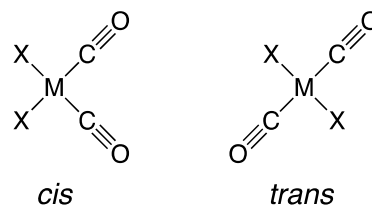


## Symmetry and Group Theory – Exercise Set 6

6.1) Prove the so-called exclusion rule, *i.e.* that in a centrosymmetric molecule no IR active mode is also Raman active and vice versa.

6.2) What are the IR and Raman active modes of the CO stretches in  $\text{MnBr}(\text{CO})_5$ ?

6.3) How can you spectroscopically distinguish the *cis* and *trans* isomers of the  $\text{MX}_2(\text{CO})_2$  complex?



6.4) Determine the symmetry species of the normal modes of  $\text{PF}_5$ . Which modes are IR and Raman active?

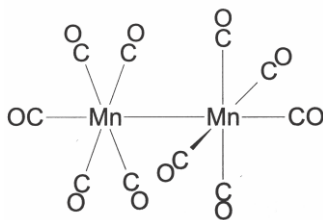
### Homework

6.5) A molecule  $\text{X}_3$  can potentially adopt two different structures, (a) an equilateral triangle (all X–X bond lengths are identical) or (b) an isosceles triangle (two X–X distances are identical, but different from the third).



How can one use IR or Raman spectroscopy to decide whether the molecule adopts structure (a) or structure (b)?

6.6) For the following carbonyl complex, determine the symmetry species of the CO stretch vibrations. Which vibrations are IR or Raman active?



Note that looking along the Mn-Mn axis, the CO ligands on the two metal centers appear staggered.

6.7) For the carbonyl complex shown below, determine the symmetry species of the CO stretch vibrations. Which vibrations are IR active and which are Raman active?

