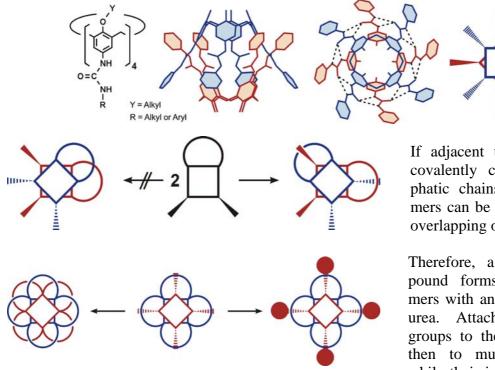
SELF-ORGANISATION OF TETRA-UREA DERIVATIVES OF CALIX[4]ARENES

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Calix[4]arenes, substituted on their wide rim by four arylurea groups form capsular dimers in apolar solvents (chloroform, benzene),¹ held together by a seam of intermolecular hydrogen bonds.



If adjacent urea residues are covalently connected by aliphatic chains, only those dimers can be formed, where no overlapping of loops occurs.

Therefore, a tetra-loop compound forms exclusively dimers with an open chain tetraurea. Attachment of bulky groups to the open end leads then to multiple rotaxanes,² while their intramolecular con-

nection creates multiple [2]catenanes.³

For mixtures of up to 11 tetra-ureas a sorting scheme has been developed, which is based on two simple rules for the selective dimerisaton:

- Dimers with overlapping loops are not formed.
- Bulky residues do not penetrate the loops.

For selected examples these two rules have been confirmed by ESI-MS using tetraethylammonium cations as guest for the dimeric capsule.⁴

¹ J. Rebek, Jr., Chem. Commun. 2000, 637-643

² O. Molokanova, M. O. Vysotsky, Y. Cao, I. Thondorf, V. Böhmer, *Angew. Chem.* **2006**, *118*, 8220-8224

³ O. Molokanova, A. Bogdan, M. O. Vysotsky, M. Bolte, T. Ikai, Y. Okamoto, V. Böhmer, *Chem. Eur. J.* **2007**, *13*, 6157-6170

⁴ D. Braekers, C. Peters, A. Bogdan, Y. Rudzevich, V. Böhmer, J. F. Desreux, *J. Org. Chem.* **2008**, *20*, 701-706