Cation Affinity Numbers in Organocatalysis Research

Boris Maryasin, Christoph Lindner, Hendrik Zipse
Department of Chemistry and Biochemistry, LMU München,
Butenandtstrasse 5-13, D-81377 München, Germany
E-mail: zipse@cup.uni-muenchen.de

The acceleration of a variety of group transfer reactions by Lewis bases such as amines and phosphines represents an important part of the field of contemporary organocatalysis, with particularly interesting applications in the area of stereoselective transformations. In recent years simple affinity numbers such as the affinity towards methyl cations (MCA) or the affinity towards acetyl cations (ACA) have been used to rationalize the catalytic performance of known pyridine bases and predict new, more highly active catalysts.\textsuperscript{1-3} These studies have also been extended to include prochiral cation probes.\textsuperscript{4}

A good number of organocatalytic transformations involve the initial reaction of neutral nucleophilic catalysts with neutral electrophiles, generating zwitterionic intermediates as the first discrete species in the catalytic cycle. Using methyl vinyl ketone (MVK) as a sample electrophile we have now evaluated theoretical methods suitable for the calculation of the corresponding affinity numbers, and have also explored the correlation of such affinity values with those derived for cationic electrophiles.

References