Protonen on Tour – DFT-Studie zur H^+-Wanderung in [1.1.1]- und [2.2.2]-Cryptanden

Protons on Tour – DFT-study of H^+-Migration in [1.1.1]- and [2.2.2]-Cryptands

Ralph Puchta, Michael Galle und Nico J. R. van Eikema Hommes

Computer-Chemie-Centrum, Nägelsbachstraße 25, D-91052 Erlangen, Deutschland

Sonderdruckanforderungen an Dr. R. Puchta. E-mail: ralph.puchta@chemie.uni-erlangen.de

Z. Naturforsch. **61b,** 1327 – 1334 (2006); eingegangen am 31. Juli 2006

DFT-calculations (RB3LYP/LANL2DZp) show that the migration of a proton inside [1.1.1]- and [2.2.2]-cryptand from one nitrogen atom to the other follows different paths. While the proton in [H⊂1.1.1]-cryptand moves *via* an ether oxygen atom (activation energy: 19.2 kcal/mol), the proton in [H⊂2.2.2]-cryptand moves directly from one nitrogenatom to the other (activation energy: 16.1 kcal/mol). Our calculations rule out the application of doubly protonated [2.2.2]-cryptands as anion hosts.

Key words: Cryptands, Proton Migration, DFT