In this program, the minimization of energy from a given molecular structure is calculated. The molecular structure consists only of hydrogen and carbon atoms. This main program is combined with four other modules: Atommod.90, Calculationmod.f90, Energymod.f90 and Minimizationmod.90. Bondlength function calculates the distance between two atoms using their cartesian coordinates. AssignBonds subroutine determines which atoms are bonded with a certain threshold and adds the bonds to the BondsArray. The CheckBonds array stores which bonds have been made so that no duplicates occur. Subroutine AddBond stores the bonds made in the AssignBonds subroutine in an array. A DummyArray is created to temporarily store the added bond. Subroutine BendAngle calculates the angle between three atoms. The first if statement makes sure the angle is being calculated with a carbon atom as centre atom. The other statements make sure that the other two atoms are connected to the same centre atom. Subroutine AddAngle stores the angle made in the BendAngle subroutine in an array. A DummyArray is created to temporarily store the added angle. Subroutine TorsionAngle calculates the torsionangle over four atoms, with two carbon atoms as the centre atoms. First, via the if statements is determined which connections can be made and makes sure no duplicate angles are calculated. Of these connections, vectors are made which are used to calculate the torsion angle which are stored The CrossProduct function calculates the cross product of two vectorsin an array. Subroutine AddTorsionAngle stores the angle made in the TorsionAngle subroutine in an array. A DummyArray is created to temporarily store the added torsion angle. The stretch energy function is a function of all pairs of atoms in the molecule. The BendingEnergy function calculates the bending energy of all triples of atoms. The TorsionEnergy function calculates the energy of all torsional angles. The NonBondedEnergy function calculates the non bonded energy of the atoms which can be divided into the Van-der Waals interactions and the electrostatic interactions. The if statements determine the use of the correct variables with the corresponding atom interactions. The j > i statements make sure that the Van der Waals interactions are counted double and the electrostatic interactions once. The TotalEnergy function calculates the total energy of the molecule by the sum of its contributions. Subroutine InputReader reads the text file and stores the coordinates in the Molecule array. The ParameterInput subroutine defines the used variables. Subroutine Minimization determines whether the new energy value is lower than the previous value. If the value is lower, the new energy value and coordinates are accepted, if the value is higher than the previous value, the value is rejected, and new coordinates are calculated. The algorithm is terminated by calculating a rejection rate. Subroutine NewCoordinates calculates the new random coordinates for one atom at the time.