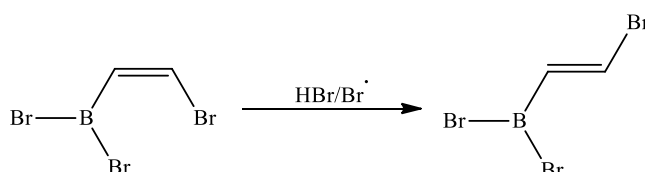


# A Quantum Chemical Study of Isomerization Step within Acetylene Bromoboration

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Haloboration reactions of alkynes represent key elements in many organic synthetic routes, as evidenced in a series of 21 papers by A. Suzuki through 1983-1992.<sup>1</sup> During an acetylene bromoboration reaction, (*Z*)-alkene is formed by the direct addition of boron tribromide to acetylene which undergoes a subsequent isomerization into (*E*)-dibromo(2-bromovinyl)borane cf. Figure 1.



**Figure 1:** *Z/E* isomerization of (*Z*)-dibromo(2-bromovinyl)borane.

Wang and Uchiyama have proposed a polar isomerization mechanism catalyzed by another  $\text{BBr}_3$  molecule with a barrier of ca.  $26 \text{ kcal mol}^{-1}$ .<sup>2</sup> This is in contrast with recent experimental findings obtained in our department.<sup>3</sup> The present study concentrates on an alternative mechanism initiated by a reaction of *Z*-alkene with the HBr molecule and with the radical  $\text{Br}\cdot$ , whose presence is expected due to the interaction with residual air humidity.

[1] Suzuki, A. *Heterocycles* 80 (2010) 15.

[2] Wang, C., Uchiyama, M. *Eur. J. Org. Chem.* (2012) 6548.

[3] Polasek, J., *Bachelor's thesis, MU Brno* (2014).