

Atomic Units

$$1\text{H} = 2625.5 \text{ kJ/mol}$$

$$1\text{H} = 627.52 \text{ kcal/mol}$$

$$1\text{H} = 27.2116 \text{ eV}$$

$$1\text{H} = 219,474.6 \text{ cm}^{-1}$$

$$a_0 = 0.529 \text{ \AA} = 52.9 \text{ pm}$$

Conversions

$$1 \text{ cal} = 4.184 \text{ J}$$

$$1 \text{ eV} = 96.485 \text{ kJ/mol}$$

$$1 \text{ eV} = 8065.5 \text{ cm}^{-1}$$

$$1 \text{ cm}^{-1} = 11.962 \text{ J/mol}$$

$$RT = 2.4790 \text{ kJ/mol} \quad \text{at } 298.2\text{K}$$

$$kT/hc = 207.226 \text{ cm}^{-1} \quad \text{at } 298.2\text{K}$$

Example: Ground state energy of H atom = $H / 2$

$$E_1 = -13.6 \text{ eV}$$

$$E_1 = -1312 \text{ kJ/mol}$$

$$E_1 = -109,737 \text{ cm}^{-1} = R_\infty$$

$$E_1 = -313.8 \text{ kcal/mol}$$