

**(I) In the Protein Data Bank ([www.rcsb.org/](http://www.rcsb.org/)) find a protein containing a “zinc finger” and open the structure in Jmol.**

1. How is the zinc ion stabilized in the structure (make a picture of the metal center and the neighboring ligands)?
2. What type of secondary structures are bound to it?
3. What is the function of the zinc finger?

You may use the following Jmol commands:

```
$ color structure  
$ select within (5, zinc)  
$ wireframe 25%  
$ color cpk  
$ select zinc  
$ cpk 100%  
$ write filename.png
```

**(II) Use Jmol to look at the metal complex in the catalase enzyme (PDB entry 1GWE).**

1. What type of metal complex is embedded in the catalase and how is it bound to the polypeptide (make a picture of the metal complex and the neighboring ligands)?
2. What is the coordination of the metal center (octahedral, tetragonal, or square-pyramidal)? Does the metal ion have a Jahn-Teller distortion (measure the metal-ligand distances).
3. Taking into account the presence (or absence) of Jahn-Teller distortion in what oxidation state could be the metal in this complex?

**(III) Transition metals**

1. Write the d-electron configuration for the ions  $\text{Cr}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Ni}^{3+}$ ,  $\text{Mn}^{3+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Cr}^{2+}$ .
2. Which of the ions above will have Jahn-Teller distortion in octahedral coordination?
3. For which of these ions high-spin complexes are possible?
4. What is the oxidation state of the manganese ion in the complexes  $[\text{Mn}(\text{H}_2\text{O})_5(\text{OH})]^{2+}$  and  $[\text{MnO}_4]^-$ ?