

teacups – Quick Reference

attribute	content	type
Sys.spin_system	define spin system: “rp” (radical pair), “doub” (doublet), “trip” (triplet), “tdp” (triplet doublet pair)	string
Sys.precursor	define precursor state: “zf”, “eigen”, “singlet”, “triplet-zf”, “triplet-pnm”	string
Sys.population	populations of the initial density matrix diagonals	list of floats
Sys.g1	diagonal elements of the g1-tensor (rp-acceptor)	list of floats
Sys.g1_frame	euler angles, rotate g1-tensor to the lab. frame	list of floats
Sys.g2	diagonal elements of the g2-tensor (rp-donor)	list of floats
Sys.g2_frame	euler angles, rotate g2-tensor to the lab. frame	list of floats
Sys.g_tri	diagonal elements of the g-tensor of a triplet	list of floats
Sys.g_tri_frame	euler angles, rotate g_tri to the lab. frame	list of floats
Sys.g	diagonal elements of the g-tensor of a doublet	list of floats
Sys.g_frame	euler angles, rotate g to the lab. frame	list of floats
Sys.width_gauss	gaussian line width in mT	float
Sys.sigma_time	time resolution in s	float
Sys.donor_list	index of cores assigned to the donor	list of str/int
Sys.acceptor_list	index of cores assigned to the acceptor	list of str/int
Sys.A _{<i>i</i>}	diagonal elements of A _{<i>i</i>} -tensor ($1 \leq i \leq 5$)	list of floats
Sys.A _{<i>i</i>} _frame	euler angles, rotate A _{<i>i</i>} -tensor to the lab. frame	list of floats
Sys.I _{<i>i</i>}	spin quantum number of core group <i>i</i> (integer or half)	float
Sys.n _{<i>i</i>}	number of cores in core group <i>i</i>	integer
Sys.A	diagonal elements of all A-tensors (assigned to spins <i>i</i> and optionally <i>j</i>)	list [[A _{<i>i</i>}], [A _{<i>j</i>}]]
Sys.A_frame	euler angles, rotate all A-tensors to the lab. frame	list [[Fr _{<i>i</i>}], [Fr _{<i>j</i>}]]
Sys.I	spin quantum numbers of all cores	list [[A _{<i>i</i>}], [A _{<i>j</i>}]]
Sys.D	axial dipolar coupling between two spins in MHz	float

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Sys.E	rhombic dipolar coupling between two spins in MHz	float
Sys.J_ex	exchange-coupling constant J of two interacting electronic species J in MHz	float
Sys.D_tri	zero-field-splitting constant D of a triplet in MHz	float
Sys.E_tri	zero-field-splitting constant E of a triplet in MHz	float
Sys.D_frame	euler angles, rotate D-tensor to lab. frame	list of floats
Sys.D_tri_frame	euler angles, rotate triplet D-tensor to lab. frame	list of floats
Sys.T_relax_1	longitudinal relaxation time in s	float
Sys.T_relax_2	transversal relaxation time in s	float
Sys.decay	decay time (exponential) for hilbert space calculations in s	float
Sys.dynamics	Matrix with rateconstants of dynamic processes in 1/s	np.ndarray
Exp.B_z	magnetic field array in mT	np.ndarray
Exp.t_scale	borders of the time variation in s	list of floats
Exp.t_points	number of time field points	integer
Exp.B_mw	amplitude of the microwave field in mT	float
Exp.freq_mw	microwave frequency in Hz	float
SimOpt.grid_points	number of points between $\vartheta = 0$ and $\vartheta = \pi/2$ on the orientational sphere	integer
SimOpt.grid	Type of grid on the sphere for powder averaging. Can be either "fibonacci" or "sophe" or "single"	string
SimOpt.theta	User-chosen orientation-angles for theta if SimOpt.grid = "single"	list
SimOpt.phi	User-chosen orientation-angles for phi if SimOpt.grid = "single"	list
SimOpt.sym	Point group of the spin system, if SimOpt.grid = "sophe"	string
SimOpt.space	define in which space the time evolution will be calculated, either "hilbert" or "liouville"	string
SimOpt.pop_evolution	Decides wether the population evolution is calculated and returned or not	boolean
SimOpt.eigval_mode	Decides wether only the eigenvalues shall be calculated	boolean

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SimOpt.cpu_cores	Number of CPU cores used for time evolution, 0 uses all available cores	integer
SimOpt.CUPY	Use GPU and Cupy for faster calculations	boolean
SimOpt.extend_t	extend the time axis to negative values to see the full baseline	boolean
