The mvac.out output file

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Brief Description

This file contains the data of mass-weighted velocity autocorrelation (VAC). The calculation itself is discussed in the VAC page.

The keyword which produces the current file

- compute_dos in run.in

File format

- The file is organized as follows:
    - column 1: correlation time (in units of ps)
    - column 2: VAC (in units of $Å^2/ps^2$) in the x direction
    - column 3: VAC (in units of $Å^2/ps^2$) in the y direction
    - column 4: VAC (in units of $Å^2/ps^2$) in the z direction

Tips

- Only the selected group in the compute_dos keyword is included in this output.

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