Input.d

Input file input.d has the following structure:

Line 1

- The total number of time steps to take.
- The number of steps to take before doing basic output (i.e. calling write_data2 in read_write.f.)
- Thermostat selector KFLAG,
  - -1 Langevin;
  - 0 none;
  - 1 Berendsen;
  - 2 zero velocity;
  - 3 Evans-Hoover;
  - 5 Berendsen after corrector;
  - 6 minimize energy;
  - 8 rescale to minimize energy

  Briefly, use -1 for isothermal and 0 for adiabatic.
- The number of steps to take before calling xmol.f to write abbreviated coord.d data (only position) to file xmol.d and energy per atom to file pair_energy.d

Line 2

- Seed for the random number generator. Ignored if a saved random number generator is found at the end of file coord.d.
- Allowed motion of the atoms before we rebuild the neighborhood lists of all atoms. Angstrom.
- Desired temperature in Kelvin, for the thermostats.

Line 3

- Switch; set to 1 for REBO (C,H,Si,Ge), to 2 for tight-binding for C

Lines 4...

Each line is of the form

- Atom number.
- Atom mass, in AMU.
- Lennard Jones parameter epsilon
- Lennard Jones parameter sigma

Records are ignored if the atom number is negative. Otherwise the atom mass will overwrite the values set in subroutine setin.
