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Quantum dynamics simulations of the thermal and light-induced high-spin to low-spin relaxation in $Fe(bpy)_3$ and $Fe(mtz)_6$ †

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1 Thermal relaxation

We add here some more detailed information about the active space, the relaxed scan and the metadynamics that we have performed to determine the thermal relaxation in $[Fe(bpy)_3]^{2+}$and $[Fe(mtz)_6]^{2+}$.

1.1 CASSCF active space

CASPT2 calculations have been performed using as reference a SA-CASSCF wave function. The active space for the reference wave function is formed by two σ orbitals formally from the ligands, five 3d-type Fe-orbitals (three t_{2g} and two e_g) and five 4d orbitals from Fe. Note that the same active space has been employed to obtain the adiabatic energies used in the fitting procedure of the model Hamiltonian. Three extra π^* orbitals from the ligands have been added in only one calculation to study the effect of the MLCT states.

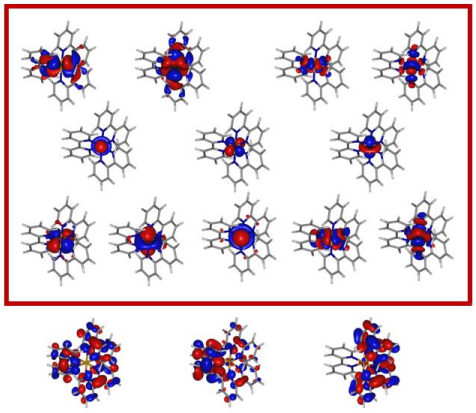

Fig. 1 Active space natural orbitals in $[Fe(bpy)_3]^{2+}$ for a CAS(10,15). Two σ orbitals in top-left, e_g orbitals in the top-right, t_{2g} orbitals in the second-row, Fe 4d orbitals in the third row and π^* at the bottom. In red the MOs that are also found in a CAS(10,12). Note that the same type orbitals are present in $[Fe(mtz)_6]^{2+}$.

1.2 Relaxed scan

The adiabatic energies are computed at CASPT2 level. Unfortunately, CASPT2 optimizations are not straightforward, therefore, we performed a relaxed scan (constrained optimization at B3LYP/def2-SVP level) along the main reaction coordinate, the Fe-N symmetric stretching mode.

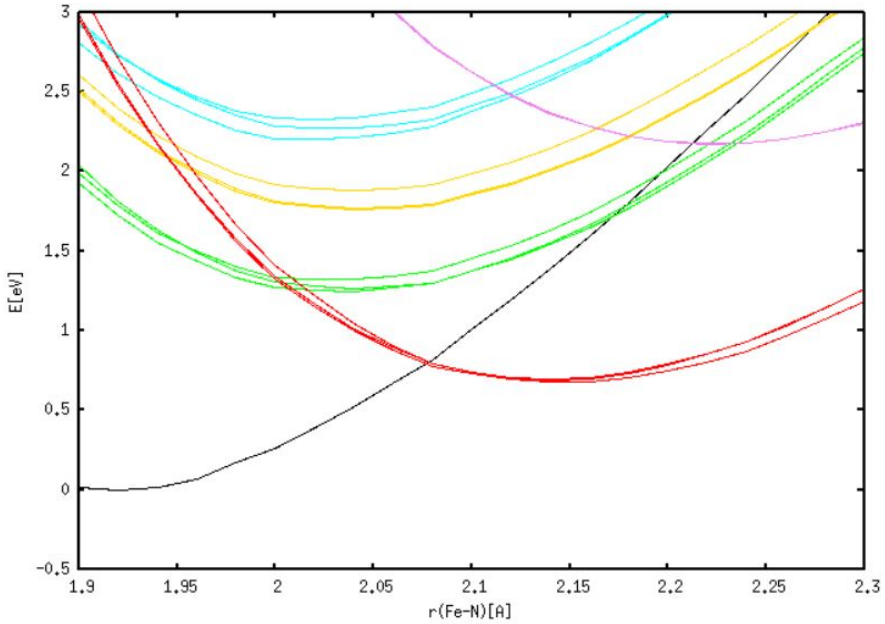

Fig. 2 Relaxed scan at CASPT2 level along the Fe-N symmetric stretching in $[Fe(bpy)_3]^{2+}$. $^1A_{1g}$ in black, $^1T_{1g}$ in cyan, $^3T_{1g}$ in green, $^3T_{2g}$ in gold, $^5T_{2g}$ in red and ^5E_g in violet.

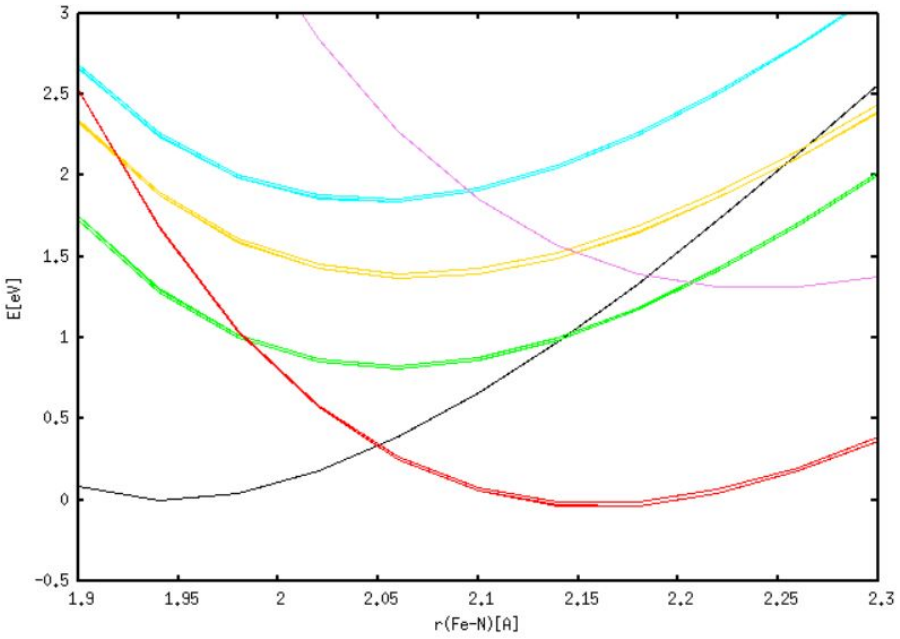

Fig. 3 Relaxed scan at CASPT2 level along the Fe-N symmetric stretching in $[Fe(bpy)_3]^{2+}$. $^1A_{1g}$ in black, $^1T_{1g}$ in cyan, $^3T_{1g}$ in green, $^3T_{2g}$ in gold, $^5T_{2g}$ in red and ^5E_g in violet.

The Fe-N distances in the minima of the relaxed scan curves are similar to those reported by Finney et al. in a CASPT2 optimization in the case of $[Fe(bpy)_3]^{2+}$.[1]

Table 1 Distances of the CASPT2 quasi-equilibrium geometries [Å] through a relaxed scan and optimized distances at (XMS-)CASPT2 level in the HS and LS of $[Fe(bpy)_3]^{2+}$ and $[Fe(mtz)_6]^{2+}$.

State	$[Fe(bpy)_3]^{2+}$		$[Fe(mtz)_6]^{2+}$
	Relaxed scan	CASPT2 opt.*	Relaxed scan
LS	1.940	1.941	1.940
HS	2.140	2.168/2.182	2.180

(*) apical and equatorial values reported for the HS.

2 Light-induced process

2.1 Model Hamiltonian

Here, we present the numerical value of the parameters of the model Hamiltonian. The nuclear kinetic energy only depends on the frequencies of the HS state: $\omega_{31} = 112$ cm^{-1}, $\omega_{33} = 115$ cm^{-1} and $\omega_{rc} = 147$ cm^{-1}. The parameters for the diabatic potentials, the non-adiabatic and the spin-orbit couplings whose expressions are defined in the main text are reported here.

2.1.1 Non-adiabatic couplings

The non-adiabatic coupling term is described as

$$W^{NA}_{n,n',S} = \sum_{i}^{N_{vib}} \lambda_i^{n,n',S} q_i \tag{1}$$

All the linear expansion terms for the non-adiabatic coupling are smaller than 0.1 cm^{-1}, therefore, they are not reported.

2.1.2 Diabatic potentials

The diabatic potentials are defined as

$$V^S_n = E^S_n + \sum_{i}^{N_{vib}} \sum_{j=1}^{4} \frac{1}{j!} k^{n,S}_{j,i} q^j_i \tag{2}$$

Table 2 Parameters for the diabatic potentials in cm^{-1}.

	E_n	$k_{1,31}$	$k_{2,31}$	$k_{3.31}$	$k_{4,31}$	$k_{1,33}$	$k_{2,33}$	$k_{3.33}$	$k_{4,33}$	$k_{1,rc}$	$k_{2,rc}$	$k_{3.rc}$	$k_{4,rc}$
$^1A_{1g}$	15522.2	17.9	24.5	4.8	2.3	36.2	20.2	2.1	2.1	-1461.6	60.7	8.0	0.7
$^1T_{1g}(1)$	22733.8	-352.2	33.8	4.8	2.6	-314.5	33.3	5.2	1.2	-936.7	94.2	9.9	0.7
$^1T_{1g}(2)$	23011.3	221.8	8.6	2.0	2.1	321.1	18.2	0.8	1.5	-970.0	90.1	9.9	0.8
$^1T_{1g}(3)$	23502.7	192.0	7.9	4.5	2.1	3.3	-11.9	3.0	2.4	-945.4	91.3	10.2	0.9
$^3T_{1g}(1)$	12871.2	225.0	-13.2	-1.2	2.4	338.4	-3.0	-3.4	2.0	-931.4	92.2	10.4	0.8
$^3T_{1g}(2)$	13126.0	-403.0	22.0	7.2	2.6	-225.7	-18.2	5.7	2.9	-902.4	94.3	10.4	0.9
$^3T_{1g}(3)$	13716.5	193.8	-22.4	1.9	2.9	18.6	-57.7	1.6	4.9	-901.1	91.6	10.8	1.0
$^3T_{2g}(1)$	17131.0	-119.0	89.3	10.0	1.1	-131.7	51.5	-1.2	0.4	-797.1	92.1	9.5	0.8
$^3T_{2g}(2)$	17377.3	368.8	22.9	4.6	2.6	237.5	29.6	1.0	1.2	-811.4	91.0	10.4	0.9
$^3T_{2g}(3)$	17595.3	-158.7	85.4	12.3	1.7	82.0	6.6	-0.3	3.8	-808.8	96.4	10.4	0.8
$^5T_{2g}(1)$	0.0	58.1	58.7	5.8	1.6	15.5	43.7	-1.1	2.2	-369.8	128.9	12.8	1.1
$^5T_{2g}(2)$	159.9	-3.4	50.6	5.6	2.3	-3.4	44.3	1.9	2.0	-365.7	127.8	12.5	1.1
$^5T_{2g}(3)$	935.9	14.5	66.2	6.9	1.7	12.9	53.1	-1.0	2.1	-332.8	129.1	12.3	1.0
$^5E_g(1)$	10936.3	-435.7	71.5	7.3	1.5	-457.3	60.5	1.8	1.6	262.6	165.6	14.7	0.9
$^5E_g(2)$	11223.0	478.2	60.2	4.0	1.6	401.0	41.2	-0.6	2.5	216.5	160.8	14.3	1.4

2.1.3 Spin-orbit coupling

The spin-orbit coupling term is defined as follows

$$W^{SO}_{nS\alpha,n'S'\alpha'} = \langle n_{S\alpha}|\hat{H}^{SO}|n'_{S'\alpha'}\rangle \tag{3}$$

Table 3 Singlet-triplet spin-orbit coupling in $cm^{-}1$.

$n_{S,\alpha}$-n'$_{S'\alpha'}$	W^{SO}	$n_{S,\alpha}$-n'$_{S'\alpha'}$	W^{SO}	$n_{S,\alpha}$-n'$_{S'\alpha'}$	W^{SO}
$^1A_{1g}$-$^3T_{1g}(1)$(MS=-1)	-16.0+236.1i	$^1A_{1g}$-$^3T_{1g}(1)$(MS=0)	-0.0-440.6i	$^1A_{1g}$-$^3T_{1g}(1)$(MS=1)	-16.0-236.1i
$^1A_{1g}$-$^3T_{1g}(2)$(MS=-1)	+77.4-320.6i	$^1A_{1g}$-$^3T_{1g}(2)$(MS=0)	+0.0-362.2i	$^1A_{1g}$-$^3T_{1g}(2)$(MS=1)	+77.4+320.6i
$^1A_{1g}$-$^3T_{1g}(3)$(MS=-1)	+397.4+52.8i	$^1A_{1g}$-$^3T_{1g}(3)$(MS=0)	+0.0+23.1i	$^1A_{1g}$-$^3T_{1g}(3)$(MS=1)	+397.4-52.8i
$^1A_{1g}$-$^3T_{2g}(1)$(MS=-1)	-4.5+18.5i	$^1A_{1g}$-$^3T_{2g}(1)$(MS=0)	-0.0-27.8i	$^1A_{1g}$-$^3T_{2g}(1)$(MS=1)	-4.5-18.5i
$^1A_{1g}$-$^3T_{2g}(2)$(MS=-1)	+22.6-1.8i	$^1A_{1g}$-$^3T_{2g}(2)$(MS=0)	+0.0-15.6i	$^1A_{1g}$-$^3T_{2g}(2)$(MS=1)	+22.6+1.8i
$^1A_{1g}$-$^3T_{2g}(3)$(MS=-1)	-2.0+35.4i	$^1A_{1g}$-$^3T_{2g}(3)$(MS=0)	-0.0-36.7i	$^1A_{1g}$-$^3T_{2g}(3)$(MS=1)	-2.0-35.4i
$^1T_{1g}(1)$-$^3T_{1g}(1)$(MS=-1)	-4.6-10.2i	$^1T_{1g}(1)$-$^3T_{1g}(1)$(MS=0)	-0.0+0.4i	$^1T_{1g}(1)$-$^3T_{1g}(1)$(MS=1)	-4.6+10.2i
$^1T_{1g}(1)$-$^3T_{1g}(2)$(MS=-1)	-56.7-10.3i	$^1T_{1g}(1)$-$^3T_{1g}(2)$(MS=0)	-0.0+0.8i	$^1T_{1g}(1)$-$^3T_{1g}(2)$(MS=1)	-56.7+10.3i
$^1T_{1g}(1)$-$^3T_{1g}(3)$(MS=-1)	+17.6-53.1i	$^1T_{1g}(1)$-$^3T_{1g}(3)$(MS=0)	+0.0-77.1i	$^1T_{1g}(1)$-$^3T_{1g}(3)$(MS=1)	+17.6+53.1i
$^1T_{1g}(1)$-$^3T_{2g}(1)$(MS=-1)	+38.4+153.6i	$^1T_{1g}(1)$-$^3T_{2g}(1)$(MS=0)	+0.0-199.3i	$^1T_{1g}(1)$-$^3T_{2g}(1)$(MS=1)	+38.4-153.6i
$^1T_{1g}(1)$-$^3T_{2g}(2)$(MS=-1)	-144.3+139.5i	$^1T_{1g}(1)$-$^3T_{2g}(2)$(MS=0)	-0.0+196.7i	$^1T_{1g}(1)$-$^3T_{2g}(2)$(MS=1)	-144.3-139.5i
$^1T_{1g}(1)$-$^3T_{2g}(3)$(MS=-1)	-10.4-1.6i	$^1T_{1g}(1)$-$^3T_{2g}(3)$(MS=0)	-0.0+36.9i	$^1T_{1g}(1)$-$^3T_{2g}(3)$(MS=1)	-10.4+1.6i
$^1T_{1g}(2)$-$^3T_{1g}(1)$(MS=-1)	+49.8-50.5i	$^1T_{1g}(2)$-$^3T_{1g}(1)$(MS=0)	+0.0-71.8i	$^1T_{1g}(2)$-$^3T_{1g}(1)$(MS=1)	+49.8+50.5i
$^1T_{1g}(2)$-$^3T_{1g}(2)$(MS=-1)	-3.4-26.1i	$^1T_{1g}(2)$-$^3T_{1g}(2)$(MS=0)	-0.0+61.1i	$^1T_{1g}(2)$-$^3T_{1g}(2)$(MS=1)	-3.4+26.1i
$^1T_{1g}(2)$-$^3T_{1g}(3)$(MS=-1)	+1.5-24.0i	$^1T_{1g}(2)$-$^3T_{1g}(3)$(MS=0)	+0.0+43.0i	$^1T_{1g}(2)$-$^3T_{1g}(3)$(MS=1)	+1.5+24.0i
$^1T_{1g}(2)$-$^3T_{2g}(1)$(MS=-1)	+157.1+73.8i	$^1T_{1g}(2)$-$^3T_{2g}(1)$(MS=0)	+0.0+165.2i	$^1T_{1g}(2)$-$^3T_{2g}(1)$(MS=1)	+157.1-73.8i
$^1T_{1g}(2)$-$^3T_{2g}(2)$(MS=-1)	+32.9-44.2i	$^1T_{1g}(2)$-$^3T_{2g}(2)$(MS=0)	+0.0+48.4i	$^1T_{1g}(2)$-$^3T_{2g}(2)$(MS=1)	+32.9+44.2i
$^1T_{1g}(2)$-$^3T_{2g}(3)$(MS=-1)	-110.0+136.1i	$^1T_{1g}(2)$-$^3T_{2g}(3)$(MS=0)	-0.0+206.3i	$^1T_{1g}(2)$-$^3T_{2g}(3)$(MS=1)	-110.0-136.1i
$^1T_{1g}(3)$-$^3T_{1g}(1)$(MS=-1)	+19.3+37.0i	$^1T_{1g}(3)$-$^3T_{1g}(1)$(MS=0)	+0.0+34.8i	$^1T_{1g}(3)$-$^3T_{1g}(1)$(MS=1)	+19.3-37.0i
$^1T_{1g}(3)$-$^3T_{1g}(2)$(MS=-1)	-2.0+26.5i	$^1T_{1g}(3)$-$^3T_{1g}(2)$(MS=0)	-0.0-46.9i	$^1T_{1g}(3)$-$^3T_{1g}(2)$(MS=1)	-2.0-26.5i
$^1T_{1g}(3)$-$^3T_{1g}(3)$(MS=-1)	+1.0-28.4i	$^1T_{1g}(3)$-$^3T_{1g}(3)$(MS=0)	+0.0+39.7i	$^1T_{1g}(3)$-$^3T_{1g}(3)$(MS=1)	+1.0+28.4i
$^1T_{1g}(3)$-$^3T_{2g}(1)$(MS=-1)	-13.4+10.4i	$^1T_{1g}(3)$-$^3T_{2g}(1)$(MS=0)	-0.0-41.8i	$^1T_{1g}(3)$-$^3T_{2g}(1)$(MS=1)	-13.4-10.4i
$^1T_{1g}(3)$-$^3T_{2g}(2)$(MS=-1)	+7.1-155.3i	$^1T_{1g}(3)$-$^3T_{2g}(2)$(MS=0)	+0.0+202.6i	$^1T_{1g}(3)$-$^3T_{2g}(2)$(MS=1)	+7.1+155.3i
$^1T_{1g}(3)$-$^3T_{2g}(3)$(MS=-1)	+204.7+60.8i	$^1T_{1g}(3)$-$^3T_{2g}(3)$(MS=0)	+0.0+75.6i	$^1T_{1g}(3)$-$^3T_{2g}(3)$(MS=1)	+204.7-60.8i

Table 4 Triplet-triplet spin-orbit coupling in cm^{-1}.

$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}	$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}
$^3T_{1g}(1)(MS=-1)$-$^3T_{1g}(2)(MS=-1)$	+0.0+8.7i	$^3T_{1g}(1)(MS=-1)$-$^3T_{1g}(2)(MS=0)$	-109.4+9.2i
$^3T_{1g}(1)(MS=0)$-$^3T_{1g}(2)(MS=-1)$	+109.4+9.2i	$^3T_{1g}(1)(MS=0)$-$^3T_{1g}(2)(MS=1)$	-109.4+9.2i
$^3T_{1g}(1)(MS=1)$-$^3T_{1g}(2)(MS=0)$	+109.4+9.2i	$^3T_{1g}(1)(MS=1)$-$^3T_{1g}(2)(MS=1)$	+0.0-8.7i
$^3T_{1g}(1)(MS=-1)$-$^3T_{1g}(3)(MS=-1)$	-0.0-126.4i	$^3T_{1g}(1)(MS=-1)$-$^3T_{1g}(3)(MS=0)$	+32.7+105.6i
$^3T_{1g}(1)(MS=0)$-$^3T_{1g}(3)(MS=-1)$	-32.7+105.6i	$^3T_{1g}(1)(MS=0)$-$^3T_{1g}(3)(MS=1)$	+32.7+105.6i
$^3T_{1g}(1)(MS=1)$-$^3T_{1g}(3)(MS=0)$	-32.7+105.6i	$^3T_{1g}(1)(MS=1)$-$^3T_{1g}(3)(MS=1)$	-0.0+126.4i
$^3T_{1g}(1)(MS=-1)$-$^3T_{2g}(1)(MS=-1)$	-0.0-124.8i	$^3T_{1g}(1)(MS=-1)$-$^3T_{2g}(1)(MS=0)$	+21.1-103.2i
$^3T_{1g}(1)(MS=0)$-$^3T_{2g}(1)(MS=-1)$	-21.1-103.2i	$^3T_{1g}(1)(MS=0)$-$^3T_{2g}(1)(MS=1)$	+21.1-103.2i
$^3T_{1g}(1)(MS=1)$-$^3T_{2g}(1)(MS=0)$	-21.1-103.2i	$^3T_{1g}(1)(MS=1)$-$^3T_{2g}(1)(MS=1)$	-0.0+124.8i
$^3T_{1g}(1)(MS=-1)$-$^3T_{2g}(2)(MS=-1)$	+0.0+84.3i	$^3T_{1g}(1)(MS=-1)$-$^3T_{2g}(2)(MS=0)$	-51.1-48.8i
$^3T_{1g}(1)(MS=0)$-$^3T_{2g}(2)(MS=-1)$	+51.1-48.8i	$^3T_{1g}(1)(MS=0)$-$^3T_{2g}(2)(MS=1)$	-51.1-48.8i
$^3T_{1g}(1)(MS=1)$-$^3T_{2g}(2)(MS=0)$	+51.1-48.8i	$^3T_{1g}(1)(MS=1)$-$^3T_{2g}(2)(MS=1)$	+0.0-84.3i
$^3T_{1g}(1)(MS=-1)$-$^3T_{2g}(3)(MS=-1)$	-0.0+38.1i	$^3T_{1g}(1)(MS=-1)$-$^3T_{2g}(3)(MS=0)$	+6.6+4.2i
$^3T_{1g}(1)(MS=0)$-$^3T_{2g}(3)(MS=-1)$	-6.6+4.2i	$^3T_{1g}(1)(MS=0)$-$^3T_{2g}(3)(MS=1)$	+6.6+4.2i
$^3T_{1g}(1)(MS=1)$-$^3T_{2g}(3)(MS=0)$	-6.6+4.2i	$^3T_{1g}(1)(MS=1)$-$^3T_{2g}(3)(MS=1)$	-0.0-38.1i
$^3T_{1g}(2)(MS=-1)$-$^3T_{1g}(3)(MS=-1)$	-0.0+138.3i	$^3T_{1g}(2)(MS=-1)$-$^3T_{1g}(3)(MS=0)$	+0.6+71.4i
$^3T_{1g}(2)(MS=0)$-$^3T_{1g}(3)(MS=-1)$	-0.6+71.4i	$^3T_{1g}(2)(MS=0)$-$^3T_{1g}(3)(MS=1)$	+0.6+71.4i
$^3T_{1g}(2)(MS=1)$-$^3T_{1g}(3)(MS=0)$	-0.6+71.4i	$^3T_{1g}(2)(MS=1)$-$^3T_{1g}(3)(MS=1)$	-0.0-138.3i
$^3T_{1g}(2)(MS=-1)$-$^3T_{2g}(1)(MS=-1)$	-0.0+60.3i	$^3T_{1g}(2)(MS=-1)$-$^3T_{2g}(1)(MS=0)$	+51.7-18.3i
$^3T_{1g}(2)(MS=0)$-$^3T_{2g}(1)(MS=-1)$	-51.7-18.3i	$^3T_{1g}(2)(MS=0)$-$^3T_{2g}(1)(MS=1)$	+51.7-18.3i
$^3T_{1g}(2)(MS=1)$-$^3T_{2g}(1)(MS=0)$	-51.7-18.3i	$^3T_{1g}(2)(MS=1)$-$^3T_{2g}(1)(MS=1)$	-0.0-60.3i
$^3T_{1g}(2)(MS=-1)$-$^3T_{2g}(2)(MS=-1)$	-0.0+108.9i	$^3T_{1g}(2)(MS=-1)$-$^3T_{2g}(2)(MS=0)$	+18.9+91.1i
$^3T_{1g}(2)(MS=0)$-$^3T_{2g}(2)(MS=-1)$	-18.9+91.1i	$^3T_{1g}(2)(MS=0)$-$^3T_{2g}(2)(MS=1)$	+18.9+91.1i
$^3T_{1g}(2)(MS=1)$-$^3T_{2g}(2)(MS=0)$	-18.9+91.1i	$^3T_{1g}(2)(MS=1)$-$^3T_{2g}(2)(MS=1)$	-0.0-108.9i
$^3T_{1g}(2)(MS=-1)$-$^3T_{2g}(3)(MS=-1)$	-0.0+103.3i	$^3T_{1g}(2)(MS=-1)$-$^3T_{2g}(3)(MS=0)$	+63.0-73.9i
$^3T_{1g}(2)(MS=0)$-$^3T_{2g}(3)(MS=-1)$	-63.0-73.9i	$^3T_{1g}(2)(MS=0)$-$^3T_{2g}(3)(MS=1)$	+63.0-73.9i
$^3T_{1g}(2)(MS=1)$-$^3T_{2g}(3)(MS=0)$	-63.0-73.9i	$^3T_{1g}(2)(MS=1)$-$^3T_{2g}(3)(MS=1)$	-0.0-103.3i
$^3T_{1g}(3)(MS=-1)$-$^3T_{2g}(1)(MS=-1)$	+0.0-77.7i	$^3T_{1g}(3)(MS=-1)$-$^3T_{2g}(1)(MS=0)$	-84.8+28.7i
$^3T_{1g}(3)(MS=0)$-$^3T_{2g}(1)(MS=-1)$	+84.8+28.7i	$^3T_{1g}(3)(MS=0)$-$^3T_{2g}(1)(MS=1)$	-84.8+28.7i
$^3T_{1g}(3)(MS=1)$-$^3T_{2g}(1)(MS=0)$	+84.8+28.7i	$^3T_{1g}(3)(MS=1)$-$^3T_{2g}(1)(MS=1)$	+0.0+77.7i
$^3T_{1g}(3)(MS=-1)$-$^3T_{2g}(2)(MS=-1)$	+0.0+47.0i	$^3T_{1g}(3)(MS=-1)$-$^3T_{2g}(2)(MS=0)$	-8.4+40.4i
$^3T_{1g}(3)(MS=0)$-$^3T_{2g}(2)(MS=-1)$	+8.4+40.4i	$^3T_{1g}(3)(MS=0)$-$^3T_{2g}(2)(MS=1)$	-8.4+40.4i
$^3T_{1g}(3)(MS=1)$-$^3T_{2g}(2)(MS=0)$	+8.4+40.4i	$^3T_{1g}(3)(MS=1)$-$^3T_{2g}(2)(MS=1)$	+0.0-47.0i
$^3T_{1g}(3)(MS=-1)$-$^3T_{2g}(3)(MS=-1)$	-0.0-32.3i	$^3T_{1g}(3)(MS=-1)$-$^3T_{2g}(3)(MS=0)$	+107.7+13.8i
$^3T_{1g}(3)(MS=0)$-$^3T_{2g}(3)(MS=-1)$	-107.7+13.8i	$^3T_{1g}(3)(MS=0)$-$^3T_{2g}(3)(MS=1)$	+107.7+13.8i
$^3T_{1g}(3)(MS=1)$-$^3T_{2g}(3)(MS=0)$	-107.7+13.8i	$^3T_{1g}(3)(MS=1)$-$^3T_{2g}(3)(MS=1)$	-0.0+32.3i
$^3T_{2g}(1)(MS=-1)$-$^3T_{2g}(2)(MS=-1)$	+0.0-47.9i	$^3T_{2g}(1)(MS=-1)$-$^3T_{2g}(2)(MS=0)$	-88.3+25.9i
$^3T_{2g}(1)(MS=0)$-$^3T_{2g}(2)(MS=-1)$	+88.3+25.9i	$^3T_{2g}(1)(MS=0)$-$^3T_{2g}(2)(MS=1)$	-88.3+25.9i
$^3T_{2g}(1)(MS=1)$-$^3T_{2g}(2)(MS=0)$	+88.3+25.9i	$^3T_{2g}(1)(MS=1)$-$^3T_{2g}(2)(MS=1)$	+0.0+47.9i
$^3T_{2g}(1)(MS=-1)$-$^3T_{2g}(3)(MS=-1)$	+0.0-70.7i	$^3T_{2g}(1)(MS=-1)$-$^3T_{2g}(3)(MS=0)$	-2.1-74.7i
$^3T_{2g}(1)(MS=0)$-$^3T_{2g}(3)(MS=-1)$	+2.1-74.7i	$^3T_{2g}(1)(MS=0)$-$^3T_{2g}(3)(MS=1)$	-2.1-74.7i
$^3T_{2g}(1)(MS=1)$-$^3T_{2g}(3)(MS=0)$	+2.1-74.7i	$^3T_{2g}(1)(MS=1)$-$^3T_{2g}(3)(MS=1)$	+0.0+70.7i
$^3T_{2g}(2)(MS=-1)$-$^3T_{2g}(3)(MS=-1)$	-0.0-100.1i	$^3T_{2g}(2)(MS=-1)$-$^3T_{2g}(3)(MS=0)$	+56.5+49.2i
$^3T_{2g}(2)(MS=0)$-$^3T_{2g}(3)(MS=-1)$	-56.5+49.2i	$^3T_{2g}(2)(MS=0)$-$^3T_{2g}(3)(MS=1)$	+56.5+49.2i
$^3T_{2g}(2)(MS=1)$-$^3T_{2g}(3)(MS=0)$	-56.5+49.2i	$^3T_{2g}(2)(MS=1)$-$^3T_{2g}(3)(MS=1)$	-0.0+100.1i

Table 5 Triplet-quintet spin-orbit coupling in cm^{-1}. (1/3)

$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}	$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}
$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(1)(MS=-2)$	-227.7+177.7i	$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(1)(MS=-1)$	-0.0+247.4i
$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(1)(MS=0)$	-92.9-72.5i	$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(1)(MS=-1)$	-161.0+125.6i
$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(1)(MS=0)$	-0.0+285.6i	$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(1)(MS=1)$	-161.0-125.6i
$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(1)(MS=0)$	-92.9+72.5i	$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(1)(MS=1)$	-0.0+247.4i
$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(1)(MS=2)$	-227.7-177.7i	$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(2)(MS=-2)$	+37.7+168.9i
$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(2)(MS=-1)$	+0.0-72.7i	$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(2)(MS=0)$	+15.4-69.0i
$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(2)(MS=-1)$	+26.7+119.4i	$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(2)(MS=0)$	+0.0-83.9i
$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(2)(MS=1)$	+26.7-119.4i	$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(2)(MS=0)$	+15.4+69.0i
$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(2)(MS=1)$	+0.0-72.7i	$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(2)(MS=2)$	+37.7-168.9i
$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(3)(MS=-2)$	+33.5+186.5i	$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(3)(MS=-1)$	+0.0-183.4i
$^3T_{1g}(1)(MS=-1)$-$^5T_{2g}(3)(MS=0)$	+13.7-76.2i	$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(3)(MS=-1)$	+23.7+131.9i
$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(3)(MS=0)$	+0.0-211.8i	$^3T_{1g}(1)(MS=0)$-$^5T_{2g}(3)(MS=1)$	+23.7-131.9i
$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(3)(MS=0)$	+13.7+76.2i	$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(3)(MS=1)$	+0.0-183.4i
$^3T_{1g}(1)(MS=1)$-$^5T_{2g}(3)(MS=2)$	+33.5-186.5i	$^3T_{1g}(1)(MS=-1)$-$^5E_g(1)(MS=-2)$	-6.4+0.2i
$^3T_{1g}(1)(MS=-1)$-$^5E_g(1)(MS=-1)$	-0.0+0.8i	$^3T_{1g}(1)(MS=-1)$-$^5E_g(1)(MS=0)$	-2.6-0.1i
$^3T_{1g}(1)(MS=0)$-$^5E_g(1)(MS=-1)$	-4.5+0.2i	$^3T_{1g}(1)(MS=0)$-$^5E_g(1)(MS=0)$	-0.0+0.9i
$^3T_{1g}(1)(MS=0)$-$^5E_g(1)(MS=1)$	-4.5-0.2i	$^3T_{1g}(1)(MS=1)$-$^5E_g(1)(MS=0)$	-2.6+0.1i
$^3T_{1g}(1)(MS=1)$-$^5E_g(1)(MS=1)$	-0.0+0.8i	$^3T_{1g}(1)(MS=1)$-$^5E_g(1)(MS=2)$	-6.4-0.2i
$^3T_{1g}(1)(MS=-1)$-$^5E_g(2)(MS=-2)$	-2.0-10.3i	$^3T_{1g}(1)(MS=-1)$-$^5E_g(2)(MS=-1)$	-0.0+7.3i
$^3T_{1g}(1)(MS=-1)$-$^5E_g(2)(MS=0)$	-0.8+4.2i	$^3T_{1g}(1)(MS=0)$-$^5E_g(2)(MS=-1)$	-1.4-7.3i
$^3T_{1g}(1)(MS=0)$-$^5E_g(2)(MS=0)$	-0.0+8.5i	$^3T_{1g}(1)(MS=0)$-$^5E_g(2)(MS=1)$	-1.4+7.3i
$^3T_{1g}(1)(MS=1)$-$^5E_g(2)(MS=0)$	-0.8-4.2i	$^3T_{1g}(1)(MS=1)$-$^5E_g(2)(MS=1)$	-0.0+7.3i
$^3T_{1g}(1)(MS=1)$-$^5E_g(2)(MS=2)$	-2.0+10.3i	$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(1)(MS=-2)$	+55.1-255.5i
$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(1)(MS=-1)$	+0.0+169.0i	$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(1)(MS=0)$	+22.5+104.3i
$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(1)(MS=-1)$	+38.9-180.6i	$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(1)(MS=0)$	+0.0+195.2i
$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(1)(MS=1)$	+38.9+180.6i	$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(1)(MS=0)$	+22.5-104.3i
$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(1)(MS=1)$	+0.0+169.0i	$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(1)(MS=2)$	+55.1+255.5i
$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(2)(MS=-2)$	+196.4+194.2i	$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(2)(MS=-1)$	+0.0+238.1i
$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(2)(MS=0)$	+80.2-79.3i	$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(2)(MS=-1)$	+138.9+137.3i
$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(2)(MS=0)$	+0.0+274.9i	$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(2)(MS=1)$	+138.9-137.3i
$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(2)(MS=0)$	+80.2+79.3i	$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(2)(MS=1)$	+0.0+238.1i
$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(2)(MS=2)$	+196.4-194.2i	$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(3)(MS=-2)$	+28.7-84.3i
$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(3)(MS=-1)$	+0.0-29.9i	$^3T_{1g}(2)(MS=-1)$-$^5T_{2g}(3)(MS=0)$	+11.7+34.4i
$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(3)(MS=-1)$	+20.3-59.6i	$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(3)(MS=0)$	+0.0-34.6i
$^3T_{1g}(2)(MS=0)$-$^5T_{2g}(3)(MS=1)$	+20.3+59.6i	$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(3)(MS=0)$	+11.7-34.4i
$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(3)(MS=1)$	+0.0-29.9i	$^3T_{1g}(2)(MS=1)$-$^5T_{2g}(3)(MS=2)$	+28.7+84.3i
$^3T_{1g}(2)(MS=-1)$-$^5E_g(1)(MS=-2)$	-0.6+1.4i	$^3T_{1g}(2)(MS=-1)$-$^5E_g(1)(MS=-1)$	-0.0-1.0i
$^3T_{1g}(2)(MS=-1)$-$^5E_g(1)(MS=0)$	-0.3-0.6i	$^3T_{1g}(2)(MS=0)$-$^5E_g(1)(MS=-1)$	-0.4+1.0i
$^3T_{1g}(2)(MS=0)$-$^5E_g(1)(MS=0)$	-0.0-1.2i	$^3T_{1g}(2)(MS=0)$-$^5E_g(1)(MS=1)$	-0.4-1.0i
$^3T_{1g}(2)(MS=1)$-$^5E_g(1)(MS=0)$	-0.3+0.6i	$^3T_{1g}(2)(MS=1)$-$^5E_g(1)(MS=1)$	-0.0-1.0i
$^3T_{1g}(2)(MS=1)$-$^5E_g(1)(MS=2)$	-0.6-1.4i	$^3T_{1g}(2)(MS=-1)$-$^5E_g(2)(MS=-2)$	-13.5+6.7i
$^3T_{1g}(2)(MS=-1)$-$^5E_g(2)(MS=-1)$	-0.0+3.0i	$^3T_{1g}(2)(MS=-1)$-$^5E_g(2)(MS=0)$	-5.5-2.7i
$^3T_{1g}(2)(MS=0)$-$^5E_g(2)(MS=-1)$	-9.6+4.8i	$^3T_{1g}(2)(MS=0)$-$^5E_g(2)(MS=0)$	-0.0+3.5i
$^3T_{1g}(2)(MS=0)$-$^5E_g(2)(MS=1)$	-9.6-4.8i	$^3T_{1g}(2)(MS=1)$-$^5E_g(2)(MS=0)$	-5.5+2.7i
$^3T_{1g}(2)(MS=1)$-$^5E_g(2)(MS=1)$	-0.0+3.0i	$^3T_{1g}(2)(MS=1)$-$^5E_g(2)(MS=2)$	-13.5-6.7i
$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(1)(MS=-2)$	-12.0-110.9i	$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(1)(MS=-1)$	-0.0+107.4i
$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(1)(MS=0)$	-4.9+45.3i	$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(1)(MS=-1)$	-8.5-78.5i
$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(1)(MS=0)$	-0.0+124.0i	$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(1)(MS=1)$	-8.5+78.5i
$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(1)(MS=0)$	-4.9-45.3i	$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(1)(MS=1)$	-0.0+107.4i
$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(1)(MS=2)$	-12.0+110.9i	$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(2)(MS=-2)$	+151.3-147.4i
$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(2)(MS=-1)$	+0.0-196.9i	$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(2)(MS=0)$	+61.8+60.2i
$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(2)(MS=-1)$	+107.0-104.2i	$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(2)(MS=0)$	+0.0-227.4i
$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(2)(MS=1)$	+107.0+104.2i	$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(2)(MS=0)$	+61.8-60.2i
$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(2)(MS=1)$	+0.0-196.9i	$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(2)(MS=2)$	+151.3+147.4i
$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(3)(MS=-2)$	-371.2-20.3i	$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(3)(MS=-1)$	-0.0-53.1i
$^3T_{1g}(3)(MS=-1)$-$^5T_{2g}(3)(MS=0)$	-151.5+8.3i	$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(3)(MS=-1)$	-262.5-14.4i
$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(3)(MS=0)$	-0.0-61.3i	$^3T_{1g}(3)(MS=0)$-$^5T_{2g}(3)(MS=1)$	-262.5+14.4i
$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(3)(MS=0)$	-151.5-8.3i	$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(3)(MS=1)$	-0.0-53.1i

Table 6 Triplet-quintet spin-orbit coupling in cm^{-1}. (2/3)

$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}	$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}
$^3T_{1g}(3)(MS=1)$-$^5T_{2g}(3)(MS=2)$	-371.2+20.3i	$^3T_{1g}(3)(MS=-1)$-$^5E_g(1)(MS=-2)$	+0.4-3.2i
$^3T_{1g}(3)(MS=-1)$-$^5E_g(1)(MS=-1)$	+0.0+5.2i	$^3T_{1g}(3)(MS=-1)$-$^5E_g(1)(MS=0)$	+0.2+1.3i
$^3T_{1g}(3)(MS=0)$-$^5E_g(1)(MS=-1)$	+0.3-2.3i	$^3T_{1g}(3)(MS=0)$-$^5E_g(1)(MS=0)$	+0.0+6.0i
$^3T_{1g}(3)(MS=0)$-$^5E_g(1)(MS=1)$	+0.3+2.3i	$^3T_{1g}(3)(MS=1)$-$^5E_g(1)(MS=0)$	+0.2-1.3i
$^3T_{1g}(3)(MS=1)$-$^5E_g(1)(MS=1)$	+0.0+5.2i	$^3T_{1g}(3)(MS=1)$-$^5E_g(1)(MS=2)$	+0.4+3.2i
$^3T_{1g}(3)(MS=-1)$-$^5E_g(2)(MS=-2)$	+19.1+10.9i	$^3T_{1g}(3)(MS=-1)$-$^5E_g(2)(MS=-1)$	+0.0+11.7i
$^3T_{1g}(3)(MS=-1)$-$^5E_g(2)(MS=0)$	+7.8-4.5i	$^3T_{1g}(3)(MS=0)$-$^5E_g(2)(MS=-1)$	+13.5+7.7i
$^3T_{1g}(3)(MS=0)$-$^5E_g(2)(MS=0)$	+0.0+13.5i	$^3T_{1g}(3)(MS=0)$-$^5E_g(2)(MS=1)$	+13.5-7.7i
$^3T_{1g}(3)(MS=1)$-$^5E_g(2)(MS=0)$	+7.8+4.5i	$^3T_{1g}(3)(MS=1)$-$^5E_g(2)(MS=1)$	+0.0+11.7i
$^3T_{1g}(3)(MS=1)$-$^5E_g(2)(MS=2)$	+19.1-10.9i	$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(1)(MS=-2)$	+170.1+78.5i
$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(1)(MS=-1)$	+0.0+96.6i	$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(1)(MS=0)$	+69.4-32.0i
$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(1)(MS=-1)$	+120.2+55.5i	$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(1)(MS=0)$	+0.0+111.6i
$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(1)(MS=1)$	+120.2-55.5i	$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(1)(MS=0)$	+69.4+32.0i
$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(1)(MS=1)$	+0.0+96.6i	$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(1)(MS=2)$	+170.1-78.5i
$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(2)(MS=-2)$	+12.8-127.3i	$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(2)(MS=-1)$	+0.0+92.8i
$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(2)(MS=0)$	+5.2+52.0i	$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(2)(MS=-1)$	+9.1-90.0i
$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(2)(MS=0)$	+0.0+107.1i	$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(2)(MS=1)$	+9.1+90.0i
$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(2)(MS=0)$	+5.2-52.0i	$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(2)(MS=1)$	+0.0+92.8i
$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(2)(MS=2)$	+12.8+127.3i	$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(3)(MS=-2)$	+7.6+122.7i
$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(3)(MS=-1)$	+0.0-81.4i	$^3T_{2g}(1)(MS=-1)$-$^5T_{2g}(3)(MS=0)$	+3.1-50.1i
$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(3)(MS=-1)$	+5.4+86.7i	$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(3)(MS=0)$	+0.0-94.0i
$^3T_{2g}(1)(MS=0)$-$^5T_{2g}(3)(MS=1)$	+5.4-86.7i	$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(3)(MS=0)$	+3.1+50.1i
$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(3)(MS=1)$	+0.0-81.4i	$^3T_{2g}(1)(MS=1)$-$^5T_{2g}(3)(MS=2)$	+7.6-122.7i
$^3T_{2g}(1)(MS=-1)$-$^5E_g(1)(MS=-2)$	+54.3-47.1i	$^3T_{2g}(1)(MS=-1)$-$^5E_g(1)(MS=-1)$	+0.0-45.3i
$^3T_{2g}(1)(MS=-1)$-$^5E_g(1)(MS=0)$	+22.2+19.2i	$^3T_{2g}(1)(MS=0)$-$^5E_g(1)(MS=-1)$	+38.4-33.3i
$^3T_{2g}(1)(MS=0)$-$^5E_g(1)(MS=0)$	+0.0-52.3i	$^3T_{2g}(1)(MS=0)$-$^5E_g(1)(MS=1)$	+38.4+33.3i
$^3T_{2g}(1)(MS=1)$-$^5E_g(1)(MS=0)$	+22.2-19.2i	$^3T_{2g}(1)(MS=1)$-$^5E_g(1)(MS=1)$	+0.0-45.3i
$^3T_{2g}(1)(MS=1)$-$^5E_g(1)(MS=2)$	+54.3+47.1i	$^3T_{2g}(1)(MS=-1)$-$^5E_g(2)(MS=-2)$	+0.3-3.1i
$^3T_{2g}(1)(MS=-1)$-$^5E_g(2)(MS=-1)$	+0.0+14.5i	$^3T_{2g}(1)(MS=-1)$-$^5E_g(2)(MS=0)$	+0.1+1.3i
$^3T_{2g}(1)(MS=0)$-$^5E_g(2)(MS=-1)$	+0.2-2.2i	$^3T_{2g}(1)(MS=0)$-$^5E_g(2)(MS=0)$	+0.0+16.8i
$^3T_{2g}(1)(MS=0)$-$^5E_g(2)(MS=1)$	+0.2+2.2i	$^3T_{2g}(1)(MS=1)$-$^5E_g(2)(MS=0)$	+0.1-1.3i
$^3T_{2g}(1)(MS=1)$-$^5E_g(2)(MS=1)$	+0.0+14.5i	$^3T_{2g}(1)(MS=1)$-$^5E_g(2)(MS=2)$	+0.3+3.1i
$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(1)(MS=-2)$	+10.2-7.3i	$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(1)(MS=-1)$	+0.0+17.6i
$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(1)(MS=0)$	+4.2+3.0i	$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(1)(MS=-1)$	+7.2-5.2i
$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(1)(MS=0)$	+0.0+20.4i	$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(1)(MS=1)$	+7.2+5.2i
$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(1)(MS=0)$	+4.2-3.0i	$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(1)(MS=1)$	+0.0+17.6i
$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(1)(MS=2)$	+10.2+7.3i	$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(2)(MS=-2)$	-183.0+51.4i
$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(2)(MS=-1)$	-0.0+74.1i	$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(2)(MS=0)$	-74.7-21.0i
$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(2)(MS=-1)$	-129.4+36.3i	$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(2)(MS=0)$	-0.0+85.6i
$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(2)(MS=1)$	-129.4-36.3i	$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(2)(MS=0)$	-74.7+21.0i
$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(2)(MS=1)$	-0.0+74.1i	$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(2)(MS=2)$	-183.0-51.4i
$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(3)(MS=-2)$	-92.6-114.4i	$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(3)(MS=-1)$	-0.0-166.8i
$^3T_{2g}(2)(MS=-1)$-$^5T_{2g}(3)(MS=0)$	-37.8+46.7i	$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(3)(MS=-1)$	-65.5-80.9i
$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(3)(MS=0)$	-0.0-192.7i	$^3T_{2g}(2)(MS=0)$-$^5T_{2g}(3)(MS=1)$	-65.5+80.9i
$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(3)(MS=0)$	-37.8-46.7i	$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(3)(MS=1)$	-0.0-166.8i
$^3T_{2g}(2)(MS=1)$-$^5T_{2g}(3)(MS=2)$	-92.6+114.4i	$^3T_{2g}(2)(MS=-1)$-$^5E_g(1)(MS=-2)$	+1.8+19.7i
$^3T_{2g}(2)(MS=-1)$-$^5E_g(1)(MS=-1)$	+0.0-31.2i	$^3T_{2g}(2)(MS=-1)$-$^5E_g(1)(MS=0)$	+0.7-8.1i
$^3T_{2g}(2)(MS=0)$-$^5E_g(1)(MS=-1)$	+1.2+14.0i	$^3T_{2g}(2)(MS=0)$-$^5E_g(1)(MS=0)$	+0.0-36.0i
$^3T_{2g}(2)(MS=0)$-$^5E_g(1)(MS=1)$	+1.2-14.0i	$^3T_{2g}(2)(MS=1)$-$^5E_g(1)(MS=0)$	+0.7+8.1i
$^3T_{2g}(2)(MS=1)$-$^5E_g(1)(MS=1)$	+0.0-31.2i	$^3T_{2g}(2)(MS=1)$-$^5E_g(1)(MS=2)$	+1.8-19.7i
$^3T_{2g}(2)(MS=-1)$-$^5E_g(2)(MS=-2)$	-60.9-32.8i	$^3T_{2g}(2)(MS=-1)$-$^5E_g(2)(MS=-1)$	-0.0-22.8i
$^3T_{2g}(2)(MS=-1)$-$^5E_g(2)(MS=0)$	-24.8+13.4i	$^3T_{2g}(2)(MS=0)$-$^5E_g(2)(MS=-1)$	-43.0-23.2i
$^3T_{2g}(2)(MS=0)$-$^5E_g(2)(MS=0)$	-0.0-26.4i	$^3T_{2g}(2)(MS=0)$-$^5E_g(2)(MS=1)$	-43.0+23.2i
$^3T_{2g}(2)(MS=1)$-$^5E_g(2)(MS=0)$	-24.8-13.4i	$^3T_{2g}(2)(MS=1)$-$^5E_g(2)(MS=1)$	-0.0-22.8i
$^3T_{2g}(2)(MS=1)$-$^5E_g(2)(MS=2)$	-60.9+32.8i	$^3T_{2g}(3)(MS=-1)$-$^5T_{2g}(1)(MS=-2)$	+87.9-96.8i
$^3T_{2g}(3)(MS=-1)$-$^5T_{2g}(1)(MS=-1)$	+0.0-127.8i	$^3T_{2g}(3)(MS=-1)$-$^5T_{2g}(1)(MS=0)$	+35.9+39.5i
$^3T_{2g}(3)(MS=0)$-$^5T_{2g}(1)(MS=-1)$	+62.2-68.4i	$^3T_{2g}(3)(MS=0)$-$^5T_{2g}(1)(MS=0)$	+0.0-147.6i

Table 7 Triplet-quintet spin-orbit coupling in cm^{-1}.(3/3)

$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}	$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}
$^3T_{2g}$(3)(MS=0)-$^5T_{2g}$(1)(MS=1)	+62.2+68.4i	$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(1)(MS=0)	+35.9-39.5i
$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(1)(MS=1)	+0.0-127.8i	$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(1)(MS=2)	+87.9+96.8i
$^3T_{2g}$(3)(MS=-1)-$^5T_{2g}$(2)(MS=-2)	+2.4+103.5i	$^3T_{2g}$(3)(MS=-1)-$^5T_{2g}$(2)(MS=-1)	+0.0-87.2i
$^3T_{2g}$(3)(MS=-1)-$^5T_{2g}$(2)(MS=0)	+1.0-42.3i	$^3T_{2g}$(3)(MS=0)-$^5T_{2g}$(2)(MS=-1)	+1.7+73.2i
$^3T_{2g}$(3)(MS=0)-$^5T_{2g}$(2)(MS=0)	+0.0-100.7i	$^3T_{2g}$(3)(MS=0)-$^5T_{2g}$(2)(MS=1)	+1.7-73.2i
$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(2)(MS=0)	+1.0+42.3i	$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(2)(MS=1)	+0.0-87.2i
$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(2)(MS=2)	+2.4-103.5i	$^3T_{2g}$(3)(MS=-1)-$^5T_{2g}$(3)(MS=-2)	+1.4+141.9i
$^3T_{2g}$(3)(MS=-1)-$^5T_{2g}$(3)(MS=-1)	+0.0-110.0i	$^3T_{2g}$(3)(MS=-1)-$^5T_{2g}$(3)(MS=0)	+0.6-57.9i
$^3T_{2g}$(3)(MS=0)-$^5T_{2g}$(3)(MS=-1)	+1.0+100.3i	$^3T_{2g}$(3)(MS=0)-$^5T_{2g}$(3)(MS=0)	+0.0-127.0i
$^3T_{2g}$(3)(MS=0)-$^5T_{2g}$(3)(MS=1)	+1.0-100.3i	$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(3)(MS=0)	+0.6+57.9i
$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(3)(MS=1)	+0.0-110.0i	$^3T_{2g}$(3)(MS=1)-$^5T_{2g}$(3)(MS=2)	+1.4-141.9i
$^3T_{2g}$(3)(MS=-1)-^5E_g(1)(MS=-2)	+24.6+10.8i	$^3T_{2g}$(3)(MS=-1)-^5E_g(1)(MS=-1)	+0.0+28.5i
$^3T_{2g}$(3)(MS=-1)-^5E_g(1)(MS=0)	+10.1-4.4i	$^3T_{2g}$(3)(MS=0)-^5E_g(1)(MS=-1)	+17.4+7.6i
$^3T_{2g}$(3)(MS=0)-^5E_g(1)(MS=0)	+0.0+32.9i	$^3T_{2g}$(3)(MS=0)-^5E_g(1)(MS=1)	+17.4-7.6i
$^3T_{2g}$(3)(MS=1)-^5E_g(1)(MS=0)	+10.1+4.4i	$^3T_{2g}$(3)(MS=1)-^5E_g(1)(MS=1)	+0.0+28.5i
$^3T_{2g}$(3)(MS=1)-^5E_g(1)(MS=2)	+24.6-10.8i	$^3T_{2g}$(3)(MS=-1)-^5E_g(2)(MS=-2)	+1.8-77.3i
$^3T_{2g}$(3)(MS=-1)-^5E_g(2)(MS=-1)	+0.0+66.2i	$^3T_{2g}$(3)(MS=-1)-^5E_g(2)(MS=0)	+0.7+31.5i
$^3T_{2g}$(3)(MS=0)-^5E_g(2)(MS=-1)	+1.3-54.6i	$^3T_{2g}$(3)(MS=0)-^5E_g(2)(MS=0)	+0.0+76.4i
$^3T_{2g}$(3)(MS=0)-^5E_g(2)(MS=1)	+1.3+54.6i	$^3T_{2g}$(3)(MS=1)-^5E_g(2)(MS=0)	+0.7-31.5i
$^3T_{2g}$(3)(MS=1)-^5E_g(2)(MS=1)	+0.0+66.2i	$^3T_{2g}$(3)(MS=1)-^5E_g(2)(MS=2)	+1.8+77.3i

Table 8 Quintet-quintet spin-orbit coupling in cm^{-1}. (1/2)

$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}	$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}
$^5T_{2g}$(1)(MS=-2)-$^5T_{2g}$(2)(MS=-2)	+0.0+63.0i	$^5T_{2g}$(1)(MS=-2)-$^5T_{2g}$(2)(MS=-1)	-81.7-22.4i
$^5T_{2g}$(1)(MS=-1)-$^5T_{2g}$(2)(MS=-2)	+81.7-22.4i	$^5T_{2g}$(1)(MS=-1)-$^5T_{2g}$(2)(MS=-1)	+0.0+31.5i
$^5T_{2g}$(1)(MS=-1)-$^5T_{2g}$(2)(MS=0)	-100.1-27.5i	$^5T_{2g}$(1)(MS=0)-$^5T_{2g}$(2)(MS=-1)	+100.1-27.5i
$^5T_{2g}$(1)(MS=0)-$^5T_{2g}$(2)(MS=1)	-100.1-27.5i	$^5T_{2g}$(1)(MS=1)-$^5T_{2g}$(2)(MS=0)	+100.1-27.5i
$^5T_{2g}$(1)(MS=1)-$^5T_{2g}$(2)(MS=1)	+0.0-31.5i	$^5T_{2g}$(1)(MS=1)-$^5T_{2g}$(2)(MS=2)	-81.7-22.4i
$^5T_{2g}$(1)(MS=2)-$^5T_{2g}$(2)(MS=1)	+81.7-22.4i	$^5T_{2g}$(1)(MS=2)-$^5T_{2g}$(2)(MS=2)	+0.0-63.0i
$^5T_{2g}$(1)(MS=-2)-$^5T_{2g}$(3)(MS=-2)	+0.0-128.1i	$^5T_{2g}$(1)(MS=-2)-$^5T_{2g}$(3)(MS=-1)	-29.0+47.1i
$^5T_{2g}$(1)(MS=-1)-$^5T_{2g}$(3)(MS=-2)	+29.0+47.1i	$^5T_{2g}$(1)(MS=-1)-$^5T_{2g}$(3)(MS=-1)	+0.0-64.1i
$^5T_{2g}$(1)(MS=-1)-$^5T_{2g}$(3)(MS=0)	-35.5+57.7i	$^5T_{2g}$(1)(MS=0)-$^5T_{2g}$(3)(MS=-1)	+35.5+57.7i
$^5T_{2g}$(1)(MS=0)-$^5T_{2g}$(3)(MS=1)	-35.5+57.7i	$^5T_{2g}$(1)(MS=1)-$^5T_{2g}$(3)(MS=0)	+35.5+57.7i
$^5T_{2g}$(1)(MS=1)-$^5T_{2g}$(3)(MS=1)	+0.0+64.1i	$^5T_{2g}$(1)(MS=1)-$^5T_{2g}$(3)(MS=2)	-29.0+47.1i
$^5T_{2g}$(1)(MS=2)-$^5T_{2g}$(3)(MS=1)	+29.0+47.1i	$^5T_{2g}$(1)(MS=2)-$^5T_{2g}$(3)(MS=2)	+0.0+128.1i
$^5T_{2g}$(1)(MS=-2)-^5E_g(1)(MS=-2)	-0.0+151.9i	$^5T_{2g}$(1)(MS=-2)-^5E_g(1)(MS=-1)	+6.2+65.9i
$^5T_{2g}$(1)(MS=-1)-^5E_g(1)(MS=-2)	-6.2+65.9i	$^5T_{2g}$(1)(MS=-1)-^5E_g(1)(MS=-1)	-0.0+75.9i
$^5T_{2g}$(1)(MS=-1)-^5E_g(1)(MS=0)	+7.6+80.7i	$^5T_{2g}$(1)(MS=0)-^5E_g(1)(MS=-1)	-7.6+80.7i
$^5T_{2g}$(1)(MS=0)-^5E_g(1)(MS=1)	+7.6+80.7i	$^5T_{2g}$(1)(MS=1)-^5E_g(1)(MS=0)	-7.6+80.7i
$^5T_{2g}$(1)(MS=1)-^5E_g(1)(MS=1)	-0.0-75.9i	$^5T_{2g}$(1)(MS=1)-^5E_g(1)(MS=2)	+6.2+65.9i
$^5T_{2g}$(1)(MS=2)-^5E_g(1)(MS=1)	-6.2+65.9i	$^5T_{2g}$(1)(MS=2)-^5E_g(1)(MS=2)	-0.0-151.9i
$^5T_{2g}$(1)(MS=-2)-^5E_g(2)(MS=-2)	-0.0+137.1i	$^5T_{2g}$(1)(MS=-2)-^5E_g(2)(MS=-1)	+147.1-81.9i
$^5T_{2g}$(1)(MS=-1)-^5E_g(2)(MS=-2)	-147.1-81.9i	$^5T_{2g}$(1)(MS=-1)-^5E_g(2)(MS=-1)	-0.0+68.6i
$^5T_{2g}$(1)(MS=-1)-^5E_g(2)(MS=0)	+180.1-100.3i	$^5T_{2g}$(1)(MS=0)-^5E_g(2)(MS=-1)	-180.1-100.3i
$^5T_{2g}$(1)(MS=0)-^5E_g(2)(MS=1)	+180.1-100.3i	$^5T_{2g}$(1)(MS=1)-^5E_g(2)(MS=0)	-180.1-100.3i
$^5T_{2g}$(1)(MS=1)-^5E_g(2)(MS=1)	-0.0-68.6i	$^5T_{2g}$(1)(MS=1)-^5E_g(2)(MS=2)	+147.1-81.9i
$^5T_{2g}$(1)(MS=2)-^5E_g(2)(MS=1)	-147.1-81.9i	$^5T_{2g}$(1)(MS=2)-^5E_g(2)(MS=2)	-0.0-137.1i
$^5T_{2g}$(2)(MS=-2)-$^5T_{2g}$(3)(MS=-2)	-0.0-138.2i	$^5T_{2g}$(2)(MS=-2)-$^5T_{2g}$(3)(MS=-1)	+1.0-83.4i
$^5T_{2g}$(2)(MS=-1)-$^5T_{2g}$(3)(MS=-2)	-1.0-83.4i	$^5T_{2g}$(2)(MS=-1)-$^5T_{2g}$(3)(MS=-1)	-0.0-69.1i
$^5T_{2g}$(2)(MS=-1)-$^5T_{2g}$(3)(MS=0)	+1.2-102.1i	$^5T_{2g}$(2)(MS=0)-$^5T_{2g}$(3)(MS=-1)	-1.2-102.1i
$^5T_{2g}$(2)(MS=0)-$^5T_{2g}$(3)(MS=1)	+1.2-102.1i	$^5T_{2g}$(2)(MS=1)-$^5T_{2g}$(3)(MS=0)	-1.2-102.1i

Table 9 Quintet-quintet spin-orbit coupling in cm^{-1}. (2/2)

$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}	$n_{S,\alpha}$-$n'_{S'\alpha'}$	W^{SO}
$^5T_{2g}$(2)(MS=1)-$^5T_{2g}$(3)(MS=1)	-0.0+69.1i	$^5T_{2g}$(2)(MS=1)-$^5T_{2g}$(3)(MS=2)	+1.0-83.4i
$^5T_{2g}$(2)(MS=2)-$^5T_{2g}$(3)(MS=1)	-1.0-83.4i	$^5T_{2g}$(2)(MS=2)-$^5T_{2g}$(3)(MS=2)	-0.0+138.2i
$^5T_{2g}$(2)(MS=-2)-^5E_g(1)(MS=-2)	+0.0+28.6i	$^5T_{2g}$(2)(MS=-2)-^5E_g(1)(MS=-1)	-130.7-36.8i
$^5T_{2g}$(2)(MS=-1)-^5E_g(1)(MS=-2)	+130.7-36.8i	$^5T_{2g}$(2)(MS=-1)-^5E_g(1)(MS=-1)	+0.0+14.3i
$^5T_{2g}$(2)(MS=-1)-^5E_g(1)(MS=0)	-160.0-45.1i	$^5T_{2g}$(2)(MS=0)-^5E_g(1)(MS=-1)	+160.0-45.1i
$^5T_{2g}$(2)(MS=0)-^5E_g(1)(MS=1)	-160.0-45.1i	$^5T_{2g}$(2)(MS=1)-^5E_g(1)(MS=0)	+160.0-45.1i
$^5T_{2g}$(2)(MS=1)-^5E_g(1)(MS=1)	+0.0-14.3i	$^5T_{2g}$(2)(MS=1)-^5E_g(1)(MS=2)	-130.7-36.8i
$^5T_{2g}$(2)(MS=2)-^5E_g(1)(MS=1)	+130.7-36.8i	$^5T_{2g}$(2)(MS=2)-^5E_g(1)(MS=2)	+0.0-28.6i
$^5T_{2g}$(2)(MS=-2)-^5E_g(2)(MS=-2)	-0.0-196.5i	$^5T_{2g}$(2)(MS=-2)-^5E_g(2)(MS=-1)	+2.1-98.4i
$^5T_{2g}$(2)(MS=-1)-^5E_g(2)(MS=-2)	-2.1-98.4i	$^5T_{2g}$(2)(MS=-1)-^5E_g(2)(MS=-1)	-0.0-98.3i
$^5T_{2g}$(2)(MS=-1)-^5E_g(2)(MS=0)	+2.6-120.5i	$^5T_{2g}$(2)(MS=0)-^5E_g(2)(MS=-1)	-2.6-120.5i
$^5T_{2g}$(2)(MS=0)-^5E_g(2)(MS=1)	+2.6-120.5i	$^5T_{2g}$(2)(MS=1)-^5E_g(2)(MS=0)	-2.6-120.5i
$^5T_{2g}$(2)(MS=1)-^5E_g(2)(MS=1)	-0.0+98.3i	$^5T_{2g}$(2)(MS=1)-^5E_g(2)(MS=2)	+2.1-98.4i
$^5T_{2g}$(2)(MS=2)-^5E_g(2)(MS=1)	-2.1-98.4i	$^5T_{2g}$(2)(MS=2)-^5E_g(2)(MS=2)	-0.0+196.5i
$^5T_{2g}$(3)(MS=-2)-^5E_g(1)(MS=-2)	+0.0+263.2i	$^5T_{2g}$(3)(MS=-2)-^5E_g(1)(MS=-1)	-59.0-108.7i
$^5T_{2g}$(3)(MS=-1)-^5E_g(1)(MS=-2)	+59.0-108.7i	$^5T_{2g}$(3)(MS=-1)-^5E_g(1)(MS=-1)	+0.0+131.6i
$^5T_{2g}$(3)(MS=-1)-^5E_g(1)(MS=0)	-72.2-133.2i	$^5T_{2g}$(3)(MS=0)-^5E_g(1)(MS=-1)	+72.2-133.2i
$^5T_{2g}$(3)(MS=0)-^5E_g(1)(MS=1)	-72.2-133.2i	$^5T_{2g}$(3)(MS=1)-^5E_g(1)(MS=0)	+72.2-133.2i
$^5T_{2g}$(3)(MS=1)-^5E_g(1)(MS=1)	+0.0-131.6i	$^5T_{2g}$(3)(MS=1)-^5E_g(1)(MS=2)	-59.0-108.7i
$^5T_{2g}$(3)(MS=2)-^5E_g(1)(MS=1)	+59.0-108.7i	$^5T_{2g}$(3)(MS=2)-^5E_g(1)(MS=2)	+0.0-263.2i
$^5T_{2g}$(3)(MS=-2)-^5E_g(2)(MS=-2)	-0.0+87.3i	$^5T_{2g}$(3)(MS=-2)-^5E_g(2)(MS=-1)	+3.2+76.6i
$^5T_{2g}$(3)(MS=-1)-^5E_g(2)(MS=-2)	-3.2+76.6i	$^5T_{2g}$(3)(MS=-1)-^5E_g(2)(MS=-1)	-0.0+43.7i
$^5T_{2g}$(3)(MS=-1)-^5E_g(2)(MS=0)	+3.9+93.8i	$^5T_{2g}$(3)(MS=0)-^5E_g(2)(MS=-1)	-3.9+93.8i
$^5T_{2g}$(3)(MS=0)-^5E_g(2)(MS=1)	+3.9+93.8i	$^5T_{2g}$(3)(MS=1)-^5E_g(2)(MS=0)	-3.9+93.8i
$^5T_{2g}$(3)(MS=1)-^5E_g(2)(MS=1)	-0.0-43.7i	$^5T_{2g}$(3)(MS=1)-^5E_g(2)(MS=2)	+3.2+76.6i
$^5T_{2g}$(3)(MS=2)-^5E_g(2)(MS=1)	-3.2+76.6i	$^5T_{2g}$(3)(MS=2)-^5E_g(2)(MS=2)	-0.0-87.3i
^5E_g(1)(MS=-2)-^5E_g(2)(MS=-2)	+0.0+30.7i	^5E_g(1)(MS=-2)-^5E_g(2)(MS=-1)	-11.6-9.9i
^5E_g(1)(MS=-1)-^5E_g(2)(MS=-2)	+11.6-9.9i	^5E_g(1)(MS=-1)-^5E_g(2)(MS=-1)	+0.0+15.3i
^5E_g(1)(MS=-1)-^5E_g(2)(MS=0)	-14.2-12.2i	^5E_g(1)(MS=0)-^5E_g(2)(MS=-1)	+14.2-12.2i
^5E_g(1)(MS=0)-^5E_g(2)(MS=1)	-14.2-12.2i	^5E_g(1)(MS=1)-^5E_g(2)(MS=0)	+14.2-12.2i
^5E_g(1)(MS=1)-^5E_g(2)(MS=1)	+0.0-15.3i	^5E_g(1)(MS=1)-^5E_g(2)(MS=2)	-11.6-9.9i
^5E_g(1)(MS=2)-^5E_g(2)(MS=1)	+11.6-9.9i	^5E_g(1)(MS=2)-^5E_g(2)(MS=2)	+0.0-30.7i

Notes and references

1 B. A. Finney, S. R. Chowdhury, C. Kirkvold and B. Vlaisavljevich, *Phys. Chem. Chem. Phys.*, 2022, **24**, 1390–1398.