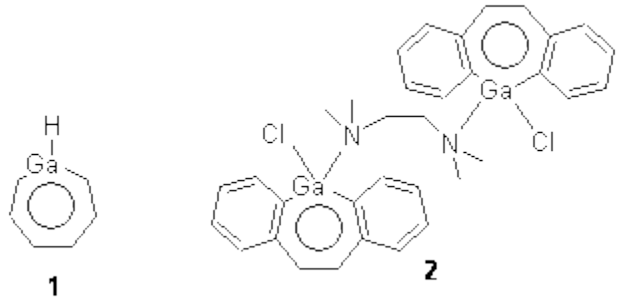
GALLEPIN

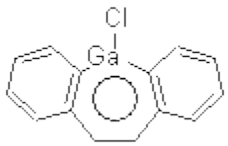
Robinson and Schleyer report the synthesis of and computations on the novel structure gallepin **1**.[1]This is the gallium analogue of tropyllium, the prototype of a seven-member aromatic ring. Robinson actually prepared the bis-benzannulated analogue **2**, which is found to coordinate to TMEDA in the crystal.



1 **2**

Schleyer computed (B3LYP/LANL2DZ) the gallepin portion of **2** in its naked form **3** and associated with trimethylamine **4**. The crystal structure of **2** reveals that the 7 member ring is boat-shaped, and this is reproduced in the computed structure of **4**. Interestingly, the naked gallepin is planar, suggestive of an aromatic structure. $NICS_{\pi ZZ}$ computations were performed to gauge the aromaticity of these compounds. The value for the 7-member ring is -9.0 in **4** and -9.9 in **3**, indicating aromatic character. These values are less then in the parent gallepin **1**, which has a value of -15.3, but this is the normal type of diminishment expected from benzannulation.

But borapin has a $NICS_{\pi ZZ}$ substantially more negative (-27.7) and so gallepins are less aromatic than borapins. Nonetheless, it is very interesting that aromaticity can be extended in this interesting way – different heteroatom and different ring size.



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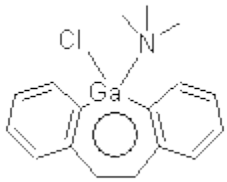

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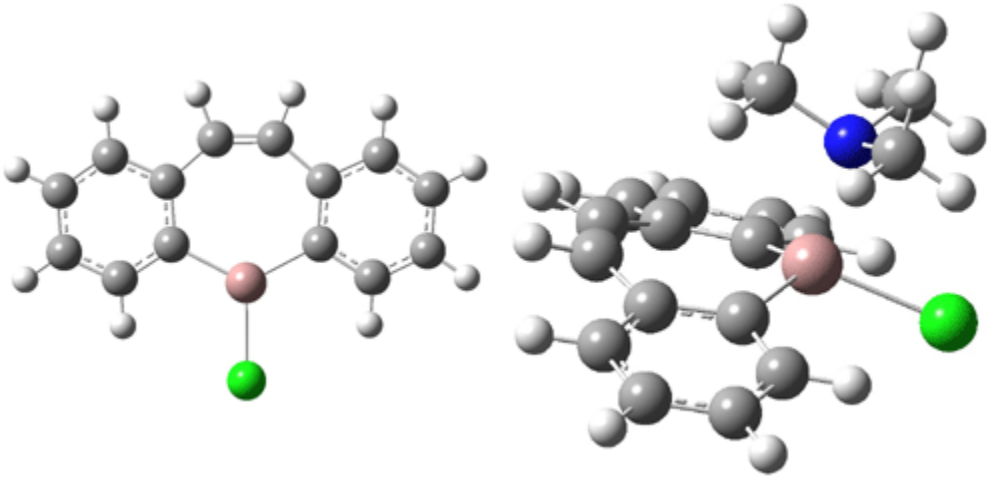

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