Table 9.1 – continued from previous page

	Table 9	9.1 – continued from previous	page			
		pairsDistances	AD	N	N	The distances of each pair
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling
		Mothod	S	N	N	constant for each pair
		Method				
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
AutoCI_Absorption_Spectrum	Y	Method	I	N	N	
[Absorption_Spectrum]		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	7 Cincianed, 3 7 Technica
		Representation	S	N	N	Possible values: Un-
				3.7		known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	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: Multi-
			_			plicity of the final state
	. -	Temperature	D	N	N	
AutoCI_ECD_Spectrum	Y	Method	I	N	N	
ECD_Spectrum]		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 continues on next page

Table 9.1 - continued from previous page

Tal	ble 9	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 Representation	S S	N N	N N	Possible values: Un-
		_				known, Length, Velocity
		PointGroup	S B	N N	N N	
		DoHigherMoments 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	Coll: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
AutoCI_MRCI_Absorption_Spectrum	Y	Method	I	N	N	m
[Absorption_Spectrum]		RelCorrection	Ι	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	Ι	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	Descible and 77
		Representation	S	N	N	Possible values: Un- known, Length, Velocity
		PointGroup	S	N	N	-
		DoHigherMoments	В	N	N	
		NTrans	I	N N	N N	
		ExcitationEnergies States	AD AI	N N	N N	The initial and Final
		States	Ai	IN	IN	states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD		N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
AutoCI MDCI ECD Ct	Y	Temperature Method	D	N N	N	
AutoCI_MRCI_ECD_Spectrum [ECD_Spectrum]	1	RelCorrection	I I	N	N N	Type of relativistic
[ECD_Spectrum]		RelCorrection	1	IN	IN	treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
						continues on next page

Table 9.1 - continued from previous page

	Table 9	0.1 – continued from previous	s 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 Representation	S S	N N	N N	Possible values: Un-
		PointGroup	S	N	N	known, Length, Velocity
		DoHigherMoments	В	N	N	
		NTrans	I	N	N	
		ExcitationEnergies		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 numOfActiveEl	I I	N N	N N	Number of active elec-
						trons
		numOfActiveOrbs	I	N	N	Number of active orbitals
		numOfFCElectrons Method	I S	N N	N N	
		totalEnergy	AD		N	Total energy of each state
		Mult	AI	Y	N	Multiplicity of each state
		Irrep	AI	Y	N	Irreducible representa-
		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 AD	N N	N N	Total energy of each state
		totalEnergy Mult	AI	Y	N	Multiplicity of each state
			471	1	T.4	manipiletty of each state

continues on next page

	Table 9	9.1 – continued from previous	s page				
		Irrep	AI	Y	N	Irreducible representa- tion 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	ΑI	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	
3 : 32,		numOfElectrons	I	N	N	2,	
		numOfActiveEl	I	N	N	Number of active electrons	
		numOfActiveOrbs numOfFCElectrons	I I	N N	N N	Number of active orbitals	
		Method	S	N	N		
		totalEnergy	AD	N	N	Total energy of each state	
		Mult	ΑI	Y	N	Multiplicity of each state	
		Irrep	AI	Y	N	Irreducible representa- tion 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	ΑI	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	TD 4 1 C 1	
		totalEnergy	AD		N	Total energy of each state	
		Mult Irrep	AI AI	Y	N N	Multiplicity of each state Irreducible representa-	
		RelCorr	S	Y	N	tion of each state 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	Y	dipoleMagnitude	D	N	N		a.u.
[Dipole_Moment]		dipoleElecContrib	AD	N	N	Electronic contribution	
						continues on nex	t nage

Table 9.1 - continued from previous page

	Table 9	9.1 – continued from previous	page				
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole atomicDipole	B AD	N Y	N N	Atomic dipoles (NAtoms	
		Makhad	C	NI	NT	* X,Y,Z)	
		Method Level	S S	N N	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	
chooci_brd_tensor[brd_tensor]		Method	S	N	N	rumber of active factor	
		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		Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y	_	
CASSCF_Polarizability	Y	isotropicPolar	D	N	N		
[Polarizability]		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD		N		
		doAtomicPolar	В	N	N		
		atomicPolarIso	AD		N	Atomic istotropic polar- izabilities	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
CLOCCE O . l l . M l	37	Irrep	I	N	N		
CASSCF_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.u.
[Quadrupole_Moment]		quadElecContrib	AD	IN	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ,	
		quadTotal	AD	N	N	XY, XZ, YZ Total. Order: XX, YY,	
		quadDiagonalized	۸D	N	NI	ZZ, XY, XZ, YZ The diagonalized tensor	0.13
		doAtomicQuad	AD B	N	N N	i ne diagonanzed tensor	a.u.
		atomicQuad	AD		N	Atomic quadrupoles (NAtoms * XX, YY, ZZ,	
		Mothod	S	N	N	XY, XZ, YZ)	
		Method 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	
[0.002]	•	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=gegNbe*bN	
						(in MHz) continues on next p	nage

Table 9.1 - continued from previous page

	Table 9	0.1 – continued from previous	page			
		ARaw	AD	N	Y	Raw tensor
		AEigenvalues	AD		Y	Eigenvalues
		orientation	AD		Y	Eigenvectors
		AIso	D	N	Y	Eigen/ectors
CASSCF_Chemical_Shift	Y	numOfNucs	I	N	N	
[Chemical_Shift]	1	Method	S	N	N	
[Chemical_Shirt]						
		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 contribu-
		SPSO	AD	N	Y	Paramagnetic contribu-
		Q	A D	N.T	37	
		STot	AD		Y	Total tensor
		orientation	AD		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	
[5_1001]	•	d_eigenvalues	AD		N	
					N	
		d_eigenvectors	AD			
		D	D	N	N	
		E	D	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
			I	N		
		Irrep			N	
CASSCF_G_Tensor[G_Tensor]	Y	g_matrix	AD		N	
		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass cor- rection
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD	N	N	
		g_iso	D	N	N	
		Delta_q	AD		N	
			D	N	N	
		Delta_g_iso				
		orientation	AD		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
[-1		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
		pairsTotalSSCIso Method	AD S	N N	N N	The Spin-Spin coupling constant for each pair

Table 9.1 - continued from previous page

	able	9.1 – continued from previou	us page		
		Level	S	N	N
		Mult	I	N	N
		State	I	N	N
		Irrep	I	N	N
D_Tensor_CASSCF_2ndOrder	Y	d_raw	AD	N	N
[D_Tensor]		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	Y	d_raw	AD	N	N
[D_Tensor]		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
		d_eigenvalues	AD		N
		d_eigenvectors	AD		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
			I	N	N
D Tongon CACCCE Hoff EC	Y	Irrep d_raw	AD		N
D_Tensor_CASSCF_Heff_ES	1		AD		N N
[D_Tensor]		d_eigenvalues			
		d_eigenvectors	AD		N
		D E	D	N	N N
			D	N	
		Method	S S	N	N N
		Level Mult		N	
			I	N	N
		State	I	N	N
D	3.7	Irrep	I	N	N
D_Tensor_NEVPT2_2ndOrder	Y	d_raw	AD		N
[D_Tensor]		d_eigenvalues	AD		N
		d_eigenvectors	AD		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	Y	d_raw	AD		N
[D_Tensor]		d_eigenvalues	AD		N
		d_eigenvectors	AD		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	_	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
					continues on next page

Table 9.1 - continued from previous page

	Table 9	9.1 – continued from previou	s page			
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
D_Tensor_NEVPT2_Heff_ES	Y	d_raw	AD	N	N	
[D_Tensor]		d_eigenvalues	AD		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	Y	d_raw	AD	N	N	
[D_Tensor]		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	Y	d_raw	AD	N	N	
[D_Tensor]		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	
<pre>D_Tensor_CUSTOM_Heff[D_Tensor]</pre>	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	Y	d_raw	AD	N	N	
[D_Tensor]		d_eigenvalues	AD		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	Y	g_matrix	AD		N	
[G_Tensor]		g_elec	D	N	N	The free electron g-value
						contribution
		g_RMC	D	N	N	The reduced mass cor-
						rection
		g_DSO	AD		N	
		g_PSO	AD		N	
		g_Tot	AD		N	
		g_iso	D	N	N	
		Delta_g	AD		N	
		Delta_g_iso	D	N	N	
		orientation	AD		N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
Q Q2 Q2Q C2	**	Irrep	I	N	N	
G_Tensor_CASSCF_Heff[G_Tensor]	Y	g_matrix	AD	N	N	
						continues on next page

Table 9.1 - continued from previous page

l	able 9	.1 – continued from previous	s page			
		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass cor- rection
		g_DSO	AD	N	N	rection
		g_PSO	AD		N	
		g_Tot	AD		N	
		g_iso	D	N	N	
		Delta_g	AD		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	Y	g_matrix	AD		N	
[G_Tensor]	•	g_elec	D	N	N	The free electron g-value
[G_TellSOT]						contribution
		g_RMC	D	N	N	The reduced mass cor- rection
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD	N	N	
		q_iso	D	N	N	
		Delta_g	AD		N	
		Delta_g_iso	D	N	N	
		orientation	AD		N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
<pre>G_Tensor_NEVPT2_Heff[G_Tensor]</pre>	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 cor- rection
		g_DSO	AD	N	N	
		g_PSO	AD		N	
		g_Tot	AD		N	
			D	N	N	
		g_iso				
		Delta_g	AD		N	
		Delta_g_iso	D	N	N	
		orientation	AD		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	Y	g_matrix	AD	N	N	
[G_Tensor]		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass correction
		q_DSO	AD	N	N	
		g_PSO	AD		N	
		g_Tot	AD		N	
		g_iso	D	N	N	
		-	AD		N	
		Delta_g				
		Delta_g_iso	D	N	N	
		orientation	AD		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

Table 9.1 - continued from previous page

T	able 9	0.1 – continued from previous	page			
		g_RMC	D	N	N	The reduced mass cor- rection
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD	N	N	
		q_iso	D	N	N	
		Delta_g	AD		N	
		Delta_g_iso	D	N	N	
		orientation	AD		N	
		Method	S	N	N	
		Level	S	N	N	
			I	N	N	
		Mult				
		State	I	N	N	
03.0007 31	37	Irrep	I	N	N	
CASSCF_Absorption_Spectrum	Y	Method	I	N	N	
[Absorption_Spectrum]		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-
		DeriType	I	N	N	>Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin Type of derivative
		Delliype	1	14	11	(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: Un- known, Length, Velocity
		PointGroup	S	N	N	, 3. ,
		DoHigherMoments	В	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD		N	
		States	AI		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	Y	Method	I	N	N	
[Absorption_Spectrum]		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

Table 9.1 - continued from previous page

	DensLevel Density_name Representation PointGroup DoHigherMoments NTrans ExcitationEnergies States		N N N N N N	N N N N N N N N N N N N N N N N N 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 // Source of density: relaxed, unrelaxed, 0->Unknown, 1->Linearized, 2->Unrelaxed, 3->Relaxed Possible values: Unknown, Length, Velocity
	Density_name Representation PointGroup DoHigherMoments NTrans ExcitationEnergies	S S B I AD	N N N N N	N N N N N	// Source of density: relaxed, unrelaxed, 0->Unknown, 1->Linearized, 2- >Unrelaxed, 3->Relaxed Possible values: Unknown, Length, Velocity The initial and Final
	Representation PointGroup DoHigherMoments NTrans ExcitationEnergies	S S B I AD	N N N N	N N N N	Possible values: Unknown, Length, Velocity The initial and Final
	Representation PointGroup DoHigherMoments NTrans ExcitationEnergies	S S B I AD	N N N N	N N N	known, Length, Velocity The initial and Final
	DoHigherMoments NTrans ExcitationEnergies	B I AD	N N N	N N N	
	NTrans ExcitationEnergies	I AD	N N	N N	
	ExcitationEnergies	AD	N	N	
	States	AI	N	N	
					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 Y	Method	I		N	
, , , ,	RelCorrection	I		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	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	// Source of density: relaxed, unrelaxed, 0->Unknown, 1->Linearized, 2- >Unrelaxed, 3->Relaxed
	Density_name	S		N	Describle andreas II
	Representation	S		N	Possible values: Un- known, Length, Velocity
	PointGroup DoHigherMoments			N N	
	DoHigherMoments	B I		N N	
	NTrans	AD		N N	
	ExcitationEnergies States			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	
CASSCF_DCD_Absorption_Spectrum Y [Absorption_Spectrum]	Method	I	N	N	

Table 9.1 - continued from previous page

Table 9	ı – continued from previous ــــــــــــــــــــــــــــــــــــ	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: Un- known, Length, Velocity
	PointGroup	S	N	N	·
	DoHigherMoments	В	N	N	
	NTrans	I	N	N	
	ExcitationEnergies		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_Spec\fmurr		I	N	N	
	RelCorrection	I	N	N	Type of relativistic
[Absorption_Spectrum]	RelCorrection			IN	treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
	DensType	Ι	N	N	Type of density (electron/spin). 0->Unknow, 1- >Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
	DeriType	Ι	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: Un- known, Length, Velocity
	PointGroup	S	N	N	, 3. ,
	DoHigherMoments	В	N	N	
	NTrans	I	N	N	
	NILGIIS	1	14	14	continues on next nage

Table :	9.1 – continued from previous	page			
	ExcitationEnergies States	AD AI	N N	N N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final
	Multiplicities	AD	N	N	Irrep Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
	Temperature	D	N	N	phony of the liner state
CASSCF_Custom_Absorption_Spectrum Y	Method	I	N	N	
[Absorption_Spectrum]	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: Un- known, Length, Velocity
	PointGroup	S	N	N	
	DoHigherMoments	В	N	N	
	NTrans	I AD	N	N N	
	ExcitationEnergies 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 Y	Method	I	N	N	TD
[ECD_Spectrum]	RelCorrection	Ι	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	Ι	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

Table 9.1 - continued from previous page

	able	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 Representation	S S	N N	N N	Possible values: Un-
		DointCrown	S	N	N	known, Length, Velocity
		PointGroup DoHigherMoments	В	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	Coll: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
CASSCF_PT_ECD_Spectrum	Y	Method	I	N	N	
[ECD_Spectrum]		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	D 111
		Representation	S	N	N	Possible values: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD		N	The initial and P' 1
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD		N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
CACCCE ODDT ECD C+	Y	Temperature Method	D	N N	N	
CASSCF_QDPT_ECD_Spectrum [ECD_Spectrum]	I	Method RelCorrection	I I	N	N N	Type of relativistic
[ECD_Spectrum]		Rescorrection	1	IN	IN	treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
						continues on next page

Table 9.1 - continued from previous page

Ta	able 9	0.1 – 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: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD		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	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
CASSCF_DCD_ECD_Spectrum	Y	Method	I	N	N	
[ECD_Spectrum]		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: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	IN	N	

	Table 9	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 RelCorrection	I I	N N	N N	Type of relativistic
[ECD_Spectrum]		Refeditection	1	11	11	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: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD		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	Y	Method	I	N	N	Trunca of malecies
[ECD_Spectrum]		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

Table 9.1 – continued from previous page

	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	> ometaxed, 5 > relaxed	
		Representation	S	N	N	Possible values: Un- known, Length, Velocity	
		PointGroup	S	N	N	, , ,	
		DoHigherMoments	В	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	r	
CIPSI_Energies	N	finalEnergy	D	N	N		
	- 1	numOfRoots	I	N	N		
		multiplicity	I	N	N		
		energies	AD		N		
CIS_Energies [Energy]	Y	e0	D	N	N	Ground state energy	
220_21019100 [2110191]	-	multP1	В	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	(B) correction augoritanin	
		totalEnergy	AD		N	Total energy of each state	
		Mult	AI	Y	N	Multiplicity of each state	
		Irrep	AI	Y	N	Irreducible representa-	
		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	ΑI	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	Y	NAtoms	I	N	N		
Nuclear_Gradient]		gradNorm	D	N	N		
		grad	AD		N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
TC Dipolo Moment [Di1- M	1 Y	Irrep dipoleMagnitude	I D	N N	N N		
CIS_Dipole_Moment[Dipole_Moment	j I	dipoleMagnitude dipoleElecContrib dipoleNucContrib	AD AD	N	N N N	Electronic contribution Nuclear contribution	a.ı
		dipoleNucContrib			N	Total	
			AD	N	N	Total	
			R				
		doAtomicDipole atomicDipole	B AD		N	Atomic dipoles (NAtoms * X V 7)	
		doAtomicDipole atomicDipole	AD	Y	N	Atomic dipoles (NAtoms * X,Y,Z)	
		doAtomicDipole atomicDipole Method	AD S	Y N	N N		
		doAtomicDipole atomicDipole	AD	Y	N		

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i abie	9. I	- continueu	110111	previous	paye

	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
		Elems	1	11	1	
			ъ	N.T	3.7	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	Y	isotropicPolar	D	N	N	
[Polarizability]	1	rawCartesian	AD		N	a.
[FOIAIIZADIIICY]		diagonalizedTensor				a.
			AD		N	
		orientation	AD		N	
		doAtomicPolar	В	N	N	
		atomicPolarIso	AD	Y	N	Atomic istotropic polar-
						izabilities
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
			I			
a.a. a. 1. 1. 1.	37	Irrep		N	N	
CIS_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N	a.
[Quadrupole_Moment]		quadElecContrib	AD	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ,
		quadTotal	AD	N	N	XY, XZ, YZ Total. Order: XX, YY,
						ZZ, XY, XZ, YZ
		quadDiagonalized	AD		N	The diagonalized tensor a.
		doAtomicQuad	В	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
				N	Y	Atomic mass
		Isotone	D			
		Isotope	D			
		I	D	N	Y	Spin of the nuclei
		I	D	N N	Y	Spin of the nuclei Prefactor PFAC=gegNbe*bN
		I PFAC ARaw	D D AD	N N	Y Y Y	Spin of the nuclei Prefactor PFAC=gegNbe*bN (in MHz) Raw tensor
		I PFAC ARaw AEigenvalues	D D AD AD	N N N	Y Y Y	Spin of the nuclei Prefactor PFAC=gegNbe*bN (in MHz) Raw tensor Eigenvalues
		I PFAC ARaw AEigenvalues orientation	D D AD AD AD	N N N N N	Y Y Y Y Y	Spin of the nuclei Prefactor PFAC=gegNbe*bN (in MHz) Raw tensor
		I PFAC ARaw AEigenvalues orientation AIso	D D AD AD AD D	N N N N N	Y Y Y Y Y	Spin of the nuclei Prefactor PFAC=gegNbe*bN (in MHz) Raw tensor Eigenvalues
	Y	I PFAC ARaw AEigenvalues orientation AIso numOfNucs	D D AD AD AD I	N N N N N N	Y Y Y Y Y Y	Spin of the nuclei Prefactor PFAC=gegNbe*bN (in MHz) Raw tensor Eigenvalues
	Y	I PFAC ARaw AEigenvalues orientation AIso numOfNucs Method	D D D AD AD D I S	N N N N N N	Y Y Y Y Y Y N N	Spin of the nuclei Prefactor PFAC=gegNbe*bN (in MHz) Raw tensor Eigenvalues
CIS_Chemical_Shift [Chemical_Shift]	Y	I PFAC ARaw AEigenvalues orientation AIso numOfNucs	D D AD AD AD I S S	N N N N N N N	Y Y Y Y Y Y N N	Spin of the nuclei Prefactor PFAC=gegNbe*bN (in MHz) Raw tensor Eigenvalues
	Y	I PFAC ARaw AEigenvalues orientation AIso numOfNucs Method	D D D AD AD D I S	N N N N N N	Y Y Y Y Y Y N N	Spin of the nuclei Prefactor PFAC=gegNbe*bN (in MHz) Raw tensor Eigenvalues

	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 contribu- tion
		SPSO	AD	N	Y	Paramagnetic contribu- tion
		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	
,		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass cor- rection
		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.
		pairsDistances	AD	N	N	Num. of B. The distances of each
		pairsTotalSSCIso	AD	N	N	pair 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	Y	Method	I	N	N	
[Absorption_Spectrum]						continues on next page

Table 9.1 - continued from previous page

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: Un- known, Length, Velocity
	PointGroup	S	N	N	, , ,
	DoHigherMoments	В	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	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 Representation	S S	N N	N N	Possible values: Un- known, Length, Velocity
	PointGroup	S	N	N	
	DoHigherMoments	В	N	N	
	NTrans	I	N	N	
					continues on next page