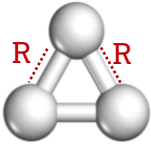


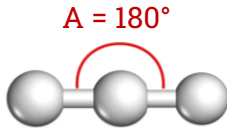
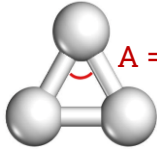
1) Dissociation Profiles



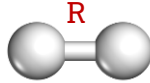
$R = 0.69 \text{ to } 2.39 \text{ \AA}, \Delta R = 0.1 \text{ \AA}.$



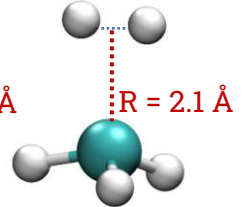
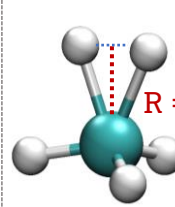
$A = 60 \text{ to } 180^\circ, \Delta A = 30^\circ.$



$R = 0.6 \text{ to } 2.7 \text{ \AA},$
 $\Delta R = 0.1 \text{ \AA}.$



$R = 1.3, 1.4, 1.6, 1.8, \text{ and } 2.1 \text{ \AA}$



2) Active Spaces

H_2 : 2 occupied and 2 unoccupied orbitals.

H_3^+ : 2 occupied and 4 unoccupied orbitals.

CH_5^+ : 2, 4, 6 and 8 occupied and unoccupied orbitals.



3) Classical Computing Methods

Theoretical level: CISD/STO-3G.

Program: Gaussian 09.



4) Quantum Simulator (VQE)

Ansätze: UCCSD, GateFabric, GRSD, k-UpCCGSD, HE-A, HE-B, HE-C and EHA.

Basis Set: STO-3G.

Library: PennyLane.