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# Directed synthesis of a halogen bonded open porphyrin network

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## Supporting information

**Table S1.** Crystallographic Data for ***compounds 1-3***

| ***Compound*** | ***1*** | ***2a*** | ***2b*** | ***2c*** | ***3*** |
|---|---|---|---|---|---|
| | *$I_2$-PFB·DABCO* | *$I_3$-PFB·DABCO* | *$I_2$-PFB·HMTA* | *$I_3$-PFB·bipy* | *$I_4$-TPFPP·HMTA* |
| Formula | $C_{12}H_{12}F_4I_2$ | $C_{12}H_{12}F_3I_3N_2$ | $C_{12}H_{12}F_3I_3N_4$ | $C_{16}H_8F_3I_3N_2$ | $C_{50}H_{22}F_{16}I_4N_8$ |
| M | 514.04 | 621.95 | 649.96 | 665.96 | 1546.36 |
| Temp/K | 250(2) | 250(2) | 250(2) | 250(2) | 298(2) |
| Crystal system | triclinic | monoclinic | monoclinic | monoclinic | monoclinic |
| Space group | P-1 (no 2) | $P2_1/c$ (no14) | Pm (no6) | Pn (no7) | P2/c (no13) |
| a/Å | 6.8359(4) | 6.2751(3) | 5.8849(13) | 4.1140(8) | 27.319(3) |
| b/Å | 10.9401(6) | 23.2198(11) | 24.903(3) | 9.0710(9) | 8.7331(7) |
| c/Å | 11.4732(7) | 11.8609(6) | 6.2247(8) | 24.104(5) | 55.699(8) |
| $\alpha$/deg | 107.204(5) | | | | |
| $\beta$/deg | 92.820(6) | 103.297(5) | 98.864(11) | 91.621(19) | 95.685(9) |
| $\gamma$/deg | 105.330(4) | | | | |
| V/Å3 | 782.88(9) | 1681.88(14) | 901.3(3) | 899.2(3) | 13223(3) |
| Z | 2 | 4 | 2 | 2 | 8 |
| $d_{calcd}$/g.cm$^{-3}$ | 2.181 | 2.456 | 2.395 | 2.460 | 1.554 |
| $\mu$/mm$^{-1}$ | 4.049 | 5.596 | 5.230 | 5.243 | 1.966 |
| $\lambda$(Mo $_{K,L2,3}$)/Å | 0.71073 | 0.71073 | 0.71073 | 0.71073 | 0.71073 |
| $\theta_{max}$/deg | 30.00 | 30.00 | 30.00 | 30.00 | 30.00 |
| Reflns collected | 14490 | 14712 | 13934 | 7515 | 148609 |
| Independent reflns (all data) | 4547 | 4766 | 4952 | 4736 | 38466 |
| Independent reflns ($I > 2\sigma(I)$) | 3082 | 3526 | 4575 | 3868 | 20516 |
| $R_{int}$(all) | 0.0462 | 0.0342 | 0.0324 | 0.0398 | 0.0643 |
| Parameters | 182 | 194 | 211 | 217 | 1406 |
| R(F), wR($F^2$) ($I > 2\sigma(I)$) | 0.0337/0.0667 | 0.0342/0.0784 | 0.0292/0.0683 | 0.0566/0.1403 | 0.0565//0.0818 |
| R(F), wR($F^2$) (all data) | 0.0680/0.756 | 0.0576/0.0972 | 0.0337/0.0699 | 0.0725/01488 | 0.1058/0.1201 |
| GOF in $F^2$ | 0.990 | 1.089 | 1.043 | 1.070 | 0.992 |
| $\rho_{max}/\rho_{min}$/e.Å$^{-3}$ | 0.57/-0.71 | 0.84/-0.75 | 1.20/-0.81 | 1.85/-2.29 | 1.32/-1.17 |

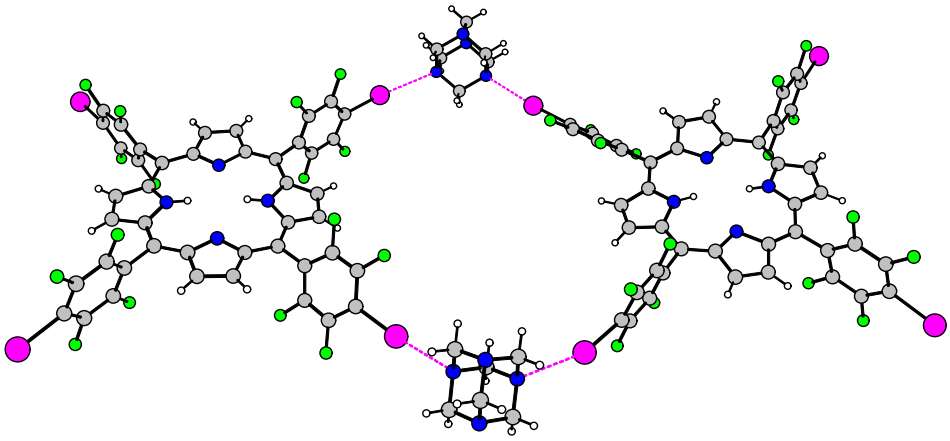

**Fig. S1.** Compound **3**: dimeric porphyrin unit linked by HMTA.

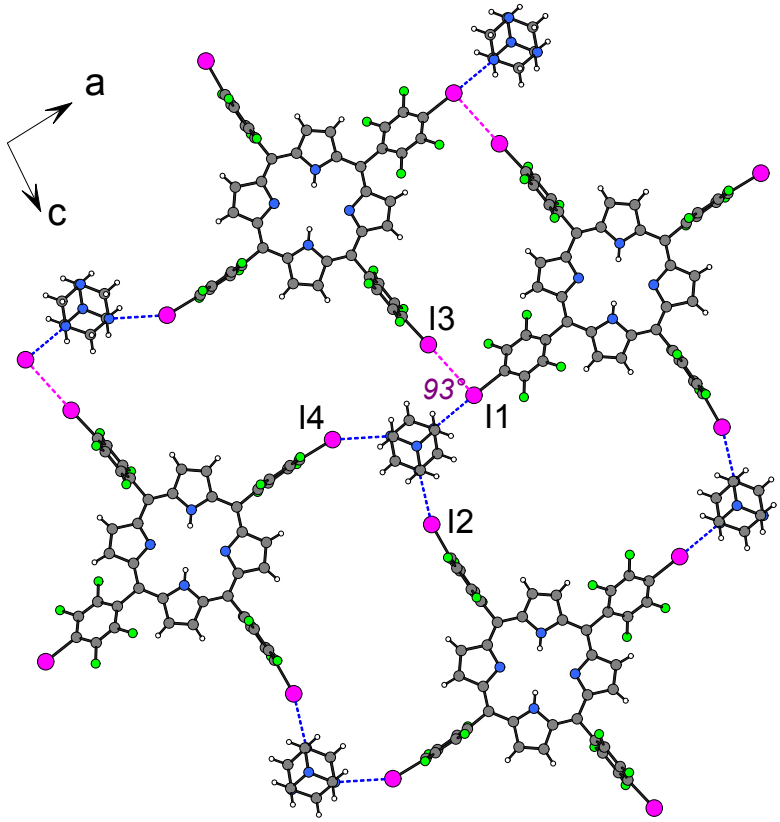


**Fig. S2**. Compound **3**. Representative cut-out of the A layer showing the N···I and I···I halogen bonds within the a,c layer. C (grey), H (white), F (green), I (pink), N (blue).

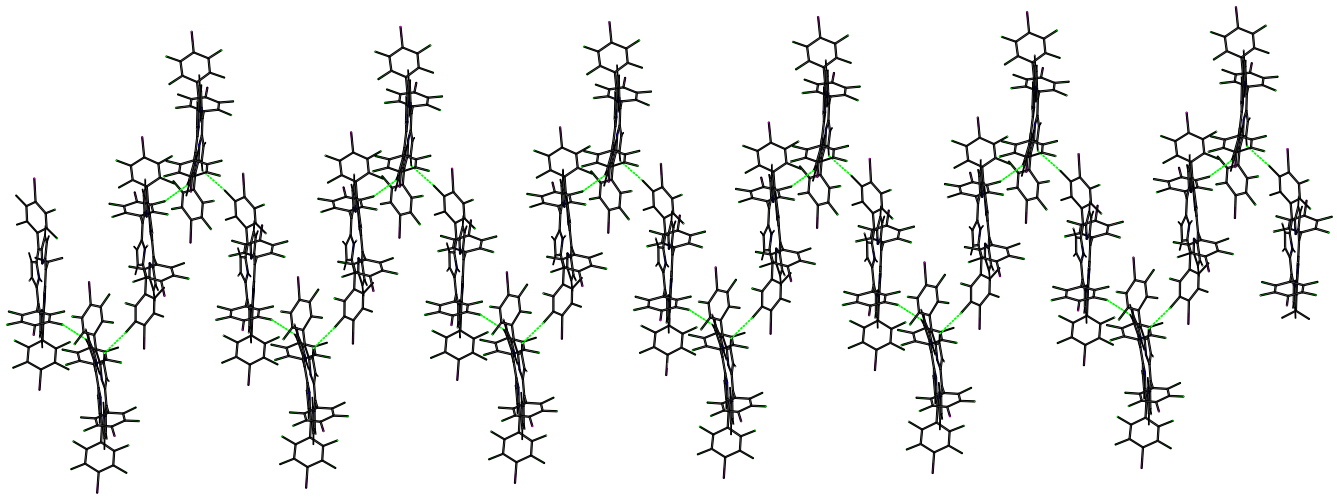

**Fig. S3**. Compound **3.** Helical structure of porphyrins forming a channel in the b direction. Short C-H···F contacts are highlighted in green.