PHI Quick Reference Guide

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Table 1 – Ion types

Keyword	Term	S	L	λ (cm^{-1})	σ	Comment
Ee	^2S	1/2	0	-	-	Radical
Ti(III)Oh	$^2T_{2g}$	1/2	1	155.0	-1.0	O_h symmetry
Ti(III)Td	^2E	1/2	0	-	-	T_d symmetry
Ti(III)FI	^2D	1/2	2	155.0	1.0	Spherical symmetry
Ti(II)Oh	$^3T_{1g}$	1	1	61.5	-1.5	O_h symmetry
Ti(II)Td	$^3A_2$	1	0	-	-	T_d symmetry
Ti(II)FI	^3F	1	3	61.5	1.0	Spherical symmetry
V(IV)Oh	$^2T_{2g}$	1/2	1	250.0	-1.0	O_h symmetry
V(IV)Td	^2E	1/2	0	-	-	T_d symmetry
V(IV)FI	^2D	1/2	2	250.0	1.0	Spherical symmetry
V(III)Oh	$^3T_{1g}$	1	1	105.0	-1.5	O_h symmetry
V(III)Td	$^3A_2$	1	0	-	-	T_d symmetry
V(III)FI	^3F	1	3	105.0	1.0	Spherical symmetry
V(II)Oh	$^4A_{2g}$	3/2	0	-	-	O_h symmetry
V(II)Td(w)	$^4T_1$	3/2	1	56.5	-1.5	T_d symmetry, weak CF
V(II)Td(s)	^2E	1/2	0	-	-	T_d symmetry, strong CF
V(II)FI	^4F	3/2	3	56.5	1.0	Spherical symmetry
Cr(III)Oh	$^4A_{2g}$	3/2	0	-	-	O_h symmetry
Cr(III)Td(w)	$^4T_1$	3/2	1	91.5	-1.5	T_d symmetry, weak CF
Cr(III)Td(s)	^2E	1/2	0	-	-	T_d symmetry, strong CF
Cr(III)FI	^4F	3/2	3	91.5	1.0	Spherical symmetry
Cr(II)Oh(w)	^5E_g	2	0	-	-	O_h symmetry, weak CF
Cr(II)Td(w)	$^5T_2$	2	1	57.5	-1.0	T_d symmetry, weak CF
Cr(II)FI	^5D	2	2	57.5	1.0	Spherical symmetry
Mn(VI)Oh	$^2T_{2g}$	1/2	1	540.0	-1.0	O_h symmetry
Mn(VI)Td	^2E	1/2	0	-	-	T_d symmetry
Mn(VI)FI	^2D	1/2	2	540.0	1.0	Spherical symmetry
Mn(IV)Oh	$^4A_{2g}$	3/2	0	-	-	O_h symmetry
Mn(IV)Td(w)	$^4T_1$	3/2	1	138.5	-1.5	T_d symmetry, weak CF
Mn(IV)Td(s)	^2E	1/2	0	-	-	T_d symmetry, strong CF
Mn(IV)FI	^4F	3/2	3	138.5	1.0	Spherical symmetry
Mn(III)Oh(w)	^5E_g	2	0	-	-	O_h symmetry, weak CF
Mn(III)Td(w)	$^5T_2$	2	1	89.0	-1.0	T_d symmetry, weak CF
Mn(III)FI	^5D	2	2	89.0	1.0	Spherical symmetry
Mn(II)Oh(w)	$^6A_{1g}$	5/2	0	-	-	O_h symmetry, weak CF
Mn(II)Oh(s)	$^2T_{2g}$	1/2	1	-300.0	-1.0	O_h symmetry, strong CF
Mn(II)Td(w)	$^6A_1$	5/2	0	-	-	T_d symmetry, weak CF
Mn(II)FI	^6S	5/2	0	-	-	Spherical symmetry
Fe(VI)Oh	$^3T_{1g}$	1	1	332.5	-1.5	O_h symmetry
Fe(VI)Td	$^3A_2$	1	0	-	-	T_d symmetry
Fe(VI)FI	^3F	1	3	332.5	1.0	Spherical symmetry
Fe(III)Oh(w)	$^6A_{1g}$	5/2	0	-	-	O_h symmetry, weak CF
Fe(III)Oh(s)	$^2T_{2g}$	1/2	1	-460.0	-1.0	O_h symmetry, strong CF
Fe(III)Td(w)	$^6A_1$	5/2	0	-	-	T_d symmetry, weak CF
Fe(III)FI	^6S	5/2	0	-	-	Spherical symmetry
Fe(II)Oh(w)	$^5T_{2g}$	2	1	-100.0	-1.0	O_h symmetry, weak CF
Fe(II)Td(w)	^5E	2	0	-	-	T_d symmetry, weak CF
Fe(II)FI	^5D	2	2	-100.0	1.0	Spherical symmetry
Co(III)Oh(w)	$^5T_{2g}$	2	1	-145.0	-1.0	O_h symmetry, weak CF
Co(III)Td(w)	^5E	2	0	-	-	T_d symmetry, weak CF

Co(III)FI	^5D	2	2	-145.0	1.0	Spherical symmetry
Co(II)Oh(w)	$^4T_{1g}$	3/2	1	-171.5	-1.5	O_h symmetry, weak CF
Co(II)Oh(s)	^2E_g	1/2	0	-	-	O_h symmetry, strong CF
Co(II)Td	$^4A_2$	3/2	0	-	-	T_d symmetry
Co(II)FI	^4F	3/2	3	-171.5	1.0	Spherical symmetry
Ni(III)Oh(w)	$^4T_{1g}$	3/2	1	-235.0	-1.5	O_h symmetry, weak CF
Ni(III)Oh(s)	^2E_g	1/2	0	-	-	O_h symmetry, strong CF
Ni(III)Td	$^4A_2$	3/2	0	-	-	T_d symmetry
Ni(III)FI	^4F	3/2	3	-235.0	1.0	Spherical symmetry
Ni(II)Oh	$^3A_{2g}$	1	0	-	-	O_h symmetry
Ni(II)Td	$^3T_1$	1	1	-315.0	-1.5	T_d symmetry
Ni(II)FI	^3F	1	3	-315.0	1.0	Spherical symmetry
Cu(II)Oh	^2E_g	1/2	0	-	-	O_h symmetry
Cu(II)Td	$^2T_2$	1/2	1	-830.0	-1.0	T_d symmetry
Cu(II)FI	^2D	1/2	2	-830.0	1.0	Spherical symmetry
Ce(J)	$^2F_{5/2}$	5/2	0	-	-	Spherical symmetry
Ce(LS)	^2F	1/2	3	Table 2.2.1	1.0	Spherical symmetry
Pr(J)	$^3H_4$	4	0	-	-	Spherical symmetry
Pr(LS)	^3H	1	5	Table 2.2.1	1.0	Spherical symmetry
Nd(J)	$^4I_{9/2}$	9/2	0	-	-	Spherical symmetry
Nd(LS)	^4I	3/2	6	Table 2.2.1	1.0	Spherical symmetry
Pm(J)	$^5I_4$	4	0	-	-	Spherical symmetry
Pm(LS)	^5I	2	6	Table 2.2.1	1.0	Spherical symmetry
Sm(J)	$^6H_{5/2}$	5/2	0	-	-	Spherical symmetry
Sm(LS)	^6H	5/2	5	Table 2.2.1	1.0	Spherical symmetry
Eu(LS)	^7F	3	3	Table 2.2.1	1.0	Spherical symmetry
Gd(III)	^8S	7/2	0	-	-	Spherical symmetry
Tb(J)	$^7F_6$	6	0	-	-	Spherical symmetry
Tb(LS)	^7F	3	3	Table 2.2.1	1.0	Spherical symmetry
Dy(J)	$^6H_{15/2}$	15/2	0	-	-	Spherical symmetry
Dy(LS)	^6H	5/2	5	Table 2.2.1	1.0	Spherical symmetry
Ho(J)	$^5I_8$	8	0	-	-	Spherical symmetry
Ho(LS)	^5I	2	6	Table 2.2.1	1.0	Spherical symmetry
Er(J)	$^4I_{15/2}$	15/2	0	-	-	Spherical symmetry
Er(LS)	^4I	3/2	6	Table 2.2.1	1.0	Spherical symmetry
Tm(J)	$^3H_6$	6	0	-	-	Spherical symmetry
Tm(LS)	^3H	1	5	Table 2.2.1	1.0	Spherical symmetry
Yb(J)	$^2F_{7/2}$	7/2	0	-	-	Spherical symmetry
Yb(LS)	^2F	1/2	3	Table 2.2.1	1.0	Spherical symmetry
1H	-	1/2	0	-	-	$g_{eff} = -3.04206422539567\times10^{-3}$
7Li	-	3/2	0	-	-	$g_{eff} = 1.18233679972407\times10^{-3}$
9Be	-	3/2	0	-	-	$g_{eff} = 4.27497106541515\times10^{-4}$
14N	-	1	0	-	-	$g_{eff} = -2.19895100623363\times10^{-4}$
19F	-	1/2	0	-	-	$g_{eff} = -2.86345235614900\times10^{-3}$
23Na	-	3/2	0	-	-	$g_{eff} = -8.05133438386439\times10^{-4}$
27Al	-	5/2	0	-	-	$g_{eff} = -7.93290633008815\times10^{-4}$
31P	-	1/2	0	-	-	$g_{eff} = -1.23257717246290\times10^{-3}$
39K	-	3/2	0	-	-	$g_{eff} = -1.42134142130333\times10^{-4}$
45Sc	-	7/2	0	-	-	$g_{eff} = -7.40129043657371\times10^{-4}$
51V	-	7/2	0	-	-	$g_{eff} = -8.01164269761082\times10^{-4}$
55Mn	-	5/2	0	-	-	$g_{eff} = -7.52279448711121\times10^{-4}$
59Co	-	7/2	0	-	-	$g_{eff} = -7.19983661185914\times10^{-4}$
75As	-	3/2	0	-	-	$g_{eff} = -5.22641694748156\times10^{-4}$

89Y	-	1/2	0	-	-	$g_{\text{eff}} = 1.49677523139677\times10^{-4}$
93Nb	-	9/2	0	-	-	$g_{\text{eff}} = -7.46778817109020\times10^{-4}$
103Rh	-	1/2	0	-	-	$g_{\text{eff}} = 9.62882838862856\times10^{-5}$
115In	-	9/2	0	-	-	$g_{\text{eff}} = -6.70586900165064\times10^{-4}$
127I	-	5/2	0	-	-	$g_{\text{eff}} = -6.12862945362421\times10^{-4}$
133Cs	-	7/2	0	-	-	$g_{\text{eff}} = -4.01775608553100\times10^{-4}$
139La	-	7/2	0	-	-	$g_{\text{eff}} = -4.33055467544589\times10^{-4}$
141Pr	-	5/2	0	-	-	$g_{\text{eff}} = -9.31403976823108\times10^{-4}$
159Tb	-	3/2	0	-	-	$g_{\text{eff}} = -7.31420617982361\times10^{-4}$
165Ho	-	7/2	0	-	-	$g_{\text{eff}} = -9.08421139832151\times10^{-4}$
169Tm	-	1/2	0	-	-	$g_{\text{eff}} = 2.51613049521855\times10^{-4}$
175Lu	-	7/2	0	-	-	$g_{\text{eff}} = -3.47356716417833\times10^{-4}$
181Ta	-	7/2	0	-	-	$g_{\text{eff}} = -3.68863641365058\times10^{-4}$
197Au	-	3/2	0	-	-	$g_{\text{eff}} = -5.29171652461937\times10^{-5}$
209Bi	-	9/2	0	-	-	$g_{\text{eff}} = -4.97453158946455\times10^{-4}$

Table 2 – ****Sus block options

Parameter	**Options/Syntax**	**Comments**
Magnetic field direction / integration	Field STR Field Powder N Field Axial N Field Vector X Y Z Field Angles θ φ	Selection of magnetic field: STR is either x, y or z for single directions or xyz for principal axes integration. If STR is ‘Powder’ then ZCW integration is used where N ≥ 0. If STR is Axial then integration with N points in the positive quadrant of the z-x plane is performed. If STR is ‘Vector’ an arbitrary single direction is given. If STR is ‘Angles’ an arbitrary single direction is given in polar coordinates in degrees. Default = “Field z” (isotropic), “Field xyz” (anisotropic).
Magnetic field	BSus A B C D …	Selects the magnetic field(s) in Tesla for the calculation. Any number of fields can be listed on the same line. Default = “BSus 0.01”.
Temperature sweep	Sweep Low High N <log>	Sets the temperature range (in Kelvin), the number of points and optionally spacing on a logarithmic scale. Default = “Sweep 1.8 300 250”.
Temperature Independent Paramagnetism	TIP X	Sets a TIP (in $\text{cm}^3\ \text{mol}^{-1}$). Default = “TIP 0”.
Intermolecular interaction	zJ X	Sets the mean-field zJ parameter (in cm^{-1}). Default = “zJ 0”.
Differential susceptibility	Differential	Calculates the true differential susceptibility, as opposed to the default $\chi = M/B$.

Table 3 – ****Tensor block options

Parameter	Options/Syntax	Comments
Magnetic field	BSus A B C D …	Selects the magnetic field(s) in Tesla for the calculation. Any number of fields can be listed on the same line. Default = "BSus 0.01".
Temperature sweep	Sweep Low High N <log>	Sets the temperature range (in Kelvin), the number of points and optionally spacing on a logarithmic scale. Default = "Sweep 1.8 300 250".

Table 4 – ****Mag block options

Parameter	Options/Syntax	Comments
Magnetic field direction / integration	Field STR Field Powder N Field Axial N Field Vector X Y Z Field Angles θ φ	Selection of magnetic field: STR is either x, y or z for single directions or xyz for principal axes integration. If STR is 'Powder' then ZCW integration is used where N ≥ 0. If STR is Axial then integration with N points in the positive quadrant of the z-x plane is performed. If STR is 'Vector' an arbitrary single direction is given. If STR is 'Angles' an arbitrary single direction is given in polar coordinates in degrees. Default = "Field z" (isotropic), "Field Powder 3" (anisotropic).
Temperature	TMag A B C D …	Selects the temperature(s) in Kelvin for the calculation. Any number of temperatures can be listed on the same line. Default = "TMag 2 4 10 20".
Magnetic field sweep	Sweep Low High N <log>	Sets the magnetic field range (in Tesla), the number of points and optionally spacing on a logarithmic scale. Default = "Sweep 0 7 10".

Table 5 – ****MCE block options

Parameter	Options/Syntax	Comments
Magnetic field direction / integration	Field STR Field Powder N Field Axial N Field Vector X Y Z Field Angles θ φ	Selection of magnetic field: STR is either x, y or z for single directions or xyz for principal axes integration. If STR is 'Powder' then ZCW integration is used where N ≥ 0. If STR is Axial then integration with N points in the positive quadrant of the z-x plane is performed. If STR is 'Vector' an arbitrary single direction is given. If STR is 'Angles' an arbitrary single direction is given in polar coordinates in degrees. Default = "Field z" (isotropic), "Field Powder 3" (anisotropic).
Magnetic field	BMCE A B C D …	Selects the magnetic field(s) in Tesla for the calculation. Any number of fields can be listed on the same line. Default = "BMCE 7".
Temperature sweep	Sweep Low High N <log>	Sets the temperature range (in Kelvin), the number of points and optionally spacing on a logarithmic scale. Default = "Sweep 1.8 50

		250”.
Molecular mass	Mass X	Sets the molecular mass for the sample in g mol^{-1}. Default = “Mass 2000”.
Integration	Integrate N	Sets the number of magnetic field integration points. Default = “Integrate 50”.

Table 6 – ****HeatCapacity block options

Parameter	**Options/Syntax**	**Comments**
Magnetic field direction / integration	Field STR Field Powder N Field Axial N Field Vector X Y Z Field Angles θ φ	Selection of magnetic field: STR is either x, y or z for single directions or xyz for principal axes integration. If STR is ‘Powder’ then ZCW integration is used where N ≥ 0. If STR is Axial then integration with N points in the positive quadrant of the z-x plane is performed. If STR is ‘Vector’ an arbitrary single direction is given. If STR is ‘Angles’ an arbitrary single direction is given in polar coordinates in degrees. Default = “Field z” (isotropic), “Field Powder 3” (anisotropic).
Magnetic field	BHeat A B C D …	Selects the magnetic field(s) in Tesla for the calculation. Any number of fields can be listed on the same line. Default = “BHeat 0.1”.
Temperature sweep	Sweep Low High N <log>	Sets the temperature range (in Kelvin), the number of points and optionally spacing on a logarithmic scale. Temperatures are on a base-10 logarithmic scale. Default = “Sweep 0.5 20 250 log”.
Debye lattice contribution	Debye T_D α	Sets the Debye temperature (in Kelvin) and exponent. Default = “Debye 0 0”

Table 7 – ****EPR block options

Parameter	**Options/Syntax**	**Comments**
Magnetic field direction / integration	Field STR Field Powder N Field Axial N Field Vector X Y Z Field Angles θ φ	Selection of magnetic field: STR is either x, y or z for single directions or xyz for principal axes integration. If STR is ‘Powder’ then ZCW integration is used where N ≥ 0. If STR is Axial then integration with N points in the positive quadrant of the z-x plane is performed. If STR is ‘Vector’ an arbitrary single direction is given. If STR is ‘Angles’ an arbitrary single direction is given in polar coordinates in degrees. Default = “Field Powder 6”.
Temperature	TEPR A B C D …	Sets the temperature(s) for the simulation, in Kelvin. Default = “TEPR 5”.
Frequency	FEPR A B C D …	Sets the frequency(ies) for the simulation, in GHz. Default = “FEPR 9.5 35 94”.
Spectrum type	Type A B C D …	Selects whether the absorption (N = 0), first derivative (N = 1), second derivative (N = 2) or integrated absorption (N = -1) spectrum is

		to be calculated, for each frequency. Default = “Type 1 1 1 1 …”.
Parallel mode	Parallel	Selects parallel mode. Default = Off.
Magnetic field sweep	Sweep Low High N <log>	Sets the magnetic field range (in Tesla), the number of points and optionally spacing on a logarithmic scale. Default = “Sweep 0 1.6 250”.
Linewidth	LW A B C D …	Sets the isotropic pseudo-voigt linewidth, in GHz, for each frequency. If only one linewidth is given and multiple frequencies are to be simulated, then all frequencies have the same linewidth. Default = “Linewidth 0.27”.
Anisotropic linewidth, x-direction	LWX A B C D …	Sets the anisotropic pseudo-voigt linewidth for the x-direction, in GHz, for each frequency. If only one linewidth is given and multiple frequencies are to be simulated, then all frequencies have the same linewidth. Default = “Linewidth 0.27”.
Anisotropic linewidth, y-direction	LWY A B C D …	Sets the anisotropic pseudo-voigt linewidth for the y-direction, in GHz, for each frequency. If only one linewidth is given and multiple frequencies are to be simulated, then all frequencies have the same linewidth. Default = “Linewidth 0.27”.
Anisotropic linewidth, z-direction	LWZ A B C D …	Sets the anisotropic pseudo-voigt linewidth for the z-direction, in GHz, for each frequency. If only one linewidth is given and multiple frequencies are to be simulated, then all frequencies have the same linewidth. Default = “Linewidth 0.27”.
Pseudo-voigt parameter	Voigt A B C D …	Sets the pseudo-voigt parameter for each frequency. If only one parameter is given and multiple frequencies are to be simulated, then all frequencies have the same parameter. Default = “Voigt 1” (Lorentzian).
Mosaicity	Mosaic A B C D …	Sets the mosacity parameter for each frequency. If only one parameter is given and multiple frequencies are to be simulated, then all frequencies have the same parameter. Default = “Mosaic 0”.
Absolute intensity	NoNorm	Gives the calculated EPR data in absolute intensity units without normalization.
Infinite order perturbation theory	Subspace N	Uses subspace perturbation theory to calculate the EPR spectrum for the N lowest lying states. Default = Off

Table 8 – Zeeman options

Parameter	Options/Syntax	Comments
Magnetic field direction	Field STR Field Vector X Y Z Field Angles θ φ	Selection of magnetic field: STR is either x, y or z for single directions or xyz for principal axes integration. If STR is 'Vector' an arbitrary single direction is given. If STR is 'Angles' an arbitrary single direction is given in polar coordinates in degrees. Default = "Field z".
Magnetic field sweep	Sweep Low High N <log>	Sets the magnetic field range (in Tesla), the number of points and optionally spacing on a logarithmic scale. Default = "Sweep 0 7 250".

Table 9 – ****Fit and ****Survey block syntax

Syntax	Comment
EX SiteA SiteB 1/2/3/4/5/6/7	Exchange coupling, third integer represents x, y, z, isotropic, antisymmetric x, antisymmetric y or antisymmetric z.
IN SiteA SiteB 1/2/3/4/5/6/7/8/9	Interaction tensor, third integer represents Jxx, Jxy, Jxz, Jyx, Jyy, Jyz, Jzx, Jzy or Jzz.
SO Site 1/2/3/4/5/6	Spin-orbit coupling, second integer is the order.
GF Site 1/2/3/4	G-factor, second integer represents x, y, z or isotropic.
CF Site Rank Order	Crystal field parameter.
RC Site 1/2/3	Reference frame rotation, second integer represents α, β or γ.
RE SiteA SiteB 1/2/3	Exchange frame rotation, third integer represents α, β or γ.
OR Site	Orbital reduction parameter.
LW Freq. 1/2/3/4	EPR linewidth, second integer selects corresponding frequency (0 applies to all frequencies), third integer represents x, y, z, or isotropic
VO Freq.	EPR pseudo-voigt parameter, second integer selects corresponding frequency, where 0 implies all frequencies.
MO Freq.	EPR mosacity, second integer selects corresponding frequency, where 0 implies all frequencies.
TI	Temperature Independent Paramagnetism.
DT	Debye temperature.
DA	Debye exponent.
ZJ	Mean-field intermolecular interaction.
IM	Monomeric impurity.
ES SiteA SiteB 1/2/3/4/5/6/7	Exchange strain, third integer represents x, y, z, isotropic, antisymmetric x, antisymmetric y or antisymmetric z.
IS SiteA SiteB 1/2/3/4/5/6/7/8/9	Interaction strain, third integer represents Jxx, Jxy, Jxz, Jyx, Jyy, Jyz, Jzx, Jzy or Jzz.
SS Site 1/2/3/4/5/6	Spin-orbit coupling strain, second integer is the order.

GS Site 1/2/3/4	G-factor strain, second integer represents x, y, z or isotropic.
CS Site Rank Order	Crystal field strain.
OS Site	Orbital reduction strain.

Table 10 – ****Params block options

Parameter	**Options/Syntax**	**Comments**
Operation mode	OpMode STR1 STR2	Selection of operation mode, STR1 and STR2 are strings, see Table 4.3.10. ***Must be present***.
Magnetism approximation	Approx	Turns on the block diagonal approximation for isotropic systems. Default = Off.
Monomeric impurity	IMP N x	Adds a monomer impurity of spin S = N/2, with fraction x, i.e. x = 1 for one uncoupled spin. Default = Off.
Zero field splitting	ZFS I J K …	Alters the convention of B_0^2 such that it equals D. Any number of sites can be listed on the same line. Default = Off.
Cubic crystal field	Cubic I J K …	Forces cubic CFP ratios for B_4^4 and B_6^4 based on B_4^0 and B_6^0. Any number of sites can be listed on the same line. Default = Off.
Static magnetic field	StaticB |B| X Y Z StaticB |B| θ φ	Includes the presence of a static magnetic field of magnitude |B| Tesla, with vector (X,Y,Z) or polar coordinates (θ,φ) in degrees. Default = Off.
Rotate reference frame	Rotate N α β γ	Rotates the reference frame (CFPs and or g) for site N, through the Euler angles α, β and γ, given in degrees. Default = Off.
Rotate exchange frame	EXRotate N M α β γ	Rotates the exchange frame for the exchange defined between sites N and M, through the Euler angles α, β and γ, given in degrees. Default = Off.
Number of CPU cores	MaxCPU N	Sets the upper limit of CPU cores available, N is an integer. Default = “MaxCPU cores-1”.
Fitting algorithm display	NoPrint	Turns off the printing of fit progress to the terminal and intermediate results to disk. Default = Off.
Full wavefunction printing	FullWF	Prints the full wavefunction in the states.res file. Default = Off.
Save survey calculations	Save	Saves a file for each step of the survey calculation. Default = Off.
Disable operator equivalent factors	NoOEF	Disables the Operator Equivalent Factors such that CF input values are assumed to contain θ_k. Default = Off.
G-tensor multiplets	Mults N A B C D …	Gives the multiplicities of the multiplets for the calculations of pseudo-spin $\tilde{S} = \frac{1}{2}$ states. N gives the number of multiplets, followed by N integers giving the multiplicity. Default = Off.

Single crystal experiment	Single	Circumvents checking for the need to integrate magnetic properties – i.e. requested single field direction is allowed. Default = Off.
Percentage completion	Percent	Prints percentage completion for command line operation. Default = Off.
Residual type	Residual STR	Selects residual calculation method. STR is a string, see Table 4.3.13. Default = Off.
G-tensor direction residual	GDir STR	Selects which directions to include in the residual calculation for g-tensors (and directions). STR is a string of x, y, z or a combination thereof. Default = “GDir xyz”.
Fitting algorithm vigour	FitVigour X	Sets how vigourous the fitting algorithm starts, as a parameter percentage. Default = “FitVigour 10”.
Fitting algorithm limiting	FitLimit X	Sets how strongly the fitting algorithm enforces parameter limits. Limiting function is $e^{X\|\Delta\|}$, where Δ is difference between the fitting parameter and its limit. Default = “FitLimit 12”.
Fitting algorithm iteration limit	FitIter N	Sets an upper limit for the number of fit iterations. Default = no limit.
Fitting algorithm tolerance	FitTolerance X	Sets the tolerance threshold for completing the fitting algorithm. Default = “FitTolerance 1E-12”.
Disable uncertainties in fit parameters	NoUncertainties	Disables the calculation of uncertainties in the fitting variables. Default = On.
Orbital Reduction in Zeeman term	ORedOnlyZeeman	Restricts the application of the orbital reduction parameter to the orbital Zeeman term only. Default = Off.
High-precision output	HighPrec	Prints results to machine precision. Default = Off.

Table 11 – Operation modes

OpMode	Comments
Sim STR2	Simulation; STR2 is a string, see below and Table 4.3.11.
Fit STR2	Fit; STR2 is a string, see below and Table 4.3.11.
Sur STR2	Survey; STR2 is a string, see below and Table 4.3.11.
Coupling Report	Reports the block diagonal structure of the matrix
Matrix Elements	Prints Hamiltonian matrix

Table 12 – Operation mode STR2

STR2	Comments
L	Energy levels
M	Magnetization
S	Susceptibility

G	G-tensors
D	G-tensors with directions
C	MCE
H	Heat capacity
E	EPR
Z	Zeeman

Table 13 – Number of directions in ZCW integration

ZCW	Number
0	21
1	34
2	55
3	89
4	144
5	233
6	377
7	610
8	987
9	1597
10	2584
11	4181
12	6765
13	10946
14	17711
15	28657
16	46368
17	75025
18	121393
19	196418
20	317811

Table 14 – Residual types

Residual type string	Comments
LowT	Low temperature bias
HighT	High temperature bias
LowB	Low field bias
HighB	High field bias
LowT/LowB	Low temperature and low field bias
LowT/HighB	Low temperature and high field bias
HighT/LowB	High temperature and low field bias
HighT/HighB	High temperature and high field bias
LowE	Low energy bias
HighE	High Energy bias

Table 15 – Optimized spin-orbit parameters for the triply ionized rare-earths

Ion		λ_1 (cm^{-1})	λ_2 (cm^{-1})	λ_3 (cm^{-1})	λ_4 (cm^{-1})	λ_5 (cm^{-1})	λ_6 (cm^{-1})
Ce$^{\mathrm{III}}$	**Ref. 1**	640	-	-	-	-	-
	Opt.	691	-	-	-	-	-
Pr$^{\mathrm{III}}$	**Ref. 1**	390	-4.63	-	-	-	-
	Opt.	421	-5.78	-	-	-	-
Nd$^{\mathrm{III}}$	**Ref. 1**	299	-2.48	0.0475	-	-	-
	Opt.	326	-2.66	0.0247	-	-	-
Pm$^{\mathrm{III}}$	**Ref. 1**	251	-1.99	0.0239	0	-	-
	Opt.	269	-1.85	0.00977	-0.000920	-	-
Sm$^{\mathrm{III}}$	**Ref. 1**	228	-2.16	0.0368	0	0	-
	Opt.	241	-2.34	0.0315	-0.000743	-0.00000883	-
Eu$^{\mathrm{III}}$	**Ref. 1**	214	-3.82	0.147	0	0	0
	Opt.	230	-3.28	0.269	0.000715	-0.00164	-0.000144
Tb$^{\mathrm{III}}$	**Ref. 1**	-252	-4.50	-0.267	0	0	0
	Opt.	-260	0.997	0.223	-0.0402	-0.00685	-0.000267
Dy$^{\mathrm{III}}$	**Ref. 1**	-357	-4.40	-0.121	0	0	-
	Opt.	-362	-2.73	-0.221	-0.00655	0.000110	-
Ho$^{\mathrm{III}}$	**Ref. 1**	-497	-7.06	-0.139	0	-	-
	Opt.	-515	-7.83	-0.121	0.00629	-	-
Er$^{\mathrm{III}}$	**Ref. 1**	-629	-18.2	-0.517	-	-	-
	Opt.	-572	-12.6	-1.85	-	-	-
Tm$^{\mathrm{III}}$	**Ref. 1**	-875	-123	-	-	-	-
	Opt.	-684	-177	-	-	-	-
Yb$^{\mathrm{III}}$	**Ref. 1**	-2910	-	-	-	-	-
	Opt.	-2957	-	-	-	-	-

Table 16 – Definition of the Stevens operators

Operator
$\hat{O}_2^{-2} = \frac{-i}{2}\left({\hat{L}_+}^2 - {\hat{L}_-}^2\right)$
$\hat{O}_2^{-1} = \frac{-i}{4}\left(\hat{L}_z(\hat{L}_+ - \hat{L}_-) + (\hat{L}_+ - \hat{L}_-)\hat{L}_z\right)$
$\hat{O}_2^{0} = 3{\hat{L}_z}^2 - \hat{L}^2$
$\hat{O}_2^{+1} = \frac{1}{4}\left(\hat{L}_z(\hat{L}_+ + \hat{L}_-) + (\hat{L}_+ + \hat{L}_-)\hat{L}_z\right)$
$\hat{O}_2^{+2} = \frac{1}{2}\left({\hat{L}_+}^2 + {\hat{L}_-}^2\right)$
$\hat{O}_4^{-4} = \frac{-i}{2}\left({\hat{L}_+}^4 - {\hat{L}_-}^4\right)$

$$\hat{O}_4^{-3} = \frac{-i}{4}\left(\hat{L}_z\left({\hat{L}_+}^3 - {\hat{L}_-}^3\right) + \left({\hat{L}_+}^3 - {\hat{L}_-}^3\right)\hat{L}_z\right)$$

$$\hat{O}_4^{-2} = \frac{-i}{4}\left(\left(7{\hat{L}_z}^2 - \hat{L}^2 - 5\right)\left({\hat{L}_+}^2 - {\hat{L}_-}^2\right) + \left({\hat{L}_+}^2 - {\hat{L}_-}^2\right)\left(7{\hat{L}_z}^2 - \hat{L}^2 - 5\right)\right)$$

$$\hat{O}_4^{-1} = \frac{-i}{4}\left(\left(7{\hat{L}_z}^3 - 3\hat{L}^2\hat{L}_z - \hat{L}_z\right)\left(\hat{L}_+ - \hat{L}_-\right) + \left(\hat{L}_+ - \hat{L}_-\right)\left(7{\hat{L}_z}^3 - 3\hat{L}^2\hat{L}_z - \hat{L}_z\right)\right)$$

$$\hat{O}_4^{0} = 35{\hat{L}_z}^4 - 30\hat{L}^2{\hat{L}_z}^2 + 25{\hat{L}_z}^2 + 3{\hat{L}^2}^2 - 6\hat{L}^2$$

$$\hat{O}_4^{+1} = \frac{1}{4}\left(\left(7{\hat{L}_z}^3 - 3\hat{L}^2\hat{L}_z - \hat{L}_z\right)\left(\hat{L}_+ + \hat{L}_-\right) + \left(\hat{L}_+ + \hat{L}_-\right)\left(7{\hat{L}_z}^3 - 3\hat{L}^2\hat{L}_z - \hat{L}_z\right)\right)$$

$$\hat{O}_4^{+2} = \frac{1}{4}\left(\left(7{\hat{L}_z}^2 - \hat{L}^2 - 5\right)\left({\hat{L}_+}^2 + {\hat{L}_-}^2\right) + \left({\hat{L}_+}^2 + {\hat{L}_-}^2\right)\left(7{\hat{L}_z}^2 - \hat{L}^2 - 5\right)\right)$$

$$\hat{O}_4^{+3} = \frac{1}{4}\left(\hat{L}_z\left({\hat{L}_+}^3 + {\hat{L}_-}^3\right) + \left({\hat{L}_+}^3 + {\hat{L}_-}^3\right)\hat{L}_z\right)$$

$$\hat{O}_4^{+4} = \frac{1}{2}\left({\hat{L}_+}^4 + {\hat{L}_-}^4\right)$$

$$\hat{O}_6^{-6} = \frac{-i}{2}\left({\hat{L}_+}^6 - {\hat{L}_-}^6\right)$$

$$\hat{O}_6^{-5} = \frac{-i}{4}\left(\left({\hat{L}_+}^5 - {\hat{L}_-}^5\right)\hat{L}_z + \hat{L}_z\left({\hat{L}_+}^5 - {\hat{L}_-}^5\right)\right)$$

$$\hat{O}_6^{-4} = \frac{-i}{4}\left(\left({\hat{L}_+}^4 - {\hat{L}_-}^4\right)\left(11{\hat{L}_z}^2 - \hat{L}^2 - 38\right) + \left(11{\hat{L}_z}^2 - \hat{L}^2 - 38\right)\left({\hat{L}_+}^4 - {\hat{L}_-}^4\right)\right)$$

$$\begin{aligned}\hat{O}_6^{-3} = \frac{-i}{4}\Big(&\left({\hat{L}_+}^3 - {\hat{L}_-}^3\right)\left(11{\hat{L}_z}^3 - 3\hat{L}^2\hat{L}_z - 59\hat{L}_z\right)\\ &+ \left(11{\hat{L}_z}^3 - 3\hat{L}^2\hat{L}_z - 59\hat{L}_z\right)\left({\hat{L}_+}^3 - {\hat{L}_-}^3\right)\Big)\end{aligned}$$

$$\begin{aligned}\hat{O}_6^{-2} = \frac{-i}{4}\Big(&\left({\hat{L}_+}^2 - {\hat{L}_-}^2\right)\left(33{\hat{L}_z}^4 - 18\hat{L}^2{\hat{L}_z}^2 - 123{\hat{L}_z}^2 + {\hat{L}^2}^2 + 10\hat{L}^2 + 102\right)\\ &+ \left(33{\hat{L}_z}^4 - 18\hat{L}^2{\hat{L}_z}^2 - 123{\hat{L}_z}^2 + {\hat{L}^2}^2 + 10\hat{L}^2 + 102\right)\left({\hat{L}_+}^2 - {\hat{L}_-}^2\right)\Big)\end{aligned}$$

$$\begin{aligned}\hat{O}_6^{-1} = \frac{-i}{4}\Big(&\left(\hat{L}_+ - \hat{L}_-\right)\left(33{\hat{L}_z}^5 - 30\hat{L}^2{\hat{L}_z}^3 + 15{\hat{L}_z}^3 + 5{\hat{L}^2}^2\hat{L}_z - 10\hat{L}^2\hat{L}_z + 12\hat{L}_z\right)\\ &+ \left(33{\hat{L}_z}^5 - 30\hat{L}^2{\hat{L}_z}^3 + 15{\hat{L}_z}^3 + 5{\hat{L}^2}^2\hat{L}_z - 10\hat{L}^2\hat{L}_z + 12\hat{L}_z\right)\left(\hat{L}_+ - \hat{L}_-\right)\Big)\end{aligned}$$

$$\begin{aligned}\hat{O}_6^{0} = 231{\hat{L}_z}^6 &- 315\hat{L}^2{\hat{L}_z}^4 + 735{\hat{L}_z}^4 + 105{\hat{L}^2}^2{\hat{L}_z}^2 - 525\hat{L}^2{\hat{L}_z}^2 + 294{\hat{L}_z}^2 - 5{\hat{L}^2}^3 + 40{\hat{L}^2}^2\\ &- 60\hat{L}^2\end{aligned}$$

$$\begin{aligned}\hat{O}_6^{+1} = \frac{1}{4}\Big(&\left(\hat{L}_+ + \hat{L}_-\right)\left(33{\hat{L}_z}^5 - 30\hat{L}^2{\hat{L}_z}^3 + 15{\hat{L}_z}^3 + 5{\hat{L}^2}^2\hat{L}_z - 10\hat{L}^2\hat{L}_z + 12\hat{L}_z\right)\\ &+ \left(33{\hat{L}_z}^5 - 30\hat{L}^2{\hat{L}_z}^3 + 15{\hat{L}_z}^3 + 5{\hat{L}^2}^2\hat{L}_z - 10\hat{L}^2\hat{L}_z + 12\hat{L}_z\right)\left(\hat{L}_+ + \hat{L}_-\right)\Big)\end{aligned}$$

$$\begin{aligned}\hat{O}_6^{+2} = \frac{1}{4}\Big(&\left({\hat{L}_+}^2 + {\hat{L}_-}^2\right)\left(33{\hat{L}_z}^4 - 18\hat{L}^2{\hat{L}_z}^2 - 123{\hat{L}_z}^2 + {\hat{L}^2}^2 + 10\hat{L}^2 + 102\right)\\ &+ \left(33{\hat{L}_z}^4 - 18\hat{L}^2{\hat{L}_z}^2 - 123{\hat{L}_z}^2 + {\hat{L}^2}^2 + 10\hat{L}^2 + 102\right)\left({\hat{L}_+}^2 + {\hat{L}_-}^2\right)\Big)\end{aligned}$$

$$\hat{O}_6^{+3} = \frac{1}{4}\left(\left({\hat{L}_+}^3 + {\hat{L}_-}^3\right)\left(11{\hat{L}_z}^3 - 3\hat{L}^2\hat{L}_z - 59\hat{L}_z\right) + \left(11{\hat{L}_z}^3 - 3\hat{L}^2\hat{L}_z - 59\hat{L}_z\right)\left({\hat{L}_+}^3 + {\hat{L}_-}^3\right)\right)$$

$$\hat{O}_6^{+4} = \frac{1}{4}\left(\left({\hat{L}_+}^4 + {\hat{L}_-}^4\right)\left(11{\hat{L}_z}^2 - \hat{L}^2 - 38\right) + \left(11{\hat{L}_z}^2 - \hat{L}^2 - 38\right)\left({\hat{L}_+}^4 + {\hat{L}_-}^4\right)\right)$$

$$\hat{O}_6^{+5} = \frac{1}{4}\left(\left({\hat{L}_+}^5 + {\hat{L}_-}^5\right)\hat{L}_z + \hat{L}_z\left({\hat{L}_+}^5 + {\hat{L}_-}^5\right)\right)$$

$$\hat{O}_6^{+6} = \frac{1}{2}\left({\hat{L}_+}^6 + {\hat{L}_-}^6\right)$$

Table 17 – Operator equivalent factors for the ground terms of the lanthanides

Ion	**Term**	**2nd Rank**	**4th Rank**	**6th Rank**
$\mathrm{Ce^{III}}$	$^2\mathrm{F}$	-2/45	2/495	-4/3861
$\mathrm{Pr^{III}}$	$^3\mathrm{H}$	-2/135	-4/10395	2/81081
$\mathrm{Nd^{III}}$	$^4\mathrm{I}$	-2/495	-2/16335	-10/891891
$\mathrm{Pm^{III}}$	$^5\mathrm{I}$	2/495	2/16335	10/891891
$\mathrm{Sm^{III}}$	$^6\mathrm{H}$	2/135	4/10395	-2/81081
$\mathrm{Eu^{III}}$	$^7\mathrm{F}$	2/45	-2/495	4/3861
$\mathrm{Gd^{III}}$	$^8\mathrm{S}$	0	0	0
$\mathrm{Tb^{III}}$	$^7\mathrm{F}$	-2/45	2/495	-4/3861
$\mathrm{Dy^{III}}$	$^6\mathrm{H}$	-2/135	-4/10395	2/81081
$\mathrm{Ho^{III}}$	$^5\mathrm{I}$	-2/495	-2/16335	-10/891891
$\mathrm{Er^{III}}$	$^4\mathrm{I}$	2/495	2/16335	10/891891
$\mathrm{Tm^{III}}$	$^3\mathrm{H}$	2/135	4/10395	-2/81081
$\mathrm{Yb^{III}}$	$^2\mathrm{F}$	2/45	-2/495	4/3861

Table 18 – Operator equivalent factors for the ground multiplets of the lanthanides

Ion	**Multiplet**	**2nd Rank**	**4th Rank**	**6th Rank**
$\mathrm{Ce^{III}}$	$^2\mathrm{F}_{5/2}$	-2/35	2/315	0
$\mathrm{Pr^{III}}$	$^3\mathrm{H}_4$	-52/2475	-4/5445	272/4459455
$\mathrm{Nd^{III}}$	$^4\mathrm{I}_{9/2}$	-7/1089	-136/467181	-1615/42513471
$\mathrm{Pm^{III}}$	$^5\mathrm{I}_4$	14/1815	952/2335905	2584/42513471
$\mathrm{Sm^{III}}$	$^6\mathrm{H}_{5/2}$	13/315	26/10395	0
$\mathrm{Eu^{III}}$	$^7\mathrm{F}_0$	0	0	0
$\mathrm{Gd^{III}}$	$^8\mathrm{S}_{7/2}$	0	0	0
$\mathrm{Tb^{III}}$	$^7\mathrm{F}_6$	-1/99	2/16335	-1/891891
$\mathrm{Dy^{III}}$	$^6\mathrm{H}_{15/2}$	-2/315	-8/135135	4/3864861
$\mathrm{Ho^{III}}$	$^5\mathrm{I}_8$	-1/450	-1/30030	-5/3864861
$\mathrm{Er^{III}}$	$^4\mathrm{I}_{15/2}$	4/1575	2/45045	8/3864861
$\mathrm{Tm^{III}}$	$^3\mathrm{H}_6$	1/99	8/49005	-5/891891
$\mathrm{Yb^{III}}$	$^2\mathrm{F}_{7/2}$	2/63	-2/1155	4/27027

Table 19 – Tesseral Harmonic coefficients for the Stevens Operators

Operator
$C_2^0 = \frac{1}{4}\sqrt{\frac{5}{\pi}}$
$C_2^{\pm 1} = \frac{1}{2}\sqrt{\frac{15}{\pi}}$
$C_2^{\pm 2} = \frac{1}{4}\sqrt{\frac{15}{\pi}}$
$C_4^0 = \frac{3}{16}\sqrt{\frac{1}{\pi}}$
$C_4^{\pm 1} = \frac{3}{4}\sqrt{\frac{5}{2\pi}}$
$C_4^{\pm 2} = \frac{3}{8}\sqrt{\frac{5}{\pi}}$
$C_4^{\pm 3} = \frac{3}{8}\sqrt{\frac{70}{\pi}}$
$C_4^{\pm 4} = \frac{3}{16}\sqrt{\frac{35}{\pi}}$
$C_6^0 = \frac{1}{32}\sqrt{\frac{13}{\pi}}$
$C_6^{\pm 1} = \frac{1}{16}\sqrt{\frac{273}{\pi}}$
$C_6^{\pm 2} = \frac{1}{64}\sqrt{\frac{2730}{\pi}}$
$C_6^{\pm 3} = \frac{1}{32}\sqrt{\frac{2730}{\pi}}$
$C_6^{\pm 4} = \frac{3}{32}\sqrt{\frac{91}{\pi}}$
$C_6^{\pm 5} = \frac{3}{32}\sqrt{\frac{2002}{\pi}}$

$$\boxed{C_6^{\pm 6} = \frac{1}{32}\sqrt{\frac{3003}{2\pi}}}$$