

Optimized synthesis and crystal growth by sublimation of 1,3,3-trichloroisoindolenines, key building blocks for crosswise phthalocyanines[†]

Mehmet Menaf Ayhan, Yunus Zorlu, Özlem Gökdemir, Ayşe Gül Gürek, Fabienne Dumoulin,*

Vefa Ahsen and Catherine Hirel*

Department of Chemistry, Gebze Institute of Technology, P. O. Box 141, 41400 Gebze Kocaeli, Turkey. Fax: +90 262 605 31 05; Tel: +90 262 605 30 22. E-mails: fdumoulin@gyte.edu.tr; chirel@gyte.edu.tr

[†]In the memory of Christian Claessens

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Table S1. Intermolecular interactions in **1** and **2**

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Compound	$\pi \cdots \pi$ interactions			
	Cg(i) \cdots Cg(j)	Symmetry	Beta ($^\circ$)	$\pi \cdots \pi$ (\AA)
1	Cg1 \cdots Cg1	1-x,-1/2+y,-z	47.09	5.0861(9)
	Cg1 \cdots Cg2	1-x,-1/2+y,-z	31.47	4.0604(7)
	Cg2 \cdots Cg2	1-x,-1/2+y,-z	32.42	4.1026(7)
2	Cg1 \cdots Cg1	-x,-1/2+y,-z	51.08	5.6568(17)
	Cg1 \cdots Cg2	-x,-1/2+y,1-z	52.36	5.8193(17)
	Cg2 \cdots Cg2	-x,-1/2+y,1-z	35.16	4.3472(12)
	C-Cl \cdots π interactions			
	C-Cl \cdots Cg(i)	Symmetry	Cl \cdots Cg (\AA)	Y-X \cdots Cg($^\circ$)
2	C8-Cl2 \cdots Cg1	-x,-1/2+y,-z	3.996(9)	110.21(5)
	C3-Cl3 \cdots Cg2	-x,-1/2+y,1-z	3.6242(5)	80.16(3)
	C=N \cdots Cl interactions			
	C-N \cdots Cl	Symmetry	N \cdots Cl (\AA)	C-N \cdots Cl ($^\circ$)
2	C7-N1 \cdots Cl4	x, y, -1+z	3.170(3)	143.3(2)

For both compounds, Cg1 and Cg2 are the centroids of the rings (N1/C7/C6/C1/C8) and (C1-C6), respectively. Beta: Angle between the planes; Cg-Cg: distance between ring centroids