

Potential energy curve for Hydrogen Fluoride

$c \in [1.1, 1.1, 1.0, 1.0, 0.9, 0.9, 0.8, 0.8, 0.7, 0.7, 0.6, 0.5, 0.5]$

Energy (Hartree)

-99.4
-99.6
-99.8
-100.0
-100.2

2

3

4

5

Atomic distance (Bohr)

- EC (13 points)
- EC (10 points)
- EC (7 points)
- EC (4 points)
- RHF,cc-pVTZ
- CCSD,cc-pVTZ