Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information for

A library of dimeric and trimeric phthalonitriles linked by a single aromatic ring : Comparative structural and DFT investigations

Muzaffer Köç,[a] Yunus Zorlu,[a] Ümit İşci,[a] Savaş Berber,[b] Vefa Ahsen,[a] Fabienne Dumoulin[a]*

[a] *Gebze Technical University, Department of Chemistry, 41400 Gebze, Kocaeli, Turkey. E-mail: fdumoulin@gtu.edu.tr. Fax: +90 262 605 31 05; Tel: +90 262 605 30 22*

[b] *Gebze Technical University, Department of Physics, 41400 Gebze, Kocaeli, Turkey*

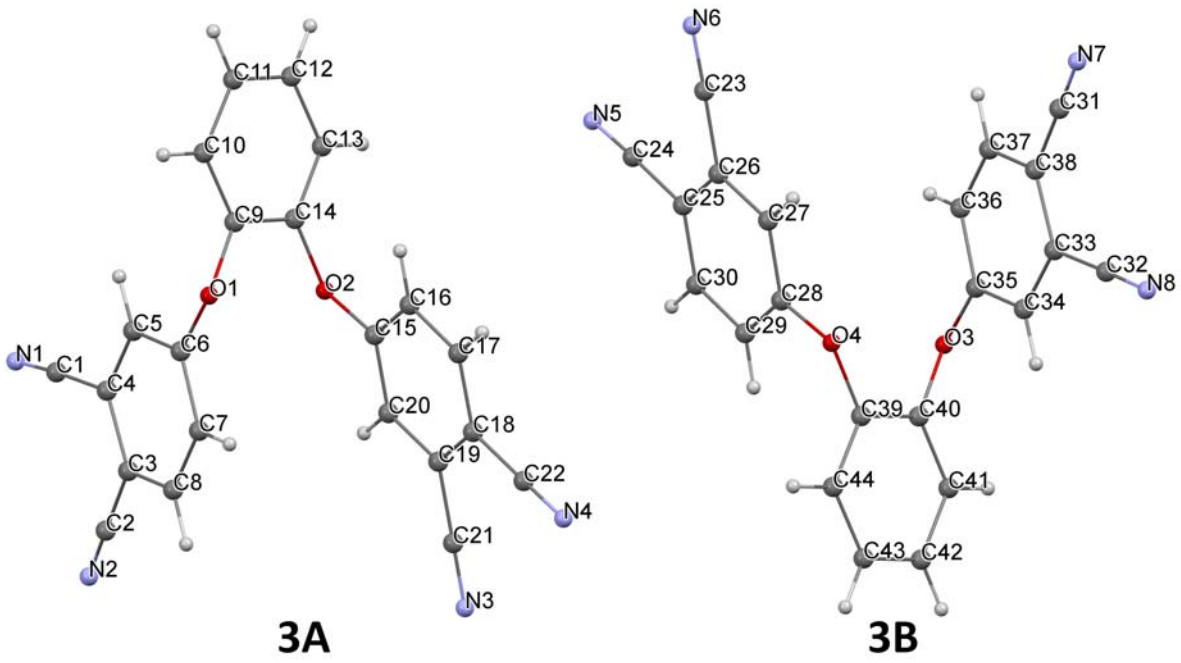

Fig. S1. The two molecules in the asymmetric unit of **3** (**3A** and **3B**) with displacement ellipsoids drawn at the 50% probability level.

Table S1. Crystal data and refinement parameters for compounds **1-5**.

Compound	**1**	**2**	**3**	**4**	**5**
CCDC	CCDC 968403	CCDC 968400	CCDC 968402	CCDC 968399	CCDC 968401
Empirical Formula	$C_{22}H_{10}N_4O_2$	$C_{22}H_{10}N_4O_2$	$C_{22}H_{10}N_4O_2$	$C_{30}H_{12}N_6O_3$	$C_{30}H_{26}N_4O_2$
Formula weight (g. mol^{-1})	362.34	362.34	362.34	504.46	474.55
Temperature (K)	148(2)	150(2)	150(2)	150(2)	150(2)
Crystal system	Monoclinic	Triclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	*C*2/c	P -1	$Pna2_1$	*C*2/c	$P2_1/n$
***a* (Å)**	13.7511(6)	8.0768(5)	20.9421(11)	14.4563(14)	10.2611(10)
***b* (Å)**	7.3953(3)	8.5809(5)	5.0644(3)	24.746(2)	13.4117(12)
***c* (Å)**	17.5013(8)	13.4764(8)	32.8970(19)	14.626(2)	18.9648(17)
α(°)	90	74.672(3)	90	90	90
β(°)	91.983(2)	88.214(3)	90	112.294(6)	101.601(6)
γ(°)	90	77.262(3)	90	90	90
Crystal size (mm)	0.12 x 0.14 x 0.25	0.10 x 0.16 x 0.17	0.04 x 0.11 x 0.16	0.04 x 0.07 x 0.08	0.06 x 0.09 x 0.21
V (Å^3)	1778.70(13)	878.24(9)	3489.0(3)	4841.1(9)	2556.6(4)
Z	4	2	8	8	4
ρ_{calcd} (g. cm^{-3})	1.353	1.370	1.380	1.384	1.233
μ (mm^{-1})	0.091	0.092	0.092	0.094	0.079
F(000)	744	372	1488	2064	1000
θ range for data collection (°)	2.33 - 24.99	2.99 - 25.00	1.24 - 25.00	1.65 - 25.00	2.92 - 25.00
h/k/l	-16/16, -8/8, -20/20	-9/9, -10/10, -16/16	-24/23, -6/6, -39/33	-16/17, -29/29, -17/17	-10/12, -15/15, -22/17
Reflections collected	12440	56718	41478	32709	20121
Independent reflections	1567 [R(int) = 0.0339]	3074 [R(int) = 0.0388]	5552 [R(int) = 0.0830]	4263 [R(int) = 0.1218]	4486 [R(int) = 0.0569]
Data/restraints/parameters	1567 / 0 / 127	3074 / 0 / 253	5552 / 1 / 505	4263 / 0 / 352	4486 / 0 / 331
Goodness-of-fit on F^2	1.109	1.099	1.035	1.039	1.080
Final *R* indices [I > 2σ(I)]	R_1 = 0.0341, wR_2 = 0.0944	R_1 = 0.0323, wR_2 = 0.0815	R_1 = 0.0450, wR_2 = 0.0815	R_1 = 0.0539, wR_2 = 0.1045	R_1 = 0.0496, wR_2 = 0.1109
***R* indices (all data)**	R_1 = 0.0384, wR_2 = 0.0980	R_1 = 0.0353, wR_2 = 0.0843	R_1 = 0.0353, wR_2 = 0.0843	R_1 = 0.1219, wR_2 = 0.1294	R_1 = 0.0909, wR_2 = 0. 0.1277
Largest diff. peak and hole (e.Å^{-3})	0.139 and -0.200	0.181 and -0.170	0.160 and -0.174	0.199 and -0.204	0.327 and -0.194