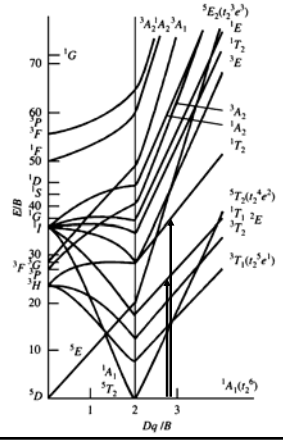
Predicting Ligand Field Transitions for $[Co(en)_3]^{3+}$

- Determine Correct Tanabe-Sugano Diagram to use
- Need
  - Electronic configuration (d^6)
  - High or low spin (low, how?)
- Look for Spin-Allowed Transitions first, if none find least Spin-Forbidden



- Predict six spin-allowed transitions
- Only two lowest in energy seen
  - $^1A_{1g} \rightarrow {}^1T_{1g}$
  - $^1A_{1g} \rightarrow {}^1T_{2g}$

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- Are Transitions Orbitally Allowed?
- In O_h
  - Electric dipole transforms as T_{1u}; all transitions are parity forbidden (intensity?)
  - Magnetic dipole as T_{1g}; calculate triple <u>direct products</u>

$A_{1g} \times T_{1g} \times T_{1g} \subset A_{1g}$

$A_{1g} \times T_{1g} \times T_{2g} \not\subset A_{1g}$

$^1A_{2g} \rightarrow {}^1T_{1g}$ allowed in CD

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- Point Group is really D_3
- Use Correlation Table to transform Term Symbols in O_h to D_3
- Predicts
  - $^1A_{1g} \rightarrow {}^1T_{1g}$ splits into $^1A_1 \rightarrow {}^1A_2$ and $^1A_1 \rightarrow {}^1E$
  - $^1A_{1g} \rightarrow {}^1T_{2g}$ splits into $^1A_1 \rightarrow {}^1A_1$ and $^1A_1 \rightarrow {}^1E$
- Using same Method find all are allowed in both CD and ABS

Experimental