Table 9.1 – continued from previous page

		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	
AutoCI_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	
AutoCI_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

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Table 9.1 – continued from previous page

		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	
AutoCI_MRCI_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	
AutoCI_MRCI_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	
CAS_DCD_Energies [Energy]	Y	finalEnergy	D	N	N	Final GS or SA energy
		numOfElectrons	I	N	N	
		numOfActiveEl	I	N	N	Number of active electrons
		numOfActiveOrbs	I	N	N	Number of active orbitals
		numOfFCElectrons	I	N	N	
		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
CAS_MSPT2_Energies [Energy]	Y	finalEnergy	D	N	N	Final GS or SA energy
		numOfElectrons	I	N	N	
		numOfActiveEl	I	N	N	Number of active electrons
		numOfActiveOrbs	I	N	N	Number of active orbitals
		numOfFCElectrons	I	N	N	
		Method	S	N	N	
		totalEnergy	AD	N	N	Total energy of each state
		Mult	AI	Y	N	Multiplicity of each state

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Table 9.1 – continued from previous page

		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	
CAS_PT2_Energies [Energy]	Y	finalEnergy	D	N	N	Final GS or SA energy	
		numOfElectrons	I	N	N		
		numOfActiveEl	I	N	N	Number of active electrons	
		numOfActiveOrbs	I	N	N	Number of active orbitals	
		numOfFCElectrons	I	N	N		
		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	
CAS_SCF_Energies [Energy]	Y	finalEnergy	D	N	N	Final GS or SA energy	
		numOfElectrons	I	N	N		
		numOfActiveEl	I	N	N	Number of active electrons	
		numOfActiveOrbs	I	N	N	Number of active orbitals	
		numOfFCElectrons	I	N	N		
		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	
CASSCF_Dipole_Moment [Dipole_Moment]	Y	dipoleMagnitude	D	N	N		a.u.
		dipoleElecContrib	AD	N	N	Electronic contribution	

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Table 9.1 – continued from previous page

		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		
CASSCF_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		
CASSCF_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		
CASSCF_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		
CASSCF_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)	

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Table 9.1 – continued from previous page

		ARaw	AD	N	Y	Raw tensor
		AEigenvalues	AD	N	Y	Eigenvalues
		orientation	AD	N	Y	Eigenvectors
		AIso	D	N	Y	
CASSCF_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	
CASSCF_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	
CASSCF_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	
CASSCF_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	

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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
D_Tensor_CASSCF_2ndOrder [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
D_Tensor_CASSCF_2ndOrder_ES [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
D_Tensor_CASSCF_Heff [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
D_Tensor_CASSCF_Heff_ES [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
D_Tensor_NEVPT2_2ndOrder [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
D_Tensor_NEVPT2_2ndOrder_ES [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
D_Tensor_NEVPT2_Heff [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

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Table 9.1 – continued from previous page

		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
D_Tensor_NEVPT2_Heff_ES [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	
D_Tensor_CUSTOM_2ndOrder [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	
D_Tensor_CUSTOM_2ndOrder_ES [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	
D_Tensor_CUSTOM_Heff [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	
D_Tensor_CUSTOM_Heff_ES [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_CASSCF_2ndOrder [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	
G_Tensor_CASSCF_Heff [G_Tensor]	Y	g_matrix	AD	N	N	

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Table 9.1 – continued from previous page

		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	
G_Tensor_NEVPT2_2ndOrder [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	
G_Tensor_NEVPT2_Heff [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	
G_Tensor_CUSTOM_2ndOrder [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	
G_Tensor_CUSTOM_Heff [G_Tensor]	Y	g_matrix	AD	N	N	
		g_elec	D	N	N	The free electron g-value contribution

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Table 9.1 – continued from previous page

		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	
CASSCF_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	
CASSCF_PT_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

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Table 9.1 – continued from previous page

		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	
CASSCF_QDPT_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	
CASSCF_DCD_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	
CASSCF_PT_Energies_Absorption_Spectrum [Absorption_Spectrum]	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	
CASSCF_Custom_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	
CASSCF_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

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Table 9.1 – continued from previous page

		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	
CASSCF_PT_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	
CASSCF_QDPT_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	
CASSCF_DCD_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	
CASSCF_PT_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	
CASSCF_Custom_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

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Table 9.1 – continued from previous page

		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		
CIPSI_Energies	N	finalEnergy	D	N	N		
		numOfRoots	I	N	N		
		multiplicity	I	N	N		
		energies	AD	N	N		
CIS_Energies [Energy]	Y	e0	D	N	N	Ground state energy	
		multP1	B	N	N	Do the higher multiplicity too?	
		mode	S	N	N	CIS mode: CIS, RPA, TDA, TD-DFT, sTDA, sTD-DFT	
		dCorr	I	N	N	(D) Correction algorithm	
		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	
CIS_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		
CIS_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		

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Table 9.1 – continued from previous page

		Irrep	I	N	N		
CIS_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		
CIS_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		
CIS_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		
CIS_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		
CIS_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		

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Table 9.1 – continued from previous page

		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	
CIS_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	
CIS_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	
CIS_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	
CIS_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	
CIS_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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