



ABSTRACT

Combustion of citrate complex has been a popular choice to synthesize nanocrystals of transition metal oxides in a single-step process. The amount of citric acid used for combustion is conventionally calculated based on the total valence of the oxidizing and reducing agents while keeping the equivalent ratio unity such that combustion energy is a maximum. This chapter demonstrates by employing quantum chemical calculations that the amount of citric acid could be reduced to nearly half if prepared for appreciable amounts. Transition metal oxides belong to quaternary double perovskites, with general formula $Ba_2REsB_6O_6$ (RE=Rare-earth), have been synthesized as nanocrystals as examples to validate the calculations.

Keywords: Perovskites, Synthesis, Characterization, Combustion.

6.1 Introduction

Perovskites-type oxides, routinely called Perovskites, have attracted considerable attention in many applied and fundamental areas of solid-state science and advanced materials research because of their technological potentials and academic interest. Traditionally, the perovskite oxides are prepared through solid state reaction of metal oxides and/or carbonates at elevated temperatures – a process called calcination. However, the resulting powder suffers from several drawbacks including:

- a. Incomplete reaction of components because the starting chemicals are micron sized granules thereby resulting in inferior phase homogeneity.
- b. Coarse grained powders of the final calcined ceramic due to prolonged high temperature processing which lead to poor sinterability.