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Supplementary material

Coordination *versus* hydrogen bonds in the structures of different tris(pyridin-2-yl)phosphoric triamide derivatives

Atekeh Tarahhomi*, Marjan Sebghati, Marjan Sadat Bozorgvar, Dan G. Dumitrescu and Arie van der Lee

Table S1 Selected bond lengths (Å) and angles (°) for compounds **1** – **3**.

1		**1**		**2**	
Co01–O007^{i}	2.011 (2)	Co02–O008^{ii}	2.013 (2)	P001–O002	1.4783 (14)
Co01–N009^{i}	2.210 (3)	Co02–N00B^{ii}	2.231 (3)	P001–N003	1.6558 (10)
Co01–N00A^{i}	2.246 (2)	Co02–N00C^{ii}	2.210 (3)	P001–N003^{i}	1.6558 (10)
P004–O007	1.498 (2)	P003–O008	1.501 (2)	P001–N003^{ii}	1.6558 (10)
P004–N00E	1.575 (3)	P003–N00D	1.571 (3)	N003–C005	1.4094 (15)
P004–N00F	1.663 (3)	P003–N00H	1.666 (3)	N004–C005	1.3403 (15)
P004–N00G	1.661 (3)	P003–N00I	1.669 (3)	N004–C007	1.3465 (16)
O007^{i}–Co01–O007	180.00 (9)	O008–Co02–O008^{ii}	180.0	O002–P001–N003	113.34 (4)
O007–Co01–N009^{i}	91.53 (9)	O008^{ii}–Co02–N00B^{ii}	88.94 (9)	O002–P001–N003^{i}	113.34 (4)
O007–Co01–N009^{i}	88.47 (9)	O008–Co02–N00B^{ii}	91.05 (9)	O002–P001–N003^{ii}	113.34 (4)
O007–Co01–N00A	88.95 (9)	O008–Co02–N00C	89.16 (10)	N003^{i}–P001–N003^{ii}	105.34 (4)
O007–Co01–N00A^{i}	91.05 (9)	O008^{ii}–Co02–N00C	90.85 (10)	N003^{i}–P001–N003	105.34 (4)
N009^{i}–Co01–N009	180.0	N00B–Co02–N00B^{ii}	180.00 (9)	N003–P001–N003^{ii}	105.34 (4)
N009^{i}–Co01–N00A	92.74 (9)	N00C^{ii}–Co02–N00B	92.76 (9)		
N009^{i}–Co01–N00A^{i}	87.26 (9)	N00C–Co02–N00B	87.24 (9)		
N00A–Co01–N00A^{i}	180.00 (11)	N00C–Co02–N00C^{ii}	180.0		
3		**3**			
P001–O004	1.4783 (14)	P002–O003	1.4805 (8)		
P001–N008	1.6456 (10)	P002–N009	1.6451 (10)		
P001–N00A	1.6562 (11)	P002–N00B	1.6559 (11)		
P001–N00C	1.6494 (11)	P002–N00D	1.6579 (10)		
N008–C00N	1.4023 (15)	N009–C00M	1.4004 (15)		
N00A–C00I	1.3969 (15)	N00B–C00K	1.3952 (14)		
N00C–C00J	1.4007 (14)	N00D–C00H	1.4013 (14)		
O004–P001–N008	114.90 (5)	O003–P002–N009	113.98 (5)		
O004–P001–N00A	112.88 (5)	O003–P002–N00B	108.46 (5)		
O004–P001–N00C	109.62 (5)	O003–P002–N00D	115.50 (5)		
N008–P001–N00A	103.35 (5)	N009–P002–N00B	110.72 (5)		
N008–P001–N00C	109.69 (5)	N009–P002–N00D	102.90 (5)		
N00A–P001–N00C	105.90 (5)	N00B–P002–N00D	104.84 (5)		

Symmetry codes for **1**: (i) –*x* + 1, –*y*, –*z* + 1; (ii) –*x*, –*y* + 1, –*z* + 1; for **2**: (i) –*x* + *y* + 1, –*x* + 1, *z*; (ii) –*y* + 1, *x* – *y*, *z*.

Table S2 Selected bond lengths (Å) and angles (°) for compounds **4** and **5**.

4		**4**		**5**	
P001–O003	1.4839 (8)	P002–O005	1.4774 (8)	Cu01–O002	2.004 (4)
P001–N008	1.6522 (9)	P002–N007	1.6459 (10)	Cu01–O002^{i}	2.004 (4)
P001–N00A	1.6444 (10)	P002–N009	1.6563 (10)	Cu01–O004^{i}	1.994 (3)
P001–N00C	1.6508 (9)	P002–N00G	1.6522 (10)	Cu01–O004	1.994 (3)
N008–C00N	1.3991 (13)	N007–C00P	1.4005 (13)	O002–C008	1.256 (5)
N00A–C00R	1.3986 (13)	N009–C00M	1.3988 (13)	O003–C006	1.232 (6)
N00C–C00O	1.3967 (13)	N00G–C00Q	1.3927 (13)	N005–C007^{ii}	1.464 (6)
O003–P001–N008	115.34 (5)	O005–P002–N007	113.87 (5)	O002–Cu01–O002^{i}	180.0
O003–P001–N00A	112.60 (5)	O005–P002–N009	114.69 (5)	O004^{i}–Cu01–O002	88.38 (13)
O003–P001–N00C	108.76 (5)	O005–P002–N00G	108.41 (5)	O004–Cu01–O002^{i}	88.38 (13)
N008–P001–N00A	103.63 (5)	N007–P002–N009	103.18 (5)	O004–Cu01–O002	91.62 (13)
N008–P001–N00C	104.53 (5)	N007–P002–N00G	110.39 (5)	O004^{i}–Cu01–O002^{i}	91.62 (13)
N00A–P001–N00C	111.68 (5)	N009–P002–N00G	105.96 (5)	O004^{i}–Cu01–O004	180.0 (2)

Symmetry codes for **5**: (i) –*x* + 1, –*y* + 1, –*z* + 2; (ii) –*x* + $\frac{1}{2}$, *y*, –*z* + 1.

Table S3 Summary of the percentage contributions of interactions, surface contacts (S_X), random contacts (R_{XX}/R_{XY}) and enrichment ratios (E_{XX}/E_{XY}) for **5** and MACUFR.

Contacts	**5**	MACUFR	S_X	H	C	O	Cu
H…H	23.7	19.3	**5**	53.95	3.70	36.40	5.65
H…C/C…H	7.4	7.3	MACUFR	51.6	3.65	38.7	5.55
H…O/O…H	53.1	57.3					
Cu…O/O…Cu	11.3	11.1					
O…O	4.2	4.5					
Atoms		H	C	O	Cu		
5	R_{XX}/R_{XY}						
H		29.11	3.99	39.27	—		
C		3.99	—	—	—		
O		39.27	—	13.25	4.11		
Cu		—	—	4.11	—		
5	E_{XX}/E_{XY}						
H		0.81	1.85	1.35	—		
C		1.85	—	—	—		
O		1.35	—	0.32	2.75		
Cu		—	—	2.75	—		
Atoms		H	C	O	Cu		
MACUFR	R_{XX}/R_{XY}						
H		26.63	3.77	39.94	—		
C		3.77	—	—	—		
O		39.94	—	14.98	4.29		
Cu		—	—	4.29	—		
MACUFR	E_{XX}/E_{XY}						
H		0.72	1.94	1.43	—		
C		1.94	—	—	—		
O		1.43	—	0.30	2.59		
Cu		—	—	2.59	—		

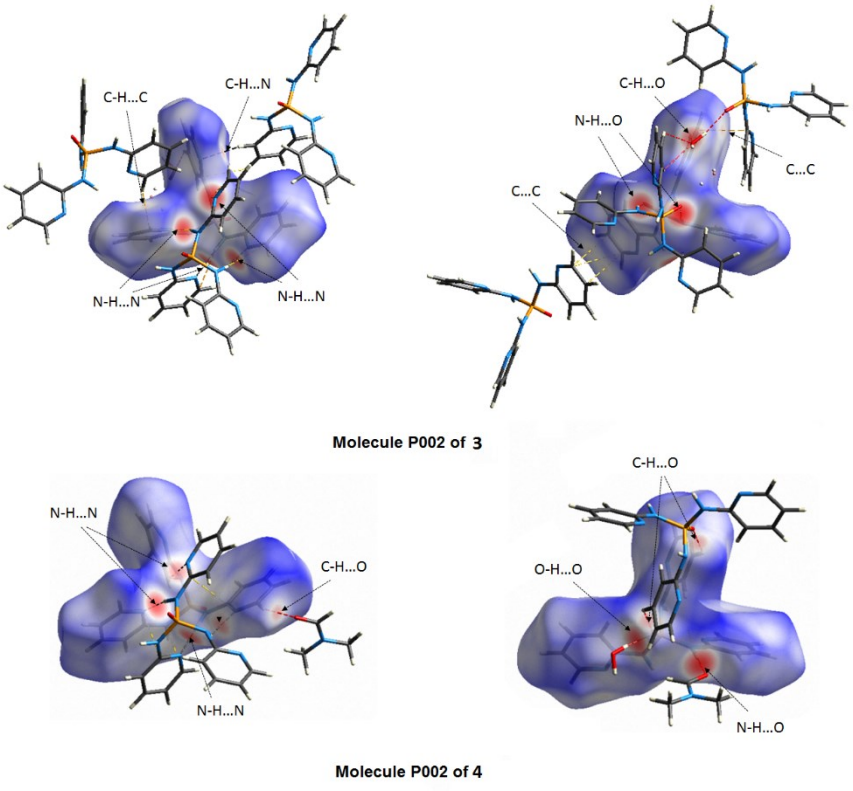

Fig. S1 Views of d_{norm} Hirshfeld surfaces plotted on the molecules P002 of **3** and **4**, in two orientations, surrounded by neighboring molecules associated with close contacts introduced in figure.

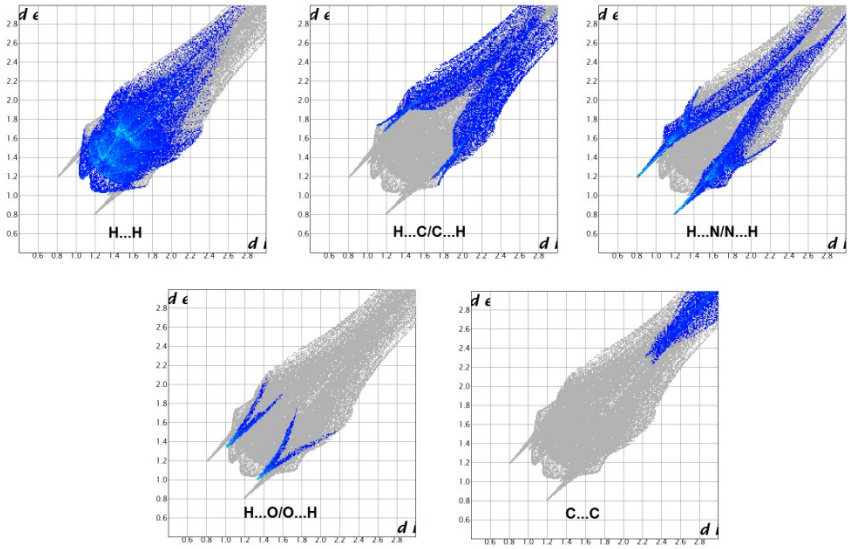

Fig. S2 Decomposed FPs of various intermolecular contacts H...H, H...C/C...H, H...N/N...H, H...O/O...H and C...C for compound **2**.

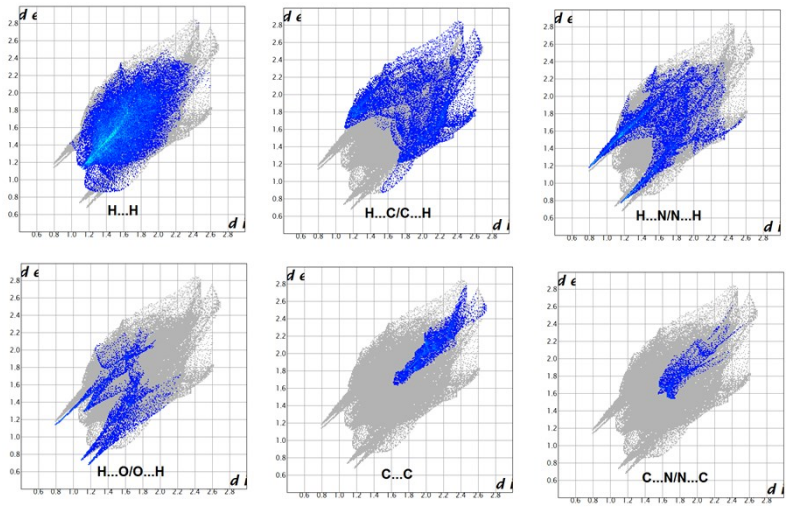

Fig. S3 Decomposed FPs of various intermolecular contacts H…H, H…C/C…H, H…N/N…H, H…O/O…H, C…C and C…N/N…C for the molecule P001 of **3**.

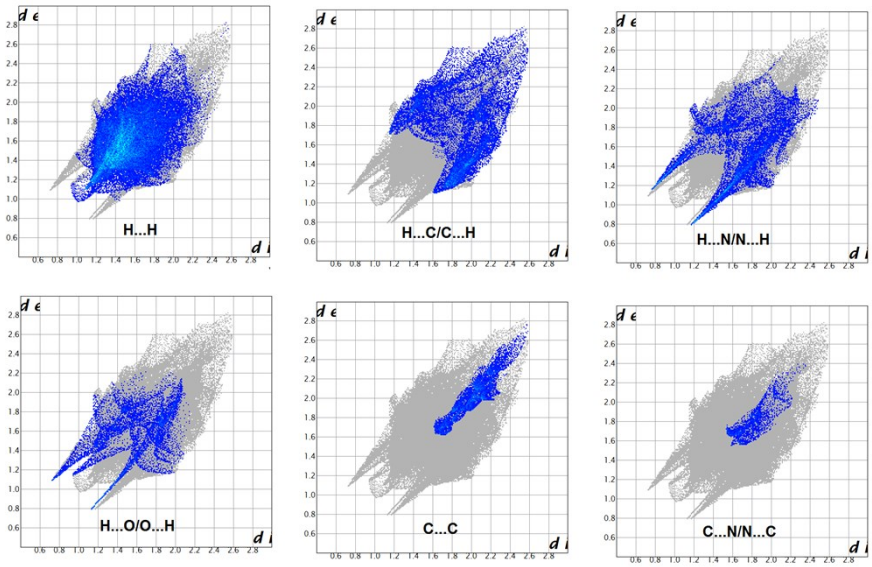

Fig. S4 Decomposed FPs of various intermolecular contacts H…H, H…C/C…H, H…N/N…H, H…O/O…H, C…C and C…N/N…C for the molecule P002 of **3**.

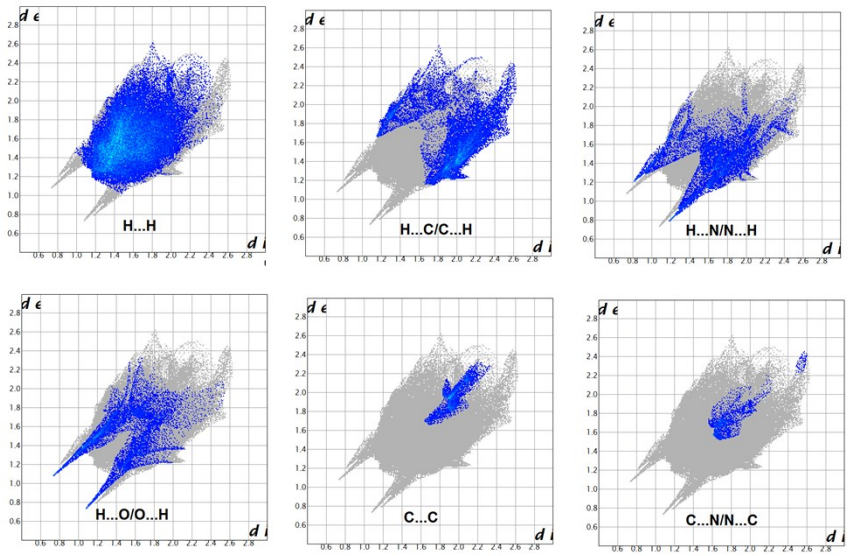

Fig. S5 Decomposed FPs of various intermolecular contacts H...H, H...C/C...H, H...N/N...H, H...O/O...H, C...C and C...N/N...C for the molecule P001 of **4**.

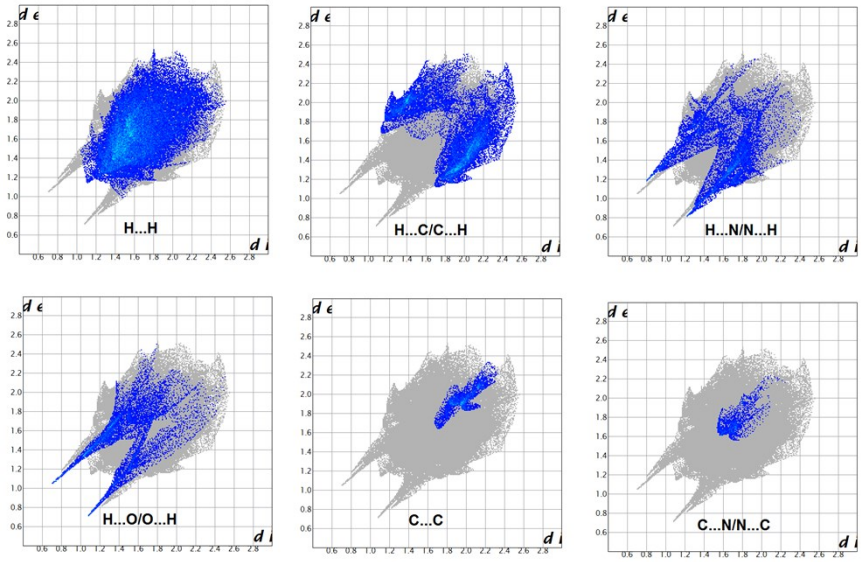

Fig. S6 Decomposed FPs of various intermolecular contacts H...H, H...C/C...H, H...N/N...H, H...O/O...H, C...C and C...N/N...C for the molecule P002 of **4**.

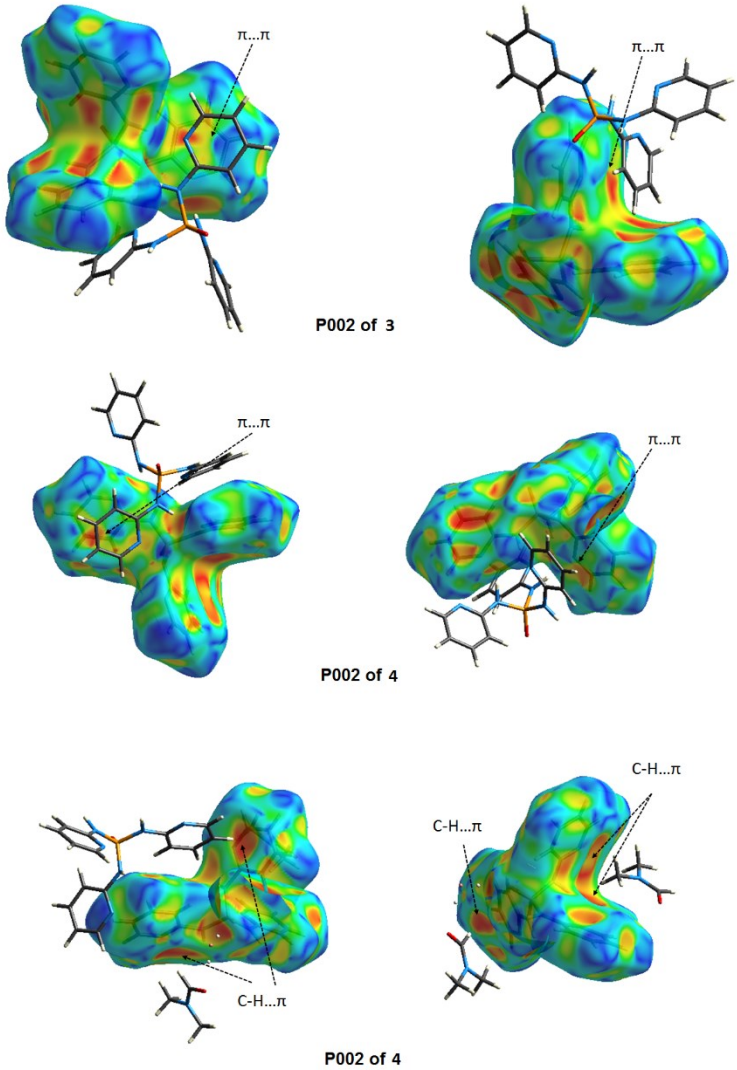

Fig. S7 Hirshfeld surfaces mapped with the shape index for the molecules P002 of **3** and **4**, surrounded by neighboring molecules associated with close contacts.

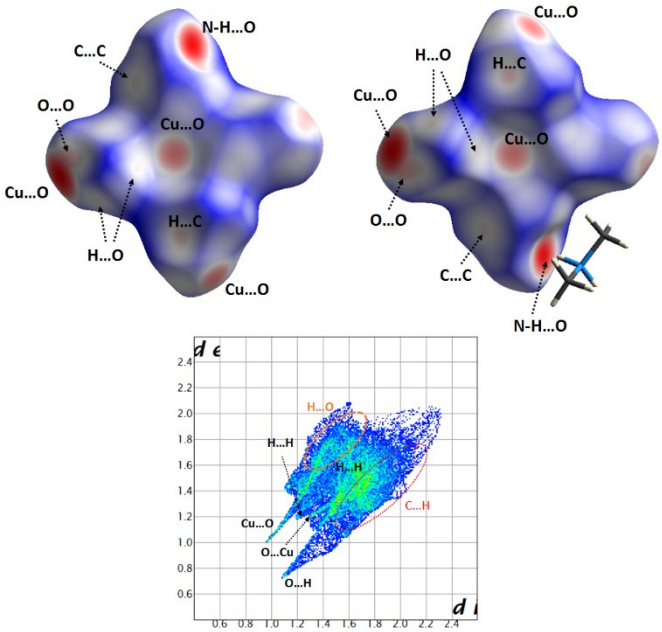

Fig. S8 Up: View of d_{norm} Hirshfeld surface plotted on the reported structure MACUFR, in two orientations, with marked close contacts; Down: Full 2D fingerprint plot highlighting the main close contacts for MACUFR has been shown.