Questions are based on the following article:


Due date: 12/20/2010

1. A range of 1,3-di(metallocenyl)allylium salts are reported by Barlow et al. where the metallocene moiety of the molecule stabilizes the carbocationic charge through resonance with the [(η⁶-fulvene)- (η⁵-cyclopentadienyl)metal] cation structures (re: Fig. 2a). It was determined that structures 1⁺ and 2⁺ are highly symmetrical not only in their design but also in their electronic properties. In contrast, complex 3⁺ shows asymmetric electronic properties.

Using the experimental and theoretical data, as well as the authors discussion of said data, in your own words discuss the following:

   a) Similarities between structures 1⁺ and 2⁺
   b) Differences between structures 1⁺ and 2⁺
   c) Similarities between structures 1⁺ and 3⁺
   d) Differences between structures 1⁺ and 3⁺

Notes:

You do not have to discuss every single technique for each comparison, only those you consider relevant.

Any conclusions made from a single set of data must be backed up by at least one more experiment.

I have not stated which particularly salts to discuss. Therefore when comparing two structures be sure to compare the same salt derivatives, e.g. UV-vis of [1][PF₆] vs [2][PF₆]. It is ok to compare a different salt as part of the same answer when discussing a different technique, e.g. electrochemistry of [1][BF₄] vs [2][BF₄].