**Supporting Information**

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**Transition Temperature Engineering of Octaalkoxycarbonyl Phthalocyanines**

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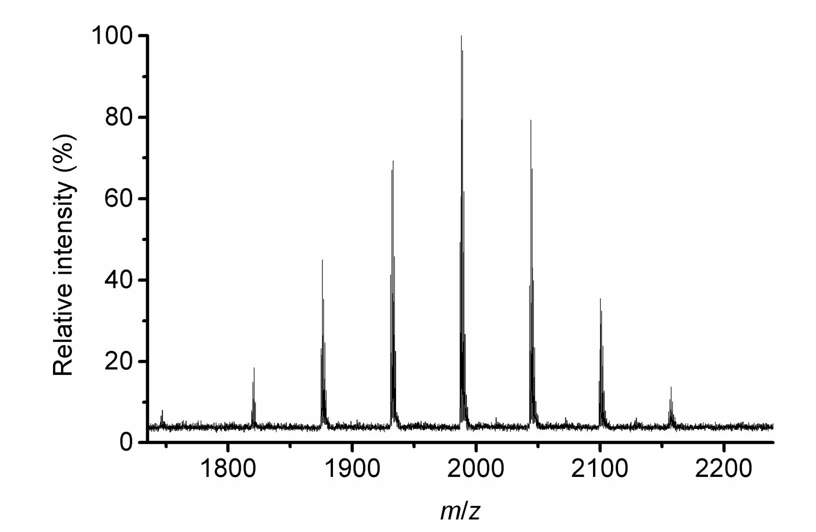


**Fig. SI 1** MALDI mass spectra of **4**

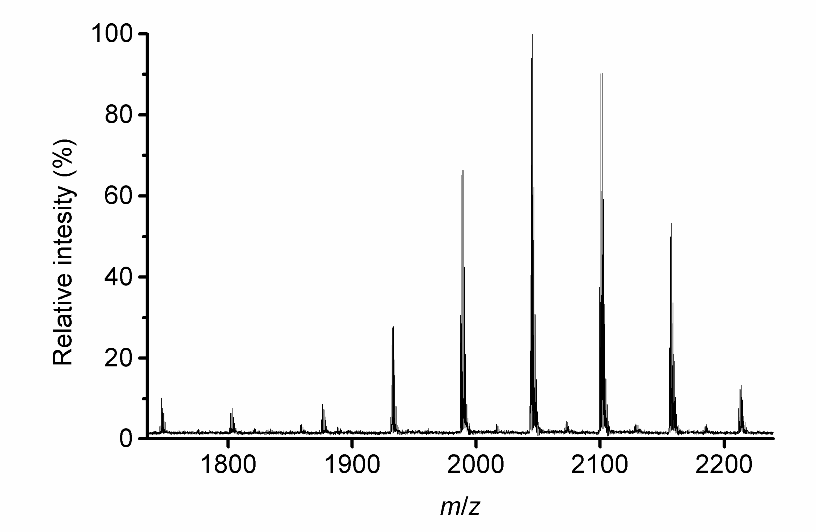


**Fig. SI 2** MALDI mass spectra of **5**

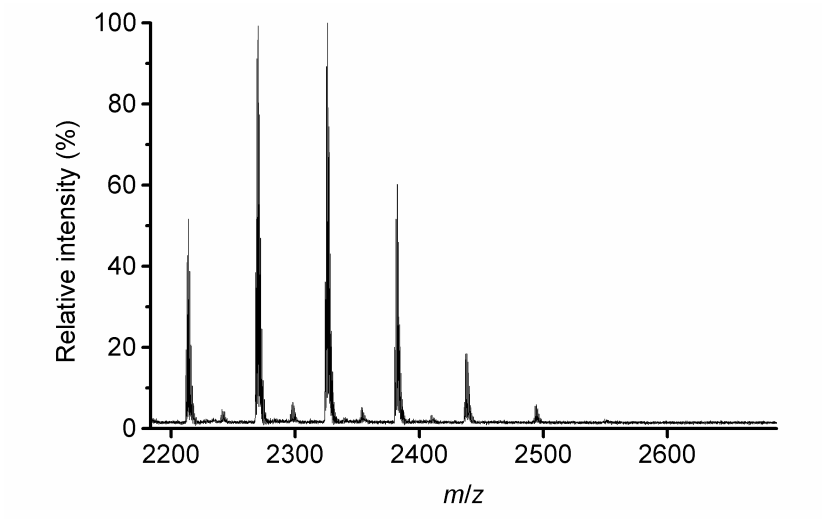


**Fig. SI 3** MALDI mass spectra of **6**

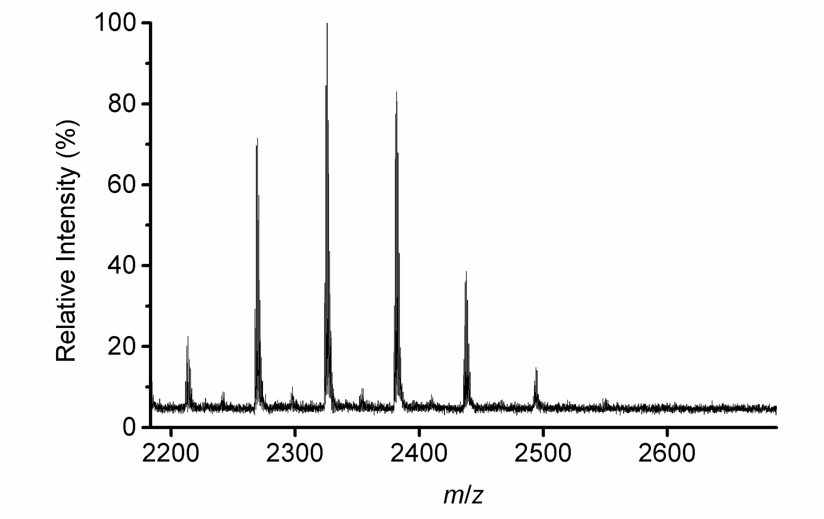


**Fig. SI 4** MALDI mass spectra of **7**

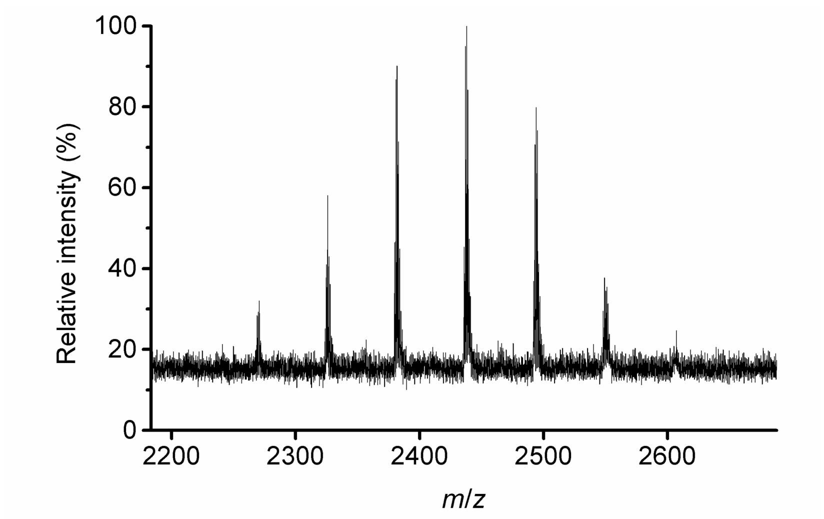


**Fig. SI 5** MALDI mass spectra of **8**

For Tables **SI 1–SI 5**, calculations have been performed as follows. Exact molecular masses and abundances of molecular ions with the lowest isotopic mass have been calculated with ChemDrawPro version 4.5 software package (CambridgeSoft Corporation). Distribution of products $Pc(COOR^1)_n(COOR^2)_{8-n}$ were calculated as coefficients of a binomial $(ax + by)^8$, where $a = 1$, $b = 1$ for **4** and **8**, $a = 1$, $b = 2$ for **5**, $a = 3$, $b = 1$ for **6**, and $a = 2$, $b = 1$ for **7**. Calculated relative intensity of signals corresponding to molecular ions with the lowest isotopic mass has been obtained by multiplying of distribution of products $Pc(COOR^1)_n(COOR^2)_{8-n}$ by the relative abundance of molecular ions with the lowest isotopic mass for each product followed by normalization (intensity of the most intense signal is taken as 100%).

**Table SI 1.** Calculated relative intensities of signals corresponding to molecular ions of individual components $Pc(COOR^1)_n(COOR^2)_{8-n}$ in **4** ($R^1 = C_{8,4}$, $R^2 = C_{6,2}$).

| *n* | Calculated exact molecular mass | Distribution of products, calculated as coefficients of binomial $(x + y)^8$ | Calculated abundance of molecular ions with the lowest isotopic mass (in % of the most intense isotopic peak) | Calculated relative intensity signals corresponding to molecular ions with the lowest isotopic mass, % |
|---|---|---|---|---|
| 0 | 1763.1 | 1.4 | 86.5 | 1.6 |
| 1 | 1819.1 | 11.4 | 83.2 | 12.7 |
| 2 | 1875.2 | 40.0 | 80.3 | 42.9 |
| 3 | 1931.3 | 80.0 | 77.5 | 82.8 |
| 4 | 1987.3 | 100.0 | 74.9 | 100 |
| 5 | 2043.4 | 80.0 | 72.5 | 77.4 |
| 6 | 2099.5 | 40.0 | 70.2 | 37.5 |
| 7 | 2155.5 | 11.4 | 68.1 | 10.4 |
| 8 | 2211.6 | 1.4 | 66.1 | 1.3 |

**Table SI 2.** Calculated relative intensities of signals corresponding to molecular ions of individual components Pc(COOR[1])$_n$(COOR[2])$_{8–n}$ in **5** ($R^1 = C_{8,4}$, $R^2 = C_{6,2}$).

| *n* | Calculated exact molecular mass | Distribution of products, calculated as coefficients of binomial $(x + 2y)^8$ | Calculated abundance of molecular ions with the lowest isotopic mass (in % of the most intense isotopic peak) | Calculated relative intensity signals corresponding to molecular ions with the lowest isotopic mass, % |
|---|---|---|---|---|
| 0 | 1763.1 | 0.06 | 86.5 | 0.07 |
| 1 | 1819.1 | 0.9 | 83.2 | 1.0 |
| 2 | 1875.2 | 6.25 | 80.3 | 6.9 |
| 3 | 1931.3 | 25 | 77.5 | 26.7 |
| 4 | 1987.3 | 62.5 | 74.9 | 64.6 |
| 5 | 2043.4 | 100 | 72.5 | 100 |
| 6 | 2099.5 | 100 | 70.2 | 96.8 |
| 7 | 2155.5 | 57.1 | 68.1 | 53.7 |
| 8 | 2211.6 | 14.3 | 66.1 | 13.0 |

**Table SI 3.** Calculated relative intensities of signals corresponding to molecular ions of individual components Pc(COOR[1])$_n$(COOR[2])$_{8–n}$ in **6** ($R^1 = C_{10,6}$, $R^2 = C_{8,4}$).

| *n* | Calculated exact molecular mass | Distribution of products, calculated as coefficients of binomial $(3x + y)^8$ | Calculated abundance of molecular ions with the lowest isotopic mass (in % of the most intense isotopic peak) | Calculated relative intensity signals corresponding to molecular ions with the lowest isotopic mass, % |
|---|---|---|---|---|
| 0 | 2211.6 | 32.1 | 66.1 | 34.0 |
| 1 | 2267.6 | 85.7 | 64.2 | 88.2 |
| 2 | 2323.7 | 100 | 62.4 | 100 |
| 3 | 2379.8 | 66.7 | 60.7 | 64.9 |
| 4 | 2435.8 | 27.8 | 59.2 | 26.4 |
| 5 | 2491.9 | 7.4 | 57.6 | 6.8 |
| 6 | 2548.0 | 1.2 | 56.2 | 1.1 |
| 7 | 2604.0 | 0.1 | 54.8 | 0.1 |
| 8 | 2660.1 | 0.005 | 53.5 | 0.004 |

**Table SI 4.** Calculated relative intensities of signals corresponding to molecular ions of individual components $Pc(COOR^1)_n(COOR^2)_{8-n}$ in **7** ($R^1 = C_{10,6}$, $R^2 = C_{8,4}$).

| *n* | Calculated exact molecular mass | Distribution of products, calculated as coefficients of binomial $(2x + y)^8$ | Calculated abundance of molecular ions with the lowest isotopic mass (in % of the most intense isotopic peak) | Calculated relative intensity signals corresponding to molecular ions with the lowest isotopic mass, % |
|---|---|---|---|---|
| 0 | 2211.6 | 14.3 | 66.1 | 15.1 |
| 1 | 2267.6 | 57.1 | 64.2 | 58.8 |
| 2 | 2323.7 | 100 | 62.4 | 100 |
| 3 | 2379.8 | 100 | 60.7 | 97.3 |
| 4 | 2435.8 | 62.5 | 59.2 | 59.3 |
| 5 | 2491.9 | 25 | 57.6 | 23.1 |
| 6 | 2548.0 | 6.25 | 56.2 | 5.6 |
| 7 | 2604.0 | 0.9 | 54.8 | 0.8 |
| 8 | 2660.1 | 0.06 | 53.5 | 0.05 |

**Table SI 5.** Calculated relative intensities of signals corresponding to molecular ions of individual components $Pc(COOR^1)_n(COOR^2)_{8-n}$ in **8** ($R^1 = C_{10,6}$, $R^2 = C_{8,4}$).

| *n* | Calculated exact molecular mass | Distribution of products, calculated as coefficients of binomial $(x + y)^8$ | Calculated abundance of molecular ions with the lowest isotopic mass (in % of the most intense isotopic peak) | Calculated relative intensity signals corresponding to molecular ions with the lowest isotopic mass, % |
|---|---|---|---|---|
| 0 | 2211.6 | 1.4 | 66.1 | 1.6 |
| 1 | 2267.6 | 11.4 | 64.2 | 12.4 |
| 2 | 2323.7 | 40.0 | 62.4 | 42.2 |
| 3 | 2379.8 | 80.0 | 60.7 | 82.0 |
| 4 | 2435.8 | 100.0 | 59.2 | 100 |
| 5 | 2491.9 | 80.0 | 57.6 | 77.8 |
| 6 | 2548.0 | 40.0 | 56.2 | 38.0 |
| 7 | 2604.0 | 11.4 | 54.8 | 10.6 |
| 8 | 2660.1 | 1.4 | 53.5 | 1.3 |

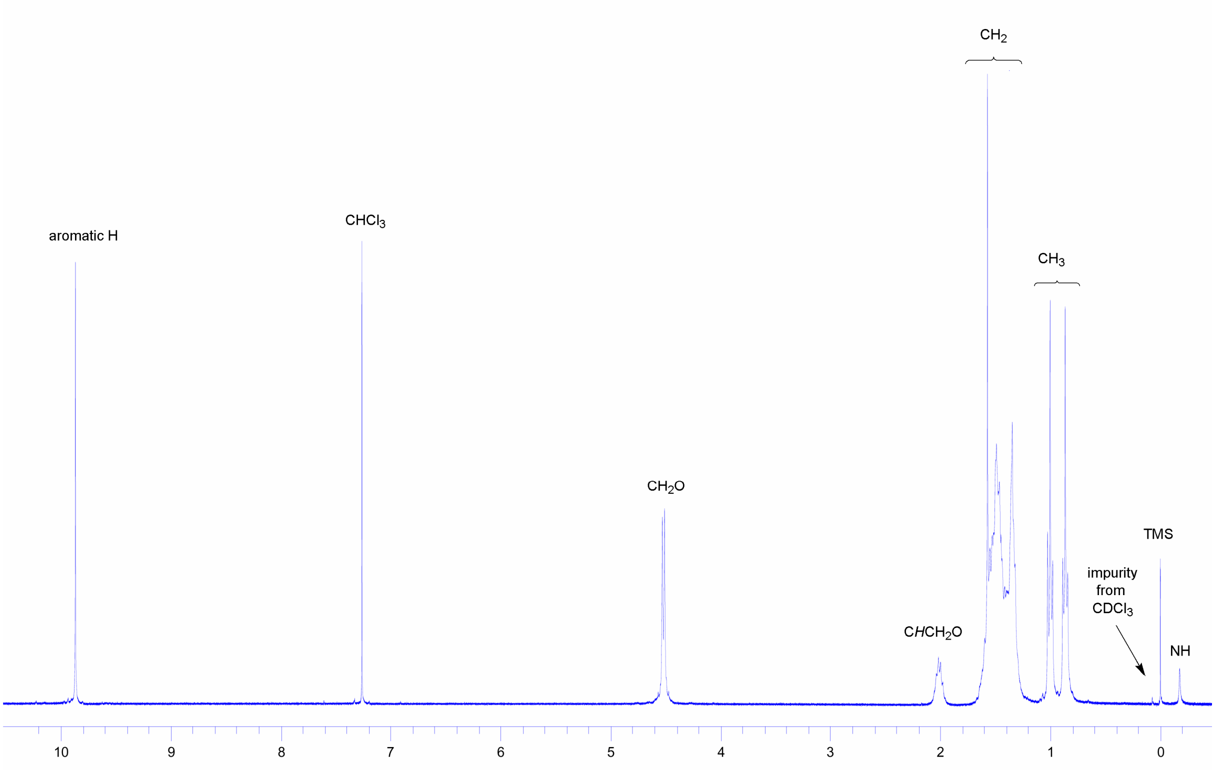


**Fig. SI 6** $^{1}$H NMR spectrum of **3b** (300 MHz, in $CDCl_3$, 25 °C)

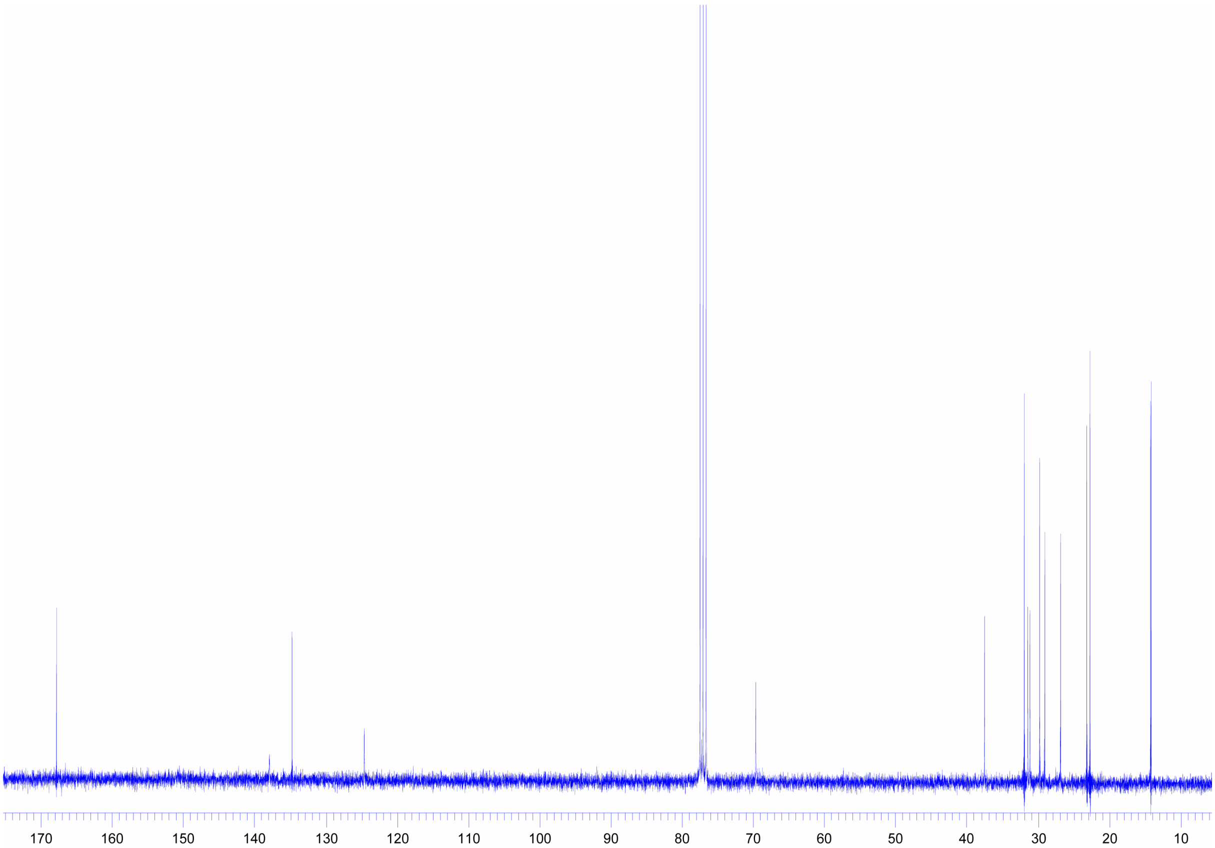


**Fig. SI 7** $^{13}$C NMR spectrum of **3b** (75 MHz, in $CDCl_3$, 25 °C)

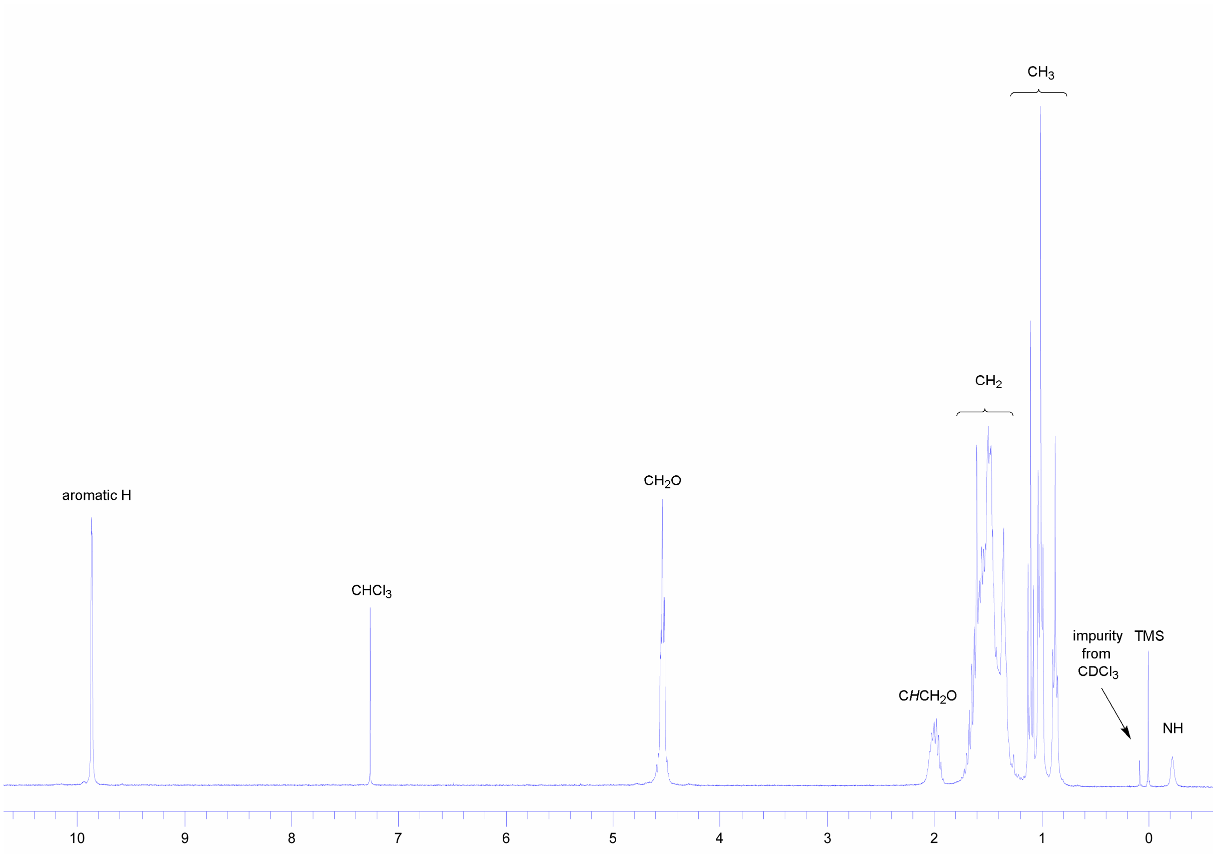


**Fig. SI 8** $^{1}$H NMR spectrum of **4** (300 MHz, in $CDCl_3$, 25 °C)

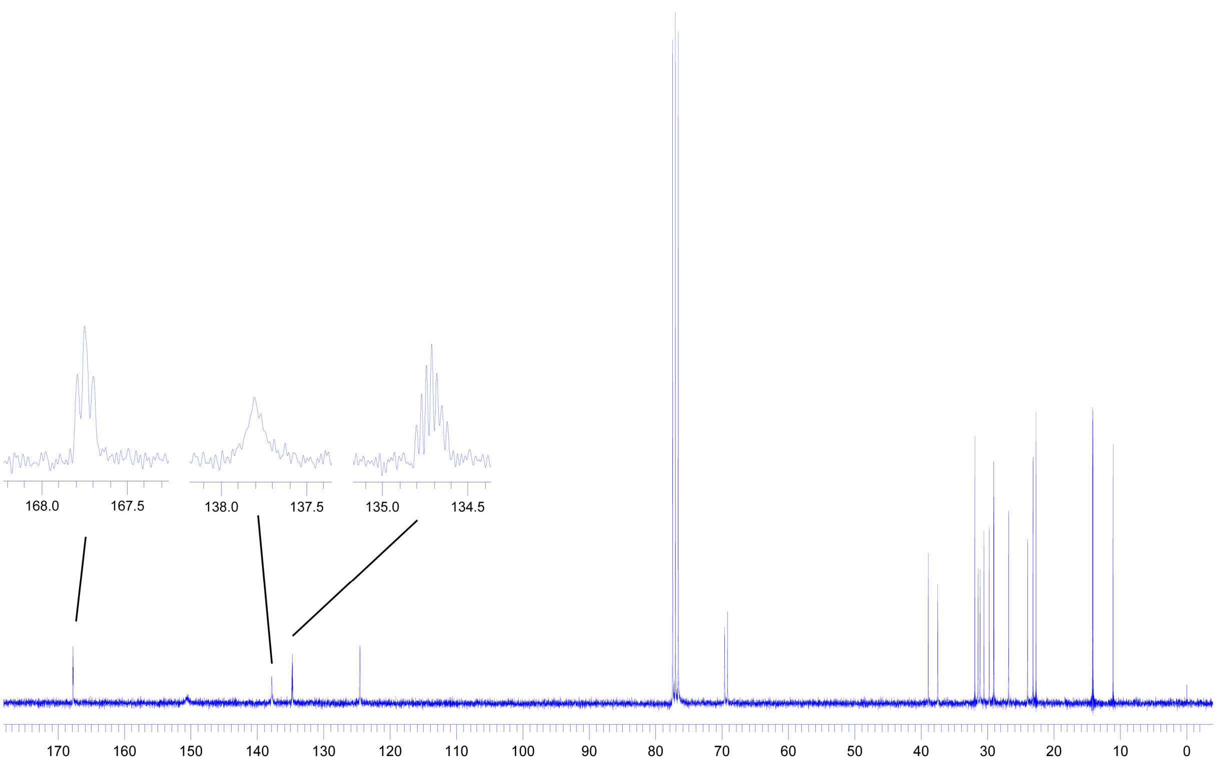


**Fig. SI 9** $^{13}$C NMR spectrum of **4** (75 MHz, in $CDCl_3$, 25 °C)

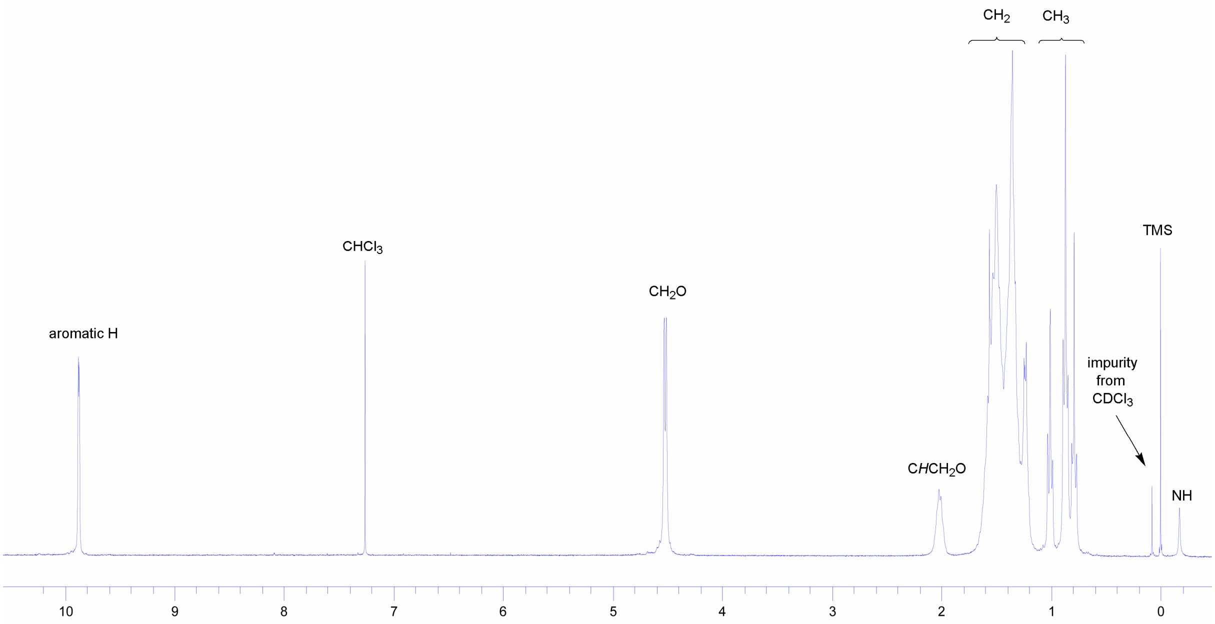


**Fig. SI 10** [1]H NMR spectrum of **8** (300 MHz, in $CDCl_3$, 25 °C)

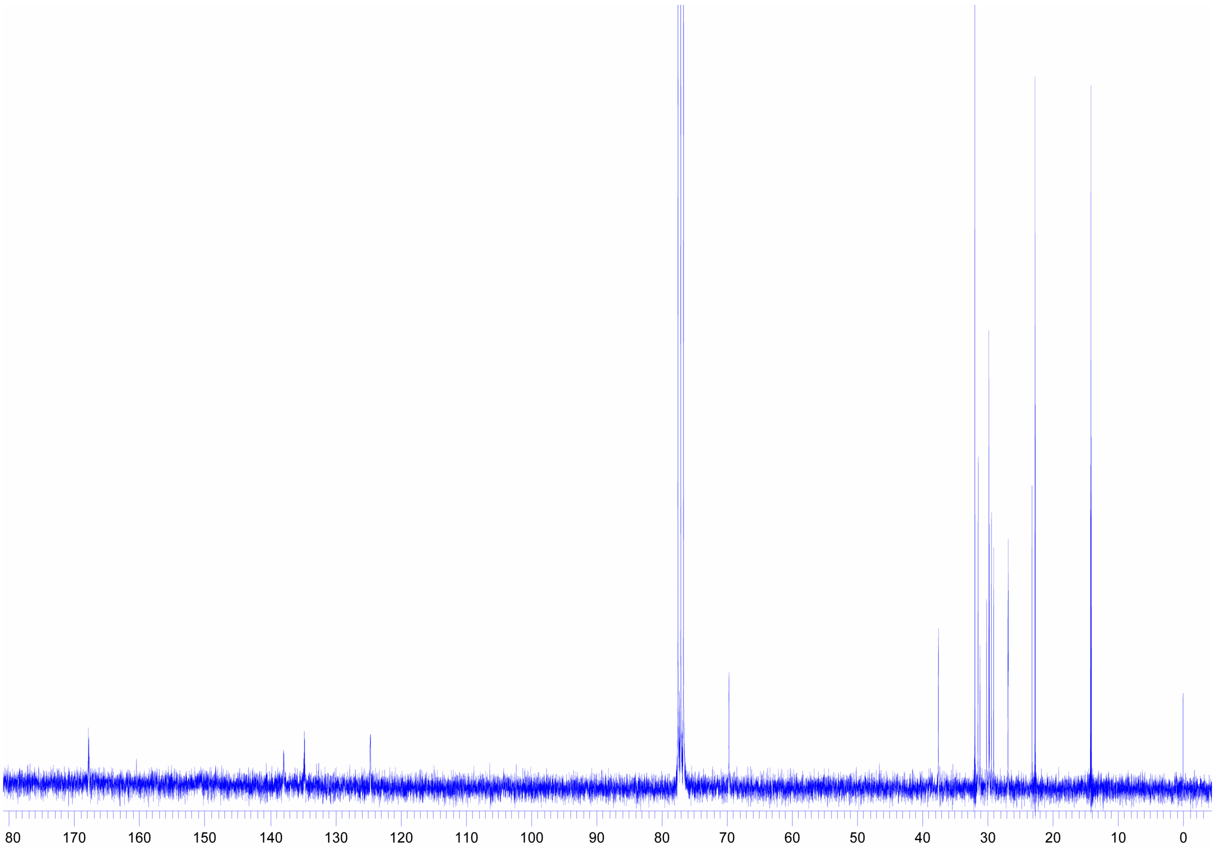


**Fig. SI 11** [13]C NMR spectrum of **8** (75 MHz, in $CDCl_3$, 25 °C)

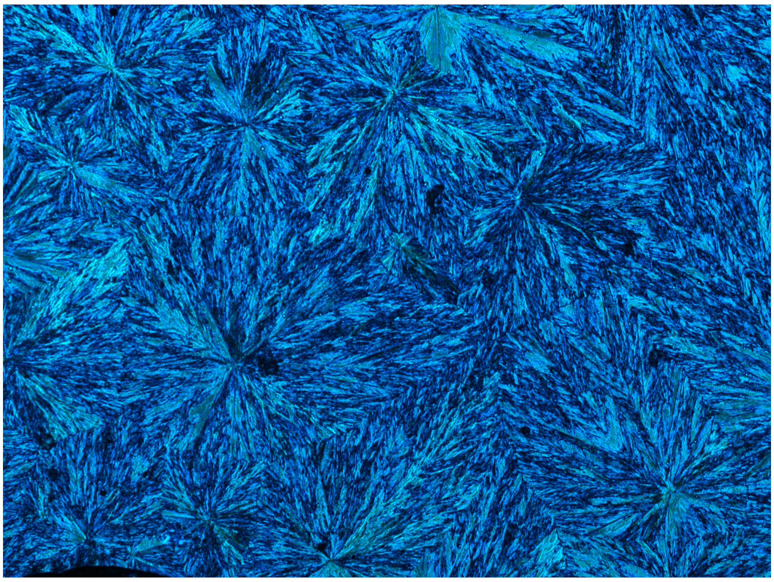

**Fig. SI 12** POM texture of **8** at 58 °C after cooling from the isotropic phase to the $Col_r$ phase.

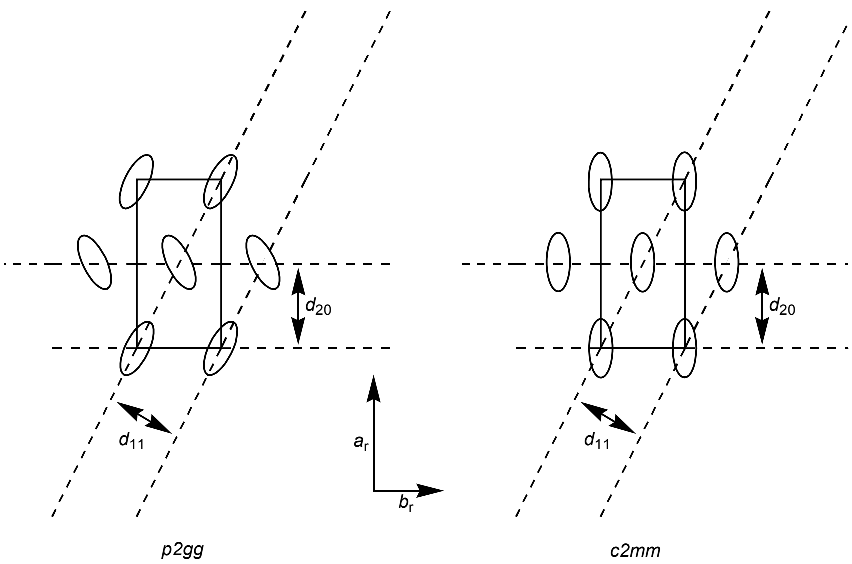


**Fig. SI 13** Schematic representation of two $Col_r$ phases possessing *p2gg* and *c2mm* plane symmetry.