



The ipso addition of OH to methylated benzenes

Paulo Alarcon (1), Birger Bohn (2), Cornelius Zetzsch (1,3)

(1) University of Bayreuth, BayCEER, Atmospheric Chemistry Research Center, Bayreuth, Germany
(c Cornelius.zetzsch@uni-bayreuth.de, +49 921 555729), (2) Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung (IEK-8), Troposphäre, Jülich, Germany, (3) Fraunhofer-Institut für Toxikologie und Experimentelle Medizin, Hannover, Germany

The reaction of OH with hexamethylbenzene has been observed to be a rapid process (Berndt and Böge, 2001) and to proceed via reversible addition (Koch et al., 2007, von Buttlar et al., 2008). Abstraction and elimination of a methyl group are only minor channels at room temperature (Loison et al., 2012). Obviously the ipso addition on an already occupied position of the ring is solely accessible for hexamethylbenzene, whereas for the lower methylated benzenes (toluene and the xylenes) this contribution is small. All three trimethylbenzenes (Bohn and Zetzsch, 2012) have been demonstrated very recently to comprise both channels.

The present study reports on the reactions of OH with toluene, p-xylene, tetramethylated benzenes and pentamethylbenzene, employing the technique of pulsed vacuum UV flash photolysis of H₂O with resonance fluorescence detection of OH. Triexponential decays of OH are observed (most clearly and pronounced for the highly symmetrical durene), and the analytical solution of the differential equation system describing the contribution of two adducts enables us to separate the two predominating addition channels for these compounds.

The consequences of ipso addition of OH to aromatics for photochemical ozone production remain uncertain, and product studies for higher methylated benzenes are missing.

References

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