Table 9.1 – continued from previous page

		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	
MRCI_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	
MRCI_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	
MRCI_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	
D_Tensor_MRCI_2ndOrder [D_Tensor]	Y	d_raw	AD	N	N	
		d_eigenvalues	AD	N	N	
		d_eigenvectors	AD	N	N	

continues on next page

Table 9.1 – continued from previous page

		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_MRCI_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_MRCI_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_MRCI_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	
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	

continues on next page

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	
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
		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	
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	
CHELPG_Population_Analysis	Y	NAtoms	I	N	N	
		ATNO	AI	N	N	
		AtomicCharges	AD	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
Hirshfeld_Population_Analysis	Y	NAtoms	I	N	N	
		ATNO	AI	N	N	
		DENSA	D	N	N	Total integrated alpha density

continues on next page

Table 9.1 – continued from previous page

		DENSB	D	N	N	Total integrated beta density
		AtomicCharges	AD	N	N	
		Spin	AD	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
Loewdin_Population_Analysis	Y	NAtoms	I	N	N	
		ATNO	AI	N	N	
		AtomicCharges	AD	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
Mayer_Population_Analysis	Y	NAtoms	I	N	N	Total number of atoms
		NBondOrdersPrint	I	N	N	The number of bond orders larger than threshold
		bondThresh	D	N	N	The threshold for printing
		components	AI	Y	N	The indices and atomic numbers of the bonding atoms
		BondOrders	AD	Y	N	The bond orders
		ATNO	AI	N	N	Atomic number of the elements
		NA	AD	N	N	Mulliken gross atomic population
		ZA	AD	N	N	Total nuclear charge
		QA	AD	N	N	Mulliken gross atomic charge
		VA	AD	N	N	Mayer's total valence
		BVA	AD	N	N	Mayer's bonded valence
		FA	AD	N	N	Mayer's free valence
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MBIS_Population_Analysis	Y	NAtoms	I	N	N	
		ATNO	AI	N	N	
		Thresh	D	N	N	
		Niter	I	N	N	
		LargePrint	B	N	N	
		DENSA	D	N	N	Total integrated alpha density
		DENSB	D	N	N	Total integrated beta density
		AtomicCharges	AD	N	N	
		Spin	AD	N	N	
		NPOPVAL	AD	N	N	
		SIGMAVAL	AD	N	N	
		AtomicDipole	AD	Y	N	
		AtomicQuadrupole	AD	Y	N	
		AtomicOctupole	AD	Y	N	
		ThirdRadialMoment	AD	Y	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
Mulliken_Population_Analysis	Y	NAtoms	I	N	N	
		ATNO	AI	N	N	
		AtomicCharges	AD	N	N	
		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

RASCI_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		
RASCI_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		
RASCI_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		
RASCI_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		
RASCI_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		
RASCI_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		

continues on next page

Table 9.1 – continued from previous page

		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	
RASCI_Chemical_Shift [Chemical_Shift]	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	
RASCI_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	
RASCI_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	
RASCI_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

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Table 9.1 – continued from previous page

		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	
RASCI_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	
RASCI_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		
ROCIS_Energies	N	refEnergy	D	N	N		
		corrEnergy	D	N	N		
		totalEnergy	D	N	N		
		numOfRoots	I	N	N		
		Energies	AD	N	N	State energies in Hartree	
		Multiplicities	AI	N	N		
ROCIS_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		
ROCIS_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		
ROCIS_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		
ROCIS_Quadrupole_Moment [Quadrupole_Moment]	Y	isotropicQuadMoment	D	N	N		a.u.
		quadElecContrib	AD	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	

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Table 9.1 – continued from previous page

		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		
ROCIS_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		
ROCIS_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		
ROCIS_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		
ROCIS_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		

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Table 9.1 – continued from previous page

		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	
ROCIS_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	
ROCIS_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

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Table 9.1 – continued from previous page

		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state	
		Temperature	D	N	N		
ROCIS_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		
RPA_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		
RPA_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	

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Table 9.1 – continued from previous page

		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y		
RPA_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		
RPA_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		
RPA_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		
RPA_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		
RPA_D_Tensor [D_Tensor]	Y	d_raw	AD	N	N		
		d_eigenvalues	AD	N	N		

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Table 9.1 – continued from previous page

		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	
RPA_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	
RPA_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	
RPA_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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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	
RPA_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	
Energy	Y	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

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Table 9.1 – continued from previous page

		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	
SCF_Energy [Energy]	Y	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	
SCF_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		
SCF_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		
SCF_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		
SCF_Polarizability [Polarizability]	Y	isotropicPolar	D	N	N		
		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	N		

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Table 9.1 – continued from previous page

		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		
SCF_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		
SCF_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		
SCF_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		
SCF_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		

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Table 9.1 – continued from previous page

		State	I	N	N	
		Irrep	I	N	N	
SCF_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	
SCF_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	
SCF_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	

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Table 9.1 – continued from previous page

		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	
SCF_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	
SOC_Energy_Correction	N	total_SOC_energy	D	N	N	
		total_non_SOC_energy	D	N	N	
		nuclear_energy	D	N	N	
		SOC_correction	D	N	N	
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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		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	
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		
THERMOCHEMISTRY_Energies	Y	temperature	D	N	N		
		pressure	D	N	N		
		totalMass	D	N	N		
		spinDegeneracy	I	N	N		
		elEnergy	D	N	N		
		transEnergy	D	N	N		
		rotEnergy	D	N	N		
		vibEnergy	D	N	N		
		numOfFreqs	I	N	N		
		freqScalingFactor	D	N	N		
		FREQ	AD	N	N		cm^-1
		zpe	D	N	N		
		innerEnergyU	D	N	N		
		enthalpyH	D	N	N		
		qEl	D	N	N		
		qRot	D	N	N		
		qVib	D	N	N		
		qTrans	D	N	N		
		entropyS	D	N	N		
		freeEnergyG	D	N	N		
		isLinear	B	N	N		
VdW_Correction	N	vdW	D	N	N		
		vdW_atomic	AD	Y	N		
Calculation_Status	N	version	S	N	N		
		progName	S	N	N		
		Status	S	N	N		
MDCI_EOM_Energies	Y	groundRefEnergy	D	N	N	Ground State Reference Energy	
		groundCorrEnergy	D	N	N	Ground State Correlation Energy	
		groundTotalEnergy	D	N	N	Ground State Total MDCI Energy	
CASPT2_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		
CAS_CUSTOM_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		
CASPT2_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	

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