

Results: 7 Search within results Go

Output | Citation tracker | Add to list | Download | References | Cited by | Select: All Page 1 to 7

Document (sort by relevance)	Author(s)	Date	Source Title	Cited By
1. **"Inject-mix-react-separate-and-quantitate" (IMReSQ) method for screening enzyme inhibitors** Abstract + Refs | View at Publisher | Find it York	Wong, E., Okhonin, V., Berezovski, M.V., Nozaki, T., Waldmann, H., Alexandrov, K., Krylov, S.N.	2008	*Journal of the American Chemical Society* 130 (36), pp. 11862-11863	1
2. **Aptamer-facilitated biomarker discovery (AptaBiD)** Abstract + Refs | View at Publisher | Find it York | Show Abstract	Berezovski, M.V., Lechmann, M., Musheev, M.U., Mak, T.W., Krylov, S.N.	2008	*Journal of the American Chemical Society* 130 (28), pp. 9137-9143	2
3. **Where does the electron go? Electron distribution and reactivity of peptide cation radicals formed by electron transfer in the gas phase** Abstract + Refs | View at Publisher | Find it York | Show Abstract	Turečček, F., Chen, X., Hao, C.	2008	*Journal of the American Chemical Society* 130 (27), pp. 8818-8833	4
4. **Are the radical centers in peptide radical cations mobile? The generation, tautomerism, and dissociation of isomeric α-carbon-centered triglycine radical cations in the gas phase** Abstract + Refs | View at Publisher | Find it York | Show Abstract	Chu, I.K., Zhao, J., Xu, M., Shiu, O.S., Hopkinson, A.C., Siu, K.W.M.	2008	*Journal of the American Chemical Society* 130 (25), pp. 7862-7872	5

Check in Web of Science

Scopus – Same last name?

View at Publisher | Find it York

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

Tureček, F.[a], Chen, X.[a b], Hao, C.[a c]

[a] Department of Chemistry, Bagley Hall, University of Washington, Seattle, WA 98195-1700, United States
[b] National Institutes of Health (NIH), 9000 Rockville Pike, Bethesda, MD 20892, United States
[c] **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 ur transfer and competitive dissociations by loss of H atoms, ammonia, and N-C_α bond cleavage in the gas phase. Doubly $(KK + 2H)^{2+}$, are each calculated to exist as two major conformers in the gas phase. Electron transfer to conformers v 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 of unpaired electron de
group in the peptide ca
attachment to ion conf
group forming dihydroxy
involving reversible prot
Lys c^+ fragments from
cleavage. This emphasi
capture. © 2008 Ameri

Make Author Selection

Author Last Name	Initials or First Name	
Hao (E.g., smith)	cunsheng (E.g., j.l.)	Show exact matches only

Affiliation (E.g., university of toronto)

Search | Clear

A link t
authors
Scopus
may no
than on
same a
More in

References (95) view in tab

Refine Results

Source Title	Affiliation	City	Country	Subject Area
Analytical Chemistry (1)	York Universite (1)	Toronto (1)	Canada (1)	Chemistry (1)

Select one or more authors and click **show documents** or **citation tracker**.

Author Results: 1

Show documents | Citation tracker | Feedback | Select: All Page

	Authors	Documents	Subject Area	Affiliation (most recent)	City	Country
1.	**Hao, Cunsheng**	1	Chemistry	York Universite	Toronto	Canada

Hide Last Title

Most recent document title:
Gas chromatographic detector for selective and sensitive detection of atmospheric organic nitrates

Show documents | Citation tracker | Feedback | Select: All Page

Web of Science - Results

Web of Science®

<< Back to results list ◄ Record 1 of 27 ►

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

Find it York | Print | E-mail | Add to Marked List | Save to EndNote Web | Save to EndNote, RefMan, ProCite | more options

Author(s): Turecek F (Turecek, Frantisek)[1], Chen XH (Chen, Xiaohong)[1], Hao CT (Hao, Changtong)[1]

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:
1. Univ Washington, Dept Chem, Seattle, WA 98195 USA

E-mail Addresses: turecek@chem.washington.edu

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

Subject Category: Chemistry, Multidisciplinary

Scopus Author Affiliation

Refine Results

Source Title	Affiliation	City	Country	Subject Area
Journal of the American Chemical Society (2)	Academia Sinica Taiwan (2)	Nankang (2)	United States (4)	Chemistry (3)
Nanotechnology (1)	York Universite (2)	Beijing (2)	Canada (3)	Engineering (3)
Materials and Manufacturing Processes (1)	Chinese Academy of Sciences (2)	New York (2)	China (2)	Biochemistry, Genetics and Mole
More...	More...	More...	More...	More...

Select one or more authors and click **show documents** or **citation tracker**.

Author Results: 5

Show documents | Citation tracker | Feedback | Select: All Page

	Authors	Documents	Subject Area	Affiliation (most recent)	City
1.	**Hao, Changtong**	Details 10 Show Last Title	Chemistry	University of Washington	Seattle
2.	**Hao, Cunsheng**	1 Show Last Title	Chemistry	York Universite	Toronto
3.	**Hao, Jingcheng Cheng** Hao, J. Hao, Jing Cheng Hao, Jingcheng	Details 103 Show Last Title	Chemistry; Materials Science; Chemical Engineering; ...	Lanzhou Institute of Chemical Physics Chinese Academy of Sciences	Lanzhou
4.	**Hao, Steven C.** Hao, Steven	Details 26 Show Last Title	Medicine; Biochemistry, Genetics and Molecular Biology; Nursing; ...	Yale University	New Haven
5.	**Hao, Zhang Cheng** Hao, Z. C. Hao, Z. Hao, ZHANG	Details 75 Show Last Title	Engineering; Computer Science; Materials Science; ...	Nanjing Forestry University	Nanjing

Not from York U

Another Author: from Munich Univ.

All Databases | Select a Database | Web of Science | Additional Resources

Search | Cited Reference Search | Advanced Search | Search History | Marked List (0)

Web of Science®

<< Back to results list ◄ Record 1 of 1 ►

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

Find it York | Print | E-mail | Add to Marked List | Save to EndNote Web | Save to EndNote, RefMan, ProCite | more options

Author(s): Siu CK (Siu, Chi-Kit), Balaj OP (Balaj, O. Petru), Bondybey VE (Bondybey, Vladimir E.), Beyer MK (Beyer, Martin K.)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 129 **Issue:** 11 **Pages:** 3238-3246 **Published:** MAR 21 2007

Times Cited: 2 **References:** 90 Citation Map

Abstract: The reactions of water cluster anions (H2O)(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 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 H2O, yielding mixed clusters Cl-(HCl)(m)(H2O)(n) until they are saturated with HCl. Those saturated clusters lose H2O 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)(H2O)(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.

Document Type: Article

Language: English

KeyWords Plus: HYDRATED ELECTRON CLUSTERS; NEGATIVELY CHARGED WATER; INITIO MOLECULAR-DYNAMICS; TOTAL-ENERGY CALCULATIONS; WAVE BASIS-SET; H ATOMS; UNIMOLECULAR DISSOCIATION; VIBRATIONAL SPECTROSCOPY; RATE CONSTANTS; PHOTOELECTRON-SPECTROSCOPY

Reprint Address: Beyer, MK (reprint author), Tech Univ Munich, Dept Chem, Lichtenbergstr 4, D-85747 Garching, Germany

Addresses:
1. Tech Univ Munich, Dept Chem, D-85747 Garching, Germany

E-mail Addresses: martin.beyer@mail.chem.tu-berlin.de

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

Subject Category: Chemistry, Multidisciplinary

IDS Number: 145WQ

Author not from York U

Quick Search Go

Journal of the American Chemical Society
Volume 129, Issue 11, 21 March 2007, Pages 3238-3246

DOI: 10.1021/ja067355o
Document Type: Article

Output Bookmark

View at Publisher Find it York

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

Siu, C.-K.[a b], Balaj, O.P.[a c], Bondybey, V.E.[a], Beyer, M.K.[a d]

[a] Department Chemie, Physikalische Chemie 2, Technische Universität München, Lichtenbergstrasse 4, 85747 Garching, Germany
[b] **Department of Chemistry, Centre for Research in Mass Spectrometry, York University, 4700 Keele Street, Toronto, Ont. M3J1P3, Canada**
[c] Ecole Polytechnique, Departement de Chimie, Laboratoire DCMR, Route de Saclay, 91128 Palaiseau Cedex, France
[d] Institut für Chemie, Technische Universität Berlin, Strasse des 17, 10623 Berlin, Germany

Abstract

The reactions of water cluster anions $(H_2O)_n^-$, n = 30-70, with hydrogen chloride have been studied by Fourier transform ion cyclotron resonance (spectrometry. The first HCl taken up by the clusters is presumably ionically dissolved. The solvated electron recombines with the proton, which is t 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 H_2O, yielding mixed clusters $Cl^-(HCl)_m(H_2O)_n$ until they are saturated with HCl. Those saturated clusters 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 t The $Cl^-(HCl)_4(H_2O)_6$ cluster represents an example for supramolecular self-organization in the gas phase: it consists of a tetrahedral $Cl^-(HCl)_4$, conn of the tetrahedron to a compact water hexamer. © 2007 American Chemical Society.