Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Consecutive reactions of small, free tantalum clusters with dioxygen controlled by relaxation dynamics

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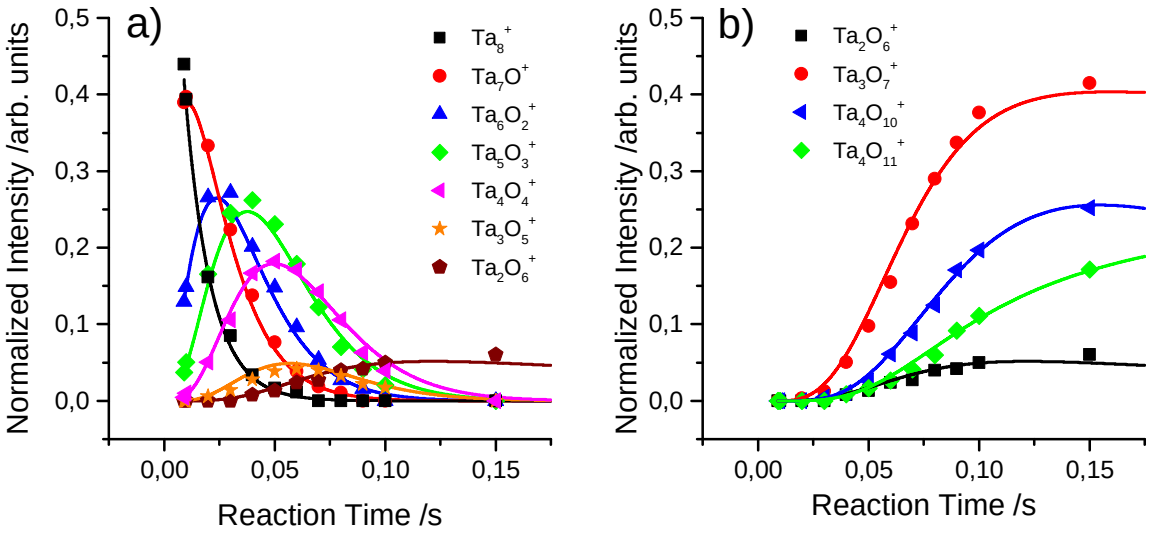

Fig. 1 Intensities of reactants in the oxidation of Ta_8^+ as a function of reaction time and the corresponding result of the kinetic simulation (solid lines). Reaction intermediates $Ta_{8-x}O_x^+$ are depleted, while $Ta_2O_6^+$ is formed (a). Other products with a high oxidation state are additionally generated over time (b).

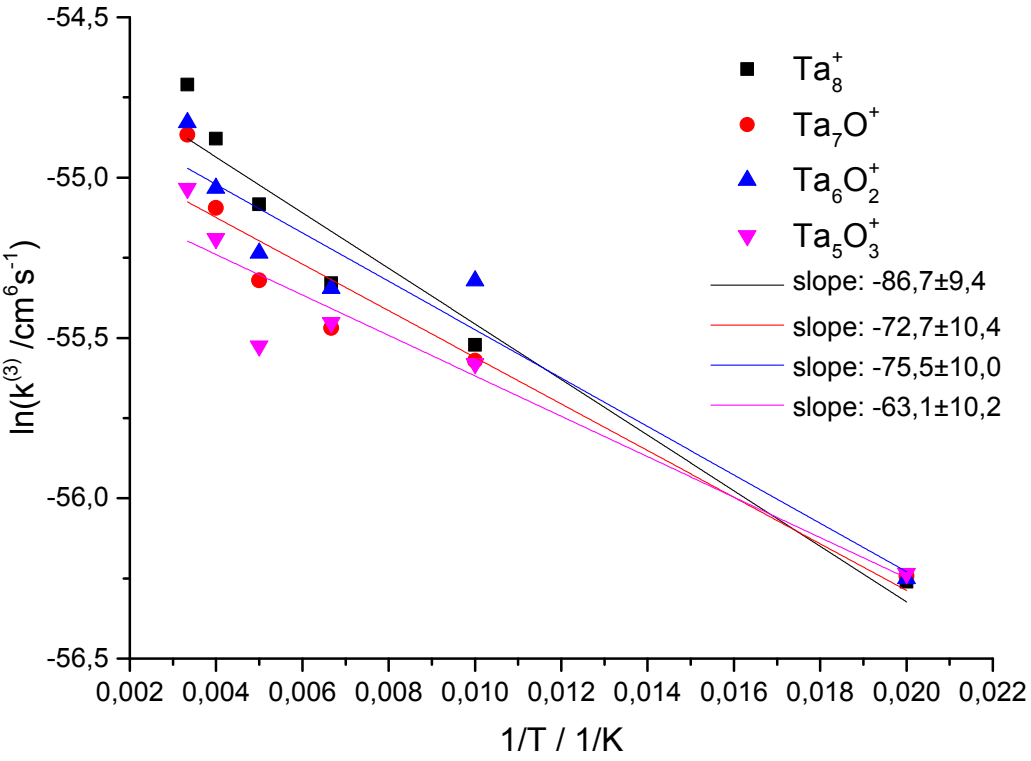

Fig. 2 Arrhenius plot of the first four oxidative degradation steps in the reaction of Ta_8^+ with dioxygen. The apparent activation energy for each reaction step is extracted from the corresponding slope.

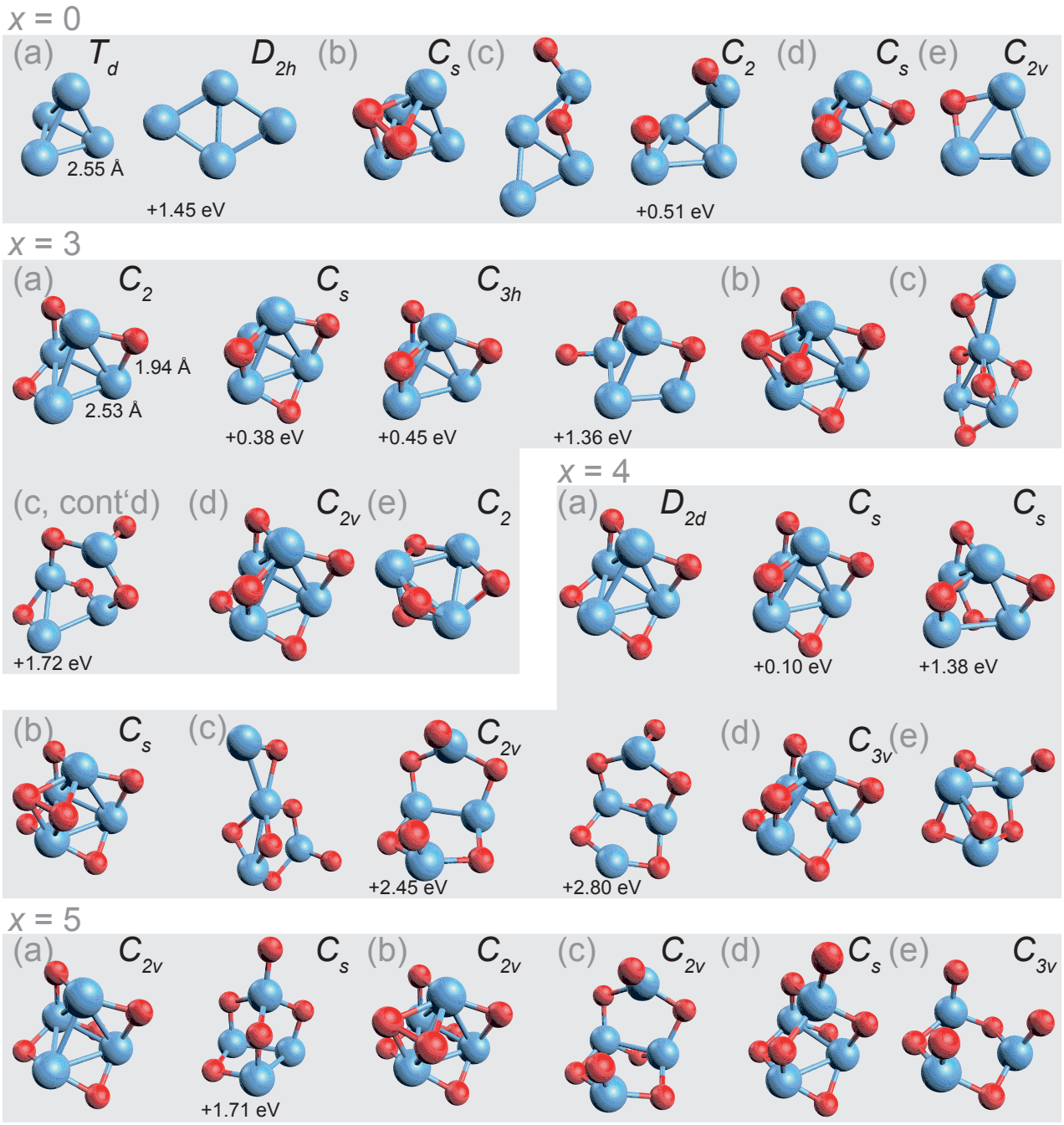

Fig. 3 Isomers of reactants and products in the reaction of $Ta_4O_x^+$ with O_2 for $x = 0, 3, 4, 5$. The initial $Ta_4O_x^+$ clusters are respectively marked with (a), followed by the intermediates with an O_2 unit (b) and the intermediates with dissociated (O,O) (c). The products of intact oxidation are labeled by (d) and products of oxidative degradation by (e). Relative energies are given with respect to the most stable isomer. Point groups are shown if they differ from C_1.