Supporting Information

Centrohexaindane: Six Benzene Rings Mutually Fixed in Three Dimensions – Solid-State Structure and Six-fold Nitration

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\(^1\text{H}\) NMR spectrum (aromatic region, 250 MHz, DMSO-\(d_6\)) of the 1 : 3 mixture of compounds 6 and 7

For further detailed interpretation and discussion of the \(^1\text{H}\) NMR spectra (500 MHz) of this mixture of isomers, see: J. Tellenbröker, D. Kuck, *Beilstein J. Org. Chem.* 2011, 7, 329–337.

\[8.66 (d, \text{ }^4J = 1.8 \text{ Hz}, 6 \text{ H}, 1\text{-H and 12-H of 7}),\]
\[8.50 (d, \text{ }^4J = 1.8 \text{ Hz}, 6 \text{ H}, 1\text{-H, 5-H and 9-H of 6 and 5-H of 7}),\]
\[8.07-8.11 (m, 12 \text{ H}, 4\text{-H, 8-H and 12-H of 6, 4-H of 7}),\]
\[7.07 (m, 6 \text{ H}, 7\text{-H and 10-H of 7}),\] partially overlapping with m at \(\delta\) 8.07-8.11
\[7.96 (d, \text{ }^3J = 8.5 \text{ Hz}, 6 \text{ H}, 8\text{-H and 9-H of 7})\]

El mass spectrum (70 eV) of the mixture of compounds 6 and 7
$^1$H NMR spectrum (aromatic region, 250 MHz, DMSO-$d_6$) of the mixture of compounds 8, 9 and 10

![NMR Spectrum](image)

8.80 (s, 6 H, 4-H of 8 and 9),
8.70 (d, $^3J = 2.0$ Hz, 2 H, 5-H of 8),
8.68 (d, $^2J = 2.1$ Hz, 6 H, 5-H and 12-H of 9, 8-H and 9-H of 10),
8.63 (s, 4 H, 1-H of 8, 1-H and 4-H of 10),
8.53 (d, $^3J = 2.0$ Hz, 2 H, 8-H of 8),
8.07–8.16 (m, 16 H, 12-H of 8 and 10, 7-H and 11-H of 8, 7-H and 10-H of 9, 6-H and 11-H of 10),
7.98 (d, $^3J = 8.6$ Hz, 4 H, 8-H and 9-H of 9)

EI mass spectrum (70 eV) of the mixture of compounds 8, 9 and 10

![EI Mass Spectrum](image)
$^1$H NMR spectrum (aromatic region, 250 MHz, DMSO-$d_6$) of compound 11

\[
\text{EI mass spectrum (70 eV) of the mixture of compound 11}
\]
$^1$H NMR spectrum (aromatic region, 250 MHz, DMSO-$d_6$) of compound 12

![NMR spectrum]

8.99 (d, $^4J = 2.1$ Hz, 1 H, 2-H),
8.89 (s, 1 H, 5-H (?)),
8.78 (s, 1 H, 8-H (?)),
8.74 (s, 1 H, 9-H (?)),
8.64 (d, $^4J = 1.9$ Hz, 1 H, 4-H),
8.06 (s, 1 H, 12-H)

El mass spectrum (70 eV) of the mixture of compound 12

![Mass spectrum graph]
$^1$H NMR spectrum of the crude mixture of compounds 14–17 (500 MHz, THF-d$_8$)

Stacked $^1$H NMR spectra of the purified isomers 14, 15, 16 and 17 (500 MHz, THF-d$_8$)
$^1$H NMR spectrum and $^1$H,$^1$H-COSY spectrum of compound 14 (500 MHz, THF-$d_8$)
$^1$H NMR spectrum and $^1$H,$^1$H-COSY spectrum of compound 15 (500 MHz, THF-d$_8$)
$^1$H NMR spectrum and $^1$H,$^1$H-COSY spectrum of compound 16 (500 MHz, THF-d$_8$)
$^1$H NMR spectrum and $^1$H, $^1$H-COSY spectrum of compound 17 (500 MHz, THF-d$_8$)
$^{13}$C NMR spectra of compound 14 (126 MHz, THF-d$_8$)

DEPT-135
Magnification of the ranges of C_{arene} and C^{\alpha} resonances (insert)

\[ f_1 (\text{ppm}) \]

13C NMR spectra of compound 15 (126 MHz, THF-d8)
DEPT-135 (with reversed sign due to the exceedingly large solvent signal)

Magnification of the ranges of C\text{arene} and C\text{α} resonances (insert)
\[13\text{C NMR spectra of compound 16 (126 MHz, THF-d}_8\text{)}\]

\[
\begin{align*}
\text{DEPT-135}
\end{align*}
\]
Magnification of the ranges of C\text{arene} and C\text{\textalpha{}} resonances (insert)

\[ f_1 (ppm) \]

1\textsuperscript{3}C NMR spectra of compound 17 (126 MHz, THF-d\textsubscript{8})
Magnification of the ranges of $C_{\text{arene}}$ and $C^\alpha$ resonances (insert)
Mass spectrum (-)-ESI (MeCN, LiCl) of compound 14

[M + Cl]^− molecular adduct ion peak group
Mass spectrum (-)-ESI (MeCN, LiCl) of compound 15

[M + Cl]− molecular adduct ion peak group
Mass spectrum (-)-ESI (MeCN, LiCl) of compound 16

[M + Cl]− molecular adduct ion peak group
Mass spectrum (-)-ESI (MeCN, LiCl) of compound 17

[M + Cl]− molecular adduct ion peak group
Solid-state structure of centrohexaindane, 1 · CHCl₃

Stacking showing six molecules of 1 and two molecules of chloroform (centre)
Solid-state structure of centrohexaindane, $1 \cdot 0.5$ para-xylene

Stacking showing six molecule of 1 and one molecule of para-xylene (centre)
Solid-state structure of centrohexaindane, 1 • NEt₃

Stacking showing five molecules of 1 and two molecules of triethylamine (lower centre)