10.1071/CH12104_AC

Australian Journal of Chemistry 2012, 65(9), 1298-1304

Supplementary Material

The magnetic dipole origins of the $^3A_{2g} \rightarrow {}^3T_{2g}$ transition in Ni(II) doped MgO

Mark J. Riley,[A,C] *Jeremy Hall,*[B] *and Elmars R. Krausz,*[B]

Table S1 C_{4h} selection rules for the MLD transitions between the $^3A_{2g} \rightarrow {}^3T_{2g}$ Zeeman components. Light is propagated along z, the magnetic field is 5Telsa ||x and the ΔA value is calculated as the $\langle m_x \rangle^2 - \langle m_y \rangle^2$, where m_α is the magnetic dipole operator, where α is the polarisation direction of the light.

O_h			$\Gamma_3(^3T_{2g})$		$\Gamma_4(^3T_{2g})$			$\Gamma_5(^3T_{2g})$			$\Gamma_2(^3T_{2g})$
	C_{4h}		Γ_1	Γ_2	Γ_3	Γ_1	Γ_4	Γ_3	Γ_2	Γ_4	Γ_2
			8016.0	8016.3	8179.5	8182.2	8184.3	8565.9	8568.5	8571.2	8725.5
$\Gamma_5(^3A_{2g})$	Γ_3	0	+1.20	+0.38	-2.21	+1.01	0	-1.72	+0.89	0	+0.48
	Γ_2	5.3	0	-2.97	+1.09	0	+1.10	+0.87	-0.00	+0.86	-1.02
	Γ_4	10.6	+1.03	+0.37	0	+1.18	-2.18	0	+0.84	-1.75	+0.54

Table S2 C_{3i} selection rules for the MLD transitions between the $^3A_{2g} \rightarrow {}^3T_{2g}$ Zeeman components. Light is propagated along the (111) direction, the magnetic field is 5Telsa ||(-110) and the ΔA value is calculated as the $\langle m_{-110} \rangle^2 - \langle m_{11\text{-}2} \rangle^2$, where m_α is the magnetic dipole operator, where α is the polarisation direction of the light.

O_h			$\Gamma_3(^3T_{2g})$		$\Gamma_4(^3T_{2g})$			$\Gamma_5(^3T_{2g})$			$\Gamma_2(^3T_{2g})$
	C_{3i}		Γ_2	Γ_3	Γ_2	Γ_1	Γ_3	Γ_3	Γ_1	Γ_2	Γ_1
			8016.2	8016.2	8179.7	8181.9	8184.5	8565.9	8568.5	8571.2	8725.5
$\Gamma_5(^3A_{2g})$	Γ_3	0	+0.80	-1.55	+1.40	+0.37	-0.68	-1.72	+0.89	0	+0.49
	Γ_1	5.3	+0.72	+0.76	+0.40	-2.92	+0.33	+0.87	-0.00	+0.86	-1.03
	Γ_2	10.6	-1.41	+0.68	-0.79	+0.36	+1.52	0	+0.84	-1.75	+0.54

Figure S1

The ligand field energy levels of d^8 system as a function of a tetragonal distortion both without a) and with b) spin-orbit coupling. The tetragonal ligand field is quantified in terms of the splitting of the e_g orbitals $\Delta_e = E(x^2-y^2) - E(z^2)$ where a positive Δ_e is an elongation. The splitting of the t_{2g} orbitals, Δ_t, is set to $\Delta_t = ¼ \Delta_e$. Other ligand field parameters indicated in the figure have been taken from B.D. Bird, *et al.* Phys. Rev. B, **1972**, *5*, 1800. The symmetry labels are those from the D_{4h} point group. The heavy lines in a) indicate triplet states. The vertical line at Δ_e=0 is octahedral symmetry.

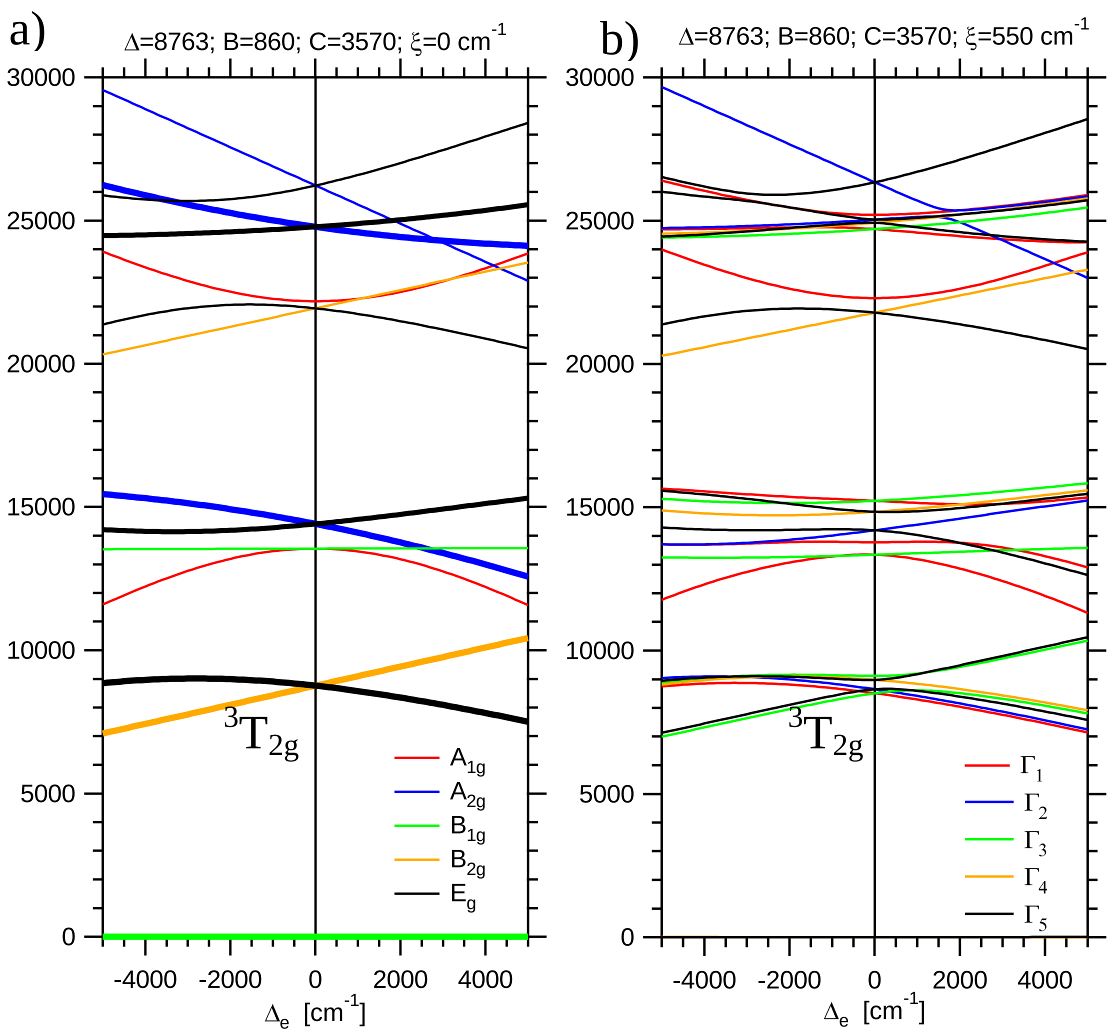

Figure s2

The ligand field energy levels of d^8 system as a function of a trigonal distortion both without a) and with b) spin-orbit coupling. The parameters are the same as given in Figure S1. The trigonal field is quantified by the distortion of all six ligands Δα from the 54.735..° they make with the trigonal axis. Positive values of Δα correspond to a trigonal elongation. The symmetry labels are those from the D_{3d} point group. The heavy lines in a) indicate triplet states. The vertical line at Δα=0 is octahedral symmetry.