

## SUPPLEMENTARY MATERIALS FOR MANUSCRIPT

### New Acentric Materials Constructed From Aminopyridines and 4-Nitrophenol

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**Table 1S.** Selected observed IR bands ( $\nu$ ,  $\text{cm}^{-1}$ ) for adducts studied

2(I)•1	2(I)•2	2(I)•3	I•4	2(I)•5	2(I)•6	Assignment
-	3446	-	3460	3430	3485	N-H stretching, O-H vibration, H-bond formation
3375	3377	-	3376	3339	3378	NH <sub>2</sub> asymmetric stretching mode
-	3286	3316	-	3221	3312	NH <sub>2</sub> symmetric stretching mode
3089	3070	-	-	-	-	aromatic CH stretching mode
-	1616	1612	-	1695	1632	pyridine ring stretching vibration
1573	1562	1586	1585	1567	1572	NO <sub>2</sub> asymmetric stretching
1321	-	1322	1330	1326	1328	NO <sub>2</sub> symmetric stretching, C-N stretching mode
1239	1247	1215	1241	1246	1243	C-O stretching vibration for substituted phenols
1153	1137	1165	-	1175	-	NH <sub>2</sub> rocking mode; O-H-in plane bending
1098	-	-	1110	1101	1104	C-C-N asymmetric stretch, ring stretching
847	-	848	842	859	849	NH <sub>2</sub> out-of plane bending mode
755	-	753	-	754	755	out-of-plane ring deformation mode
697	668	-	687	694	-	C-H out-of-plane deformation mode

**Table 2S. Selected Structural Data for Multicomponent Complexes Containing 4-Nitrophenol.**

Compound	Sp. Gr.	CSD code	Reference
4-Aminopyridine	$P2_12_12_1$	AMPYRE	[71]
3,4-Diaminopyridine	$P2_12_12_1$	REWBOL	[72]
2,3-Diaminopyridine	$P4_2bc$	EVODEZ	[73]
3-Aminopyridine	$Cc$	AMIPYR	[74]
2-Amino,6-methylpyridine	$P2_1/c$	-	[75]
2,4-Diaminopyrimidine acetone solvate	$P2_1/c$	-	[76]
<b>4-Aminopyridinium 4-nitrophenolate 4-nitrophenol</b>	$P2_1$	-	<b>This work</b>
<b>2-Amino,6-methylpyridinium 4-nitrophenolate 4-nitrophenol</b>	$Pna2_1$	-	<b>This work</b>
<b>3,4-Diaminopyridinium 4-nitrophenolate 4-nitrophenol</b>	$P2_1$	-	<b>This work</b>
<b>2,3-Diaminopyridinium 4-nitrophenolate 4-nitrophenol</b>	$P2_1$	-	<b>This work</b>
4-(Dimethylamino)pyridinium 4-nitrophenolate 4-nitrophenol	$P2_12_12_1$	PUMQAP PUMQAP01	[49] [77]
2-Aminopyridinium 4-nitrophenolate 4-nitrophenol	$Pna2_1$	KAPFEN	[50]
2,6-Diaminopyridinium 4-nitrophenolate 4-nitrophenol	$Pna2_1$	KAPFIR	[50]
<i>L</i> -Histidine-4-nitrophenolate 4-nitrophenol	$P2_1$	EMUROU	[53]
<i>L</i> -Arginine 4-nitrophenolato 4-nitrophenol dihydrate	$P2_1$	-	[56]
1,5,7-Triazabicyclo(4.4.0)dec-5-ene bis(4-nitrophenol)	$P2_1$	OFECAD	[78]
<b>2,3-Diaminopyrimidinium 4-nitrophenolate 4-nitrophenol</b>	$P2_1/c$	-	<b>This work</b>
1,3,5-triazine-2,4,6-triamine bis(4-nitrophenol) monohydrate	$P-1$	XECBEON	[70]
Imidazolium 4-nitrophenolate 4-nitrophenol monohydrate	$P2_1/c$	HILMAR	[79]
2-( <i>N,N</i> -Diethylamino)methyl-4-nitrophenol 4-nitrophenol	$Pbca$	NUDLON	[80]
Hexa-aqua-(4-nitrophenol- <i>O</i> )-calcium bis(4-nitrophenolate) 4-nitrophenol dihydrate	$P2_1/n$	FEDWIU	[81]
Hexa-aqua-(4-nitrophenol- <i>O,O'</i> )-strontium bis(4-nitrophenolate) 4-nitrophenol dihydrate	$P2_1/c$	FEDWUG	[81]
(4-Nitrophenolato)-(tetramethylethylenediamine)-methyl-palladium(II) 4-nitrophenol solvate	$P2_1/c$	ZIHWOC	[82]
Dimethylammonium 4-nitrophenolate 4-nitrophenol	$P2_1/n$	KUSWOL	[83]
(3-Pyridyl)methanaminium 4-nitrophenolate 4-nitrophenol	$P-1$	QUYZOA	[84]
<i>L</i> -Tryptophan (tris)(4-nitrophenol solvate)	$P2_1$	LAQXIM	[85]
<b>3-Aminopyridine 4-nitrophenol</b>	$P2_1$	-	<b>This work</b>
4-Pyridone 4-nitrophenol	$Pna2_1$	PUMQET	[49]
<i>L</i> -Argininium 4-nitrophenolate monohydrate	$P2_12_12_1$	OFIWUW	[55]
<i>L</i> -Phenylalanine 4-nitrophenol	$P2_1$	XETLIS	[86]
4-Nitropyridine <i>N</i> -oxide 4-nitrophenol	$Pna2_1$	JUDNAX	[87]
2-Pyridone 4-nitrophenol	$P2_1/c$	OFUGUR	[88]
Pyridine <i>N</i> -oxide 4-nitrophenol	$P2_1/c$	NILZOX	[89]
2-Picoline <i>N</i> -oxide 4-nitrophenol	$P2_1/c$	WIRWID	[90]
4-Methylpyridine 4-nitrophenol	$Pbca$	CAXNOE	[91]
Acetamide 4-nitrophenol	$P2_1/c$	LOCHOB	[92]
<i>Cis,trans</i> -Diacetamide 4-nitrophenol	$P-1$	VIVYUU	[93]
<i>N</i> -Butyrylbenzamide 4-nitrophenol	$P-1$	VIVZAB	[93]
Urea 4-nitrophenol	$P-1$	GAVHUH	[94]
2,3,5,6-Tetramethylpyrazine 4-nitrophenol	$P-1$	FIQBAJ	[95]
Methylammonium nitrophenolate	$Pbca$	NUZKAU	[96]
1-Adamantylammonium 4-nitrophenolate monohydrate	$P2_1/n$	FIRNEA	[97]
Benzyltrimethylammonium <i>p</i> -nitrophenolate trihydrate	$P2_12_12_1$	FITZEN	[98]
<i>O</i> -(1-adamantoyl)- <i>N</i> -(9-anthracenylmethyl)dihydrocinchoninium 4-nitrophenolate acetonitrile solvate tetrahydrate	$P2_12_12_1$	HEXPOQ	[99]
<i>O</i> -Allyl-9-anthracenylmethyl cinchonidinium <i>p</i> -nitrophenoxide dichloromethane solvate	$P2_12_12_1$	NEDDEF	[100]
Theophylline <i>p</i> -nitrophenol	$P-1$	TOPPNP	[101]

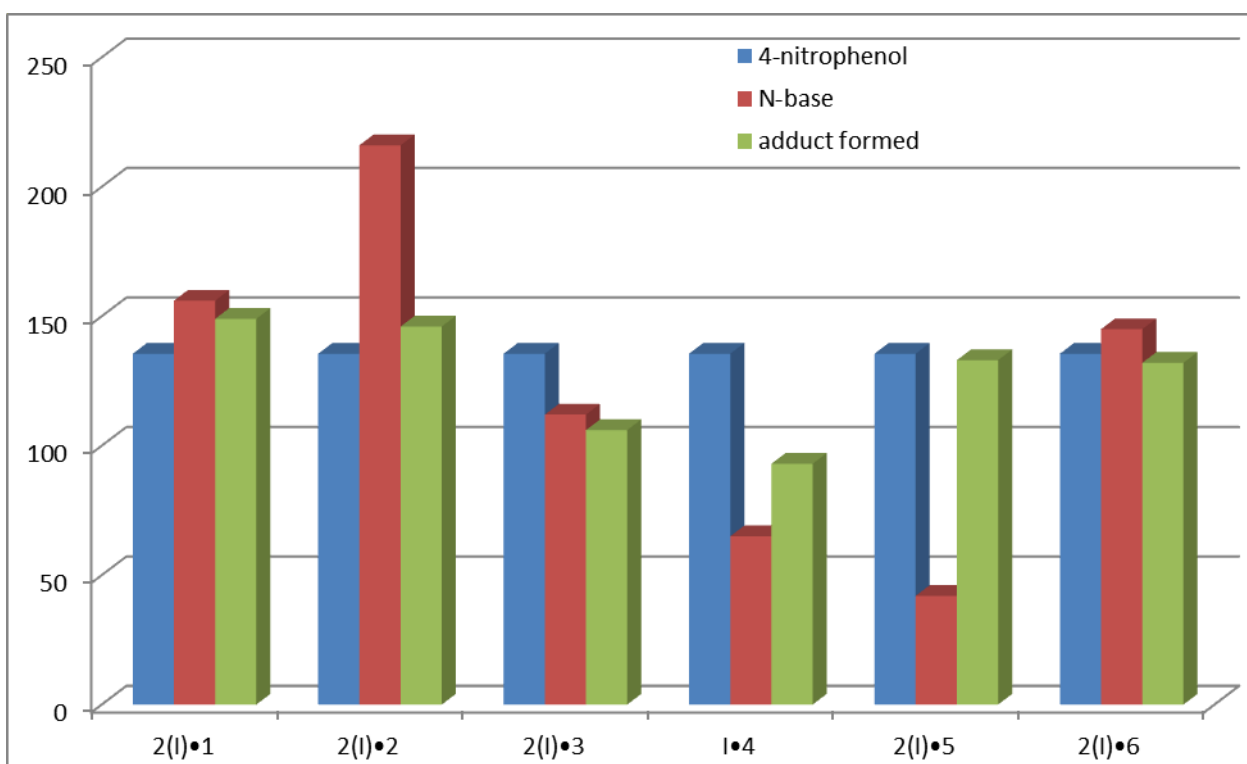
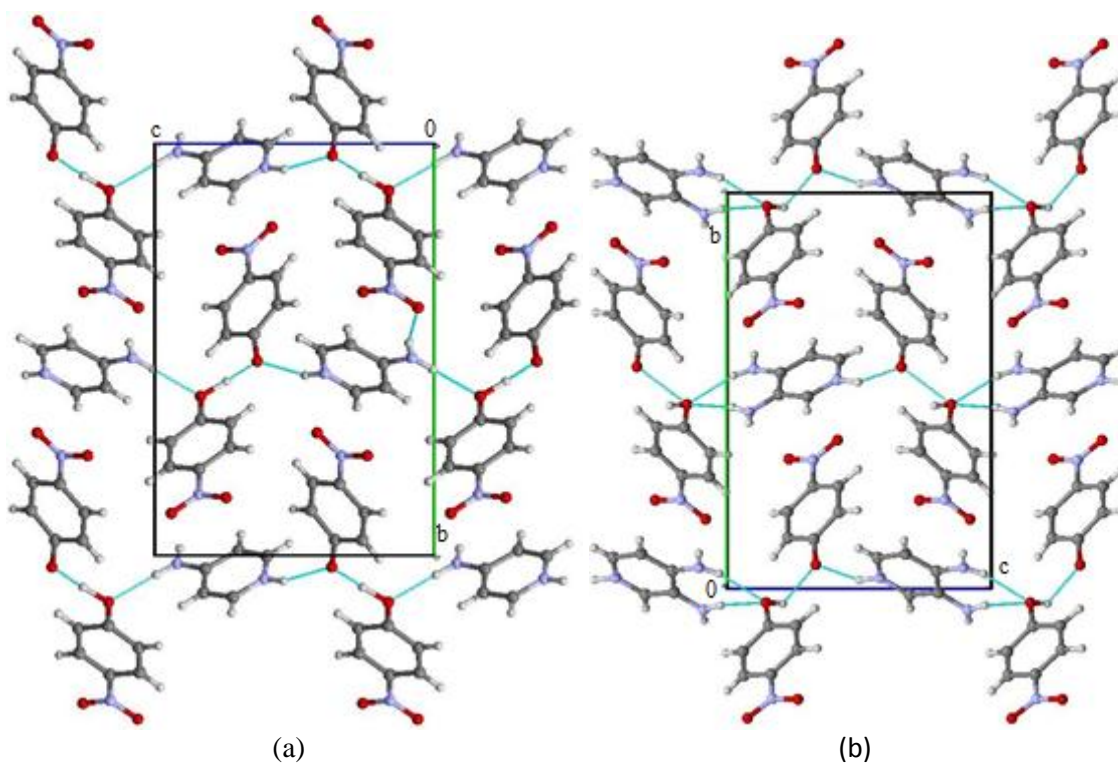
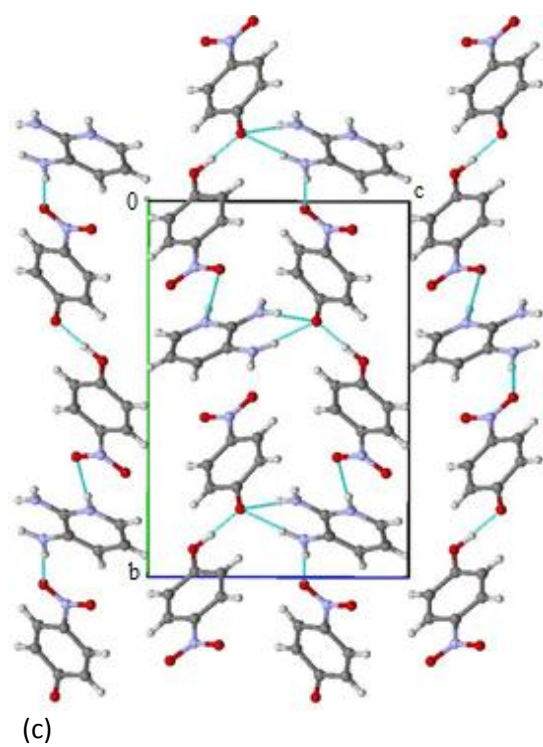
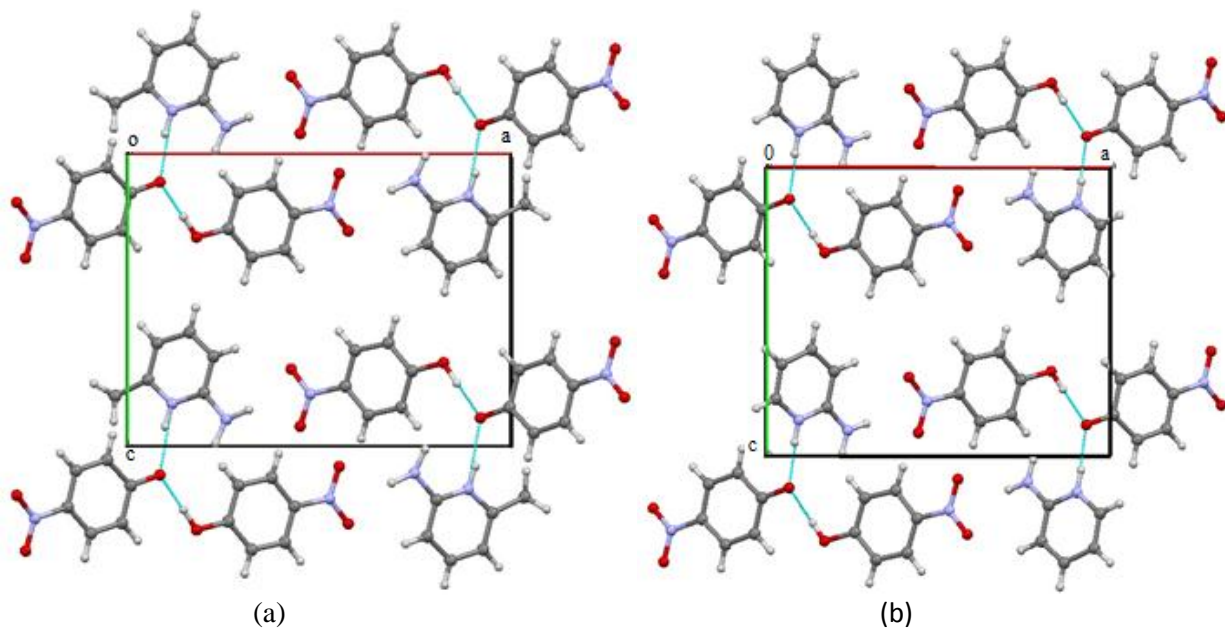


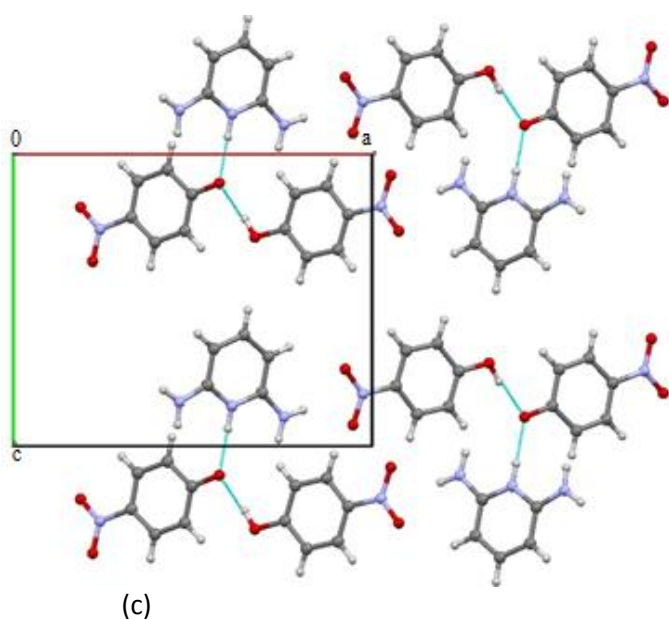
Fig. 1S. Melting points for new and initial compounds.





**Figure 2S.** Fragments of crystal packing in 2(I)•1(a), 2(I)•2 (b), 2(I)•3 (c).





**Figure 3S.** Fragments of crystal packing in 2(I)•5 (a), KAPFEN(b) and KAPFIR(c) [50].