**QM Lab 2 - Quantum Espresso**

1. Total energy as a function of cutoff energy, which ranged from 10 to 140 Ryd by increments of 10 Ryd. The convergence value was calculated to be 110 Ryd. This means the change from 100 to 110 Ryd is less than 5 meV/atom.

Chart, histogram

Description automatically generated

1. Total energy as a function of k-point grid size. The k values ranged from 1 to 8 by increments of 1, resulting in the grid sizes 1, 3, 4, 8, 10, 16, 20, and 29 respectively. Convergence was calculated to occur at a grid size of 20 using the same method as the previous problem.

Chart

Description automatically generated

1. A C atom was displaced by +0.05 in the z direction resulting in the plotted force on atom 1 as a function of the cutoff energy. The force on atom 2 is equal in magnitude but the opposite sign, for this reason only atom 1 is plotted. Convergence was calculated with the condition that a change in force of less than 10 meV/Angstrom signifies convergence. The cutoff energy value for convergence is 100 Ryd.

Chart, line chart

Description automatically generated

1. Total energies for both the lattice parameters of 6.74 and 6.70 Bohr were calculated with cutoff energies ranging from 10 to 140 Ryd by increments of 10 Ryd. Plotted below is the difference between these total energies for each lattice parameter versus the respective cutoff energy. The condition for convergence is a change less than 5 meV/atom. This first occurs at a cutoff energy of 30 Ryd, but larger changes occur at 40 and 50 Ryd. Thus the total energy is converged at a cutoff energy value of 60 because all subsequent changes are less than 5 meV/atom.

Chart, line chart

Description automatically generated