Rate constants for the reaction of OH with durene (1,2,4,5-tetramethylbenzene), leading to two types of adducts: ortho and ipso.

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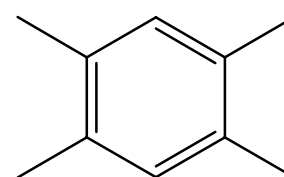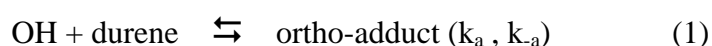[2] Forschungszentrum Jülich GmbH, IEK-8: Troposphäre, Jülich, Germany
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The high symmetry of durene (1,2,4,5-tetramethylbenzene) leads to identical electronic configurations at the four positions of the aromatic ring occupied by methyl groups - different from the two unoccupied positions, which are identical as well. The addition of OH radicals to these two types of positions (ortho and ipso) was studied by VUV flash photolysis of H_2O in the presence of durene between 300 and 353 K in He, monitoring OH by time resolved resonance fluorescence.

Reversible addition in competition with abstraction leads to biexponential decays of OH in general and has hitherto been observed for almost every aromatic in the temperature range where addition becomes reversible on the time scale of the observation. A rapid, reversible addition of OH to the six ipso positions of hexamethylbenzene is already known (Koch et al., 2006). Two types of reversible addition (ortho and ipso) have been recently distinguished for mesitylene (1,3,5-trimethylbenzene) by quantitative evaluation of triexponential decays of OH (Bohn and Zetzsch, 2012). The other isomeric trimethylbenzenes (1,2,3 and 1,2,4) follow a similar behavior with two predominating adducts (Bohn and Zetzsch, 2012). Measurements for OH + durene follow the same mechanism

$$\text{OH} + \text{durene} \quad \rightleftarrows \quad \text{ortho-adduct } (k_a , k_{-a}) \qquad (1)$$

$$\text{OH} + \text{durene} \quad \rightleftarrows \quad \text{ipso-adduct } (k_b , k_{-b}) \qquad (2)$$

$$\text{OH} + \text{durene} \quad \rightarrow \quad \text{products } (k_c) \qquad (3)$$

Durene: 1,2,4,5 - tetramethylbenzene

and are   evaluated for the total of the abstraction and both addition paths $(k_a+k_b+k_c)$, decreasing from 5.3 x 10^{-11} cm^3 s^{-1} at room temperature to 2.5 x 10^{-11} cm^3 s^{-1} at 353 K. Activation energies for the product of the forward and backward reaction of each adduct were measured. Using some approximations, activation energies for each reaction can be estimated, as well as the equilibrium constant for the more energetic adduct.

R. Koch, R. Knispel, M. Elend, M. Siese, C. Zetzsch (2007) **Atmos. Chem. Phys.,** 7, 2057-2071

B.Bohn, C.Zetzsch (2012). Submitted for publication.