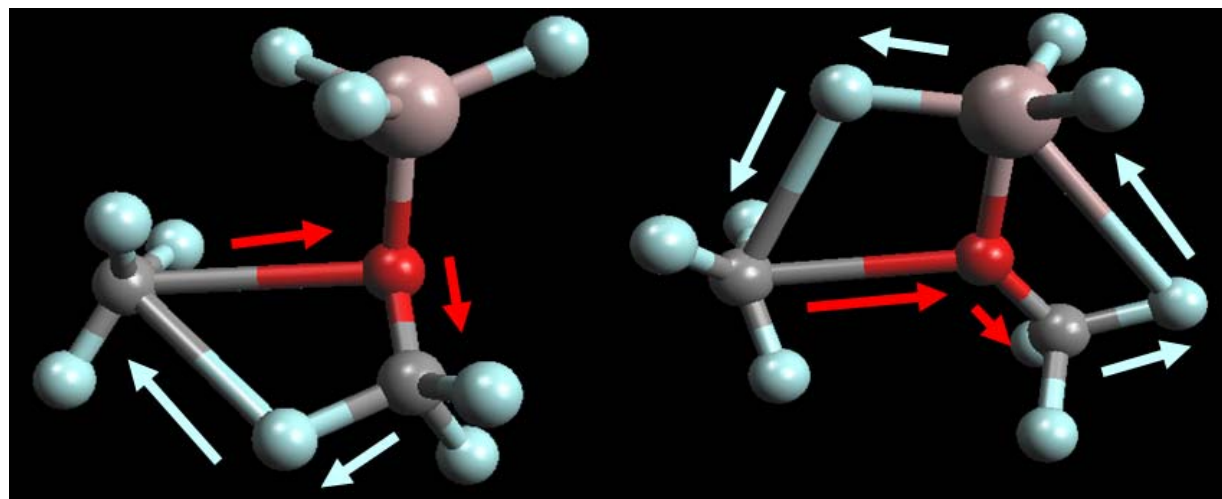
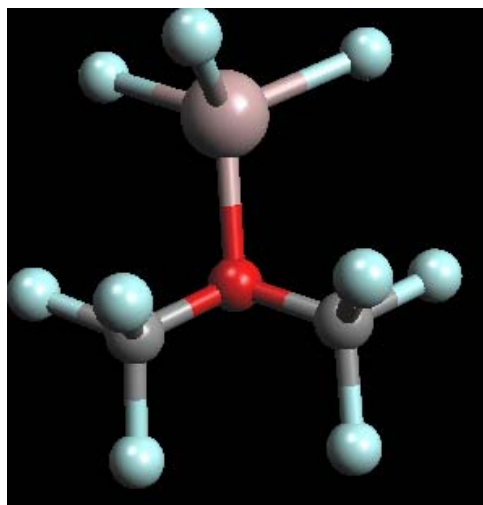


# Reaction Pathways and Kinetics



old transition state

new transition state

red: O;  
blue: F;  
dark grey: C;  
light grey: Al

Two fundamentally different transition structures identified  
In TS<sub>1</sub>, AlF<sub>3</sub> strictly stabilizes O  
In TS<sub>2</sub>, AlF<sub>3</sub> acts as a carrier of F from one C to another C

The new transition state lowers the activation energy from 228 to 199 kJ/mole, making the reaction 100,000 times faster at room temperature.

Jiang, B., Keffer, D.J., Edwards, B.J., J. Phys. Chem. A 112(12) 2008 pp. 2604-2609.