Coord.d

Atom state file coord.d has the following structure:

Line 1

- A descriptive header string

Line 2

- The number of atoms NP.
- Variable IDUM. IDUM is set to 0 by make_tube, and to 3 by xmol.f. IDUM was undefined in overwr.f and read_write.f, so I set it to 0 there, which is what some compilers would (improperly) do by default anyway. As a result, when IDUM is 3, the .d file does not have the Nordsieck parameters beyond the first, position, in it.
- 0 (an unused variable)
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Line 3

- The total time that the simulation has run before creating this file.
- The time step in picoseconds.

Line 4

- The size of the periodic box in the x-direction. Set to a large number such as 1.d20 to get a nonperiodic computation. Angstrom.
- The size of the periodic box in the y-direction. Set to a large number such as 1.d20 to get a nonperiodic computation. Angstrom.
- The size of the periodic box in the z-direction. Set to a large number such as 1.d20 to get a nonperiodic computation. Angstrom.

Next NP lines:
Each line is of the form

- Atom counter.
- Atom number.
- Atom x-position in A.
- Atom y-position in A.
- Atom z-position in A.
- Switch, normally 1. Set it to 2 to prevent the atom from moving, to anything else to prevent the thermostat to affect the atom.

Next NP lines:
Each line is of the form

- Atom counter.

- Atom x-velocity component in A/ps.
- Atom y-velocity component in A/ps.
- Atom z-velocity component in A/ps.

Next NP lines:

Each line is of the form

- Atom counter.
- Atom x-Nordsieck parameter 3 in A.
- Atom y-Nordsieck parameter 3 in A.
- Atom z-Nordsieck parameter 3 in A.

Next NP lines:

Each line is of the form

- Atom counter.
- Atom x-Nordsieck parameter 4 in A.
- Atom y-Nordsieck parameter 4 in A.
- Atom z-Nordsieck parameter 4 in A.

Next NP lines:

Each line is of the form

- Atom counter.
- Atom x-Nordsieck parameter 5 in A.
- Atom y-Nordsieck parameter 5 in A.
- Atom z-Nordsieck parameter 5 in A.

Note that the 5th Nordsieck parameter is not used and will always be zero.
