In class exercise
Ch112
Nov. 10, 2016

Consider a d^2 ion in a *strong* tetrahedral ligand field.

1. Write down all possible electronic *configurations* for this ion and arrange them in order of increasing energy. Provide the total number of microstates for each electronic configuration.

e^2: 4×3/2 = 6 microstates

$t_2^1e^1$: 6×4 = 24 microstates

t_2^2: 6×5/2 = 15 microstates

2. For each configuration, a new set of *states* (or *terms*) will be obtained as the electrons start to feel each other's presence. The symmetry properties of these states can be determined by taking the direct products of the representations of the single electrons (*e.g.* $e_g \times e_g$). Reduce each electronic configuration found in part 1 to a sum of irreducible representations.

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$	xyz
A_2	+1	+1	+1	-1	-1	-	-	-
E	+2	-1	+2	0	0	-	$(2z^2-x^2-y^2, x^2-y^2)$	-
T_1	+3	0	-1	+1	-1	(R_x, R_y, R_z)	-	$[x(z^2-y^2), y(z^2-x^2), z(x^2-y^2)]$
T_2	+3	0	-1	-1	+1	(x, y, z)	(xy, xz, yz)	(x^3, y^3, z^3) $[x(z^2+y^2), y(z^2+x^2), z(x^2+y^2)]$

T_d	E	C_3	C_2	S_4	σ_d	
$t_2 \times t_2$	9	0	1	1	1	$A_1 + E + T_1 + T_2$
$t_2 \times e$	6	0	-2	-1	1	$T_1 + T_2$
$e \times e$	4	1	4	0	0	$A_1 + A_2 + E$

3. The total number of microstates must be conserved. Assign spin multiplicities for each state found in part 2.

T_d	
$e \times e$	${}^1A_1 + {}^3A_2 + {}^1E$
$t_2 \times e$	${}^1T_1 + {}^1T_2 + {}^3T_1 + {}^3T_2$
$t_2 \times t_2$	${}^1A_1 + {}^1E + {}^3T_1 + {}^1T_2$

(see class notes)