

# Spontaneous Formation of Strained Anti-Bredt Bridgehead Alkenes upon Computational Geometry Optimization of Bicyclic $\beta$ -Halo Carbanions

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## 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*