

SUPPLEMENTARY MATERIALS FOR MANUSCRIPT

New Acentric Materials Constructed From Aminopyridines and 4-Nitrophenol

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Table 1S. Selected observed IR bands (ν , 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 ₂ asymmetric stretching mode
-	3286	3316	-	3221	3312	NH ₂ symmetric stretching mode
3089	3070	-	-	-	-	aromatic CH stretching mode
-	1616	1612	-	1695	1632	pyridine ring stretching vibration
1573	1562	1586	1585	1567	1572	NO ₂ asymmetric stretching
1321	-	1322	1330	1326	1328	NO ₂ symmetric stretching, C-N stretching mode
1239	1247	1215	1241	1246	1243	C-O stretching vibration for substituted phenols
1153	1137	1165	-	1175	-	NH ₂ rocking mode; O-H-in plane bending
1098	-	-	1110	1101	1104	C-C-N asymmetric stretch, ring stretching
847	-	848	842	859	849	NH ₂ 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]
4-Aminopyridinium 4-nitrophenolate 4-nitrophenol	$P2_1$	-	This work
2-Amino,6-methylpyridinium 4-nitrophenolate 4-nitrophenol	$Pna2_1$	-	This work
3,4-Diaminopyridinium 4-nitrophenolate 4-nitrophenol	$P2_1$	-	This work
2,3-Diaminopyridinium 4-nitrophenolate 4-nitrophenol	$P2_1$	-	This work
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]
2,3-Diaminopyrimidinium 4-nitrophenolate 4-nitrophenol	$P2_1/c$	-	This work
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]
3-Aminopyridine 4-nitrophenol	$P2_1$	-	This work
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]

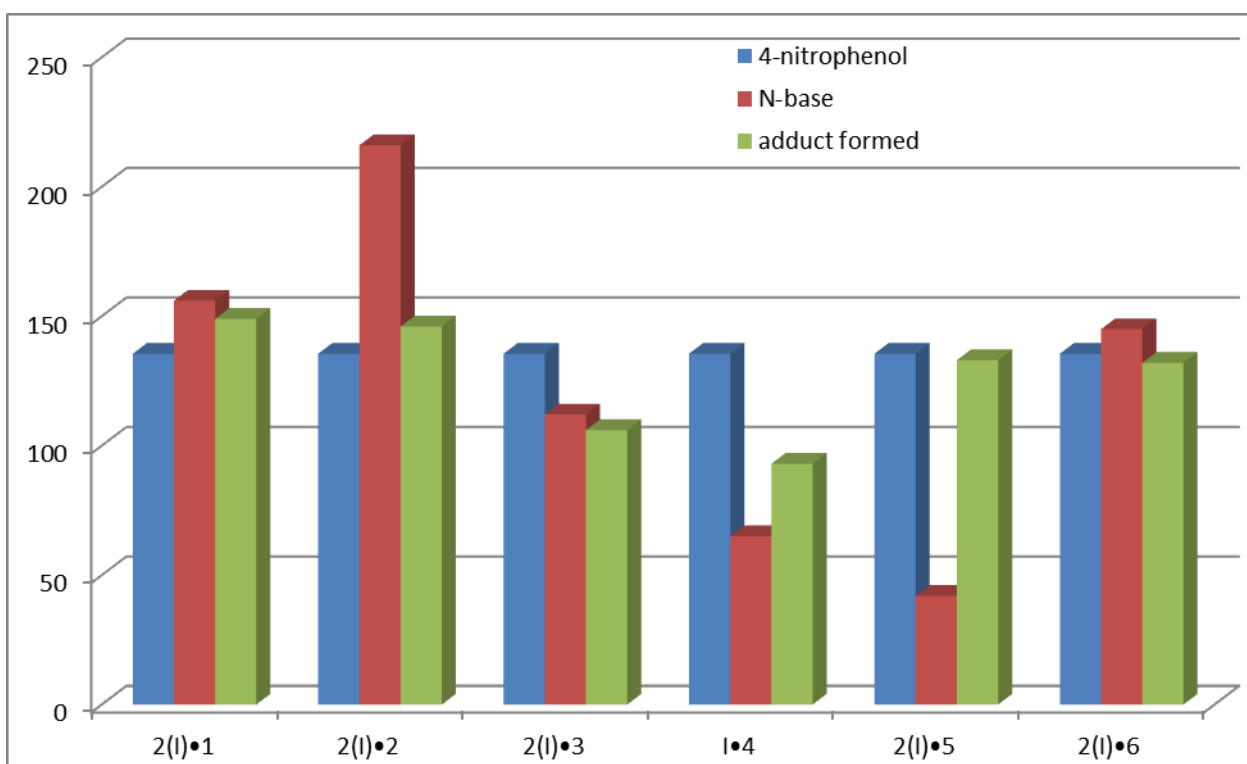
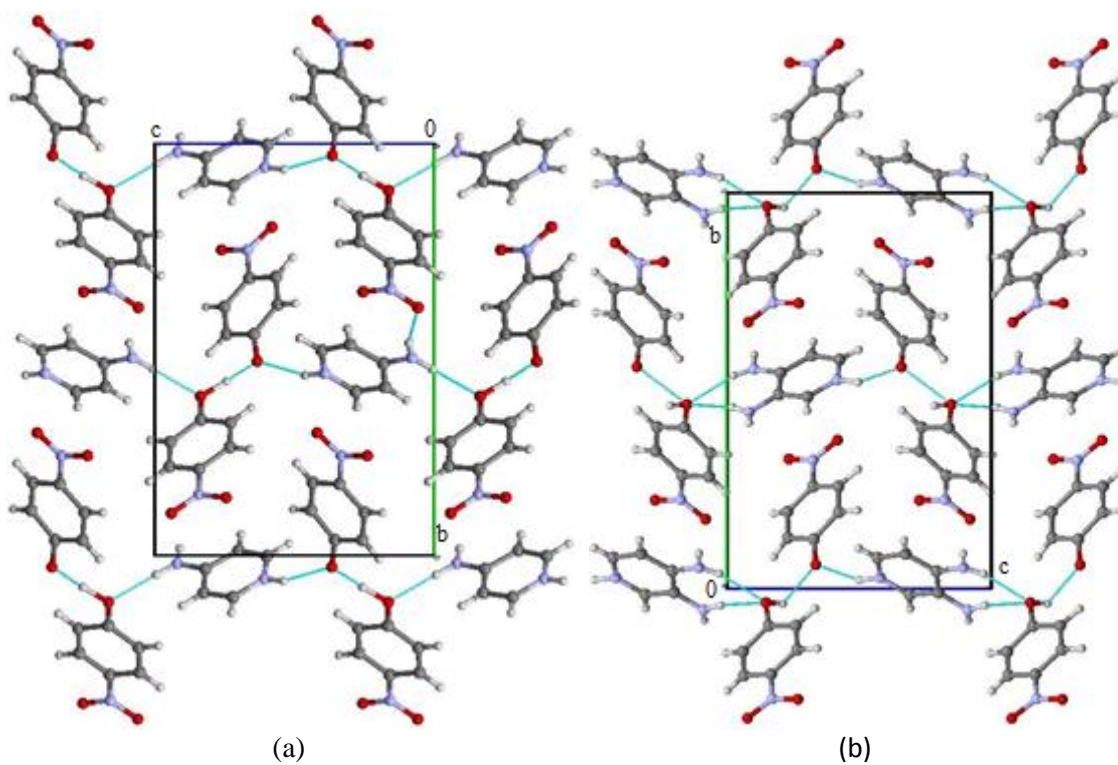


Fig. 1S. Melting points for new and initial compounds.



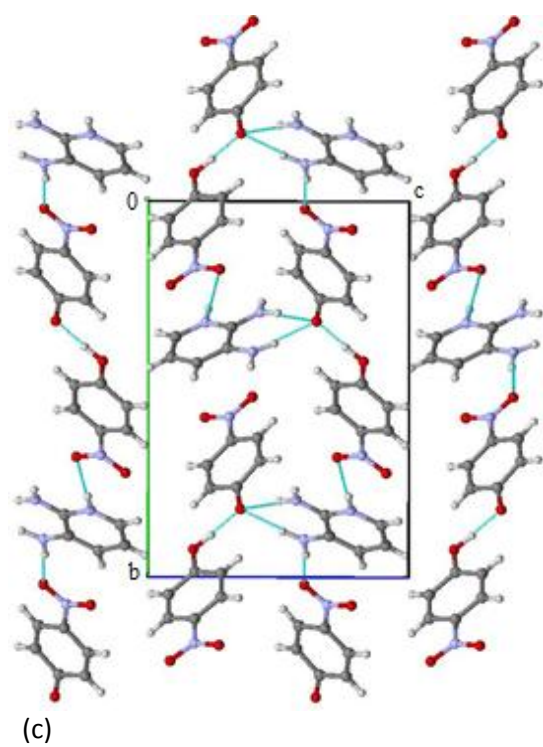
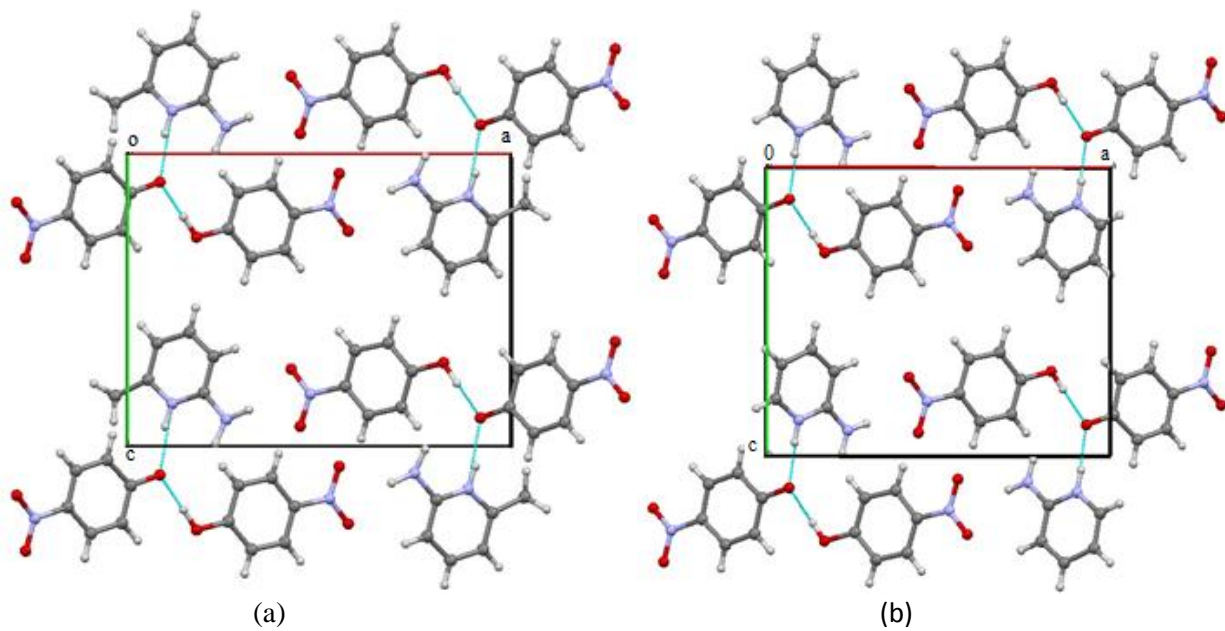


Figure 2S. Fragments of crystal packing in 2(I)•1(a), 2(I)•2 (b), 2(I)•3 (c).



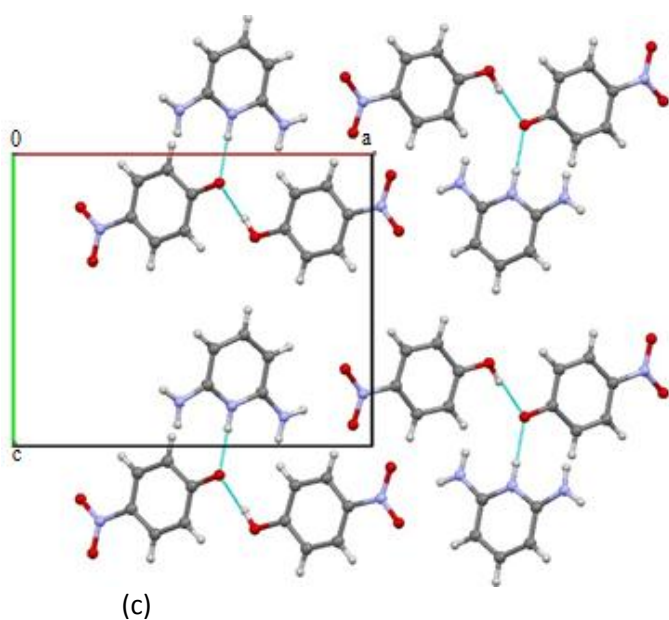


Figure 3S. Fragments of crystal packing in 2(I)•5 (a), KAPFEN(b) and KAPFIR(c) [50].