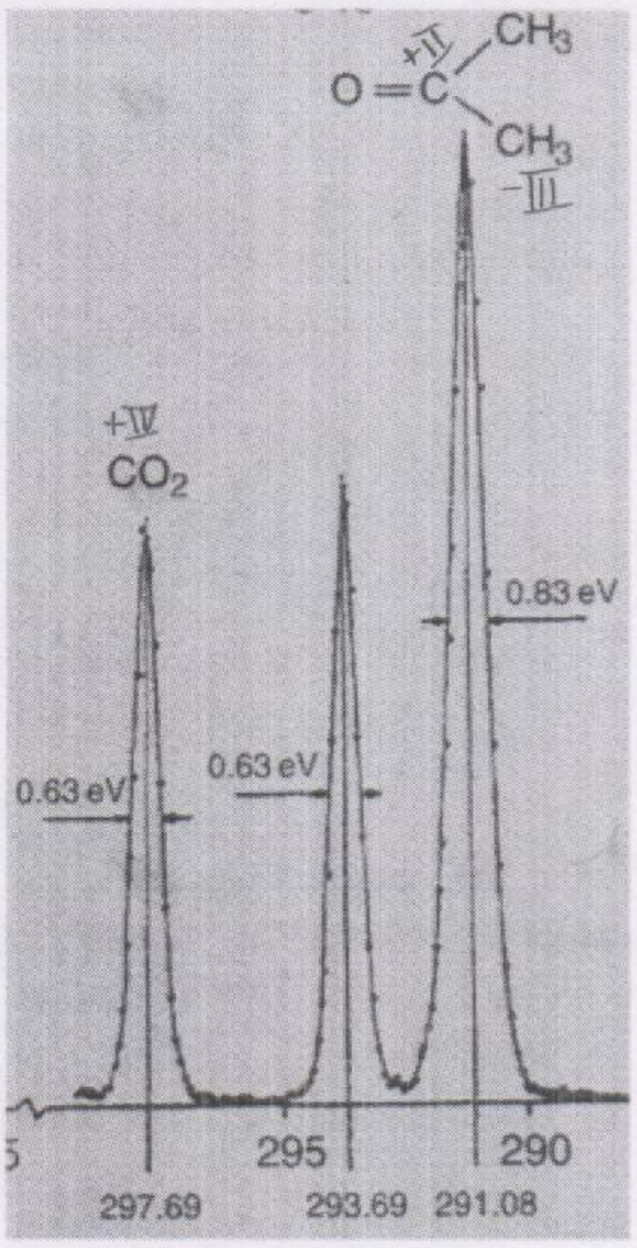
CH314 – Structural Analysis
Part III : X-ray Tools

Exercise 4, Dec 14

1) Below you see a photoelectron spectrum of a carbon dioxide / acetone gas mix converted to binding energies.



a) Carbon K-edge

b) 297,69 eV
→ Carbon in CO_2 (Oxidation state +IV)

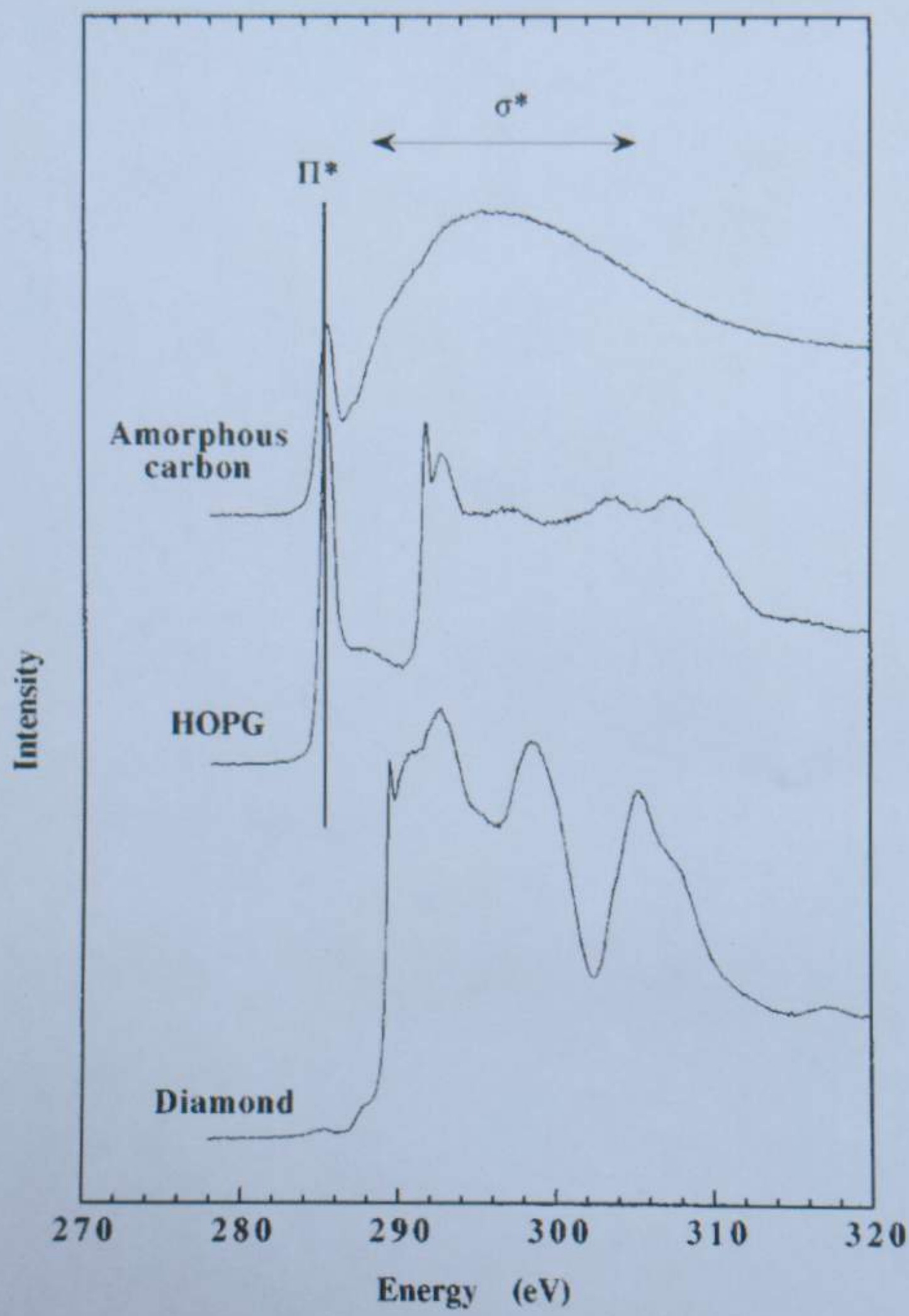
293,69 eV
→ Carbon in acetone with oxidation state +II

291,08 eV
→ Carbon in acetone with oxidation state -III

a) To which element does the spectrum belong? Which core level is targeted?
b) Which peaks belong to which gas? Explain the middle peak.
c) Describe the peaks from the right to the left in terms of their chemical shift.

c) From the right to the left the oxidation state of the carbon increases and therefore, the chemical shift increases as well.

2) The figure below displays the X-ray absorption near-edge (XANES) spectra of fully sp^3 hybridized diamond, sp^2 hybridized graphite, and amorphous carbon.



a) Which electronic transitions are we observing?
b) Assign the resonances and fill in the circles.
c) Which spectra belongs to which form of carbon? Fill in the boxes and explain.

a) Carbon K-edge
→ Carbon 1s electrons to vacant σ^* and π^* valence orbitals