Table Documentation

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NOTE: Unless otherwise noted, columns are `NOT NULL`.

orders

PK	Column Name	Type	Description
✓	`id`	`INTEGER`	The order identifier
	`name`	`VARCHAR`	The name of the order
	`hash`	`VARCHAR`	A hash of the order file contents
	`eleanor_version`	`VARCHAR`	The version of eleanor used to run the order
	`raw`	`JSON`	The raw, JSON-encoded contents of the order

PK	Column Name	Type	Description
	`create_date`	`DATETIME`	The datetime at which the order was created

huffer

PK	Column Name	Type	References	Description
✓	`id`	`INTEGER`	`orders.id`	The huffer entry identifier corresponds to the order id
	`exit_code`	`INTEGER`		The exit code generated by the huffer (non-zero for failure)
	`zip`	`BLOB`		A zip archive of the input files used and output files generated when running the huffer. This includes a traceback when an error occurs

variable_space

PK	Column Name	Type	References	Unit	Description
✓	`id`	`INTEGER`			The variable space point identifier
	`order_id`	`INTEGER`	`orders.id`		The order id for which the point was generated
	`temperature`	`DOUBLE`		$^{\circ}C$	The temperature
	`pressure`	`DOUBLE`		bar	The pressure
	`exit_code`	`INTEGER`			The exit code generated by the kernel (non-zero for failure)
	`create_date`	`DATETIME`			The datetime when variable space was created
	`start_date`	`DATETIME`			The datetime when the equilibration started
	`complete_date`	`DATETIME`			The datetime when the equilibration completed

scratch

PK	Column Name	Type	References	Description
✓	`id`	`INTEGER`	`variable_space.id`	The scratch entry identifier corresponds to the variable space id
	`zip`	`BLOB`		A zip archive of the input files used and output files generated when equilibrating the variable space point. This includes a traceback when an error occurs

kernel

PK	Column Name	Type	References	Description
✓	`id`	`INTEGER`	`variable_space.id`	The kernel entry identifier corresponds to the variable space point
	`type`	`VARCHAR`		The type of the kernel used, e.g. `eq36`

PK	Column Name	Type	References	Description
	`settings`	`JSON`		A json-encoded object of the settings passed to the kernel

elements

PK	Column Name	Type	References	Unit	Description
✓	`id`	`INTEGER`			The element identifier, specific to the variable space point
	`variable_space_id`	`INTEGER`	`variable_space.id`		The id of the variable space point for which elemental molality was generated
	`name`	`VARCHAR`			The name of the element (atomic symbol)
	`log_molality`	`DOUBLE`		$\log molal$	The log molality of the element in the variable space solution

species

PK	Column Name	Type	References	Unit	Description
✓	`id`	`INTEGER`			The species identifier, specific to the variable space point
	`variable_space_id`	`INTEGER`	`variable_space.id`		The id of the variable space point for which the species molality/activity/fugacity was generated
	`name`	`VARCHAR`			The name of the species (formula)
	`value`	`DOUBLE`		variable	The log molality/activity/fugacity of the species in the variable space solution

aqueous_reactants

PK	Column Name	Type	References	Unit	Description
✓	`id`	`INTEGER`			The aqueous reactant identifier, specific to the variable space point
	`variable_space_id`	`INTEGER`	`variable_space.id`		The id of the variable space point for which the aqueous reactant amount and titration rate were generated
	`name`	`VARCHAR`			The name of the aqueous reactant
	`log_moles`	`DOUBLE`		$\log mole$	The log amount of the reactant to be reacted with the fluid
	`titration_rate`	`DOUBLE`		$mole/\xi$	The rate (in ξ) at which the reactant will be titrated into the fluid

element_reactants

PK	Column Name	Type	References	Unit	Description
✓	`id`	`INTEGER`			The element reactant identifier, specific to the variable space point

PK	Column Name	Type	References	Unit	Description
	variable_space_id	INTEGER	variable_space.id		The id of the variable space point for which the element reactant amount and titration rate were generated
	name	VARCHAR			The name of the element reactant
	log_moles	DOUBLE		$\log mole$	The log amount of the reactant to be reacted with the fluid
	titration_rate	DOUBLE		$mole/\xi$	The rate (in ξ) at which the reactant will be titrated into the fluid

fixed_gas_reactants

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The fixed gas reactant identifier, specific to the variable space point
	variable_space_id	INTEGER	variable_space.id		The id of the variable space point for which the fixed gas reactant amount and fugacity were generated
	name	VARCHAR			The name of the fixed gas reactant
	log_moles	DOUBLE		$\log mole$	The log amount of the reactant to be reacted with the fluid
	log_fugacity	DOUBLE		$mole/\xi$	The log fugacity of will be titrated into the fluid

gas_reactants

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The gas reactant identifier, specific to the variable space point
	variable_space_id	INTEGER	variable_space.id		The id of the variable space point for which the gas reactant amount and titration rate were generated
	name	VARCHAR			The name of the gas reactant
	log_moles	DOUBLE		$\log mole$	The log amount of the reactant to be reacted with the fluid
	titration_rate	DOUBLE		$mole/\xi$	The rate (in ξ) at which the reactant will be titrated into the fluid

mineral_reactants

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The mineral reactant identifier, specific to the variable space point
	variable_space_id	INTEGER	variable_space.id		The id of the variable space point for which the mineral reactant amount and titration rate were generated
	name	VARCHAR			The name of the mineral reactant

PK	Column Name	Type	References	Unit	Description
	log_moles	DOUBLE		$\log mole$	The log amount of the reactant to be reacted with the fluid
	titration_rate	DOUBLE		$mole/\xi$	The rate (in ξ) at which the reactant will be titrated into the fluid

special_reactants

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The special reactant identifier, specific to the variable space point
	variable_space_id	INTEGER	variable_space.id		The id of the variable space point for which the special reactant amount and titration rate were generated
	name	VARCHAR			The name of the special reactant
	log_moles	DOUBLE		$\log mole$	The log amount of the reactant to be reacted with the fluid
	titration_rate	DOUBLE		$mole/\xi$	The rate (in ξ) at which the reactant will be titrated into the fluid

solid_solution_reactants

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The solid solution identifier, specific to the variable space point
	variable_space_id	INTEGER	variable_space.id		The id of the variable space point for which the solid solution amount and titration rate were generated
	name	VARCHAR			The name of the solid solution
	log_moles	DOUBLE		$\log mole$	The log amount of the reactant to be reacted with the fluid
	titration_rate	DOUBLE		$mole/\xi$	The rate (in ξ) at which the reactant will be titrated into the fluid

solid_solution_reactant_end_members

PK	Column Name	Type	References	Description
✓	id	INTEGER		The solid solution end member id, specific to the solid solution
	solid_solution_reactant_id	INTEGER	solid_solution_reactants.id	The id of the solid solution for which this is an end member
	name	VARCHAR		The name of the end member
	fraction	DOUBLE		The mole-fraction of the end member in the solid solution

- CONSTRAINT fraction_in_range CHECK (0.0 <= fraction AND fraction <= 1.0)

special_reactant_compositions

PK	Column Name	Type	References	Description
✓	id	INTEGER		The special reactant composition identifier
	special_reactant_id	INTEGER	special_reactants.id	The id of the special reactant
	element	VARCHAR		The name of the element in the special reactant
	count	INTEGER		The stoichiometric count of the element in the special reactant

suppressions

PK	Column Name	Type	Nullable	References	Description
✓	id	INTEGER			The suprression identifier
	variable_space_id	INTEGER		variable_space.id	The id of the variable space point
	name	VARCHAR	✓		The name of the species/phase to suppress, e.g. H2O2, methane, olivine
	type	VARCHAR	✓		The type of species/phase to suppress, e.g. “solid solutions”

- CONSTRAINT suppressions_well_defined CHECK (name is not null or type is not null)

suppression_exceptions

PK	Column Name	Type	References	Description
✓	id	INTEGER		The suppression exception identifier
	name	VARCHAR		The name the species/phase to except, e.g. H2O2, methane, olivine
	suppression_id	INTEGER	suppressions.id	The id of the suppression for which to except

equilibrium_space

PK	Column Name	Type	Nullable	References	Unit	Description
✓	id	INTEGER				The equilibrium space point identifier
	variable_space_id	INTEGER	✓	variable_space.id		The id of the variable space point for which the equilibrium was found
	stage	VARCHAR				The stage of the equilibration, e.g. eq3, eq6
	log_xi	DOUBLE	✓		unitless	The logarithm of the ξ-step at which this equilibrium was found
	temperature	DOUBLE			C	The temperature

PK	Column Name	Type	Nullable	References	Unit	Description
	pressure	DOUBLE			bar	The pressure
	"pH"	DOUBLE			unitless	The pH on the NBS scale
	"log_fO2"	DOUBLE			log bar	The logarithm of the oxygen (O_2) fugacity
	log_activity_water	DOUBLE			unitless	The logarithm of the activity of water
	mole_fraction_water	DOUBLE			unitless	The mole fraction of the fluid that is water
	log_gamma_water	DOUBLE			unitless	The logarithm of the activity coefficient of water
	"Eh"	DOUBLE			volt	The redox potential
	pe	DOUBLE			unitless	The negative logarithm of the hypothetical electron activity
	"Ah"	DOUBLE			kcal	The redox affinity
	"pcH"	DOUBLE	✓		unitless	The pH based on the molarity of the hydrogen ion (H+)
	"pHCl"	DOUBLE	✓		unitless	The pHCl = pH + pCl, the sum of the negative logarithms of the activity of H+ and Cl- respectively
	log_ionic_strength	DOUBLE			log molal	The logarithm of the ionic strength of the solution
	log_stoichiometric_ionic_strength	DOUBLE			log molal	The logarithm of the stoichiometric ionic strength of the solution
	log_ionic_asymmetry	DOUBLE			log molal	The logarithm of the ionic asymmetry
	log_stoichiometric_ionic_asymmetry	DOUBLE			log molal	The logarithm of the stoichiometric ionic asymmetry

PK	Column Name	Type	Nullable	References	Unit	Description
	osmotic_coefficient	DOUBLE			unitless	The osmotic coefficient of the solution
	stoichiometric_osmotic_coefficient	DOUBLE			unitless	The stoichiometric osmotic coefficient of the solution
	log_sum_molalities	DOUBLE			molal	The logarithm of the sum of the molalities of all non-water species in the solution
	log_sum_stoichiometric_molalities	DOUBLE			molal	The logarithm of the sum of the stoichiometric molalities of all non-water species in the solution
	charge_imbalance	DOUBLE			eq	The charge imbalance of the solution
	expected_charge_imbalance	DOUBLE	✓		eq	The charge imbalance of the solution before mass transfer
	sigma	DOUBLE	✓		eq	
	charge_discrepancy	DOUBLE	✓		eq	The charge discrepancy of the solution
	anions	DOUBLE	✓		eq/kg H2O	The total charge of anions per kilogram of water (z_+)
	cations	DOUBLE	✓		eq/kg H2O	the total charge of cations per kilogram of water (z_-)
	total_charge	DOUBLE	✓		eq/kg H2O	The total charge of the solution per kilogram of water ($z_\pm = z_+ - z_-$)
	mean_charge	DOUBLE	✓		eq/kg H2O	The mean charge of the solution per kilogram of water ($0.5 z_\pm$)
	solute_mass	DOUBLE				The total mass of all dissolved species
	solvent_mass	DOUBLE				The mass of the solvent (water)
	solution_mass	DOUBLE				The mass of the solution
	solution_volume	DOUBLE	✓			The volume of the solution
	tds	DOUBLE			mg/kg sol	The total dissolved solute (TDS)

PK	Column Name	Type	Nullable	References	Unit	Description
	solute_fraction	DOUBLE				The fraction of the solution mass from dissolved species
	solvent_fraction	DOUBLE				The fraction of the solution mass from the solvent (water)
	extended_alkalinity	DOUBLE	✓			
	overall_affinity	DOUBLE	✓			
	reactant_mass_reacted	DOUBLE	✓			The total mass reacted into the system up to this ξ step
	reactant_mass_remaining	DOUBLE	✓			The total mass remaining to be reacted
	solid_mass_change	DOUBLE	✓			The change of the solid mass of the system up to this ξ step
	solid_mass_created	DOUBLE	✓			The solid mass created up to this ξ step
	solid_mass_destroyed	DOUBLE	✓			The solid mass destroyed up to this ξ step
	solid_volume_change	DOUBLE	✓			The change of the solid volume of the system up to this ξ step
	solid_volume_created	DOUBLE	✓			The solid volume created up to this ξ step
	solid_volume_destroyed	DOUBLE	✓			The solid volume destroyed up to this ξ step
	start_date	DATETIME				The datetime when the equilibration started
	complete_date	DATETIME				The datetime when the equilibration completed
	custom_properties	JSON				A json-encoded field for equilibrium properties computed by the kernel

equilibrium_reactants

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The equilibrium reactant identifier
	equilibrium_space_id	INTEGER	equilibrium_space.id		The id of the equilibrium space point
	name	VARCHAR			The name of the reactant
	affinity	DOUBLE			The affinity of the reactant
	relative_rate	DOUBLE		mole/mole	The molar rate of reactant titration relative to the total molar quantity of all reactants
	log_moles_reacted	DOUBLE		log mole	The moles of reactant that have been reacted up to this ξ step
	log_moles_remaining	DOUBLE		log mole	The moles of reactant that remain to be reacted

PK	Column Name	Type	References	Unit	Description
	log_mass_reacted	DOUBLE		log kg	The mass of the reactant that have been reacted up to this ξ step
	log_mass_remaining	DOUBLE		log kg	The mass of the reactant that remain to be reacted

equilibrium_elements

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The equilibrium element identifier
	equilibrium_space_id	INTEGER	equilibrium_space.id		The id of the equilibrium space point
	name	VARCHAR			The name of the element (atomic symbol)
	log_molality	DOUBLE		log molal	The molality of the element in solution
	mass_fraction	DOUBLE		unit less	The fraction of solution mass accounted for by ths element

equilibrium_aqueous_species

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The equilibrium aqueous species identifier
	equilibrium_space_id	INTEGER	equilibrium_space.id		The id of the equilibrium space point
	name	VARCHAR			The name of the aqueous species, e.g. “H2O2”
	log_molality	DOUBLE		log molal	The logarithm of the molality of that species in solution
	log_activity	DOUBLE		unitless	The logarithm of the activity of that species in solution
	log_gamma	DOUBLE		unitless	The logarithm of the activity coefficient of that species in solution

equilibrium_gases

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The equilibrium gas identifier
	equilibrium_space_id	INTEGER	equilibrium_space.id		The id of the equilibrium space point
	name	VARCHAR			The name of the gas, e.g. “H2(g)”
	log_fugacity	DOUBLE		log bar	The logarithm of the fugacity of the gas at this ξ step

equilibrium_pure_solids

PK	Column Name	Type	References	Unit	Description
✓	`id`	`INTEGER`			The equilibrium pure solid id
	`equilibrium_space_id`	`INTEGER`	`equilibrium_space.id`		The id of the equilibrium space point
	`name`	`VARCHAR`			The name of the pure solid, e.g. “fayalite”
	`log_qk`	`DOUBLE`			The saturation index of the pure solid phase
	`affinity`	`DOUBLE`		kcal	the affinity of the pure solid
	`log_moles`	`DOUBLE`		log mole	The logarithm of the net moles of the solid that have precipitated up to this ξ step
	`log_mass`	`DOUBLE`		log mass	The logarithm of the net mass of the solid that has precipitated up to this ξ step
	`log_volume`	`DOUBLE`		log cm^3	The logarithm of the volume of the solid that has precipitated

equilibrium_solid_solutions

PK	Column Name	Type	References	Unit	Description
✓	`id`	`INTEGER`			The equilibrium solid solution identifier
	`equilibrium_space_id`	`INTEGER`	`equilibrium_space.id`		The id of the equilibrium space point
	`name`	`VARCHAR`			The name of the solid solution, e.g. “olivine”
	`log_qk`	`DOUBLE`			The saturation index of the solid solution
	`affinity`	`DOUBLE`		kcal	The affinity of the solid solution
	`log_moles`	`DOUBLE`		log mole	The logarithm of the net moles of the solid solution that have precipitated up to this ξ step
	`log_mass`	`DOUBLE`		log mass	The logarithm of the net mass of the solid solution that has precipitated up to this ξ step
	`log_volume`	`DOUBLE`		log cm^3	The logarithm of the volume of the solid solution that has precipitated

equilibrium_end_members

PK	Column Name	Type	References	Unit	Description
✓	`id`	`INTEGER`			The equilibrium solid solution end member identifier
	`equilibrium_solid_solution_id`	`INTEGER`	`equilibrium_solid_solution.id`		The id of the equilibrium solid solution
	`name`	`VARCHAR`			The name of the end member, e.g. “fayalite”

PK	Column Name	Type	References	Unit	Description
	log_qk	DOUBLE			The saturation index of the end member
	affinity	DOUBLE			
	log_moles	DOUBLE		log mole	The logarithm of the net moles of the end member that have precipitated up to this ξ step
	log_mass	DOUBLE		log mass	The logarithm of the net mass of the end member that has precipitated up to this ξ step
	log_volume	DOUBLE		log cm^3	The logarithm of the volume of the end member that has precipitated

equilibrium_redox_reactions

PK	Column Name	Type	References	Unit	Description
✓	id	INTEGER			The equilibrium redox reaction identifier
	equilibrium_space_id	INTEGER	equilibrium_space.id		The id of the equilibrium space point
	couple	VARCHAR			The name of the redox couple
	"Eh"	DOUBLE		volt	The redox potential
	pe	DOUBLE		unitless	The negative logarithm of the hypothetical electron activity
	"log_fO2"	DOUBLE		log bar	The logarithm of the oxygen (O_2) fugacity
	"Ah"	DOUBLE		kcal	The redox affinity