Q6.32 The catalytic activity of palladium–gold alloys for cyclotrimerization of acetylene (ethyne) to benzene is thought to depend on the size of the Pd-atom clusters present in the surface layer. A series of disordered alloys with different Pd compositions was prepared by evaporating a gold film onto a palladium substrate and annealing at various temperatures to intermix the two metals. The relative numbers of isolated Pd atoms, Pd-atom pairs and Pd-atom triplets at the surface could then be estimated by adsorbing CO and determining the amounts of linearly, 2-fold bridge- and 3-fold bridge-bonded species using EELS (Figure 6.4). Select from the key the *two* statements that are **incorrect**.

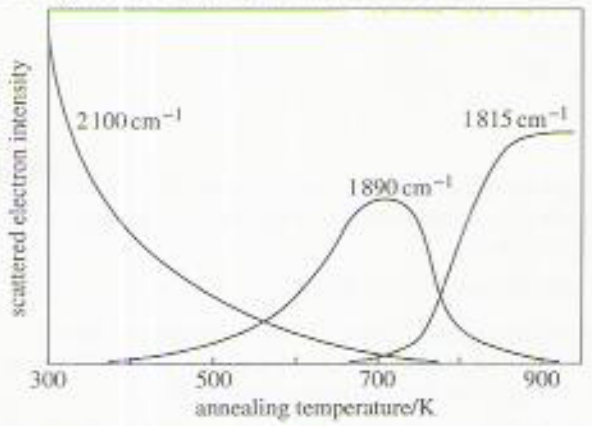

Figure 6.4 Variation of EELS peak intensities for CO species adsorbed on Au–Pd alloys annealed at various temperatures.

KEY for Q6.32

A An increase in the electron density in the $2\pi^*$ LUMO (lowest unoccupied molecular orbital) in adsorbed CO will lower the force constant of the C—O bond.

B The C—O vibrational frequency in CO adsorbed on Pd varies with adsorption site due to differing degrees of back-donation of charge from the metal conduction band to the 5σ HOMO (highest occupied molecular orbital) in the adsorbate.

C The surfaces of Au–Pd alloys annealed at temperatures below 500 K contain a significant number of Pd-atom triplets.

D The number of Pd-atom triplets in Au–Pd alloy surfaces increases with annealing temperature beyond 700 K to reach a plateau at 900 K.

E In Au-Pd alloy surfaces annealed at temperatures below 500 K, palladium is predominantly in the form of isolated atoms surrounded by Au atoms.

F With increasing annealing temperature, the number of Pd-atom pairs in Au–Pd alloy surfaces increases to a maximum and then falls again.

Q6.33 The orientation of the molecular plane of adsorbed benzene with respect to a Ni(110) substrate can be determined by monitoring the π-electron system in the adsorbate. Select from the key the *one* technique that would be *most* suitable for carrying out this experiment.

KEY for Q6.33

A Work function measurement

B Low-energy electron diffraction (LEED)

C Surface extended X-ray absorption fine structure (SEXAFS)

D X-ray photoelectron spectroscopy (XPS)

E Ultraviolet photoelectron spectroscopy (UPS)

F Auger electron spectroscopy (AES)

Q6.34 Following benzene adsorption on Ni(110), heating to 630 K causes decomposition of the adsorbate to leave the surface covered by an ordered carbon layer with the unit mesh shown in Figure 6.5. Select from the key the *two* statements that are **correct**.

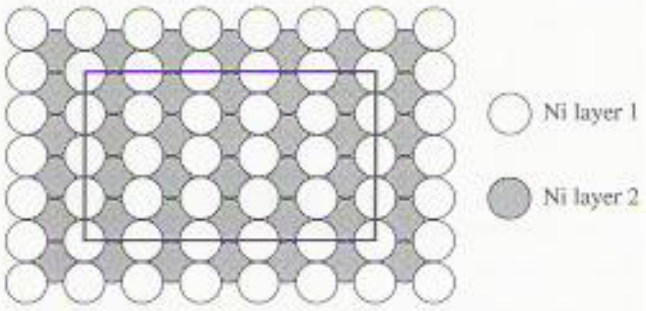

Figure 6.5 The unit mesh of the carbon layer formed on Ni(110) by decompositon of adsorbed benzene. Note that the positions of the adsorbed carbon atoms are *not* shown.

KEY for Q6.34

A In terms of the $(m \times n)$ notation, the carbon structure is Ni(110)(4×5).

B In terms of the $(m \times n)$ notation, the carbon structure is Ni(110)(5×4).

C In terms of the $(m \times n)$ notation, the carbon structure is Ni(110)c(5×4).

D The fractional surface coverage of carbon must be 0.05.

E The fractional surface coverage of carbon must be 0.10.

F There is insufficient information to determine the fractional surface coverage of carbon.

Q6.35 Select from the key the *two* statements that are **incorrect**.

KEY for Q6.35

A The $L_1M_1M_{2,3}$ Auger transition in a vanadium atom involves electrons in the 2s, 3s and 3p levels.

B Because vibration of the N_2 molecule is not accompanied by a change in dipole moment, adsorbed dinitrogen, N_2(ad), is not detected by infrared reflection absorption spectroscopy.

C Adsorbed dinitrogen, N_2(ad), is detectable by electron energy loss spectroscopy when the scattering is observed in the specular direction.

D Extended X-ray absorption fine structure provides information on the coordination shells surrounding the absorbing atom.

E Scanning tunnelling microscopy and scanning Auger electron spectroscopy are comparable in their sensitivity to the chemical identity of different species at a surface.