Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

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

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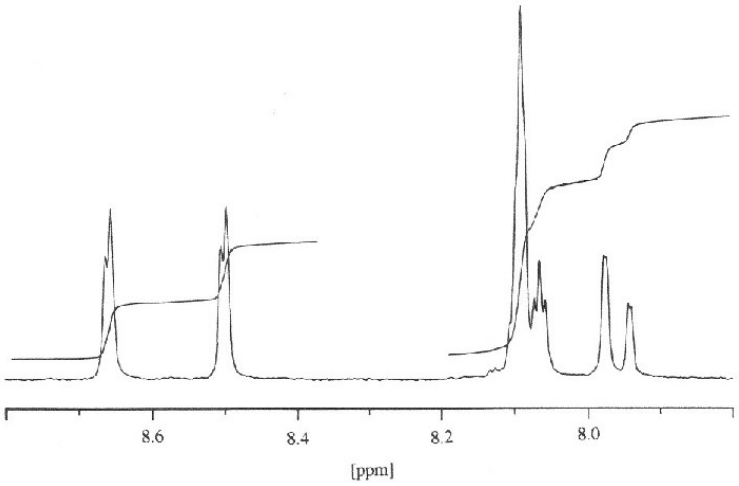
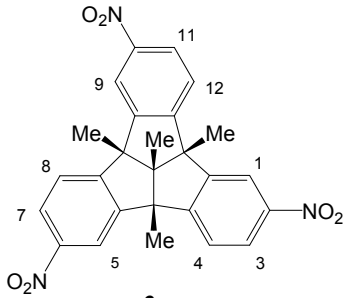
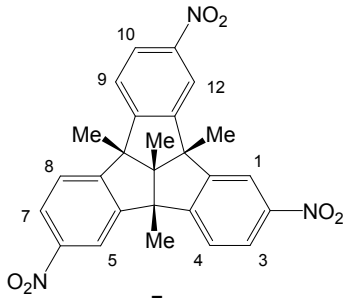
^{1}H NMR spectrum (aromatic region, 250 MHz, DMSO-d_6) of the 1 : 3 mixture of compounds **6** and **7**

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





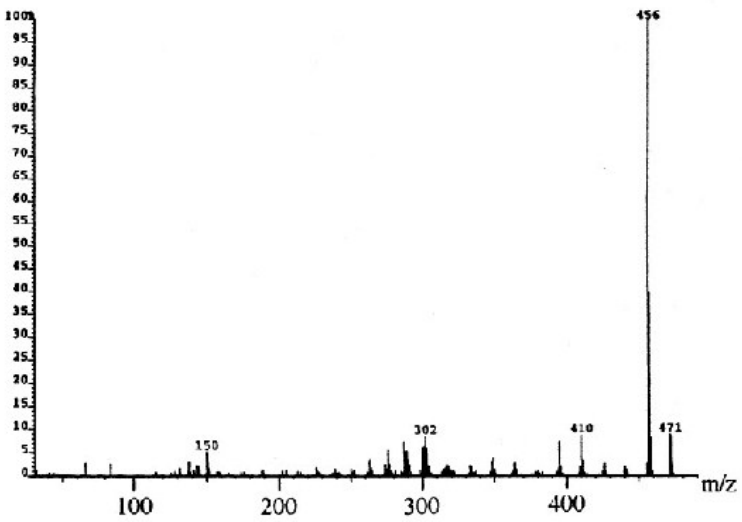
6



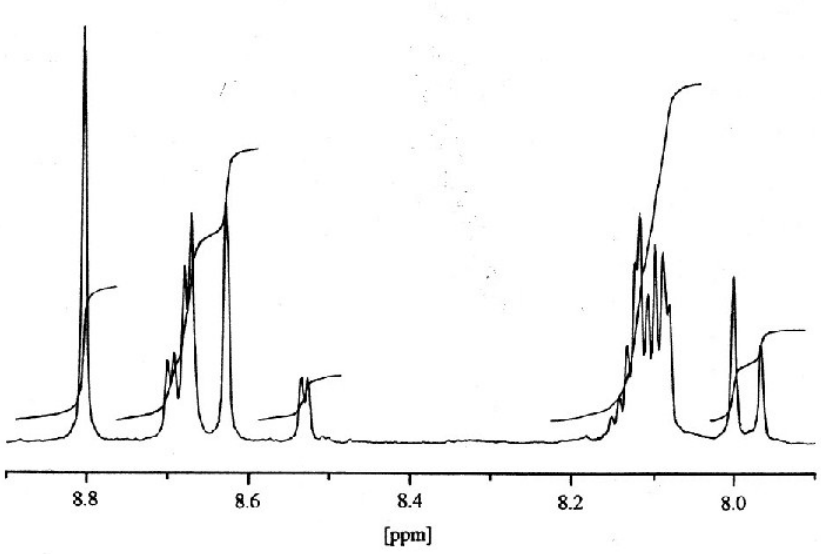
7

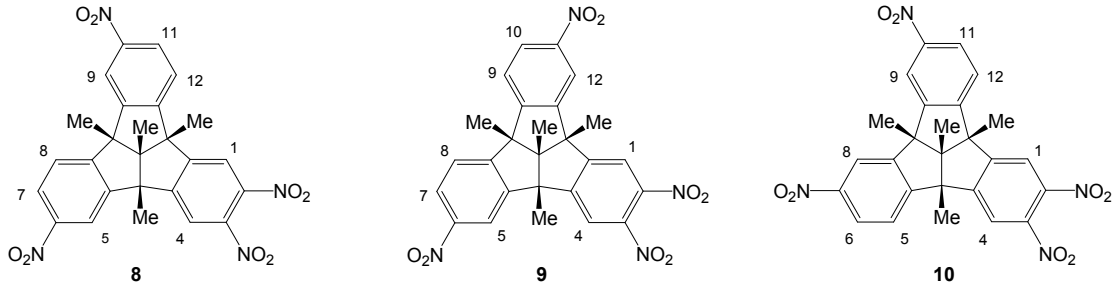
8.66 (d, ^4J = 1.8 Hz, 6 H, 1-H and 12-H of **7**,
8.50 (d, ^4J = 1.8 Hz, 6 H, 1-H, 5-H and 9-H of **6** and 5-H of **7**),
8.07-8.11 (m, 12 H, 4-H, 8-H and 12-H of **6**, 4-H of **7**),
7.07 (m, 6 H, 7-H and 10-H of **7**), partially overlapping with m at δ 8.07-8.11
7.96 (d, ^3J = 8.5 Hz, 6 H, 8-H and 9-H of **7**)

EI mass spectrum (70 eV) of the mixture of compounds **6** and **7**



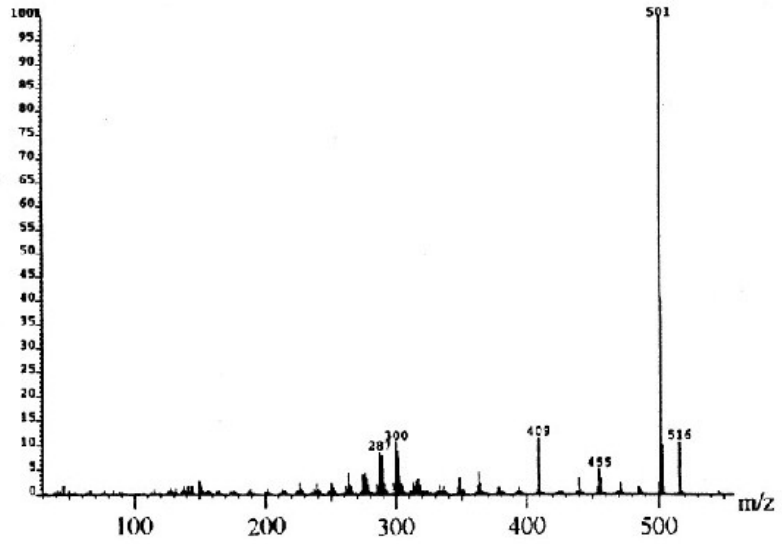
^{1}H NMR spectrum (aromatic region, 250 MHz, DMSO-d_6) of the mixture of compounds **8**, **9** and **10**



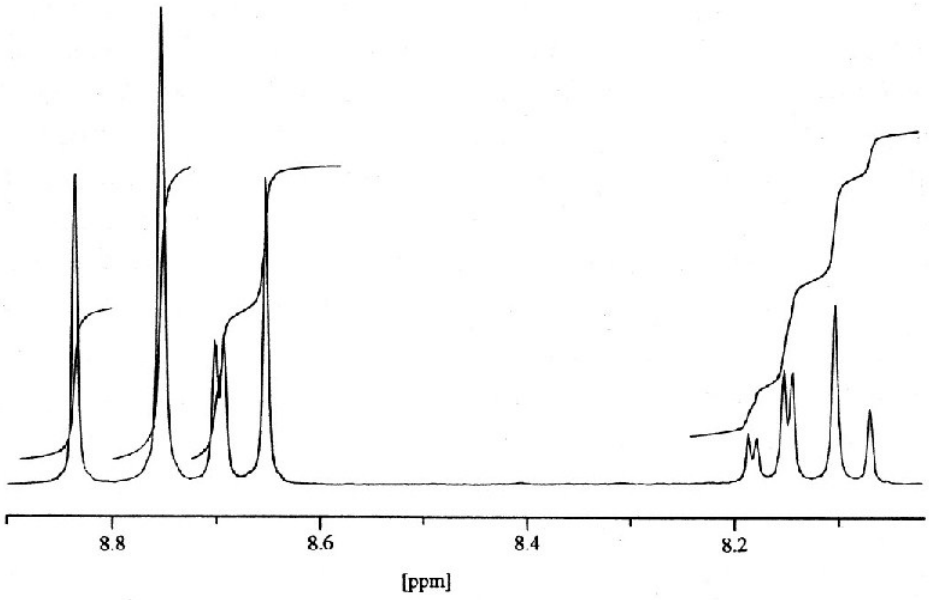


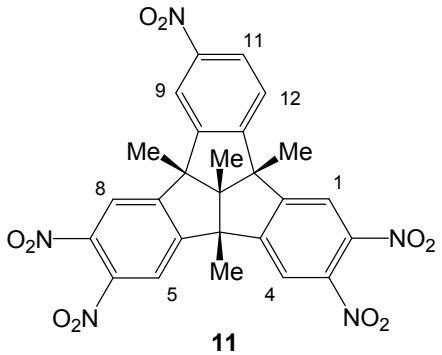
8.80 (s, 6 H, 4-H of **8** and **9**),
8.70 (d, ^4J = 2.0 Hz, 2 H, 5-H of 8),
8.68 (d, ^4J = 2.1 Hz, 6 H, 5-H and 12-H of **9**, 8-H and 9-H of **10**),
8.63 (s, 4 H, 1-H of **8**, 1-H and 4-H of **10**),
8.53 (d, ^4J = 2.0 Hz, 2 H, 8-H of **8**),
8.07–8.16 (m, 16 H, 12-H of **8** and **10**, 7-H and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



^{1}H NMR spectrum (aromatic region, 250 MHz, DMSO-d_6) of compound **11**

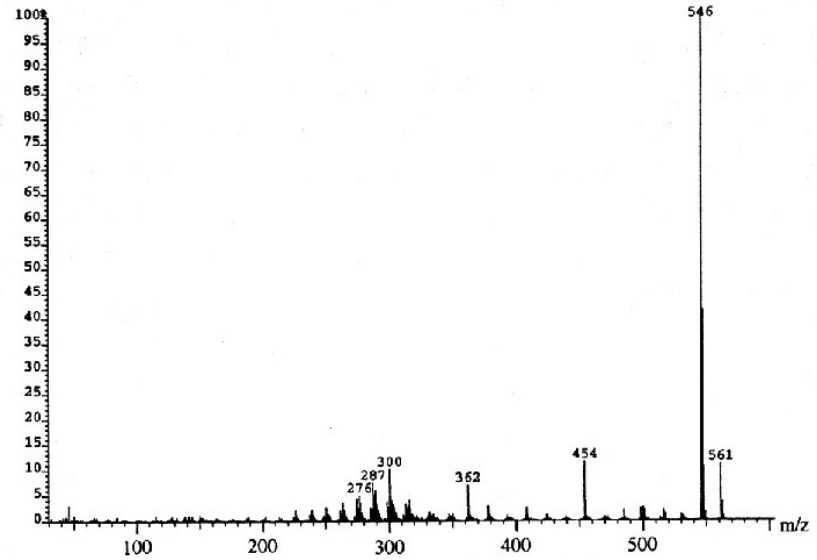




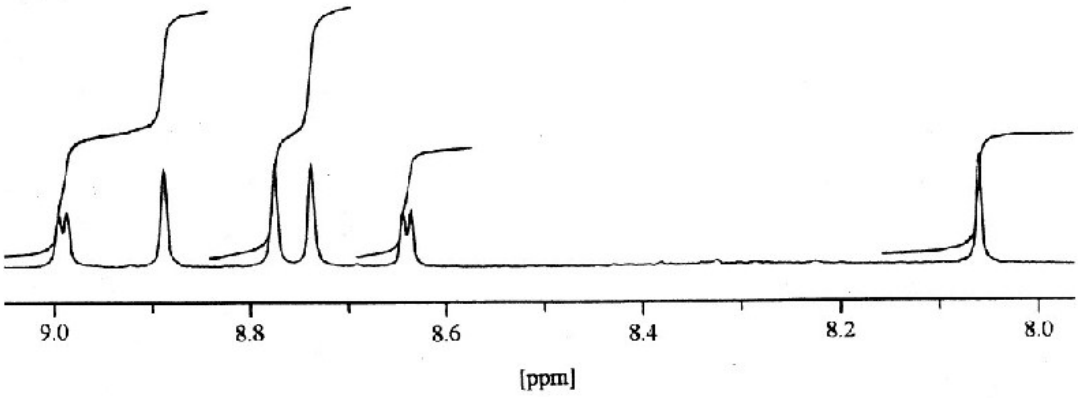
11

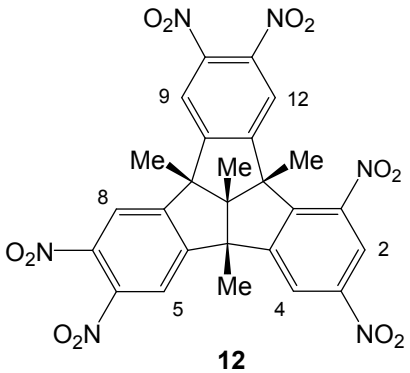
8.84 (s, 1 H, 8-H),
8.75 (s, 2 H, 4- and 5-H),
8.70 (d, ^4J = 2.0 Hz, 1 H, 9-H),
8.65 (s, 1 H, 1-H),
8.17 (dd, ^3J = 8.5 Hz, ^4J = 2.1 Hz , 1 H, 11-H),
8.09 (d, ^3J = 8.6 Hz, 1 H, 12-H)

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**

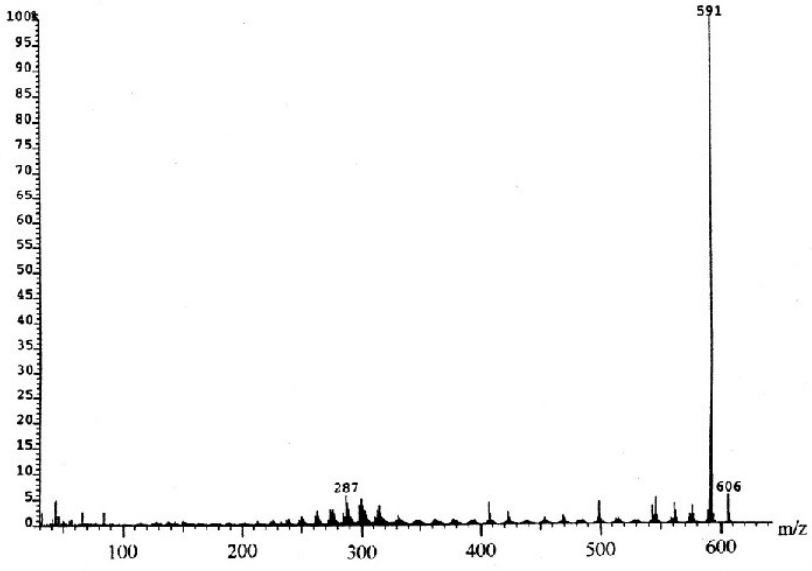




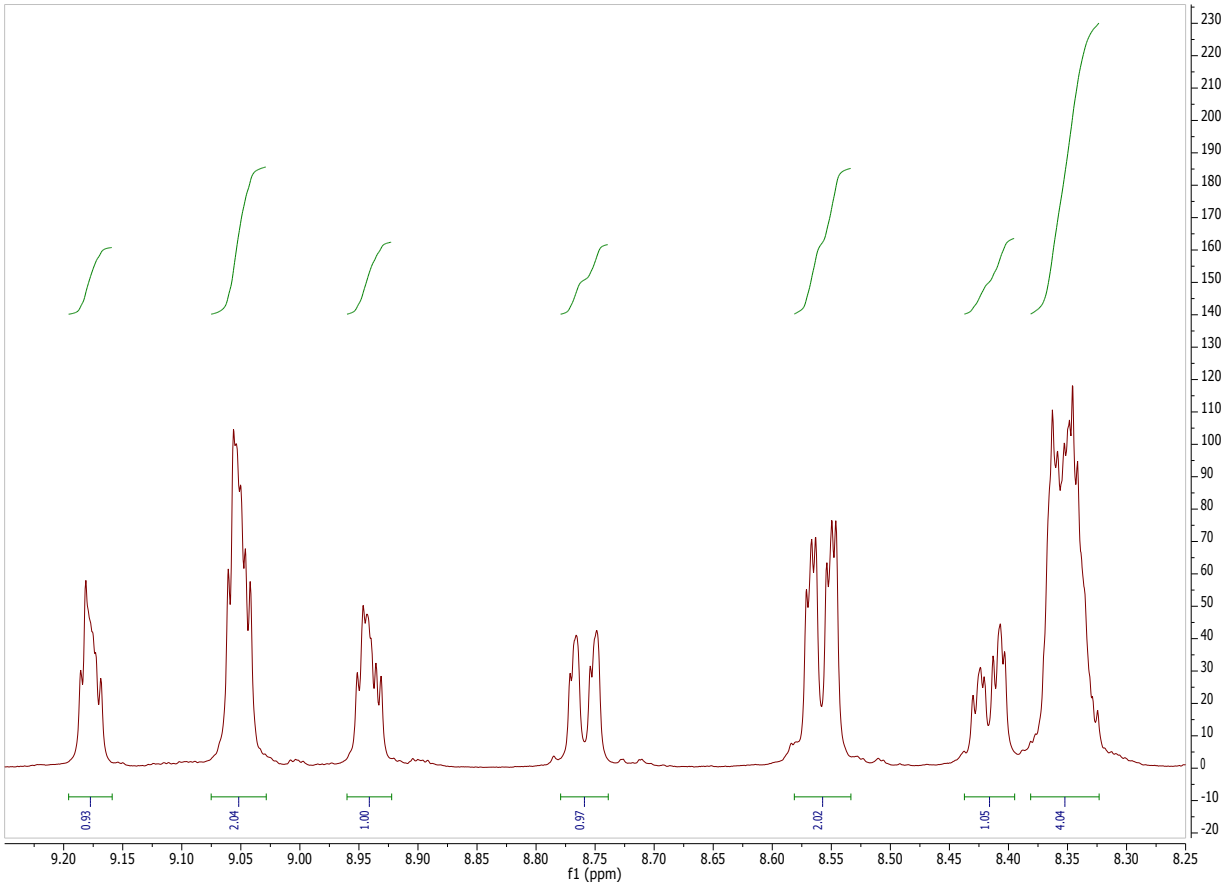
12

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)

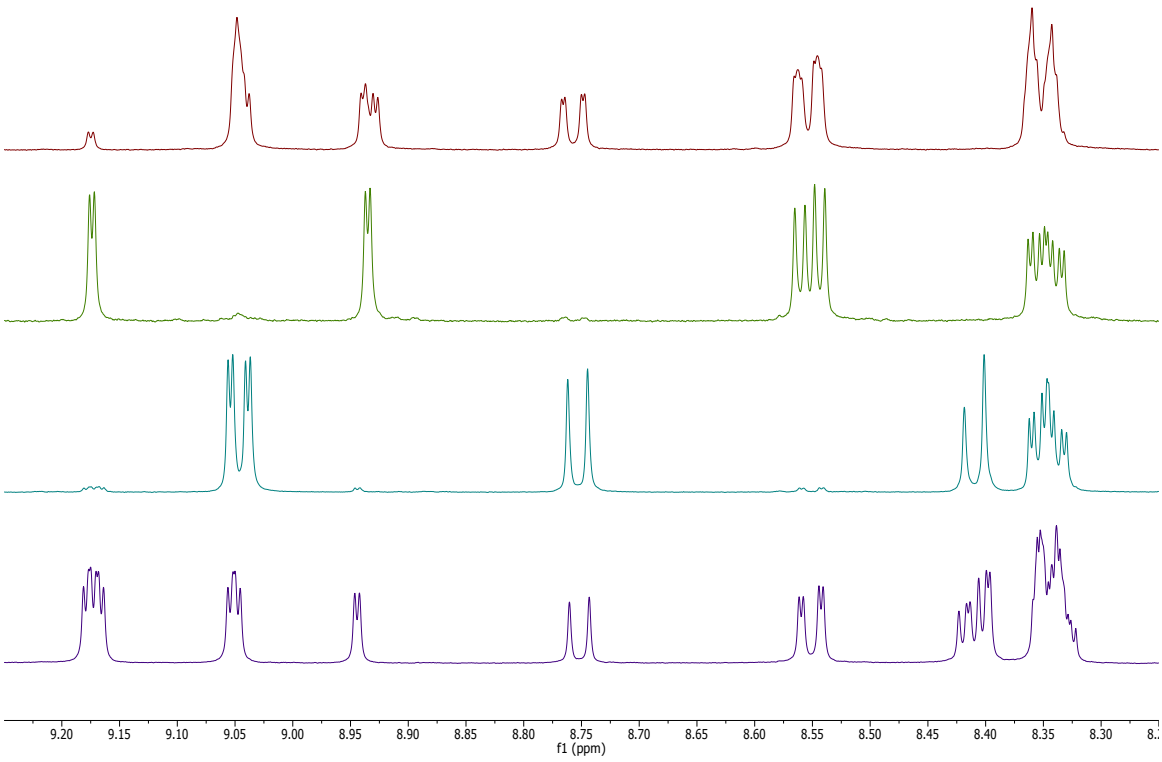
EI mass spectrum (70 eV) of the mixture of compound **12**



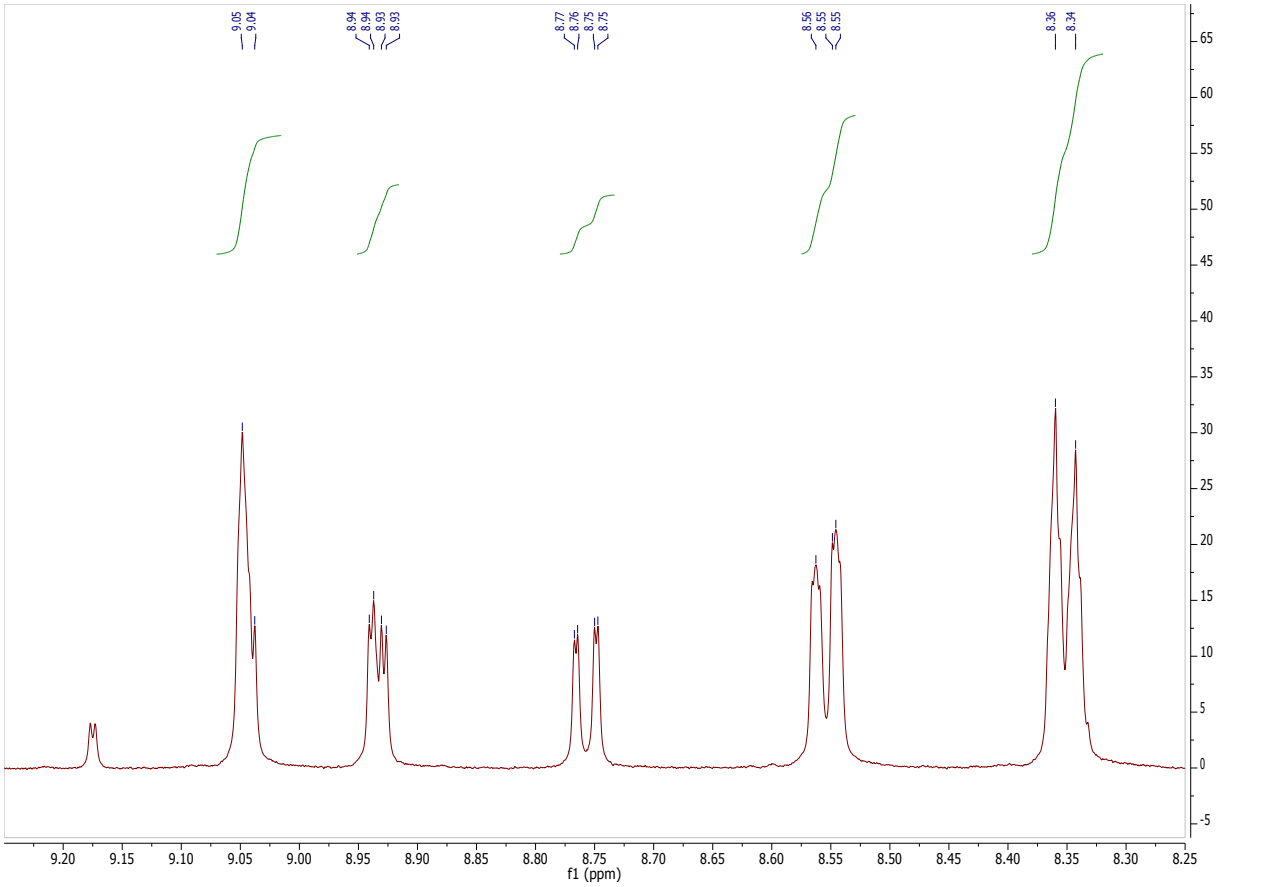
^{1}H NMR spectrum of the crude mixture of compounds **14**–**17** (500 MHz, THF-d_8)

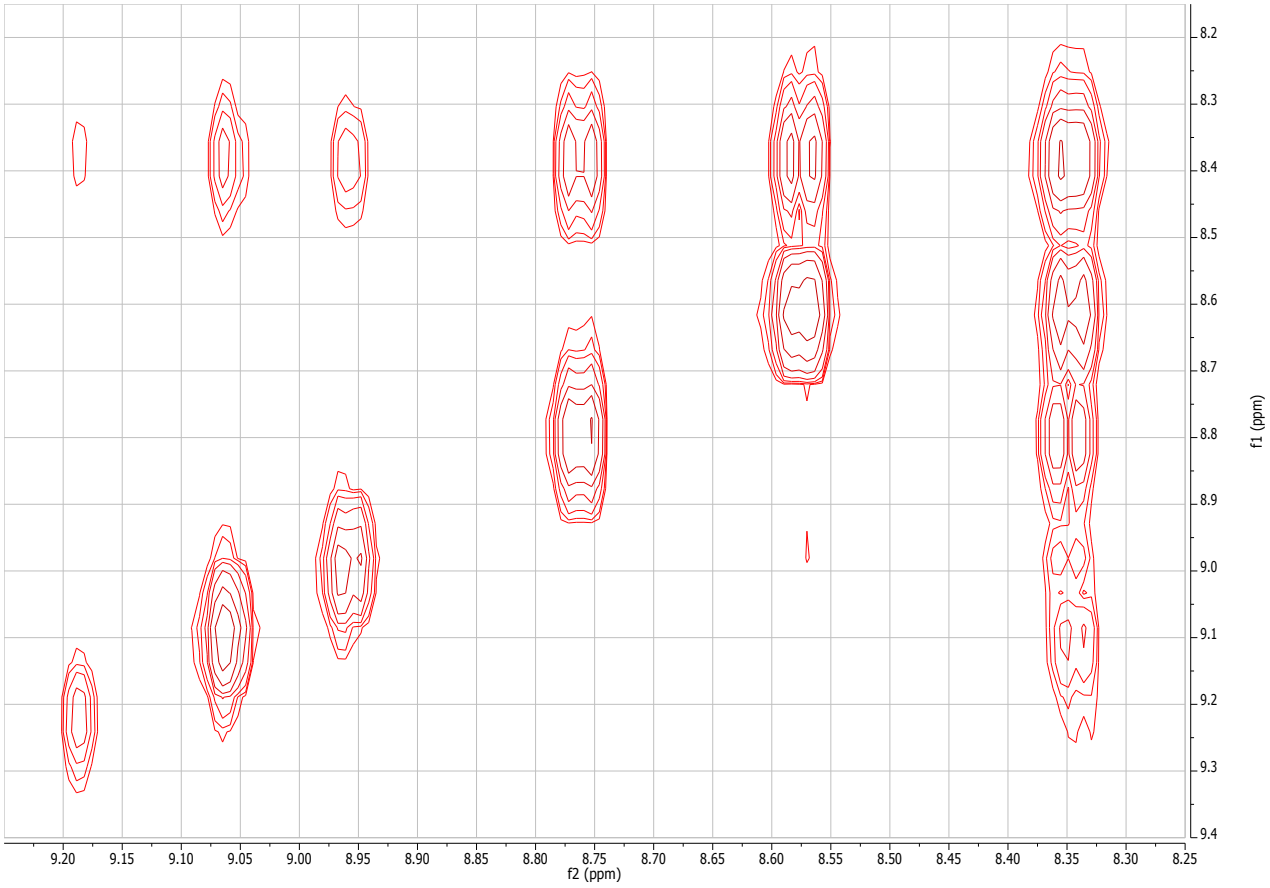


Stacked ^{1}H NMR spectra of the purified isomers **14**, **15**, **16** and **17** (500 MHz, THF-d_8)

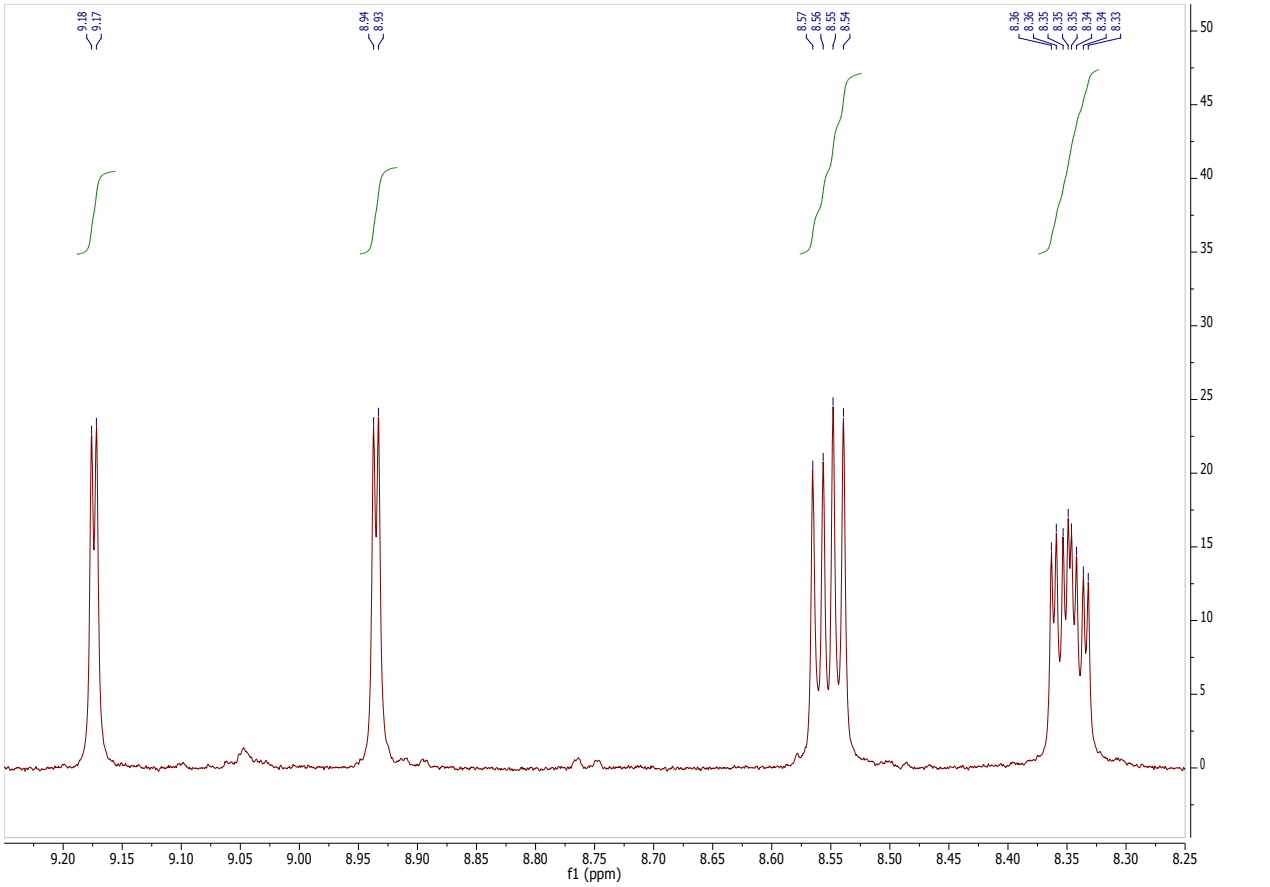


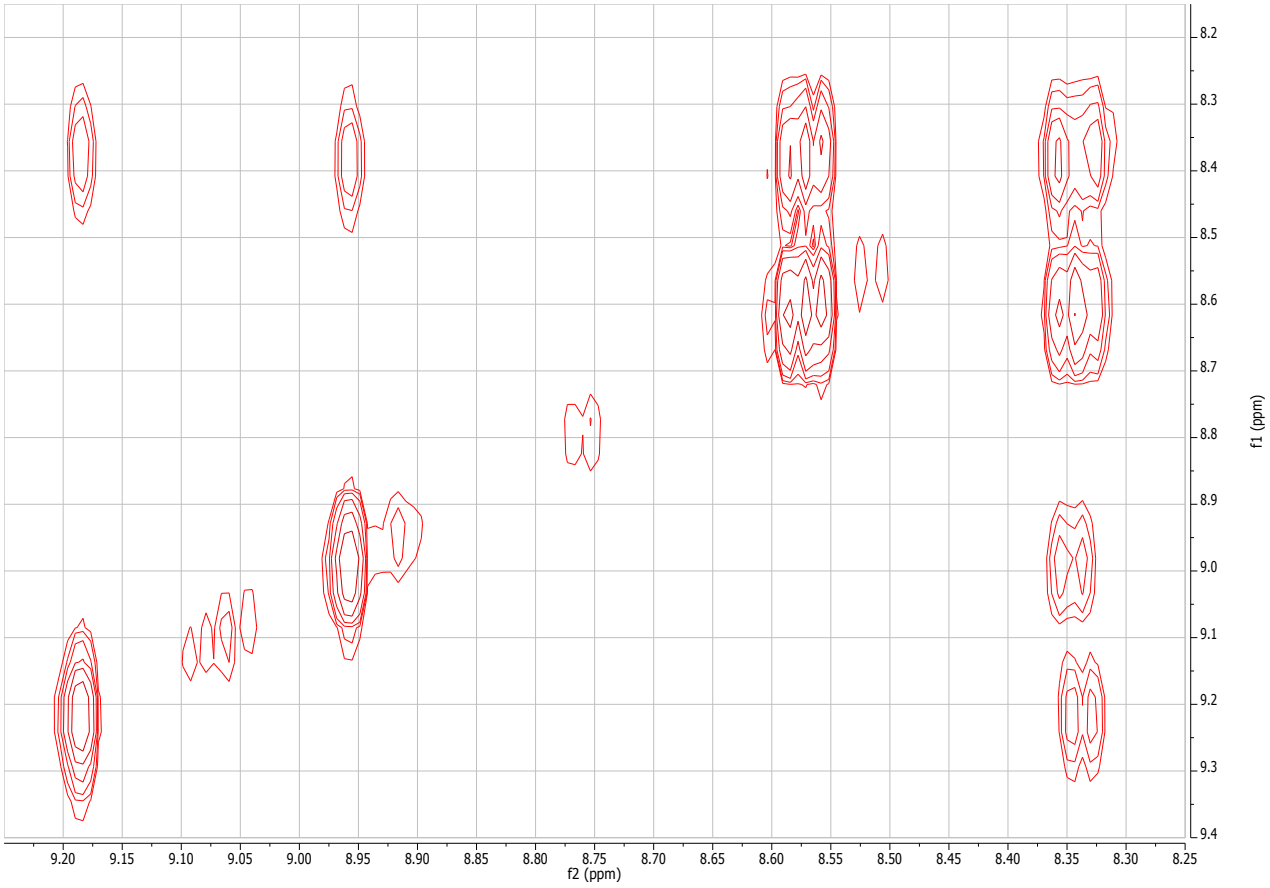
^{1}H NMR spectrum and ^{1}H,^{1}H-COSY spectrum of compound **14** (500 MHz, THF-d_8)



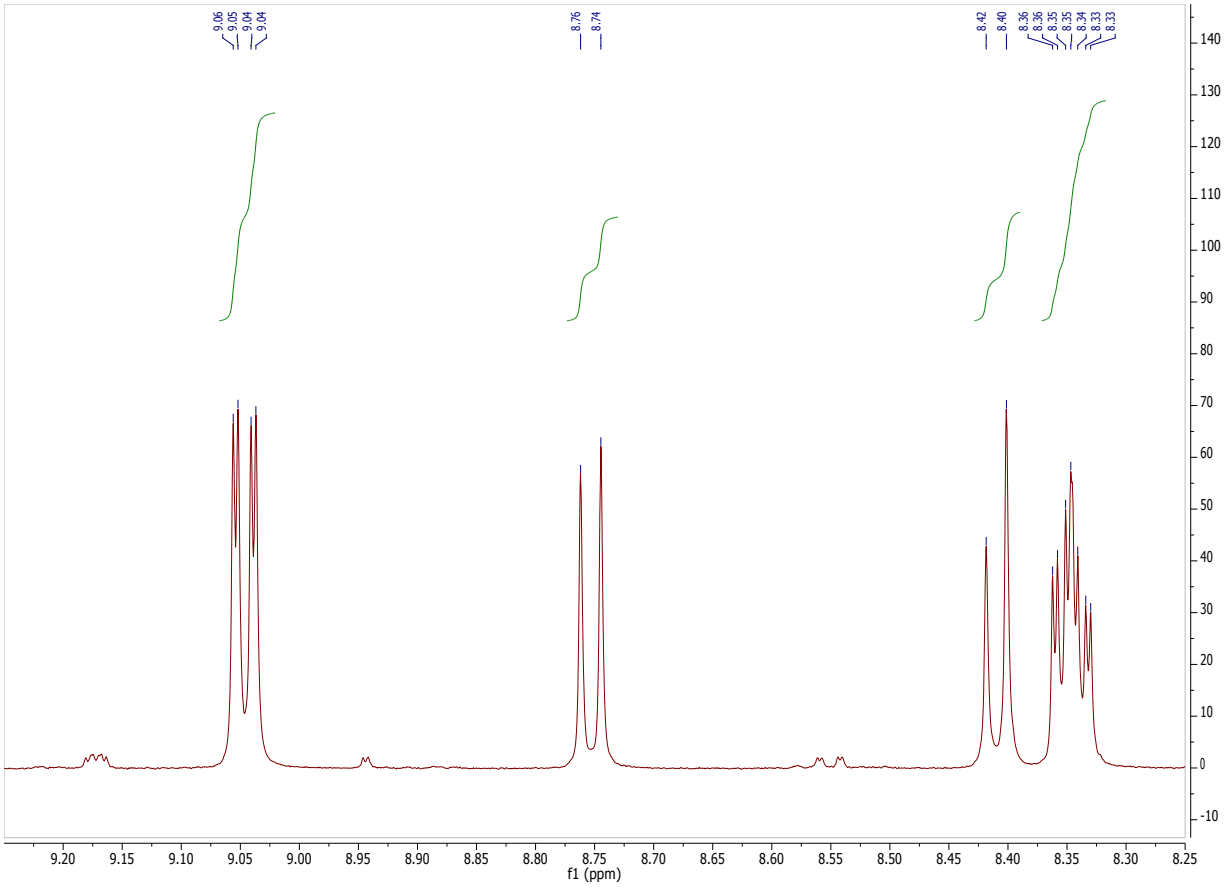


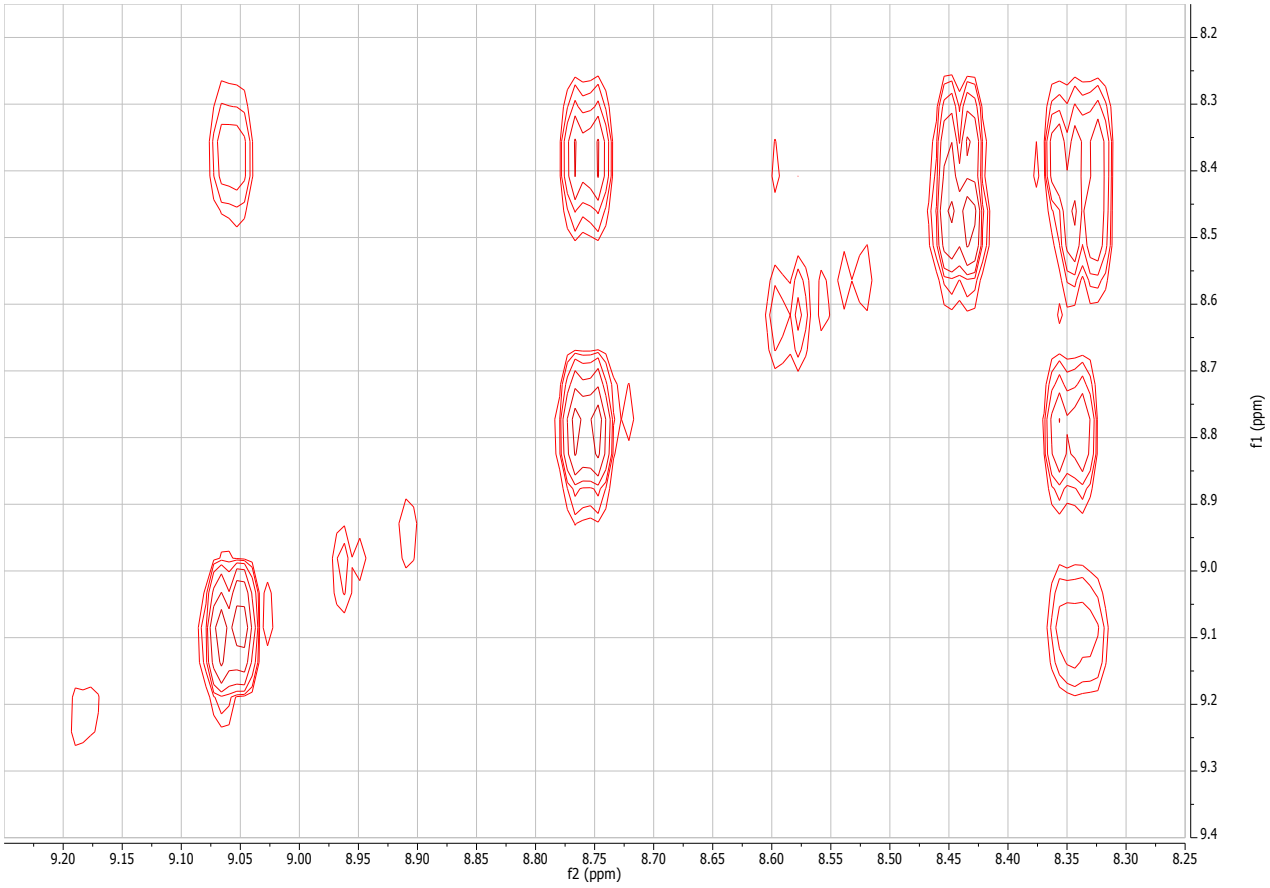
^{1}H NMR spectrum and ^{1}H,^{1}H-COSY spectrum of compound **15** (500 MHz, THF-d_8)



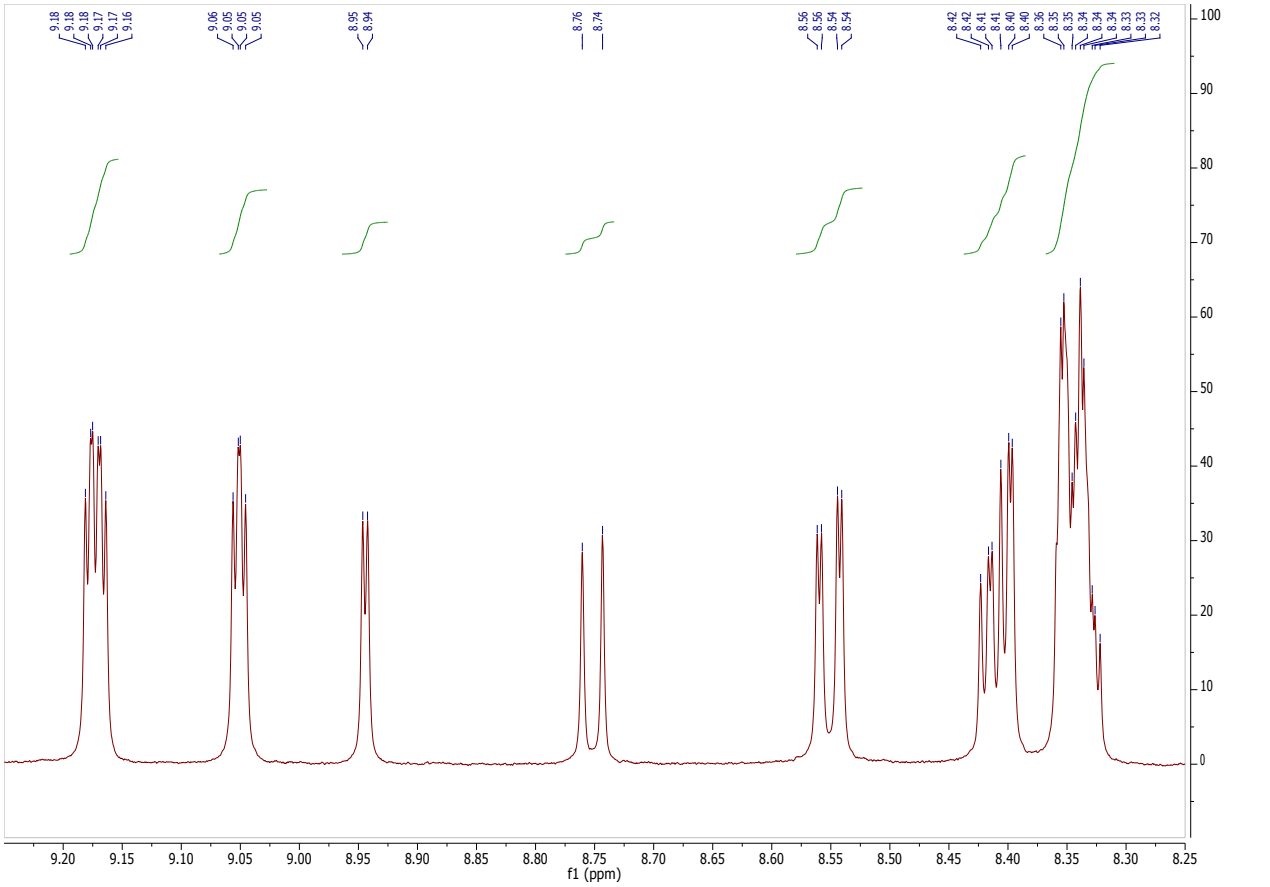


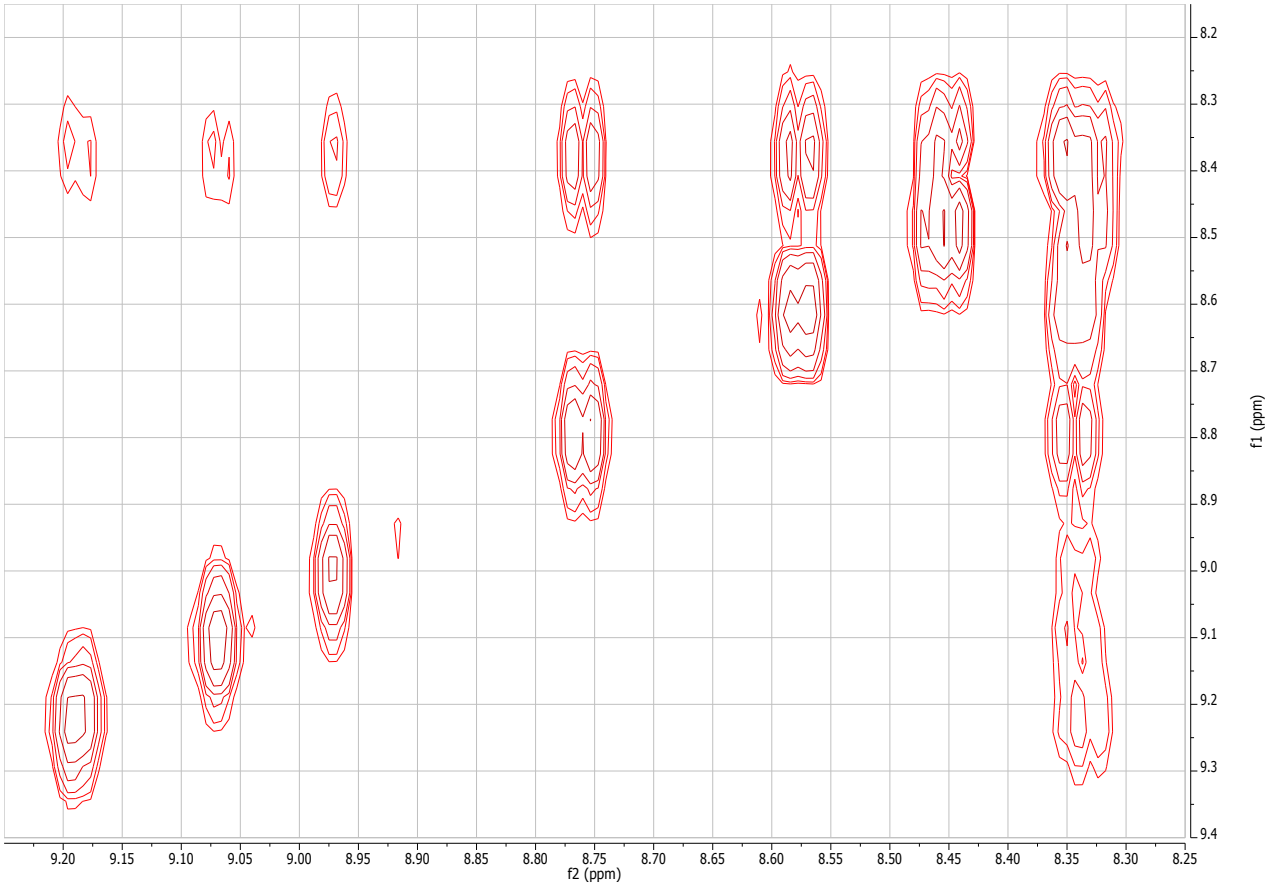
^{1}H NMR spectrum and ^{1}H,^{1}H-COSY spectrum of compound **16** (500 MHz, THF-d_8)



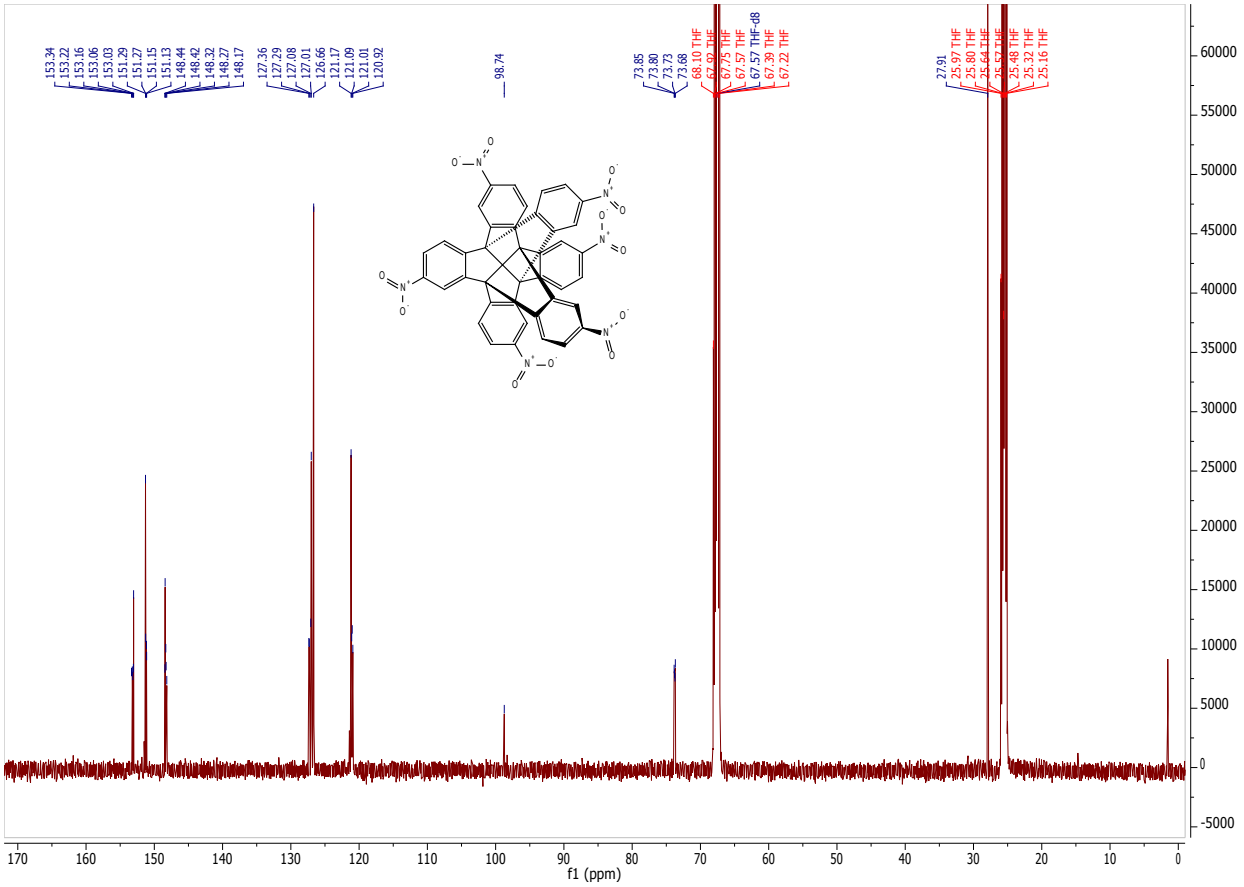


^{1}H NMR spectrum and ^{1}H,^{1}H-COSY spectrum of compound **17** (500 MHz, THF-d_8)

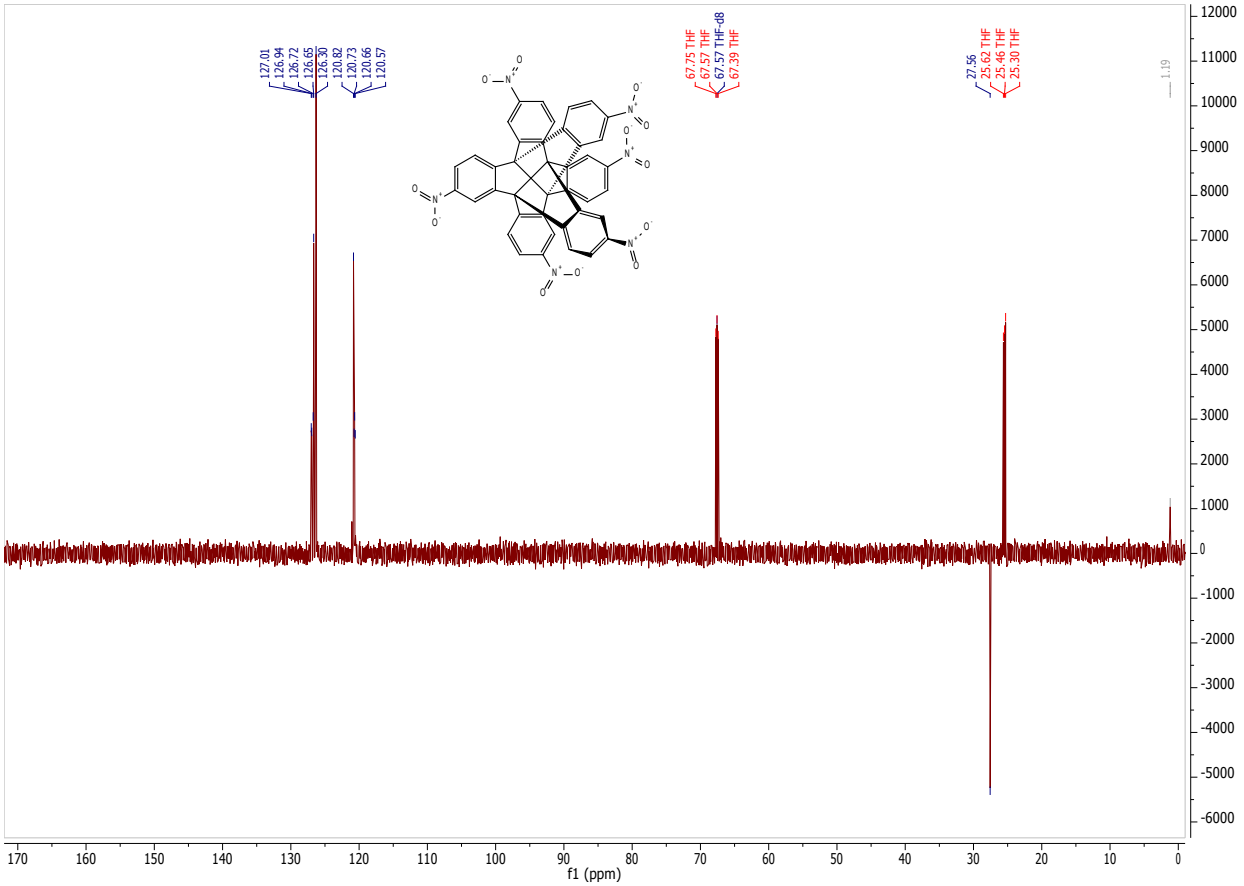




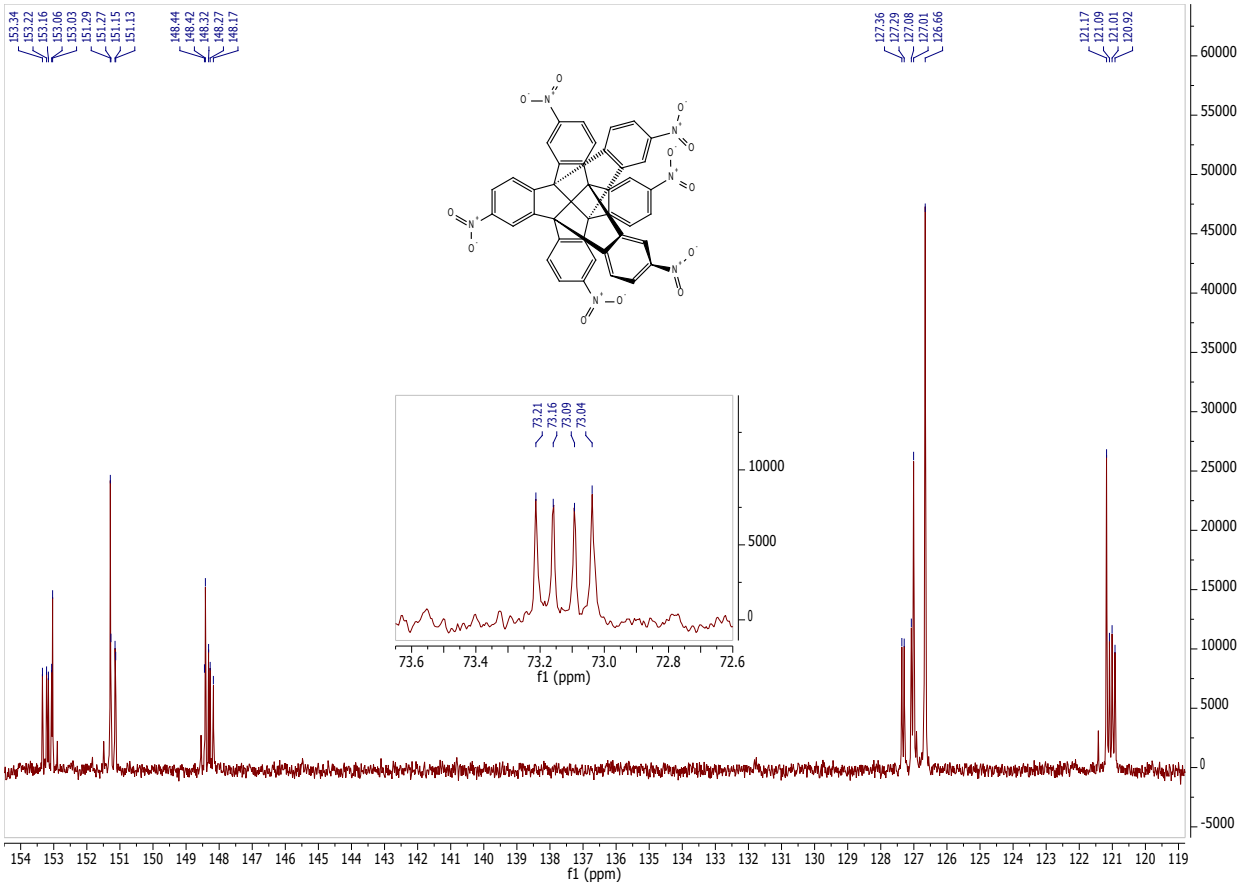
^{13}C NMR spectra of compound **14** (126 MHz, THF-d_8)



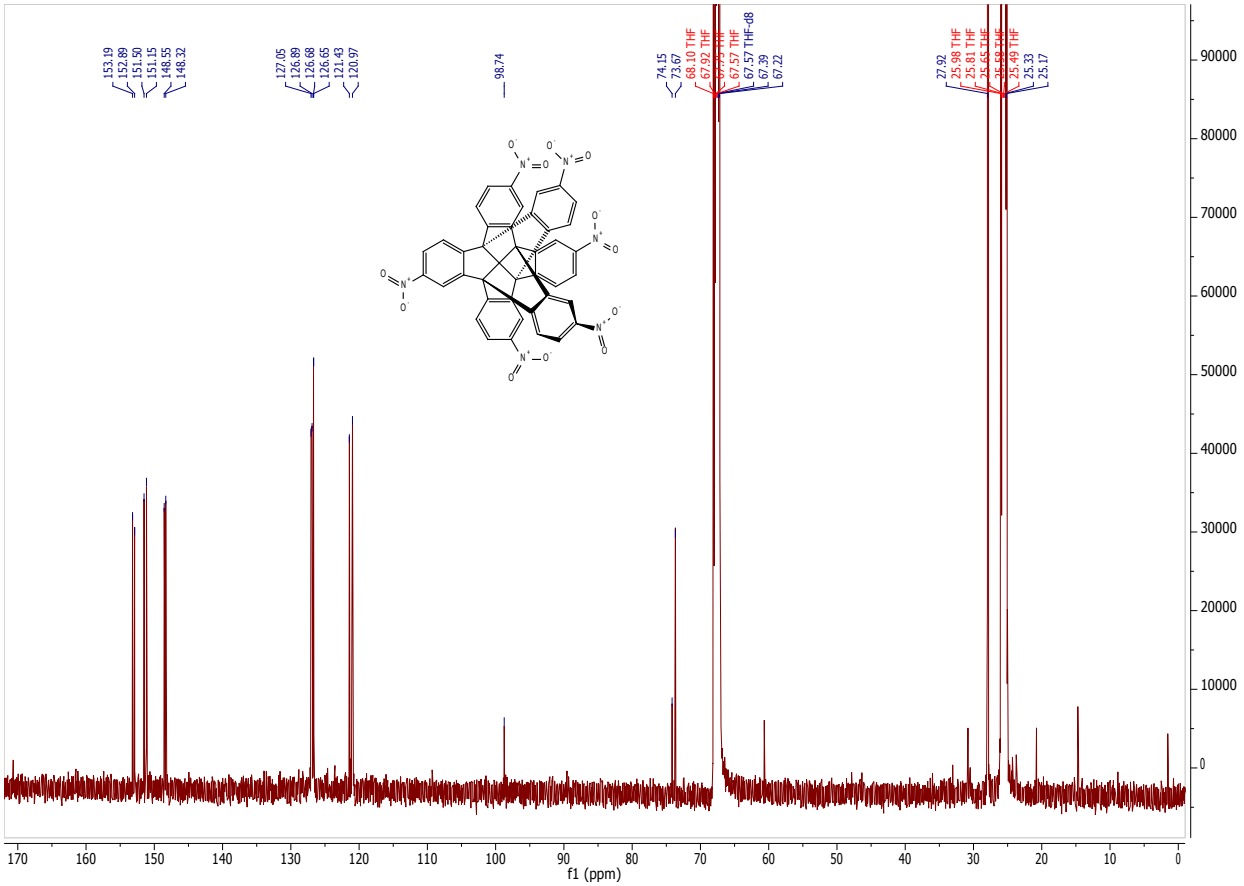
DEPT-135



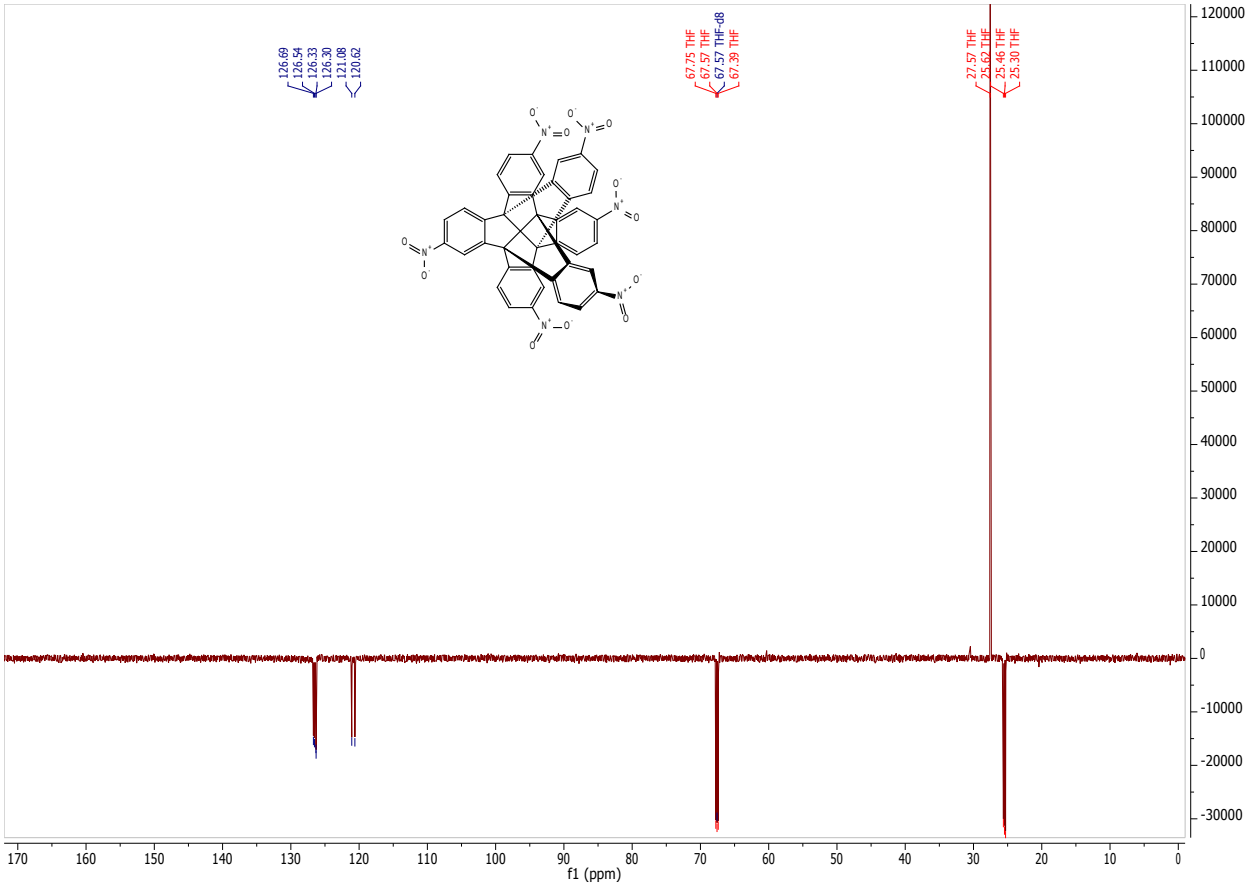
Magnification of the ranges of C^{arene} and C^{α} resonances (insert)



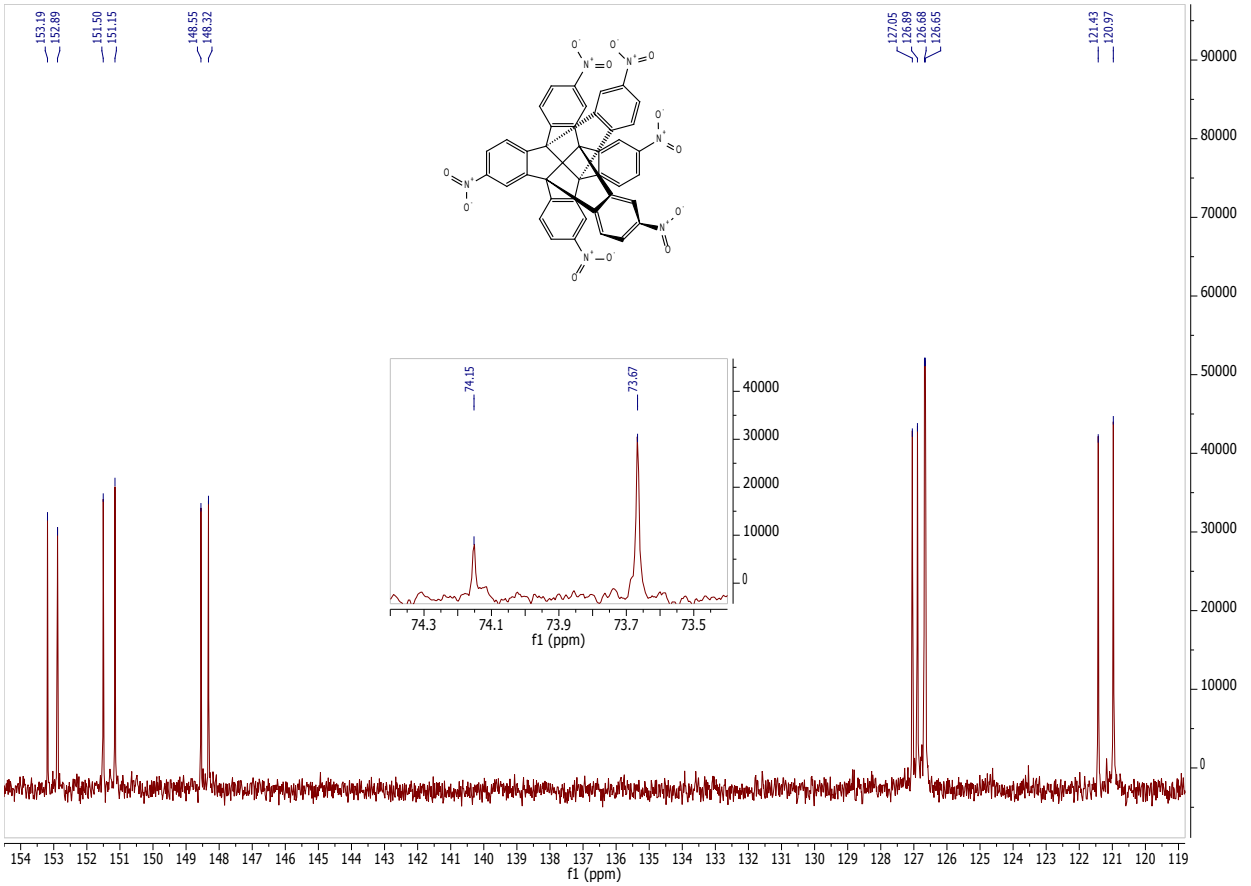
^{13}C NMR spectra of compound **15** (126 MHz, THF-d_8)



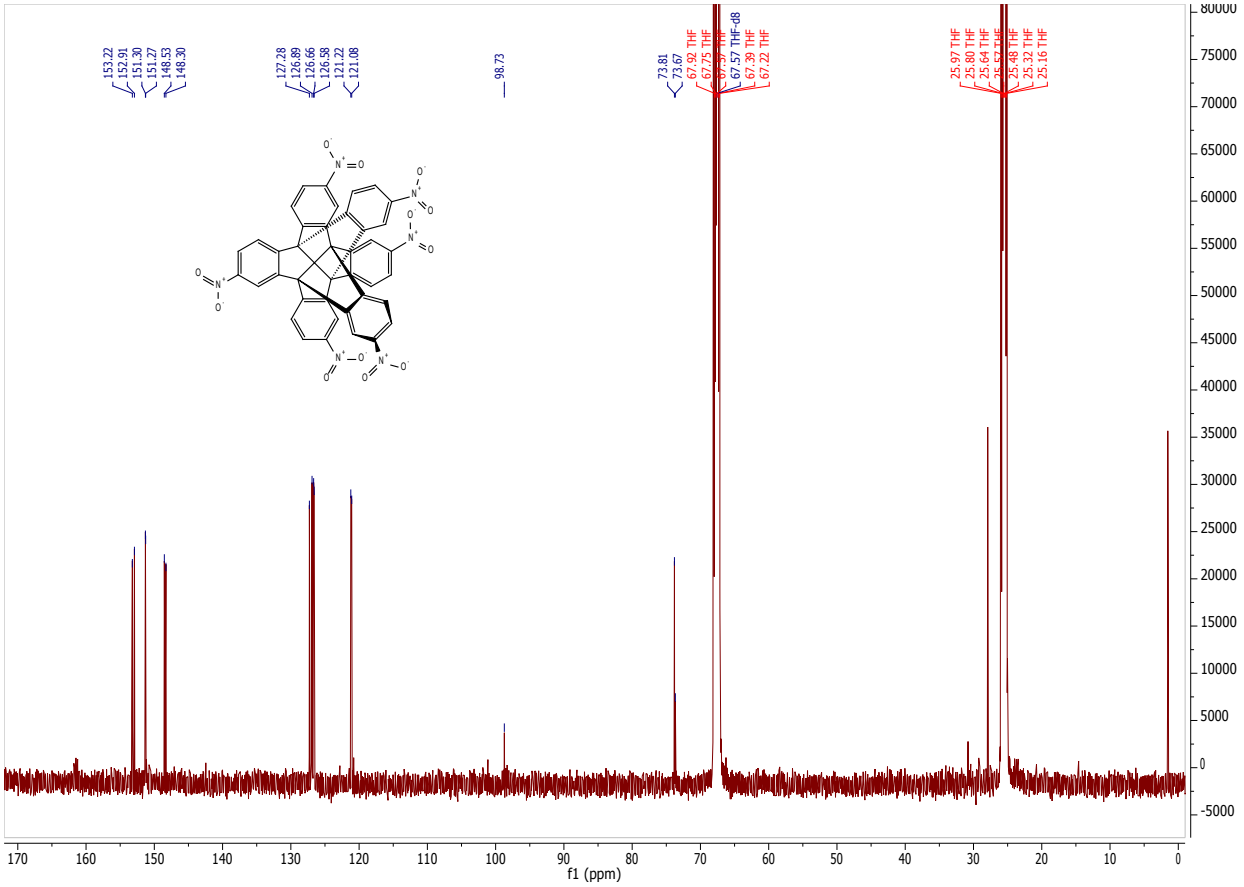
DEPT-135 (with reversed sign due to the exceedingly large solvent signal)



Magnification of the ranges of C^{arene} and C^{α} resonances (insert)



^{13}C NMR spectra of compound **16** (126 MHz, THF-d_8)



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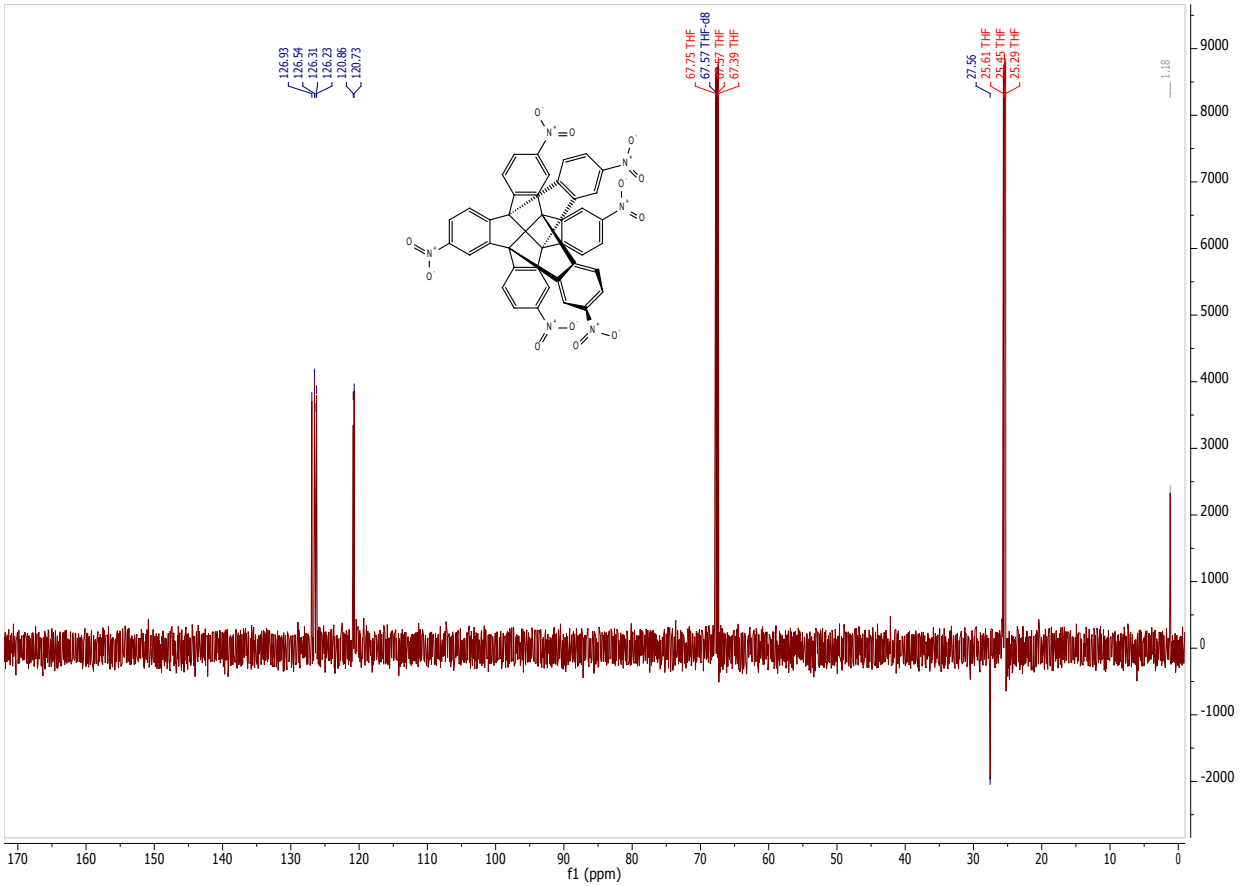
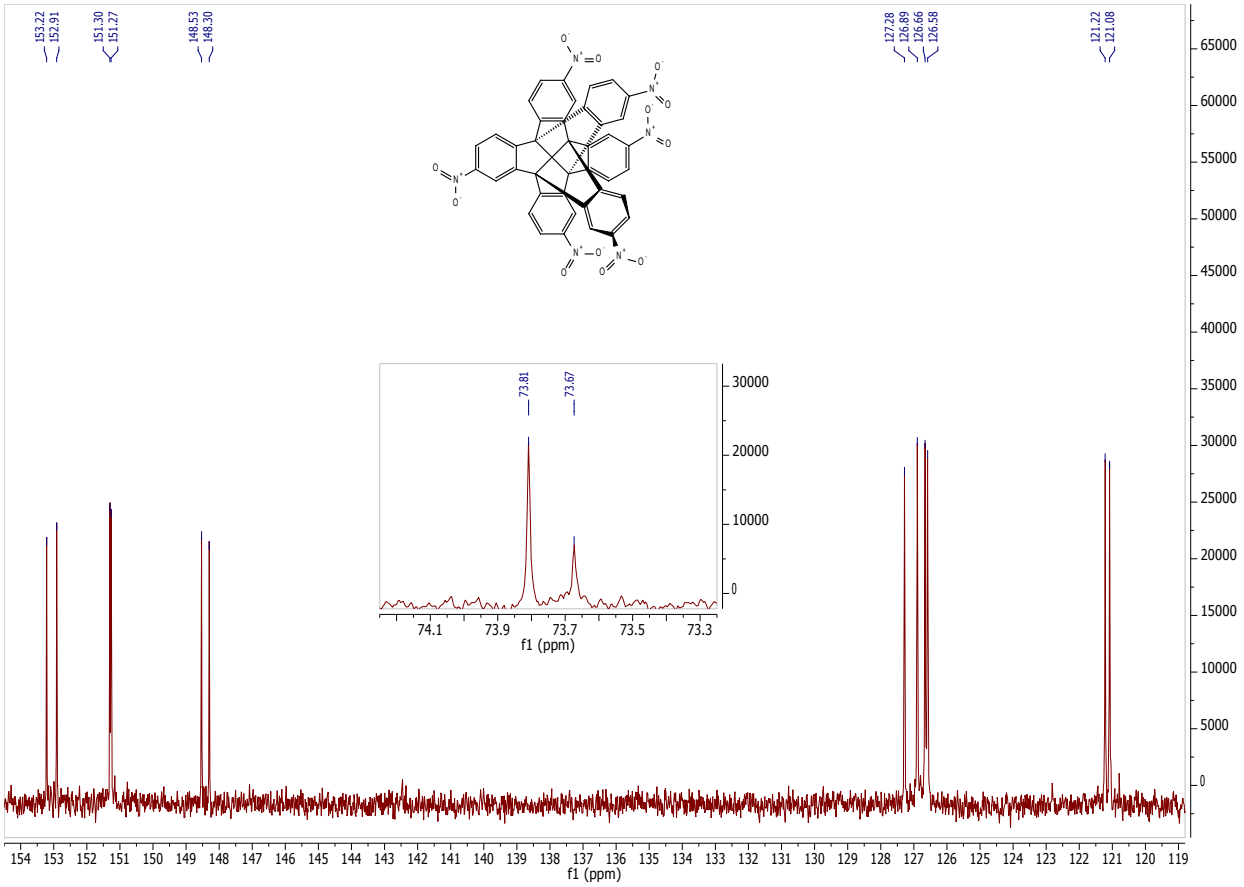
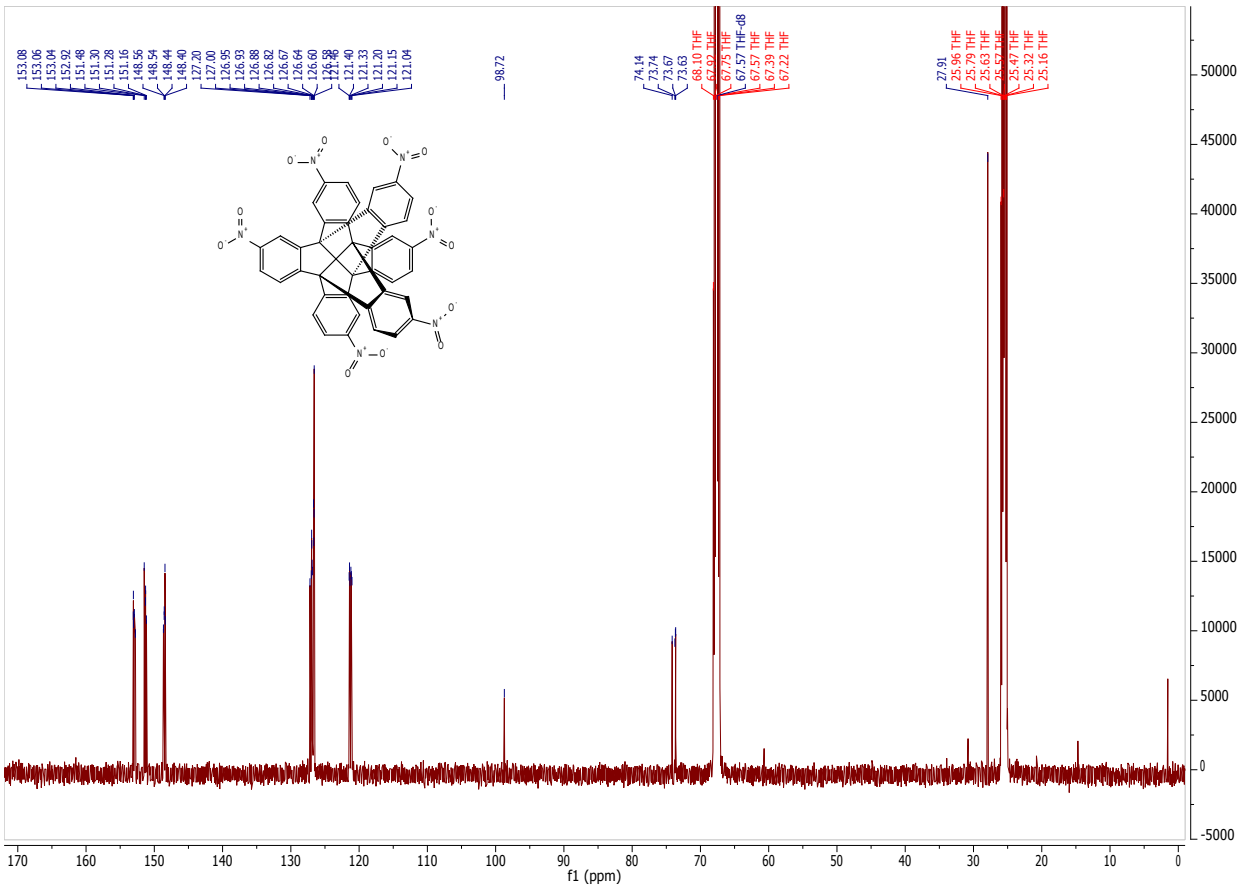


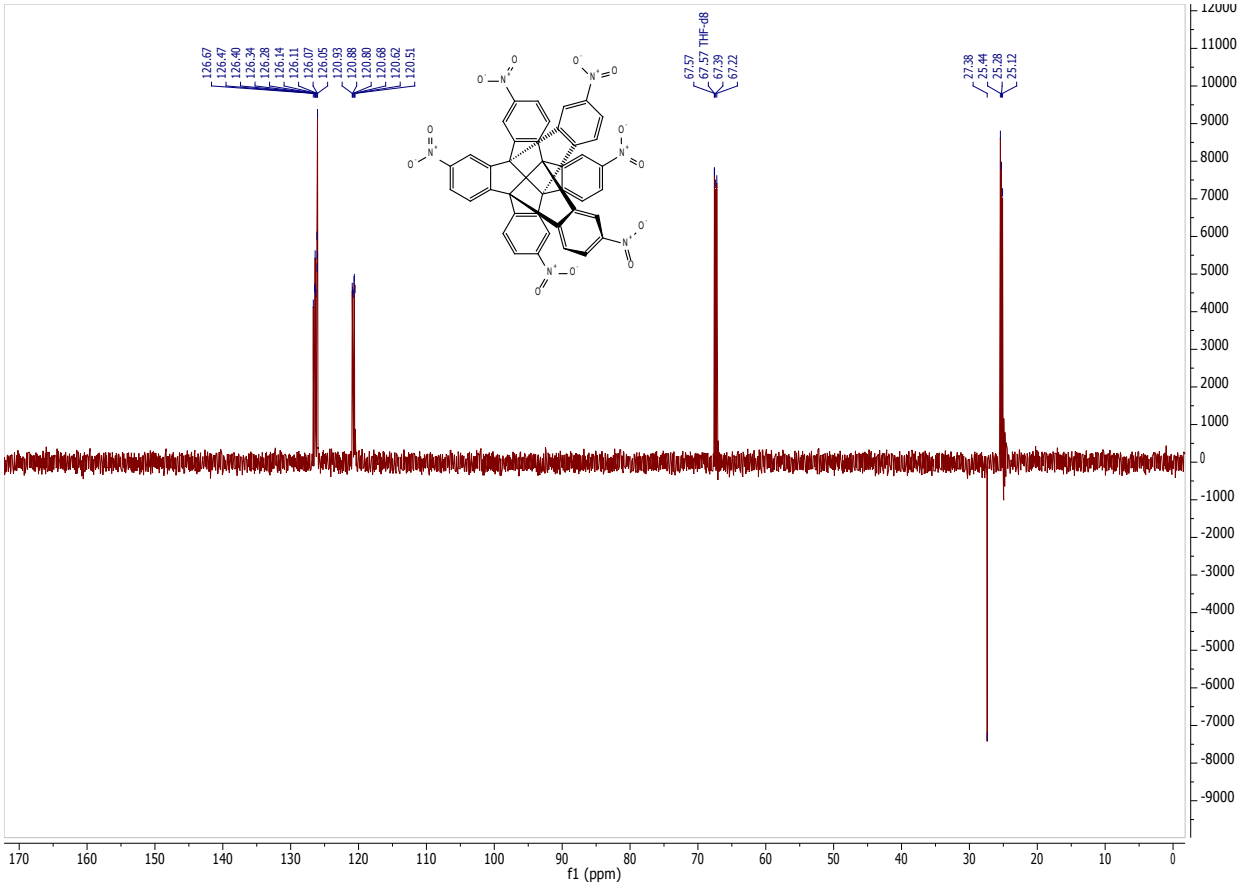
Magnification of the ranges of C^{arene} and C^{α} resonances (insert)



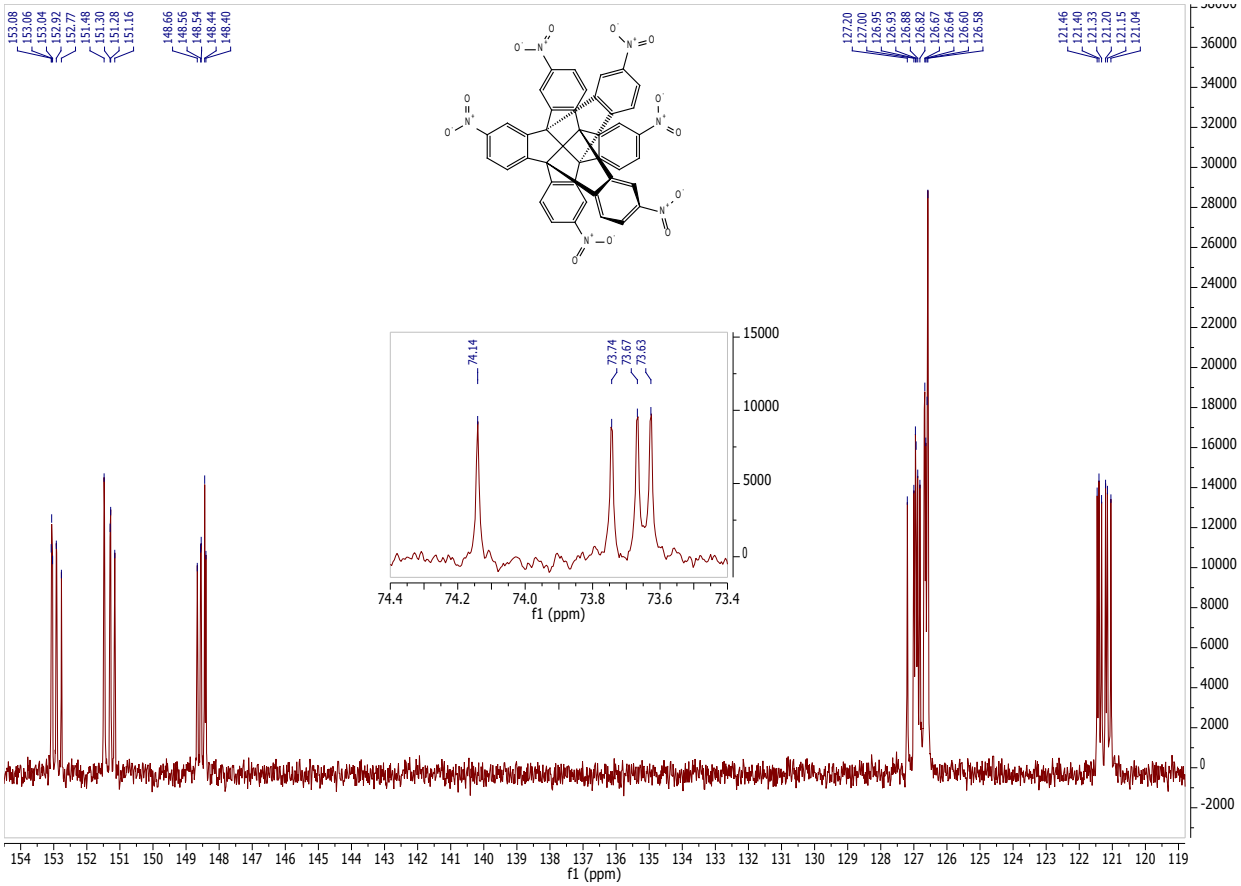
^{13}C NMR spectra of compound **17** (126 MHz, THF-d_8)



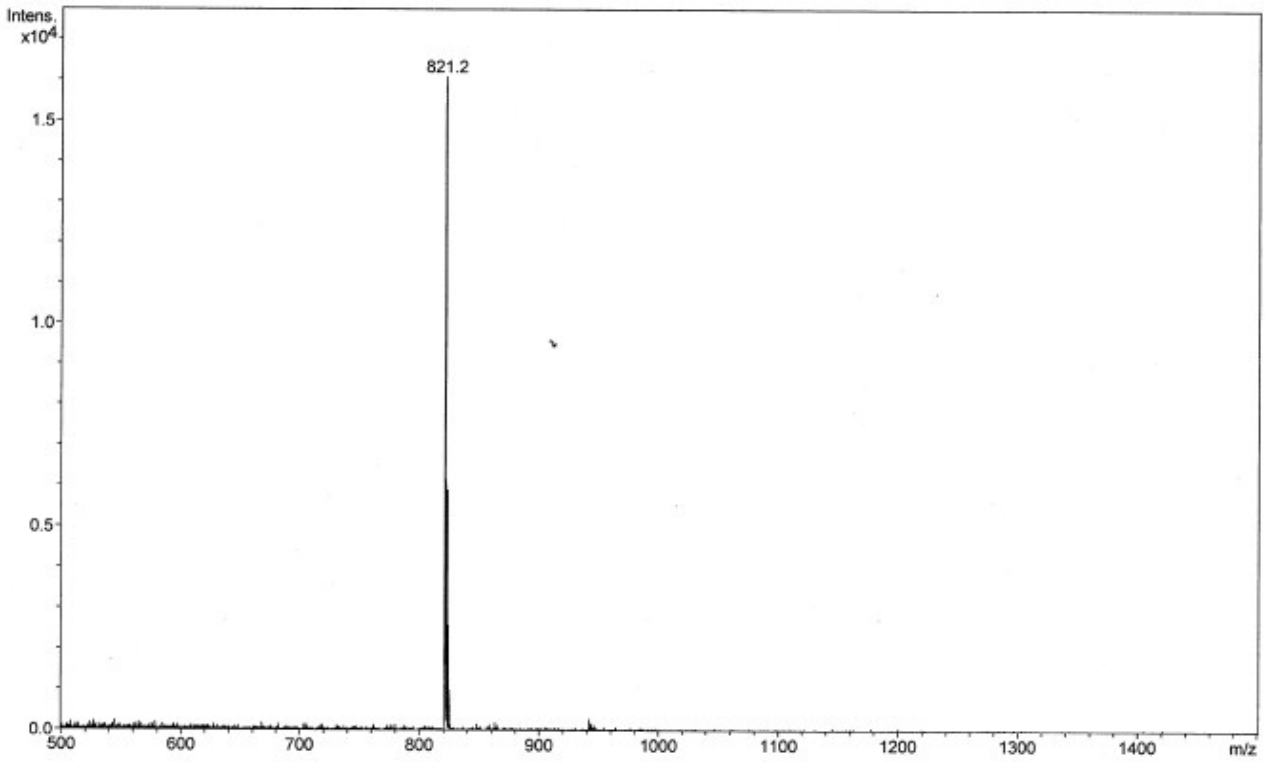
DEPT-135



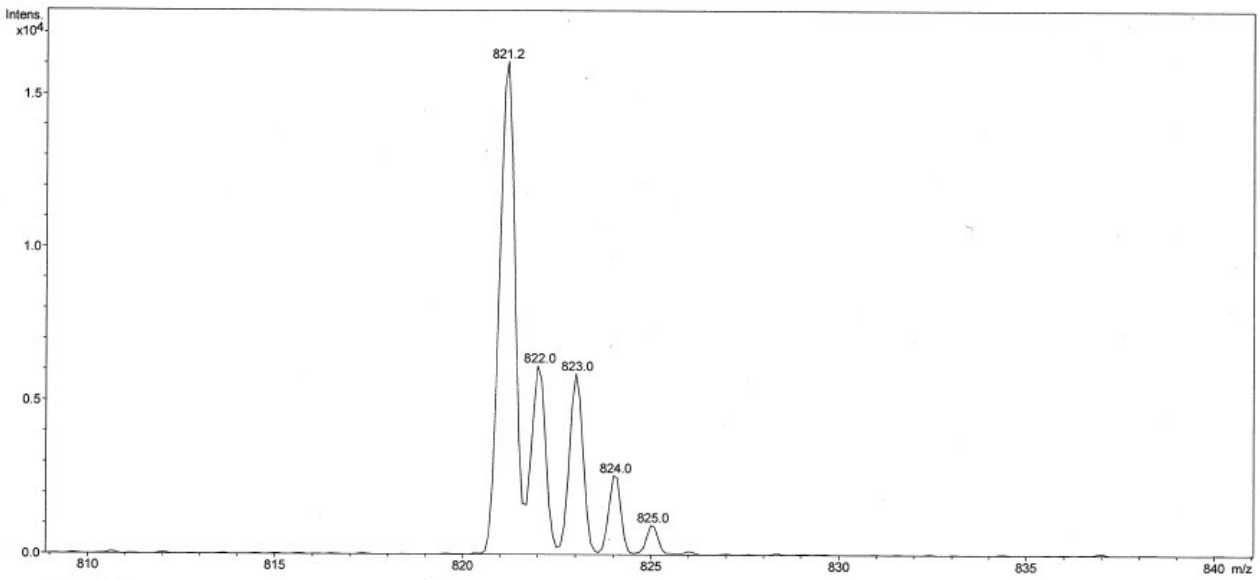
Magnification of the ranges of C^{arene} and C^{α} resonances (insert)



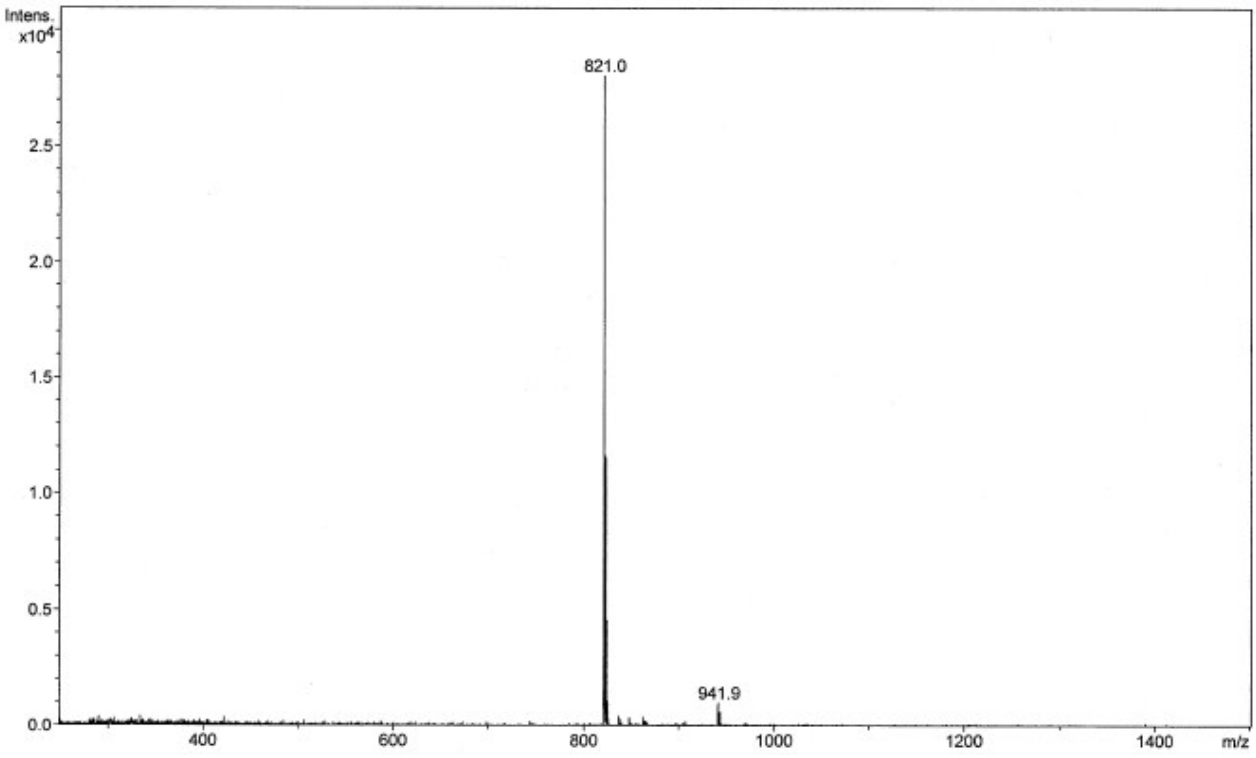
Mass spectrum (-)-ESI (MeCN, LiCl) of compound **14**



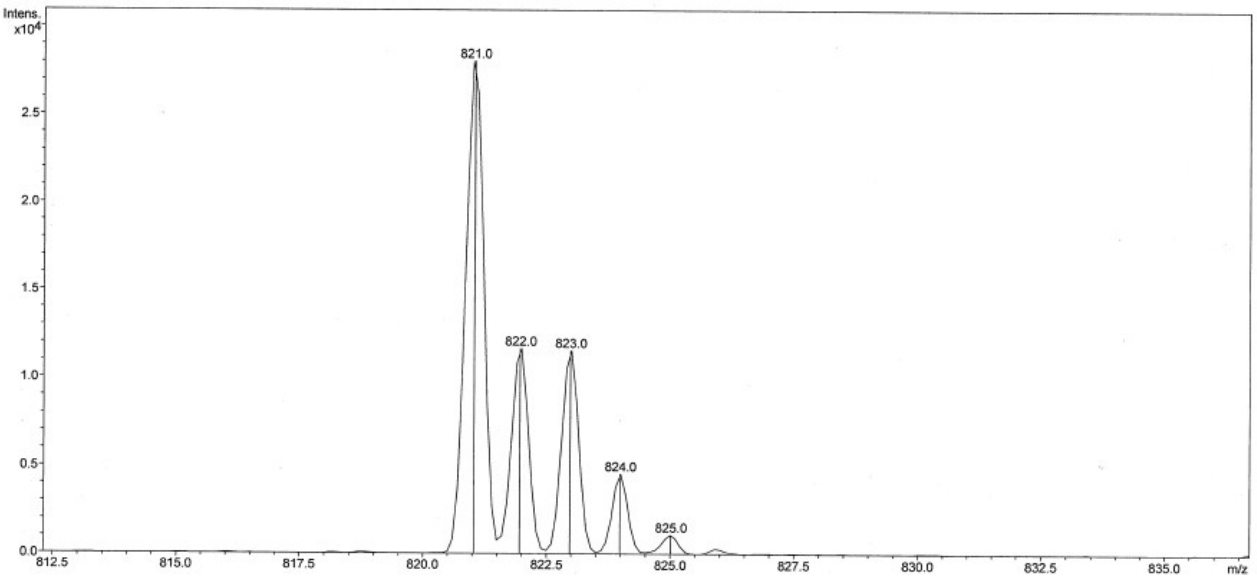
$[M + Cl]^-$ molecular adduct ion peak group



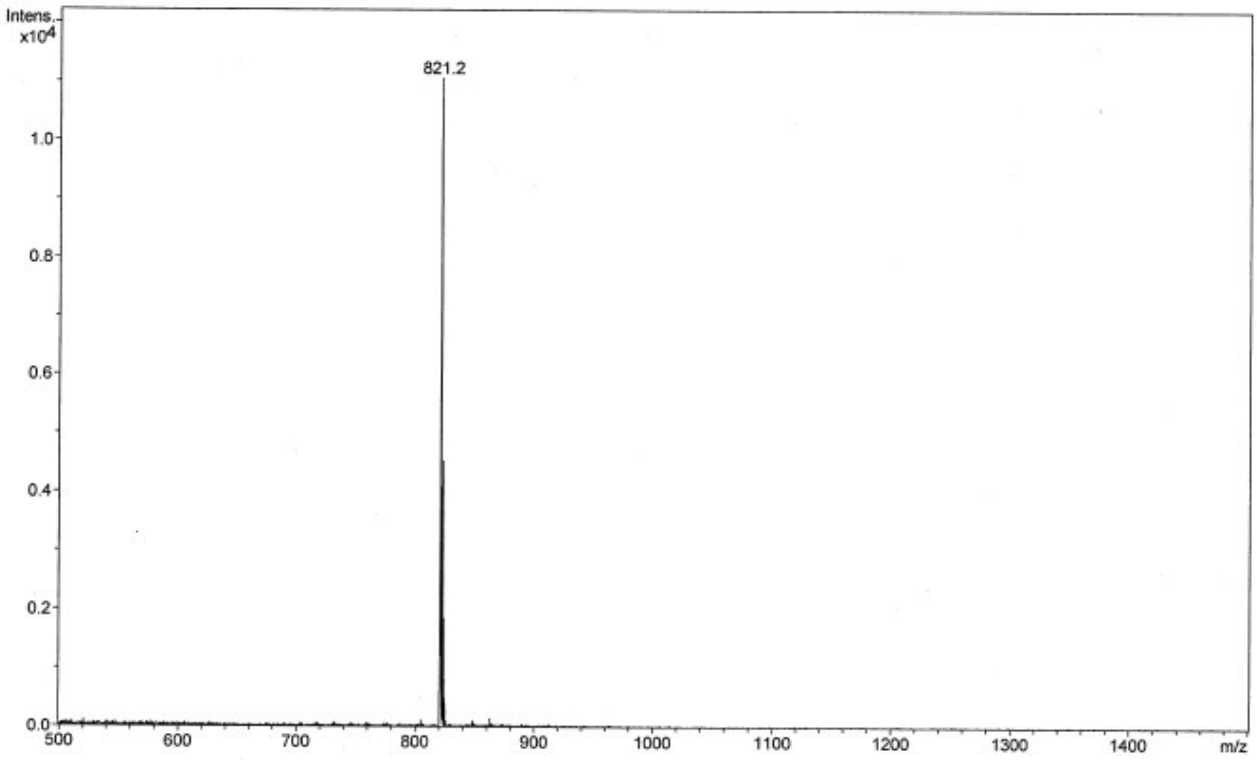
Mass spectrum (-)-ESI (MeCN, LiCl) of compound **15**



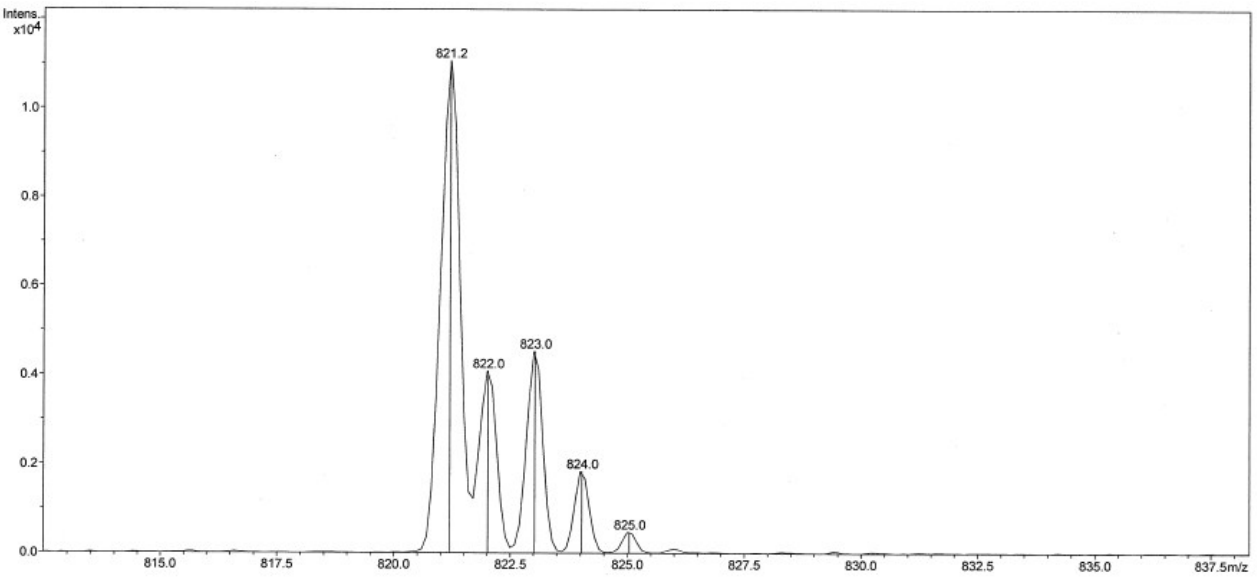
$[M + Cl]^-$ molecular adduct ion peak group



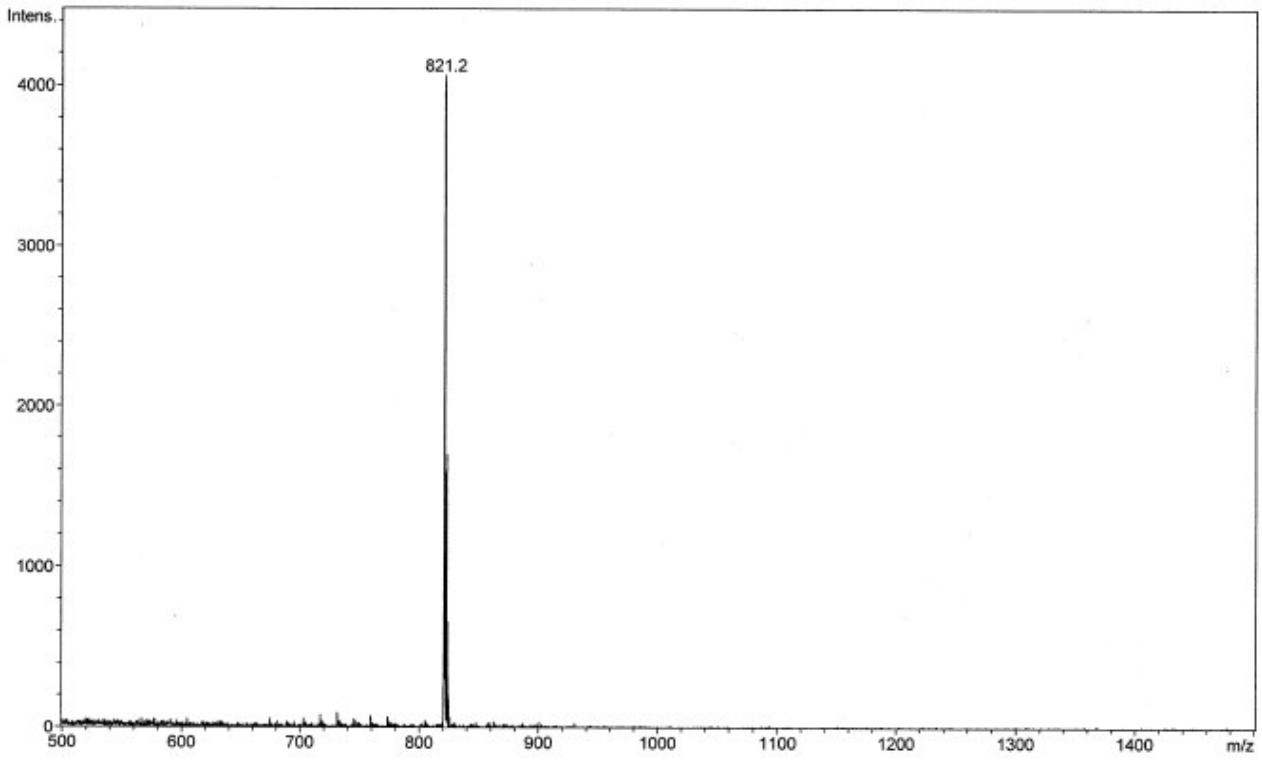
Mass spectrum (-)-ESI (MeCN, LiCl) of compound **16**



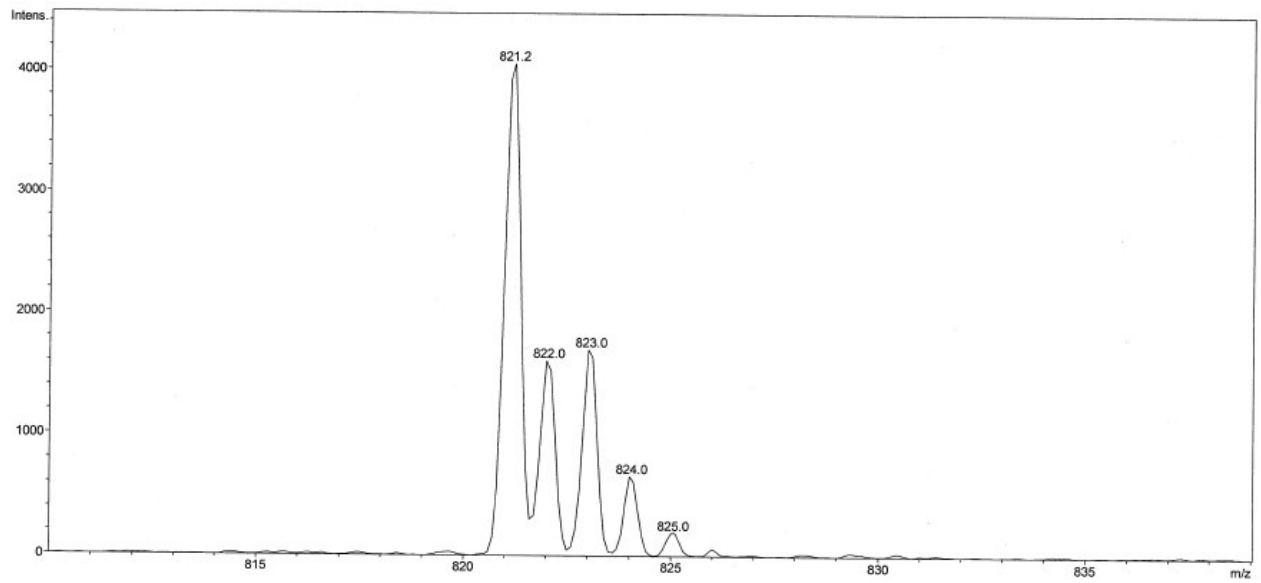
$[M + Cl]^-$ molecular adduct ion peak group



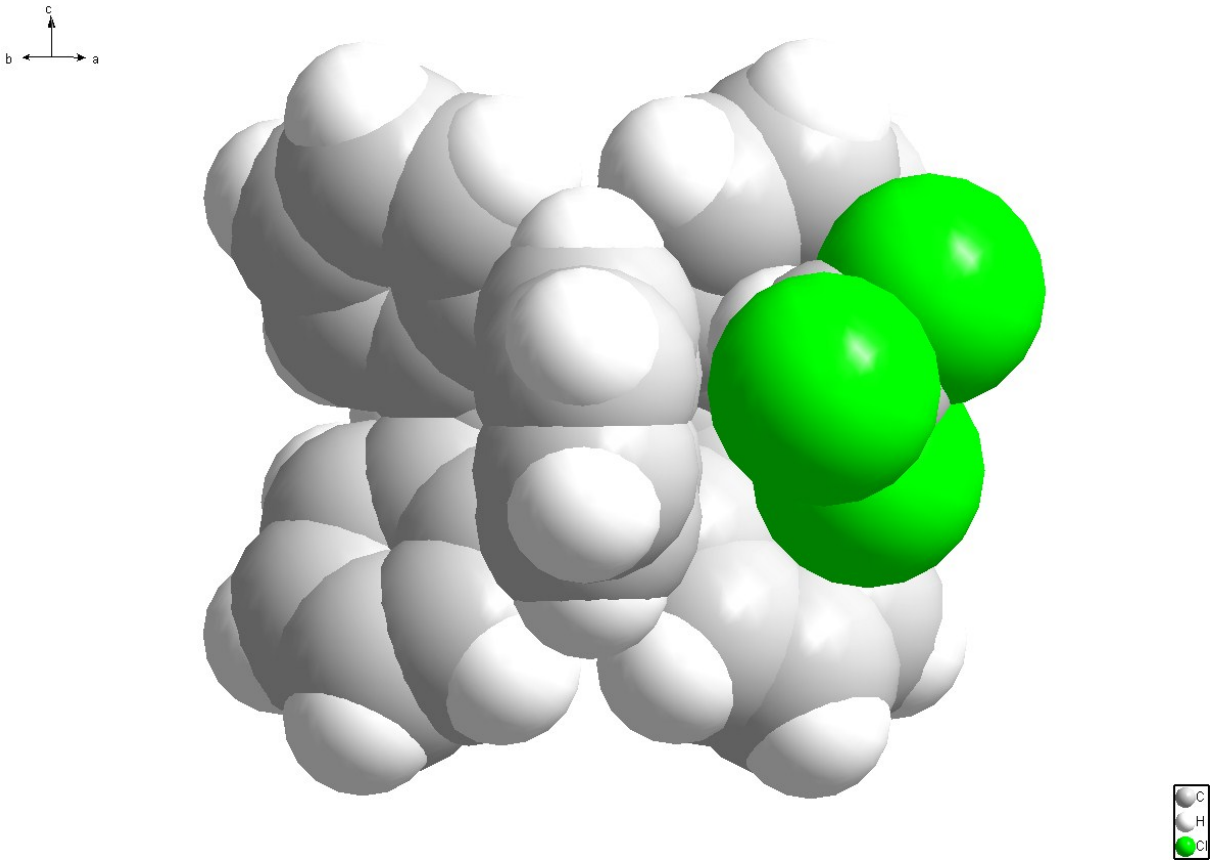
Mass spectrum (-)-ESI (MeCN, LiCl) of compound **17**



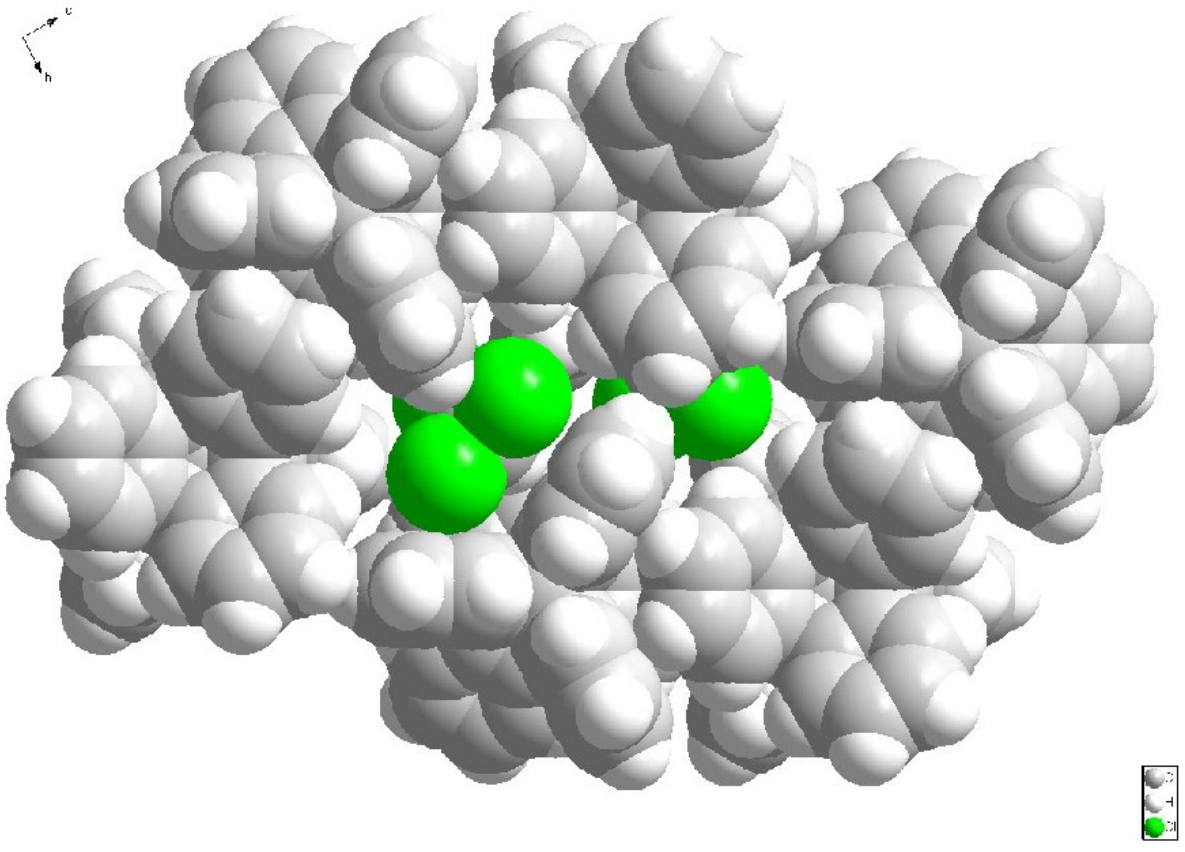
$[M + Cl]^-$ molecular adduct ion peak group



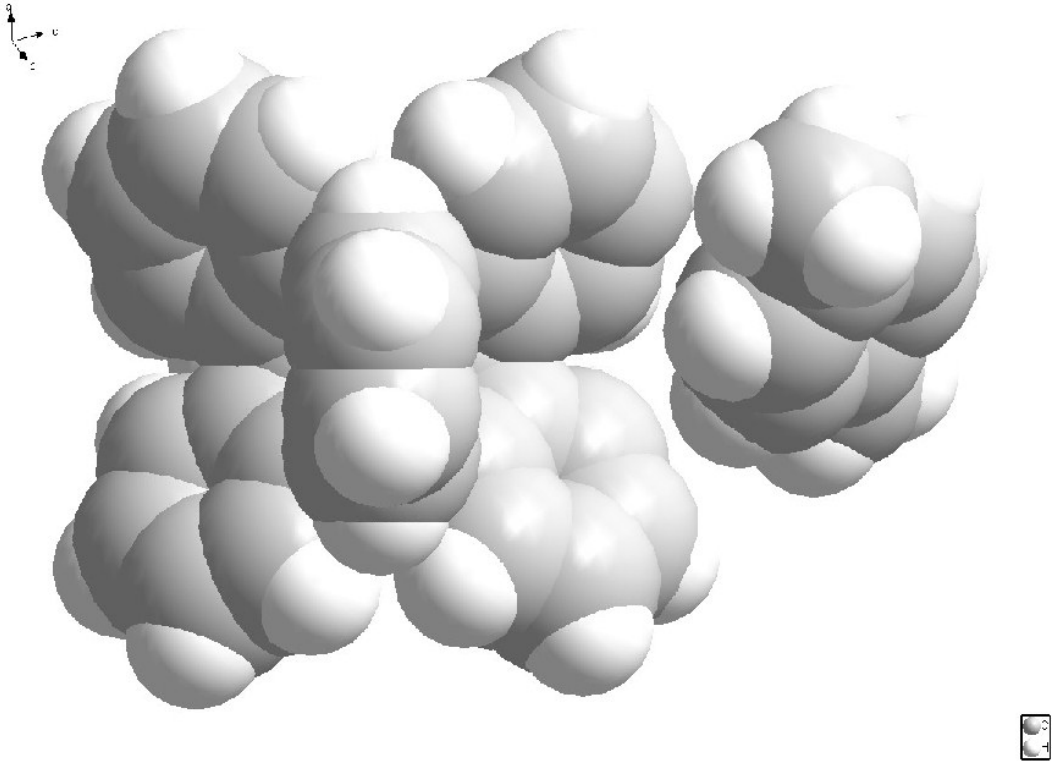
Solid-state structure of centrohexaindane, 1 · $CHCl_3$



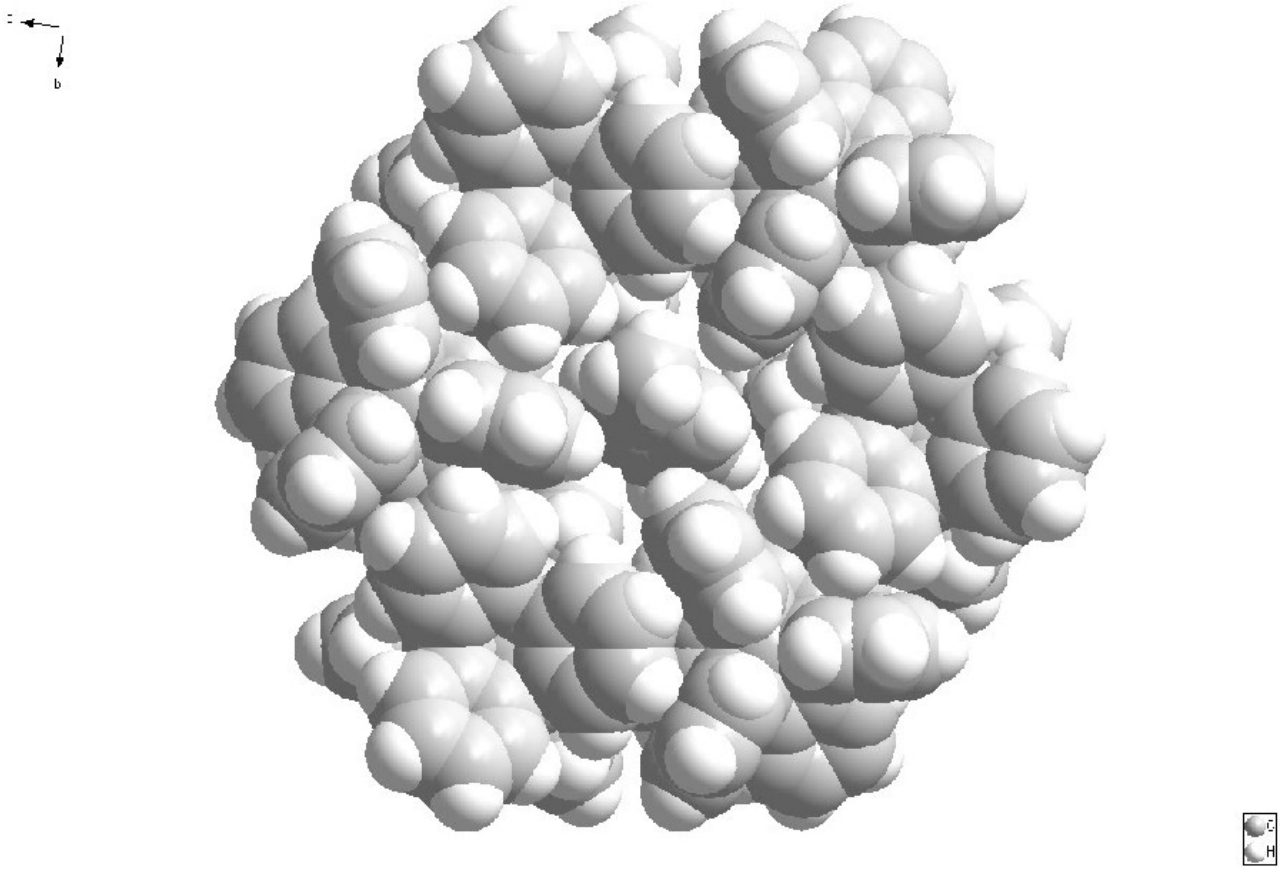
Stacking showing six molecules of **1** and two molecules of chloroform (centre)



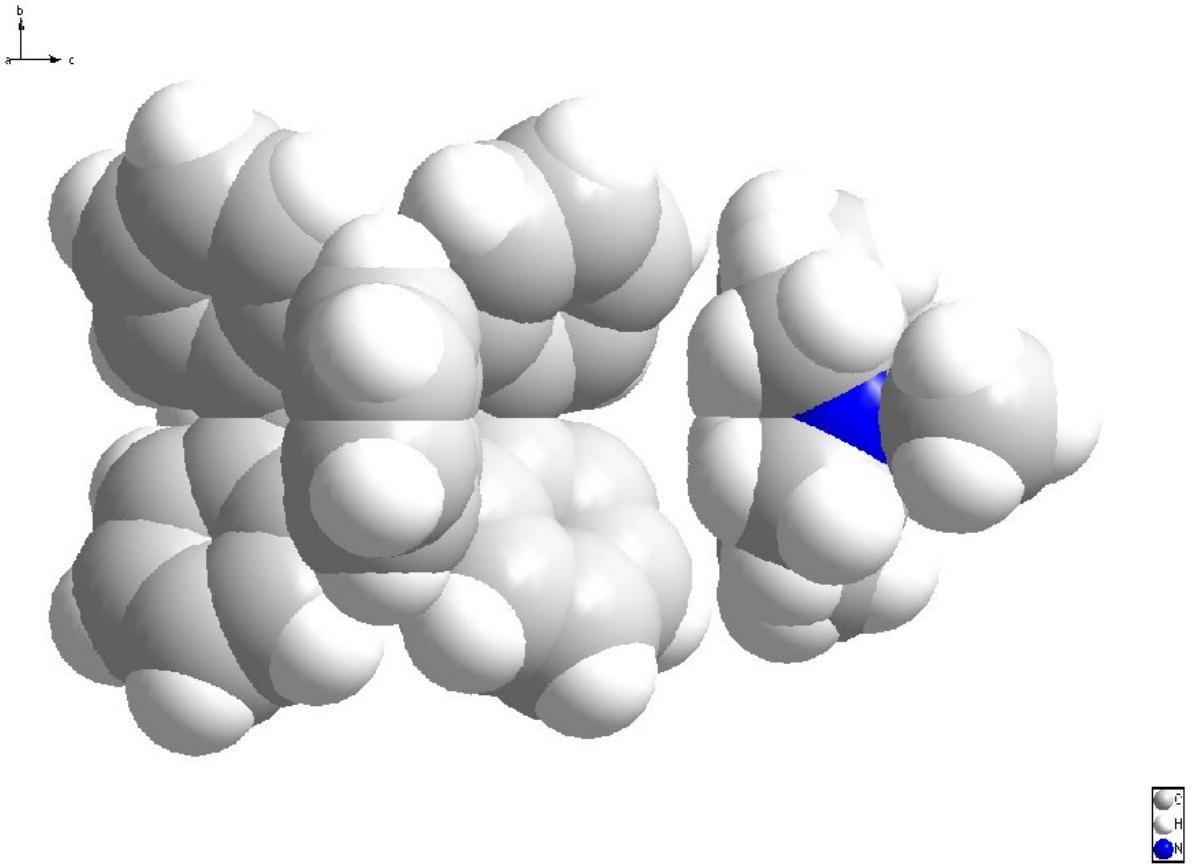
Solid-state structure of centrohexaindane, 1 · 0.5 *para*-xylene



Stacking showing six molecule of **1** and one molecule of *para*-xylene (centre)



Solid-state structure of centrohexaindane, 1 · NEt_3



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