

Family name, First name: Gschwind, Ruth M.Researcher ID:I-4639-2015; http://orcid.org/0000-0003-3052-0077H-index: 23(please note there are articles with R.M. and R. Gschwind)Publications: 82(68 in peer-reviewed journals, only Angew. Chemie Int. Ed.)Citations: 1613(1463 without self citations; 23,7 Citations / article)High impact research articles: 1 Nature Chemistry; 10 Angew. Chemie (6 single corresp. author (1 VIP), 1 shared corr. authorship (VIP); 14 JACS (10 single corresp.

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Nationality: German

Date of birth: 29.11.1969 URL for web site: <u>http://www-oc.chemie.uni-regensburg.de/gschwind/index.html</u>

• EDUCATION

PhD, Department of Chemistry, Technical Univ. of Munich, Germany (*summa cum laude*)
Diplom, Department of Chemistry, Technical Univ. of Munich, Germany (*summa cum laude*)

• CURRENT POSITION

2005 – Professor of Organic Chemistry Faculty of Chemistry and Pharmacy / University or Regensburg / Germany

• **PREVIOUS POSITIONS**

- 2002 2005 Professor of Organic Chemistry, University of Bonn
- 1997 2002 Head of NMR department / Habilitation in Organic Chemistry Department of Chemistry, University of Marburg, Germany

• AWARDS AND FELLOWSHIPS

2013	ERC Consolidator Grant "IonPairs@Catalysis"
	Thieme journal award
1999 / 2000	Visiting Professor at INSA/IRCOF University of Rouen, France
1989 – 1994	Grant of the German National Academic Foundation

• SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

2000 – 2015 8 Postdocs / 19 PhD students / 23 Master/diploma students at the University of Bonn, Germany (until 2002) and at the Faculty of Chemistry and Pharmacy, University of Regensburg, Germany

• TEACHING ACTIVITIES

Since 1998 Teaching chemistry at all levels from first year organic class to specialized graduate seminars.

• COMMISSIONS OF TRUST, MEMBERSHIPS

since 2011 Associate director of the Center for Magnetic Resonance in Chemistry and Biomedicine in Regensburg

- since 2011 Member of the DECHEMA (Society for Chemical Engineering and Biotechnology) committee Kinetics and Reaction Mechanisms
- 2008-2011 Board member of the Liebig Vereinigung (organic chemistry division of the german chemical society GDCh)
- 2005-2006 Chairwoman of the GDCh chapter Regensburg
- since 2005 Member of national and international appointment committees e.g. for professorships, NMR positions or awards.

• MEMBERSHIPS OF SCIENTIFIC SOCIETIES

German Chemical Society (GDCh), Liebig Vereinigung and Fachgruppe NMR Spektroskopie

• INTERNATIONAL AND NATIONAL COLLABORATIONS

International: Prof. E. Nakamura (Tokyo), Japan; Prof. Dr. P. I. Dem'yanov (Moskau) Russia; Dr. R. Cibulka (Prague), Czech Republic.

National (without University of Regensburg): Prof. P. Knochel (Munich); Prof. M. Rueping (Aachen); Prof. K. Zeitler (Leipzig); Prof. S. Bräse (Karlsruhe); Prof. H. Zipse (Munich); Prof. E. Riedle (Munich); Prof. E. Niecke (Bonn); Prof. C. A. Schalley (Berlin); Prof. N. Krause (Dortmund) Prof. J. Sundermeyer (Marburg).

• **RESEARCH PROFILE**

NMR-spectroscopic investigations of structure/ reactivity or selectivity correlations in bioorganic, organocatalytic and organometallic systems.

Stabilization and structure elucidation of hydrogen bridged systems and reaction intermediates e.g. hydrogen bridged systems and preferred conformations of arginines and acyl-guanidines, hydrogen bridge properties and structures in organocatalytic Brønsted acid catalysts, enamine intermediates in proline catalysed aldol reactions, Cu(I) and Cu(III) intermediates in organo-cuprates, Cu(I) phosphoramidite precatalysts and intermediates.

Scientific achievements (The numbers refer to the five representative publications): A characteristic of my research projects is to enter structurally uncharted territory in various synthetically highly important fields, in which the structures, species, intermediates or intermolecular interaction pattern remained elusive despite a long standing and international effort. To state only the most prominent examples, together with my coworkers I • solved the long standing scientific discussion about the supramolecular structure of organocuprates, their structure/reactivity relation and the potential reactivity differences between iodo- and cyanocuprates; • elucidated the first structures of phosphoramidite copper complexes in solution revealing an so far unprecedented precatalyst structure and succeded in the first direct NMR detection of their transmetallation intermediates; \bullet detected the elusive highly charged Zintl anions Si₄⁴⁻ and Sn₄⁴⁻; \bullet reported concurrently with Bertz and Oagle the first Cu(III) reaction intermediate in substitution reactions of organocuprates; $^{1} \bullet$ revealed intermediate structures in Negishi cross-coupling reactions $^{2} \bullet$ detected the long time elusive enamine intermediates with proline,³ prolinol and prolinolether catalysts in situ and revealed their formation trends, conformational preferences, and mechanistic pathways; • detected the first through hydrogen bond scalar couplings for bioorganic ion pairs in classical organic solvents; • revealed the hydrogen bond/ion pair properties in Brønsted acid imine complexes;⁴ • developed the supramolecular balance for transition metal complexes allowing for the first time to measure interligand supramolecular interactions in transition metal complexes; • developed an improved LED illumination device for NMR spectroscopic studies allowing to measure not only the first reaction profiles of photocatalytic reactions but to differentiate between one and two electron transfer processes.⁵

Based on these achievements, in the NMR community I am currently regarded as the leader in the field of NMR of small reactive species and reaction intermediates.

1. Five representative publications

- NMR-Detection of Cu(III) Intermediates in Substitution Reactions of Alkyl Halides with Gilman Cuprates (Times Cited: 55), T. Gärtner, W. Henze, R. M. Gschwind, J. Am. Chem. Soc., 2007, 129, 11362-11363. DOI: 10.1021/ja074788y
- Highly diastereoselective Csp3-Csp2 Negishi cross-coupling with 1,2-, 1,3- and 1,4-substituted cycloalkylzinc compounds (Times Cited: 53) T. Thaler, B. Haag, A. Gavryushin, K. Schober, E. Hartmann, R. M. Gschwind, H. Zipse, P. Mayer, P. Knochel, Nature Chemistry, 2010, 2, 125-130. DOI: 10.1038/NCHEM.505
- 3) The Elusive Enamine Intermediate in Proline-Catalyzed Aldol Reactions NMR Detection, Formation Pathway, and Stabilization Trends (Times Cited: 83) M. Schmid, K. Zeitler, R. M. Gschwind, Angew. Chem. Int. Ed., 2010, 49, 4997-5003. DOI: 10.1002/anie.200906629
- Brønsted Acid Catalysis: Hydrogen Bonding versus Ion Pairing in Imine Activation (Times Cited: 56) M. Fleischmann, D. Drettwan, E. Sugiono, M. Rueping, R. M. Gschwind, Angew. Chem. Int. Ed., 2011, 50, 6364–6369. DOI: 10.1002/anie.201101385
- 5) LED-illuminated NMR-Studies of Flavine-Catalyzed Photooxidations Reveal Solvent Control of the Electron-Transfer Mechanism (Times Cited: 0) C. Feldmeier, H. Bartling, K. Magerl, R. M. Gschwind, Angew. Chem. Int. Ed., 2015, 54, 1347-1351. DOI: 10.1002/anie.201409146

2. Contributions to Research monographs

"NMR Spectroscopic Aspects", F. von Rekowski, C. Koch, R. M. Gschwind, in: "*Copper-Catalyzed Asymmetric Synthesis*", A. Alexakis, N. Krause, S. Woodward (Eds.), Wiley-VCH, Weinheim, Germany, 2014, 353–372. ISBN 378-3-527-33204-5

"NMR of Organocopper Compounds", T. Gärtner, R. M. Gschwind, in: *"The Chemistry of Organocopper Compounds"*, Z. Rappoport, I. Marek, (Eds.), John Wiley & Sons Ltd., Chichester, England, **2009**, 163–215. ISBN: 978-0-470-77296-6.

4. Invited lectures on international conferences (*no upgraded posters, sorted by date*):

Since 2010 I declined several invited plenary lectures on international conferences due to personnel reasons e.g. a key note lecture in the Organocatalysis section at the ICC at Munich 2012. In addition, often my PhD students are invited or upgraded to give talks on international and national conferences and meetings.

- 1. International Society of Magnetic Resonance ISMAR, Shanghai, China, plenary lecture, 20.08.2015.
- 2. Physical Organic Chemistry Gordon Research Conference, Holderness NH, United States, 2015.
- 3. 15th NMR Meeting (AUREMN), Angra dos Reis, RJ Brasilien, plenary lecture, 09.06.2015.
- 4. 10th Euromar, Zürich, Schweiz, 02.07.2014.
- 5. 55th Experimental Nuclear Magnetic Resonance Conference (ENC), Boston, USA, 27.03.14.
- 6. 5th ORCA Meeting, Alicante, Spain, 17.10.13.
- 7. GDCh FGMR: 35th Annual Discussion Meeting, Frauenchiemsee, Germany, plenary lecture, 09/2013.
- 8. ORCHEM, 18. Lecture Conference, Weimar, Germany, 09/2012
- 9. Department of Organic Chemistry, Chennai, India, 2/2012.
- 10. 1st Germany-Japan Organocatalytic Symposium, Kyoto, Japan, 10/2011
- 11. XXXIII Finnish NMR Symposium, Jyväskylä, Finnland, 07.06 and 08.06.2011. (2 Lectures).
- 12. 7th Euromar (Magnetic Resonance Conference), Frankfurt, Germany, 2011.
- 13. Euract-NMR, Karlsruhe, Germany, 01/2010.
- 14. GDCh FGMR: 29th Annual Discussion Meeting, Göttingen, Germany, 09/2007.

- 15. 8th Int. Symposium on Carbanion Chemistry (ISCC-8), Madison, Wisconsin, USA, 06/2007.
- 16. GAFOC III (German-American Symposium: Frontiers of Chemistry), Kloster Seeon, 07/2004.
- 17. 6th International Symposium on Carbanion Chemistry (ISCC-6), Marburg, Germany, 07/2001.

Invited lectures at foreign universities (sorted by date):

- 1. Department of Organic Chemistry, ETH-Zürich, Switzerland, 09. 11. 2015.
- 2. Institute of Organic Chemistry, University of Innsbruck, Austria, November 2015.
- 3. Department of Organic Chemistry, Univerzita Komenského v Bratislave, Slovakia, 26.04.2012.
- 4. Department of Organic Chemistry University of Oxford, Oxford, England, 01.12.2011.
- 5. Institut Català d'Investigació Química (ICIQ), Tarragona, Spain, 11.11.2011.
- 6. Université de Genève, Genève, Switzerland, 21.01.2010.
- 7. GÖCh Lecture, Universität Linz, Linz, Austria, 17.06.2008.
- 8. Institut de Recherche en Chimie Organique Fine de Rouen, Mont St. Aignan, France, 2000 (2 lectures)

About 40 invited lectures at german universities or meetings.