

# Snapshot of content, retrieval, and quality of some chemical information systems

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# **TECHNOLOGY DOES NOT IMPROVE CONTENT !**

- 1. Author name: bad CAS record**
- 2. Record is missing for a full paper in a core journal**
- 3. Records exist but cannot be retrieved**
- 4. Supplementary material not indexed (Beilstein)**
- 5. Indexing by CAS does not reflect keywords given by author**

# TECHNOLOGY DOES NOT IMPROVE CONTENT !

## Author name: bad CAS record

**Summary:** A paper authored by A. Stephen K. Hashmi (1) cannot be found in CAplus (2). The record has been accidentally located in a substance search by structure (3). The author's name is NOT **Hashimi** but **Hashmi**.

**Conclusion:** Publish or or perish? Better send your own publication list when applying for a job.

There are authors who change their initials in a random way. Authors as well as editors should be more watchful.

# EXAMPLE FOR AUTHOR NAME: BAD CAS RECORD (1/3)

*Wiley InterScience*

Journal für praktische Chemie Volume 342, Issue 1, 2000.

Pages: 40 51

**Mercury(II)-Catalyzed Synthesis of Spiro[4.5]deca-  
trienediones from Allenyl Ketones and Comparison  
with Silver(I)-, Palladium(II)- and Brønsted Acid-  
Catalyzed Reactions**

**Stephen K. Hashmi,  
Lothar Schwarz, J. W. Bats**



# EXAMPLE FOR AUTHOR NAME: BAD CAS RECORD (2/3)

*Aug 10, 2002*

Explored by Author in CAPLUS.

Hashmi

Selected 7 of 103 candidates

<b>HASHMI A</b>	<b>( 2 references)</b>	<b>-</b>
<b>HASHMI A S</b>	<b>( 5 references)</b>	<b>-</b>
<b>HASHMI A S K</b>	<b>( 3 references)</b>	<b>+</b>
<b>HASHMI A STEPHEN K</b>	<b>(42 references)</b>	<b>+</b>
<b>HASHMI STEPHAN</b>	<b>( 1 reference)</b>	<b>+</b>
<b>HASHMI STEPHEN</b>	<b>( 2 references)</b>	<b>+</b>
<b>HASHMI STEPHEN K</b>	<b>( 1 reference)</b>	<b>+</b>

**Analyze**

**Analyzed 56 of 56 by Author Name**

## EXAMPLE FOR AUTHOR NAME: BAD CAS RECORD (3/3)

*SFS Jul 25, 2002*

**Mercury(II)-catalyzed synthesis of spiro[4.5]deca-trienediones from allenyl ketones and comparison with silver(I)-, palladium(II)- and Bronsted acid-catalyzed reactions.**

**Hashimi, A. Stephen K.;**



Schwarz, Lothar; Bats, J. W.

Inst. Organische Chemie, Johann Wolfgang Goethe Univ., Frankfurt am Main, Germany. Journal fuer Praktische Chemie (2000), 342(1), 40-51.

**Citations:** 7) Hashimi, A; Tetrahedron Lett 1998, 39, 8969



# TECHNOLOGY DOES NOT IMPROVE CONTENT

## Record is missing for a full paper in a core journal

**Summary:** The full paper (9 pages) by Reiner Luckenbach in 1981 (when celebrating the centennial of BEILSTEIN's Handbook of Organic Chemistry" he was the director of the BEILSTEIN Institute) cannot be located in CPlus. The paper has been published in Angew. Chem., also available in the Int. Edit. in Engl., without doubt a core journal of chemistry (1). Author searches in CPlus and CA show 13% of the name entries to be wrong. CPlus results correctly in one more hit as does a search in CA (2,3). Two other search strategies (4,5) verify the absence of a record of the publication in question (1) which should have been in Section 20. *(Just for curiosity: note the accounts used when searching STN/MESSENGER : They are still in use).*

**Conclusion:** How much is really missed in CA/CPlus? Tell CAS, if you have examples. Ask them to correct. CAS does correct! Authors should always check if the records of their publications are searchable in CPlus. If they know indexing rules they should even check the indexing. Are all substances registered and is the stereochemistry correct? Learn from indexing on how to write your abstract.

**Ist kritische Sichtung und Bewertung naturwissenschaftlicher Untersuchungsergebnisse ohne Informationsverlust möglich?**

**Von Reiner Luckenbach,  
Reinhard Ecker und Josef Sunkel**

***Angew. Chem.*93, 876-885 (1981) ←**

**Volume Author Index shows: [I.E. 841] ←**



# RECORD IS MISSING FOR A FULL PAPER IN A CORE JOURNAL (2/5)

*Jul 26, 2002*

Explored by Author in **CAPLUS**.

luckenbach, r

Selected 5 of 9 candidates

<b>LUCHENBACH REINER</b>	<b>( 1 reference)</b>	<b>←</b>	<b>+</b>
LUCKENBACH R	(40 references)	←	+
LUCKENBACH REINER	(46 references)	←	+
<b>LUCKENBACK R</b>	<b>( 5 references)</b>	<b>←</b>	<b>+</b>
<b>LUCKENBACK REINER</b>	<b>( 6 references)</b>	<b>←</b>	<b>+</b>

Analyzed 98 of 98 by Journal Name **←**

Actual. Chim. 1

Beilstein Syst. 1

Book of Abstracts, 210th ACS Nat.Meeting... 1

Chem. Ber. ....

# RECORD IS MISSING FOR A FULL PAPER IN A CORE JOURNAL (3/5)

Welcome to STN International! Enter x:z

LOGINID:ssscol03



**FILE 'CA' ENTERED ON 08 AUG 2002**

<b>L1</b>	<b>1 S LUCHENBACH REINER/AU</b>	<b>+</b>
L2	39 S LUCKENBACH R/AU	+
L3	46 S LUCKENBACH REINER/AU	+
L4	5 S LUCKENBACK R/AU	+
<b>L5</b>	<b>6 S LUCKENBACK REINER/AU</b>	<b>+</b>
<b>L6</b>	<b>97 S L1-5</b>	<b>←</b>

## RECORD IS MISSING FOR A FULL PAPER IN A CORE JOURNAL (4/5)

*Jul 26, 2002*

Explored by Author in CAPLUS.

luckenbach, r

Selected 5 of 9 candidates

Refine by Document Type started

Analyzed 48 of 48 by Publication Year

Selected 1981 (3 references) ← shown below

**Straightforward procedure for locating chemical compounds in the Beilstein Handbook.** J. Chem. Educ. (1981), 58(12), 982-6

**The Beilstein Handbook of Organic Chemistry: the first hundred years.** J. Chem. Inf. Comput. Sci. (1981), 21(2), ...

**Do you know Beilstein?** Chem. Unserer Zeit (1981), 15(2), 47-51.

# RECORD IS MISSING FOR A FULL PAPER IN A CORE JOURNAL (5/5)

Welcome to STN International! Enter x:z

LOGINID: sssunv01 ←

=> file caplus

=> s (angew? chem?)/so and 1981/py

39273 ANGEW?/SO

2420355 CHEM?/SO

28146 (ANGEW? CHEM?)/SO

((ANGEW?(W)CHEM?)/SO)

508024 1981/PY

L1 377 (ANGEW? CHEM?)/SO AND 1981/PY

=> s l1 and luckenba?/au

293 LUCKENBA?/AU

L2 0 L1 AND LUCKENBA?/AU ← !

# TECHNOLOGY DOES NOT IMPROVE CONTENT !

## Records exist but cannot be retrieved

**Summary:** This concerns searching by research topics with SFS as well as searches with STN/MESSENGER. There are 18 papers indexed for flourescence only but not for fluorescence. At present the newest one is from 2001.

For the records relating to “Abstracts of Papers” of the ACS meetings the authors themselves may be responsible if they used the electronic submission. By the way: Not all records have a CODEN assigned.

***Conclusion:*** Since electronic submission of papers will become the standard procedure, authors should be aware that mistakes they make when typing are documented. Don't forget: *proofreading the old way is gone!*

## RECORDS EXIST BUT CANNOT BE RETRIEVED (1/2)

*Sat Aug 3, 2002*

“flourescence not fluorescence”

2 Research Topic candidates were identified in CAPLUS  
using the phrase "flourescence not fluorescence"

18 references were found containing the concept

"flourescence", but not containing the concept "fluorescence". ←

**The synergistic antioxidative effect of ascorbyl 2-phosphate and alpha-tocopheryl acetate.**

Jentzsch, Axel; Streicher, Harald; Engelhart, Karin.

BASF Aktiengesellschaft, Ludwigshafen, Germany.

Cosmetics & Toiletries (2001), 116(6), 55-58,60,62,64.

**Abstract** ... a human keratinocyte cell line and a flourescencebased assay system.

## RECORDS EXIST BUT CANNOT BE RETRIEVED (2/2)

*Aug 3, 2002*

18 references were found containing the concept "flourescence", but not containing the concept "fluorescence".

Abstracts of Papers, **222**nd ACS National Meeting, Chicago, IL, United States, August 26 - 30, 2001 (2001), Publisher: American Chemical Society

**Also: 222nd, 217th, 215th ,210th**



# TECHNOLOGY DOES NOT IMPROVE CONTENT !

## Supplementary material not indexed

### Part 1-Beilstein

**Summary:** Dr. R. Siegfried (Ruhr University Bochum, DE) had been interested in data of the compound shown on the Xfire Beilstein record (16); 2 references attached to (2;3). Field Availability (4) shows data available only for reactions and NMR (5). Reference/Citation 1 not 2 is linked to NMR data (5, 2).

**Conclusion:** If spectroscopical and reaction data are given I would in principle expect more physical data. What happened?

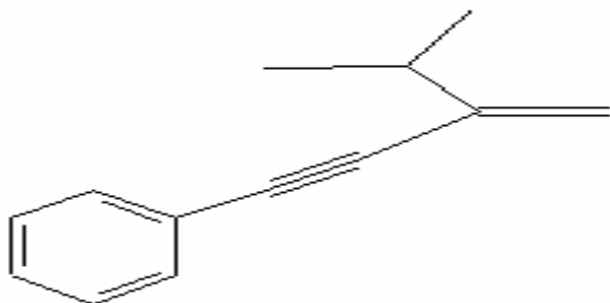


## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (1/11)

*XfireBeilstein*

Substance BRN ([3537493](#))

<b>Chemical Name</b>	<b>2-Isopropyl-4-phenyl-1-buten-3-yne</b>
<b>Autoname</b>	<b>(3-isopropyl-but-3-en-1-ynyl)-benzene</b>
<b>Molecular Formula</b>	<b>C<sub>13</sub>H<sub>14</sub></b>
<b>Lawson Number</b>	<b>4364</b>
<b>Beilstein Reference</b>	<b>6-05</b>
<b>Entry Date</b>	<b>1991/10/23</b>
<b>Update Date</b>	<b>2000/10/23</b>



## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (2/11)

*XfireBeilstein*                      Substance                      BRN ([3537493](#))

<b>Chemical Name</b>	<b>2-Isopropyl-4-phenyl-1-buten-3-yne</b>
<b>Beilstein Registry Number</b>	<a href="#">3537493</a>

Reference (1 of 2)                      Citation Number                      [5508114](#)

<b>Authors</b>	<b>Kuznetsov, M. A.; Semenovskii, V. V; Belov, V. N.; Gindin, V. A</b>
<b>CODEN</b>	<b>CHCCAL; KGSSAQ</b>
<b>Journal Title</b>	<b>Chem.Heterocycl.Compound.(Engl.Transl.); Khim.Geterotsikl.Soedin.</b>
<b>Language Code</b>	<b>EN; RU</b>
<b>(Series) Volume</b>	<b>25; 25    Number 2; 2    Publication Year 1989; 1989</b>
<b>Page</b>	<b>136-142; 173-179</b>

## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (3/11)

*XfireBeilstein*

Substance

BRN ([3537493](#))

Beilstein Registry Number	<a href="#">3537493</a>
Chemical Name	2-Isopropyl-4-phenyl-1-buten-3-yne
Page	136-142; 173-179

Reference (2 of 2)

Citation Number [6238400](#)

Citation Number	<a href="#">6238400</a>
Authors	Dash, Aswini K.; Eisen, Moris S.
CODEN	ORLEF7
Journal Title	Org.Lett.
Language Code	EN
(Series) Volume	2 Number 6
Number	6 Page 737 - 740
Publication Year	2000

## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (4/11)

*XfireBeilstein*

Substance BRN ([3537493](#))

Field Availability List 1-3 of 3: BRN [3537493](#) ←

Code	Field Name	Occ.
RX	Reaction	2
<b>NMR</b>	<b>Nuclear Magnetic Resonance</b>	<b>1</b> ←
CNR	Reference	2

## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (5/11)

*XfireBeilstein* Substance BRN ([3537493](#))

Nuclear Magnetic Resonance (1 of 1)

← No other data in  
BEILSTEIN!

Description	Chemical shifts
Nucleus	1H
Solvents	CDCl3
Citation Pointer	<a href="#">5508114</a> ; Journal; Kuznetsov, M. A.; Semenovskii, V. V; Belov, V. N.; Gindin, V. A; CHCCAL; Chem.Heterocycl.Compound.(Engl.Transl.); EN; 25; 2; 1989; 136-142; KGSSAQ; Khim.Geterotsikl.Soedin.; RU; 25; 2; 1989; 173-179;

# TECHNOLOGY DOES NOT IMPROVE CONTENT !

## Supplementary material not indexed

### Part 2

**Summary:** (6) shows Citation 2. Author's abstract displays a reaction scheme. The BEILSTEIN abstract (7) does not display the scheme but the abstract still refers to it (see arrows).

Abstract in CPlus omits scheme as generally done and changes text. (8) shows part of the indexing. Record for citation 1 (9;10;11) looks like this paper does not deal with the compound in question.

**Conclusion:** Reading the English translation of this Russian paper reveals that a Markush type formula may have been interpreted wrong. So the compound in question should not be referenced to citation1 at all.

**Citation 2 of 2**

**ACS Publications**

*Org. Lett.*, **2** (6), 737- 740, 2000. 10.1021/ol9903584  
S1523 7060(99)00358 2

**Web Release Date:** February 19, 2000

**Chemo- and Regioselective Dimerization of Terminal Alkynes Promoted by Methylaluminumoxane**

*Department of Chemistry and Institute of Catalysis Science and Technology, Technion-Israel Institute of Technology, Haifa 32000 Israel*

**Aswini K. Dash and Moris S. Eisen\***



[chmoris@techunix.technion.ac.il](mailto:chmoris@techunix.technion.ac.il)

*Received November 15, 1999*

## Chemo- and Regioselective Dimerization of Terminal Alkynes Promoted by Methylaluminoxane

AUTHORS

Dash, Aswini K.; Eisen, Moris S.

SOURCE

*Org.Lett.* 2000, 2: 6 737 - 740

CODEN

ORLEF7

ABSTRACT

(scheme). Methylalumoxane (MAO) was found to be an active catalytic precursor for the chemo- and regioselective dimerization of a wide range of aryl- and alkyl-substituted terminal alkynes yielding the corresponding geminal dimers **A**. ←

For an olefin-functionalized terminal alkyne (RC(\*)CH, R = MeC=CH<sub>2</sub>), the geminal dimer undergoes an intermolecular [4 + 2] cycloaddition **forming compound B**. ←



## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (8/11)

*Citation 2 of 2 in CAplus*

*Aug 10, 2002*

Explored by Author in CAPLUS.

Chemo- and Regioselective Dimerization of Terminal Alkynes Promoted by Methylaluminumoxane.

Dash, Aswini K.; Eisen, Moris S.

Organic Letters (2000), 2(6), 737-740.

CAN 132:264735 AN 2000:118819 CAPLUS

### Abstract

Methylaluminumoxane (MAO) was found to be an active catalytic precursor for the chemo- and regioselective dimerization of a wide range of aryl- and alkyl-substituted terminal alkynes yielding the corresponding geminal dimers A. ←

For an olefin-functionalized terminal alkyne (RC.tplbond.CH, R = MeC:CH<sub>2</sub>), the geminal dimer undergoes an intermol. [4 + 2] cycloaddn forming compound B ←

## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (9/11)

*Indexing by CA (in part):*

**Indexing -- Section 21-2 (General Organic Chemistry)**

**Aluminoxanes**

**Role: CAT (Catalyst use); USES (Uses)**

**Chemoselectivity**

**Dimerization**

**Dimerization catalysts**

**Dimerization kinetics**



**Regiochemistry**

**(chemo- and regioselective dimerization of terminal alkynes promoted by methylaluminoxane)**

.....

**263394-39-4P**

**←** *RN of compound in question*

.....

**Role: SPN (Synthetic preparation); PREP (Preparation)**

**(.....)**

## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (10/11)

***Citation 1 of 2:***

***Aug 10, 2002***

**Explored by Author in CAPLUS.**

**Reaction of phthalimidonitrene with phenylbutenyne.**

**Kuznetsov, M. A.; Semenovskii, V. V.; Belov, V. N.; Gindin, V. A. ←**

**Khim. Geterotsykl. Soedin. (1989), (2), 173-9. ←**

**CODEN: KGSSAQ. Journal written in Russian.**

**CAN 112:35575 AN 1990:35575 CAPLUS**

### **Abstract**

Aziridines I (.....) were prepd. in 63-89% yield by adding PhthN: (Phth = phthalimido), prepd. in situ by oxidn. of PhthNH<sub>2</sub> with Pb(OAc)<sub>4</sub>, to RC.tplbond.CCR<sub>1</sub>:CR<sub>2</sub>R<sub>3</sub>. The latter were prepd. by thermal dehydration of RC.tplbond.CC(OH)R<sub>1</sub>CHR<sub>2</sub>R<sub>3</sub>.

## SUPPLEMENTARY MATERIAL NOT INDEXED (BEILSTEIN) (11/11)

Citation 1 of 2:

Indexing -- Section 27-3 (Heterocyclic Compounds)  
(One Hetero Atom)

Cycloaddition reaction

(of phthalimidonitrene to phenylbutenyne, aziridine derivs. from)

<u>RNs:</u> 75-07-0	78-84-2	78-94-4
935-01-3	1463-04-3	1875-48-5
13343-79-8P	13633-26-6P	19016-83-2P
124475-73-6P	5876-76-6P	5923-02-4P
89458-21-9P	886-66-8P	124475-74-7P
124475-75-8P	24475-76-9P	124475-77-0P
124475-78-1P	124475-79-2P	124475-80-5P
536-74-3		

Supplementary Terms

addn phthalimidonitrene enyne; aziridine phthalimido;  
phthalimide aziridino

# TECHNOLOGY DOES NOT IMPROVE CONTENT !

**Supplementary material ? How do producers of secondary information deal with that problem?**

**BEILSTEIN**: In the discussion the audience was informed by Dr. Hellwich, member of the “Chemie Daten- und Software GmbH”, that **BEILSTEIN** does not cover Supplementary Material at present.

I hope that changes will be in the future.

**Of course, this costs money but if not done the value of the content of the database will decrease.**

**Open question to CAS**: Please tell us: Do abstractors and indexers take into account the sometimes really long Supplementary Material authors submit? Seems to be a general problem in the future:

**Number of journals offering Supplementary Material will increase. A publisher can increase the number of accepted papers moving experimental details into the Supplementary Material. Technology does support this. Do we want that? My answer would be: “No, we don’t.”**

# TECHNOLOGY DOES NOT IMPROVE CONTENT !

**Indexing by CAS does not reflect keywords given by author**

**Summary:** Journals often show keywords selected by the author or editors (1). The indexing done by CAS staff is deep, but very often the keywords of the author are not present at all (2).

**Conclusion:** Would it not be better that CAS accepts all these keywords given by author as part of the Supplementary Terms?

SciFinderScholar analyzing pops up Supplementary Terms as single words (if I remember correctly!). But those keywords have been and still are often “strings of words”.

**Indexing by CAS does not reflect keywords given by author (1/2)**

**Chemistry - A European Journal Volume 7, Issue 20,  
2001. Pages: 4386 – 4394**

The Cyclization of Parent and Cyclic Hexa-1,3-dien-5-ynes- A Combined Theoretical and Experimental Study  
Matthias Prall, Dipl.-Chem. 1, Anke Krüger, Dr. 2, Peter R. Schreiner, Prof. Dr. 1 \*, Henning Hopf, Prof. Dr. 2 \*

**Indexing....etc.**

## **Keywords**

ab initio calculations; cycloaromatization; enynes; isobenzene; macrocycles

**Abstract etc...**

## Indexing by CAS does not reflect keywords given by author (2/2)

Aug 4, 2002

*Explored by Author in CAPLUS and MEDLINE.*

The cyclization of parent and cyclic hexa-1,3-dien-5-ynes- a combined theoretical and experimental study.

CAN 136:102006 AN 2001:790482 CAPLUS

Indexing -- Section 22-5 (Physical Organic Chemistry)  
124869-33-6, Isobenzene



Supplementary Terms

dienyne thermal cyclization exptl theor study

*Keywords in Journal by Autor or Editor* and in CAplus:

Enynes ( ✓ )    cycloaromatization ( ✓ )    Isobenzene ✓



(alkenynes)    (cycloisomerization)

(dienynes)

*ab initio* ( - )    *macrocycles* ( - )

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# **TECHNOLOGY DOES NOT IMPROVE CONTENT !**

**Therefore it is still necessary, to use chemical information as a real effective tool, to teach students how to use it ! So-called “end user systems” are intelligently used technology but do not replace knowledge of content structures totally.**

**“I think it is important for every chemist to have a fair appreciation of the literature, history and chemistry. I have observed that superior chemists have gained this knowledge, but by self-education. To ensure every chemist having an opportunity to become educated in these areas, each academic chemistry department should offer a chemical information science course....preferably as a required course.”**

**HERMAN SKOLNIK**

***J. Chem. Inf. Comput. Sci., Vol. 20, No. 2, 1980***

# TECHNOLOGY DOES NOT IMPROVE CONTENT !

**Last question: Does faculty really know this?**

*Dieter Rehm*



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See also: [CHMINF-L](#)      [CINF Member Directory](#)