

The mechanism of adsorption of Rh(III) bromide complex ions on activated carbon

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1. TD-DFT calculations.

Additionally, TD-DFT calculations were performed to optimize the structure of the dominant Rh (III) complex and to calculate the theoretical UV-Vis spectrum of this complex. It should be noted, that the TD-DFT calculation gives also oscillation strengths. The peaks with oscillation strengths equal to 0, were excluded. Thanks to that it was possible to reduce the number of the peaks.

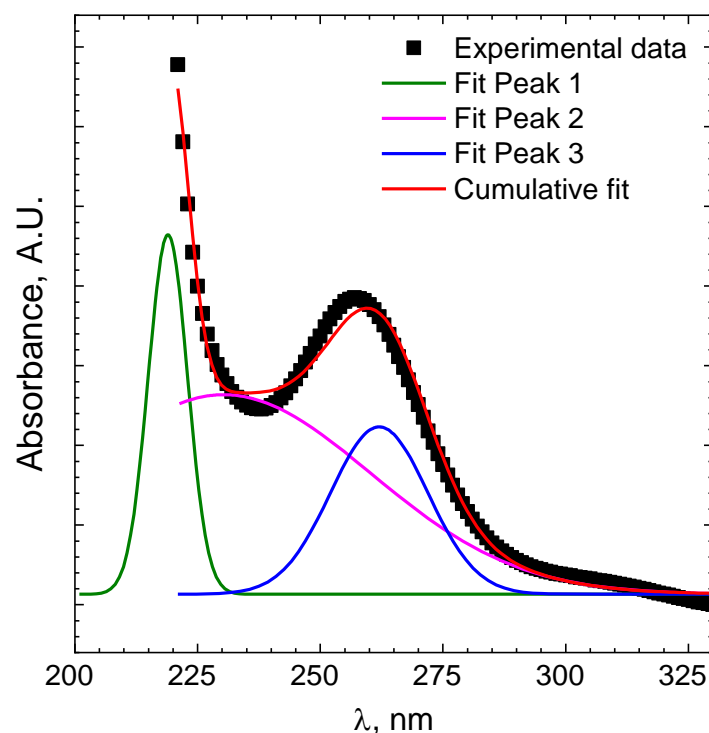


Figure S1. Comparison of experimental and calculated UV-Vis spectra of Rh(III) bromide complex ions.

It may be observed that the fit is not perfect. This is possibly related to the presence of other equilibrium forms of RhBr_x .

Additionally, only peaks located within the recorded spectrum were taken into account. The analyzes included a fragment of the UV-Vis spectrum with distinct peaks, i.e. the range from 220nm - 330nm. After taking into account described above assumption 4 peaks were fitted to registered UV-Vis spectra. Obtained results are shown in **Error! Reference source not found.**.

Table S1. The location of absorption maximum peaks.

Peak location calculated using DFT, nm	Peak location fitted, nm	Related species
219.91	218.94	RhBr_3^-
231	230.43	RhBr_3^-
264.63	352	RhBr_3^-
305.06	305	RhBr_3^-
305.19		

2. XPS analysis

XPS measurements were performed on two samples. Crude, i.e. the starting material, and for the carbon sample after the adsorption of Rh (III) ions. The results of C1s peak, analysis are gathered in Table S2.

Table S2. Surface composition of activated carbon.

Structure description	Binding energy, eV	Fraction, % Sample before adsorption	Fraction, % Sample after adsorption
Carbide	283.2	4.9±0.4	4.9±0.2
C-C sp ²	284.2	59.7±1.3	58.6±0.9
C-C sp ³	285.0	22.0±1.5	22.7±1.0
C-O	286.5	9.1±0.3	9.1±0.4
COO	288.0	4.2±0.3	4.7±0.4
π - π^*	290.3	-	-

There is no statistically significant differences. This confirms that the carbon and its functional groups do not react with HBr and water. However, due to the small amount of Rh (III) on the surface, it is not visible which functional groups are involved