j-j Coupling

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heavy atoms (large Z)

→ spin-orbit coupling for each electron becomes large

spin-orbit coupling of 1e	>	Coulomb energy of 2 electrons

L, S are not good quantum numbers

instead: $\vec{j}_i = \vec{l}_i + \vec{s}_i$

$$\vec{J} = \sum_{i=1}^{Z} \vec{j}$$

opt. dipole selection rules for j-j-coupling

$\Delta J = 0, \pm 1$ but not $J = 0 \rightarrow 0$

Optical selection rules (Dipole transitions)

$\Delta J = 0, \pm 1$ but NOT $J = 0 \rightarrow 0$

$\Delta m_J = 0, \pm 1$ but NOT $m_J = 0 \rightarrow 0$ for $\Delta J = 0$

$\Delta S = 0$ } for the atom

$\Delta L = 0, \pm 1$ }

$\Delta l = \pm 1$ for the electron

} LS coupling

$\Delta j = 0, \pm 1$ " jj coupling

Hund's rules

1. Full shells $s^2, p^6, d^{10}, \ldots$ $S=0, L=0, J=0$
2. lowest energy with max. multiplicity $2S+1$
3. for a given mult., lowest energy for largest L
4. outermost shell
   $\frac{1}{2}$ full or less: lowest energy for <u>minimal</u> J
   more than $\frac{1}{2}$ full: maximal J

$2e^-$: $S=0$ singlett
$S=1$ triplett

$3e^-$: $S=\frac{1}{2}$ doublett
$S=3/2$ quartett

$4e^-$: $S=0,1$
$S=2$ quintett

$5e^-$: $S=\frac{1}{2}, 3/2$
$S=5/2$ sextett