Dicarboxylic Acid-*based* Co-crystals of Pyridine Derivatives involving Structure guiding Unconventional Synthons: Experimental and Theoretical Studies

Pranay Sharma[1], Rosa M. Gomila[2], Antonio Frontera*[2], Miquel Barcelo-Oliver[2], Manjit K. Bhattacharyya*[1]

[1]*Department of Chemistry, Cotton University, Guwahati-781001, Assam, India*
[2]*Departament de Química, Universitat de les Illes Balears, Crta de Valldemossa km 7.7, 07122 Palma de Mallorca (Baleares), Spain*
**Corresponding authors E-mail:* *manjit.bhattacharyya@cottonuniversity.ac.in*
toni.frontera@uib.es

Supplementary Information

Table S1. Comparison of crystal parameters of compound **1** with the already reported compound

Crystal Parametres	Compound **1**	CCDC **1453483**
Emprical formula	$C_7H_5N_2O_2$	$C_{14}H_{10}N_4O_4$
Formula weight	149.13	298.26
Temperature (K)	100.0	173(2)
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	3.664(2)	3.7569(17)
b/Å	13.887(8)	13.997(6)
c/Å	13.455(6)	13.549(7)
α °	90	90
β°	91.55(2)	91.97(3)
γ °	90	90
Volume (Å^3)	684.5(6)	712.0(6)
Z	4	2
Calculated density (Mgm^{-3})	1.447	1.391
Absorption coefficient (mm^{-1})	0.927	0.106
F(000)	908	308
Crystal size (mm^3)	0.49 × 0.20 × 0.19	0.20×0.10×0.10
θ range for data collection(°)	6.378 to 66.541	3.277 to 24.984
Index ranges	-3 ≤ h ≤ 4, -16 ≤ k ≤ 16, -16 ≤ l ≤ 16	-4<=h<=4, -16<=k<=16, -16<=l<=16
Reflections collected	1166	1256
Independent reflections	1114	942
Refinement method	Full-matrix least squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	1166/0/105	1256/0/105
Goodness-of-fit on F^2	1.088	1.043
Final *R* indices[$I>2\sigma(I)$] *R*1/ *wR*2	0.0433/0.1140	0.0654/0.1606
R indices(all data) *R*1/ *wR*2	0.0449/0.1153	0.0858/0.1763

Table S2. Comparison of crystal parameters of compound **2** with the already reported compound

Crystal Parametres	Compound **2**	CCDC **1453486**
Emprical formula	$C_{18}H_{18}N_4O_4$	$C_{18}H_{18}N_4O_4$
Formula weight	354.36	354.36
Temperature (K)	100.0	293(2)
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a/Å	3.8849(3)	3.9764(3)
b/Å	10.5878(9)	10.5803(10)
c/Å	11.7569(10)	11.7777(13)
α º	63.760(4)	64.472(10)
βº	86.193(5)	85.454(7)
γ º	85.953(5)	86.796(7)
Volume ($Å^3$)	432.34(6)	445.60(8)
Z	1	1
Calculated density (Mgm^{-3})	1.361	1.321
Absorption coefficient (mm^{-1})	0.818	0.096
F(000)	186	186
Crystal size (mm^3)	0.45 × 0.39 × 0.33	0.20×0.10×0.10
θ range for data collection(º)	8.39 to 134.446	3.5 to 14.8
Index ranges	-4 ≤ h ≤ 3, -12 ≤ k ≤ 12, -14 ≤ l ≤ 13	-4<=h<=4, -11<=k<=12, -13<=l<=13
Reflections collected	5081	1547
Independent reflections	1541	1235
Refinement method	Full-matrix least squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	1541/0/119	1571/0/122
Goodness-of-fit on F^2	1.063	1.045
Final *R* indices[$I>2\sigma(I)$] *R*1/ *wR*2	0.0479/0.1327	0.0488/ 0.1310
R indices(all data) *R*1/ *wR*2	0.0539/0.1376	0.0610/ 0.1451

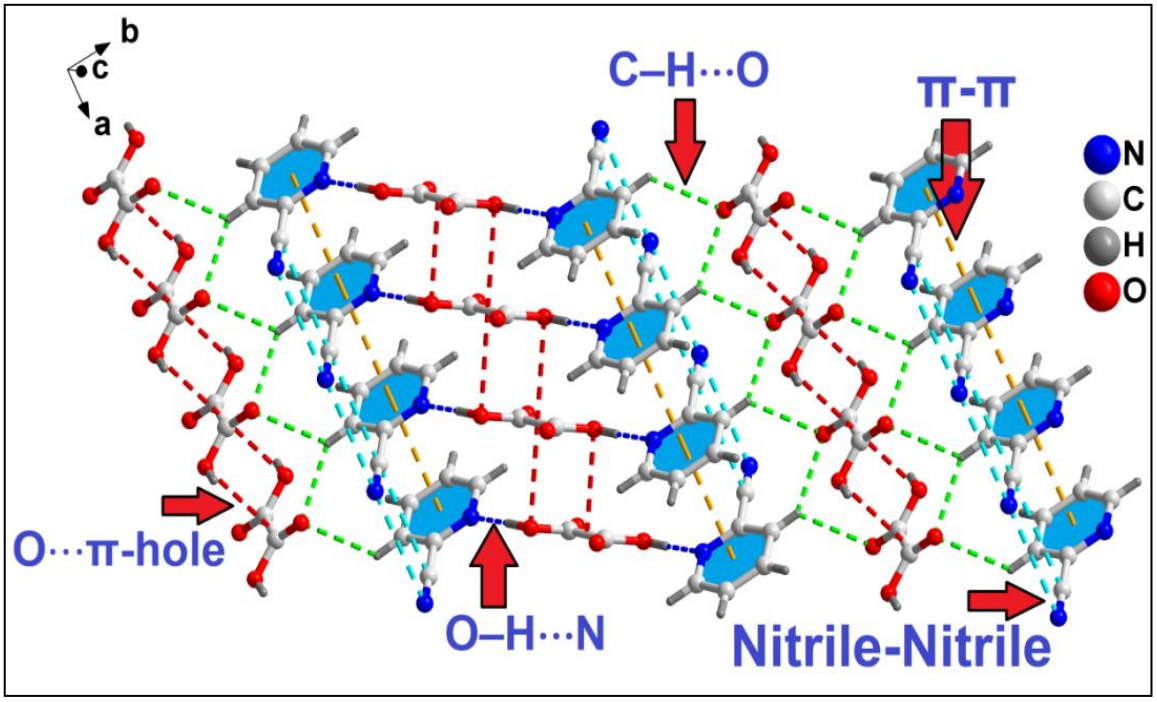

Figure S1. Layered assembly of **1** along the crystallographic *ab* plane assisted by unconventional O···π-hole, unusual parallel nitrile-nitrile, π-stacking, O–H···N and C–H···O hydrogen bonding interactions.

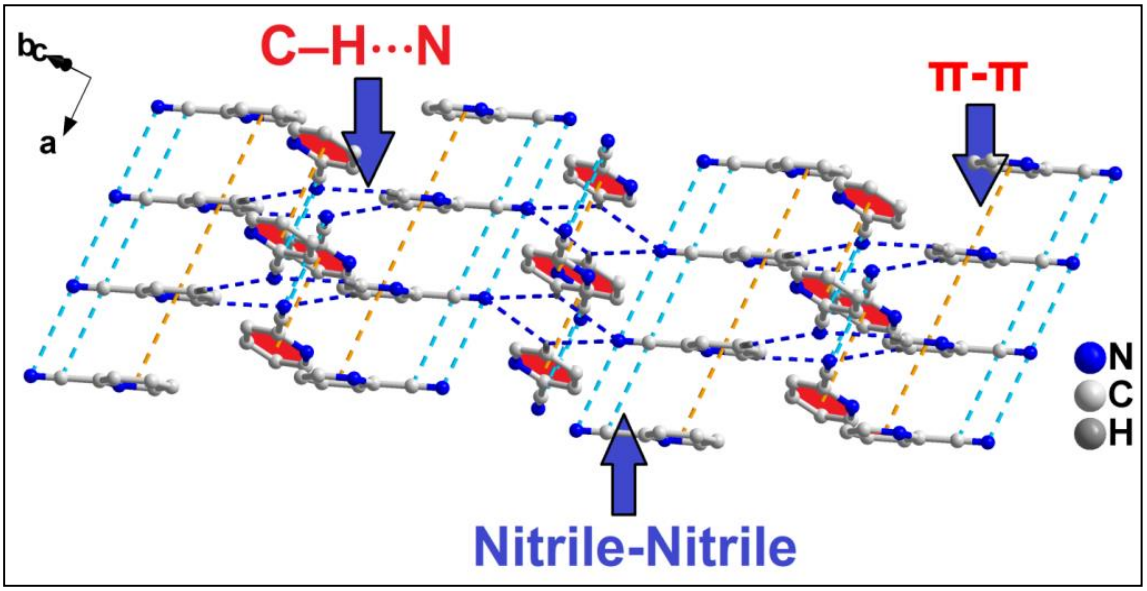

Figure S2. Layered assembly of **1** along the crystallographic *ac* plane.

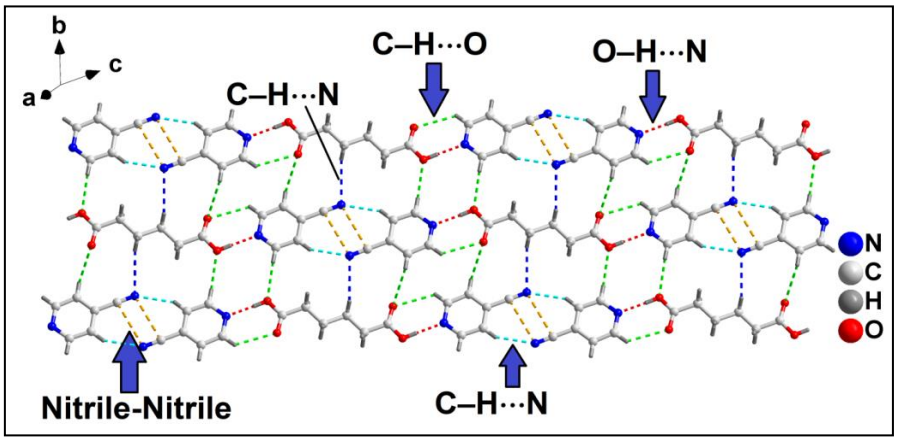

Figure S3. Layered assembly of **2** assisted by nitrile-nitrile, C–H···N, O–H···N and C–H···O hydrogen bonding interactions

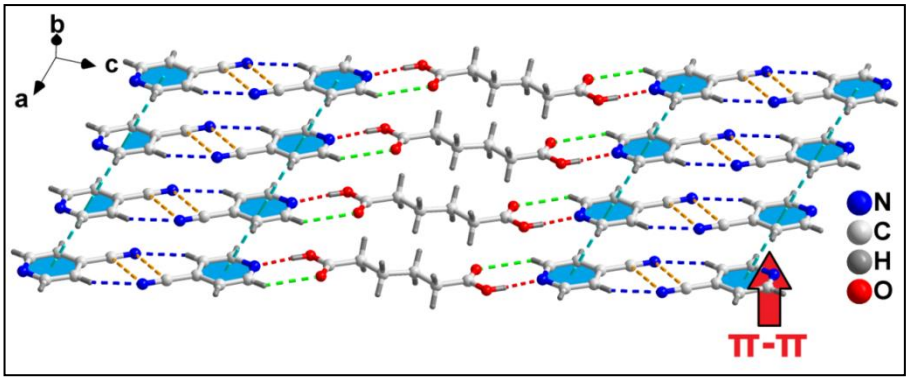

Figure S4. Layered architecture of **2** along the crystallographic *ac* plane assisted by aromatic π-stacking interaction.

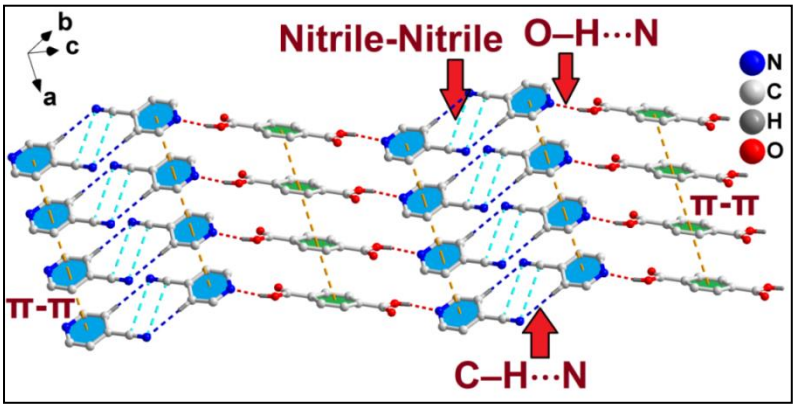

Figure S5. Layered assembly of co-crystal **3** along the crystallographic *ac* plane assisted by antiparallel nitrile-nitrile, aromatic π-stacking, C–H···N and O–H···N hydrogen bonding interactions.

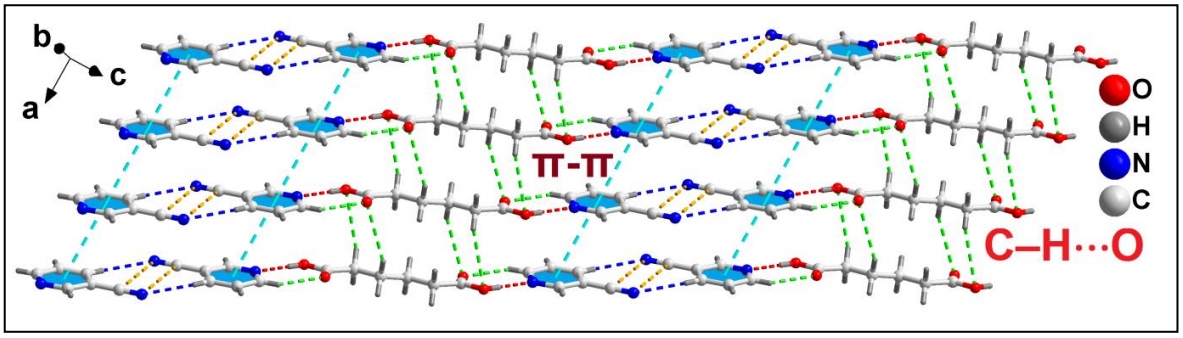

Figure S6. Layered assembly of co-crystal **4** along the crystallographic *ac* plane.