

**Chemistry 5.04 (F04)**  
**Problem Set 8**

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Due Monday, 29 November

1. The octahedral and tetrahedral ligand fields may be generalized in a cubic field. As derived in class and discussed in the foregoing problem, the potential energy for a cubic crystal field is:

$$V_{cubic}(r_i) = A_{0,0}r^0Y_{0,0} + A_{4,0}r^4 \left[ Y_{4,0} + \sqrt{\frac{5}{14}}(Y_{4,+4} + Y_{4,-4}) \right]$$

In class, the general expression was applied to the specific case of six ligands in an octahedral crystal field (i.e., on the face of a cube). Derive the case for four ligands in a tetrahedral field (i.e. opposite corners of a cube). You should obtain the answer shown on pg 25.7 of the notes.

2. (a) Determine the terms of a  $d^3$  ion.  
(b) Determine the  $\Psi(L,2,S,1/2)$  eigenfunctions for the  ${}^2H$  term.  
(c) Determine the energy of the  ${}^2H$  term.