ISEELS

Inner Shell Electron Energy Loss Spectroscopy

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INTRODUCTION TO ISEELS

- ISEELS provides systematic analysis of K shell excitation spectroscopy of gas phase molecules containing B,C,N,O & F.

- It correlates the position of the characteristic K shell excitation, its features, the б shape resonance and the intra molecular bond length.

- The position of the shape resonance (w.r.t. 1s ionization) vary linearly with the inter nuclear distances.

- In ISEELS, the structures above the excitation threshold of a core e^- arises from the intramolecular scattering processes of the created photo electron.

BASIC SPECTRUM

Molecules with unoccupied π* orbital will have 1s $\longrightarrow$ π* excitation.

The second molecular resonance observed at higher energy is referred to as the б Shape resonance.

$(1s^{-1}, б^*)$

This arises due to the back & forth scattering of the photo electron resonantly along the inter nuclear axis between the absorbed atom and its neighbour.

EXPERIMENTAL APPARATUS

- Spectra are produced by inelastic scattering of electrons by gases (at 10^{-2} pa)

- Scattering angles will lie between 1 – 2° creating final electron energy of 2.5 keV

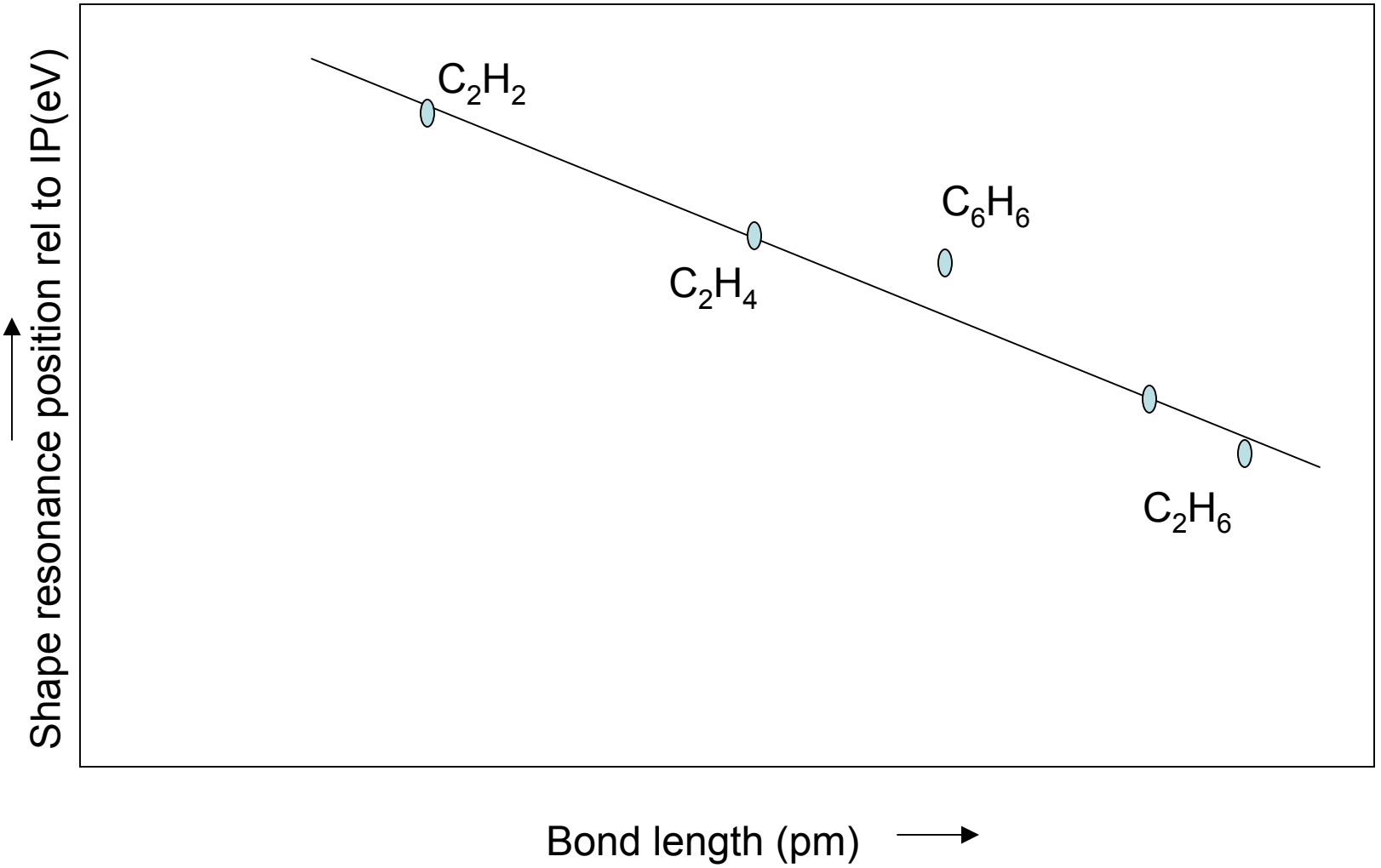
- Resolution is limited to 0.7eV & is determined by the thermal spread of e^- energies in the unmonochromated incident beam.

ISEELS developed in McMaster university, Canada

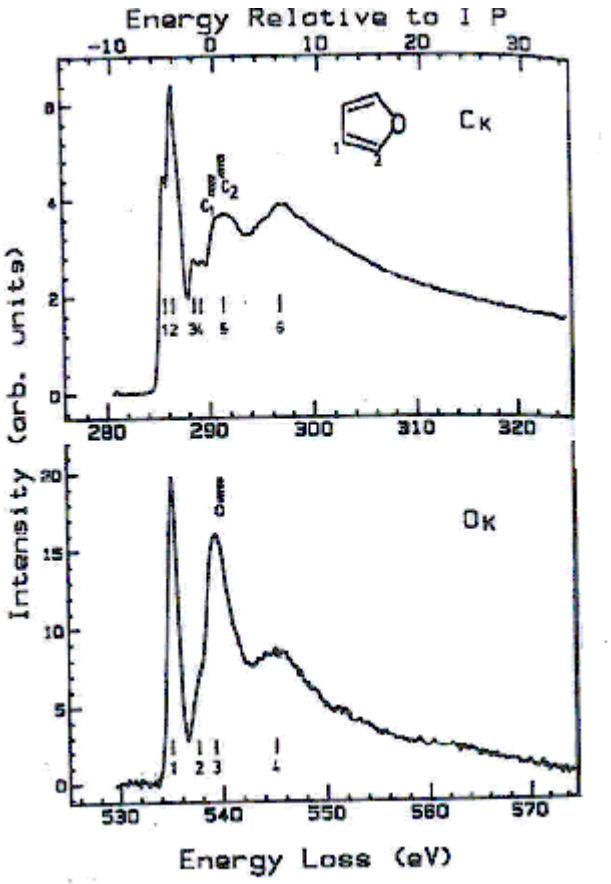
- Absolute energy scales were determined by calibrating the spectra relative to
  C 1s $\longrightarrow$ π* in
  CO (287.40 eV), C_2H_4 (284.7eV) or CO_2 (290.7 eV).

  N 1s $\longrightarrow$ π* in N_2 (401.10 eV).
  O 1s $\longrightarrow$ π* in CO (534.12 eV).

Relationship between position of shape resonance and bond distance.



Carbon K shell spectrum of furan



The Carbon & Oxygen K-Shell ISEELS spectra of gaseous furan at 0.7 eV FWHM resolution by e^- energy loss with 2.5 keV final electron energy.

- First 4 features are attributed to 1s $\longrightarrow \pi^*$ transitions.
- Two diff C environments and 2 unoccupied π* levels which lead to 4 possible C 1s $\longrightarrow$ π* transitions with

  0.86 eV separation between 1—2

  0.80 eV separation between 3—4
- This may represent the separation of C1s leve

  (1.2 eV) or $3b_1$ and $2a_2$ π* levels(1.8ev)
- (1.2 eV) ~ close to 0.83 so it reflects the separation of core levels rather than π* levels.
- The avg 0.83 eV is the difference in the IP's of

  C_1 's and C_2 's

  $3b_1$ orbital has greater density on C_2 and O

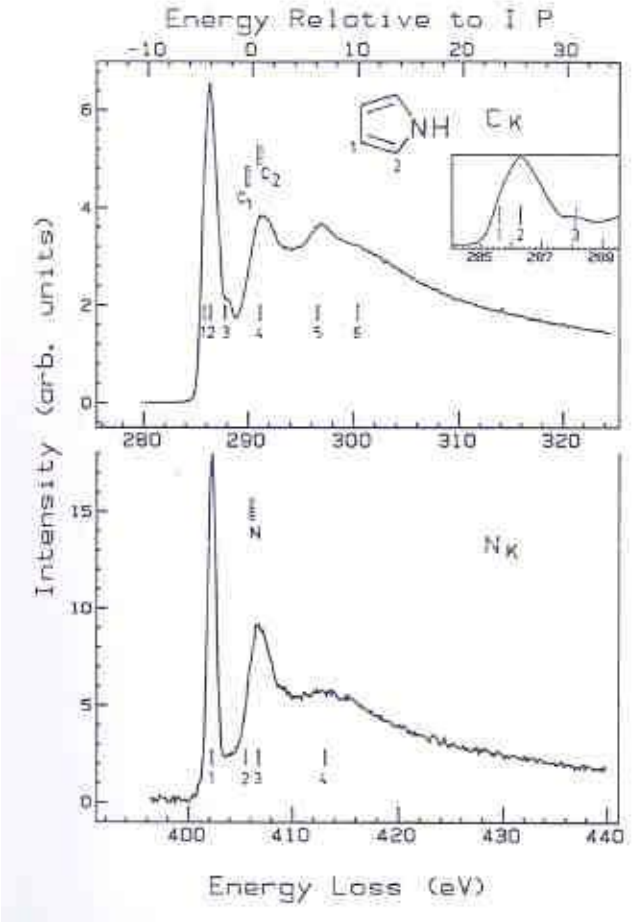
  $2a_2$ orbital has roughly equal density on C_1 and C_2 atoms.

- Features 5 and 6 correspond to C1s---- б* transition
- Furan has two diff bond C-C lengths (136.1, 143.1)

and one O-C bond length (136.2) so bond length correlation predicts shell spectrum around 10.6,6.8,2.8 eV above IP but only two continuum resonances are observed at 0.4 & 6.0 eV above IP because furan is aromatic.

Oxygen K-shell spectrum of FURAN

Feature	Energy eV	Term value eV	Assignment
1	535.3	4.7	π*(3b1)
2	537.6	2.4	3p or(2a2)
0IP	540.0		
3	539.4	0.6	б*(C----O)
4	545.3	-5.3	б*(C---O)



The carbon and Nitrogen K-shell ISEELS spectra of pyrrole recorded by electron energy loss.

Energies & term values for features observed in carbon 1s K-Shell spectra of pyrrole

Feature	Energy eV	Term value eV		Assignment	
		C_1	C_2	C_1	C_2
1	285.6	4.2		$\pi^*(3b_1)$	
2	286.3		4.5		$\pi^*(3b_1)$
3	288.1	2.2		$\pi^*(2a_2)$	$\pi^*(2a_2)$
C_1IP	289.8				
C_2 IP	290.8				
4	291.3	-1.0		б*(C---N)	
5	296.8	-6.5		б*(C---C)	
6	300.5(8)	-10		б*(C═C)	

Energies & term values for features observed in Nitrogen 1s K-Shell spectra of pyrrole

Feature	Energy (eV)	Term value (eV)	Assignment
1	402.3	3.8	$\pi^*(3b_1)$
2	405.9	0.2	4p
N IP	406.1		
3	406.7	-0.6	б*(C---N)
4	413.4	-7.3	б*(C---N)

References

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