Table 9.1 – continued from previous page

		ExcitationEnergies	AD	N	N		
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep	
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state	
		Temperature	D	N	N		
DBOC_Energy	N	DBOC_Energy	D	N	N		
DFT_Energy	N	nAlphaEl	I	N	N		
		nBetaEl	I	N	N		
		nTotalEl	I	N	N		
		finalEn	D	N	N	No Van der Waals correction	
		eExchange	D	N	N		
		eCorr	D	N	N		
		eXC	D	N	N		
		eCNL	D	N	N		
		eEmbed	D	Y	N		
BROKEN_SYMMETRY	N	enHighSpin	D	N	N	The High Spin Energy	
		enBrokenSym	D	N	N	The Broken Symmetry Energy	
		SHighSpin	D	N	N	The High Spin Spin	
		S2HighSpin	D	N	N	The Expectation value of S**2 for the High Spin case	
		S2BrokenSym	D	N	N	The Expectation value of S**2 for the Broken symmetry case	
Dipole_Moment	Y	dipoleMagnitude	D	N	N		a.u.
		dipoleElecContrib	AD	N	N	Electronic contribution	
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole	B	N	N		
		atomicDipole	AD	Y	N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
EFG_Tensor	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		QFAC	D	N	Y	Prefactor	
		V	AD	N	Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y		
Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.u.
		quadElecContrib	AD	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadTotal	AD	N	N	Total. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadDiagonalized	AD	N	N	The diagonalized tensor	a.u.
		doAtomicQuad	B	N	N		

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Table 9.1 – continued from previous page

		atomicQuad	AD	Y	N	Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
Polarizability	Y	isotropicPolar	D	N	N		
		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	N		
		doAtomicPolar	B	N	N		
		atomicPolarIso	AD	Y	N	Atomic istotropic polarizabilities	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
Hyperpolarizability	Y	rawCartesian	AD	N	N		a.u
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
Excited_States_Dynamics	N	fluorRateConstant	D	N	N		
Energy_Extrapolation	N	doEp1	B	N	N	Extrapolation using only one method	
		doEp2	B	N	N	Extrapolation using two different methods (same small basis Set)	
		doEp3	B	N	N	Extrapolation using two different methods (use three basis Sets for the cheap method)	
		doGradients	B	N	N	Extrapolate energy gradients	
		scfEnergies	AD	N	N		
		scfCBS	D	N	N		
		scfGradients	AD	Y	N	The SCF Gradients	
		corrEnergies	AD	N	N		
		corrCBS	D	N	N		
		ccsdtEnergyX	D	Y	N		
		totalCBS	D	N	N		
		cardinalNumbers	AI	N	N		
		alphas	AD	N	N		
		betas	AD	N	N		
		numOfEnergies	I	N	N	How many energies we are going to use (e.g. two-point scheme).	
		basisName	S	N	Y		
gCP_Energy	N	gCP_Energy	D	N	N		
Hessian	N	HESSIAN	AD	N	N	The Hessian	
		MODES	AD	N	N	The modes of vibrations	
ICE_Dipole_Moment [Dipole_Moment]	Y	dipoleMagnitude	D	N	N		a.u.
		dipoleElecContrib	AD	N	N	Electronic contribution	
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole	B	N	N		
		atomicDipole	AD	Y	N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
ICE_EFG_Tensor [EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		

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Table 9.1 – continued from previous page

		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		QFAC	D	N	Y	Prefactor	
		V	AD	N	Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y		
ICE_Polarizability [Polarizability]	Y	isotropicPolar	D	N	N		
		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	N		
		doAtomicPolar	B	N	N		
		atomicPolarIso	AD	Y	N	Atomic istotropic polarizabilities	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
ICE_Quadrupole_Moment [Quadrupole_Moment]	Y	isotropicQuadMoment	D	N	N		a.u.
		quadElecContrib	AD	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadTotal	AD	N	N	Total. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadDiagonalized	AD	N	N	The diagonalized tensor	a.u.
		doAtomicQuad	B	N	N		
		atomicQuad	AD	Y	N	Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
ICE_A_Tensor [A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elem	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		PFAC	D	N	Y	Prefactor PFAC=g$_e$g$_N$be*bN (in MHz)	
		ARaw	AD	N	Y	Raw tensor	
		AEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		AIso	D	N	Y		
ICE_Chemical_Shift [Chemical_Shift]	Y	numOfNucs	I	N	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	

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Table 9.1 – continued from previous page

		SDSO	AD	N	Y	Diamagnetic contribution
		SPSO	AD	N	Y	Paramagnetic contribution
		STot	AD	N	Y	Total tensor
		orientation	AD	N	Y	Eigenvectors
		sTotEigen	AD	N	Y	Eigenvalues
		siso	D	N	Y	
		saniso	D	N	Y	
ICE_D_Tensor [D_Tensor]	Y	d_raw	AD	N	N	
		d_eigenvalues	AD	N	N	
		d_eigenvectors	AD	N	N	
		D	D	N	N	
		E	D	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
ICE_G_Tensor [G_Tensor]	Y	g_matrix	AD	N	N	
		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass correction
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD	N	N	
		g_iso	D	N	N	
		Delta_g	AD	N	N	
		Delta_g_iso	D	N	N	
		orientation	AD	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
ICE_Spin_Spin_Coupling [Spin_Spin_Coupling]	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to calculate
		numOfNucPairsDSO	I	N	N	number of nuclear pairs to calculate DSO
		numOfNucPairsPSO	I	N	N	number of nuclear pairs to calculate PSO
		numOfNucPairsFC	I	N	N	number of nuclear pairs to calculate FC
		numOfNucPairsSD	I	N	N	number of nuclear pairs to calculate SD
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs to calculate SD/FC
		pairsInfo	AI	N	N	Pairs Info: Col1->Index of A. Col2->Atom. Num. of A. Col3->Index of B. Col4->Atom. Num. of B.
		pairsDistances	AD	N	N	The distances of each pair
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling constant for each pair
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
ICE_Absorption_Spectrum [Absorption_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC

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Table 9.1 – continued from previous page

		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Unknown, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	B	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	N	N	
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
ICE_ECD_Spectrum [ECD_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Unknown, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	B	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	N	N	

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Table 9.1 – continued from previous page

		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
Calculation_Info	N	Mult	I	N	N	
		Charge	I	N	N	
		NumOfAtoms	I	N	N	
		NumOfElectrons	I	N	N	
		NumOfBasisFuncts	I	N	N	
		NumOfAuxCBasisFuncts	I	N	N	
		NumOfAuxJBasisFuncts	I	N	N	
		NumOfAuxJKBasisFunct	I	N	N	
		NumOfCABSBasisFuncts	I	N	N	
Single_Point_Data	N	FinalEnergy	D	N	N	Final single point energy
		Converged	B	N	N	
LFT_Absorption_Spectrum [Absorption_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Unknown, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	B	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	N	N	
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
LFT_ECD_Spectrum [ECD_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC

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Table 9.1 – continued from previous page

		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Unknown, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	B	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	N	N	
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
A_Tensor	Y	numOfNucs	I	N	N	Number of active nuclei
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
		NUC	I	N	Y	Index of the nuclei
		Elem	I	N	Y	Atomic number of the nuclei
		Isotope	D	N	Y	Atomic mass
		I	D	N	Y	Spin of the nuclei
		PFAC	D	N	Y	Prefactor PFAC=g*e*g*N*be*bN (in MHz)
		ARaw	AD	N	Y	Raw tensor
		AEigenvalues	AD	N	Y	Eigenvalues
		orientation	AD	N	Y	Eigenvectors
		AIso	D	N	Y	
Chemical_Shift	Y	numOfNucs	I	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
		NUC	I	N	Y	Index of the nuclei
		Elems	I	N	Y	Atomic number of the nuclei
		SDSO	AD	N	Y	Diamagnetic contribution
		SPSO	AD	N	Y	Paramagnetic contribution
		STot	AD	N	Y	Total tensor
		orientation	AD	N	Y	Eigenvectors
		sTotEigen	AD	N	Y	Eigenvalues
		siso	D	N	Y	
		saniso	D	N	Y	

continues on next page

Table 9.1 – continued from previous page

D_Tensor	Y	d_raw	AD	N	N		
		d_eigenvalues	AD	N	N		
		d_eigenvectors	AD	N	N		
		D	D	N	N		
		E	D	N	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
G_Tensor	Y	g_matrix	AD	N	N		
		g_elec	D	N	N	The free electron g-value contribution	
		g_RMC	D	N	N	The reduced mass correction	
		g_DSO	AD	N	N		
		g_PSO	AD	N	N		
		g_Tot	AD	N	N		
		g_iso	D	N	N		
		Delta_g	AD	N	N		
		Delta_g_iso	D	N	N		
		orientation	AD	N	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
Spin_Spin_Coupling	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to calculate	
		numOfNucPairsDSO	I	N	N	number of nuclear pairs to calculate DSO	
		numOfNucPairsPSO	I	N	N	number of nuclear pairs to calculate PSO	
		numOfNucPairsFC	I	N	N	number of nuclear pairs to calculate FC	
		numOfNucPairsSD	I	N	N	number of nuclear pairs to calculate SD	
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs to calculate SD/FC	
		pairsInfo	AI	N	N	Pairs Info: Col1->Index of A. Col2->Atom. Num. of A. Col3->Index of B. Col4->Atom. Num. of B.	
		pairsDistances	AD	N	N	The distances of each pair	
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling constant for each pair	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MCRPA_Dipole_Moment [Dipole_Moment]	Y	dipoleMagnitude	D	N	N		a.u.
		dipoleElecContrib	AD	N	N	Electronic contribution	
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole	B	N	N		
		atomicDipole	AD	Y	N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MCRPA_EFG_Tensor [EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		

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Table 9.1 – continued from previous page

		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		QFAC	D	N	Y	Prefactor	
		V	AD	N	Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y		
MCRPA_Polarizability [Polarizability]	Y	isotropicPolar	D	N	N		
		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	N		
		doAtomicPolar	B	N	N		
		atomicPolarIso	AD	Y	N	Atomic istotropic polarizabilities	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MCRPA_Quadrupole_Moment [Quadrupole_Moment]	Y	isotropicQuadMoment	D	N	N		a.u.
		quadElecContrib	AD	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadTotal	AD	N	N	Total. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadDiagonalized	AD	N	N	The diagonalized tensor	a.u.
		doAtomicQuad	B	N	N		
		atomicQuad	AD	Y	N	Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MCRPA_A_Tensor [A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elem	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		PFAC	D	N	Y	Prefactor PFAC=ge*g*Nbe*bN (in MHz)	
		ARaw	AD	N	Y	Raw tensor	
		AEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		AIso	D	N	Y		
MCRPA_Chemical_Shift [Chemical_Shift]	Y	numOfNucs	I	N	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		SDSO	AD	N	Y	Diamagnetic contribution	

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Table 9.1 – continued from previous page

		SPSO	AD	N	Y	Paramagnetic contribution
		STot	AD	N	Y	Total tensor
		orientation	AD	N	Y	Eigenvectors
		sTotEigen	AD	N	Y	Eigenvalues
		siso	D	N	Y	
		saniso	D	N	Y	
MCRPA_D_Tensor [D_Tensor]	Y	d_raw	AD	N	N	
		d_eigenvalues	AD	N	N	
		d_eigenvectors	AD	N	N	
		D	D	N	N	
		E	D	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MCRPA_G_Tensor [G_Tensor]	Y	g_matrix	AD	N	N	
		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass correction
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD	N	N	
		g_iso	D	N	N	
		Delta_g	AD	N	N	
		Delta_g_iso	D	N	N	
		orientation	AD	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MCRPA_Spin_Spin_Coupling [Spin_Spin_Coupling]	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to calculate
		numOfNucPairsDSO	I	N	N	number of nuclear pairs to calculate DSO
		numOfNucPairsPSO	I	N	N	number of nuclear pairs to calculate PSO
		numOfNucPairsFC	I	N	N	number of nuclear pairs to calculate FC
		numOfNucPairsSD	I	N	N	number of nuclear pairs to calculate SD
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs to calculate SD/FC
		pairsInfo	AI	N	N	Pairs Info: Col1->Index of A. Col2->Atom. Num. of A. Col3->Index of B. Col4->Atom. Num. of B.
		pairsDistances	AD	N	N	The distances of each pair
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling constant for each pair
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MCRPA_Absorption_Spectrum [Absorption_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC

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Table 9.1 – continued from previous page

		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Unknown, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	B	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	N	N	
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
MCRPA_ECD_Spectrum[ECD_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Unknown, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	B	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	N	N	

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Table 9.1 – continued from previous page

		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep	
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state	
		Temperature	D	N	N		
MDCI_Energies [Energy]	Y	numOfEl	I	N	N		
		numOfCorrEl	I	N	N		
		numOfAlphaCorrEl	I	N	N		
		numOfBetaCorrEl	I	N	N		
		refEnergy	AD	N	N	Reference Energy	
		corrEnergy	AD	N	N	Total Correlation Energy	
		aaCorrEn	AD	N	N	Alpha-Alpha Pairs Correlation Energy (No (T))	
		bbCorrEn	AD	N	N	Beta-Beta Pairs Correlation Energy (No (T))	
		abCorrEn	AD	N	N	Alpha-Beta Pairs Correlation Energy (No (T))	
		CorrDS	AD	Y	N	Singlet pairs energy of double amplitudes (No (T))	
		CorrDT	AD	Y	N	Triplet pairs energy of double amplitudes (No (T))	
		CorrSS	AD	Y	N	Singlet pairs energy of quadratic single amplitudes (No (T))	
		CorrST	AD	Y	N	Triplet pairs energy of quadratic single amplitudes (No (T))	
		triplesEnergy	AD	N	N	Triples Correction Energy	
		Method	S	N	N		
		totalEnergy	AD	N	N	Total energy of each state	
		Mult	AI	Y	N	Multiplicity of each state	
		Irrep	AI	Y	N	Irreducible representation of each state	
		RelCorr	S	Y	N	Relativistic correction (SOC and/or SSC)	
		NBlocks	I	Y	N	Number of multiplicity blocks	
		NRoots	AI	Y	N	Number of roots in each block	
		NTotalRoots	I	Y	N	Total number of roots	
		Block	AI	Y	N	Block index of each state	
		Root	AI	Y	N	Root index within the block	
		FollowIRoot	I	Y	N	Index of the followed root	
		AvgMult	AD	Y	N	Average multiplicity of each SO-/SS-coupled state	
MDCI_Nuc_Gradient [Nuclear_Gradient]	Y	NAtoms	I	N	N		
		gradNorm	D	N	N		
		grad	AD	N	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MDCI_Dipole_Moment [Dipole_Moment]	Y	dipoleMagnitude	D	N	N		a.u.
		dipoleElecContrib	AD	N	N	Electronic contribution	
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole	B	N	N		
		atomicDipole	AD	Y	N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		

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Table 9.1 – continued from previous page

		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MDCI_EFG_Tensor [EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		QFAC	D	N	Y	Prefactor	
		V	AD	N	Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y		
MDCI_Polarizability [Polarizability]	Y	isotropicPolar	D	N	N		
		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	N		
		doAtomicPolar	B	N	N		
		atomicPolarIso	AD	Y	N	Atomic istotropic polarizabilities	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MDCI_Quadrupole_Moment [Quadrupole_Moment]	Y	isotropicQuadMoment	D	N	N		a.u.
		quadElecContrib	AD	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadTotal	AD	N	N	Total. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadDiagonalized	AD	N	N	The diagonalized tensor	a.u.
		doAtomicQuad	B	N	N		
		atomicQuad	AD	Y	N	Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MDCI_A_Tensor [A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elem	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		PFAC	D	N	Y	Prefactor PFAC=g$_e$g$_N$be*bN (in MHz)	
		ARaw	AD	N	Y	Raw tensor	
		AEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		AIso	D	N	Y		
MDCI_Chemical_Shift [Chemical_Shift]	Y	numOfNucs	I	N	N		
		Method	S	N	N		

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Table 9.1 – continued from previous page

		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
		NUC	I	N	Y	Index of the nuclei
		Elems	I	N	Y	Atomic number of the nuclei
		SDSO	AD	N	Y	Diamagnetic contribution
		SPSO	AD	N	Y	Paramagnetic contribution
		STot	AD	N	Y	Total tensor
		orientation	AD	N	Y	Eigenvectors
		sTotEigen	AD	N	Y	Eigenvalues
		siso	D	N	Y	
		saniso	D	N	Y	
MDCI_D_Tensor [D_Tensor]	Y	d_raw	AD	N	N	
		d_eigenvalues	AD	N	N	
		d_eigenvectors	AD	N	N	
		D	D	N	N	
		E	D	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MDCI_G_Tensor [G_Tensor]	Y	g_matrix	AD	N	N	
		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass correction
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD	N	N	
		g_iso	D	N	N	
		Delta_g	AD	N	N	
		Delta_g_iso	D	N	N	
		orientation	AD	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MDCI_Spin_Spin_Coupling [Spin_Spin_Coupling]	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to calculate
		numOfNucPairsDSO	I	N	N	number of nuclear pairs to calculate DSO
		numOfNucPairsPSO	I	N	N	number of nuclear pairs to calculate PSO
		numOfNucPairsFC	I	N	N	number of nuclear pairs to calculate FC
		numOfNucPairsSD	I	N	N	number of nuclear pairs to calculate SD
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs to calculate SD/FC
		pairsInfo	AI	N	N	Pairs Info: Col1->Index of A. Col2->Atom. Num. of A. Col3->Index of B. Col4->Atom. Num. of B.
		pairsDistances	AD	N	N	The distances of each pair
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling constant for each pair
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MDCI_Absorption_Spectrum [Absorption_Spectrum]	Y	Method	I	N	N	

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Table 9.1 – continued from previous page

		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Unknown, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	B	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	N	N	
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
MDCI_ECD_Spectrum[ECD_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Unknown, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	B	N	N	
		NTrans	I	N	N	

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Table 9.1 – continued from previous page

		ExcitationEnergies	AD	N	N		
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep	
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state	
		Temperature	D	N	N		
MP2_Energies [Energy]	Y	refEnergy	AD	N	N	Reference energy for each state	
		corrEnergy	AD	N	N	MP2 correlation energy for each state	
		Method	S	N	N		
		totalEnergy	AD	N	N	Total energy of each state	
		Mult	AI	Y	N	Multiplicity of each state	
		Irrep	AI	Y	N	Irreducible representation of each state	
		RelCorr	S	Y	N	Relativistic correction (SOC and/or SSC)	
		NBlocks	I	Y	N	Number of multiplicity blocks	
		NRoots	AI	Y	N	Number of roots in each block	
		NTotalRoots	I	Y	N	Total number of roots	
		Block	AI	Y	N	Block index of each state	
		Root	AI	Y	N	Root index within the block	
		FollowIRoot	I	Y	N	Index of the followed root	
		AvgMult	AD	Y	N	Average multiplicity of each SO-/SS-coupled state	
MP2_Nuc_Gradient [Nuclear_Gradient]	Y	NAtoms	I	N	N		
		gradNorm	D	N	N		
		grad	AD	N	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MP2_Dipole_Moment [Dipole_Moment]	Y	dipoleMagnitude	D	N	N		a.u.
		dipoleElecContrib	AD	N	N	Electronic contribution	
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole	B	N	N		
		atomicDipole	AD	Y	N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MP2_EFG_Tensor [EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		QFAC	D	N	Y	Prefactor	
		V	AD	N	Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y		
MP2_Polarizability [Polarizability]	Y	isotropicPolar	D	N	N		

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Table 9.1 – continued from previous page

		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	N		
		doAtomicPolar	B	N	N		
		atomicPolarIso	AD	Y	N	Atomic istotropic polarizabilities	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MP2_Quadrupole_Moment [Quadrupole_Moment]	Y	isotropicQuadMoment	D	N	N		a.u.
		quadElecContrib	AD	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadTotal	AD	N	N	Total. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadDiagonalized	AD	N	N	The diagonalized tensor	a.u.
		doAtomicQuad	B	N	N		
		atomicQuad	AD	Y	N	Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MP2_A_Tensor [A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elem	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		PFAC	D	N	Y	Prefactor PFAC=g*e*g*N*be*bN (in MHz)	
		ARaw	AD	N	Y	Raw tensor	
		AEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		AIso	D	N	Y		
MP2_Chemical_Shift [Chemical_Shift]	Y	numOfNucs	I	N	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		SDSO	AD	N	Y	Diamagnetic contribution	
		SPSO	AD	N	Y	Paramagnetic contribution	
		STot	AD	N	Y	Total tensor	
		orientation	AD	N	Y	Eigenvectors	
		sTotEigen	AD	N	Y	Eigenvalues	
		siso	D	N	Y		
		saniso	D	N	Y		
MP2_D_Tensor [D_Tensor]	Y	d_raw	AD	N	N		
		d_eigenvalues	AD	N	N		
		d_eigenvectors	AD	N	N		
		D	D	N	N		
		E	D	N	N		

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Table 9.1 – continued from previous page

		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MP2_G_Tensor [G_Tensor]	Y	g_matrix	AD	N	N	
		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass correction
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD	N	N	
		g_iso	D	N	N	
		Delta_g	AD	N	N	
		Delta_g_iso	D	N	N	
		orientation	AD	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MP2_Spin_Spin_Coupling [Spin_Spin_Coupling]	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to calculate
		numOfNucPairsDSO	I	N	N	number of nuclear pairs to calculate DSO
		numOfNucPairsPSO	I	N	N	number of nuclear pairs to calculate PSO
		numOfNucPairsFC	I	N	N	number of nuclear pairs to calculate FC
		numOfNucPairsSD	I	N	N	number of nuclear pairs to calculate SD
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs to calculate SD/FC
		pairsInfo	AI	N	N	Pairs Info: Col1->Index of A. Col2->Atom. Num. of A. Col3->Index of B. Col4->Atom. Num. of B.
		pairsDistances	AD	N	N	The distances of each pair
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling constant for each pair
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MP2_Absorption_Spectrum [Absorption_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad

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		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed	
		Density_name	S	N	N		
		Representation	S	N	N	Possible values: Unknown, Length, Velocity	
		PointGroup	S	N	N		
		DoHigherMoments	B	N	N		
		NTrans	I	N	N		
		ExcitationEnergies	AD	N	N		
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep	
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state	
		Temperature	D	N	N		
MP2_ECD_Spectrum [ECD_Spectrum]	Y	Method	I	N	N		
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC	
		DensType	I	N	N	Type of density (electron/spin …). 0->Unknow, 1->Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin	
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad	
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, … 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed	
		Density_name	S	N	N		
		Representation	S	N	N	Possible values: Unknown, Length, Velocity	
		PointGroup	S	N	N		
		DoHigherMoments	B	N	N		
		NTrans	I	N	N		
		ExcitationEnergies	AD	N	N		
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep	
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state	
		Temperature	D	N	N		
MRCI_Dipole_Moment [Dipole_Moment]	Y	dipoleMagnitude	D	N	N		a.u.
		dipoleElecContrib	AD	N	N	Electronic contribution	
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole	B	N	N		
		atomicDipole	AD	Y	N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
		Level	S	N	N		

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Table 9.1 – continued from previous page

		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MRCI_EFG_Tensor [EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		QFAC	D	N	Y	Prefactor	
		V	AD	N	Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y		
MRCI_Polarizability [Polarizability]	Y	isotropicPolar	D	N	N		
		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	N		
		doAtomicPolar	B	N	N		
		atomicPolarIso	AD	Y	N	Atomic istotropic polarizabilities	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MRCI_Quadrupole_Moment [Quadrupole_Moment]	Y	isotropicQuadMoment	D	N	N		a.u.
		quadElecContrib	AD	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadTotal	AD	N	N	Total. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadDiagonalized	AD	N	N	The diagonalized tensor	a.u.
		doAtomicQuad	B	N	N		
		atomicQuad	AD	Y	N	Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MRCI_A_Tensor [A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elem	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		PFAC	D	N	Y	Prefactor PFAC=g*e*g*N*be*bN (in MHz)	
		ARaw	AD	N	Y	Raw tensor	
		AEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		AIso	D	N	Y		
MRCI_Chemical_Shift [Chemical_Shift]	Y	numOfNucs	I	N	N		
		Method	S	N	N		
		Level	S	N	N		

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