MS15-2-13 Charge-density studies of single and transient (single to double) boron-oxygen bonds #MS15-2-13

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Abstract
Issues in boron chemistry are still less described than those of the chemistry of carbon. One of such issue seems to be bonds between boron and oxygen. It is already known that except singular, double and triple B-O bonds, there are also claimed a transient type between a single and double B-O bonds [1]. To analyze this phenomena topologically, DFT calculations and electron localization function (ELF) were adopted on wide set of relatively simple molecules containing boron [2,3]. Those theoretically optimized structures were also characterized from the point of view of properties at their bond critical points (BCPs). In this work, on the basis of $(H_4B_4O_9)^{2-}$ ion, we would like to look deeper into the phenomenon of existence of single and multiple bonds. Presented result originate from high-resolution, single crystal, X-ray diffraction experiment. High quality of collected data allowed to obtain experimental charge density distribution. Multipole model refinement according to Hansen-Coppens theory was adopted.
In a nutshell, the ion $(H_4B_4O_9)^{2-}$, which is a component of $(NH_4)_2B_4O_5(OH)_4$ x $2H_2O$ crystal structure, has two types of boron-oxygen bond, i.e. single B-O bond and the other one intermediary between single and double B-O bond. Differences between those two bond types are visible not only cause they differ by their lengths but also a topology of electron density distribution differs. Experimental results based on multipole model refinement give excellent agreement with theoretical DFT calculation as well as with literature data. Properties such as electron density and Laplacian of electron densitycal obtained at bond critical points for both types of B-O bonds could work also as a kind of hint helping us to categorise B-O bonds previously reported in the literature (in the case when electron density and Laplacian at bond critical points are known).

References
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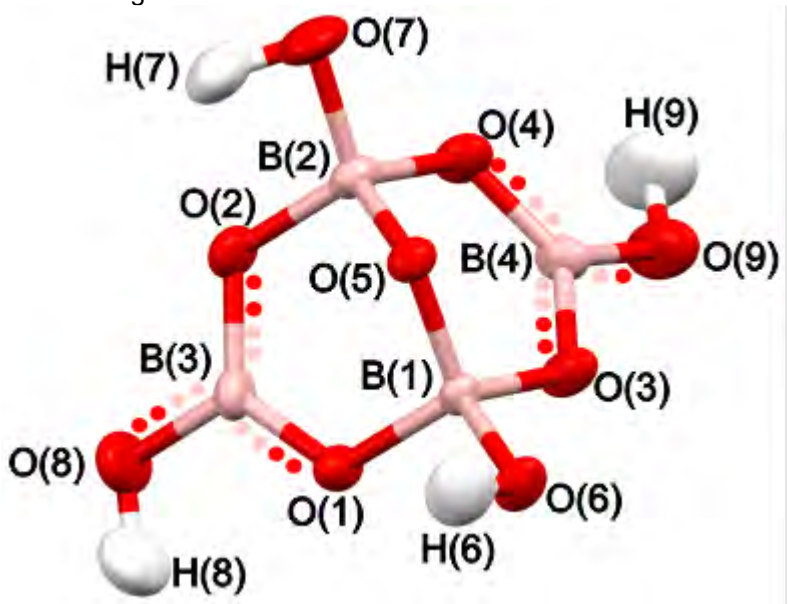
The investigated ion.



Laplacian of the experimental electron density.