

# Synthesis, Crystal Structure and Supramolecular Features of Novel 2,4-Diaminopyrimidine Salts

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## Supplementary Materials:

**Table S1.** Geometric parameters of  $\pi\cdots\pi$  interactions observed in the crystals **1** - **4** (only distances Cg $\cdots$ Cg < 5 Å are shown).

Cg...Cg	Symmetry code	Cg...Cg distance	P	Q	R	S	alpha	beta	gamma	CgI-perp	CgJ-perp	slippage
1												
Cg1...Cg1	-1+x, y, z	4.7895(10)	0.6582	0.7374	0.1518	-3.2330	0.00(8)	48.8	48.8	3.1526(7)	3.1526(7)	3.606
2												
Cg1...Cg1	1-x, 1-y, 1-z	4.6924(7)	-0.6162	0.5336	0.5792	10.2047	0.00(6)	47.3	47.3	3.1816(5)	3.1816(5)	
Cg1...Cg1	-1+x, y, z	4.8526(8)	0.6162	-0.5336	-0.5792	-10.0135	0.00(6)	52.0	52.0	2.9904(5)	2.9904(5)	
3												
Cg1...Cg1	1-x, 2-y, 1-z	4.1620(7)	-0.7740	-0.6295	-0.0684	-17.3739	0.00(5)	36.5	36.5	3.3449(5)	3.3449(5)	2.477
4												
Cg1...Cg1	1-x, -y, -z	4.2894(11)	0.5417	-0.6043	-0.5843	3.0752	0.00(9)	40.9	40.9	3.2434(8)	3.2334(8)	2.807

**Table S2.** Geometric parameters of C-O $\cdots\pi$  interactions observed in the crystals **1** – **4**.

[illegible]

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C1-O2...Cg1	1+x, 1+y, z	3.2750(13)	0.6582	0.7374	0.1518	9.1654	-3.234	9.12	120.94(9)	4.0850(18)	24.74
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**3**

C6-O3...Cg1	½+x, -1/2+y, z	3.0468(11)	0.7740	0.6295	0.684	24.6772	-2.982	11.86	126.62(8)	3.8934(13)	25.19
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**4**

C5-O3...Cg1	X, y, z	3.5305(17)	-0.5417	0.6043	0.5843	0.1681	3.369	17.40	104.97(13)	4.030(2)	0.83
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**Table S3.** Gallery of H-bonding supramolecular synthons containing 2,4-diaminopyrimidine moiety.

<b>1</b>	
$D(2)$	$^{*}_{(\text{NH}_2)}\text{N4-H4A}\cdots\text{O2}(\text{COO}^-)$ $^{*}_{(\text{NH}_2)}\text{N4-H4A}\cdots\text{O4}(\text{COOH})$ $^{*}_{(\text{NH})}\text{N2-H2}\cdots\text{O2}(\text{COO}^-)$ $^{*}_{(\text{NH}_2)}\text{N3-H3A}\cdots\text{O4}(\text{COOH})$ $^{*}_{(\text{NH}_2)}\text{N3-H3B}\cdots\text{O5}(\text{H}_2\text{O})$
$R^2_2(8)$	$[(\text{NH}_2)\text{N4-H4A}\cdots\text{N1}_{(\text{cycl})}]_2$
<i>Level 2</i>	
$R^1_2(6)$	$(\text{NH}_2)\text{N4-H4A}\cdots\text{O2}(\text{COO}^-)$ & $(\text{NH}_{\text{cycl}})\text{N2-H2}\cdots\text{O2}(\text{COO}^-)$
$R^2_4(16)$	$(\text{NH}_2)\text{N3-H3A}\cdots\text{O4}(\text{C=O})$ & $(\text{NH}_2)\text{N4-H4A}\cdots\text{O4}(\text{C=O})_2$
$R^4_2(16)$	$(\text{NH}_2)\text{N4-H4A}\cdots\text{O2}(\text{COO}^-)$ & $(\text{NH}_2)\text{N4-H4A}\cdots\text{O4}(\text{COOH})_2$
$C^2_2(14)$	$^{*}_{(\text{NH}_2)}\text{N4-H4A}\cdots\text{O2}(\text{COO}^-)$ & $(\text{NH}_2)\text{N3-H3A}\cdots\text{O4}(\text{COOH})$ $^{*}_{(\text{NH}_2)}\text{N2-H2}\cdots\text{O2}(\text{COO}^-)_2$ & $(\text{NH}_2)\text{N3-H3A}\cdots\text{O4}(\text{COOH})$
$D^1_2(3)$	$(\text{NH}_2)\text{N3-H3B}\cdots\text{O5}(\text{H}_2\text{O})$ & $(\text{CH}_2)\text{C2-H2A}\cdots\text{O5}(\text{H}_2\text{O})$
$D^2_2(4)$	$(\text{NH}_2)\text{N3-H3B}\cdots\text{O5}(\text{H}_2\text{O})$ & $(\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O1}(\text{COO}^-)$
$D^2_2(5)$	$(\text{NH}_2)\text{N4-H4A}\cdots\text{O2}(\text{COO}^-)$ & $(\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O1}(\text{COO}^-)$ $^{*}_{(\text{NH}_{\text{cycl}})}\text{N2-H2}\cdots\text{O2}(\text{COO}^-)$ & $(\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O1}(\text{COO}^-)$ $^{*}_{(\text{NH}_2)}\text{N3-H3A}\cdots\text{O4}(\text{COOH})$
$D^2_2(6)$	$^{*}_{(\text{NH}_2)}\text{N4-H4A}\cdots\text{O2}(\text{COO}^-)$ & $(\text{CH}_2)\text{C2-H2A}\cdots\text{O5}(\text{H}_2\text{O})$ $^{*}_{(\text{NH}_2)}\text{N2-H2}\cdots\text{O2}(\text{COO}^-)$ & $(\text{CH}_2)\text{C2-H2A}\cdots\text{O5}(\text{H}_2\text{O})$
$D^2_2(8)$	$^{*}_{(\text{NH}_2)}\text{N4-H4A}\cdots\text{O4}(\text{COOH})$ & $(\text{CH}_2)\text{C2-H2A}\cdots\text{O5}(\text{H}_2\text{O})$ $^{*}_{(\text{NH}_2)}\text{N3-H3A}\cdots\text{O4}(\text{COOH})$ & $(\text{CH}_2)\text{C2-H2A}\cdots\text{O5}(\text{H}_2\text{O})$
$D^2_2(9)$	$^{*}_{(\text{NH}_2)}\text{N4-H4A}\cdots\text{O4}(\text{COOH})$ & $(\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O1}(\text{COO}^-)$ $^{*}_{(\text{NH}_2)}\text{N3-H3A}\cdots\text{O4}(\text{COOH})$ & $(\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O1}(\text{COO}^-)$ $^{*}_{(\text{NH}_2)}\text{N4-H4A}\cdots\text{O2}(\text{COO}^-)$ & $(\text{NH}_2)\text{N3-H3B}\cdots\text{O5}(\text{H}_2\text{O})$ $^{*}_{(\text{NH}_2)}\text{N4-H4A}\cdots\text{O4}(\text{COOH})$ & $(\text{NH}_2)\text{N3-H3B}\cdots\text{O5}(\text{H}_2\text{O})$ $^{*}_{(\text{NH}_{\text{cycl}})}\text{N2-H2}\cdots\text{O2}(\text{COO}^-)$ & $(\text{NH}_2)\text{N3-H3B}\cdots\text{O5}(\text{H}_2\text{O})$

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$D^2_3(5)$	$[(\text{NH}_2)\text{N}3\text{-H}3\text{B}\cdots\text{O}5_{(\text{H}_2\text{O})}]_2 \& (\text{H}_2\text{O})\text{O}5\text{-H}5\text{C}\cdots\text{O}5_{(\text{H}_2\text{O})}$
$D^2_3(7)$	$*[(\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{O}4_{(\text{COOH})}]_2 \& (\text{CH}_2)\text{C}3\text{-H}3\text{C}\cdots\text{O}4_{(\text{COOH})}$  $*[(\text{NH}_2)\text{N}3\text{-H}3\text{A}\cdots\text{O}4_{(\text{COOH})}]_2 \& (\text{CH}_2)\text{C}3\text{-H}3\text{C}\cdots\text{O}4_{(\text{COOH})}$
$D^2_3(11)$	$[(\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{O}2_{(\text{COO}^-)}]_2 \& (\text{COOH})\text{O}3\text{-H}3\cdots\text{O}2_{(\text{COO}^-)}$
$D^3_3(9)$	$(\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{O}2_{(\text{COO}^-)}]_2 \& (\text{NH}_2)\text{N}4\text{-H}4\text{B}\cdots\text{N}1_{(\text{cycl})}$  $*(\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{O}4_{(\text{COOH})}]_2 \& (\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{N}1_{(\text{cycl})}$
$D^3_3(11)$	$*(\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{O}4_{(\text{COOH})}]_2 \& (\text{CH}_2)\text{C}2\text{-H}2\text{B}\cdots\text{O}3_{(\text{COOH})}$  $*(\text{NH}_2)\text{N}3\text{-H}3\text{A}\cdots\text{O}4_{(\text{COOH})}]_2 \& (\text{CH}_2)\text{C}2\text{-H}2\text{B}\cdots\text{O}3_{(\text{COOH})}$  $*(\text{NH}_2)\text{N}2\text{-H}2\cdots\text{O}2_{(\text{COO}^-)}]_2 \& (\text{NH}_2)\text{N}4\text{-H}4\text{B}\cdots\text{N}1_{(\text{cycl})}$
$D^3_3(13)$	$*[(\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{O}4_{(\text{COOH})}]_2 \& (\text{COOH})\text{O}3\text{-H}3\cdots\text{O}2_{(\text{COO}^-)}$  $*(\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{O}2_{(\text{COO}^-)}]_2 \& (\text{CH}_2)\text{C}2\text{-H}2\text{B}\cdots\text{O}3_{(\text{COOH})}$  $*(\text{NH}_{\text{cycl}})\text{N}2\text{-H}2\cdots\text{O}2_{(\text{COO}^-)}]_2 \& (\text{CH}_2)\text{C}2\text{-H}2\text{B}\cdots\text{O}3_{(\text{COOH})}$
$D^3_3(15)$	$*[(\text{NH}_2)\text{N}4\text{-H}4\text{A}\cdots\text{O}2_{(\text{COO}^-)}]_2 \& (\text{CH}_2)\text{C}3\text{-H}3\text{C}\cdots\text{O}4_{(\text{COOH})}$  $*[(\text{NH}_{\text{cycl}})\text{N}2\text{-H}2\cdots\text{O}2_{(\text{COO}^-)}]_2 \& (\text{CH}_2)\text{C}3\text{-H}3\text{C}\cdots\text{O}4_{(\text{COOH})}$

## 2

$D(2)$	$*(\text{NH}_{\text{cycl}})\text{N}1\text{-H}1\cdots\text{O}3_{(\text{COO}^-)}$  $*(\text{NH}_2)\text{N}4\text{-H}4\text{C}\cdots\text{O}5_{(\text{H}_2\text{O})}$  $*(\text{NH}_2)\text{N}4\text{-H}4\text{D}\cdots\text{O}1_{(\text{COOH})}$  $*(\text{NH}_2)\text{N}3\text{-H}3\text{D}\cdots\text{O}1_{(\text{COOH})}$  $*(\text{NH}_2)\text{N}3\text{-H}3\text{D}\cdots\text{O}3_{(\text{COO}^-)}$
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$R^2_2(8)$	$(\text{NH}_2)\text{N}3\text{-H}3\text{C}\cdots\text{N}2_{(\text{N}_{\text{cycl}})}]_2$
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### Level 2

$R^1_2(6)$	$(\text{NH}_2)\text{N}3\text{-H}3\text{D}\cdots\text{O}3_{(\text{cycl})} \& (\text{cycl})\text{N}1\text{-H}1\cdots\text{O}3_{(\text{COO}^-)}]_2$
$R^2_4(16)$	$(\text{NH}_2)\text{N}4\text{-H}4\text{D}\cdots\text{O}1_{(\text{COOH})} \& (\text{NH}_2)\text{N}3\text{-H}3\text{D}\cdots\text{O}1_{(\text{COOH})}$
$C^2_1(8)$	$(\text{NH}_2)\text{N}3\text{-H}3\text{D}\cdots\text{O}1_{(\text{COOH})} \& (\text{NH}_2)\text{N}3\text{-H}3\text{D}\cdots\text{O}3_{(\text{COO}^-)}]_2$
$C^2_2(12)$	$(\text{NH}_{\text{cycl}})\text{N}1\text{-H}1\cdots\text{O}3_{(\text{COO}^-)} \& (\text{NH}_2)\text{N}3\text{-H}3\text{D}\cdots\text{O}1_{(\text{COOH})}$
$C^2_2(14)$	$(\text{NH}_{\text{cycl}})\text{N}1\text{-H}1\cdots\text{O}3_{(\text{COO}^-)} \& (\text{NH}_2)\text{N}4\text{-H}4\text{D}\cdots\text{O}1_{(\text{COOH})}$

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$D^2_2(4)$	$(\text{NH}_2)\text{N4-H4C}\cdots\text{O5}(\text{H}_2\text{O}) \& (\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O4}(\text{COO}^-)$
$D^2_2(5)$	$*(\text{NH}_{\text{cycl}})\text{N1-H1}\cdots\text{O3}(\text{COO}^-) \& (\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O4}(\text{COO}^-)$
	$*(\text{NH}_2)\text{N3-H3D}\cdots\text{O3}(\text{COO}^-) \& (\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O4}(\text{COO}^-)$
$D^2_2(9)$	$(\text{NH}_2)\text{N4-H4D}\cdots\text{O1}(\text{COOH}) \& (\text{H}_2\text{O})\text{O5-H5A}\cdots\text{O4}(\text{COO}^-)$
$D^2_3(11)$	$(\text{NH}_{\text{cycl}})\text{N1-H1}\cdots\text{O3}(\text{COO}^-)]_2 \& (\text{COOH})\text{O2-H2}\cdots\text{O3}(\text{COO}^-)$
$D^3_3(9)$	$(\text{NH}_2)\text{N3-H3C}\cdots\text{N2}_{(\text{cycl})} \& (\text{NH}_2)\text{N3-H3D}\cdots\text{O3}(\text{COO}^-)]_2$
$D^3_3(11)$	$(\text{NH}_2)\text{N3-H3C}\cdots\text{N2}_{(\text{cycl})} \& (\text{cycl})\text{N1-H1}\cdots\text{O3}(\text{COO}^-)]_2$
$D^3_3(13)$	$(\text{NH}_2)\text{N4-H4D}\cdots\text{O1}(\text{COOH})]_2 \& (\text{COOH})\text{O2-H2}\cdots\text{O3}(\text{COO}^-)$

### 3

$D(2)$	$*(\text{NH}_{\text{cycl}})\text{N2-H2}\cdots\text{O2}(\text{COO}^-)$
	$*(\text{NH}_2)\text{N4-H4C}\cdots\text{O1}(\text{COO}^-)$
	$*(\text{NH}_2)\text{N3-H3C}\cdots\text{O1}(\text{COO}^-)$
	$*(\text{CH}_{\text{cycl}})\text{C10-H10}\cdots\text{O1}(\text{COO}^-)$
	$*(\text{CH}_{\text{cycl}})\text{C9-H9}\cdots\text{O3}(\text{COOH})$
$R^2_2(8)$	$(\text{NH}_2)\text{N3-H3D}\cdots\text{N1}_{(\text{cycl})}]_2$

#### Level 2

$R^1_2(6)$	$(\text{NH}_2)\text{N3-H3C}\cdots\text{O1}(\text{COO}^-) \& (\text{NH}_2)\text{N3-H3C}\cdots\text{O1}(\text{COO}^-)$
$R^2_2(8)$	$(\text{NH}_{\text{cycl}})\text{N2-H2}\cdots\text{O2}(\text{COO}^-) \& (\text{NH}_2)\text{N4-H4C}\cdots\text{O1}(\text{COO}^-)$
$C^1_2(8)$	$*(\text{NH}_2)\text{N4-H4C}\cdots\text{O1}(\text{COO}^-) \& (\text{CH}_{\text{cycl}})\text{C10-H10}\cdots\text{O1}(\text{COO}^-)$
	$*(\text{NH}_2)\text{N4-H4C}\cdots\text{O1}(\text{COO}^-) \& (\text{NH}_2)\text{N3-H3C}\cdots\text{O1}(\text{COO}^-)$
$C^2_2(8)$	$(\text{NH}_{\text{cycl}})\text{N2-H2}\cdots\text{O2}(\text{COO}^-) \& (\text{CH}_{\text{cycl}})\text{C10-H10}\cdots\text{O1}(\text{COO}^-)$
$C^2_2(10)$	$(\text{NH}_{\text{cycl}})\text{N2-H2}\cdots\text{O2}(\text{COO}^-) \& (\text{NH}_2)\text{N3-H3C}\cdots\text{O1}(\text{COO}^-)$
$C^2_2(16)$	$(\text{NH}_2)\text{N4-H4C}\cdots\text{O1}(\text{COO}^-) \& (\text{CH}_{\text{cycl}})\text{C9-H9}\cdots\text{O3}(\text{COOH})$
$D^1_2(3)$	$*(\text{NH}_2)\text{N4-H4C}\cdots\text{O1}(\text{COO}^-) \& (\text{H}_2\text{O})\text{O5-H5C}\cdots\text{O1}(\text{COO}^-)$
	$*(\text{CH}_{\text{cycl}})\text{C10-H10}\cdots\text{O1}(\text{COO}^-) \& (\text{H}_2\text{O})\text{O5-H5D}\cdots\text{O1}(\text{COO}^-)$
	$*(\text{NH}_2)\text{N3-H3C}\cdots\text{O1}(\text{COO}^-) \& (\text{H}_2\text{O})\text{O5-H5D}\cdots\text{O1}(\text{COO}^-)$
$D^2_2(5)$	$(\text{NH}_{\text{cycl}})\text{N2-H2}\cdots\text{O2}(\text{COO}^-) \& (\text{H}_2\text{O})\text{O5-H5C}\cdots\text{O1}(\text{COO}^-)$

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$D^2_2(12)$	(CHcycl)C9-H9...O3(COOH) & (H2O)O5-H5D...O1(COO-)
$D^2_3(6)$	*(CHcycl)C10-H10...O1(COO-) & (H2O)O5-H5D...O1(COO-) & (H2O)O5-H5C...O1(COO-)
	*(NH2)N3-H3C...O1(COO-) & [(H2O)O5-H5D...O1(COO-)]2
$D^2_3(14)$	[(NHcycl)N2-H2...O2(COO-)]2 & (COOH)O4-H4...O2(COO-)
$D^3_3(8)$	(NHcycl)N2-H2...O2(COO-) & (H2O)O5-H5C...O1(COO-)]2
$D^3_3(9)$	(NH2)N3-H3C...O1(COO-) & (NH2)N3-H3D...N1(cycl)
$D^3_3(11)$	(NH2)N3-H3D...N1(cycl) & (CHcycl)C10-H10...O1(COO-)]2
$D^3_3(13)$	(NHcycl)N2-H2...O2(COO-)]2 & (CH2)C3-H3A...S2
$D^3_3(15)$	(CHcycl)C9-H9...O3(COOH)]2 & (CH2)C3-H3A...S2
$D^3_3(16)$	(NH2)N4-H4C...O1(COO-)]2 (COOH)O4-H4...O2(COO-)

#### 4

$R^2_2(8)$	(NH2)N3-H3B...N2(cycl)]2
$D(2)$	(NH2)N4-H4A...O5(H2O)
$D^2_2(12)$	*(CHcycl)C12-H12...O3(COOH)]2
	*(NH2)N3-H3A...O1(COO-)]2

#### Level 2

$R^2_2(8)$	(NH2)N3-H3A...O1(COO-) & (NHcycl)N1-H1...O2(COO-)
$R^2_4(14)$	(CHcycl)C12-H12...O3(COOH) & (NH2)N4-H4B...O3(COOH)
$D^1_2(3)$	*(NHcycl)N1-H1...O2(COO-) & (COOH)O4-H4...O2(COO-)
	*(NH2)N4-H4A...O5(H2O) & (CH2)C6-H6B...O5(H2O)
	*(NH2)N4-H4A...O5(H2O) & (CH2)C2-H2B...O5(H2O)
$D^2_2(4)$	*(NH2)N4-H4A...O5(H2O) & (H2O)O5-H5A...O1(COO-)
$D^2_2(5)$	*(NH2)N3-H3A...O1(COO-) & (COOH)O4-H4...O2(COO-)
	*(CHcycl)C12-H12...O3(COOH) & (CH2)C2-H2A...O4(COOH)
$D^2_2(6)$	*(NH2)N4-H4B...O3(COOH) & (COOH)O4-H4...O2(COO-)
	*(NH2)N4-H4B...O3(COOH) & (CH2)C6-H6B...O5(H2O)
	*(NHcycl)N1-H1...O2(COO-) & (CH2)C2-H2A...O4(COOH)

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$D^2_2(8)$	(CH <sub>cycl</sub> )C12-H12...O3(COOH) & (NH <sub>2</sub> )N3-H3A...O1(COO-)
$D^2_2(9)$	(NH)N1-H1...O2(COO-) & (NH <sub>2</sub> )N4-H4A...O5(H <sub>2</sub> O)
$D^2_2(11)$	*(CH <sub>cycl</sub> )C12-H12...O3(COOH) & (CH <sub>2</sub> )C6-H6B...O5(H <sub>2</sub> O) *(NH <sub>cycl</sub> )N1-H1...O2(COO-) & (CH <sub>2</sub> )C2-H2A...O4(COOH)
$D^2_2(12)$	(NH <sub>cycl</sub> )N1-H1...O2(COO-) & (COOH)O4-H4...O2(COO-)
$D^2_2(13)$	(NH <sub>2</sub> )N4-H4B...O3(COOH) & (COOH)O4-H4...O2(COO-)
$D^2_3(11)$	(NH <sub>2</sub> )N4-H4A...O5(H <sub>2</sub> O) & (CH <sub>2</sub> )C2-H2B...O5(H <sub>2</sub> O)
$D^3_3(11)$	(NH <sub>2</sub> )N4-H4A...O5(H <sub>2</sub> O) & (CH <sub>2</sub> )C6-H6B...O5(H <sub>2</sub> O)
$D^3_3(13)$	(NH <sub>2</sub> )N4-H4A...O5(H <sub>2</sub> O) & (NH <sub>2</sub> )N3-H3B...N2(cycl)
$D^3_3(15)$	[(NH <sub>2</sub> )N4-H4B...O3(COOH)] <sub>2</sub> & (NH <sub>2</sub> )N4-H4A...O5(H <sub>2</sub> O)

**Table S4.** Percentage contributions of close intermolecular contacts in the crystals **1 - 4** (Hirshfeld surface analysis for 2,4-diaminopyrimidine motif).

	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>
H...H	30	34.5	40	36.7
O...H/H...O	27.2	22.4	21.3	20.7
N...H/H...N	15.1	19.3	16	18.2
C...H/H...C	13.1	15.1	9.6	14.7
N...C/C...N	2.9	3.8	5.7	2.8
O...N/N...O	2	1.3	1.9	2.4
O...C/C...O	2	2.1	3.2	1.7
N...N	1.7	0.8	1.1	1.5
C...C	0.3	0.7	0.6	1.4
S...C/C...S	1.4			
S...H/H...S	3.1		0.6	
S...N/N...S	1.2			