

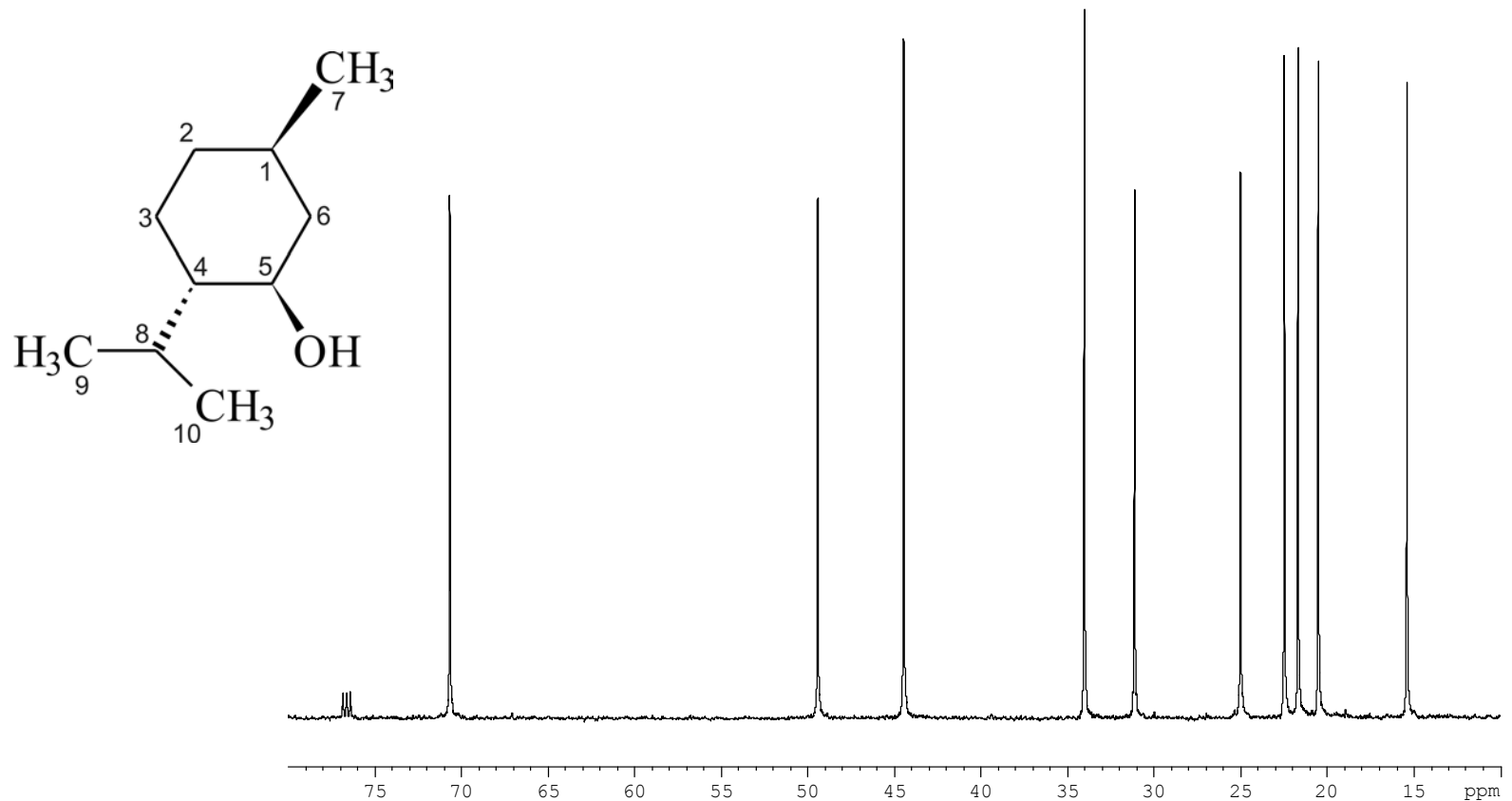
DEPT

(Distortionless Enhancement by Polarization Transfer)

Lit: M.R. Bendall, D.M. Doddrell, D.T. Pegg,
J.Am.Chem.Soc. **1981** (103) 4603-4605

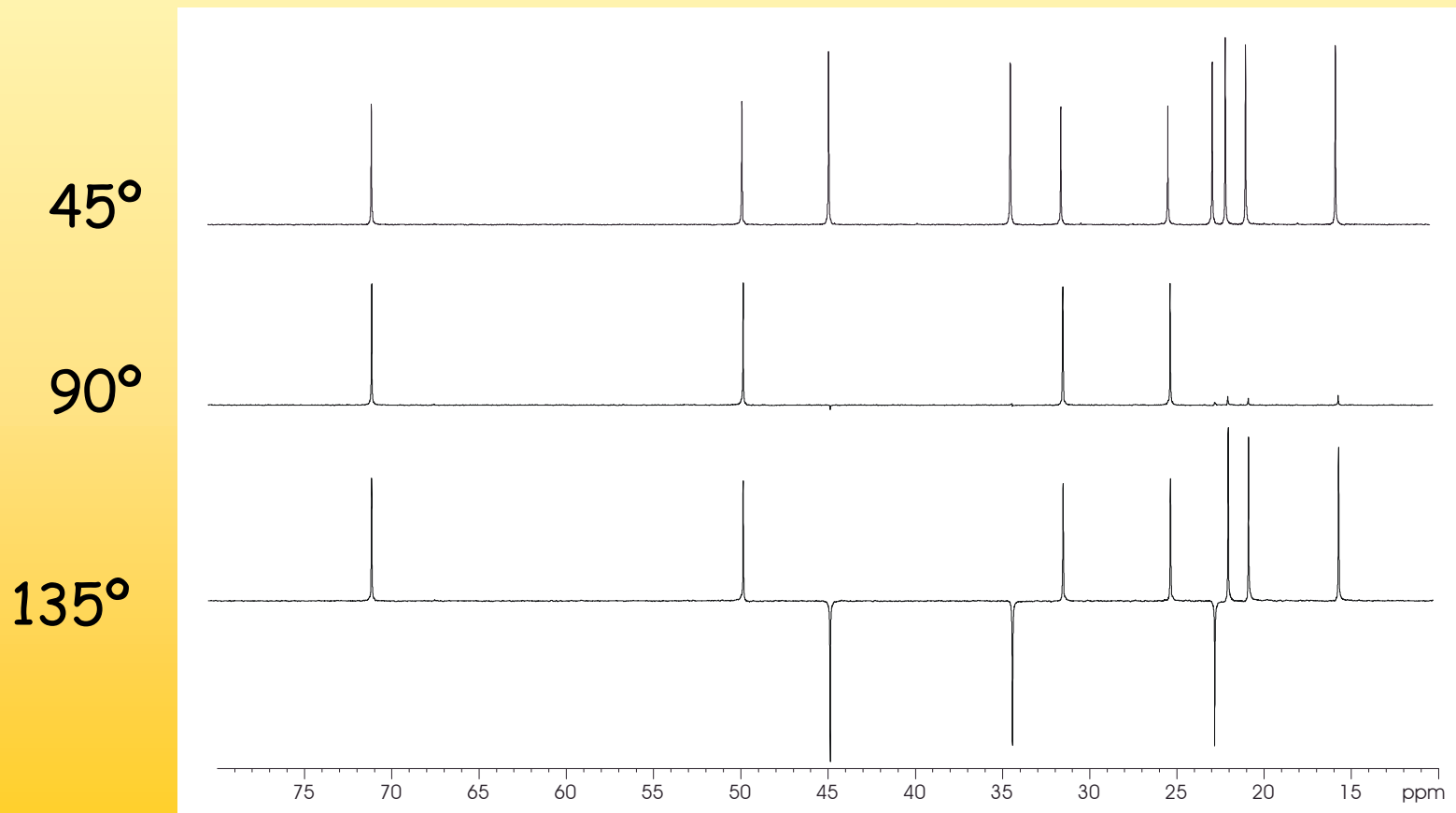
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Die DEPT Sequenz: (-)-Menthol



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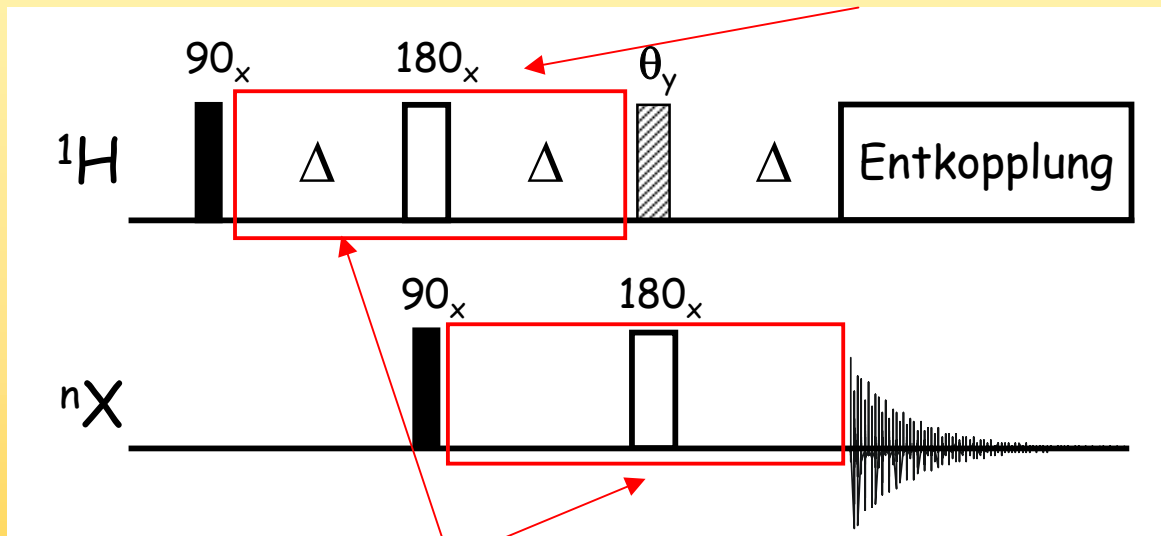
Die DEPT Sequenz: Menthol



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Berechnung der DEPT Sequenz

„building block“



$$\Delta = 1/(2J_{HC})$$

$$J_{HC} \sim 130 \text{ Hz}$$

$$\Delta = 3.85 \text{ msec}$$

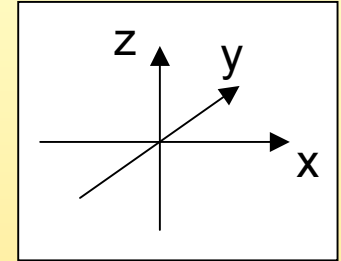
$$J_{HH} \text{ unbedeutend}$$

keine chemische Verschiebung

$$H_{1y} \cos \pi J_{HH} 2\Delta - 2H_{1x} H_{2z} \sin \pi J_{HH} 2\Delta$$

$$= 0.96 (H_{1y}) - 0.04 (2H_{1x} H_{2z})$$

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Berechnung der DEPT Sequenz

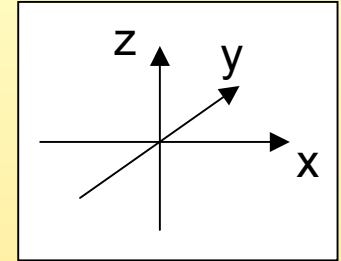
$$H_z \xrightarrow{90^\circ H_x} -H_y \xrightarrow{\pi J_{HC}\Delta} -H_y \cos \pi J_{HC}\Delta + 2H_x C_z \sin \pi J_{HC}\Delta$$

$$\Delta = 1/(2J_{HC}): \cos \pi J_{HC}\Delta = 0, \sin \pi J_{HC}\Delta = 1$$

$$\longrightarrow 2H_x C_z \xrightarrow[90^\circ C_x]{180^\circ H_x} -2H_x C_y$$

Ab hier ergeben sich
unterschiedliche Berechnungen für
CH, CH₂ und CH₃

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Berechnung der DEPT Sequenz

CH:

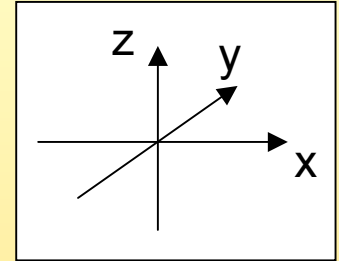
$$-2H_x C_y \xrightarrow{\pi J_{HC}\Delta} -2H_x C_y \xrightarrow[180^\circ C_x]{\theta^\circ H_y} 2(H_x \cos \theta - H_z \sin \theta) C_y$$

$= 2H_x C_y \cos \theta - 2H_z C_y \sin \theta$: Multiquanten und anti-phase

$$\xrightarrow{\pi J_{HC}\Delta} 2H_x C_y \cos \theta + C_x \sin \theta$$

detektierbar

DEPT



Berechnung der DEPT Sequenz

CH_2 :

$$-2 H_{1x} C_y \xrightarrow{\pi J_{HC} \Delta} 4 H_{1x} C_x H_{2z} \xrightarrow[180^\circ C_x]{\theta^\circ H_y}$$

$$4 (H_{1x} \cos \theta - H_{1z} \sin \theta) C_x (H_{2z} \cos \theta - H_{2x} \sin \theta)$$

$$= 4 (H_{1x} C_x H_{2z} \cos^2 \theta - H_{1z} C_x H_{2z} \sin \theta \cos \theta$$

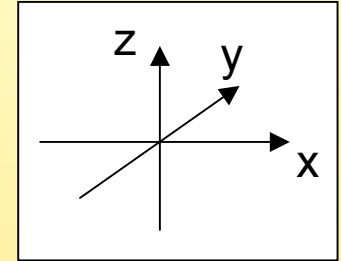
$$- H_{1x} C_x H_{2x} \cos \theta \sin \theta + H_{1z} C_x H_{2x} \sin^2 \theta)$$

$$\xrightarrow{\pi J_{HC} \Delta} 2 H_{1x} C_y \cos^2 \theta + C_x \sin \theta \cos \theta$$

detektierbar

$$+ H_{1x} C_x H_{2x} \cos \theta \sin \theta - 2 C_y H_{2x} \sin^2 \theta$$

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Berechnung der DEPT Sequenz

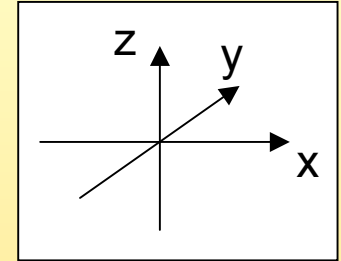
CH_3 :

$$-2 H_{1x} C_y \xrightarrow{\pi J_{HC} \Delta} 8 H_{1x} C_y H_{2z} H_{3z} \xrightarrow[180^\circ C_x]{\theta^\circ H_y}$$

$$- 8 (H_{1x} \cos \theta - H_{1z} \sin \theta) C_y (H_{2z} \cos \theta - H_{2x} \sin \theta) \\ \times (H_{3z} \cos \theta - H_{3x} \sin \theta)$$

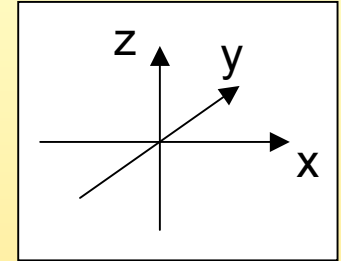
$$= \dots - 8 H_{1z} C_y H_{2z} H_{3z} \sin \theta \cos \theta \cos \theta \dots$$

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$$\begin{aligned}
 = & - 8 H_{1x} C_y H_{2z} H_{3z} \cos \theta \cos \theta \cos \theta \\
 & + 8 H_{1x} C_y H_{2z} H_{3x} \cos \theta \cos \theta \sin \theta \\
 & + 8 H_{1x} C_y H_{2x} H_{3z} \cos \theta \sin \theta \cos \theta \\
 & - 8 H_{1x} C_y H_{2x} H_{3x} \cos \theta \sin \theta \sin \theta \\
 & + 8 H_{1z} C_y H_{2z} H_{3z} \sin \theta \cos \theta \cos \theta \\
 & - 8 H_{1z} C_y H_{2z} H_{3x} \sin \theta \cos \theta \sin \theta \\
 & - 8 H_{1z} C_y H_{2x} H_{3z} \sin \theta \sin \theta \cos \theta \\
 & + 8 H_{1z} C_y H_{2x} H_{3x} \sin \theta \sin \theta \sin \theta
 \end{aligned}$$

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$$\begin{aligned}
 \xrightarrow{\pi J_{HC}\Delta} & + 2 H_{1x} C_y \cos \theta \cos \theta \cos \theta \\
 & - 4 H_{1x} C_x H_{3x} \cos \theta \cos \theta \sin \theta \\
 & - 2 H_{1x} C_x H_{2x} \cos \theta \sin \theta \cos \theta \\
 & - 8 H_{1x} C_y H_{2x} H_{3x} \cos \theta \sin \theta \sin \theta \\
 & + C_x \sin \theta \cos \theta \cos \theta \\
 & + 2 C_y H_{3x} \sin \theta \cos \theta \sin \theta \\
 & + 2 C_y H_{2x} \sin \theta \sin \theta \cos \theta \\
 & - 4 C_x H_{2x} H_{3x} \sin \theta \sin \theta \sin \theta
 \end{aligned}$$

← detektierbar

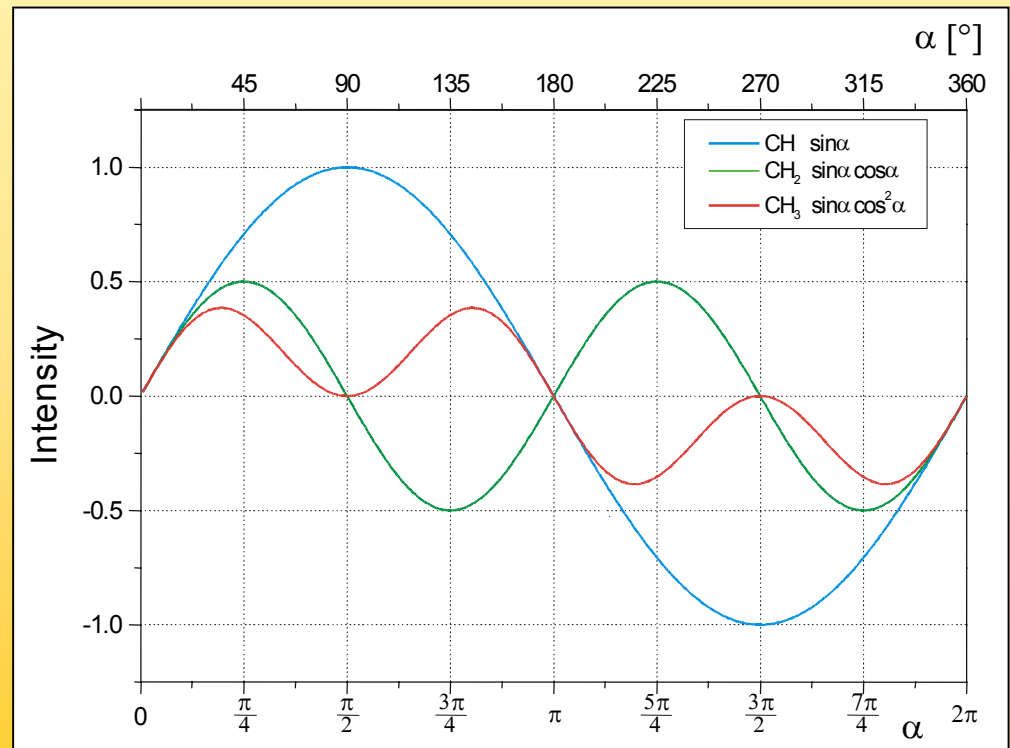
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DEPT: Intensitäten vs. Pulswinkel

$$C_x \sin \theta$$

$$C_x \sin \theta \cos \theta$$

$$C_x \sin \theta \cos \theta \cos \theta$$



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	45°	90°	135°
CH	$\frac{1}{2} \sqrt{2}$	1	$\frac{1}{2} \sqrt{2}$
CH ₂	$\frac{1}{2}$	0	$-\frac{1}{2}$
CH ₃	$\frac{1}{4} \sqrt{2}$	0	$\frac{1}{4} \sqrt{2}$

DEPT: Sub-Spektren
mit reiner
Multiplizität

$$\text{CH} = [90^\circ]$$

$$\text{CH}_2 = [45^\circ] - [135^\circ]$$

$$\text{CH}_3 = ([45^\circ] + [135^\circ]) - \sqrt{2} [90^\circ]$$

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DEPT: Sub-Spektren von Menthol

