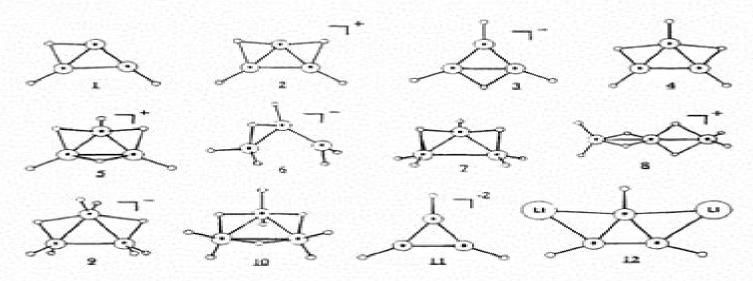
#### THE AROMATICITY IN THREE MEMBERED BORON SPECIES.

#### A.A. Korkin, 'M.L. McKee' and P.v.R. Schleyer'

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Department of Chemistry, Auburn University, Auburn, Alabama 36849-5312

The considerable current interest in three membered boron rings is documented by numerous experimental and theoretical papers. Our ab initio study of B,H, (1), B,H, (2), B,H, (3), B,H, (4), B,H, (5), B,H, (6), B,H, (7), B,H, (8), B,H, (2), B,H, (9), B,H, (10), B,H, (11), and B,H,Li, (12) summarizes and extends earlier investigations. We have elucidated: 1) the potential energy surfaces of B,H, species (1-10) at MP2/6-31+G'; 2) and have estimated the aromatic stabilization energies (SEs) of 3-5, 11 and 12.



We demonstrate that the aromatic SEs in 1-5, 10 and 11 approach the large value (78 kcal/mol [1]) in the  $2\pi$  electron aromatic cyclopropenium ion. The lowest energy structures of the electron and hydrogen deficient three boron hydride ions and molecules considered are governed by their aromatic stabilizations.

[1] (a) A.A. Korkin, M.N. Glukhovtsev, P.v.R. Schleyer Int. J. Quant. Chem., 1992, 46, 137; (b) U.v. Arx, R. Lauber, R. Keese, A.A. Korkin, P.v.R. Schleyer Angew. Chem. (submitted for publication).

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Fukushima, Young-Wook Kim, Kiyoshi
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