Supporting information for the Communication "New symmetrically substituted 1,3,5-triazines as host compounds for channel-type inclusion formation"

General procedure for the cyclotrimerization of aromatic nitriles:
The neat benzonitrile and zinc chloride, in a molar ratio as specified in Table 01, were filled into an ampoule under inert gas and sealed under vacuum. The ampoule was heated in a furnace for the given time and broken after cooling to room temperature. The zinc chloride was removed from the reaction mixture by mixing with water and treatment in an ultrasonic bath for 1 h. The aqueous solution was removed by suction and the product purified by soxhlet extraction and subsequent recrystallization from chloroform.

Selected data for triazines:
2,4,6-Tris(4-fluorophenyl)-1,3,5-triazine. (**1**) Mp 303 °C. ^{1}H-NMR (300 MHz, CDCl$_3$) $\delta = 7.25$ (m); 8.76 (m). ^{13}C-NMR (75 MHz, CDCl$_3$) $\delta = 115.76$, 131.29, 132.19, 164.22/167.58, 170.70 (NCN). EI(+)-MS: *m/z*: found 363; calc. 363.33. ν(KBr)/cm^{-1}: 3086, 3071, 1667, 1602, 1523, 1506, 1414, 1371, 1226, 1142, 859, 816, 581, 510.

2,4,6-Tris(4-chlorophenyl)-1,3,5-triazine. (**2**) Mp 343 °C. ^{1}H-NMR (300 MHz, CDCl$_3$) $\delta = 8.69$ (6H, d, $^{3}J_{HH} = 8.6$ Hz); 7.55 (6H, d, $^{3}J_{HH} = 8.7$ Hz). ^{13}C-NMR (75 MHz, CDCl$_3$) $\delta = 129.03$, 130.32, 134.40, 139.16, 170.97 (NCN). EI(+)-MS: *m/z*: found 412; calc. 412.68. ν(KBr)/cm^{-1}: 3072, 1583, 1520, 1487, 1405, 1367, 1350, 1089, 1013, 804, 512, 479.

2,4,6-Tris(4-bromophenyl)-1,3,5-triazine. (**3**) Mp 360 °C. ^{1}H-NMR (300 MHz, CDCl$_3$) $\delta = 8.61$ (6H, d, $^{3}J_{HH} = 8.6$ Hz); 7.71 (6H, d, $^{3}J_{HH} = 8.7$ Hz). ^{13}C-NMR (75 MHz, CDCl$_3$) $\delta = 127.84$, 130.49, 132.03, 134.81, 171.13 (NCN). EI-MS: *m/z*: found 546; calc. 546.03. ν(KBr)/cm^{-1}: 3069, 3039, 1579, 1514, 1486, 1401, 1370, 1355, 1067, 1010, 805, 495.

2,4,6-Tris(4-iodophenyl)-1,3,5-triazine. (**4**) Mp 378 °C. ^{1}H-NMR (300 MHz, CDCl$_3$) $\delta = 7.98$ (6H, d, $^{3}J_{HH} = 8.5$ Hz); 8.52 (6H, d, $^{3}J_{HH} = 8.7$ Hz). ^{13}C-NMR (75 MHz, CDCl$_3$) $\delta = 101.41$, 131.48, 136.66, 139.17, 172.50 (NCN). EI(+)-MS: *m/z*: found 688; calc. 687.03. ν(KBr)/cm^{-1}: 3062, 3033, 1584, 1574, 1526, 1508, 1396, 1367, 1176, 1055, 1005, 803, 492.

2,4,6-Tris(4-bromo-3-fluorophenyl)-1,3,5-triazine. (**5**) Mp 278 °C. ^{1}H-NMR (300 MHz, CDCl$_3$) $\delta = 7.48$ (m); 8.34 (t, $^{3}J_{HH} = 8.3$ Hz). ^{13}C-NMR (75 MHz, CDCl$_3$) $\delta = 121.01$, 123.26, 127.39, 127.90, 133.26, 160.41/163.94, 170.20 (NCN). EI(+)-MS: *m/z*: found 601; calc. 600.00. ν(KBr)/cm^{-1}: 1618, 1601, 1578, 1522, 1358, 1225, 1215, 1072, 892, 808, 563.

2,4,6-Tris(4-bromo-3,5-difluorophenyl)-1,3,5-triazine. (**6**) Mp 366 °C. ^{1}H-NMR (300 MHz, THF-d$_8$) $\delta = 8.57$ (d, $^{3}J_{HF} = 8.3$ Hz). ^{19}F-NMR (376.5 MHz, THF-d$_8$) $\delta = -106.89$ (m). ^{13}C-NMR (75 MHz, THF-d$_8$) $\delta = 104.45$, 113.53, 138.68, 160.13/163.35, 171.38 (NCN). MALDI-TOF-MS: *m/z*: found 655; calc. 653.97. ν(KBr)/cm^{-1}: 1637, 1526, 1474, 1379, 1193, 1032, 826, 730, 584.

2,4,6-Tris(4-bromo-2,3,5,6-tetrafluorophenyl)-1,3,5-triazine. (**7**) Mp 183 °C. ^{19}F-NMR (376.5 MHz, CDCl$_3$) $\delta = -131.16$ (d, $^{3}J_{FF} = 10.43$ Hz, F3); -139.58 (d, $^{3}J_{FF} = 12.12$ Hz, F2). ^{13}C-NMR (75 MHz, CDCl$_3$) $\delta = 104.41$ (t, $^{2}J_{CF} = 22.3$ Hz); 115.37 (t, $^{2}J_{CF} = 13.6$ Hz); 143.66/147.15 (d, $^{1}J_{CF} = -167.4$ Hz); 167.4 (t, $^{3}J_{CF} = -3.11$ Hz, NCN). GC-MS: *m/z*: 762.1 [M]$^{+}$, 683 [M-Br]$^{+}$, 254 [BrC$_6$F$_4$CN]$^{+}$. ν(KBr)/cm^{-1}: 1641, 1527, 1497, 1411, 1355, 1154, 988, 838, 708.

2,4,6-Tris(4'-bromobiphenylyl)-1,3,5-triazine. (**8**) Mp *decomp*. ^{1}H-NMR (300 MHz, CDCl$_3$) δ = 7.56 (d, $^3J_{HH}$ = 8.7 Hz); 7.63 (d, $^3J_{HH}$ = 8.6 Hz); 7.76 (d, $^3J_{HH}$ = 8.5 Hz); 8.83 (d, $^3J_{HH}$ = 8.3 Hz). ^{13}C-NMR (75 MHz, CDCl$_3$) δ = 122.42; 127.12; 128.83; 129.60; 132.09; 135.51; 139.26; 143.97; 171.31 (NCN). MALDI-TOF-MS: *m/z*: found 775.5; calc. 774.3. ν(KBr)/cm^{-1}: 3064, 1607, 1581, 1560, 1512, 1481, 1416, 1371, 1074, 1002, 804, 657.

2,4,6-Tris(4'-bromo-2',3',5',6'-tetrafluorobiphenylyl)-1,3,5-triazine. (**9**) Mp 358 °C. ^{1}H-NMR (300 MHz, THF-d$_8$) δ = 7.80 (d, $^3J_{HH}$ = 8.7 Hz); 9.00 (d, $^3J_{HH}$ = 8.7 Hz). ^{19}F-NMR (376.5 MHz, THF-d$_8$) δ = -137.10 (m), -144.84 (m). ^{13}C-NMR (75 MHz, THF-d$_8$) δ = 100.37, 120.99, 130.41, 131.71, 132.59, 138.26, 147.20/143.69 (d, $^1J_{CF}$ = -264.8 Hz), 148.39/145.12 (d, $^1J_{CF}$ = - 245.3 Hz), 172.66 (NCN). MALDI-TOF-MS: *m/z*: found 991.6; calc. 990.2. ν(KBr)/cm^{-1}: 3247, 1576, 1522, 1480, 1406, 1374, 1192, 1160, 1020, 974, 817, 798, 519.

2,4,6-Tris(2',3',4',5',6'-pentafluorobiphenylyl)-1,3,5-triazine. (**10**) Mp decomposition. ^{1}H-NMR (300 MHz, THF-d$_8$) δ = 7.70 (d, $^3J_{HH}$ = 8.5 Hz); 8.91 (d, $^3J_{HH}$ = 8.7 Hz). ^{19}F-NMR (376.5 MHz, THF-d$_8$) δ = -144.30 (m), -157.75 (7, $^3J_{FF}$ = 19.9 Hz), -164.53 (m). EI(+)-MS: *m/z*: found 809; calc. 807.5. ν(KBr)/cm^{-1}: 3179, 1657, 1613, 1531, 1489, 1411, 1283, 1065, 988, 861, 761.

Crystal-Structure Determination:

A crystal of **8** · (toluene)$_{0.69}$ was mounted with Paratone-N^1 in a MiTeGen loop and used for X-ray structure determination at 90 K. All measurements were made on a *Bruker APEX II* area-detector diffractometer^2 using graphite monochromated MoK_α radiation (λ = 0.71073 Å). The unit cell constants and an orientation matrix for data collection were obtained from a least-squares refinement of the setting angles of 8056 reflections in the range 2.30° < θ < 28.00°. A total of 1429 frames were collected using ω and φ scans, 240 seconds exposure time and a rotation angle of 0.5° per frame, and a crystal-detector distance of 59.5 mm.

Crystal data for **8** · *(toluene)*$_{0.69}$

Empirical formula	C$_{43.80}$H$_{29.49}$Br$_3$N$_3$
Formula weight	837.54
Temperature	90(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*I*2/a
Unit cell dimensions	a = 39.8459(11) Å α = 90°
	b = 3.84340(10) Å β = 104.3980(10)°
	c = 46.6728(18) Å γ = 90°
Volume	6923.2(4) Å^3
Z	8
Density (calculated)	1.607 Mg/m^3
Absorption coefficient	3.534 mm^{-1}
F(000)	3346
Crystal size	0.31 x 0.12 x 0.05 mm^3
Theta range for data collection	1.55 to 28.57°.
Index ranges	-53 ≤ h ≤ 51, -5 ≤ k ≤ 4, -62 ≤ l ≤ 58
Reflections collected	31239

Independent reflections 8626 [R(int) = 0.0407]

Completeness to theta = 27.00° 99.7 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.9281 and 0.7137

Refinement method Full-matrix least-squares on F^2

Data / restraints / parameters 8626 / 57 / 474

Goodness-of-fit on F^2 1.028

Final R indices [I>2sigma(I)] R1 = 0.0581, wR2 = 0.1421

R indices (all data) R1 = 0.0881, wR2 = 0.1567

Largest diff. peak and hole 1.130 and -2.058 e.Å^{-3}

A crystal of **8** · (*p*-xylene)$_{0.72}$ was mounted with Paratone-N on a glass needle and used for X-ray structure determination at -100 °C. All measurements were made on a *Oxford Diffraction SuperNova* area-detector diffractometer[3] using mirror optics monochromated MoK_α radiation (λ = 0.71073 Å). The unit cell constants and an orientation matrix for data collection were obtained from a least-squares refinement of the setting angles of 23023 reflections in the range $1.50° < \theta < 28.17°$. A total of 2236 frames were collected using ω scans, 80 seconds exposure time and a rotation angle of 0.5° per frame, and a crystal-detector distance of 65.0 mm.

Crystal data for **8** · *(p-xylene)$_{0.72}$*

Empirical formula $C_{44.77}H_{31.21}Br_3N_3$

Formula weight 850.85

Temperature 173(2) K

Wavelength 0.71073 Å

Crystal system Monoclinic

Space group *I*2/a

Unit cell dimensions a = 39.9115(7) Å α = 90°

b = 3.86753(7) Å β = 103.6149(15)°

c = 46.7250(7) Å γ = 90°

Volume 7009.7(2) Å^3

Z 8

Density (calculated) 1.612 Mg/m^3

Absorption coefficient 3.491 mm^{-1}

F(000) 3406.3

Crystal size 0.46 x 0.23 x 0.07 mm^3

Theta range for data collection 1.53 to 28.23°.

Index ranges $-50 \leq h \leq 50, -5 \leq k \leq 4, -60 \leq l \leq 60$

Reflections collected 54702

Independent reflections 7995 [R(int) = 0.0320]

Completeness to theta = 26.00° 100.0 %

Refinement method Full-matrix least-squares on F^2

Data / restraints / parameters 7995 / 12 / 454

Goodness-of-fit on F^2 1.042

Final R indices [I>2sigma(I)] R1 = 0.0809, wR2 = 0.2554

| R indices (all data) | R1 = 0.0890, wR2 = 0.2643 |
| Largest diff. peak and hole | 1.258 and -2.125 e.Å^{-3} |

A crystal of **8** · (mesitylene)$_{2.0}$ was mounted with Paratone in a MiTeGen loop and used for X-ray structure determination at -50 °C. All measurements were made on a *Oxford Diffraction SuperNova* area-detector diffractometer[3] using mirror optics monochromated MoK_α radiation ($\lambda = 0.71073$ Å). The unit cell constants and an orientation matrix for data collection were obtained from a least-squares refinement of the setting angles of 17273 reflections in the range $1.51° < \theta < 28.25°$. A total of 5958 frames were collected using ω scans, 80 seconds exposure time and a rotation angle of 0.5° per frame, and a crystal-detector distance of 65.0 mm.

*Crystal data for **8** · (mesitylene)$_{2.0}$*

Empirical formula	$C_{57}H_{48}Br_3N_3$	
Formula weight	1014.71	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 3.86154(9) Å	$\alpha = 67.429(3)°$
	b = 22.1115(7) Å	$\beta = 88.114(2)°$
	c = 27.1691(7) Å	$\gamma = 87.127(2)°$
Volume	2139.20(10) Å^3	
Z	2	
Density (calculated)	1.575 Mg/m^3	
Absorption coefficient	2.874 mm^{-1}	
F(000)	1032	
Crystal size	0.446 x 0.1475 x 0.0172 mm^3	
Theta range for data collection	1.51 to 28.31°.	
Index ranges	$-4 \leq h \leq 5$, $-27 \leq k \leq 28$, $-35 \leq l \leq 35$	
Reflections collected	99271	
Independent reflections	9845 [R(int) = 0.0955]	
Completeness to theta = 26°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.52964	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9845 / 0 / 406	
Goodness-of-fit on F^2	1.118	
Final R indices [I>2sigma(I)]	R1 = 0.1229, wR2 = 0.3324	
R indices (all data)	R1 = 0.1685, wR2 = 0.3607	
Largest diff. peak and hole	1.012 and -1.385 e.Å^{-3}	

[1] Hampton Research, Catalog Number HR2-643; H. Hope, *Acta Cryst*, **1988**, *B44*, 22.
[2] Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
[3] Oxford Diffraction (2010). *CrysAlisPro* (Version 1.171.34.36). Oxford Diffraction Ltd., Yarnton, Oxfordshire, UK.