Application of FTICR-MS analysis to soil organic matter

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Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) has an ultrahigh resolution which makes it possible that respective organic molecules detected are accurately assigned to a molecular formula. Soil organic matter plays important roles associated with crop productivity and carbon sequestration. However, the chemical structure is still unknown. We applied this technique to some humic and fulvic acids that were chemically extracted and separated from some typical soils in Japan.

Materials and methods

Humic acids (HAs) were prepared from ten Japanese soils to cover varying degrees of humification and fulvic acids (FAs) were prepared from four Japanese and one Chinese soils according to NAGOYA method or IHSS method. The degree of humification of HAs was evaluated with the absorbance at 600 nm per mg C mL^{-1} (A_{600}/C) and the ratio of absorbances at 400 and 600 nm on a logarithmic scale [$\log(A_{400}/A_{600})$]. Based on these two variables, HAs were classified into four types: Rp < P < B < A, with the degree of humificaiton increasing in this order. The FTICR-MS was performed according to Sleighter and Hatcher (2008). The molecular formulas assigned were examined using the van Krevelen diagram, double bond equivalent (DBE), and Kendrick mass defect (KMD) analysis that focusing on condensed aromatic structure.

Results

1) The number of molecular formulas in the condensed aromatic region increased from Type Rp (124-374) HAs to Type A HAs (751-1008). The sum of the peak magnitudes of the condensed aromatic components increased with increasing degree of humification.

2) The largest DBE values tended to be larger in the order: Type A (33) > Type B (30) > Type P (27) > Type Rp (25) HAs.

3) The KMD analysis indicated that potential structures of condensed aromatic components having 2-10 rings could occur in the soil HAs. The largest number of the rings increased in the order: Types Rp and P (7) < Type B (9) < Type A (10) HAs.

4) The KMD analysis indicated that potential structures of condensed aromatic components having up to 7 rings could occur in the five FAs.

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