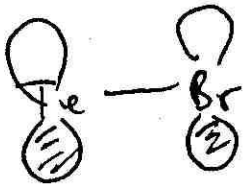
Problem Set 13 (It's almost summer!)

1. One point which I hope has been made clear in this course, is that one way (perhaps the only way) we know a theory is on to something useful is when it can make verifiable predictions. As an example let us consider $TeBr_6^{2-}$, a known ion.

(a) This compound by electron counting has 7 pairs of e^- around the central atom. Draw what you expect the structure of $TeBr_6^{2-}$ might be using VSEPR reasoning.

(b) Now consider this ion from an MO viewpoint. Assume (as we discussed in class) that the s orbitals for Te and Br are fairly inert. Note also that heavy main group atoms do not form π bonds with eachother. ∴ Assume



interaction can be ignored.

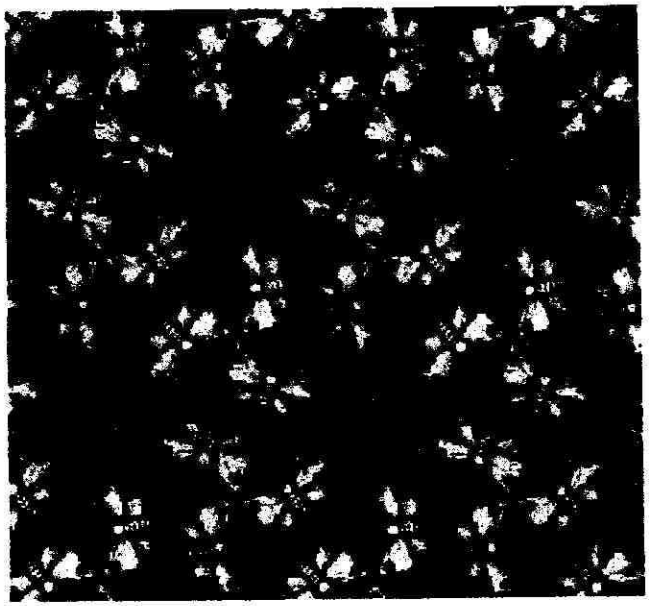
Draw an MO diagram for $TeBr_6^{2-}$ using these assumptions. for $TeBr_6^{2-}$ in an octahedral geometry. (Assumes orbitals are inert!)

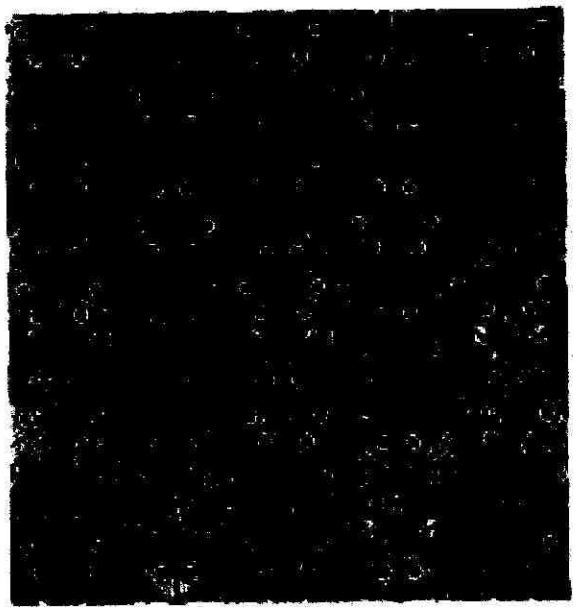
Assume $E(Te\ p) = -13$ eV and $E(Br\ p) = -14$ V

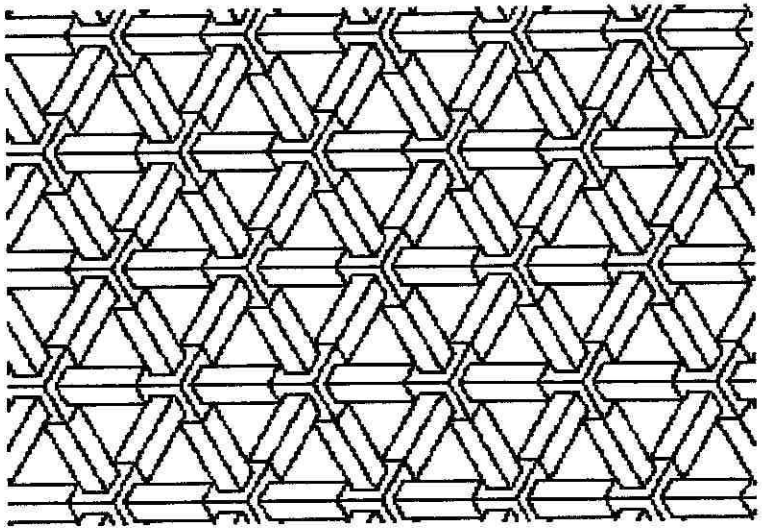
Show $TeBr_6^{2-}$ in the octahedral geometry has all bonding and non-bonding orbitals might filled and all antibonding orbitals empty & ∴ $TeBr_6^{2-}$ be expected by simple MO theory to be of octahedral symmetry.

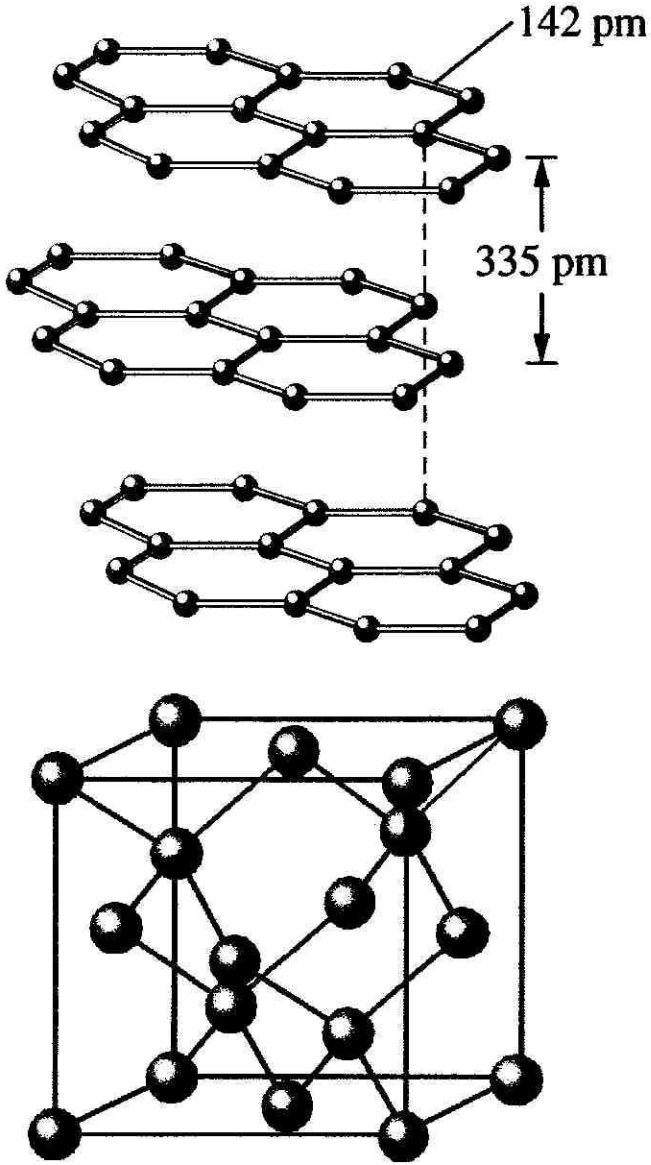
The structure of $TeBr_6^{2-}$ can ∴ be used to distinguish the relative merits of the MO and VSEPR pictures

2. Find the primtive unit cells of each pattern . How many faces, butterflies, animals or rods are there in each unit cell?



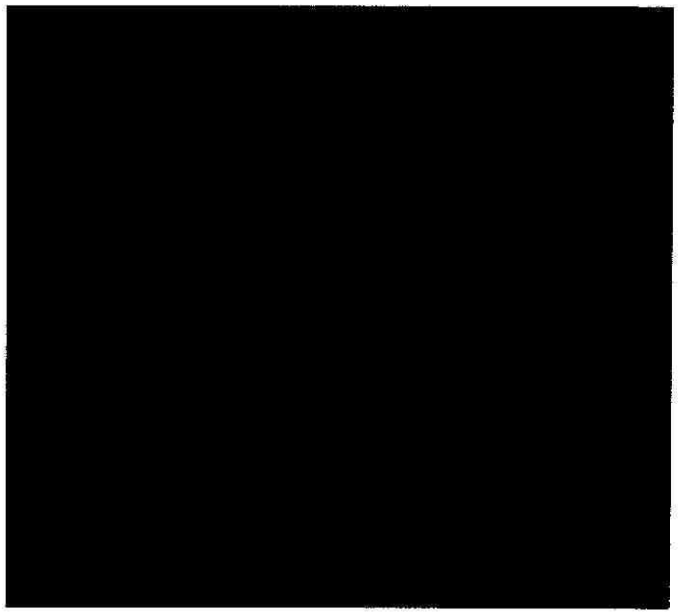


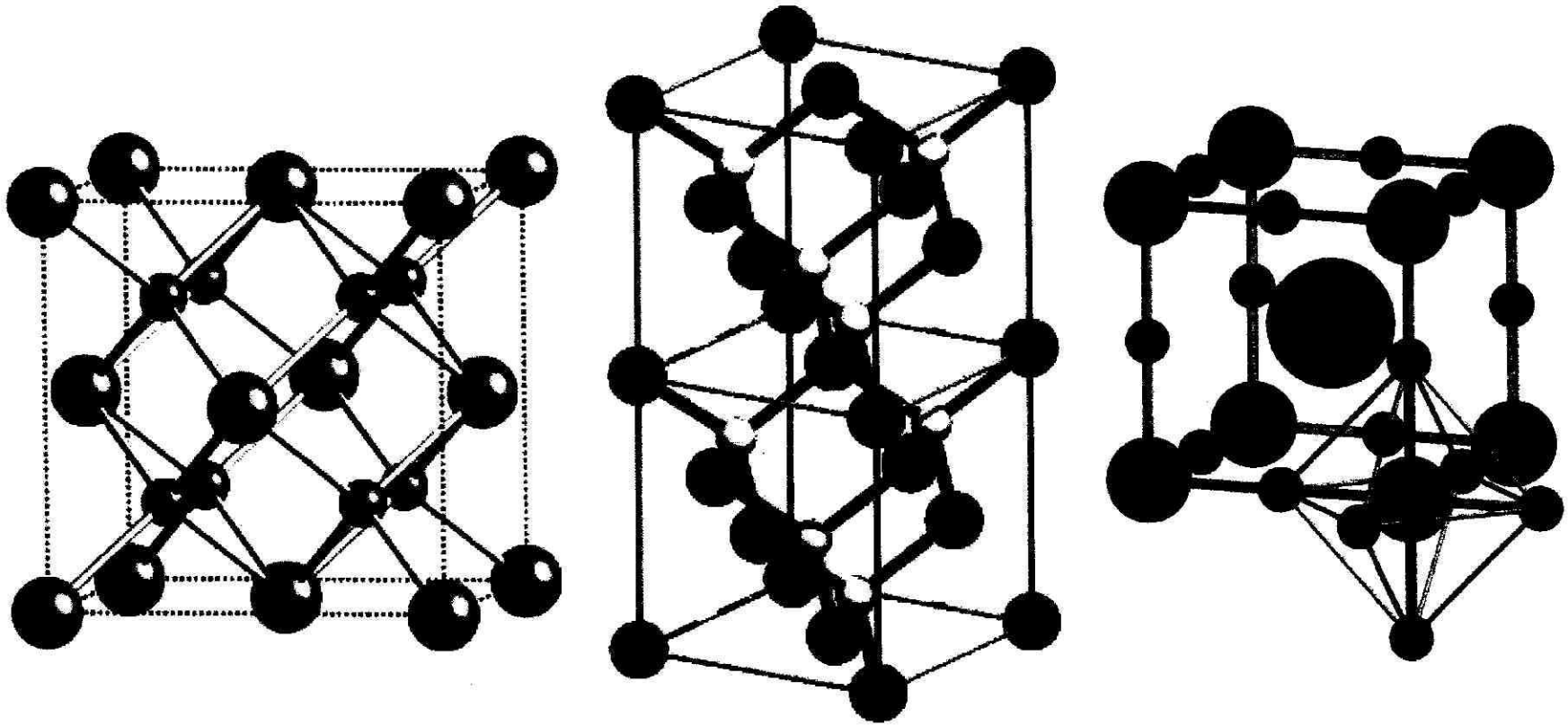




3. The pictures on this page are three of the known forms of carbon: diamond, graphite and fullerene. Which picture goes with which type of carbon? In the picture on the left find a unit cell with three orthogonal axes.

How many carbon atoms are there in each unit cell? For the picture on the bottom right is there a relationship between this structure and fcc, bcc or hcp? If so to which one, and what is the relationship? Finally, for each of the three types, which localization scheme sp, sp^2 or sp^3 is most appropriate?





4. Find the number of (a) green and red balls (b) white, blue and red balls and © red, blue and aqua balls per unit cell. What is the coordination environmment of each atom (consider only nearest neighbors)? How many first nearest neighbors does each atom have? What are the stoichiometries of each crystal? And finally, and this is hard, guess for each crystal structure what true compound might adopt these structures. Specify here exact elements.