Table 9.1 - continued from previous page

	Table 9	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	1 7	
DBOC_Energy	N	DBOC_Energy	D	N	N		
DFT_Energy	N	nAlphaEl	I	N	N		
_ 31		nBetaEl	I	N	N		
		nTotalEl	I	N	N		
		finalEn	D	N	N	No Van der Waals cor- rection	
		eExchange	D	N	N	rection	
		eCorr	D	N	N		
		eXC	D	N	N		
		eCNL	D	N	N		
		eEmbed	D	Y	N		
ROKEN_SYMMETRY	N	enHighSpin	D	N	N	The High Spin Energy	
.com_ornabilit	11	enBrokenSym	D	N	N	The Broken Symmetry	
						Energy	
		SHighSpin	D	N	N	The High Spin Spin	
		S2HighSpin	D	N	N	The Expectation value of S**2 for the High Spin case	
		S2BrokenSym	D	N	N	The Expectation value of S**2 for the Broken symmetry case	
ipole_Moment	Y	dipoleMagnitude	D	N	N		a.ı
		dipoleElecContrib	AD	N	N	Electronic contribution	
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole	В	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		
G_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 Elems	I I	N N	Y Y	Index of the nuclei Atomic number of the	
		Isotope	D	N	Y	nuclei 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		
adrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.
		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	
		quadTotal quadDiagonalized	AD AD		N N	Total. Order: XX, YY,	a.ı

Table 9.1 - continued from previous page

		.1 – continued from previous	page				
		atomicQuad	AD	Y	N	Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	Ī	N	N		
		State	I	N	N		
		Irrep	I	N	N		
D-1	Y		D	N	N		
Polarizability	1	isotropicPolar					
		rawCartesian	AD		N		a.u
		diagonalizedTensor	AD		N		
		orientation	AD	N	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		N		
TT	3.7	Irrep		N			
Hyperpolarizability	Y	rawCartesian	AD		N		a.u
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
Excited_States_Dynamics	N	fluorRateConstant	D	N	N		
Energy_Extrapolation	N	doEp1	В	N	N	Extrapolation using only one method	
		doEp2	В	N	N	Extrapolation using two different methods (same small basis Set)	
		doEp3	В	N	N	Extrapolation using two different methods (use three basis Sets for the	
		doGradients	В	N	N	cheap method) Extrapolate energy gradients	
		scfEnergies	AD	N	N		
		scfCBS	D	N	N		
		scfGradients	AD		N	The SCF Gradients	
			AD		N	The SCI Gradients	
		corrEnergies					
			D	N	N		
		corrCBS					
		corrCBS ccsdtEnergyX	D	Y	N		
				Y N	N N		
		ccsdtEnergyX	D				
		ccsdtEnergyX totalCBS cardinalNumbers	D D	N N	N		
		ccsdtEnergyX totalCBS cardinalNumbers alphas	D D AI AD	N N N	N N N		
		ccsdtEnergyX totalCBS cardinalNumbers	D D AI	N N N	N N	How many energies we are going to use (e.g.	
		ccsdtEnergyX totalCBS cardinalNumbers alphas betas	D D AI AD AD	N N N	N N N		
gCP Energy	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies basisName	D D AI AD AD I	N N N N	N N N N	are going to use (e.g.	
		ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy	D D AI AD AD I S D	N N N N N	N N N N Y	are going to use (e.g. two-point scheme).	
	N N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN	D D AI AD AD I S D AD	N N N N N	N N N N Y	are going to use (e.g. two-point scheme).	
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES	D D AI AD AD I S D AD AD AD AD	N N N N N N	N N N N Y N N	are going to use (e.g. two-point scheme).	
Hessian		ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude	D D AI AD AD I S D AD AD AD D	N N N N N N N	N N N N Y N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib	D D AI AD AD I S D AD AD D AD	N N N N N N N N	N N N N Y N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations Electronic contribution	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib	D D AI AD AD I S D AD AD AD AD AD AD AD	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 N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib dipoleTotal	D D AI AD AD I S D AD AD D AD	N N N N N N N N N N N N N N N N N N N	N N N N Y N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations Electronic contribution	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib	D D AI AD AD I S D AD AD AD AD AD AD AD	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 N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib dipoleTotal	D D AI AD AD I S D AD AD AD AD AD AD AD AD AD	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 N N N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib dipoleTotal doAtomicDipole	D D AI AD AD I S D AD AD AD AD AD AD AD AD AD B	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 N N N N N N N N N N N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib dipoleTotal doAtomicDipole atomicDipole Method	D D AI AD AD I S D AD AD D AD AD AD B AD S	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 N N N N N N N N N N N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleTotal doAtomicDipole atomicDipole Method Level	D D AI AD AD D AD AD AD AD B AD S S	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 N N N N N N N N N N N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib dipoleTotal doAtomicDipole atomicDipole Method Level Mult	D D AI AD AD I S D AD AD AD AD AD AD AD AD AD S S I	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 N N N N N N N N N N N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms	a.u.
Hessian	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib dipoleTotal doAtomicDipole atomicDipole Method Level Mult State	D D AI AD AD I S D AD AD AD AD B AD S S I I	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 N N N N N N N N N N N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms	a.u.
Hessian  ICE_Dipole_Moment[Dipole_Moment]	N Y	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleTotal doAtomicDipole atomicDipole Method Level Mult State Irrep	D D AI AD AD I S D AD AD AD AD AD AD S S I I I		N N N N N N N N N N N N N N N N N N N	are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms * X,Y,Z)	a.u.
Hessian  ICE_Dipole_Moment[Dipole_Moment]	N	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleNucContrib dipoleTotal doAtomicDipole atomicDipole Method Level Mult State	D D AI AD AD D AD AD B AD S S I I I I I I			are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms	a.u.
gCP_Energy Hessian ICE_Dipole_Moment[Dipole_Moment] ICE_EFG_Tensor[EFG_Tensor]	N Y	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleTotal doAtomicDipole atomicDipole Method Level Mult State Irrep	D D AI AD AD D AD AD B AD I I I I I S			are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms * X,Y,Z)	a.u.
Hessian  ICE_Dipole_Moment[Dipole_Moment]	N Y	ccsdtEnergyX totalCBS cardinalNumbers alphas betas numOfEnergies  basisName gCP_Energy HESSIAN MODES dipoleMagnitude dipoleElecContrib dipoleTotal doAtomicDipole atomicDipole Method Level Mult State Irrep numOfNucs	D D AI AD AD D AD AD B AD S S I I I I I I			are going to use (e.g. two-point scheme).  The Hessian The modes of vibrations  Electronic contribution Nuclear contribution Total  Atomic dipoles (NAtoms * X,Y,Z)	a.u.

Table 9.1 - continued from previous page

	Table	9.1 – continued from previous	page				
		State	I	N	N		
		Irrep	I	N	N	I. d	
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N		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		Y	Eigenvalues	
		orientation	AD		Y	Eigenvectors	
	37	VIso	D	N	Y		
ICE_Polarizability	Y	isotropicPolar	D	N	N		
[Polarizability]		rawCartesian	AD		N		a.u
		diagonalizedTensor	AD		N		
		orientation	AD		N		
		doAtomicPolar	В	N	N	A	
		atomicPolarIso	AD		N	Atomic istotropic polar- izabilities	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
ICE_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.u.
[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, 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	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		
ICE_A_Tensor[A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elem	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		PFAC	D	N	Y	Prefactor PFAC=gegNbe*bN (in MHz)	
		ARaw	AD	N	Y	Raw tensor	
		AEigenvalues	AD		Y	Eigenvalues	
		orientation	AD		Y	Eigenvectors	
		AIso	D	N	Y	<i>3</i>	
ICE_Chemical_Shift	Y	numOfNucs	I	N	N		
[Chemical_Shift]	-	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	
			I	N	Y	Atomic number of the	

continues on next page

Table	9.1 -	<ul> <li>continued</li> </ul>	from	previous page
-------	-------	-------------------------------	------	---------------

	Table 9	9.1 – continued from previous	page			
		SDSO	AD	N	Y	Diamagnetic contribu-
		SPSO	AD	N	Y	Paramagnetic contribu-
		STot	AD	N	Y	Total tensor
		orientation	AD		Y	Eigenvectors
		sTotEigen	AD	N	Y	Eigenvalues
		siso	D	N	Y	
		saniso	D	N	Y	
<pre>ICE_D_Tensor[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	
<pre>ICE_G_Tensor[G_Tensor]</pre>	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	
		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	
<pre>ICE_Spin_Spin_Coupling [Spin_Spin_Coupling]</pre>	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	, pui
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
ICE_Absorption_Spectrum	Y	Method	I	N	N	
[Absorption_Spectrum]		RelCorrection	Ī	N	N	Type of relativistic 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	.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	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	
		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	
ICE_ECD_Spectrum[ECD_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	I	N	N	Type of density (electron/spin). 0->Unknow, 1- >Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, 0->Unknown, 1->Linearized, 2- >Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	N	N	
		NTrans	I	N	N	
		ExcitationEnergies	AD	IN	N	

T:	able 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	1 7
Calculation_Info	N	Mult	I	N	N	
_		Charge	I	N	N	
		NumOfAtoms	I	N	N	
		NumOfElectrons	I	N	N	
		NumOfBasisFuncts	I	N	N	
		NumOfAuxCBasisFuncts	I	N	N	
		NumOfAuxJBasisFuncts	I	N	N	
		NumOfAuxJKBasisFunct		N	N	
		NumOfCABSBasisFuncts		N	N	
Single_Point_Data	N	FinalEnergy	D	N	N	Final single point energy
3 · · · - · · · · ·		Converged	В	N	N	0 1
LFT_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 Representation	S S	N N	N N	Possible values: Un- known, Length, Velocity
		PointGroup	S	N	N	<u> </u>
		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	
LFT_ECD_Spectrum[ECD_Spectrum]	Y	Method RelCorrection	I	N N	N N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC

Table 9.1 - continued from previous page

	able 9	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 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		N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	
A_Tensor	Y	numOfNucs	I	N	N	Number of active nuclei
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
		NUC	I	N	Y	Index of the nuclei
		Elem	I	N	Y	Atomic number of the nuclei
		Isotope	D	N	Y	Atomic mass
		I PFAC	D D	N N	Y	Spin of the nuclei Prefactor
		ARaw	AD	N	Y	PFAC=gegNbe*bN (in MHz) Raw tensor
		AEigenvalues	AD		Y	Eigenvalues
		orientation	AD		Y	Eigenvectors
		AIso	D	N	Y	2.5011100015
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		Y	Diamagnetic contribu- tion
			AD	N	Y	Paramagnetic contribu-
		SPSO			3.7	tion
		STot	AD		Y	Total tensor
		STot orientation	AD AD	N	Y	Total tensor Eigenvectors
		STot orientation sTotEigen	AD AD AD	N N	Y Y	Total tensor
		STot orientation	AD AD	N	Y	Total tensor Eigenvectors

Table 9.1 - 0	continued from	previous page
---------------	----------------	---------------

	Table 9	0.1 – continued from previous	page				
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		
		Irrep	I	N	N		
G_Tensor	Y	g_matrix	AD		N		
		g_elec	D	N	N	The free electron g-value	
		g_RMC	D	N	N	contribution 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		
		Irrep	I	N	N		
Spin_Spin_Coupling	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to calculate	
		numOfNucPairsDSO	I	N	N	number of nuclear pairs to calculate DSO	
		numOfNucPairsPSO	I	N	N	number of nuclear pairs to calculate PSO	
		numOfNucPairsFC	I	N	N	number of nuclear pairs to calculate FC	
		numOfNucPairsSD	I	N	N	number of nuclear pairs to calculate SD	
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs to calculate SD/FC	
		pairsInfo	AI	N	N	Pairs Info: Col1->Index of A. Col2->Atom.	
						Num. of A. Col3->Index of B. Col4->Atom. Num. of B.	
		pairsDistances	AD	N	N	The distances of each pair	
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling constant for each pair	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MCRPA_Dipole_Moment	Y	dipoleMagnitude	D	N	N		a.u.
[Dipole_Moment]		dipoleElecContrib	AD	N	N	Electronic contribution	
-		dipoleNucContrib	AD		N	Nuclear contribution	
		dipoleTotal	AD		N	Total	
		doAtomicDipole	В	N	N		
		atomicDipole	AD	Y	N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MCRPA_EFG_Tensor[EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
						continues on next	page

Table 9.1 - continued from previous page

	Table 9	0.1 – continued from previous	page				
		NUC	I	N	Y	Index of the nuclei	
		Elems	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		QFAC	D	N	Y	Prefactor	
		V	AD	N	Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y	_	
MCRPA_Polarizability	Y	isotropicPolar	D	N	N		
[Polarizability]		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	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		
		Irrep	I	N	N		
MCRPA_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.u.
[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	N	The diagonalized tensor	a.u.
		doAtomicQuad	В	N	N	The diagonalized tensor	u.u.
		atomicQuad	AD		N	Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MCRPA_A_Tensor[A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC Elem	I	N N	Y Y	Index of the nuclei Atomic number of the	
		Tastons	D	NI	Y	nuclei	
		Isotope	D D	N N	Y	Atomic mass	
		I PFAC	D	N	Y	Spin of the nuclei Prefactor PFAC=gegNbe*bN	
		10.	4 F	N.T	37	(in MHz)	
		ARaw	AD		Y	Raw tensor	
		AEigenvalues	AD		Y	Eigenvalues	
		orientation	AD		Y	Eigenvectors	
MCDDA Chomical Chift	Y	AIso	D	N N			
MCRPA_Chemical_Shift [Chemical_Shift]	ĭ	numOfNucs Method	I S	N N	N N		
[CHEMICAI_DHILLE]		Level	S	N	N		
		Mult	I	N	N		
			I	N	N		
		State		4.4	T 4		
		State Trrep		N	N		
		Irrep	I	N N	N Y	Index of the nuclei	
				N N N	N Y Y	Index of the nuclei Atomic number of the nuclei	

	Table 9	0.1 – continued from previous	page			
		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	8
		saniso	D	N	Y	
MCRPA_D_Tensor[D_Tensor]	Y	d_raw	AD		N	
MCNTA_D_Tell301 [D_Tell301]	1	d_eigenvalues	AD		N	
		_	AD		N	
		d_eigenvectors				
		D	D	N	N	
		E	D	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MCRPA_G_Tensor[G_Tensor]	Y	g_matrix	AD	N	N	
		g_elec	D	N	N	The free electron g-value
		g_RMC	D	N	N	contribution The reduced mass cor-
				, ,		rection
		g_DSO	AD		N	
		g_PSO	AD		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	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MCRPA_Spin_Spin_Coupling [Spin_Spin_Coupling]	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to calculate
		numOfNucPairsDSO	I	N	N	number of nuclear pairs to calculate DSO
		numOfNucPairsPSO	I	N	N	number of nuclear pairs to calculate PSO
		numOfNucPairsFC	I	N	N	number of nuclear pairs to calculate FC
		numOfNucPairsSD	I	N	N	number of nuclear pairs to calculate SD
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs to calculate SD/FC
		pairsInfo	ΑI	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	
MCDDA Absorption Coastwor	Y	_	I	N		
MCRPA_Absorption_Spectrum	I	Method			N	Type of relativistic
[Absorption_Spectrum]		RelCorrection	Ι	N	N	Type of relativistic 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

Tab	ble 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: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	N	N	
		NTrans	I AD	N N	N N	
		ExcitationEnergies States		N	N	The initial and Final
		States	Ai	IN	11	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	
MCRPA_ECD_Spectrum[ECD_Spectrum]	Y	Method	I	N	N	TD 0 1 1 1 1 1
		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 9.1 - continued from previous page

	Table 9	.1 – continued from previou	s page				
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep	
		Multiplicities	AD	N	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state	
		Temperature	D	N	N		
MDCI_Energies [Energy]	Y	numOfEl	I	N	N		
		numOfCorrEl	I	N	N		
		numOfAlphaCorrEl	I	N	N		
		numOfBetaCorrEl refEnergy	I AD	N N	N N	Reference Energy	
		corrEnergy	AD		N	Total Correlation Energy	
		aaCorrEn	AD		N	Alpha-Alpha Pairs Cor- relation Energy (No (T))	
		bbCorrEn	AD	N	N	Beta-Beta Pairs Correlation Energy (No (T))	
		abCorrEn	AD	N	N	Alpha-Beta Pairs Correlation Energy (No (T))	
		CorrDS	AD	Y	N	Singlet pairs energy of double amplitudes (No (T))	
		CorrDT	AD	Y	N	Triplet pairs energy of double amplitudes (No (T))	
		CorrSS	AD	Y	N	Singlet pairs energy of quadratic single amplitudes (No (T))	
		CorrST	AD	Y	N	Triplet pairs energy of quadratic single amplitudes (No (T))	
		triplesEnergy	AD	N	N	Triples Correction Energy	
		Method	S	N	N		
		totalEnergy	AD		N	Total energy of each state	
		Mult Irrep	AI AI	Y	N N	Multiplicity of each state 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	AI	Y	N	Block index of each state	
		Root	AI	Y	N	Root index within the block Index of the followed	
		FollowTDoot	т	v	NT		
		FollowIRoot	I	Y	N	root	
		FollowIRoot AvgMult	AD	Y	N		
	Y	AvgMult NAtoms	AD I	Y N	N N	root Average multiplicity of each SO-/SS-coupled	
	Y	AvgMult  NAtoms gradNorm	AD I D	Y N N	N N N	root Average multiplicity of each SO-/SS-coupled	
	Y	AvgMult  NAtoms gradNorm grad	AD  I D AD	Y N N N	N N N N	root Average multiplicity of each SO-/SS-coupled	
	Y	AvgMult  NAtoms gradNorm grad Method	AD I D AD S	Y N N N N	N N N N	root Average multiplicity of each SO-/SS-coupled	
	Y	AvgMult  NAtoms gradNorm grad Method Level	AD  I D AD S S	Y N N N N N	N N N N N	root Average multiplicity of each SO-/SS-coupled	
MDCI_Nuc_Gradient [Nuclear_Gradient]	Y	AvgMult  NAtoms gradNorm grad Method	AD I D AD S	Y N N N N	N N N N	root Average multiplicity of each SO-/SS-coupled	
MDCI_Nuc_Gradient [Nuclear_Gradient]	Y	AvgMult  NAtoms gradNorm grad Method Level Mult State	I D AD S S I	Y N N N N N N	N N N N N	root Average multiplicity of each SO-/SS-coupled	
[Nuclear_Gradient]	Y Y	AvgMult  NAtoms gradNorm grad Method Level Mult	I D AD S S I I I	Y N N N N N N N N	N N N N N N	root Average multiplicity of each SO-/SS-coupled	a.u.
[Nuclear_Gradient]		AvgMult  NAtoms gradNorm grad Method Level Mult State Irrep	I D AD S S I I I I	Y  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	root Average multiplicity of each SO-/SS-coupled	a.u.
[Nuclear_Gradient]  MDCI_Dipole_Moment		AvgMult  NAtoms gradNorm grad Method Level Mult State Irrep dipoleMagnitude dipoleElecContrib dipoleNucContrib	AD  I D AD S S I I I D	Y  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 N N N N N N N	root Average multiplicity of each SO-/SS-coupled state	a.u.
[Nuclear_Gradient]  MDCI_Dipole_Moment		AvgMult  NAtoms gradNorm grad Method Level Mult State Irrep dipoleMagnitude dipoleElecContrib dipoleNucContrib dipoleTotal	I D AD S S I I I D AD AD AD AD AD	Y  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 N N N N N N N N N N N N	root Average multiplicity of each SO-/SS-coupled state  Electronic contribution	a.u.
<pre>[Nuclear_Gradient]  MDCI_Dipole_Moment</pre>		AvgMult  NAtoms gradNorm grad Method Level Mult State Irrep dipoleMagnitude dipoleElecContrib dipoleNucContrib	I D AD S S I I I D AD AD AD	Y  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 N N N N N N N N N N N N	root Average multiplicity of each SO-/SS-coupled state  Electronic contribution Nuclear contribution	a.u.

	Table 9	.1 – continued from previous	page				
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MDCI_EFG_Tensor[EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elems	Ι	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		QFAC	D	N	Y	Prefactor	
		V	AD	N	Y	Raw tensor	
		VEigenvalues	AD	N	Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		VIso	D	N	Y		
MDCI_Polarizability	Y	isotropicPolar	D	N	N		
[Polarizability]		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD		N		
		orientation	AD		N		
		doAtomicPolar	В	N	N		
		atomicPolarIso	AD		N	Atomic istotropic polar- izabilities	
		Mot bod	C	NT	N	izaomues	
		Method	S	N			
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MDCI_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.u.
[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, 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	В	N	N	The diagonalized tensor	a.u.
		atomicQuad	AD		N	Atomic quadrupoles (NAtoms * XX, YY, ZZ,	
		Mot hod	C	N	NI	XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N	N. 1 C	
MDCI_A_Tensor[A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
		NUC	I	N	Y	Index of the nuclei	
		Elem	I	N	Y	Atomic number of the nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		PFAC	D	N	Y	Prefactor PFAC=gegNbe*bN (in MHz)	
		ARaw	AD	N	Y	Raw tensor	
		AEigenvalues	AD		Y	Eigenvalues	
		J			Y	Eigenvectors	
		orientation	AD				
		orientation Also	AD D			Eigenvectors	
MDCI Chemical Shift	Y	AIso	D	N	Y	Ligenvectors	
MDCI_Chemical_Shift [Chemical_Shift]	Y					Eigenvectors	

continues on next page

l able	9.1	<ul> <li>continued</li> </ul>	trom	previous page

1	able 9	9.1 – continued from previous	page			
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
		NUC	I	N	Y	Index of the nuclei
		Elems	I	N	Y	Atomic number of the nuclei
		SDSO	AD	N	Y	Diamagnetic contribu-
		SPSO	AD	N	Y	Paramagnetic contribu-
		STot	AD	N	Y	Total tensor
		orientation	AD		Y	Eigenvectors
		sTotEigen	AD	N	Y	Eigenvalues
		siso	D	N	Y	2
		saniso	D	N	Y	
MDCI_D_Tensor[D_Tensor]	Y	d_raw	AD	N	N	
,		d_eigenvalues	AD	N	N	
		d_eigenvectors	AD	N	N	
		D	D	N	N	
		E	D	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MDCI_G_Tensor[G_Tensor]	Y	g_matrix	AD	N	N	
		g_elec	D	N	N	The free electron g-value contribution
		g_RMC	D	N	N	The reduced mass 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	
MDCI_Spin_Spin_Coupling [Spin_Spin_Coupling]	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to calculate
		numOfNucPairsDSO	I	N	N	number of nuclear pairs to calculate DSO
		numOfNucPairsPSO	I	N	N	number of nuclear pairs to calculate PSO
		numOfNucPairsFC	I	N	N	number of nuclear pairs to calculate FC
		numOfNucPairsSD	I	N	N	number of nuclear pairs to calculate SD
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs to calculate SD/FC
		pairsInfo	AI	N	N	Pairs Info: Col1->Index of A. Col2->Atom. Num. of A. Col3->Index of B. Col4->Atom. Num. of B.
		pairsDistances	AD	N	N	The distances of each pair
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling constant for each pair
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MDCI_Absorption_Spectrum	Y	Method	I	N	N	
[Absorption_Spectrum]		<u> </u>				continues on next page

Table 9.1 - continued from previous page

Tab	ole 9	0.1 – 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	
		States		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
		Temperature	D	N	N	
MDCI_ECD_Spectrum[ECD_Spectrum]	Y	Method	I	N	N	
		RelCorrection	I	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
		DensType	I	N	N	Type of density (electron/spin). 0->Unknow, 1- >Electronic, 2->Spin, 3->Trans/Electronic, 4->Tran/Spin
		DeriType	I	N	N	Type of derivative (w.r.t. to what perturbation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4->Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	// Source of density: relaxed, unrelaxed, 0->Unknown, 1->Linearized, 2- >Unrelaxed, 3->Relaxed
		Density_name	S	N	N	
		Representation	S	N	N	Possible values: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	N	N	
		NTrans	I	N	N	
						continues on next page

Table 9.1 - continued from previous page

Та	able 9	.1 – continued from previous	page			
		ExcitationEnergies States	AD 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	F,
MP2_Energies[Energy]	Y	refEnergy	AD		N	Reference energy for
_ 3 , 31,		corrEnergy	AD	N	N	each state MP2 correlation energy
						for each state
		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
MP2_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	
		Irrep	I	N	N	
MP2_Dipole_Moment[Dipole_Moment]	Y	dipoleMagnitude	D	N	N	a.u.
		dipoleElecContrib	AD	N	N	Electronic contribution
		dipoleNucContrib	AD		N	Nuclear contribution
		dipoleTotal	AD		N	Total
			В	N	N	
		doAtomicDipole			TAT .	Atomia dinolog (NIAtomo
		atomicDipole	AD		N	Atomic dipoles (NAtoms * X,Y,Z)
		atomicDipole Method	AD S	N	N	
		atomicDipole  Method Level	AD S S	N N	N N	
		atomicDipole  Method Level Mult	AD S S I	N N N	N N N	
		atomicDipole  Method Level Mult State	AD S S I	N N N	N N N	
/D2 FEG Tonsor [FEG Tonsor]	v	Method Level Mult State Irrep	AD S S I I	N N N N	N N N N	* X,Y,Z)
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs	S S I I I	N N N N N	N N N N N	
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method	S S I I I I S	N N N N N N	N N N N N N	* X,Y,Z)
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level	S S I I I I S S S	N N N N N N	N N N N N N	* X,Y,Z)
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult	S S I I I I S	N N N N N N N	N N N N N N N	* X,Y,Z)
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult State	S S I I I S S I I I I	N N N N N N N N	N N N N N N N N	* X,Y,Z)
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult	S S I I I S S I I	N N N N N N N	N N N N N N N	* X,Y,Z)  Number of active nuclei
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult State Irrep	S S I I I S S I I I I I I I I I I I I I	N N N N N N N N N	N N N N N N N N N	* X,Y,Z)
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult State Irrep NUC	S S I I I S S I I I I I I I I I I I I I	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 N N N Y Y	Number of active nuclei  Index of the nuclei Atomic number of the nuclei Atomic mass
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult State Irrep Nuc Elems Isotope I	S S I I I S S I I I I I I D	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 N N N Y	* X,Y,Z)  Number of active nuclei  Index of the nuclei Atomic number of the nuclei Atomic mass Spin of the nuclei
MP2_EFG_Tensor [EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult State Level Mult State Irrep NUC Elems	S S I I I I S S I I I I I I I D D D	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 N N N Y Y	Number of active nuclei  Index of the nuclei Atomic number of the nuclei Atomic mass
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult State Irrep NuC Elems  Isotope I QFAC	S S I I I I S S I I I I I I D D D D D	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 N N N N Y Y Y Y Y Y Y	* X,Y,Z)  Number of active nuclei  Index of the nuclei Atomic number of the nuclei Atomic mass Spin of the nuclei Prefactor Raw tensor
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult State Irrep NUC Elems  Isotope I QFAC V	S S I I I S S I I I I I I D D D AD	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 N N N N Y Y Y Y Y Y Y Y Y Y	* X,Y,Z)  Number of active nuclei  Index of the nuclei Atomic number of the nuclei Atomic mass Spin of the nuclei Prefactor
MP2_EFG_Tensor[EFG_Tensor]	Y	Method Level Mult State Irrep numOfNucs Method Level Mult State Irrep NUC Elems Isotope I QFAC V VEigenvalues	S S I I I S S I I I I I I D D D AD AD AD	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 N N N Y Y Y Y Y Y Y Y Y Y Y	* X,Y,Z)  Number of active nuclei  Index of the nuclei Atomic number of the nuclei Atomic mass Spin of the nuclei Prefactor Raw tensor Eigenvalues

Table 9.1 - continued from previous page

	Table 9	9.1 – continued from previous	page				
		rawCartesian	AD	N	N		a.u
		diagonalizedTensor	AD	N	N		
		orientation	AD	N	N		
		doAtomicPolar	В	N	N		
		atomicPolarIso	AD	Y	N	Atomic istotropic polar-	
				_	- '	izabilities	
		Method	S	N	N	<u> </u>	
		Level	S	N	N		
			I				
		Mult		N	N		
		State	I	N	N		
		Irrep	I	N	N		
MP2_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.u.
[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, 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	В	N	N		a.u.
		atomicQuad	AD		N	Atomic quadrupoles	
		atomicyuad	AD	ĭ	IN	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		
			I	N	N		
	37	Irrep				N 1 C .: 1:	
MP2_A_Tensor[A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
			I	N	N		
		Irrep				I., J.,	
		NUC Elem	I I	N N	Y Y	Index of the nuclei 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)	
		ARaw	AD		Y	Raw tensor	
		AEigenvalues	AD		Y	Eigenvalues	
		orientation	AD	N	Y	Eigenvectors	
		AIso	D	N	Y		
MP2_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		Y	Diamagnetic contribu-	
		SPSO STot	AD AD		Y Y	Paramagnetic contribu- tion Total tensor	
		orientation			Y		
			AD			Eigenvectors	
		sTotEigen	AD		Y	Eigenvalues	
		siso		N	Y		
		saniso	D	N	Y		
MP2_D_Tensor[D_Tensor]	Y	d_raw	AD	N	N		
. –		d_eigenvalues	AD		N		
		d_eigenvectors	AD		N		
			, 11				
		_	D	N	N		
		D E	D D	N N	N N		

Table 9.1	<ul> <li>continued</li> </ul>	from	previous page	
-----------	-------------------------------	------	---------------	--

Та	able 9	9.1 – continued from previous	page			
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MP2_G_Tensor[G_Tensor]	Y	g_matrix	AD	N	N	
		g_elec	D	N	N	The free electron g-value
		3=				contribution
		g_RMC	D	N	N	The reduced mass cor-
		3				rection
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		q_Tot	AD		N	
		g_iso	D	N	N	
		Delta_g	AD	N	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	
MP2_Spin_Spin_Coupling	Y	numOfNucPairs	I	N	N	Number of nuclei pairs to
[Spin_Spin_Coupling]	-					calculate
7.7 - 7		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
		namornaor arror o	•	- '	- '	to calculate FC
		numOfNucPairsSD	I	N	N	number of nuclear pairs
		namornaor arroop	-	- '		to calculate SD
		numOfNucPairsSD_FC	I	N	N	number of nuclear pairs
		namornaci arrabb_r c	•	11	11	to calculate SD/FC
		pairsInfo	ΑI	N	N	Pairs Info: Col1->Index
		parisinio		- 1	- 1	of A. Col2->Atom.
						Num. of A. Col3->Index
						of B. Col4->Atom.
						Num. of B.
		pairsDistances	AD	N	N	The distances of each
		parisbiscances	AD	11	14	pair
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling
		pairsiocaissciso	AD	11	11	constant for each pair
		Method	S	N	N	constant for each pan
		Level	S	N	N	
		Mult	I	N	N	
			I	N	N	
		State	I	N	N	
MP2_Absorption_Spectrum	Y	Irrep Method	I	N	N	
[Absorption_Spectrum]	1	RelCorrection	I	N	N	Type of relativistic
[wnanthetou_abecerum]		Mercorrection	1	IA	IN	treatment in QDPT.
						0->Unknow, 1->None,
						· · · · · · · · · · · · · · · · · · ·
						2->SOC, 3->SSC,
		DonaTimo	т	NT	NT	4->SOC/SSC Type of density
		DensType	I	N	N	71
						(electron/spin).
						0->Unknow, 1-
						>Electronic, 2->Spin,
						3->Trans/Electronic,
		D	T	NT	NT.	4->Tran/Spin
		DeriType	I	N	N	Type of derivative
						(w.r.t. to what pertur-
						bation). 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

Т	able 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	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		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	priority of the iniai state	
MP2_ECD_Spectrum[ECD_Spectrum]	Y	Method	I	N	N		
ET 5 DECD OPECCI UM [DCD Specci UM]	1	RelCorrection	I	N	N	Type of relativistic	
		VETCOTTECTION	1	IN	14	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		
		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		
MRCI_Dipole_Moment	Y	dipoleMagnitude	D	N	N		a.u.
[Dipole_Moment]		dipoleElecContrib	AD	N	N	Electronic contribution	
		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD	N	N	Total	
		doAtomicDipole	В	N	N		
		atomicDipole	AD		N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
		Level	S	N	N		
						continues on nex	t nage

Table 9.1 - continued from previous page

	Table 9	9.1 – continued from previous	page				
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MRCI_EFG_Tensor[EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
			I	N	N		
		Irrep				I d£ 411-:	
		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	<i>G</i>	
MRCI_Polarizability	Y	isotropicPolar	D	N	N		
[Polarizability]		rawCartesian	AD		N		a.u
[IOIAIIZADIIICY]			AD		N		a.u
		diagonalizedTensor	AD		N		
		orientation					
		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		
		Irrep	I	N	N		
MRCI Ouadrupole Moment	Y	isotropicQuadMoment	D	N	N		a.u.
MRCI_Quadrupole_Moment [Quadrupole_Moment]	1	quadElecContrib	AD		N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ	a.u.
		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 doAtomicQuad	AD B	N N	N N	The diagonalized tensor	a.u.
		atomicQuad	AD		N	Atomic quadrupoles	
		acomicquad	AD	1	11	(NAtoms * XX, YY, ZZ, XY, XZ, YZ)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
MRCI_A_Tensor[A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
	•	Method	S	N	N	- Emoti of delive fidelet	
		Level	S	N	N		
			I				
		Mult		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)	
		ARaw	AD	N	Y	Raw tensor	
		AEigenvalues	AD		Y	Eigenvalues	
		orientation	AD		Y	Eigenvectors	
			D	N	Y	G	
		ATso					
MRCI Chemical Shift	v	AIso					
MRCI_Chemical_Shift	Y	numOfNucs	I	N	N		
MRCI_Chemical_Shift [Chemical_Shift]	Y						