Table 9.1 - continued from previous page

Ta	ble 9	0.1 – continued from previous	page			
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
			I			Index of the musici
		NUC		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-
		STot	AD		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	
rate1_b_render[b_render]	1	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	
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 cor- rection
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD		N	
		_	D	N	N	
		g_iso				
		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	
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	The Spin-Spin coupling constant for each pair
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
				N	N	
		Trron				
D. Tarrana MDGT 20120 1 FD T	<b>1</b> 7	Irrep	I			
D_Tensor_MRCI_2ndOrder[D_Tensor]	Y	d_raw	AD	N	N	
D_Tensor_MRCI_2ndOrder[D_Tensor]	Y	-		N N		

Table 9.1 - 0	continued from	previous page
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T;	able 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	Ī	N	N	
		Irrep	Ī	N	N	
D_Tensor_MRCI_2ndOrder_ES	Y	d_raw	AD		N	
[D_Tensor]	1	d_eigenvalues	AD		N	
[5_1011301]		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	
	3.7	Irrep	I	N	N	
D_Tensor_MRCI_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	
		Irrep	I	N	N	
D_Tensor_MRCI_Heff_ES[D_Tensor]	Y	d_raw	AD		N	
5_10.001m.01011_20 (5_10.001)	-	d_eigenvalues	AD		N	
		d_eigenvectors	AD		N	
		D D	D	N	N	
		E	D	N	N	
			S			
		Method		N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
MRCI_Absorption_Spectrum	Y	Method	I	N	N	
[Absorption_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	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
		Density name	I	N	N	// Source of density: relaxed, unrelaxed, 0->Unknown, 1->Linearized, 2- >Unrelaxed, 3->Relaxed
		Density_name	S	N	N	Dessible vel II
		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	
						continues on next page

Table 9.1 – continued from previous page

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	• •
MRCI_ECD_Spectrum[ECD_Spectrum]	Y	Method	I	N	N	
		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	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	Coll: 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	
		Method	S	N N	N N	
		Level Mult	S I	N N	N N	
		State	I	N	N N	
		Irrep	I	N	N	
CHELPG_Population_Analysis	Y	NAtoms	I	N	N	
		ATNO	AI	N	N	
		AtomicCharges	AD		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 DENSA	AI D	N N	N N	Total integrated alpha density
						continues on next page

Table 9.1 - continued from previous page

	Table	9.1 – continued from previous	s 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	
			I	N	N	
T	<b>3</b> 7	Irrep				
Loewdin_Population_Analysis	Y	NAtoms	I	N	N	
		ATNO	AI	N	N	
		AtomicCharges	AD		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 or- ders larger than threshold
		bondThresh	D	N	N	The threshold for print-
		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 el- ements
		NA	AD	N	N	Mulliken gross atomic population
		ZA	AD	N	N	Total nuclear charge
		QA	AD		N	Mulliken gross atomic
						charge
		VA	AD		N	Mayer's total valence
		BVA	AD		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	
MDIS_1 OPUIACION_ANALYSIS	1		AI	N	N	
		ATNO				
		Thresh	D	N	N	
		Niter	I	N	N	
		LargePrint	В	N	N	
		DENSA	D	N	N	Total integrated alpha
			Ъ			density
		DENSB	D	N	N	density Total integrated beta density
		DENSB			N N	Total integrated beta
		DENSB AtomicCharges	D AD	N	N	Total integrated beta
		DENSB AtomicCharges Spin	D AD AD	N N	N N	Total integrated beta
		DENSB AtomicCharges Spin NPOPVAL	D AD AD AD	N N N	N N N	Total integrated beta
		DENSB AtomicCharges Spin NPOPVAL SIGMAVAL	D AD AD AD AD AD	N N N	N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole	D AD AD AD AD AD AD AD	N N N N	N N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole	D AD AD AD AD AD AD AD AD	N N N N Y	N N N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole	D AD	N N N N Y Y	N N N N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole	D AD	N N N N Y Y	N N N N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole	D AD	N N N N Y Y	N N N N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment	D AD	N N N Y Y Y	N N N N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method	D AD S	N N N N Y Y Y Y	N N N N N N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult	AD AD AD AD AD AD AD AD S S I	N N N Y Y Y Y N N	N N N N N N N N	Total integrated beta
		DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult State	D AD AD AD AD AD AD AD AD S S I I	N N N Y Y Y Y Y N N N	N N N N N N N N N	Total integrated beta
Mullikan Papulation Apolusis	V	DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult State Irrep	AD AD AD AD AD S S I I I I	N N N Y Y Y Y Y N N N N	N N N N N N N N N N N N N N N N N N N	Total integrated beta
Mulliken_Population_Analysis	Y	DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicQctupole ThirdRadialMoment Method Level Mult State Irrep NAtoms	D AD AD AD AD AD AD AD AD I I I I	N N N Y Y Y Y N N N N N		Total integrated beta
Mulliken_Population_Analysis	Y	DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult State Irrep NAtoms ATNO	AD AD AD AD AD S S I I I I AI	N N N N Y Y Y Y N N N N N N N N N N N N		Total integrated beta
Mulliken_Population_Analysis	Y	DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult State Irrep NAtoms ATNO AtomicCharges	D AD AD AD AD AD AD AD I I I I AI AD	N N N N Y Y Y 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	Total integrated beta
Mulliken_Population_Analysis	Y	DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult State Irrep NAtoms ATNO	D AD AD AD AD AD AD AD I I I I AI AD S	N N N N Y Y Y 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	Total integrated beta
Mulliken_Population_Analysis	Y	DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult State Irrep NAtoms ATNO AtomicCharges	D AD AD AD AD AD AD AD I I I I AI AD	N N N N Y Y Y 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	Total integrated beta
Mulliken_Population_Analysis	Y	DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult State Irrep NAtoms ATNO AtomicCharges Method	D AD AD AD AD AD AD AD I I I I AI AD S	N N N N Y Y Y 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	Total integrated beta
Mulliken_Population_Analysis	Y	DENSB  AtomicCharges Spin NPOPVAL SIGMAVAL AtomicDipole AtomicQuadrupole AtomicOctupole ThirdRadialMoment Method Level Mult State Irrep NAtoms ATNO AtomicCharges Method Level	D AD AD AD AD AD AD AD I I I I AI AD S S S	N N N N Y Y Y 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	Total integrated beta

	Table 9	.1 – continued from previous	page				
RASCI_Nuc_Gradient	Y	NAtoms	I	N	N		
[Nuclear_Gradient]		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	Y	dipoleMagnitude	D	N	N		a.u.
[Dipole_Moment]		dipoleElecContrib	AD	N	N	Electronic contribution	
,		dipoleNucContrib	AD	N	N	Nuclear contribution	
		dipoleTotal	AD		N	Total	
		doAtomicDipole	В	N	N	2.4.000	
		atomicDipole	AD		N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N	,-,-,	
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
DACCI BEC To the IRRO TO 1	37	Irrep	I	N	N	Number of	
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 V	AD		Y	Raw tensor	
		V VEigenvalues	AD		Y	Eigenvalues	
		orientation	AD		Y		
						Eigenvectors	
	3.7	VIso	D	N	Y		
RASCI_Polarizability	Y	isotropicPolar	D	N	N		
[Polarizability]		rawCartesian	AD		N		a.u
		diagonalizedTensor	AD		N		
		orientation	AD	N	N		
		doAtomicPolar	В	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	Y	isotropicQuadMoment	D	N	N		a.u.
[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	AD		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		
			I	N	N		
			1	1.4			
DAGGI A T-11 - 12 T-1 - 1	37	Irrep	T	NT	TA.T	Manahan -ft'- 1 '	
RASCI_A_Tensor[A_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei	
RASCI_A_Tensor[A_Tensor]	Y	numOfNucs Method	S	N	N	Number of active nuclei	
RASCI_A_Tensor[A_Tensor]	Y	numOfNucs				Number of active nuclei	

continues on next page

Table 9.1 - continued from previous page

	Table 9	0.1 – 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=gegNbe*bN (in MHz)
		ARaw	AD		Y	Raw tensor
		AEigenvalues	AD		Y	Eigenvalues
		orientation	AD		Y	Eigenvectors
D3.007.01. 1. 01.1.01	37	AIso	D	N	Y	
RASCI_Chemical_Shift	Y	d_raw	AD		N	
[Chemical_Shift]		d_eigenvalues	AD AD		N 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	
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 I	N N	N N	
RASCI_G_Tensor[G_Tensor]	Y	Irrep g_matrix	AD		N	
RASCI_G_TellSOT [G_TellSOT]	1	g_macrix g_elec	D	N	N	The free electron g-value
			D	N	N	contribution The reduced mass cor-
		g_RMC				rection
		g_DSO	AD		N	
		g_PSO	AD AD		N N	
		g_Tot 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	Ī	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	Ι	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 continues on next page

Table 9.1 - continued from previous page

	able a	1.1 – continued from previous	page			
		pairsTotalSSCIso	AD	N	N	The Spin-Spin coupling constant for each pair
		Method	S	N	N	1
		Level	S	N	N	
		Mult	I	N	N	
			I			
		State		N	N	
		Irrep	I	N	N	
RASCI_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	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	
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

Table 9.1 - continued from previous page

	Table 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	AD		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		
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	ΑI	N	N		
ROCIS_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		
		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 NUC	I I	N N	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	Y	isotropicPolar	D	N	N		
[Polarizability]		rawCartesian	AD		N		a.u
		diagonalizedTensor	AD		N		
		orientation	AD		N		
		doAtomicPolar	В	N	N		
		atomicPolarIso	AD		N	Atomic istotropic polar- izabilities	
		Method	S	N N	N N		
		Level Mult	S I	N N	N N		
		Mult State	I	N N	N N		
		Irrep	I	N	N		
ROCIS_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.u.
[Quadrupole_Moment]	I	quadElecContrib	AD		N	Electronic contribution. Order: XX, YY, ZZ,	a.u.
						XY, XZ, YZ continues on nex	t page

Table 9.1 – continued from previous page

	Table 9	0.1 – continued from previou	s page			
		quadNucContrib	AD	N	N	Nuclear contribution. Order: XX, YY, ZZ, XY, XZ, YZ
		quadTotal	AD	N	N	Total. Order: XX, YY,
		quadDiagonalized	AD		N	ZZ, XY, XZ, YZ The diagonalized tensor a.u.
		doAtomicQuad atomicQuad	B AD	N Y	N N	Atomic quadrupoles (NAtoms * XX, YY, ZZ,
		Method	S	N	N	XY, XZ, YZ)
		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=gegNbe*bN (in MHz)
		ARaw	AD	N	Y	Raw tensor
		AEigenvalues	AD	N	Y	Eigenvalues
		orientation	AD	N	Y	Eigenvectors
		Also	D	N	Y	
ROCIS_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
		Elems	I	N	Y	Atomic number of the nuclei
		SDSO	AD AD		Y Y	Diamagnetic contribu- tion Paramagnetic contribu-
		SPSO				tion
		STot	AD		Y	Total tensor
		orientation	AD		Y	Eigenvectors
		sTotEigen	AD		Y	Eigenvalues
		siso	D	N	Y Y	
OCIS_D_Tensor[D_Tensor]	v	saniso	D AD	N N	Y N	
OCIS_D_lensor[D_lensor]	Y	d_raw d_eigenvalues	AD		N N	
		d_eigenvalues d_eigenvectors	AD		N N	
		D D	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 cor- rection
		g_DSO	AD		N	
		g_PSO	AD		N	
		g_Tot	AD		N	
		g_iso	D AD	N	N N	
		Delta_g			INI	

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i abie	9.1	- continued from	previous	page

	Table 3	.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	1
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
ROCIS_Absorption_Spectrum	Y	Method	I	N	N	
Absorption_Spectrum]		RelCorrection	Ī	N	N	Type of relativistic
nboorperon_opecerumj						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	
		Representation	S	N	N	Possible values: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments	В	N	N	
				N	N	
		NTrans	I			
		ExcitationEnergies	AD		N	
		States	AI	N	N	The initial and Final states. Col1: Initial State Col2: Initial Irrep Col3: Final State Col4: Final Irrep

Table 9.1 - continued from previous page

Ta	able 9	0.1 – 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	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	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	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	
RPA_EFG_Tensor[EFG_Tensor]	Y	numOfNucs	I	N	N	Number of active nuclei
- <u>-</u> .		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		Y	Raw tensor
		VEigenvalues	AD		Y	Eigenvalues
						continues on next page

Tahla	<b>Q 1</b>	<ul> <li>continued</li> </ul>	from	nravious	nana
i abie	9. I	- continueu	110111	previous	paye

	Table 9	9.1 – continued from previous	page				
		orientation	AD		Y	Eigenvectors	
		VIso	D	N	Y		
RPA_Polarizability	Y	isotropicPolar	D	N	N	Electronic contribution. Order: XX, YY, ZZ, XY, XZ, YZ Nuclear contribution. Order: XX, YY, ZZ, XY, XZ, YZ Total. Order: XX, YY, ZZ, XY, XZ, YZ The diagonalized tensor Atomic quadrupoles (NAtoms * XX, YY, ZZ, XY, XZ, YZ)  Number of active nuclei Atomic number of the nuclei Atomic number of the nuclei Prefactor PFAC=geg/be*bN (in MHz) Raw tensor Eigenvalues Eigenvectors	
[Polarizability]		rawCartesian	AD		N		a.u
		diagonalizedTensor	AD		N		
		orientation	AD		N		
		doAtomicPolar	В	N	N		
		atomicPolarIso	AD	Y	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N		
RPA_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N		a.u.
[Quadrupole_Moment]		quadElecContrib	AD	N	N	Order: XX, YY, ZZ,	
		quadNucContrib	AD	N	N	Order: XX, YY, ZZ,	
		quadTotal	AD	N	N	Total. Order: XX, YY,	
		quadDiagonalized	AD	N	N		a.u.
		doAtomicQuad	В	N	N		
		atomicQuad	AD		N	(NAtoms * XX, YY, ZZ,	
		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	Ī	N	N	Number of active nuclei	
nan_n_remoor (n_remoor)	•	Method	S	N	N	N	
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
		Irrep	I	N	N	T 1 C.1 1.	
		NUC	I	N	Y		
		Elem	I	N	Y	nuclei	
		Isotope	D	N	Y	Atomic mass	
		I	D	N	Y	Spin of the nuclei	
		PFAC	D	N	Y	PFAC=gegNbe*bN (in MHz)	
		ARaw	AD		Y		
		AEigenvalues	AD		Y		
		orientation	AD		Y	Eigenvectors	
		AIso	D	N	Y		
RPA_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	
		Elems	I	N	Y	nuclei	
		SDSO	AD		Y	Diamagnetic contribu-	
		SPSO	AD		Y	Paramagnetic contribu-	
		STot	AD		Y	Total tensor	
		orientation	AD		Y	Eigenvectors	
		sTotEigen	AD		Y	Eigenvalues	
		siso	D	N	Y		
		saniso	D	N	Y		
				N.T.	NT		
RPA_D_Tensor[D_Tensor]	Y	d_raw	AD	IN	N		

Table 9.1 – continued from previous page

	1 4010 0	.1 – continued from previous	page			
		d_eigenvectors	AD		N	
		D	D	N	N	
		E	D	N	N	
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
			I		N	
		State		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 cor- rection
		g_DSO	AD	N	N	
		g_PSO	AD	N	N	
		g_Tot	AD		N	
		_	D	N	N	
		g_iso				
		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	
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	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	
DDA Abgomptice Conti	37	=	I	N	N	
RPA_Absorption_Spectrum [Absorption_Spectrum]	Y	Method RelCorrection	I	N	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

Ta	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	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	N	Col1: Multiplicity of the initial state Col2: Multiplicity of the final state
		Temperature	D	N	N	phony of the illiai state
RPA_ECD_Spectrum[ECD_Spectrum]	Y	Method	I I	N	N	
vrv-eop-phecerum[Eop-phecerum]	1	RelCorrection	I	N	N	Type of relativistic
		RefCoffection	1	IN	IN	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	
Energy	Y	Method	S	N	N	
		totalEnergy	AD		N	Total energy of each state
		Mult		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
						continues on next page

Table 9.1 - continued from previous page

Та	able 9	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	ΑI	Y	N	Block index of each state	
		Root	ΑI	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	ΑI	Y	N	Multiplicity of each state	
		Irrep	ΑI	Y	N	Irreducible representa-	
		-1				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	v	N	Average multiplicity of	
		Avgnate	AD		11	each SO-/SS-coupled state	
SCF_Nuc_Gradient	Y	NAtoms	I	N	N		
[Nuclear_Gradient]		gradNorm	D	N	N		
		grad		N	N		
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
			I	N	N		
		State	I	N			
COR D' - 1 - M   [D' ] - M	37	Irrep			N		
<pre>SCF_Dipole_Moment[Dipole_Moment]</pre>	Y	dipoleMagnitude	D	N	N	E1	a.u.
		dipoleElecContrib	AD		N	Electronic contribution	
		dipoleNucContrib	AD		N	Nuclear contribution	
		dipoleTotal	AD		N	Total	
		doAtomicDipole	В	N	N		
		atomicDipole	AD		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		Y	Raw tensor	
		VEigenvalues	AD		Y	Eigenvalues	
		orientation	AD		Y	Eigenvectors	
		VIso	D	N	Y	2.5011001010	
SCE Polarizability	Y	isotropicPolar	D	N	N		
SCF_Polarizability	1	rawCartesian	AD		N		9.11
[Dolarizahili+v1			AD	IN	1.4		a.u
[Polarizability]			۸D	N	N		
[Polarizability]		diagonalizedTensor orientation	AD AD		N N		

	Table 9	.1 – continued from previous	page			
		doAtomicPolar atomicPolarIso	B AD	N Y	N N	Atomic istotropic polar-
		Method	S	N	N	izabilities
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
		Irrep	I	N	N	
SCF_Quadrupole_Moment	Y	isotropicQuadMoment	D	N	N	a.u
[Quadrupole_Moment]		quadElecContrib	AD		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, XY, XZ, YZ)
		Method	S	N	N	
		Level	S	N	N	
		Mult	I	N	N	
		State	I	N	N	
			I		N	
		Irrep		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=gegNbe*bN (in MHz)
		ARaw	AD	N	Y	Raw tensor
		AEigenvalues	AD	N	Y	Eigenvalues
		orientation	AD		Y	Eigenvectors
						Eigenvectors
		AIso	D	N	Y	
CF_Chemical_Shift	Y	numOfNucs	I	N	N	
Chemical_Shift]		Method	S	N	N	
-		Level	S	N	N	
		Mult	I	N	N	
			I		N	
		State		N		
		Irrep	I	N	N	
		NUC Elems	I	N N	Y Y	Index of the nuclei Atomic number of the
						nuclei
		SDSO	AD	N	Y	Diamagnetic contribu- tion
		SDSO SPSO	AD	N	Y	Paramagnetic contribu-
		SDSO		N		tion Paramagnetic contribution Total tensor
		SDSO SPSO	AD	N N	Y	Paramagnetic contribu-
		SDSO SPSO STot orientation	AD AD AD	N N N	Y Y Y	tion Paramagnetic contribution Total tensor Eigenvectors
		SDSO SPSO STot orientation sTotEigen	AD AD AD AD	N N N	Y Y Y Y	tion Paramagnetic contribution Total tensor
		SDSO SPSO STot orientation sTotEigen siso	AD AD AD AD D	N N N N	Y Y Y Y Y Y	tion Paramagnetic contribution Total tensor Eigenvectors
		SDSO SPSO STot orientation sTotEigen siso saniso	AD AD AD AD D	N N N N N	Y Y Y Y Y Y Y Y	tion Paramagnetic contribution Total tensor Eigenvectors
CF_D_Tensor[D_Tensor]	Y	SDSO SPSO STot orientation sTotEigen siso saniso d_raw	AD AD AD D AD AD	N N N N N	Y Y Y Y Y Y Y N	tion Paramagnetic contribution Total tensor Eigenvectors
CF_D_Tensor[D_Tensor]	Y	SDSO SPSO STot orientation sTotEigen siso saniso	AD AD AD AD D	N N N N N	Y Y Y Y Y Y Y Y	tion Paramagnetic contribution Total tensor Eigenvectors
CF_D_Tensor[D_Tensor]	Y	SDSO SPSO STot orientation sTotEigen siso saniso d_raw d_eigenvalues	AD AD AD D AD AD	N N N N N N	Y Y Y Y Y Y Y N	tion Paramagnetic contribution Total tensor Eigenvectors
CF_D_Tensor[D_Tensor]	Y	SDSO SPSO STot orientation sTotEigen siso saniso d_raw d_eigenvalues d_eigenvectors	AD AD AD D AD AD AD AD AD AD	N N N N N N N	Y Y Y Y Y Y N N N	tion Paramagnetic contribution Total tensor Eigenvectors
CF_D_Tensor[D_Tensor]	Y	SDSO  SPSO  STot orientation sTotEigen siso saniso d_raw d_eigenvalues d_eigenvectors D	AD AD AD D AD AD AD AD AD D	N N N N N N N	Y Y Y Y Y Y N N N N	tion Paramagnetic contribution Total tensor Eigenvectors
SCF_D_Tensor[D_Tensor]	Y	SDSO  SPSO  STot orientation sTotEigen siso saniso d_raw d_eigenvalues d_eigenvectors D E	AD AD AD D AD AD AD AD D D D	N N N N N N N N N	Y Y Y Y Y Y N N N N	tion Paramagnetic contribution Total tensor Eigenvectors
SCF_D_Tensor[D_Tensor]	Y	SDSO  SPSO  STot orientation sTotEigen siso saniso d_raw d_eigenvalues d_eigenvectors D E Method	AD AD AD D AD AD AD AD D D S		Y Y Y Y Y Y N N N N N N	tion Paramagnetic contribution Total tensor Eigenvectors
SCF_D_Tensor[D_Tensor]	Y	SDSO  SPSO  STot orientation sTotEigen siso saniso d_raw d_eigenvalues d_eigenvectors D E	AD AD AD D AD AD AD AD D D D	N N N N N N N N N	Y Y Y Y Y Y N N N N	tion Paramagnetic contribution Total tensor Eigenvectors

Table	9.1 -	<ul> <li>continued</li> </ul>	from	previous page
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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 cor- rection
		g_DSO	AD	N	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	
CCE Crin Crin Counling	Y	numOfNucPairs	I	N	N	Number of pueloi pairs to
SCF_Spin_Spin_Coupling [Spin_Spin_Coupling]	1					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 to calc N Pairs I of A Num. of I	number of nuclear pairs to calculate SD/FC
		pairsInfo	AI	N	N	Num. of A. Col3->Index
		pairsDistances	AD	N	N	The distances of each
		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	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	,
		<u> </u>				continues on next page

Table 9.1 - continued from previous page

Та	ble 9	.1 – continued from previous	oage			
		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	mi '''' i i m' '
		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	
per Teen obsect au [Fen obsect au]	1		I	N		Type of relativistic
		RelCorrection	1	IN	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	
		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	mi trata
		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		N	N	
			D	N	N	
		nuclear_energy				
		SOC_correction	D	N	N	
Absorption_Spectrum	Y	Method	I	N	N	
		RelCorrection	Ι	N	N	Type of relativistic treatment in QDPT. 0->Unknow, 1->None, 2->SOC, 3->SSC, 4->SOC/SSC
						continues on port page

Table 9.1 - continued from previous page

	ibic o	.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	<b>5</b>
		Representation	S	N	N	Possible values: Un- known, Length, Velocity
		PointGroup	S	N	N	
		DoHigherMoments NTrans	B I	N N	N N	
		Nirans ExcitationEnergies	AD		N	
		States		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	
ECD_Spectrum	Y	Method	I	N	N	T
		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 pertur-
						bation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4- >Magnetic/Dipole, 5->Magnetic/Quad
		DensLevel	I	N	N	bation). 0->Unknown, 1->No Derivative, 2->Electric/Dipole, 3->Electric/Quad, 4- >Magnetic/Dipole,
		Density_name	S	N	N	bation). 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
		Density_name Representation	S S	N N	N N	bation). 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-
		Density_name Representation PointGroup	S S	N N	N N	bation). 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: Un-
		Density_name Representation PointGroup DoHigherMoments	S S S B	N N N	N N N	bation). 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: Un-
		Density_name Representation PointGroup	S S	N N N N	N N	bation). 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: Un-

Table 9.1 - continued from previous page

	Table 9	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	1 . 3	
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 D	N N	N N		
		rotEnergy vibEnergy	D	N	N		
		numOfFreqs	I	N	N		
		freqScalingFactor	D	N	N		
		FREQ	AD		N		cm^-
		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 D	N N	N N		
		entropyS freeEnergyG	D	N	N		
		isLinear	В	N	N		
VdW_Correction	N	vdW	D	N	N		
. un_00110001011		vdW_atomic		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	
GRODEO D'anda Manada	V	groundTotalEnergy	D	N	N	Ground State Total MDCI Energy	
CASPT2_Dipole_Moment	Y	dipoleMagnitude dipoleElecContrib	D AD	N N	N N	Electronic contribution	a.u.
[Dipole_Moment]		dipoleElecContrib dipoleNucContrib	AD AD		N N	Nuclear contribution	
		dipoleTotal	AD		N	Total	
		doAtomicDipole	В	N	N	10111	
		atomicDipole	AD		N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
		Level	S	N	N		
		Mult	I	N	N		
		State	I	N	N		
CAS_CUSTOM_Dipole_Moment	Y	Irrep dipoleMagnitude	I D	N N	N N		a.u.
Dipole_Moment]	I	dipoleElecContrib	AD		N	Electronic contribution	a.u.
[p.tbo.te_i.ouenc]		dipoleNucContrib	AD		N	Nuclear contribution	
		dipoleTotal	AD		N	Total	
		doAtomicDipole	В	N	N		
		atomicDipole	AD		N	Atomic dipoles (NAtoms * X,Y,Z)	
		Method	S	N	N		
				N	N		
		Level	S				
		Level Mult	I	N	N		
		Level Mult State	I I	N N	N N		
CARDES O Townselforms of the	v	Level Mult State Irrep	I I I	N N N	N N N		
CASPT2_G_Tensor[G_Tensor]	Y	Level Mult State	I I	N N N	N N	The free electron g-value contribution	