

- ①. Running HF/3-21G calculations for water, explaining the definition of the basis set in terms of primitive GTOs.

Use: GFPrint option

- ②. File 2-06 from G03 folder, energy calculation of C<sub>60</sub>, use

SCF = Tight option.

Requests stricter convergence criteria for the SCF wavefunction

- ③ Running RHF/3-21G on O<sub>2</sub> with geometry optimization (Opt job type)

$$E = -148.687 \text{ a.u.}$$

$$R_{O-O} = 1.2419 \text{ \AA}$$

Testing SCF stability: Stable = Opt

RHF → UHF instability!

Run UHF/3-21G

Opt (Spin = Triplet)

$$E = -148.769$$

$$R_{O-O} = 1.2396 \text{ \AA}$$

$$\begin{aligned} \Delta E &= E_{\text{singlet}} - E_{\text{triplet}} = \\ &= 52 \text{ kcal/mol} \end{aligned}$$

④. Dissociation of hydrogen from  $H_2O$ : L2-2

Job Type: Scan

Method: HF/3-21G

Edit file:

OH PES Scan

B1	0.7	10	0.1
	<u>        </u>	<u>        </u>	<u>        </u>
	initial	number	step
	distance	of points	