A Gas Phase Study of the Reactivity of $V_mO_nH_O^+$ Clusters

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A quadrupole-based mass spectrometer equipped with an electrospray ionization source was used to examine the gas-phase reactivity of various vanadium-oxide cations which mediate the oxidative dehydrogenation (ODH) of small alkenes and alkanes.

For ion generation, a solution of $V_6O_7(OMe)_{12}$ dissolved in deuterated methanol was subjected electrospray under very harsh conditions to obtain smaller vanadium-oxide clusters $V_mO_nH_o^+$ (m = 1-4, n = 1-11, o = 0-2) [1]. The reactivity of the resulting cations was studied towards isomeric butenes [2] and different small alkanes. For butene, the ODH activity strongly depends on the valence as well as on the state of protonation. $V_4O_{10}^+$ was found to be the most reactive one towards alkenes and is the only of the ions investigated which oxidizes alkanes, too.

The implications of these results as well as the prospects of electrospray ionization for the generation of more complex vanadium-oxide clusters are discussed.

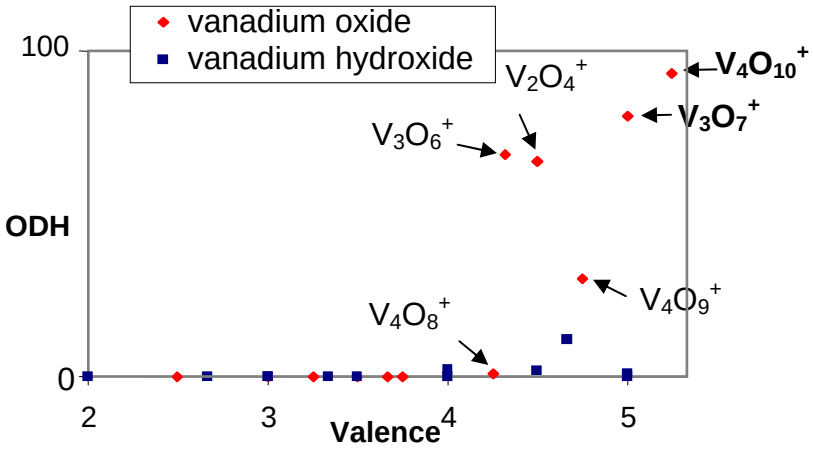

Figure: ODH-activities of $V_mO_nH_0^+$ versus valence

[1] D. Schröder, M. Engeser, M. Bronstrup, C. Daniel, J. Spandl, H. Hartl, *Int. J. of Mass Spectrom.*, **2003**, 228 (2-3), 743-757

[2] R. C. Bell, A. W. Castleman, Jr., *J. Phys. Chem. A*, **2002**, 106, 9893-9899