Application Note 4

Identify the Correct Heptachlor Epoxide Isomer by Capillary GC

Heptachlor epoxide exists in two isomer forms, each having specific behavior characteristics. Often analysts use the wrong isomer as a reference sample in their labwork. Supelco offers both isomers in high purity concentration form.

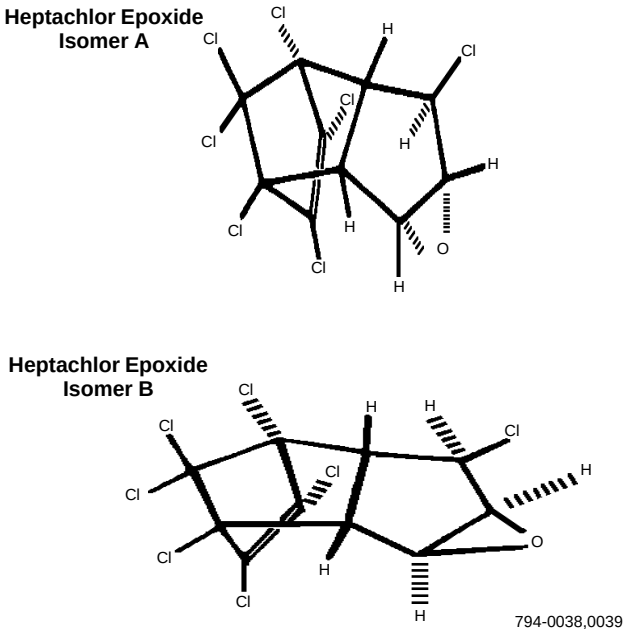
Key Words:

- heptachlor epoxide
- isomer

For many decades, heptachlor was used routinely in agriculture as a pest control agent. Within the environment, heptachlor does not remain in its natural state, but metabolizes to form heptachlor epoxide. Heptachlor has been found to convert to heptachlor epoxide in animal species as well as in plants. Heptachlor epoxide is far more stable than heptachlor, and thus is more suitable for environmental testing (1).

Heptachlor epoxide exists in two isomeric forms (Figure A). Isomer A is readily synthesized and is commercially available from a variety of sources. It is water insoluble, and breaks down relatively quickly in nature. Isomer B is the more stable form of heptachlor epoxide. It is of greater concern to environmental scientists because of its ability to persist in the environment. This isomer is not generally available in the commercial market.

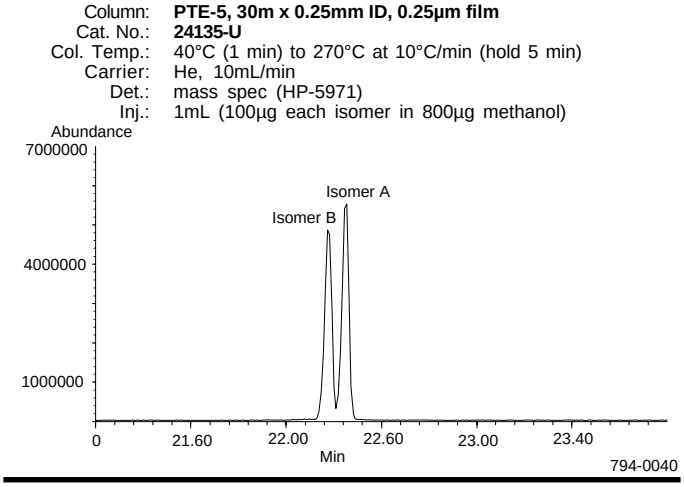
Figure A. Heptachlor Epoxide Isomers



Analysts commonly and erroneously use isomer A as a reference sample in their environmental analyses, when isomer B actually is the compound of their concern. Realizing this common laboratory error, Supelco now offers both isomers in high purity concentration form.

Attempts to separate the two heptachlor epoxide isomers using packed column gas chromatography have not been successful. However, capillary GC completes this separation quite readily. We achieved the isomer separation using a 30m x 0.25mm ID x 0.25µm film PTE™ -5 fused silica capillary column, under conditions described in US Environmental Protection Agency Method 8270 for semivolatile organics. The total ion chromatogram (TIC) shows a 90% separation of the isomer peaks (Figure B).

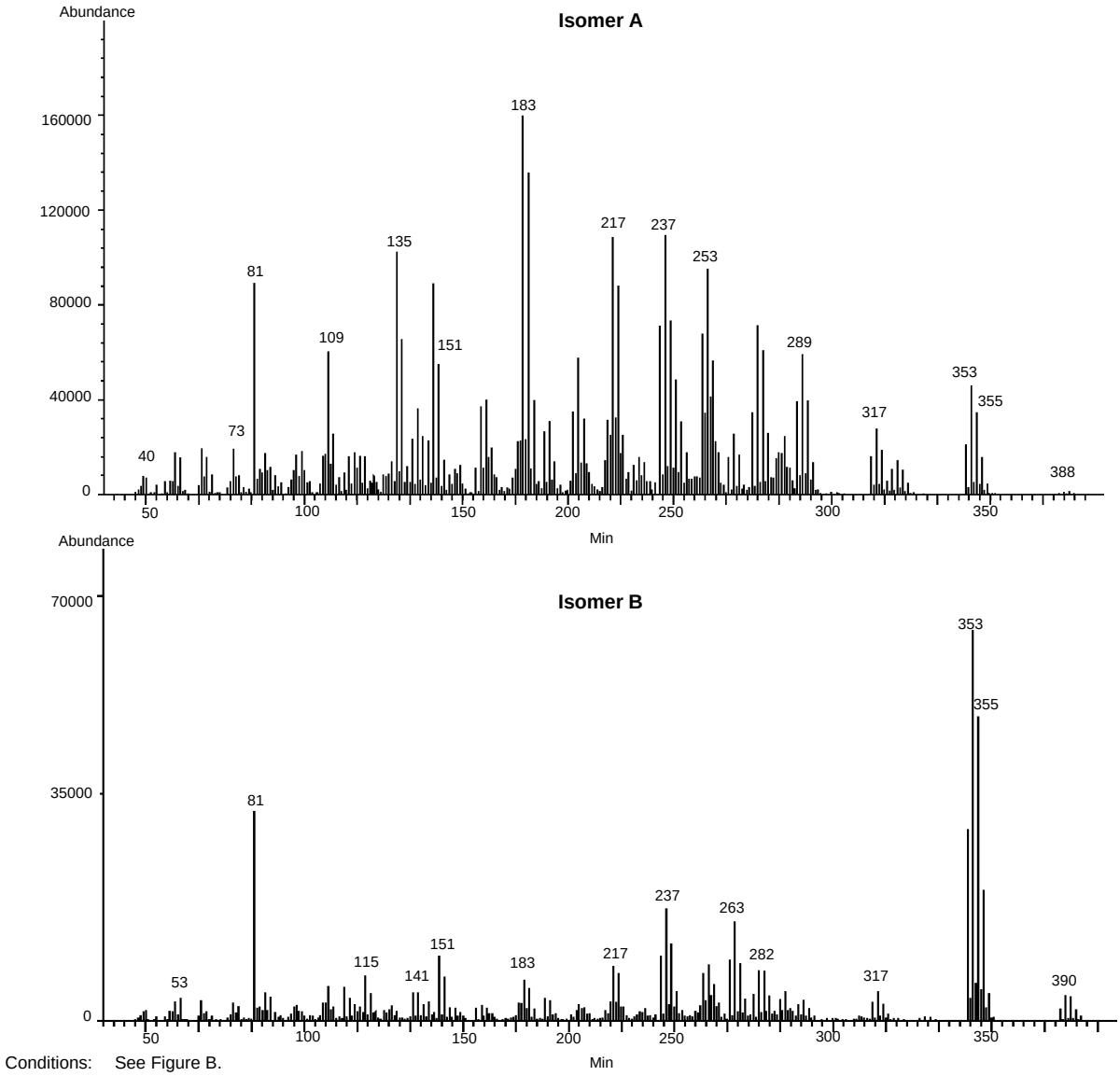
Figure B. Total Ion Chromatogram of Heptachlor Isomers A and B



Minor differences in the retention times of heptachlor epoxide between the analytical standard and the reference standard are sometimes observed This is often the result of the reference standard isomer selected. If the system is calibrated using isomer A, a difference between an environmental sample retention, typically isomer B, and the calibration retention times is to be expected.

Further demonstration of the difference between the two heptachlor epoxide isomer forms is illustrated through consideration of the fragmentation patterns for these isomers. Fragmentation patterns were collected for the two peaks present in the TIC. The fragmentation patterns of the isomers are distinct and easily differentiated (Figure C). A search of the spectra at the National Institute of Standards and Testing (NIST) library identified the peak for isomer B, but not for isomer A. While it is possible that

Figure C. Fragmentation Patterns of Heptachlor Epoxide Isomers



Conditions: See Figure B.

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isomer A could be found in the environment, it is more likely that this isomer is not readily observed.

Supelco has identified the important isomer B form of heptachlor epoxide, and made it available in both neat and single-analyte solution form.

If you are analyzing heptachlor epoxide, we strongly recommend that you examine the source of the reference material to determine its isomeric character. Then select the standard most appropriate for your analytical needs.

Contact our Technical Service Department (phone 800-359-3041 or 814-359-3041, FAX 814-359-5468) for expert answers to your questions.

Ordering Information:

Description	Cat. No.
Heptachlor Epoxide Isomer A, 1mL 1000µg/mL in methanol	**48198**
Heptachlor Epoxide Isomer B, 1mL 1000µg/mL in methanol	**40099**
PTE-5 Fused Silica Capillary Column 30m x 0.25mm ID, 0.25µm film	**24135-U**

Reference

1. Donnelly, Joseph R., G. Wayne Sovocool, and Richard L. Titus, Structures and Environmental Significance of Heptachlor Epoxide Isomers, Journal of AOAC International, Vol. 76, No. 5 (1993).

Fused silica columns manufactured under HP US Pat. No. 4,293,415.

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