WHAT IS CLAIMED IS:

1. A method to determine the model-of-composition of a heavy petroleum or hydrocarbon samples comprising:

(a) obtaining molecular ions or pseudo molecular ions, such as protonated ions, deprotonated ions, cation or anion adduct of parent molecule of said heavy petroleum or hydrocarbon sample by soft ionization method;

(b) determining elemental formula of said molecular ions or pseudo molecular ions and quantifying corresponding concentrations using high resolution mass spectrometry; and

(c) reconciling the output from step (b) with other analytical measurements that determine hydrocarbon and petroleum properties to obtain a model-of-composition.

2. The method of claim 1, wherein said heavy petroleums or hydrocarbon samples are separated into asphaltenes and deasphalted oils (DAO).

3. The method of claim 2,wherein said DAO are separated into chemical meaningful classes including saturates, aromatics, sulfides and polars to improve certainty in assigning chemical structures to the molecular formulas obtained by mass spectrometry.

4. The method of claim 3 wherein said aromatics are separated into aromatic ring class fractions including 1-ring aromatics (ARC1), 2-ring aromatics (ARC2), 3-ring aromatics (ARC3), 4-ring+ aromatics (ARC4+) to improve certainty in assigning chemical structures to the molecular formulas obtained by mass spectrometry.

5. The method according to anyone of the preceding claims, wherein said heavy petroleums or hydrocarbon samples are separated by on-line chromatography-high resolution mass spectrometry.

6. The method according to anyone of the preceding claims, wherein ionization is performed by one or multiple ionization methods with or without chromatographic separation.

7. The method according to anyone of the claims 1-5, wherein said ionization step is a soft ionization where molecular ion or pseudo molecular ion structures remain intact after ionization.

8. The method according to anyone of the claims 1-5, wherein said ionization step is performed by one of electrospray ionization, atmospheric pressure chemical ionization, atmospheric pressure photoionization (or photon ionization), matrix assisted laser desorption ionization, direct laser desorption ionization, and field desorption ionization.

9. The method according to anyone of the preceding claims, wherein high resolution is defined as $M/\Delta M_{FWHM} > 10{,}000$.

10. The method according to anyone of the preceding claims, wherein average resolution is greater than 100,000.

11. The method of claim 10, wherein average resolution is greater than 300,000.

12. The method of claim 11, wherein average resolution is greater than 500,000.

13. The method according to anyone of the preceding claims, wherein heavy petroleum and hydrocarbon sample is a vacuum gas oil, vacuum resid or petroleum products of similar boiling point range.

14. The method according to anyone of the preceding claims, wherein said reconsolidation step uses lumps to normalize concentrations.

15. The method according to anyone of claims 1-13, wherein said reconciliation step use bulk elemental properties include: hydrogen, sulfur, nitrogen, nickel and vanadium content.

16. The method according to anyone of claims 1-13, wherein said reconciliation step uses bulk composition and structural properties including at least one of % Aromatic carbon (Ca), Average aromatic cluster size (C#), Amount of C in long chains, Degree of chain branching, organic forms of sulfur, pyrrolic, pyridinic and quaternary nitrogens.

WHAT IS CLAIMED IS:

1. A method to determine the model-of-composition of a sample of petroleum resid comprising:

(a) separating the resid sample into asphaltenes and deasphalted oils (DAO) and separating the deasphalted oils (DAO) into chemical meaningful classes including saturates, aromatics, sulfides and polars; wherein said aromatics are separated into aromatic ring class fractions including 1-ring aromatics (ARC1), 2-ring aromatics (ARC2), 3-ring aromatics (ARC3), 4-ring+ aromatics (ARC4+);

(b) obtaining molecular ions or pseudo molecular ions of each of the asphaltenes, separated DAO and separated classes using a combination of Atmospheric Pressure Photoionization (APPI) or Atmospheric Pressure Chemical Ionization (APCI) and Field Desorption/Field Ionization and Electrospray Ionization (ESI) in high resolution mass spectrometry; wherein using ESI includes using positive ion electrospray ionization Fourier-transform ion cyclotron resonance mass spectrometry (PESI FTICR-MS) to ionize basic nitrogen molecules and by means of negative ion electrospray ionization Fourier-transform ion cyclotron resonance mass spectrometry (NESI FTICR-MS) to ionize acidic molecules;

(c) determining elemental formula and assigning structure of said molecular ions or pseudo molecular ions and quantifying their corresponding concentrations in the asphaltenes, separated DAO and separated fractions from the high resolution mass spectrometry; and

(d) combining compositions of separated fractions from act (c);

(e) directly measuring bulk properties, average structures, and molecular weight distribution of the resid, asphaltenes and separated DAO and separated fractions;

(f) minimally adjusting the molecular compositions obtained from acts (a) – (d) to match the properties the directly measured by act (e) to obtain a model-of-composition.

2. The method of claim 1, in which the resid separation and spectrometry analyses are performed by on-line chromatography-mass spectrometry.

3. The method of claim 1, in which the molecular ion or pseudo molecular ion structures remain intact after the ionization.

4. The method of claim 1 which includes the step of superimposing the PESI FTICR-MS and NESI FTICR-MS analyses.

5. The method of claim 1 in which the molecular weight of each separated classis matched to the molecular weight distribution of field-desorption ionization mass spectrometry (FDMS) analysis.

6. The method of claim 1 in which the ionization of molecules boiling above 1300°F is by means of laser desorption ionization.

7. The method of claim 1 in which the ionization of molecules boiling above 1300°F is by means of matrix assisted laser desorption.

8. The method of claim 1 in which the consolidation uses lumps to normalize concentrations.

9. The method of claim 1 in which the bulk properties include bulk elemental properties, which include hydrogen, sulfur, nitrogen, nickel and vanadium content.

10. The method of claim 9 in which the bulk properties include bulk composition and structural properties, which include:% Aromatic carbon (Ca), Average aromatic cluster size (C#), amount of C in long chains, degree of chain branching, organic forms of sulfur, pyrrolic, pyridinic and quaternary nitrogens.

11. The method of claim 10 in which the adjusting step uses molecular properties including Microcarbon Residue (MCR) or Conradson Carbon Residue (CCR) content, molecular weight distribution by FDMS and boiling point distribution by SIMDIS.