

Interpretation of CID Mass Spectra

I. API BASICS FOR THE INTERPRETATION OF CID MASS SPECTRA

1. Interpretation Introduction and Isotopes.
2. Masses of Isotopes and Compound MW'S.
3. Ions: Even vs. Odd Electron; Positive vs. Negative Ions.
4. Mass Resolution, Nitrogen Rule and Rings plus Double Bonds.

II. COLLISION-INDUCED DISSOCIATION

5. Collision-Induced Dissociation.
6. Tandem Mass Spectrometry and Chemical Bonds.
7. CID Thermodynamics.
8. Precursor Ions and Compound Molecular Weight.

III. INDUCTIVE CLEAVAGE AND PRODUCT ION STABILITY

9. The Nitrogen Rule.
10. Favored Ionization Sites.
11. Cation Stabilization.
12. Inductive Cleavage.
13. Molecular Weight Determination.

IV. SINGLE BOND CLEAVAGES

14. Types of Bond Cleavages.
15. Product Ion Stability.
16. Stabilization Factors.
17. Stable Product Ions.
18. Lecture 4 Questions.

V. RING OPENING AND FRAGMENTATION

19. Ring Opening.
20. Retro Diels Alder Reaction.
21. Steroid Fragmentation.
22. RDA from more Complex Molecules.

VI. MULTIPLE BOND CLEAVAGES

23. Multiple bond Cleavages of Amines.
24. Alicyclic Hydrogen Rearrangements.
25. Oleandrin and Oleandrogenin.
26. N-alkyl Amine Fragmentation.
27. Deuteriated Amphetamine Scrambling.
28. Melamine, Sulfa Drugs and Triacyl Glycerides.

VII. HYDROGEN REARRANGEMENTS

29. Hydrogen Rearrangements / MS/MS Behavior of Even-Electron Ions.
30. Common Neutral Losses / Hydrogen Rearrangement Problems.
31. Relative Stability of Organic Cations.

VIII. CYCLISATIONS

32. Cyclization of Even-Electron Phthlate Cations.
33. Intramolecular Cyclization Reactions.
34. Structures for Carnitines.
35. Lecture 8 Questions.

IX. CID OF NEGATIVE IONS

36. CID of Negative Ions.
37. Problem – Loss of SO₂.
38. Problem – Loss of Phosphoric Acid.
39. CID of Negative Ions (Cont'd).
40. Lecture 9 Questions.

X. PEPTIDE FRAGMENTATION BEHAVIOR

41. Peptide Fragmentation Behavior.
42. Summary of Fragmentation Behavior and Other Examples.

XI. PROBLEM SOLVING OF CID MASS SPECTRA

43. Dexamethasone.

44. Problem – Succinyl Choline.

45. Problems – Reserpine and Tetrahydrolipstatin.