



Sijbren Otto is awarded a TA-NEWPOL grant

Sijbren Otto is awarded a 250.000 TA-NEWPOL grant. These grants aim at developing new polymer materials which meet the social and industrial need for sustainability and multifunctionality.

Self-synthesizing gels

This research aims to develop new gels that form from simple building blocks. The build-up process can be controlled so that the gels have the desired structure and properties. The investigators wish to apply the resulting materials as media for the growth of cells in three dimensions.

Highlights by Prof. dr. Jan B.F.N.Engberts

- Three organic chemists from the Technical University of Munich wrote an interesting review about self-assembled supramolecular structures that can be used as catalysts for reactions that occur via cationic transition states. Such catalysts are highly necessary since otherwise the cationic transition states may be attacked by counterions and/or solvent molecules. The supramolecular structures contain aromatic, hydrophobic reaction pockets and make it possible to perform cationic reactions outside the scope of standard solution chemistry. A number of such processes have been discussed in some detail. However, several problems have still to be solved and a variety of new host structures have to be designed and prepared. Such structures should be easily obtainable, tailored towards a particular transformation and highly modifiable. *Catti, L., Zhang, Q., Tiefenbacher, K., Synthesis 2016, 48, 313.*
- SN₂ nucleophilic substitution processes are significantly dependent on nucleophile, solvent and the leaving group. Physical-organic chemists from Institutes in Austria and Hungary argue that the role of the leaving group on the reaction dynamics has remained rather unclear. The effect of the leaving group on the gas-phase dynamics of SN₂ reactions has now been investigated in a combined approach of crossed-beam imaging and dynamics simulations. A comparison was made of the reaction of F⁻ with CH₃Cl and CH₃I. An important factor that was identified was the relative orientation of the approaching reactants. This effect occurs on short timescales and may also prevail in solution chemistry. *Stel, M., Carrascosa, E., Kainz, M.A., Kelkar, A.H., Meyer, J., Szabó, I., Czakó, G., Wester, R., Nature Chem. 2016, 8, 151.*
- Four Chinese synthetic chemists have accomplished the total synthesis of three antituberculosis diterpenoids, ileabethoxazole, pseudopteroxazole and seco-pseudopteroxazole, in a collective fashion. The key step in their approach was a one-pot 6π electrocyclization/aromatization sequence, leading to the required multisubstituted arene scaffold from a geometry-defined hexasubstituted triene. The five- and six-membered rings of ileabethoxazole and pseudopteroxazole were obtained with the desired stereochemistry. Seco-

pseudopteroxazole was formed using a straightforward side-chain elongation. Further biological studies will substantially benefit from these novel synthetic procedures. *Yang, M., Yang, X., Sun, H., Li, A., Angew.Chem.Int.Ed. 2015, DOI 10.1002/anie.201510568.*

- David Leigh and four coworkers at the University of Manchester, UK, have reported a completely artificial small-molecule robotic arm that is able to selectively transport a molecular cargo in either direction between two spatially distinct (2 nm apart), chemically similar, sites on a molecular platform. The arm can pick up or release a 3-mercaptopropanehydrazide cargo by formation/breakage of a disulfide bond. Dynamic hydrazine chemistry controls binding of the cargo to the platform. Selectively-induced conformational and configurational changes within an embedded hydrazine rotary switch, that steer the robotic arm, provides the control of transport. The transport does occur without the cargo at any time fully dissociating from the arm nor exchanging with other molecules in the bulk. Possible applications of these molecular-sized machines are discussed. The paper has been reviewed by Aprahamian in the same journal. *Kassem, Sh., Lee, A.T.L., Leigh, D.A., Markevicius, A., Sola, J., Nature Chemistry, 2016, 8, 138. Aprahamian, I., Nature Chemistry, 2016, 8, 97.*
- A detailed study, performed at two research centers and at Northwestern University, Evanston, USA, highlighted the relevance of molecular weight tuning of both donor and acceptor polymers for all-polymer solar cell performance. The authors described a promising strategy and matrix approach as well as useful synthetic tools for optimizing future efficiencies of these types of solar cells. The proposed synthetic methodologies allow a predictable access to conjugated polymers with desired number-average molecular weights (M_n) and stress the importance of optimizing M_n for both polymer components. *Zhou, N., Dudnik, A.S., Li, T.I.N.G., Manley, E.F., Aldrich, T.J., Guo, P., Liao, H-C., Chen, Z., Chen, L.X., Chang, R.P.H., Facchetti, A., Olivera de la Cruz, M., Marks, T.J. J.Am.Chem.Soc. 2016, 138, 1240.*
- Cycloaddition reactions using visible light photoredox catalysis are a useful tool in organic chemistry. Three Chinese synthetic chemists have recently reviewed the area with particular emphasis on [2+2], [3+2], [4+2] and [2+2+2] cycloadditions for the preparation of four-, five- or six-membered cycles and polycycles. Reaction mechanisms are discussed, in which visible light photoredox catalysis leads to the formation of radical intermediates. Further developments of these transformations are a challenge, but it is assumed that they may be useful in sequences to prepare various bioactive compounds. *Liu, Y., Song, R., Li, J., Science China, Chemistry, 2016, DOI 10.1007/s11426-015-5516-5.*
- Recently there has been considerable interest in halogen bonding interactions. In a joint project of The Chinese Academy of Sciences and UCB Biopharma in Belgium, the characteristics and stability of anion-anion complex formation was studied using quantum chemical calculations. Perhaps unexpectedly, complex formation between halobenzoates and propiolate revealed that anion-anion halogen bonding is unstable in vacuum but attractive in solvents. Also unexpected was the finding that the optimal halogen bonding distance between the two anions is shorter than that in a neutral system, suggesting a stronger halogen bonding interaction. Calculations were also carried out on four protein-ligand complexes from the protein data bank and showed that halogen bonding could contribute to the ligands' binding affinity up to about 3 kcal/mol. *Wang, G., Chen, Z., Xu, Z., Wang, J., Yang, Y., Cai, T., Shi, J., Zhu, W., J.Phys.Chem.B, 2016, DOI 10.1021/acs.jpcc.5b08139.*
- The final item this month is concerned with a topic that receives much attention in recent physical, chemical, biological and also philosophic studies: the zero-point energy (ZPE). This is the ground state of every quantum mechanical physical system. Every system is in motion, even at absolute zero, and empty space is filled with zero-point electromagnetic radiation. The Dutch physical chemist H.B.G. Casimir found experimental evidence for the ZPE that is responsible for the creation of virtual particles. Interestingly, the ZPE may well have relevance for biological systems. I cannot go into further detail, but only draw your attention to a recent study at Okayama University and a research center at Okayama that showed rather convincingly that the thermodynamic stability of ice II and its hydrogen-disordered counterpart is, at least in part, determined by differences in the ZPE. *Nakamura, T., Matsumoto, M., Yagasaki, T., Tanaka, H., J.Phys.Chem.B 2016, DOI 10.1021/acs.jpcc.5b09544.*

Jan Engberts

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The Stratingh Office is located on the ground floor of building 16—Nijenborgh 4— and it consists of Hilda, Alphons and Cristina. We handle a range of responsibilities and provide help and advice on various aspect of University regulations.



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Werkbespreking: Thursday morning 8.30 hrs, room 5111.0080

March 3rd—Francesco Mecozi (PhD Browne): "Selective oxidation of alkenes and vicinal diols to acyloins with H₂O₂ in multistep one-pot reactions using a simple Mn catalyst"

March 10th—Nabil Tahiri (PhD Minnaard): "Regioselective modifications on aminoglycoside antibiotics"

March 17th— Xingchen Yan (PhD Harutyunyan): "Title to be announced"

March 24th— Manuela Bersellini (PhD Roelfes): "Title to be announced"

March 31st—Peter Stacko (PhD Feringa): "Machines based on molecular motors"

If you have items for the next issue of this Newsletter, please send an e mail to the Stratingh Institute office: Stratingh@rug.nl