

Molecular Mechanics project

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The program will be divided into three modules.

- The **Atom** module
 - Subroutine to read/ store the input data
 - Creates the atom type
 - declaring the parameters in data block
- The **Energy** module
 - Total energy function/subroutine which calculates the total energy
 - Functions/subroutines to calculate the contributions to the total energy
- The **Minimalization** module
 - Moves the configuration to calculate a new energy position
 - Checks the energy difference between old and new value
 - Terminates if multiple iterations of no energy difference are achieved

