

A fourth rubber oligomer isomer of $C_{13}H_{23}Cl$ and $C_{13}H_{23}Br$

In a recent post by Gyorgy Vas, the existence of a fourth rubber oligomer isomer of $C_{13}H_{23}Cl$ and $C_{13}H_{23}Br$ was described ([link](#)).

The structure of 3 isomers is known, but the structure of isomer 4 not.

I took a closer look at my raw GC-MS data of bromobutyl rubber extracts and indeed there was an additional peak with M^+ 258/260 matching $C_{13}H_{23}Br$.

Even though this peak is insignificant (about 1 % of all $C_{13}H_{23}Br$ isomers in the given rubber formulation) and is unlikely to be relevant for E&L toxicity evaluations, I am interested in the structure elucidation.

Below is the EI spectrum of isomer 4 and a schematic of its possible formation.

I look forward to hearing the experts suggestions on the possible structure.

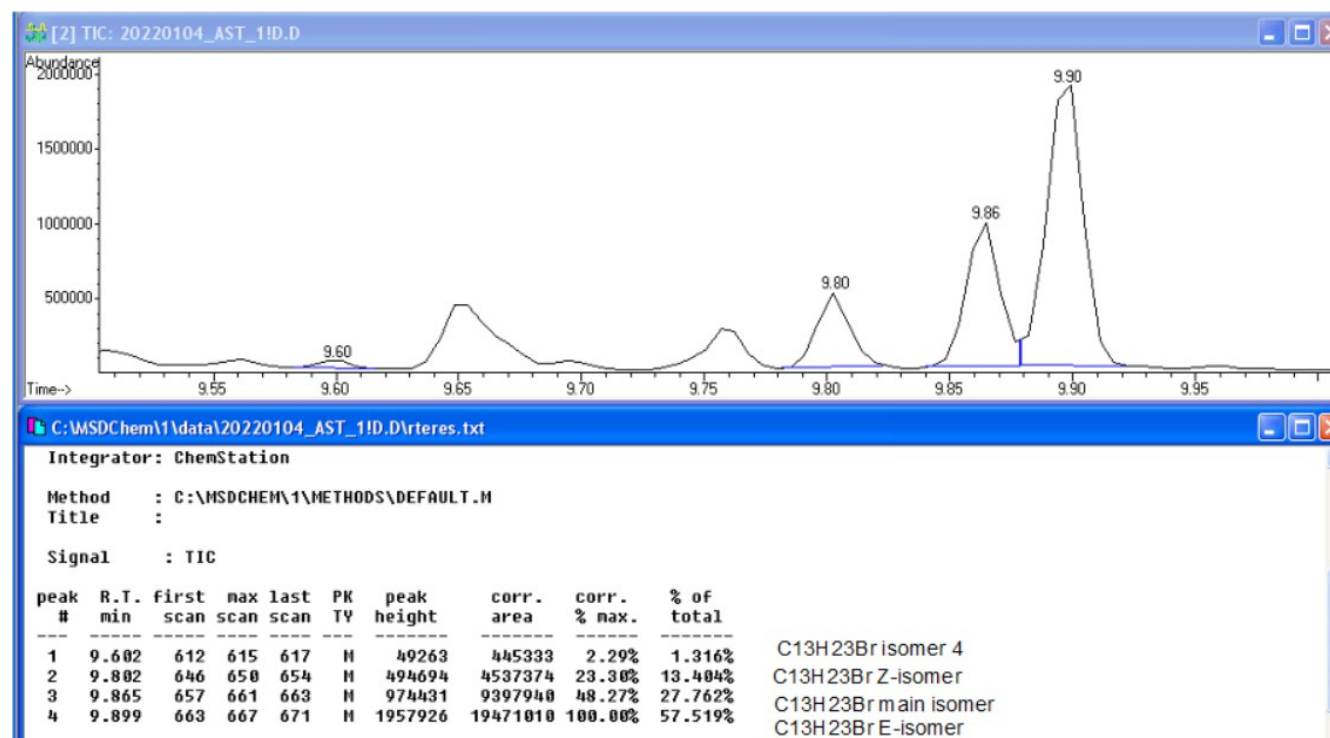


Fig. 1: GC-MS chromatogram (TIC) of a bromobutyl rubber extract

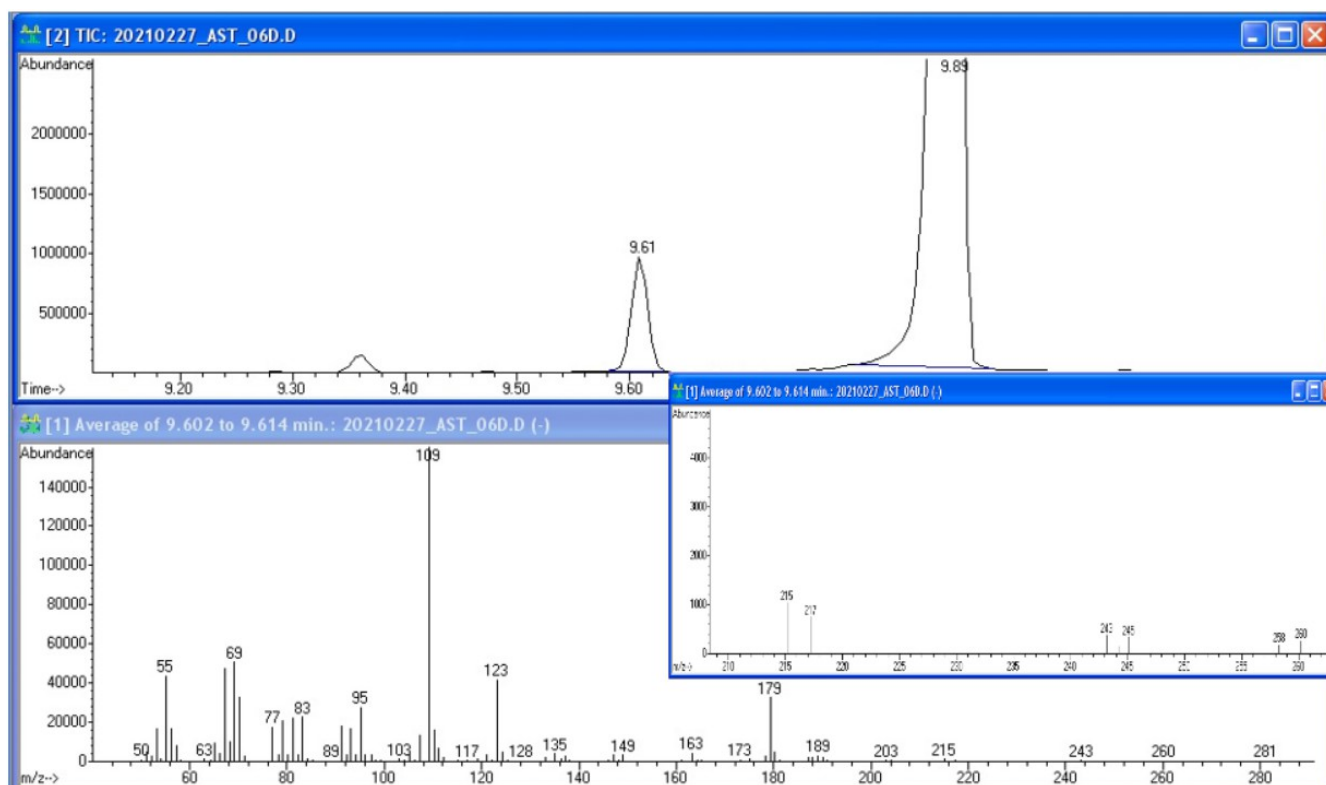
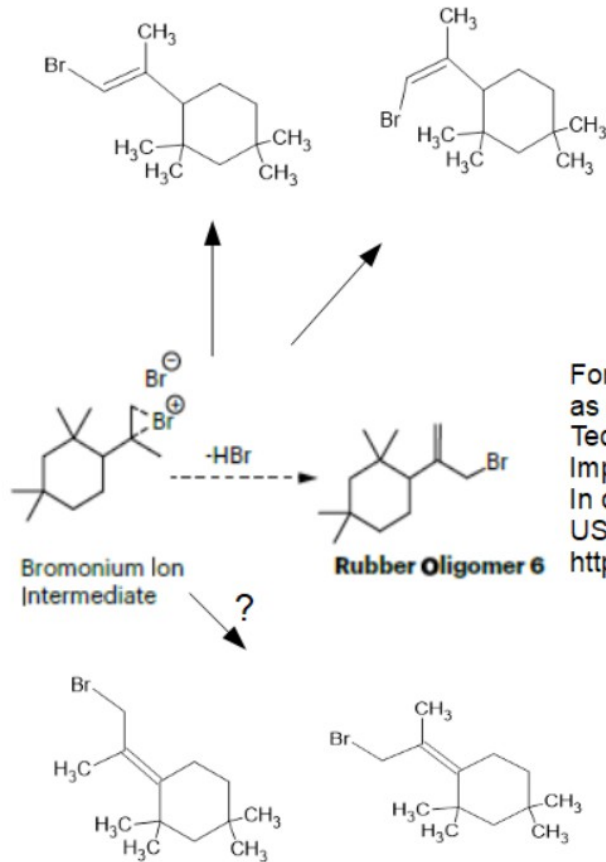


Fig. 2: EI-MS spectrum of unknown rubber oligomer isomer (peak 9.61 min), region around the molecular ion zoomed

C₁₃H₂₃Br E-isomer of vinyl analog

C₁₃H₂₃Br Z-isomer of vinyl analog



Formation of rubber oligomer 6 (C₁₃H₂₃Br main isomer as described in:
 Technical Guide
 Importance of evaluating rubber oligomers
 In drug products-the why, how and what
 USP

<https://www.usp.org/impurities/extractables-and-leachables>

Fig. 3: Possible formation and proposed structure of unknown rubber oligomer