Problem R-12E \((C_5H_8Br_2)\)

200 MHz \(^1H\) NMR spectrum (CDCl\(_3\))

Source: J. Holladay/Reich digitized hard copy 10/23 g

90 MHz \(^{13}C\) NMR spectrum (CDCl\(_3\))

IR Spectrum
Problem R-12E \((C_5H_8Br_2)\). Determine the structure (or part structure) of R-12E from the \(^1\text{H} \text{NMR}, \ ^{13}\text{C} \text{NMR} \text{ and IR spectra provided.}

(a) DBE\_. (b) Analyze the \(^1\text{H} \text{NMR signals, in particular the multiplet at } \delta \text{ 2.6. Report } \delta, \text{ multiplicities and } J \text{ values. Show the structure of R-12E.}

\[
\begin{align*}
&2.7 \quad 2.6 \quad 2.5
&Hz
\end{align*}
\]

(c) Assign the \(^{13}\text{C} \text{NMR signals (write them on a structure). Explain the signal at } \delta \text{ 86.8 ppm.}

\[
\begin{align*}
&21.19
&33.14
&86.84
&145.10
\end{align*}
\]

(d) IR spectrum.

Problem R-12E \((C_5H_8Br_2)\)
90 MHz \(^{13}\text{C} \text{NMR spectrum (CDCl}_3)\)
(Source: J. Holladay/Reich 10/23)

Problem R-12E \((C_5H_8Br_2)\)
IR spectrum (CDCl\textsubscript{3})
(Source: J. Holladay/Reich 10/23)
Problem R-12E (C₅H₈Br₂)
200 MHz ¹H NMR spectrum (CDCl₃)
(Source: J. Holladay/Reich 10/23)
Problem R-12E \((C_5H_8Br_2)\). Determine the structure (or part structure) of \(R-12E\) from the \(^1H\) NMR, \(^{13}C\) NMR and IR spectra provided.

(a) DBE 1. (b) Analyze the \(^1H\) NMR signals, in particular the multiplet at \(\delta 2.6\). Report \(\delta\), multiplicities and \(J\) values. Show the structure of \(R-12E\).

\(\delta 2.6, 1H, d\) septets, \(J = 8.5, 7\) Hz  
\(\delta 6.2, 1H, d, J = 8.5\) Hz  
\(\delta 1.0, 6H, d, J = 7\) Hz

4 other structures, none fit the data

(c) Assign the \(^{13}C\) NMR signals (write them on a structure). Explain the signal at \(\delta 86.8\) ppm.

Heavy atoms (like iodine, and to a lesser extent bromine) cause unusual upfield shifts of attached carbons.

(d) IR spectrum.