New structural properties of trees with minimal atom-bond connectivity index

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The *atom-bond connectivity (ABC) index* is a degree-based graph topological index that found chemical applications, including those of predicting the stability of alkanes and the strain energy of cycloalkanes. Several structural properties of the trees with minimal *ABC* index were proved recently, however the complete characterization of the minimal-ABC trees is still an open problem. It is known that minimal-ABC trees can have at most one pendent path of length 3. It is also known that the minimal-ABC trees that have a pendent path of length 3 do not contain so-called B_k-branches, with $k \geq 4$, and do not contain more than two B_2-branches. Here, we improve the later result by showing that minimal-ABC trees of order larger than 168 and with a pendent path of length 3 do not contain B_2-branches.

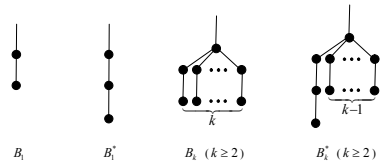

Figure 1: The B_k-branch for $k \geq 1$, and B_k^*-branch for $k \geq 1$.

Moreover, we show that trees with minimal ABC index with a pendent path of length 3 do not contain B_1-branches.

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