Table 1. Structure of the input file `root_chem.dat` (free format)

Line	First Value	Second Value	Third Value	Fourth Value	
1	nº of phases (*nphases*)	nº of components (*nc*)			
2	Blank line				
3	Name of the liquid phase	Numeric name of the liquid phase: 1	Total nº of species in the liquid phase		
3 + 1	Name species in liquid phase #1	Ion size param. $\hat{a}$ of the species #1 ($\hat{a}_1$)	Ion size param. $\hat{b}$ of the species #1 ($\hat{b}_1$)	Charge number of the species #1 (z_1)	
⋮	⋮	⋮	⋮	⋮	
3 + …	Name species in liquid phase #last	Ion size param. $\hat{a}$ of the species i ($\hat{a}_i$)	Ion size param. $\hat{b}$ of the species i ($\hat{b}_i$)	Charge number of the species i (z_i)	
	Blank line				
	Name of the gas phase	Numeric name of the gas phase: 2	Total nº of species in the gas phase		
	Name species in gas #1	0	0	0	
⋮	⋮	⋮	⋮	⋮	
	Name of species in gas phase #last	0	0	0	
	Blank line				
	Name of the solid phase	Numeric name of the solid phase: 3	Total nº of species in the gas phase		
	Name species in solid #1	0	0	0	
⋮	⋮	⋮	⋮	⋮	
	Name of species in solid phase #last	0	0	0	
… + …	Blank line				
…	number of chemical equilibrium equations (nr_{equi})				
	Blank line				
…	number of chemical kinetic equations (nr_{kin})				
	Blank line				

Table 1. Structure of the input file `root_chem.dat` (free format) (continuation)

Line	First Value	Second Value	Third Value	Fourth Value	Fifth Value
	S(1,1)	S(1,2)	…	S(1, *ns_total*)	0 `irtype(1)`
	k parameter of chemical reaction 1				
	Blank line				
	S(2,1)	S(2,2)	…	S(2,*ns_total*)	0
	k parameter of chemical reaction 2				
	Blank line				
⋮	⋮	⋮	…	⋮	
	Blank line				
	S(nr_{equi},1)	S(nr_{equi},2)		S(nr_{equi}, *ns_total*)	0 `irtype(`nr_{equi}`)`
	k parameter of chemical reaction nr_{equi}				
	Blank line				
	S(nr_{equi}+*1*,1)	S(nr_{equi}+*1*,2)		S(nr_{equi}+*1*, *ns_total*)	1 `irtype(`nr_{equi}+*1*`)`
	akinetics (1) parameter of chemical reaction nr_{equi}+*1*	akinetics (2) parameter of chemical reaction nr_{equi}+*1*		akinetics (nparamk) parameter of chemical reaction nr_{equi}+*1*	
	Blank line				
⋮	⋮	⋮	…	⋮	
	Blank line				
	S(nr_{equi}+nr_{kin},1)	S(nr_{equi}+ nr_{kin},2)		S(nr_{equi}+ nr_{kin}, *ns_total*)	1 `irtype(`nr_{equi}+ nr_{kin}`)`
	akinetics (1) parameter of chemical reaction nr_{equi}+ nr_{kin}	akinetics (2) parameter of chemical reaction nr_{equi}+ nr_{kin}		akinetics (10) parameter of chemical reaction nr_{equi}+ nr_{kin}	
	Blank line				
	U(1 , 1)	...	U(1 , *ns_total*)		
	⋮	...	⋮		
	U(*nc* , 1)	...	U(*nc* , *ns_total*)		
	Blank line				

Table 1. Structure of the input file `root_chem.dat` (free format) (continuation)

Line	First Value	Second Value	Third Value	Fourth Value	Fifth Value
	Phase indicator for each species: *isphase(1)*				
	⋮				
	isphase(ns_total)				
	Blank line				
	Index of primary species (1)				
	⋮				
	Index of primary species (*nc*)				
	Blank line				
	Index of secondary species (*nc*+1) (Only if there are secondary species)				
	⋮				
	Index of secondary species (*ns_total-nc*) (Only if there are secondary species)				