Li<inf>7</inf>(BH)<inf>5</inf>+: a new thermodynamically favored star-shaped molecule

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The potential energy surfaces (PESs) of Li<inf>n</inf>(BH)<inf>5</inf>n-6 systems (where n = 5, 6, and 7) were explored using the gradient embedded genetic algorithm (GEGA) program, in order to find their global minima conformations. This search predicts that the lowest-energy isomers of Li<inf>6</inf>(BH)<inf>5</inf> and Li<inf>7</inf>(BH)<inf>5</inf>+ contain a (BH)<inf>5</inf>6- pentagonal fragment, which is isoelectronic and structurally analogous to the prototypical aromatic hydrocarbon anion C<inf>5</inf>H<inf>5</inf>-. Li<inf>7</inf>(BH)<inf>5</inf>+, along with Li<inf>7</inf>C<inf>5</inf>+, Li<inf>7</inf>Si<inf>5</inf>+ and Li<inf>7</inf>Ge<inf>5</inf>+, joins a select group of clusters that adopt a seven-peak star-shape geometry, which is favored by aromaticity in the central five-membered ring, and by the preference of Li atoms for bridging positions. The theoretical analysis of chemical bonding, based on magnetic criteria, supports the notion that electronic delocalization is an important stabilization factor in all these star-shaped clusters. This journal is © the Owner Societies.