

## What is the Most Stable Isomer of Ammonia – Methyl Trifluorogermane Complex ( $\text{H}_3\text{N}-\text{GeF}_3-\text{CH}_3$ )?

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We have undertaken a computational study (m06/6-31+G(d)) of the stability of various isomers of  $\text{H}_3\text{N} - \text{GeF}_3-\text{CH}_3$ , considering not only coordination site, axial or equatorial, but also the various conformations for each of four possible configurations (Figure 1). We will assess the stability by relative energies and the occurrence of imaginary frequencies. Another key issue is the Lewis acid strength of  $\text{GeF}_3\text{CH}_3$  relative to  $\text{GeF}_4$ . We expect the methyl group to reduce the acid strength, and we will compare to results for  $\text{H}_3\text{N}-\text{GeF}_3-\text{CH}_3$  to those for  $\text{H}_3\text{N}-\text{GeF}_4$ . Recent results for analogous compounds and those from higher levels of theory will also be discussed.

