20.11 (a) ^3F (b) ^5D (c) ^6S

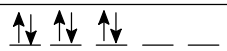
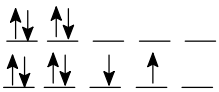
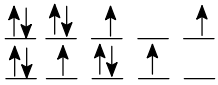
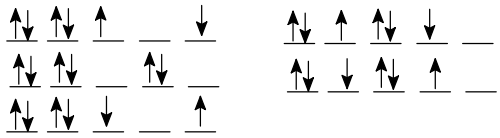
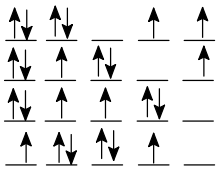
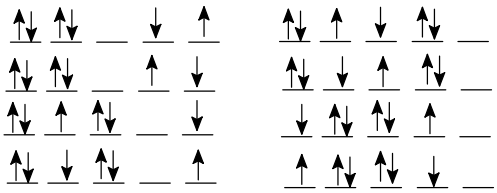
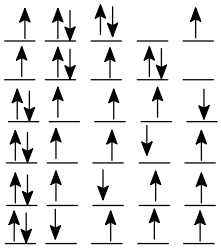
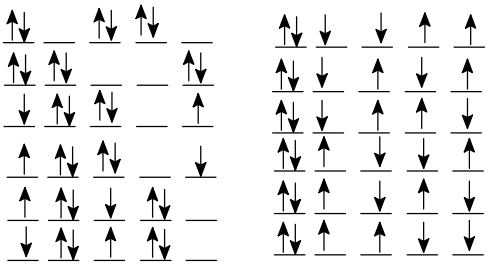
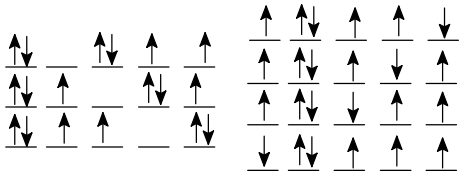
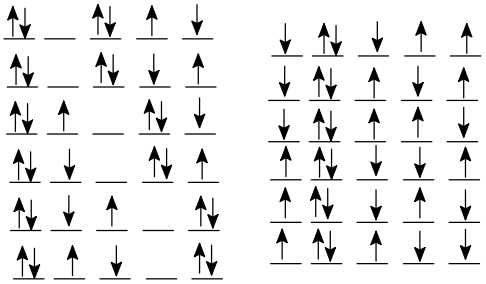
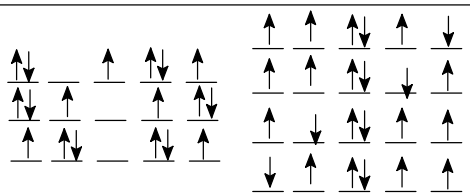
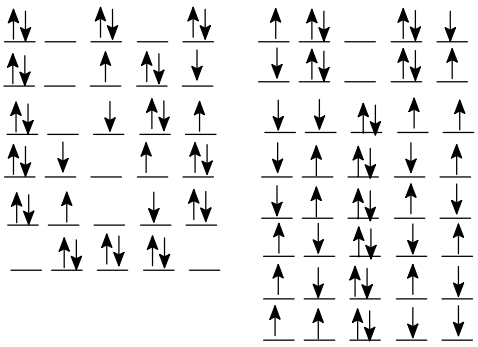
20.15 This is a d^8 system, therefore, the lowest energy transition will be Δ_O (the ground state and first lines are not curved).
(a) 8500 cm^{-1} (b) 10 750 cm^{-1}

20.16 This is a d^6 system. It must be low spin because the high spin case (small Δ_O/B) has only one spin-allowed transition. By the description of the peak intensities, one "very weak" and two "moderate," it would appear that there are two spin-allowed transitions. If that is the case, the very weak peak is likely $^5T_{2g} \leftarrow {}^1A_{1g}$, (a slightly arbitrary choice, rather than excitation to either of the triplet states) while the two moderate peaks are $^1T_{1g} \leftarrow {}^1A_{1g}$, and $^1T_{2g} \leftarrow {}^1A_{1g}$,

20.23 Since Mn^{7+} is d^0, there are no *d-d* transitions! However, it does mean that there is a filled orbital below it, and if we make the assumption (as we always do) that transitions arise from the ground state HOMO, the two transitions must be LUMO (e) ← HOMO and LUMO + 1 (t_2) ← HOMO. Thus, the energy Δ_T is the difference between the two transitions, or 32200-18500 = 13700 cm^{-1}.

Question: find the microstates and terms for a *d*6 configuration.

This is the "$^{1}/_{4}$ table" for the microstates:

	2	1	0
6			
5			
4			
3			
2			
1			
0			

highest $M_S = 2$, its largest $M_L = 2$ ==> ^{5}F term (25 terms, or 9 from our part-table)
next highest $M_S = 1$, its largest $M_L = 5$ ==> ^{3}H term (33 terms, or 12 from our part-table)
next highest $M_S = 1$, its largest $M_L = 4$ ==> ^{3}G term (27 terms, or 10 from our part-table)
next highest $M_S = 1$, its largest $M_L = 3$ ==> ^{3}F term (21 terms, or 8 from our part-table)
next highest $M_S = 1$, its largest $M_L = 3$ ==> another ^{3}F term (21 terms, or 8 from our part-table)
next highest $M_S = 1$, its largest $M_L = 2$ ==> ^{3}D term (15 terms, or 6 from our part-table)
next highest $M_S = 1$, its largest $M_L = 1$ ==> ^{3}P term (9 terms, or 4 from our part-table)
next highest $M_S = 0$, its largest $M_L = 6$ ==> ^{1}I term (13 terms, or 7 from our part-table)
next two terms are both $M_S = 0$, $M_L = 4$ ==> two ^{1}G term (9 terms each, or 10 total from our part-table)
next highest $M_S = 0$, its largest $M_L = 3$ ==> ^{1}F term (7 terms, or 4 from our part-table)
next highest $M_S = 0$, its largest $M_L = 2$ ==> ^{1}D term (5 terms, or 3 from our part-table)
last remaining terms (2 of them) are both ^{1}S

this makes 14 terms, and a total of 196 microstates (if I added this all up correctly!)

Question: Number of I-F vibrations in T-shaped IF_3.

Solution: there are 4(3) = 12 degrees of freedom, also 12 arrows on the 4 atoms.

FOR C_{2v}: Reducible representation (assuming the molecule lies in the *xz* plane):

$E = 12$ $C_2 = -2$ $\sigma_v = 4$ $\sigma_v' = 2$

Using the reduction formula should give the irreducible representations as,

$4\ A_1 + A_2 + 4\ B_1 + 3\ B_2$ (= 12 modes)

Removing $A_1 + A_2 + 2\ B_1 + 2\ B_2$ (for three rotation and three translation modes) leaves:

$3\ A_1 + 2\ B_1 + B_2$ (= six vibrations)

All are IR active, all are Raman active, all lines match up.