Synthesis, Crystal Structure and Vibrational Characterization of Cesium Carbonate Triperoxido Hydrate, Cs$_2$CO$_3$ · 3 H$_2$O

Introduction
Carbonate peroxo compounds such as Na$_2$CO$_3$ · 1.5 H$_2$O$_2$[1] are well known as bleaching agents. The oxidizing effect of these so-called “percarbonates” is also used in chemical treatments. In addition to this usage, reactions of percarbonates are ecologically more harmless than those with perborates, which were usually used as bleaching agents in the past.

By variation of the cation it is possible to achieve new alkali metal carbonate peroxo hydrates. In this publication we present the structure of a new cesium carbonate triperoxido hydrate, Cs$_2$CO$_3$ · 3 H$_2$O$_2$.

Experimental
The title compound was prepared by adding cesium carbonate to cold, concentrated hydrogen peroxide (ca 76% solution). The resulting solution was layered with ethanol (approximately half the volume of the solution) and allowed to stand at -15°C. After a few days Cs$_2$CO$_3$ · 3 H$_2$O$_2$ precipitated. Due to the fact, that the obtained product is unstable at room temperature, the structure was verified by X-ray structure analysis and Raman spectroscopy at low temperatures (223 K).

Structure description
Cesium carbonate triperoxido hydrate crystallizes in the orthorhombic space group Pnma (No. 56) with eight formula units per unit cell and cell parameters a = 5.859(1) Å, b = 16.826(2) Å, c = 17.651(2) Å and V = 1798.82(8) Å (Tab. 1).

The crystal structure consists of three crystallographically different cesium ions, one carbonate group and four hydrogen peroxide molecules, which are involved in a hydrogen bonding network. The corresponding bond lengths and angles are presented in Tab. 2.

In Fig. 1 the crystal structure is shown along [001]. Along a-axis two layers of [H$_2$O$_2$]CO$_3$(H$_2$O)$_4$(Cs) are connected by one layer of [H$_2$O$_2$]CO$_3$(Cs)$^+$, which is the coordination number of cesium ions coordantion by eight oxygen atoms (Tab. 2). In Fig. 2 and 3 the coordination polyhedra of the cesium ions are presented. The Cs$^+$ polyhedra are connected by hydrogen peroxide molecules. The face-sharing Cs$_2$Cs$^+$ polyhedra are connected by H$_2$O$_2$ molecules to adjacent Cs$_2$Cs$^+$ polyhedra on both sides.

The title compound crystallizes in the same orthorhombic space group as the known rubidium carbonate triperoxido hydrate, Rb$_2$CO$_3$ · 3 H$_2$O$_2$ and shows similairities in the structure setting.

### References

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