

In this assignment you will calculate the energy of the wavefunction

$$\psi(1,2,3,4) = C_1 \mathcal{A}1s\alpha1s\beta2s\alpha2s\beta + C_2 \mathcal{A}1s\alpha1s\beta2p_x\alpha2p_x\beta \\ + C_3 \mathcal{A}1s\alpha1s\beta2p_y\alpha2p_y\beta + C_4 \mathcal{A}1s\alpha1s\beta2p_z\alpha2p_z\beta$$

Where 1s and 2s are the 1s and 2s orbitals of <sup>1</sup>S Be and the 2p<sub>i</sub> are the Be 2p orbitals.

Note that by symmetry C<sub>2</sub> = C<sub>3</sub> = C<sub>4</sub>. The required integrals have been calculated using the Gaussian program and are collected below.