Hydroxy-1*H*-imidazole-3-oxides – Synthesis, Kinetic Acidity, and Application in Catalysis and Supramolecular Anion Recognition

Susan Bartz[a], Bettina Blumenröder[a], Anika Kern[b], Julia Fleckenstein[b], Sabine Frohnapfel[b], Jürgen Schatz[a,b], and Alexander Wagner[b]

[a] Organic Chemistry 1, Department of Chemistry and Pharmacy, University of Erlangen, Henkestraße 42, D-91054 Erlangen, Germany
[b] Department of Chemistry and Biochemistry, Ludwig-Maximilians-Universität Munich, Butenandtstraße 5 – 13 (Haus F), D-81377 München-Grosshadern, Germany

Reprint requests to Prof. Dr. Jürgen Schatz. Fax: +49 9131 85 24707.
E-mail: juergen.schatz@chemie.uni-erlangen.de

Z. Naturforsch. **2009**, *64b,* 629 – 638; received March 27, 2009

Dedicated to Professor Gerhard Maas on the occasion of his 60th birthday

Using *ab initio* calculations (B3LYP 6-31G*) the geometries of diethyl, dimethoxy and dimethylamino imidazolium salts were studied as representative models of imidazolium salts bearing heteroatoms directly attached to the ring nitrogen atoms of the imidazolium core units. In all cases the *syn* and *anti* arrangement of the substituents could be identified. In addition to the theoretical studies, eleven dialkoxy imidazolium salts were prepared by alkylation of six 1-hydroxy-imidazole-3-oxides using dimethyl or diethyl sulfate as strong alkylating reagents. The kinetic acidities of these compounds were studied by measuring the pseudo-first order reaction rates of the H/D exchange process of the C^2-H proton of compounds **3** – **9**. The observed kinetic acidities are much higher than reaction rates observed for simple imidazolium salts; half-lifes of the H/D exchange are usually in the range of minutes. Similar to dialkyl/aryl imidazolium salts, all prepared dialkoxy imidazolium salts could be used as precatalysts in standard aqueous Suzuki coupling reactions. In addition, two representative dialkoxy imidazolium salts could be used in supramolecular anion recognition, as demonstrated by binding studies towards iodide as guest.

Key words: Imidazolium Salts, Kinetic Acidity, Catalysis, Suzuki Reaction, Anion Receptors