

POSCAR File Structure in VASP

Section	Number of Lines	Required?	Content	Comments
Scaling factor(s)	1	Mandatory	Universal lattice scaling factor or in	
Lattice	3	Mandatory	Three lines defining the lattice vect	
Species names	1	Optional	Species of the present ions, order s	
Ions per species	1	Mandatory	Number of ions of each species, or	
Selective dynamics	1	Optional	Enables selective dynamics feature	
Ion positions	1 + #atoms	Mandatory	Ion positions in direct or Cartesian	
Lattice velocities	8	From CONTCAR only	Lattice vectors and their velocities.	
Ion velocities	1 + #atoms	Optional	Initial velocities for all ions.	
MD extra	Variable	From CONTCAR only	Predictor-corrector coordinates.	