

Spontaneous Formation of Strained Anti-Bredt Bridgehead Alkenes upon Computational Geometry Optimization of Bicyclic β -Halo Carbanions

Gary W. Breton* and Jazmine V. Riddlehoover

Department of Chemistry and Biochemistry, Berry College, 2277 Martha Berry HWY, Mount Berry, GA 30149, USA; jazmine.riddlehoover@vikings.berry.edu

* Correspondence: gbreton@berry.edu; Phone: 706-290-2661; fax: 706-238-7855

Supporting Information

1. Please find sample GAMESS output files corresponding to select optimizations performed as described in the manuscript with Br as leaving group. These may be viewed with any program capable of visualizing such as MacMolPlt (for MAC) and wxMacMolPlt (for Windows).

Included files (all with standard .out file names):

1a
1b
2a_endo
2b_endo
3a
3b
5a
5b
8a
8b
10a
10b
11a_exo
11a_endo
12aexo_exo
12aendo_exo
13aeq
13beq
15a
15b
16a
16b
17
18
19
20
21
22

2. Expanded basis set used in Spartan'20 calculations for molecules containing iodine:

Iodine_PVDZ_expandedbasisset.bas